



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:23 AM UTC

PDB ID : 7OD9 / pdb_00007od9
Title : Crystal structure of activated CheY fused to the C-terminal domain of CheF
Authors : Altegoer, F.; Weiland, P.; Bange, G.
Deposited on : 2021-04-29
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

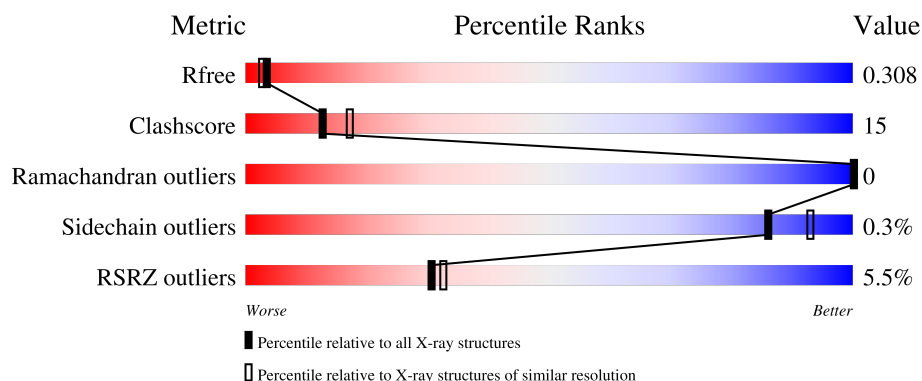
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	142	5% 55% 30% 14%
1	B	142	5% 73% 18% 9%
2	C	115	6% 49% 30% 22%
2	F	115	6% 45% 25% 30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3374 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 Response regulator receiver protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	129	Total	C	N	O	S	0	0	0
			994	635	162	189	8			
1	A	122	Total	C	N	O	S	0	0	0
			935	596	150	181	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	initiating methionine	UNP G0H061
B	-4	GLY	-	expression tag	UNP G0H061
B	-3	HIS	-	expression tag	UNP G0H061
B	-2	HIS	-	expression tag	UNP G0H061
B	-1	HIS	-	expression tag	UNP G0H061
B	0	HIS	-	expression tag	UNP G0H061
B	1	HIS	-	expression tag	UNP G0H061
B	2	HIS	-	expression tag	UNP G0H061
B	124	VAL	-	expression tag	UNP G0H061
B	125	LEU	-	expression tag	UNP G0H061
B	126	PHE	-	expression tag	UNP G0H061
B	127	GLN	-	expression tag	UNP G0H061
B	128	GLY	-	expression tag	UNP G0H061
B	129	PRO	-	expression tag	UNP G0H061
B	130	SER	-	expression tag	UNP G0H061
B	131	ALA	-	expression tag	UNP G0H061
B	132	GLY	-	expression tag	UNP G0H061
B	133	LEU	-	expression tag	UNP G0H061
B	134	VAL	-	expression tag	UNP G0H061
B	135	PRO	-	expression tag	UNP G0H061
B	136	ARG	-	expression tag	UNP G0H061
A	-5	MET	-	initiating methionine	UNP G0H061
A	-4	GLY	-	expression tag	UNP G0H061
A	-3	HIS	-	expression tag	UNP G0H061
A	-2	HIS	-	expression tag	UNP G0H061

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP G0H061
A	0	HIS	-	expression tag	UNP G0H061
A	1	HIS	-	expression tag	UNP G0H061
A	2	HIS	-	expression tag	UNP G0H061
A	124	VAL	-	expression tag	UNP G0H061
A	125	LEU	-	expression tag	UNP G0H061
A	126	PHE	-	expression tag	UNP G0H061
A	127	GLN	-	expression tag	UNP G0H061
A	128	GLY	-	expression tag	UNP G0H061
A	129	PRO	-	expression tag	UNP G0H061
A	130	SER	-	expression tag	UNP G0H061
A	131	ALA	-	expression tag	UNP G0H061
A	132	GLY	-	expression tag	UNP G0H061
A	133	LEU	-	expression tag	UNP G0H061
A	134	VAL	-	expression tag	UNP G0H061
A	135	PRO	-	expression tag	UNP G0H061
A	136	ARG	-	expression tag	UNP G0H061

- Molecule 2 is a protein called C-terminal domain of CheF from *Methanococcus maripaludis*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	90	Total	C	N	O	S	0	0	0
			711	449	112	146	4			
2	F	81	Total	C	N	O	S	0	0	0
			641	406	102	130	3			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	234	GLY	-	expression tag	UNP G0H062
C	235	SER	-	expression tag	UNP G0H062
C	236	GLY	-	expression tag	UNP G0H062
C	237	GLY	-	expression tag	UNP G0H062
C	238	ILE	-	expression tag	UNP G0H062
C	239	GLU	-	expression tag	UNP G0H062
C	240	GLY	-	expression tag	UNP G0H062
C	241	GLY	-	expression tag	UNP G0H062
C	242	SER	-	expression tag	UNP G0H062
C	243	MET	-	expression tag	UNP G0H062
C	244	GLY	-	expression tag	UNP G0H062
F	234	GLY	-	expression tag	UNP G0H062
F	235	SER	-	expression tag	UNP G0H062

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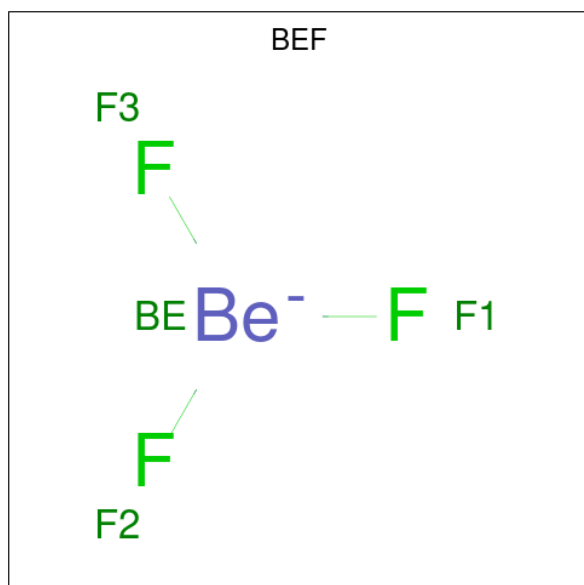
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Chain	Residue	Modelled	Actual	Comment	Reference
F	236	GLY	-	expression tag	UNP G0H062
F	237	GLY	-	expression tag	UNP G0H062
F	238	ILE	-	expression tag	UNP G0H062
F	239	GLU	-	expression tag	UNP G0H062
F	240	GLY	-	expression tag	UNP G0H062
F	241	GLY	-	expression tag	UNP G0H062
F	242	SER	-	expression tag	UNP G0H062
F	243	MET	-	expression tag	UNP G0H062
F	244	GLY	-	expression tag	UNP G0H062

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

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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



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

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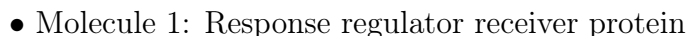
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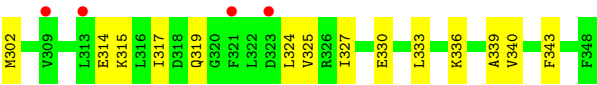
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Be 1	F 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	43	Total 43	O 43	0	0
5	A	27	Total 27	O 27	0	0
5	C	5	Total 5	O 5	0	0
5	F	8	Total 8	O 8	0	0

- Molecule 1: Response regulator receiver protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.29Å 70.87Å 59.82Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	44.07 – 2.30 44.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.07-2.30) 99.9 (44.07-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.249 , 0.307 0.250 , 0.308	Depositor DCC
R_{free} test set	1086 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3374	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	1/946 (0.1%)	0.58	0/1277
1	B	0.19	0/1009	0.39	0/1363
2	C	0.21	0/718	0.44	0/967
2	F	0.19	0/646	0.42	0/869
All	All	0.23	1/3319 (0.0%)	0.47	0/4476

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	GLN	C-O	5.05	1.26	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	74	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	935	0	976	38	0
1	B	994	0	1031	17	0
2	C	711	0	715	39	0
2	F	641	0	655	31	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	1	0
4	B	4	0	0	0	0
5	A	27	0	0	5	0
5	B	43	0	0	1	0
5	C	5	0	0	0	0
5	F	8	0	0	1	0
All	All	3374	0	3377	101	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 15.

All (101) 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:C:285:ILE:HG13	2:C:302:MET:HE1	1.49	0.91
2:C:296:LEU:HB3	2:F:296:LEU:HD13	1.61	0.82
2:F:293:ILE:HG21	2:F:301:MET:HE1	1.63	0.81
1:A:105:ILE:HD13	1:A:114:ILE:HD13	1.63	0.79
2:F:343:PHE:O	5:F:401:HOH:O	2.01	0.78
1:A:28:ASN:ND2	5:A:301:HOH:O	2.18	0.75
1:A:85:THR:O	1:A:107:LYS:N	2.22	0.72
1:A:85:THR:C	1:A:107:LYS:HG2	2.14	0.72
2:C:295:SER:OG	2:F:330:GLU:HA	1.91	0.71
2:C:279:ALA:HB3	2:C:282:GLU:HG3	1.74	0.68
2:C:272:LYS:HA	2:C:275:VAL:HG12	1.74	0.67
1:B:105:ILE:HG21	1:B:114:ILE:HD12	1.77	0.66
2:C:335:GLU:HA	2:C:338:ARG:HE	1.60	0.65
2:C:275:VAL:HG11	2:F:343:PHE:CE1	2.31	0.65
2:C:340:VAL:HG13	2:F:275:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:NZ	1:A:122:PHE:O	2.34	0.61
1:A:39:GLY:HA3	1:A:63:THR:HB	1.82	0.61
2:C:325:VAL:HG12	2:C:326:ARG:HG2	1.81	0.60
1:A:53:LEU:HD12	5:A:302:HOH:O	2.01	0.59
2:C:326:ARG:HG3	2:F:330:GLU:OE1	2.03	0.59
2:F:285:ILE:HG13	2:F:302:MET:HE1	1.83	0.59
2:C:274:GLU:O	2:C:278:LEU:HD13	2.03	0.59
2:C:296:LEU:HD13	2:F:296:LEU:HB3	1.85	0.59
1:B:19:ILE:HD13	2:C:301:MET:HE1	1.84	0.59
1:B:28:ASN:HD21	1:A:32:VAL:HG13	1.68	0.58
2:C:313:LEU:O	2:C:317:ILE:HG13	2.04	0.57
2:F:280:PRO:O	2:F:284:GLU:HG3	2.05	0.57
1:A:58:ILE:HG23	1:A:66:ILE:HG12	1.86	0.56
2:C:295:SER:HA	2:C:298:LEU:CD2	2.36	0.56
2:C:321:PHE:CE1	2:F:340:VAL:HG21	2.41	0.54
2:C:336:LYS:O	2:C:340:VAL:HG23	2.07	0.54
1:A:6:LYS:HB3	1:A:33:ILE:HD13	1.89	0.54
1:B:58:ILE:HD12	1:B:85:THR:HG21	1.90	0.54
2:C:281:GLU:O	2:C:285:ILE:HD12	2.07	0.54
1:A:15:PHE:CE1	2:F:284:GLU:HB3	2.43	0.53
1:A:113:LYS:HE3	1:A:116:GLU:OE1	2.08	0.53
1:A:113:LYS:HD2	1:A:113:LYS:N	2.23	0.53
2:C:321:PHE:HE1	2:F:340:VAL:HG21	1.73	0.53
2:C:296:LEU:HD22	2:F:296:LEU:HD22	1.90	0.52
1:B:75:LYS:HD2	1:B:76:THR:HG23	1.91	0.52
2:C:278:LEU:HD11	2:C:321:PHE:CE2	2.45	0.52
1:A:17:ARG:O	1:A:21:LYS:HG3	2.10	0.52
1:B:22:ARG:NH1	5:B:305:HOH:O	2.43	0.51
1:A:80:LYS:O	5:A:302:HOH:O	2.18	0.51
1:A:81:ILE:HA	5:A:302:HOH:O	2.09	0.51
2:C:278:LEU:HD11	2:C:321:PHE:CZ	2.45	0.51
2:C:275:VAL:HG11	2:F:343:PHE:HE1	1.75	0.50
2:F:314:GLU:HA	2:F:317:ILE:HG12	1.93	0.50
1:B:89:GLN:HA	1:B:89:GLN:OE1	2.11	0.50
1:A:39:GLY:O	1:A:42:ALA:N	2.41	0.50
1:A:93:MET:O	1:A:97:VAL:HG23	2.12	0.50
1:A:108:PRO:HB2	2:F:290:TYR:CE2	2.48	0.49
1:A:58:ILE:HA	1:A:65:GLY:HA3	1.94	0.48
2:F:294:THR:OG1	2:F:297:GLU:OE1	2.18	0.48
2:F:315:LYS:O	2:F:319:GLN:HG3	2.13	0.48
1:A:15:PHE:CE2	1:A:19:ILE:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HB2	1:A:99:ALA:HB1	1.96	0.47
2:F:289:ILE:HD11	2:F:298:LEU:HD21	1.95	0.47
1:A:73:LYS:HE2	1:A:100:GLY:O	2.14	0.47
2:C:333:LEU:HD11	2:F:290:TYR:HB2	1.96	0.47
1:A:57:ASP:OD1	4:A:202:BEF:F1	2.22	0.47
1:A:59:VAL:HG12	5:A:304:HOH:O	2.15	0.46
2:F:336:LYS:O	2:F:340:VAL:HG23	2.15	0.46
1:A:16:MET:HA	1:A:16:MET:HE2	1.98	0.46
2:C:305:ASP:HB2	2:C:308:GLU:HG3	1.96	0.46
2:C:340:VAL:O	2:C:344:ILE:HG12	2.15	0.46
2:C:335:GLU:N	2:C:338:ARG:HH21	2.14	0.45
1:A:57:ASP:O	1:A:65:GLY:HA3	2.16	0.45
2:C:275:VAL:HG23	2:F:340:VAL:HG13	1.99	0.45
2:C:298:LEU:HB3	2:C:302:MET:HE2	1.99	0.45
2:C:271:LEU:HD11	2:F:339:ALA:HB1	1.99	0.45
1:B:73:LYS:HE3	1:B:100:GLY:O	2.16	0.45
1:A:85:THR:HA	1:A:107:LYS:HE3	1.99	0.45
1:A:15:PHE:HE2	1:A:19:ILE:HD11	1.82	0.45
1:A:12:ASP:HB3	1:A:61:PRO:HD2	1.98	0.45
1:B:116:GLU:O	1:B:120:LYS:HG2	2.17	0.44
2:F:279:ALA:HB1	2:F:280:PRO:HD2	2.00	0.43
1:B:93:MET:HE2	1:B:93:MET:HB2	1.67	0.43
1:A:58:ILE:HD11	1:A:85:THR:HG21	1.99	0.43
1:B:121:LEU:HD12	1:B:121:LEU:H	1.83	0.43
1:A:10:VAL:HG22	1:A:36:ALA:HB3	2.01	0.43
1:A:88:ASP:O	1:A:93:MET:HE3	2.19	0.43
2:C:327:ILE:HG12	2:F:327:ILE:HD11	2.01	0.42
1:A:39:GLY:O	1:A:43:ILE:HD12	2.19	0.42
1:B:61:PRO:O	1:B:63:THR:N	2.52	0.42
1:B:53:LEU:HD21	1:B:118:PHE:CD2	2.54	0.42
2:C:329:LYS:HG2	2:F:324:LEU:CD1	2.50	0.42
2:C:282:GLU:HA	2:C:285:ILE:HD13	2.02	0.42
1:A:43:ILE:HD12	1:A:43:ILE:H	1.85	0.41
1:A:107:LYS:HG3	2:C:345:ILE:HD11	2.02	0.41
1:B:83:MET:HG3	1:B:96:ALA:HB1	2.02	0.41
2:C:332:ASP:OD2	2:F:325:VAL:HG21	2.21	0.41
2:C:290:TYR:HB2	2:F:333:LEU:HD11	2.02	0.41
1:B:19:ILE:O	1:B:23:ILE:HG13	2.20	0.41
1:A:107:LYS:CG	2:C:345:ILE:HD11	2.51	0.41
2:C:272:LYS:O	2:C:276:GLU:HG3	2.21	0.41
2:F:277:GLN:HA	2:F:277:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PHE:O	2:C:291:THR:HA	2.21	0.40
1:A:73:LYS:NZ	1:A:79:ILE:O	2.31	0.40
2:F:279:ALA:O	2:F:283:GLN:HG3	2.21	0.40
1:B:85:THR:OG1	1:B:87:VAL:HG22	2.22	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	120/142 (84%)	112 (93%)	8 (7%)	0	100	100
1	B	127/142 (89%)	125 (98%)	2 (2%)	0	100	100
2	C	88/115 (76%)	86 (98%)	2 (2%)	0	100	100
2	F	79/115 (69%)	77 (98%)	2 (2%)	0	100	100
All	All	414/514 (80%)	400 (97%)	14 (3%)	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	105/121 (87%)	104 (99%)	1 (1%)	68	82
1	B	111/121 (92%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	80/99 (81%)	80 (100%)	0	100	100
2	F	72/99 (73%)	72 (100%)	0	100	100
All	All	368/440 (84%)	367 (100%)	1 (0%)	86	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	ASN
1	B	117	GLN
1	A	28	ASN
1	A	89	GLN
2	C	273	ASN
2	C	283	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	BEF	A	202	-	0,3,3	-	-	-		
4	BEF	B	202	1	0,3,3	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

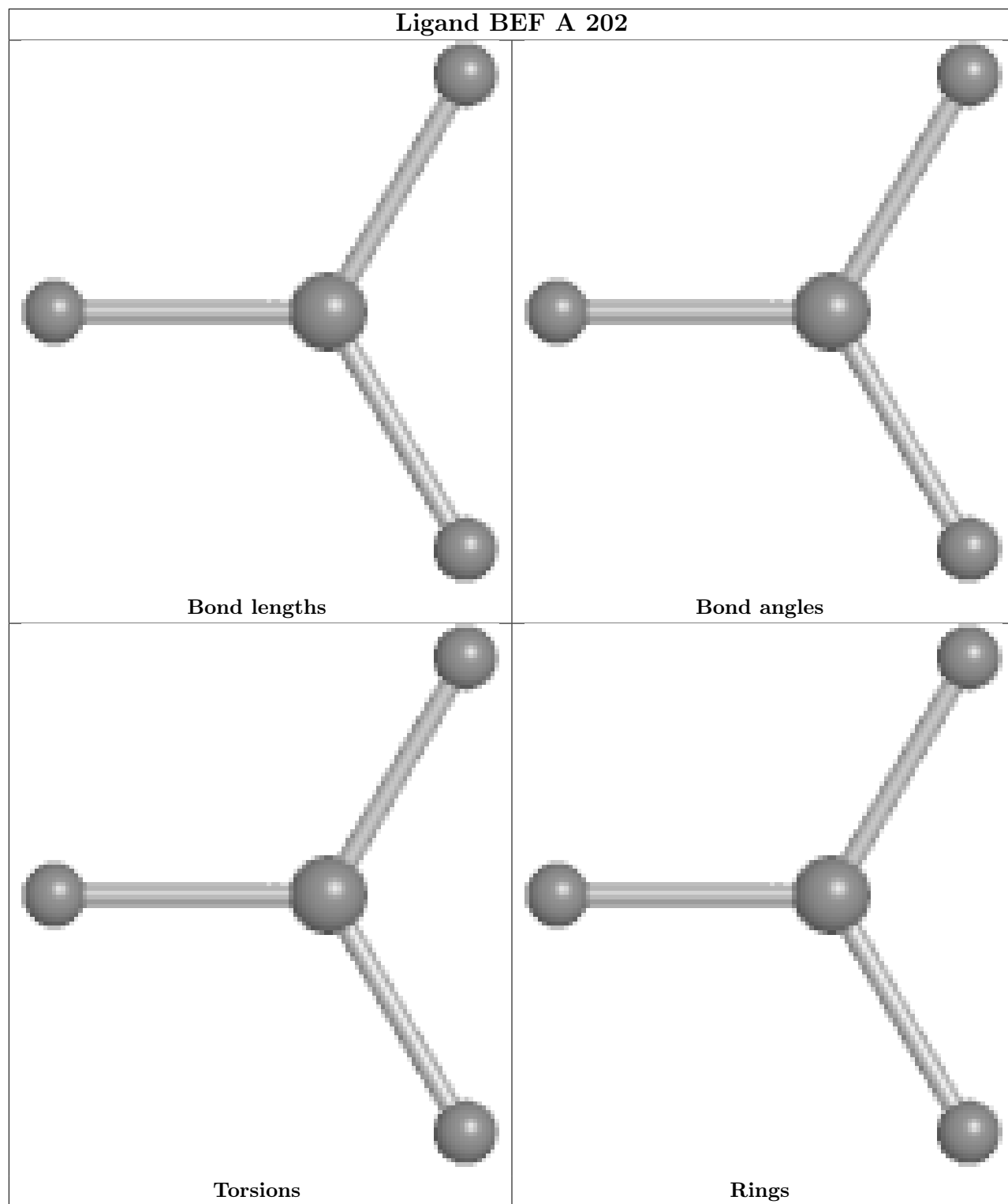
There are no torsion outliers.

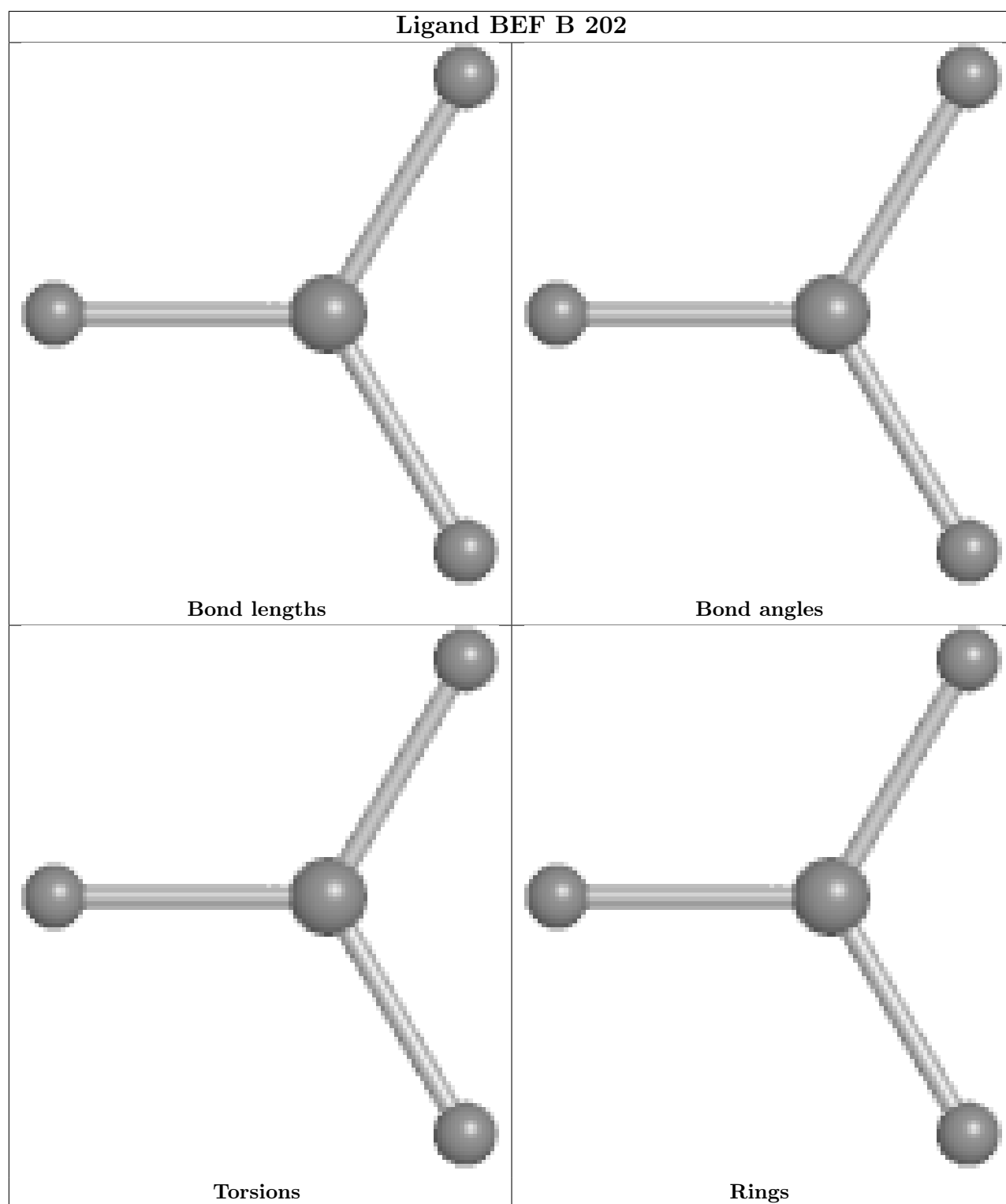
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	202	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	122/142 (85%)	0.68	2 (1%) 70 72	51, 72, 98, 131	0
1	B	129/142 (90%)	0.66	7 (5%) 31 33	42, 59, 85, 112	0
2	C	90/115 (78%)	0.97	7 (7%) 19 21	60, 97, 122, 131	0
2	F	81/115 (70%)	0.99	7 (8%) 16 17	59, 98, 119, 129	0
All	All	422/514 (82%)	0.79	23 (5%) 30 32	42, 76, 113, 131	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	THR	3.5
1	A	124	VAL	3.3
2	F	271	LEU	3.3
2	C	296	LEU	3.2
2	F	298	LEU	2.9
2	C	259	SER	2.9
2	F	313	LEU	2.7
1	B	114	ILE	2.6
2	C	271	LEU	2.5
1	B	1	HIS	2.5
2	F	309	VAL	2.4
2	C	324	LEU	2.3
1	B	117	GLN	2.3
2	F	296	LEU	2.3
2	C	327	ILE	2.3
1	B	37	ALA	2.2
2	F	321	PHE	2.2
1	B	72	ILE	2.1
2	C	287	THR	2.1
2	C	300	GLY	2.1
1	A	58	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	125	LEU	2.0
2	F	323	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

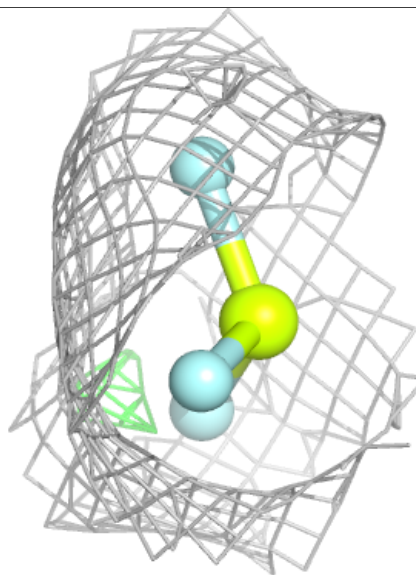
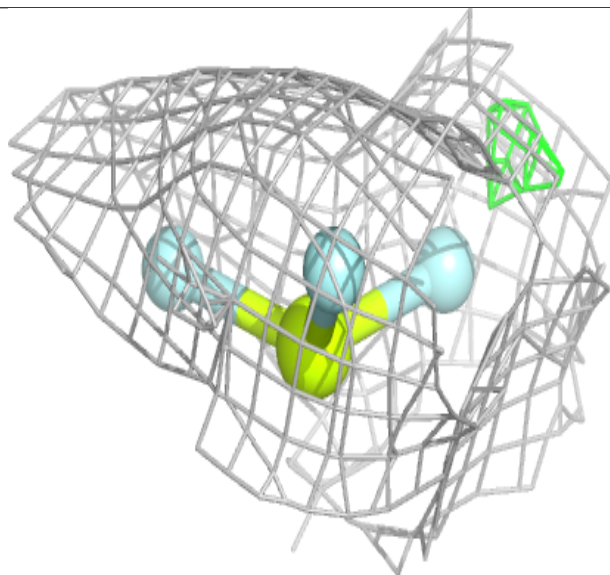
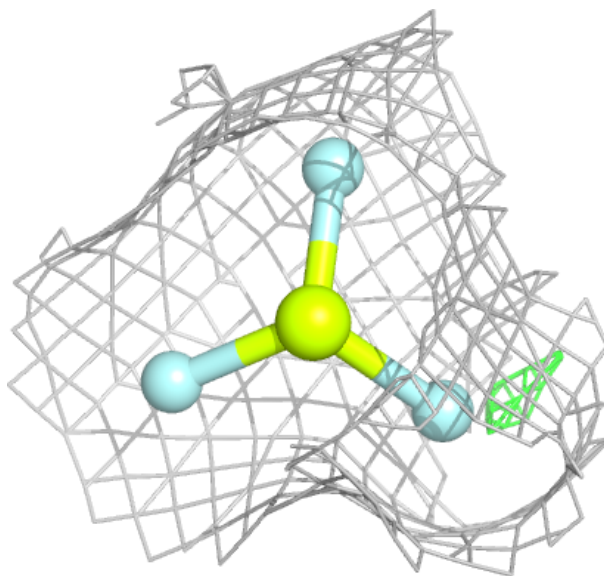
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BEF	B	202	4/4	0.91	0.07	37,43,49,54	0
4	BEF	A	202	4/4	0.91	0.08	69,73,75,88	0
3	MG	B	201	1/1	0.95	0.07	50,50,50,50	0
3	MG	A	201	1/1	0.96	0.06	80,80,80,80	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.

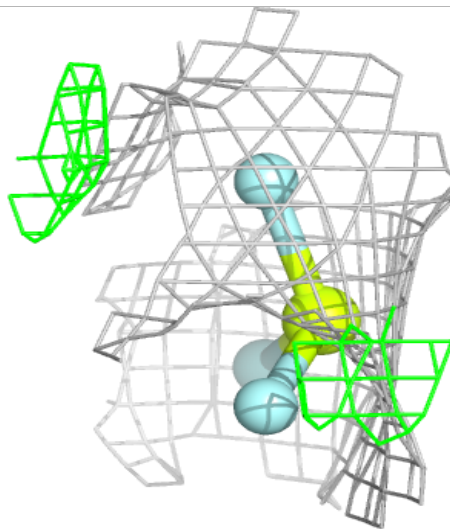
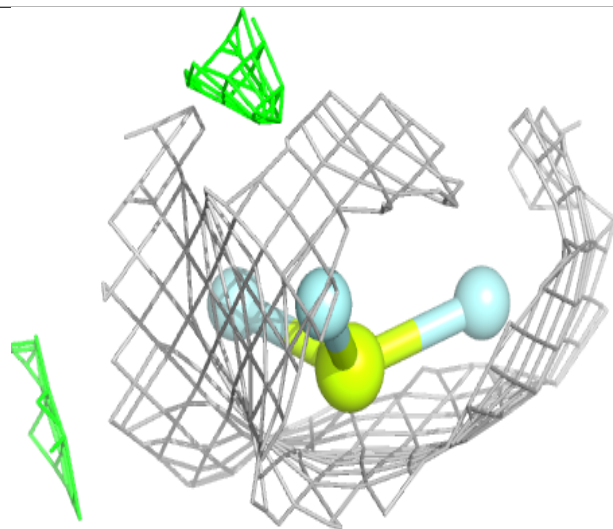
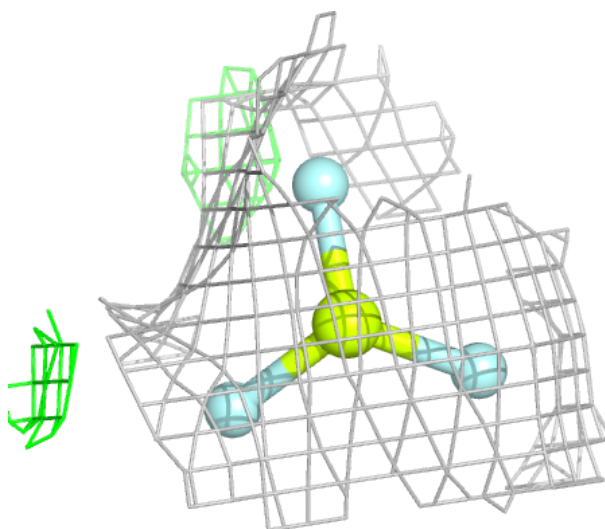
Electron density around BEF B 202:

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



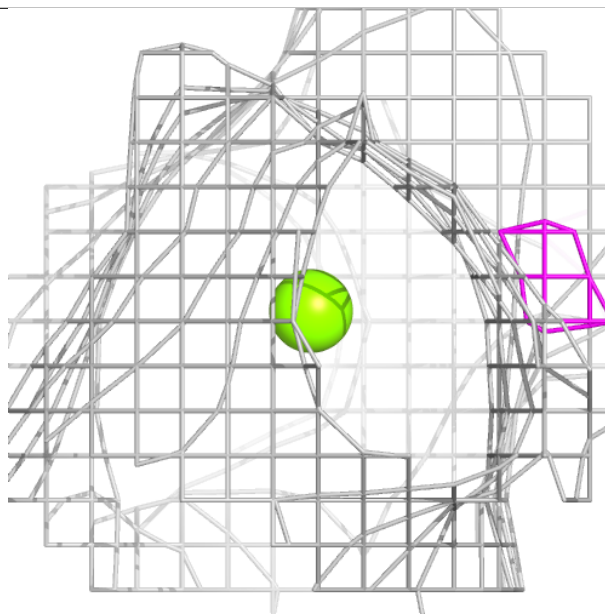
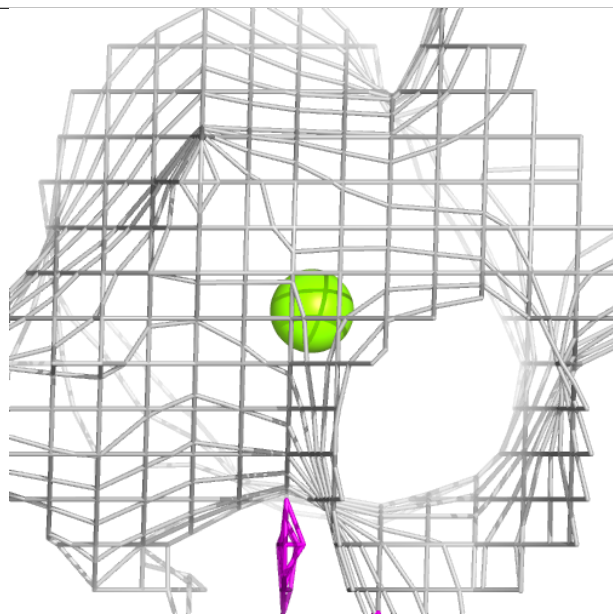
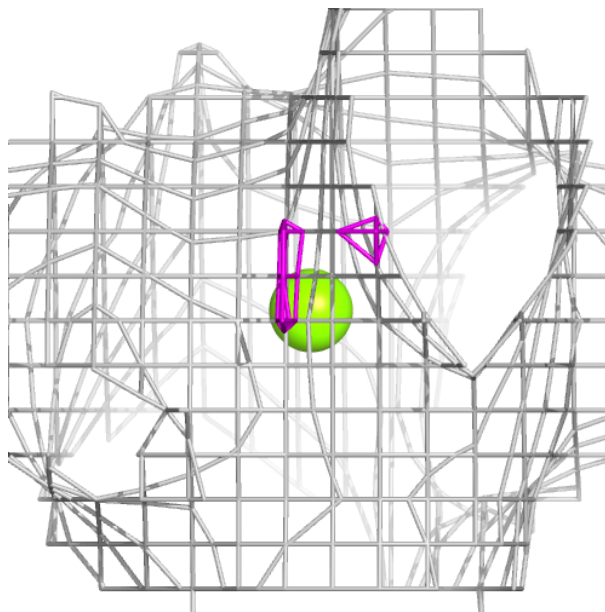
Electron density around BEF A 202:

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



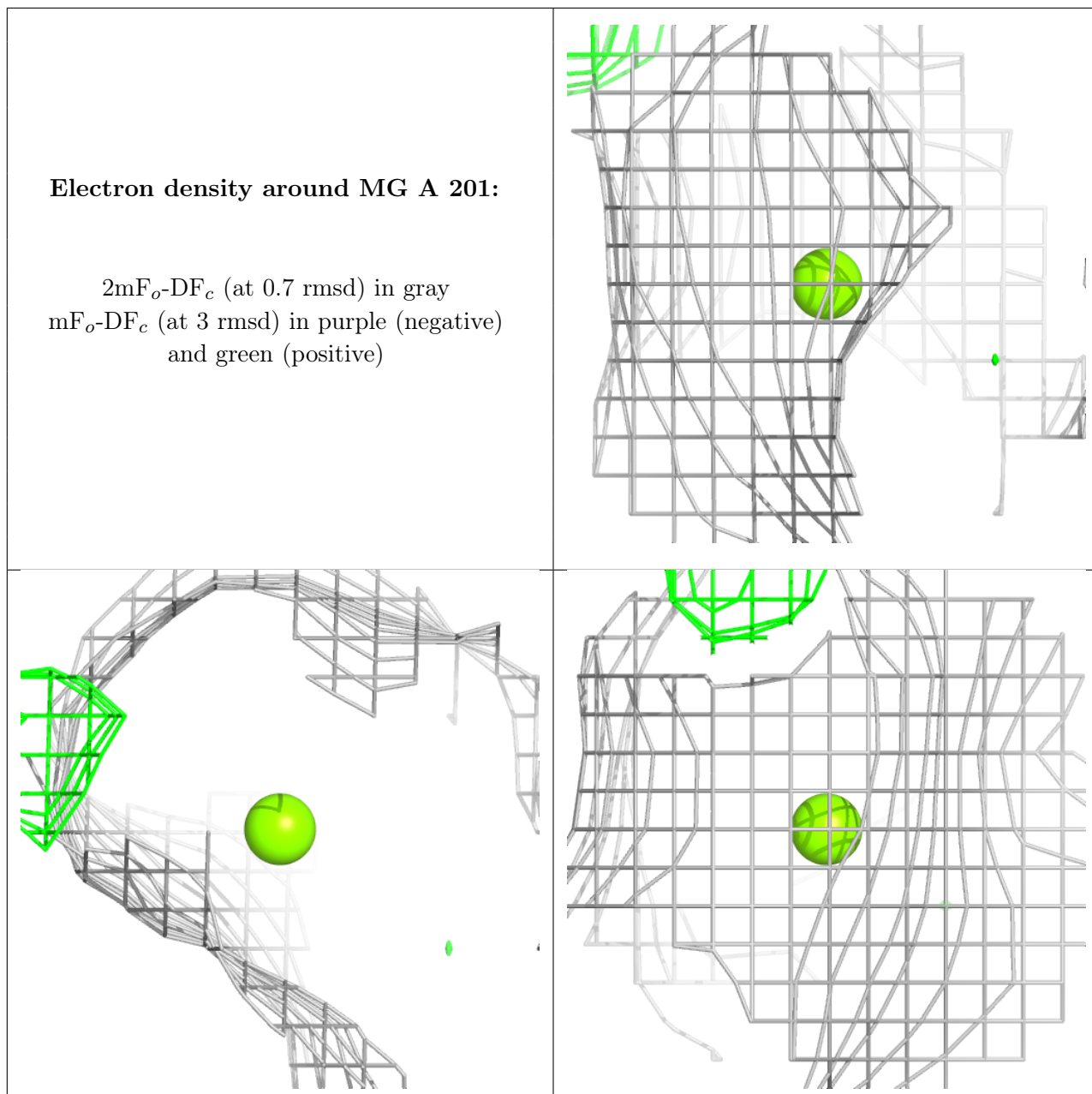
Electron density around MG B 201:

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



Electron density around MG A 201:

$2mF_o-DF_c$ (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.