wwPDB X-ray Structure Validation Summary Report (i)

Oct 6, 2026 – 07:31 pm BST

PDB ID	:	9QGT / pdb_00009qgt
Title	:	Crystal Structure of human MLH1 N-terminal domain I219V with ADP-BeF3
Authors	:	Thomsen, M.; Ganichkin, O.; Thieulin-Pardo, G.; Bandera, A.M.; Boudet, J.; Finley, M.; Felsenfeld, D.; Haque, T.; Prasad, B.C.; Monteagudo, E.; Vogt, T.; Stamford, A.
Deposited on	:	2025-03-14
Resolution	:	1.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

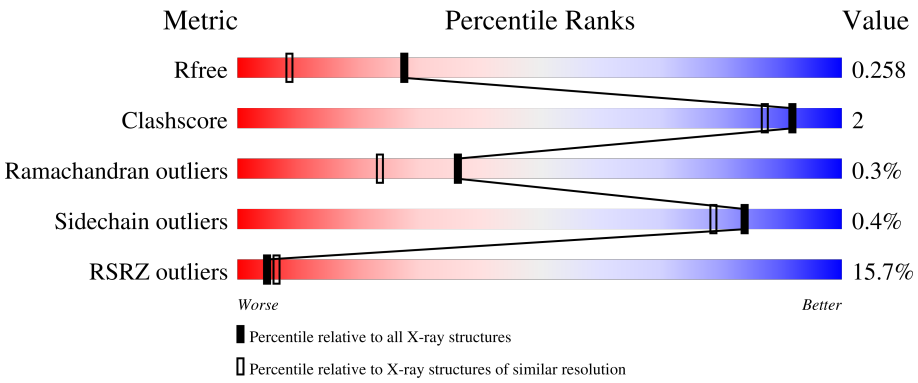
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.75 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	A1	341	11% 96%
1	B1	341	18% 94%
1	C1	341	18% 91% 7%
1	D1	341	15% 95%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 12169 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

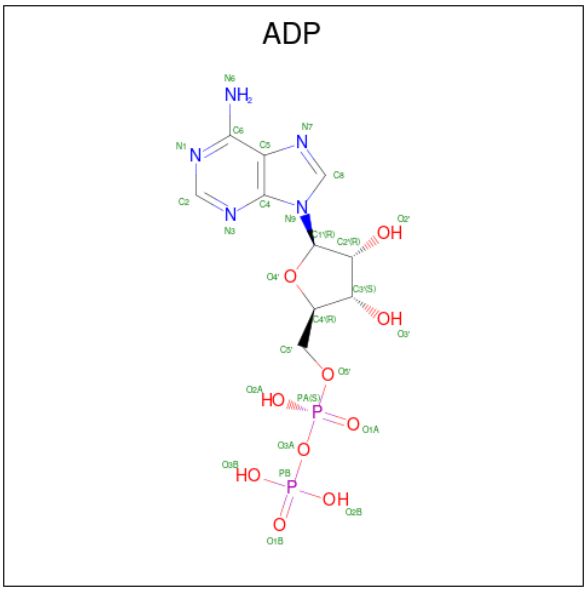
- Molecule 1 is a protein called DNA mismatch repair protein Mlh1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A1	334	2695	1701	475	511	8	25	11	0
1	B1	334	2659	1677	468	506	8	36	7	0
1	C1	334	2675	1687	472	508	8	42	8	0
1	D1	337	2707	1702	476	519	10	45	11	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	0	GLY	-	expression tag	UNP P40692
A1	219	VAL	ILE	variant	UNP P40692
B1	0	GLY	-	expression tag	UNP P40692
B1	219	VAL	ILE	variant	UNP P40692
C1	0	GLY	-	expression tag	UNP P40692
C1	219	VAL	ILE	variant	UNP P40692
D1	0	GLY	-	expression tag	UNP P40692
D1	219	VAL	ILE	variant	UNP P40692

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

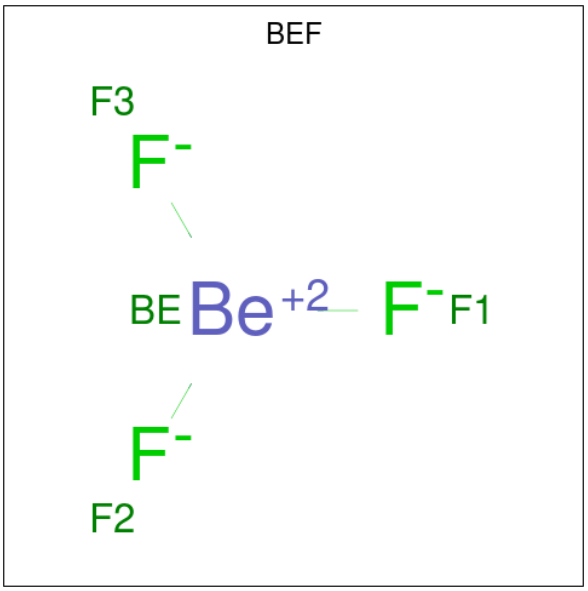


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A1	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B1	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C1	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D1	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A1	1	Total	Mg	0	0
			1	1		
3	B1	1	Total	Mg	0	0
			1	1		
3	C1	1	Total	Mg	0	0
			1	1		
3	D1	1	Total	Mg	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
4	A1	1	4	1	3	0	0
4	B1	1	4	1	3	0	0
4	C1	1	4	1	3	0	0
4	D1	1	4	1	3	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A1	1	1	1	0	0
5	B1	1	1	1	0	0
5	C1	1	1	1	0	0
5	D1	1	1	1	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A1	2	2	2	0	0

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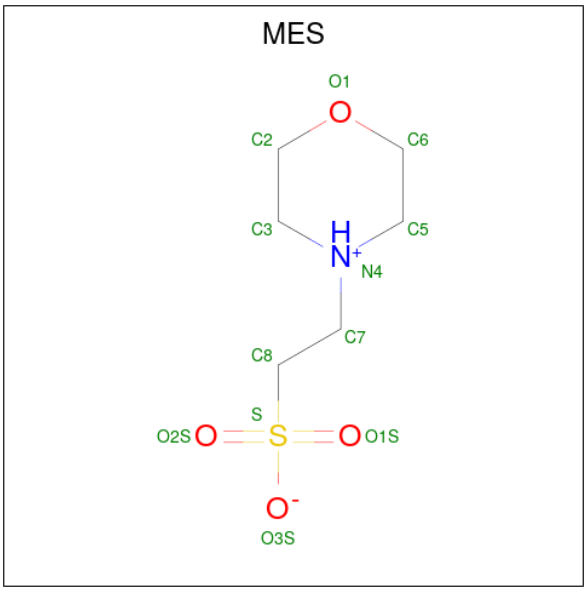
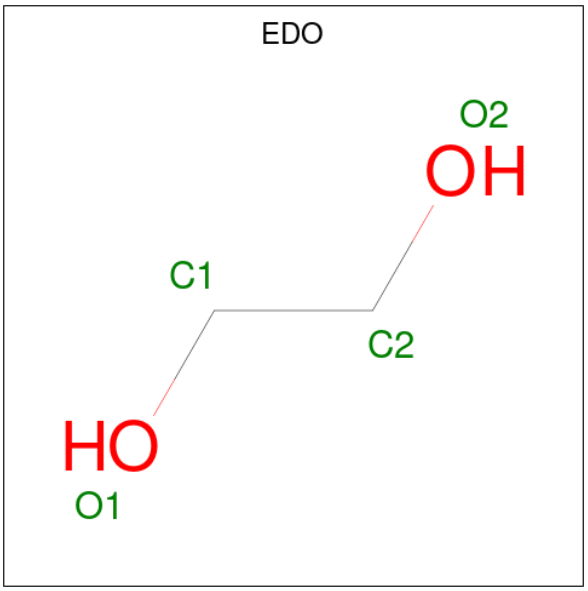
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	B1	1	1	1	0	0
			Total	Ca		
6	C1	1	1	1	0	0
			Total	Ca		
6	D1	1	1	1	0	0

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



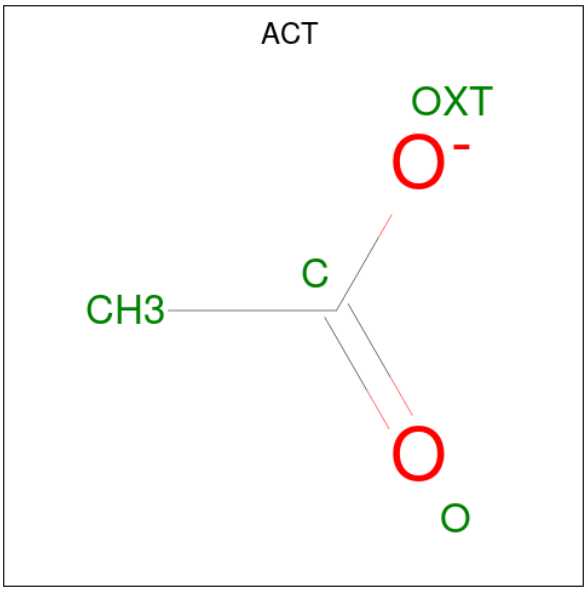
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	A1	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
7	B1	1	12	6	1	4	1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



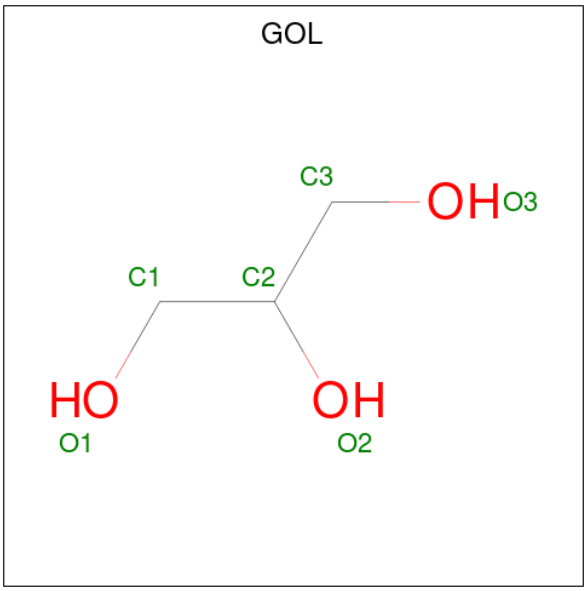
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A1	1	4	2	2	0	0
8	A1	1	4	2	2	0	0
8	A1	1	4	2	2	0	0
8	A1	1	4	2	2	0	0
8	B1	1	4	2	2	0	0
8	B1	1	4	2	2	0	0
8	B1	1	4	2	2	0	0
8	C1	1	4	2	2	0	0
8	C1	1	4	2	2	0	0
8	D1	1	4	2	2	0	0
8	D1	1	4	2	2	0	0

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A1	1	4	2	2	0	0
			Total	C	O		
9	A1	1	4	2	2	0	0
			Total	C	O		
9	A1	1	4	2	2	0	0
			Total	C	O		
9	B1	1	4	2	2	0	0
			Total	C	O		
9	C1	1	4	2	2	0	0
			Total	C	O		
9	D1	1	4	2	2	0	0
			Total	C	O		
9	D1	1	4	2	2	0	0

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A1	1	6	3	3	0	0
			Total	C	O		
10	A1	1	6	3	3	0	0
			Total	C	O		
10	C1	1	6	3	3	0	0
			Total	C	O		
10	D1	1	6	3	3	0	0
			Total	C	O		
10	D1	1	6	3	3	0	0

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
11	B1	2	2	2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A1	325	325	325	0	0
			Total	O		
12	B1	285	285	285	0	0
			Total	O		
12	C1	272	272	272	0	0

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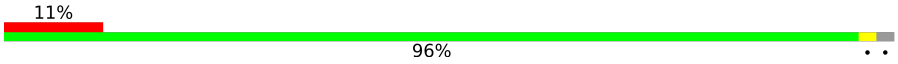
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	D1	285	286	286	0	1

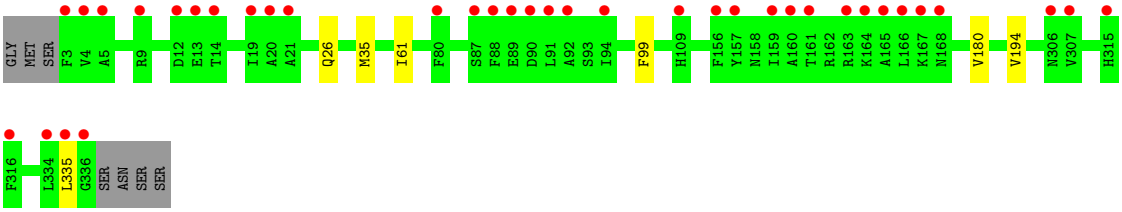
3 Residue-property plots (i)

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

• Molecule 1: DNA mismatch repair protein Mlh1

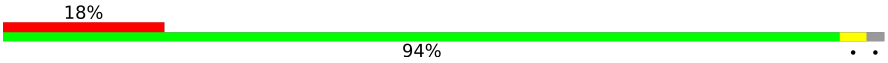
Chain A1:

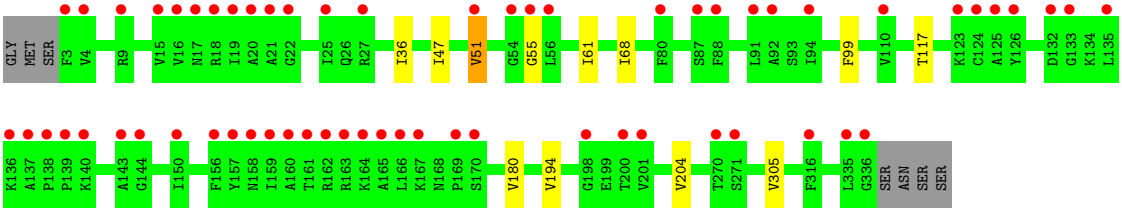




• Molecule 1: DNA mismatch repair protein Mlh1

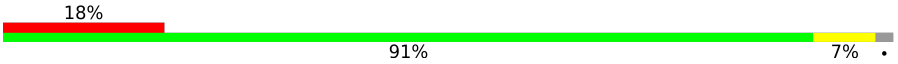
Chain B1:

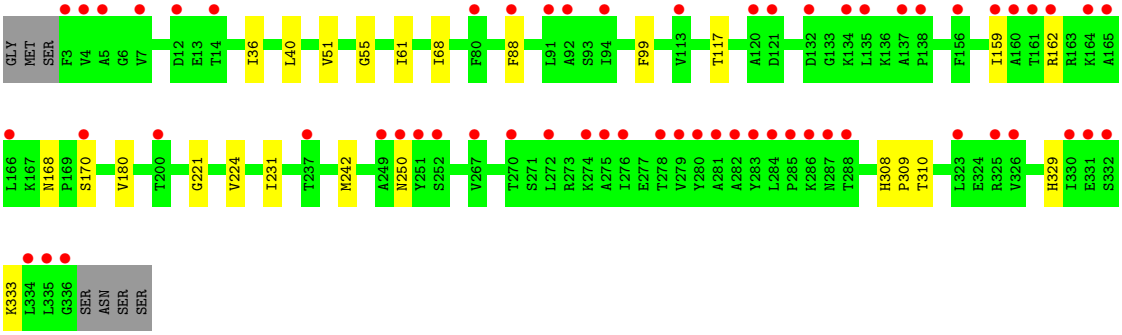




• Molecule 1: DNA mismatch repair protein Mlh1

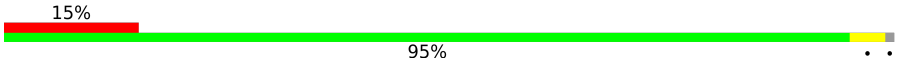
Chain C1:

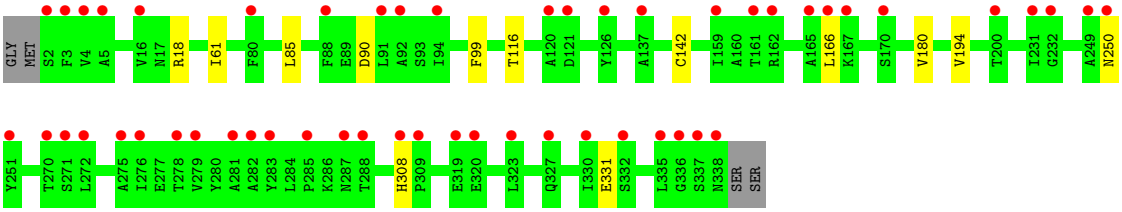




• Molecule 1: DNA mismatch repair protein Mlh1

Chain D1:


15%
95%


GLY MET S2 F3 V4 A5 V16 N17 R18 I61 F80 L85 F88 E89 D90 L91 A92 S93 I94 F99 T116 A120 D121 Y126 A137 C142 I159 A160 T161 R162 A165 L166 K167 S170 V180 V194 T200 I231 G232 A249 N250
Y251 T270 S271 L272 A275 I276 E277 T278 V279 Y280 A281 A282 Y283 L284 P285 K286 N287 T288 H308 P309 E319 E320 L323 Q327 I330 E331 S332 L335 G336 S337 N338 SER SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.07Å 178.78Å 73.78Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	89.39 – 1.75 89.39 – 1.75	Depositor EDS
% Data completeness (in resolution range)	72.9 (89.39-1.75) 72.9 (89.39-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.218 , 0.258 0.223 , 0.258	Depositor DCC
R_{free} test set	2120 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12169	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ACT, CL, CA, MES, EDO, NA, BEF, MG, GOL

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	A1	1.06	0/2738	1.39	0/3703
1	B1	1.06	0/2702	1.39	0/3654
1	C1	1.05	0/2718	1.41	0/3675
1	D1	1.05	0/2750	1.41	1/3719 (0.0%)
All	All	1.06	0/10908	1.40	1/14751 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D1	331	GLU	CB-CG-CD	6.05	122.88	112.60

There are no chirality outliers.

There are no planarity outliers.

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	A1	2695	0	2738	3	0
1	B1	2659	0	2696	12	0
1	C1	2675	0	2716	13	0
1	D1	2707	0	2729	9	0
2	A1	27	0	12	0	0
2	B1	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C1	27	0	12	0	0
2	D1	27	0	12	0	0
3	A1	1	0	0	0	0
3	B1	1	0	0	0	0
3	C1	1	0	0	0	0
3	D1	1	0	0	0	0
4	A1	4	0	0	0	0
4	B1	4	0	0	0	0
4	C1	4	0	0	0	0
4	D1	4	0	0	0	0
5	A1	1	0	0	0	0
5	B1	1	0	0	0	0
5	C1	1	0	0	0	0
5	D1	1	0	0	0	0
6	A1	2	0	0	0	0
6	B1	1	0	0	0	0
6	C1	1	0	0	0	0
6	D1	1	0	0	0	0
7	A1	12	0	13	0	0
7	B1	12	0	13	0	0
8	A1	16	0	24	0	0
8	B1	12	0	18	0	0
8	C1	8	0	12	0	0
8	D1	8	0	12	1	0
9	A1	12	0	9	0	0
9	B1	4	0	3	0	0
9	C1	4	0	3	0	0
9	D1	8	0	6	0	0
10	A1	12	0	16	0	0
10	C1	6	0	8	0	0
10	D1	12	0	16	0	0
11	B1	2	0	0	0	0
12	A1	325	0	0	1	0
12	B1	285	0	0	0	0
12	C1	272	0	0	0	0
12	D1	286	0	0	0	0
All	All	12169	0	11080	35	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 2.

The worst 5 of 35 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:B1:180[A]:VAL:HG11	1:B1:194[A]:VAL:CG2	1.81	1.10
1:B1:180[A]:VAL:HG11	1:B1:194[A]:VAL:HG23	1.56	0.86
1:D1:116[B]:THR:HG23	1:D1:142:CYS:SG	2.32	0.69
1:C1:36[B]:ILE:O	1:C1:40[B]:LEU:HD13	1.97	0.64
1:C1:308[B]:HIS:NE2	1:D1:308:HIS:ND1	2.46	0.62

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	A1	343/341 (101%)	336 (98%)	6 (2%)	1 (0%)	36	23
1	B1	339/341 (99%)	331 (98%)	7 (2%)	1 (0%)	36	23
1	C1	341/341 (100%)	335 (98%)	5 (2%)	1 (0%)	36	23
1	D1	346/341 (102%)	339 (98%)	6 (2%)	1 (0%)	36	23
All	All	1369/1364 (100%)	1341 (98%)	24 (2%)	4 (0%)	36	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	99	PHE
1	B1	99	PHE
1	C1	99	PHE
1	D1	99	PHE

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	A1	299/294 (102%)	298 (100%)	1 (0%)	86	82
1	B1	295/294 (100%)	294 (100%)	1 (0%)	86	82
1	C1	297/294 (101%)	294 (99%)	3 (1%)	68	54
1	D1	302/294 (103%)	300 (99%)	2 (1%)	76	67
All	All	1193/1176 (101%)	1186 (99%)	7 (1%)	84	71

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C1	61[B]	ILE
1	C1	250	ASN
1	D1	61[B]	ILE
1	D1	61[A]	ILE
1	C1	61[A]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C1	48	GLN
1	C1	329	HIS
1	C1	209	ASN
1	D1	149	GLN
1	C1	315	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 15 are monoatomic - leaving 33 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	D1	403	2	0,3,3	-	-	-		
9	ACT	D1	406	-	3,3,3	0.90	0	3,3,3	0.87	0
2	ADP	B1	401	3,4	27,29,29	0.55	0	42,45,45	0.50	0
4	BEF	A1	403	2	0,3,3	-	-	-		
9	ACT	D1	408	-	3,3,3	1.07	0	3,3,3	0.72	0
2	ADP	A1	401	3,4	27,29,29	0.46	0	42,45,45	0.54	0
8	EDO	C1	409	-	3,3,3	0.12	0	2,2,2	0.32	0
8	EDO	A1	416	-	3,3,3	0.17	0	2,2,2	0.47	0
9	ACT	A1	411	-	3,3,3	1.00	0	3,3,3	0.79	0
8	EDO	D1	409	-	3,3,3	0.15	0	2,2,2	0.18	0
2	ADP	C1	401	3,4	27,29,29	0.37	0	42,45,45	0.50	1 (2%)
8	EDO	A1	410	-	3,3,3	0.23	0	2,2,2	0.51	0
8	EDO	B1	410	-	3,3,3	0.11	0	2,2,2	0.24	0
9	ACT	B1	411	-	3,3,3	1.02	0	3,3,3	0.69	0
8	EDO	B1	409	-	3,3,3	0.06	0	2,2,2	0.23	0
9	ACT	A1	409	-	3,3,3	0.83	0	3,3,3	0.91	0
10	GOL	A1	413	-	5,5,5	0.13	0	5,5,5	0.44	0
9	ACT	C1	406	-	3,3,3	0.99	0	3,3,3	0.81	0
10	GOL	D1	410	-	5,5,5	0.12	0	5,5,5	0.40	0
8	EDO	A1	412	-	3,3,3	0.17	0	2,2,2	0.45	0
10	GOL	D1	407	-	5,5,5	0.11	0	5,5,5	0.35	0
7	MES	A1	407	-	12,12,12	0.73	0	14,16,16	0.70	0
8	EDO	C1	408	-	3,3,3	0.09	0	2,2,2	0.15	0
8	EDO	A1	408	-	3,3,3	0.16	0	2,2,2	0.35	0
7	MES	B1	406	-	12,12,12	0.72	0	14,16,16	0.56	0
9	ACT	A1	415	-	3,3,3	0.90	0	3,3,3	0.95	0
4	BEF	B1	403	2	0,3,3	-	-	-		
4	BEF	C1	403	2	0,3,3	-	-	-		
10	GOL	A1	414	-	5,5,5	0.13	0	5,5,5	0.36	0
8	EDO	B1	412	-	3,3,3	0.10	0	2,2,2	0.33	0
10	GOL	C1	407	-	5,5,5	0.12	0	5,5,5	0.33	0
8	EDO	D1	411	-	3,3,3	0.20	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	D1	401	3,4	27,29,29	0.47	0	42,45,45	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B1	401	3,4	-	2/16/32/32	0/3/3/3
2	ADP	A1	401	3,4	-	1/16/32/32	0/3/3/3
8	EDO	C1	409	-	-	1/1/1/1	-
8	EDO	A1	416	-	-	1/1/1/1	-
8	EDO	D1	409	-	-	1/1/1/1	-
2	ADP	C1	401	3,4	-	1/16/32/32	0/3/3/3
8	EDO	A1	410	-	-	1/1/1/1	-
8	EDO	B1	410	-	-	1/1/1/1	-
8	EDO	B1	409	-	-	1/1/1/1	-
10	GOL	A1	413	-	-	0/4/4/4	-
10	GOL	D1	410	-	-	2/4/4/4	-
8	EDO	A1	412	-	-	1/1/1/1	-
10	GOL	D1	407	-	-	2/4/4/4	-
7	MES	A1	407	-	-	0/6/14/14	0/1/1/1
8	EDO	C1	408	-	-	0/1/1/1	-
8	EDO	A1	408	-	-	0/1/1/1	-
7	MES	B1	406	-	-	0/6/14/14	0/1/1/1
10	GOL	A1	414	-	-	2/4/4/4	-
8	EDO	B1	412	-	-	1/1/1/1	-
10	GOL	C1	407	-	-	4/4/4/4	-
8	EDO	D1	411	-	-	1/1/1/1	-
2	ADP	D1	401	3,4	-	1/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C1	401	ADP	O2A-PA-O1A	2.01	122.16	112.24

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A1	401	ADP	PA-O3A-PB-O3B
2	C1	401	ADP	PA-O3A-PB-O3B
2	D1	401	ADP	PA-O3A-PB-O3B
10	A1	414	GOL	O1-C1-C2-C3
10	C1	407	GOL	O1-C1-C2-C3

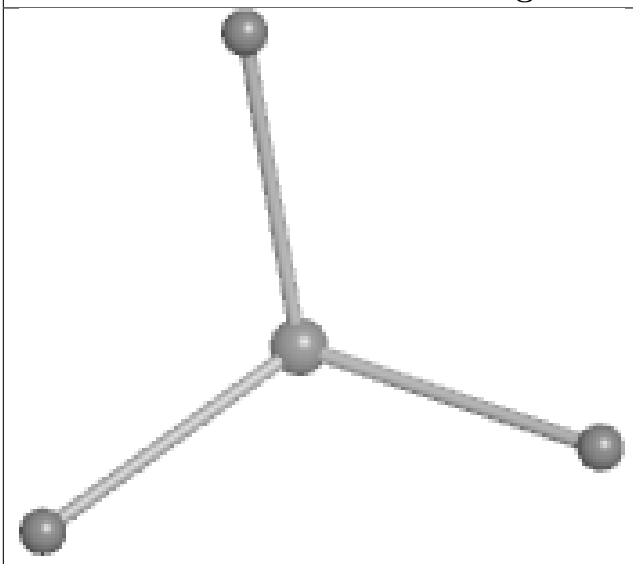
There are no ring outliers.

1 monomer is involved in 1 short contact:

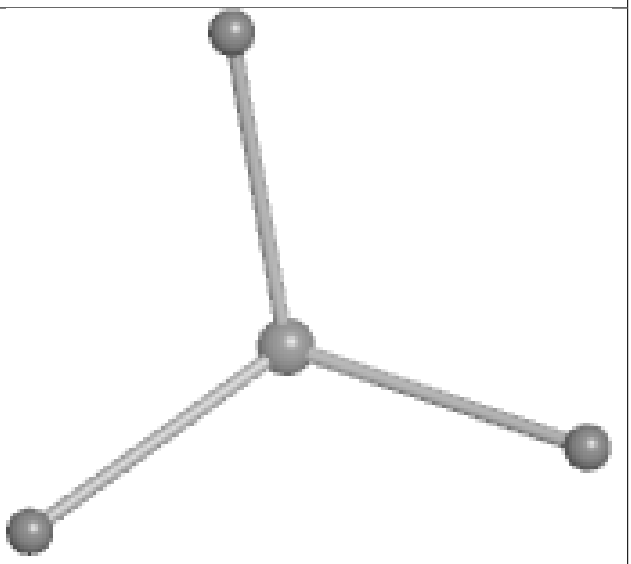
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D1	409	EDO	1	0

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.

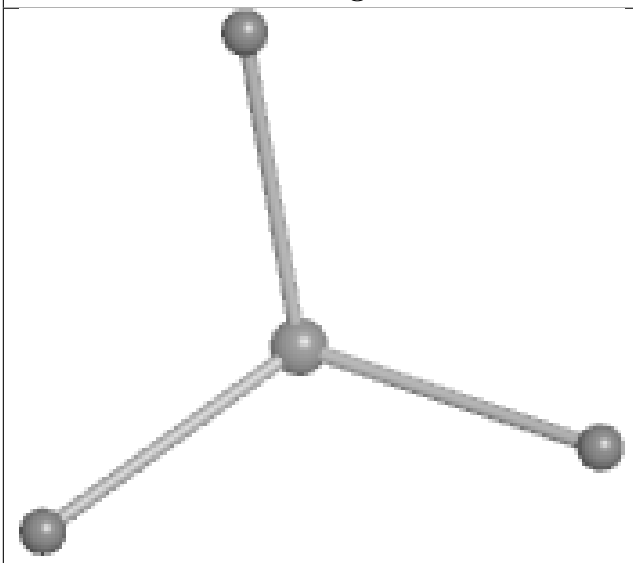
Ligand BEF D1 403



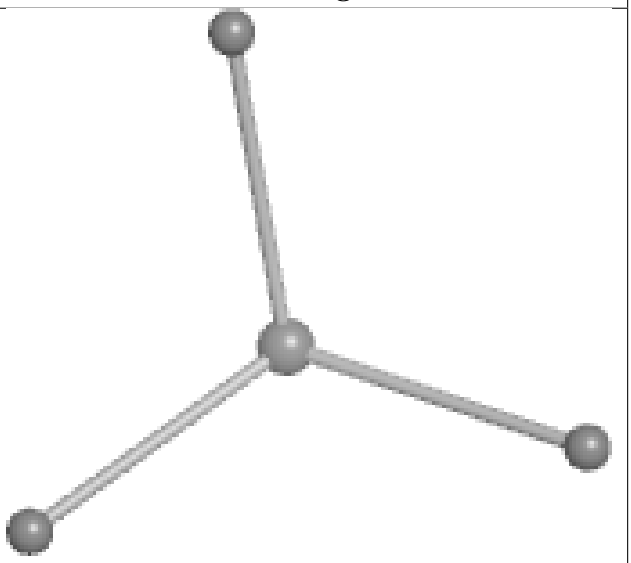
Bond lengths



Bond angles

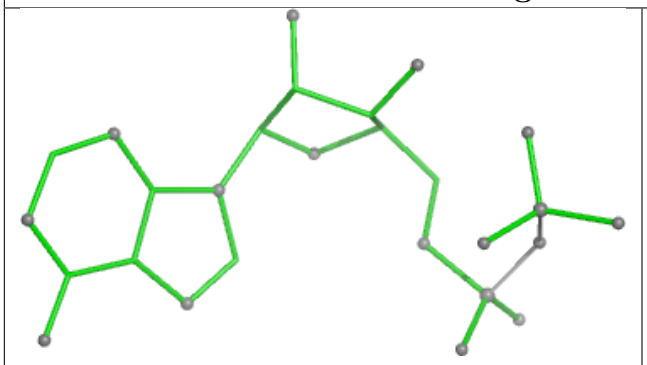


Torsions



Rings

Ligand ADP B1 401



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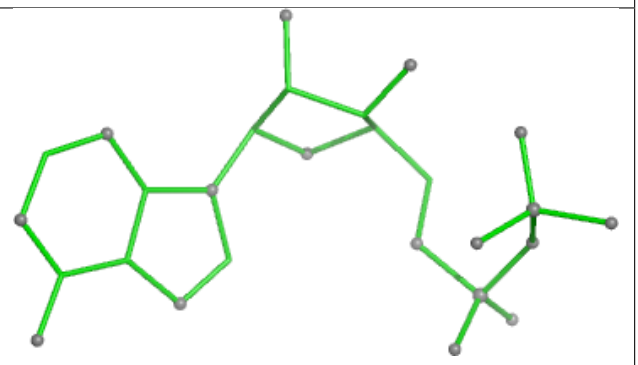

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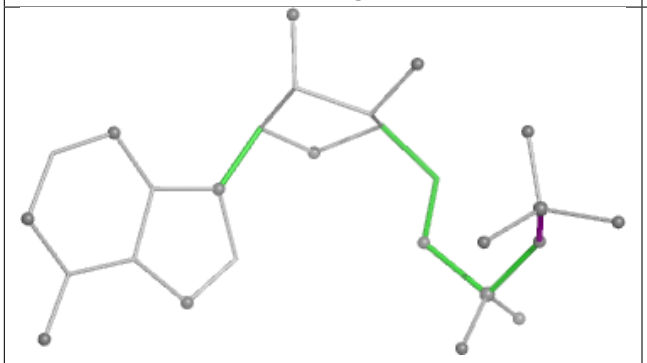
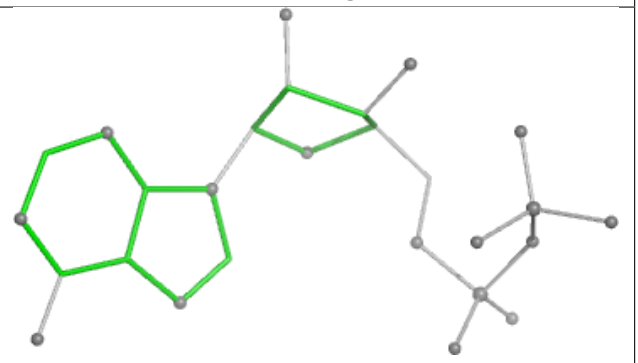
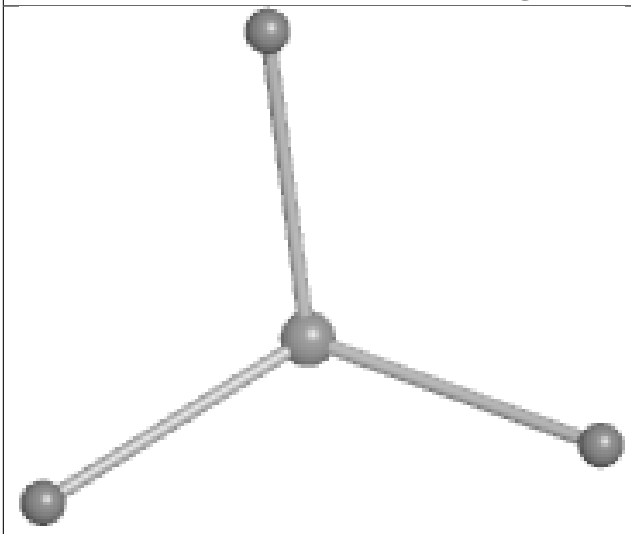


Torsions



Rings

Ligand BEF A1 403



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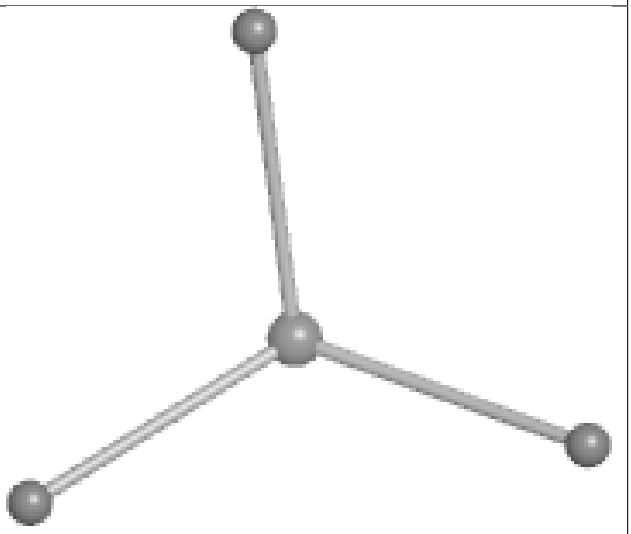

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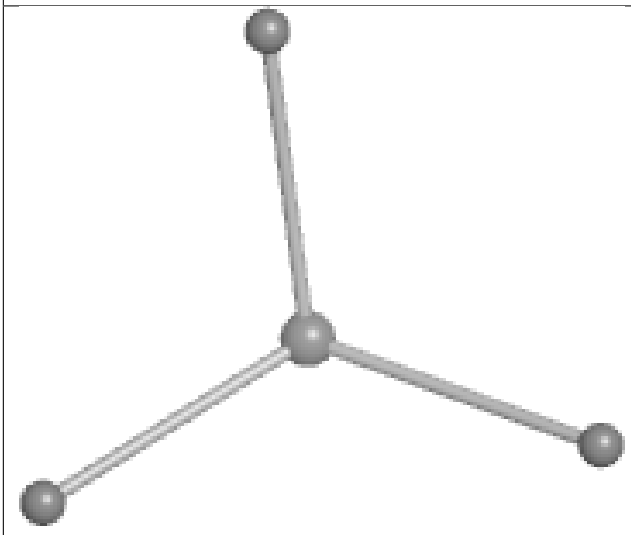

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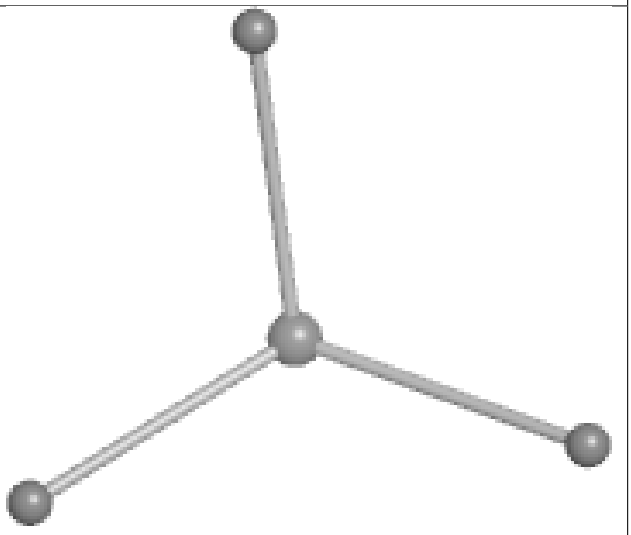
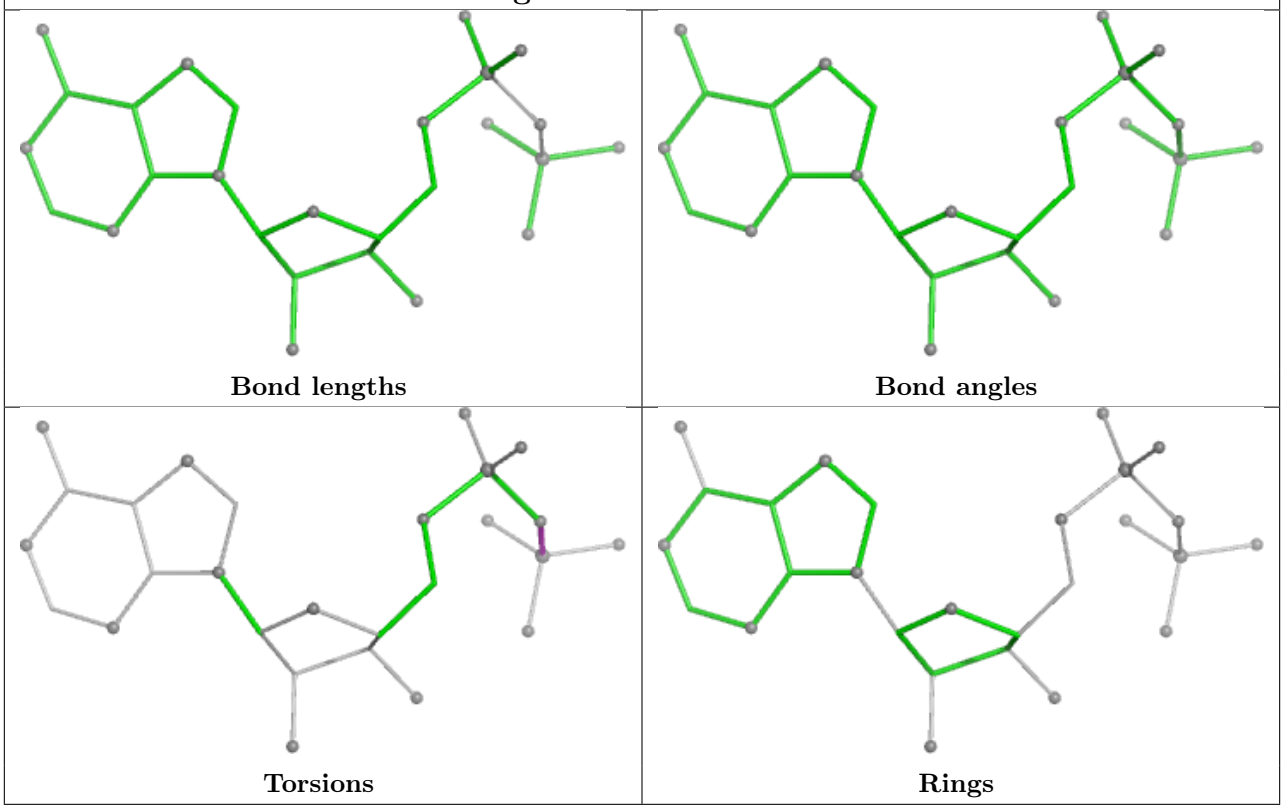


Rings

Ligand ADP A1 401



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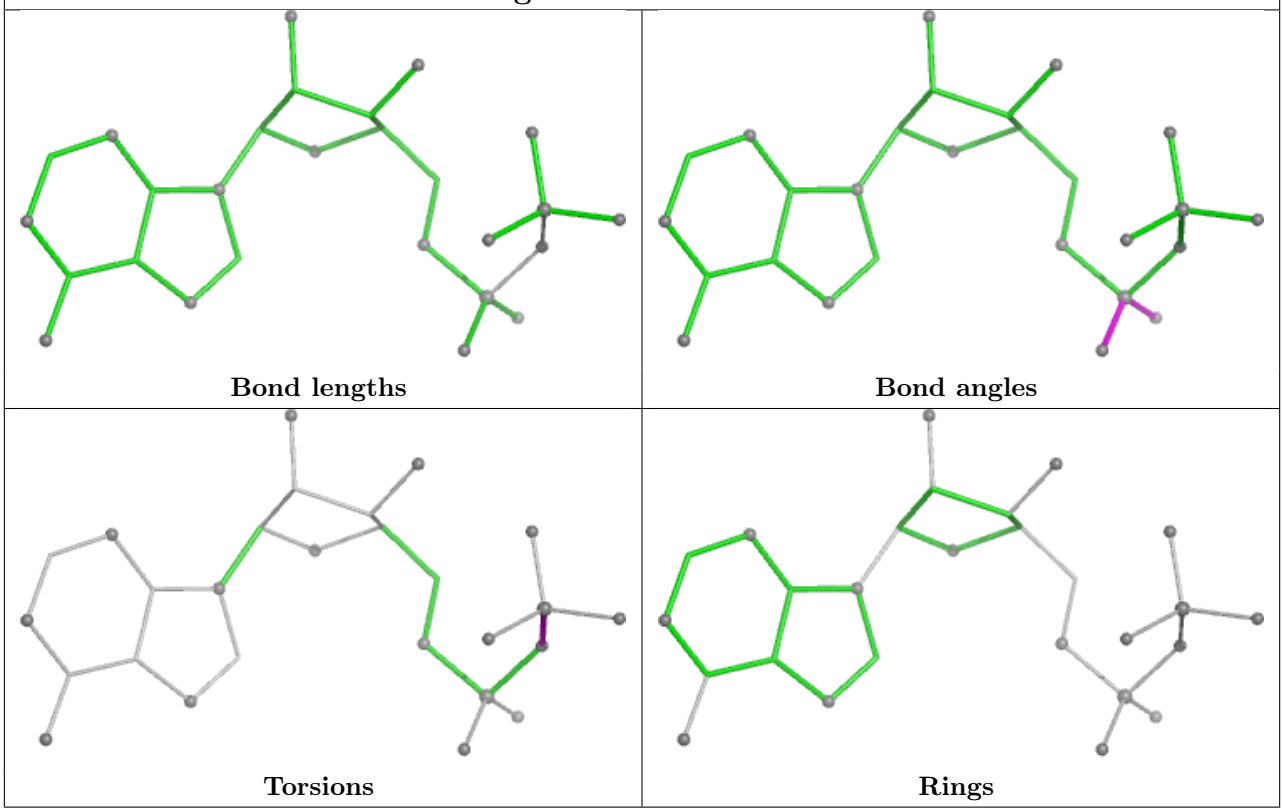

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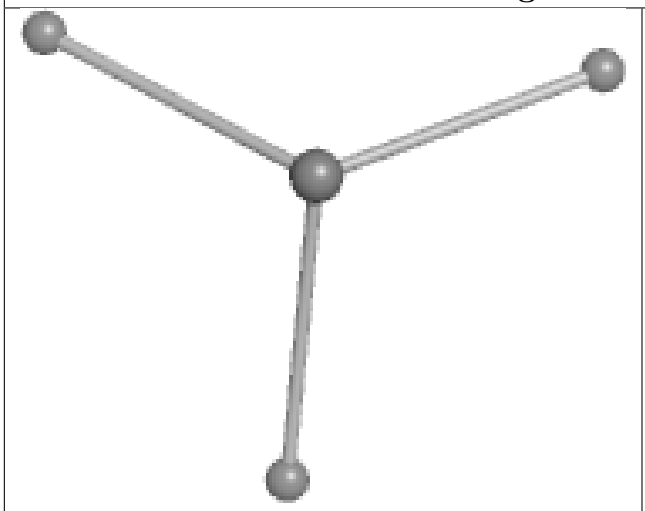
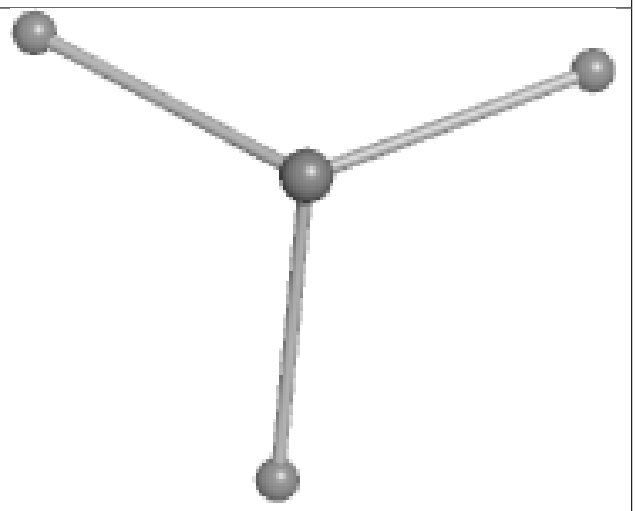
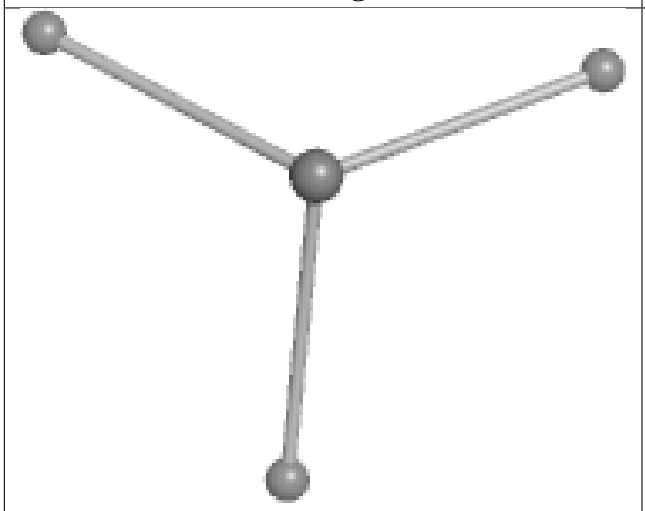


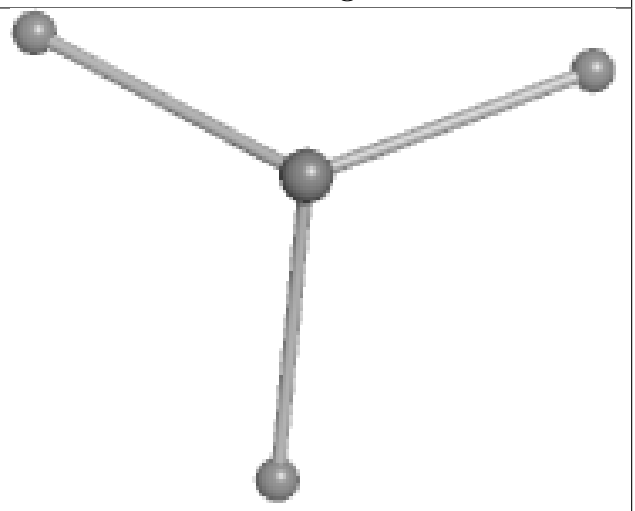
Bond lengths



Bond angles

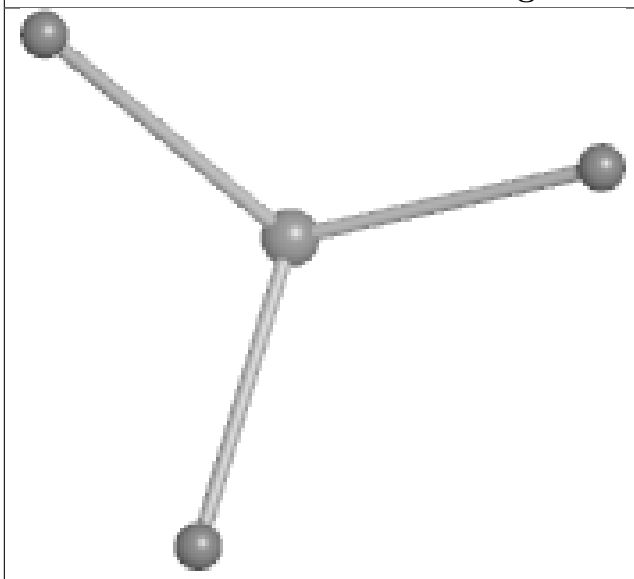


Torsions



Rings

Ligand BEF C1 403



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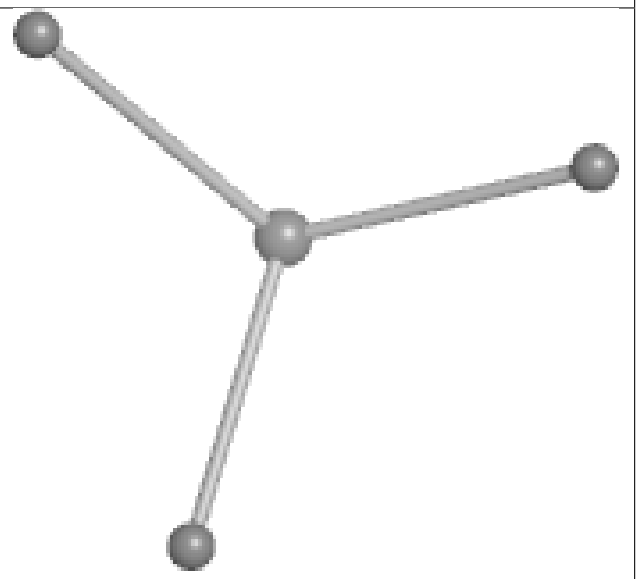
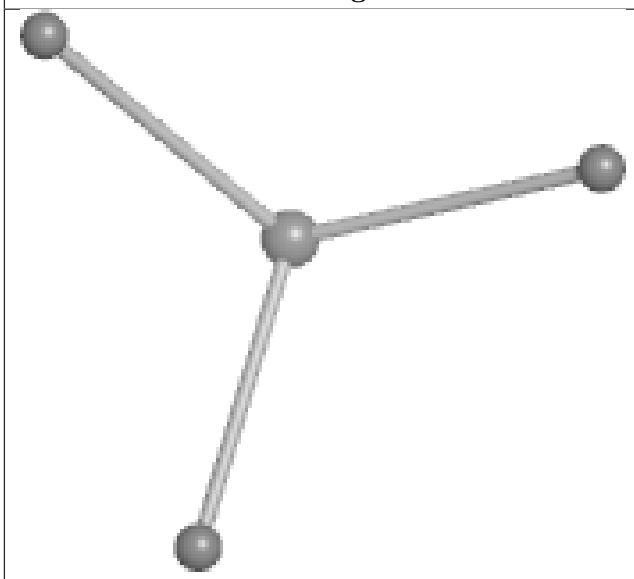


Bond angles



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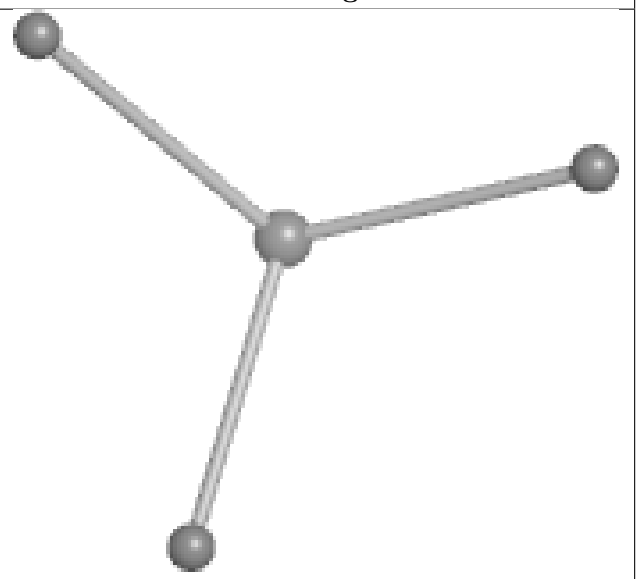
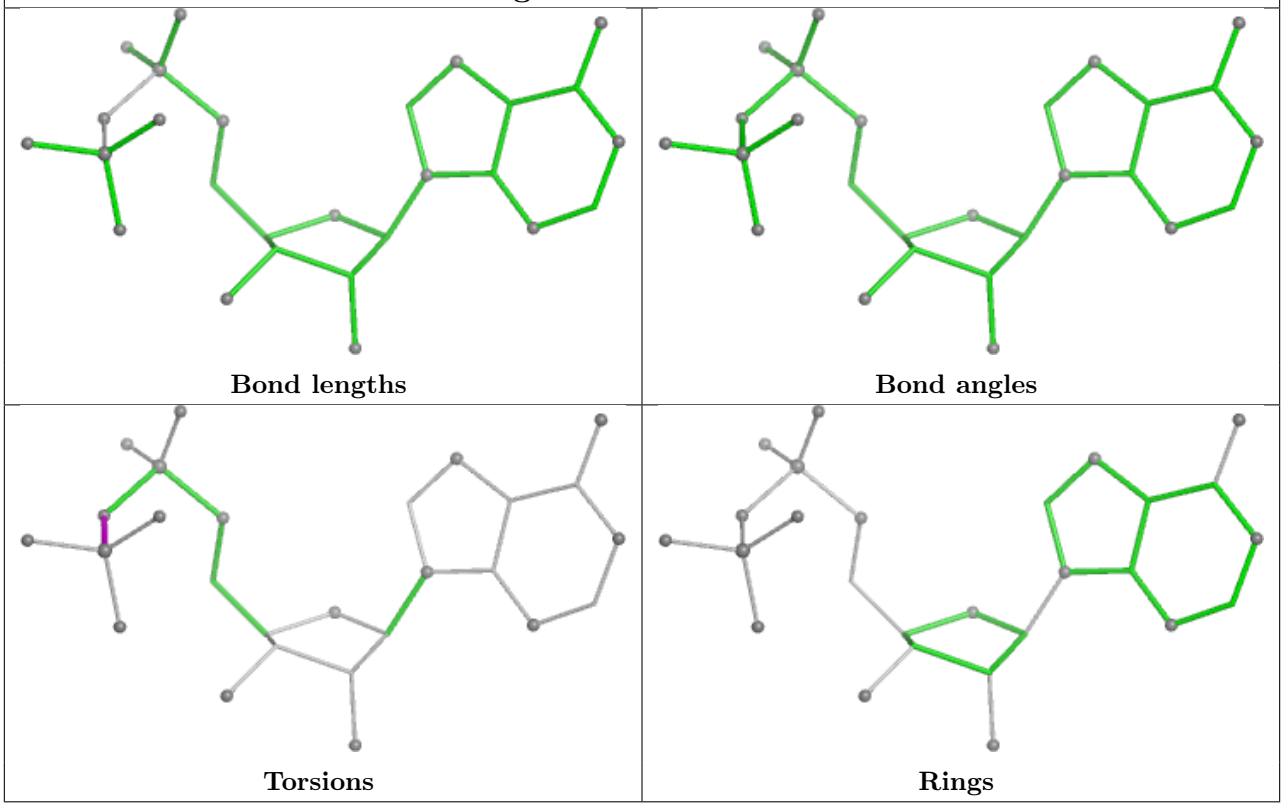


Rings

Ligand ADP D1 401



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	A1	334/341 (97%)	0.82	37 (11%)	10	14	8, 23, 43, 69	22 (6%)
1	B1	334/341 (97%)	1.19	61 (18%)	3	4	8, 26, 49, 74	24 (7%)
1	C1	334/341 (97%)	1.10	60 (17%)	3	4	7, 28, 51, 62	25 (7%)
1	D1	337/341 (98%)	0.99	52 (15%)	5	7	8, 27, 46, 81	29 (8%)
All	All	1339/1364 (98%)	1.02	210 (15%)	5	6	7, 26, 48, 81	100 (7%)

The worst 5 of 210 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B1	3	PHE	6.4
1	B1	165	ALA	5.5
1	A1	166	LEU	5.4
1	A1	3	PHE	5.4
1	C1	88	PHE	5.3

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(Å^2)	Q<0.9
10	GOL	D1	407	6/6	0.52	0.23	81,83,85,85	0
9	ACT	A1	409	4/4	0.55	0.28	56,57,60,60	0
10	GOL	C1	407	6/6	0.68	0.25	65,66,67,68	0
8	EDO	A1	416	4/4	0.71	0.24	45,47,48,52	0
9	ACT	D1	406	4/4	0.72	0.18	40,46,47,50	0
9	ACT	B1	411	4/4	0.75	0.20	36,39,40,41	0
10	GOL	A1	413	6/6	0.75	0.22	40,42,44,46	0
8	EDO	C1	408	4/4	0.76	0.23	44,45,47,47	0
10	GOL	D1	410	6/6	0.77	0.19	53,56,57,58	0
8	EDO	A1	412	4/4	0.78	0.26	53,55,58,60	0
9	ACT	A1	411	4/4	0.78	0.19	41,46,47,47	0
8	EDO	A1	410	4/4	0.79	0.20	38,43,46,47	0
8	EDO	B1	410	4/4	0.80	0.13	53,54,54,55	0
8	EDO	B1	409	4/4	0.81	0.21	57,58,59,60	0
8	EDO	D1	409	4/4	0.81	0.21	46,48,48,50	0
9	ACT	C1	406	4/4	0.82	0.18	57,57,58,58	0
9	ACT	A1	415	4/4	0.83	0.14	35,37,37,37	0
10	GOL	A1	414	6/6	0.85	0.13	40,46,48,52	0
5	NA	C1	404	1/1	0.85	0.10	29,29,29,29	0
9	ACT	D1	408	4/4	0.86	0.14	38,39,40,40	0
11	CL	B1	407	1/1	0.86	0.16	64,64,64,64	0
11	CL	B1	408	1/1	0.87	0.16	78,78,78,78	0
5	NA	D1	404	1/1	0.89	0.09	26,26,26,26	0
8	EDO	C1	409	4/4	0.91	0.10	26,29,30,31	0
5	NA	A1	404	1/1	0.92	0.07	20,20,20,20	0
8	EDO	A1	408	4/4	0.92	0.09	26,28,28,30	0
8	EDO	B1	412	4/4	0.94	0.07	26,26,27,28	0
3	MG	C1	402	1/1	0.94	0.04	25,25,25,25	0
8	EDO	D1	411	4/4	0.95	0.07	28,28,28,30	0
4	BEF	C1	403	4/4	0.95	0.06	15,16,18,20	0
7	MES	B1	406	12/12	0.95	0.08	21,25,26,26	0
7	MES	A1	407	12/12	0.96	0.08	17,20,21,21	0
2	ADP	B1	401	27/27	0.96	0.06	12,17,19,22	0
5	NA	B1	404	1/1	0.96	0.07	20,20,20,20	0
4	BEF	B1	403	4/4	0.97	0.07	14,15,15,19	0
2	ADP	C1	401	27/27	0.97	0.06	18,21,24,24	0
2	ADP	D1	401	27/27	0.97	0.06	15,19,20,21	0
2	ADP	A1	401	27/27	0.97	0.05	12,14,19,19	0
3	MG	D1	402	1/1	0.97	0.09	23,23,23,23	0
4	BEF	A1	403	4/4	0.97	0.05	15,15,16,18	0
6	CA	A1	406	1/1	0.97	0.04	31,31,31,31	0
6	CA	C1	405	1/1	0.97	0.04	37,37,37,37	0
6	CA	D1	405	1/1	0.97	0.06	38,38,38,38	0

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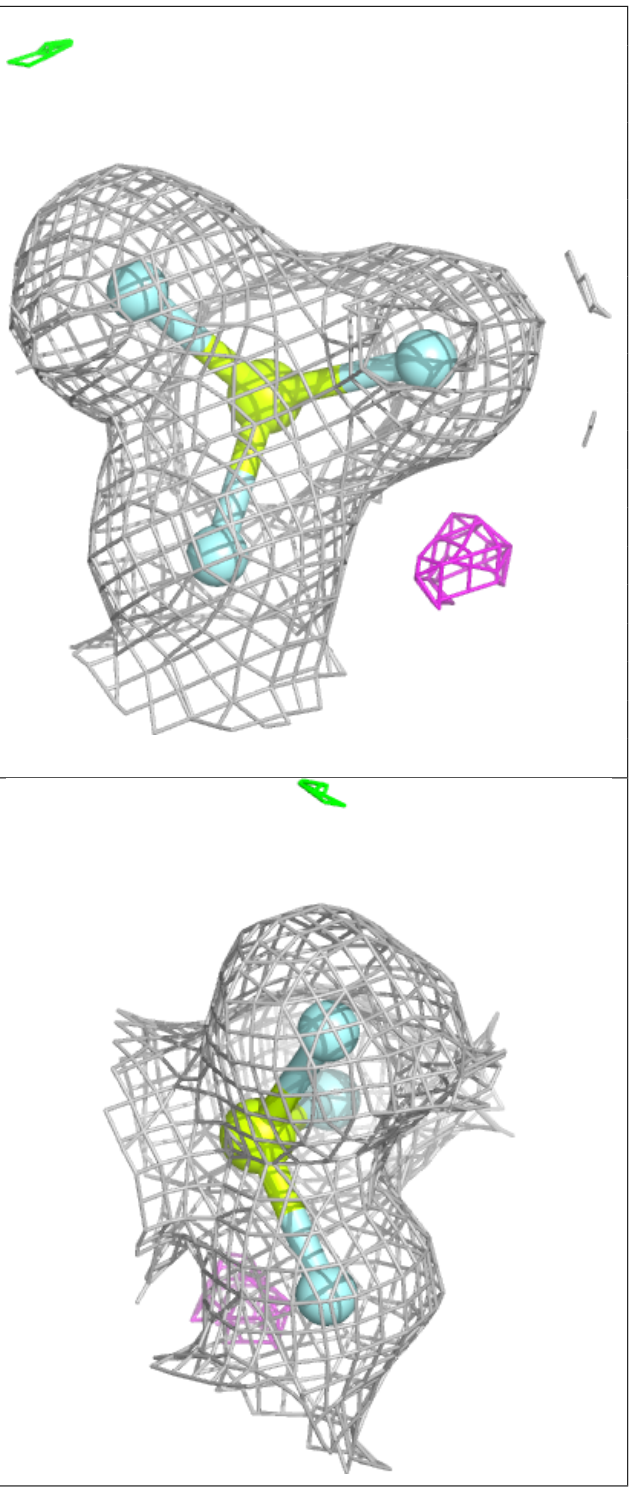
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B1	402	1/1	0.98	0.04	20,20,20,20	0
4	BEF	D1	403	4/4	0.98	0.04	17,17,18,22	0
6	CA	B1	405	1/1	0.99	0.03	22,22,22,22	0
3	MG	A1	402	1/1	0.99	0.04	21,21,21,21	0
6	CA	A1	405	1/1	1.00	0.01	21,21,21,21	0

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.

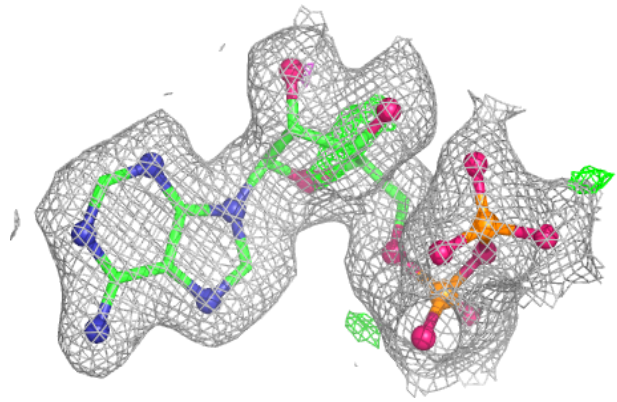
Electron density around BEF C1 403:

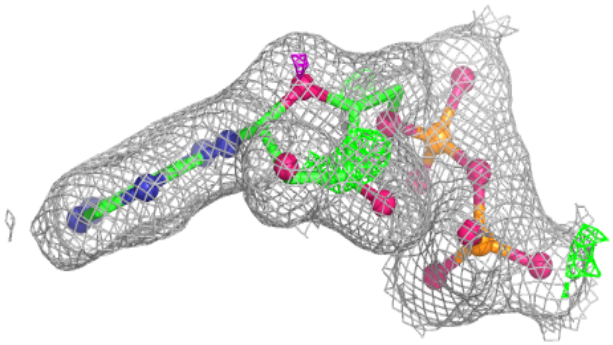
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

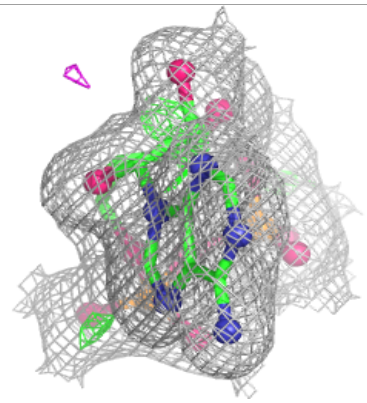


Electron density around ADP B1 401:

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

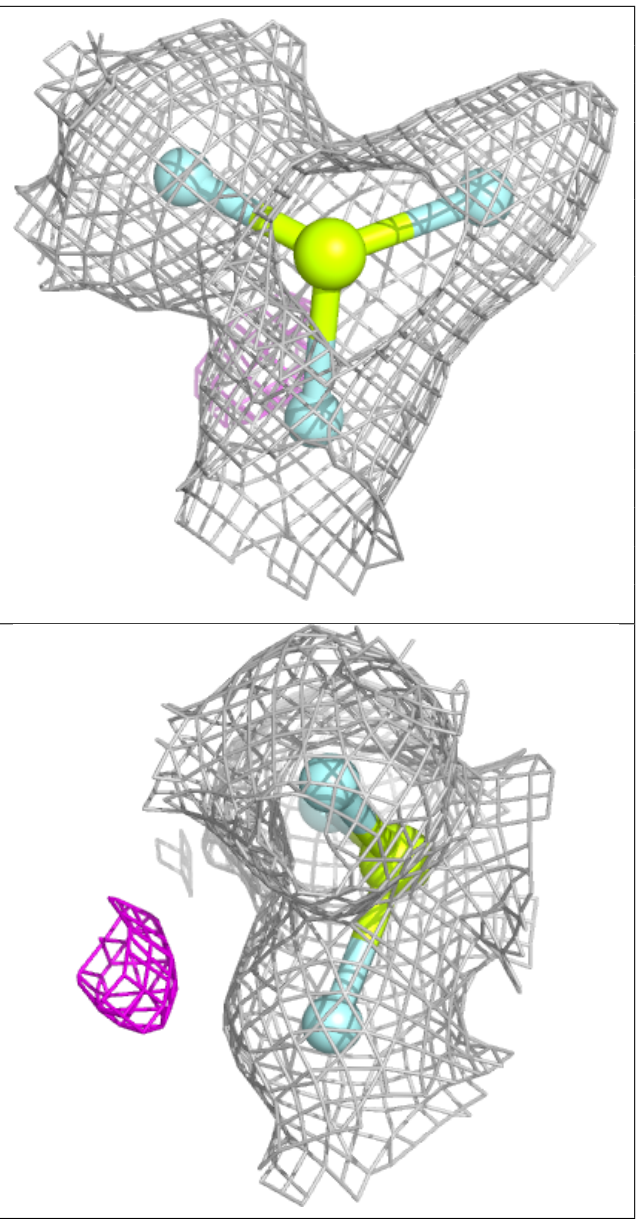






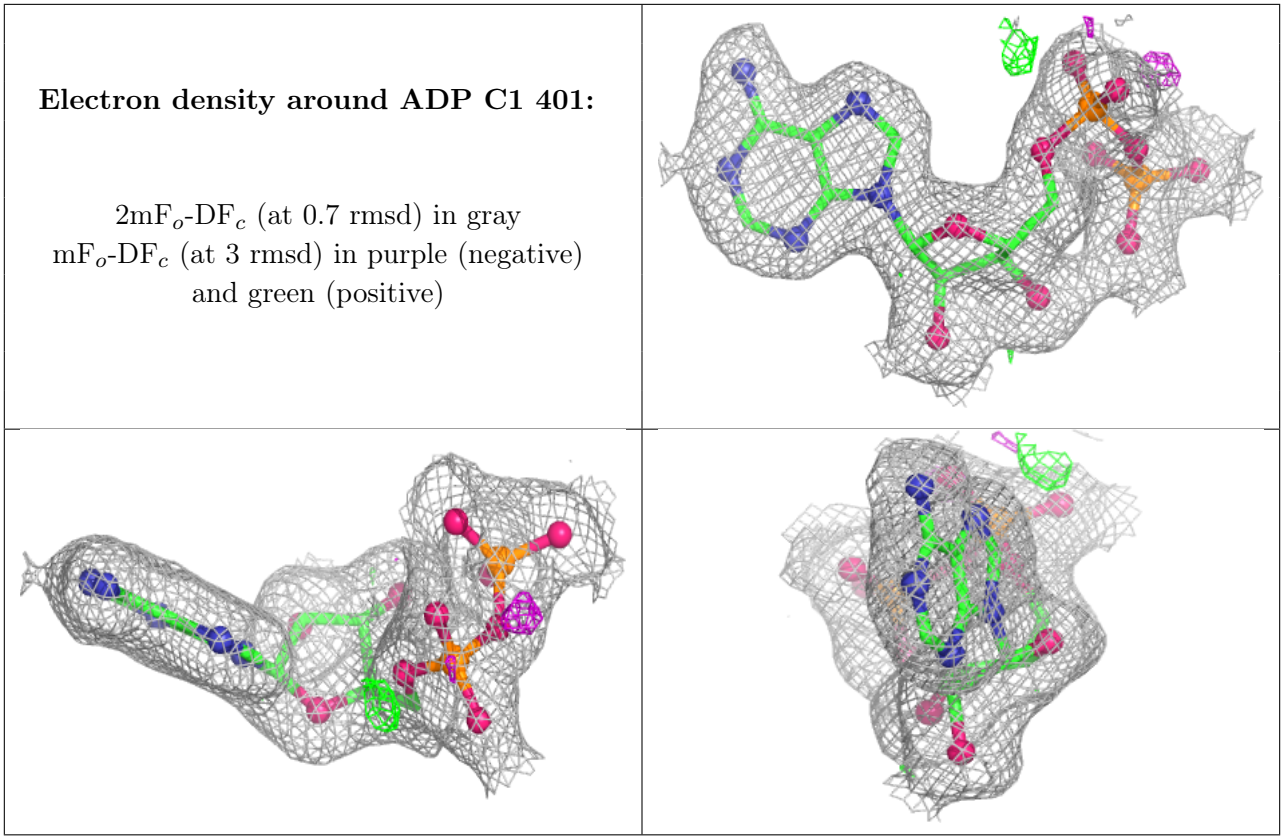
Electron density around BEF B1 403:

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



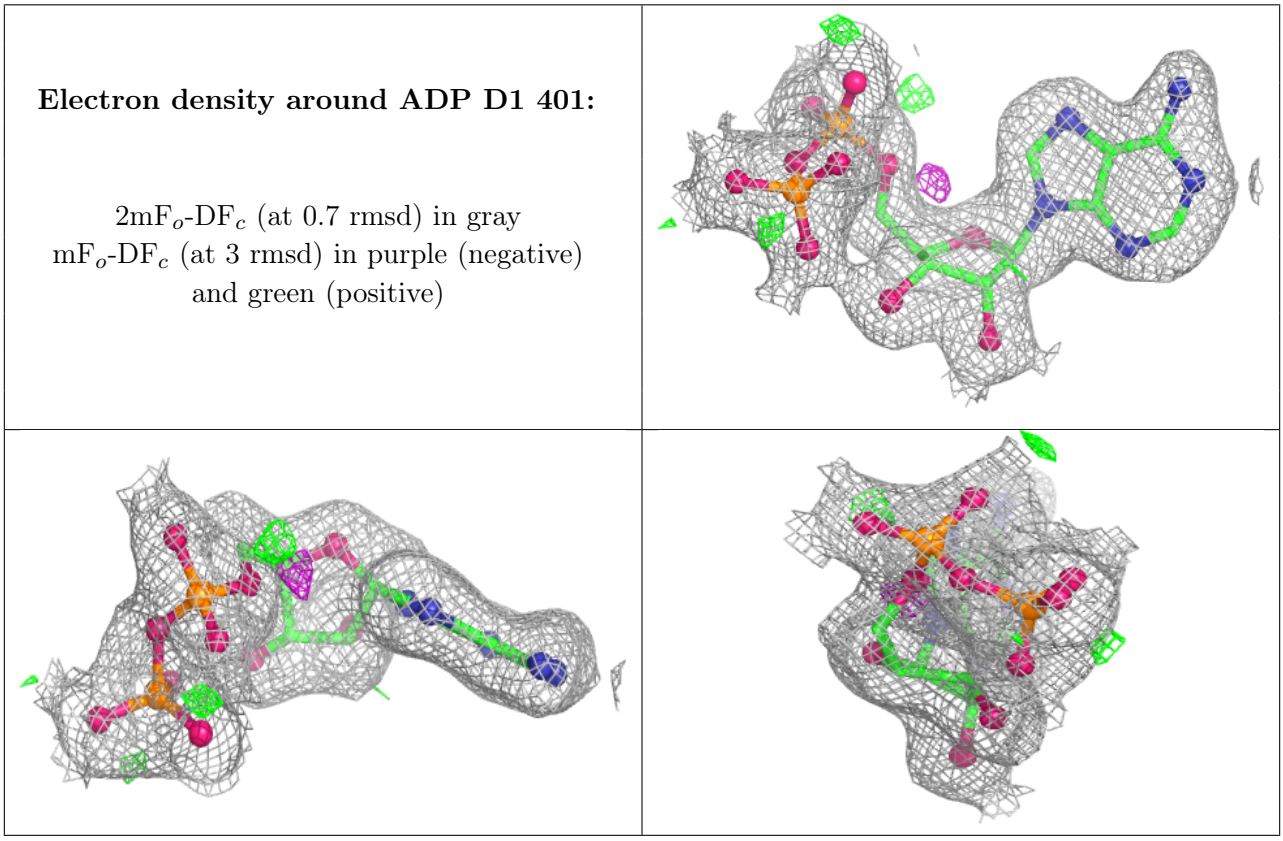
Electron density around ADP C1 401:

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



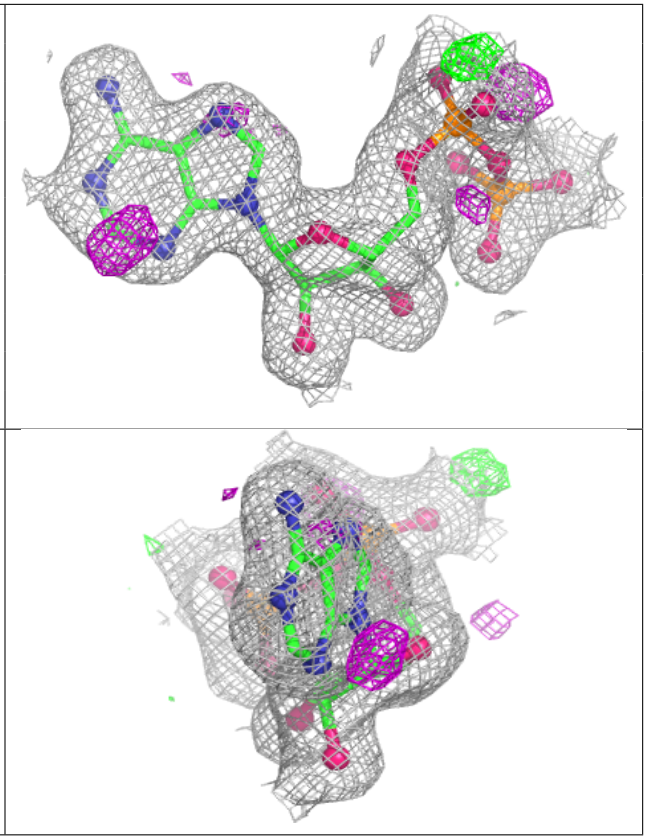
Electron density around ADP D1 401:

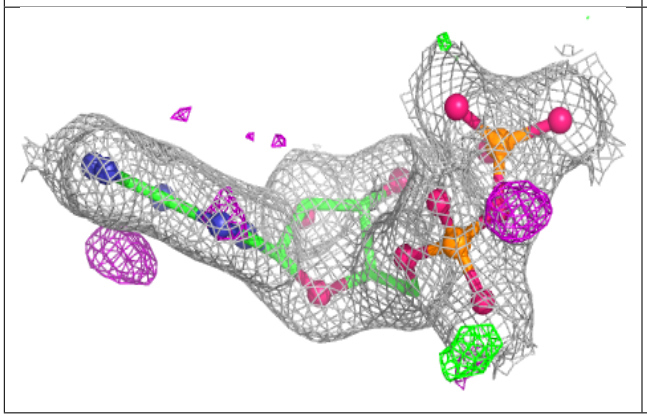
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A1 401:

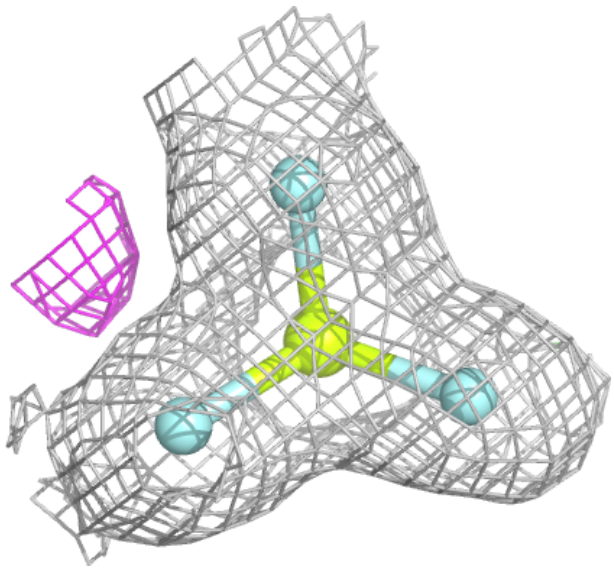
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

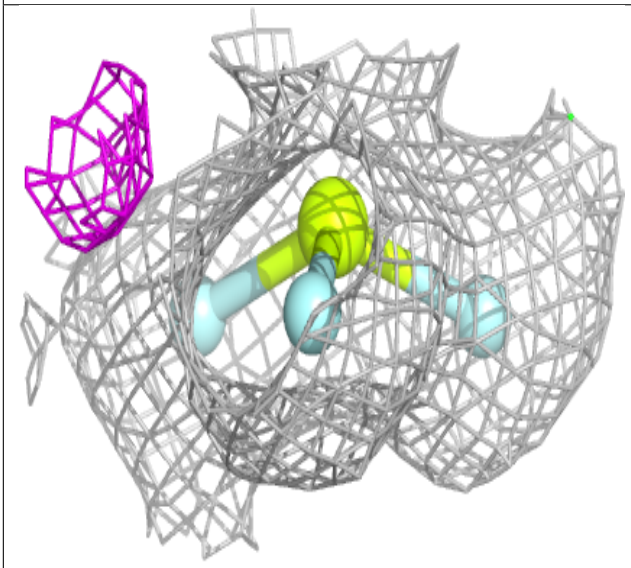


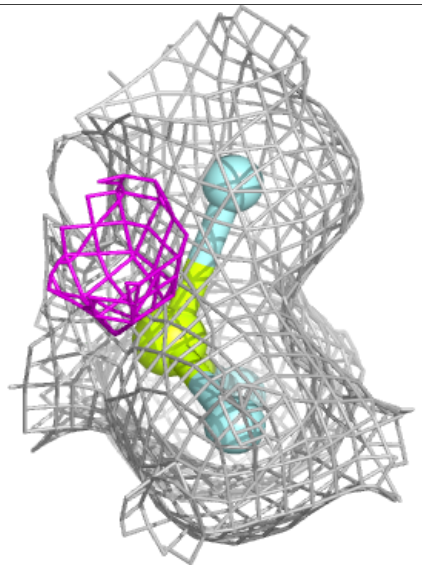


Electron density around BEF A1 403:

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

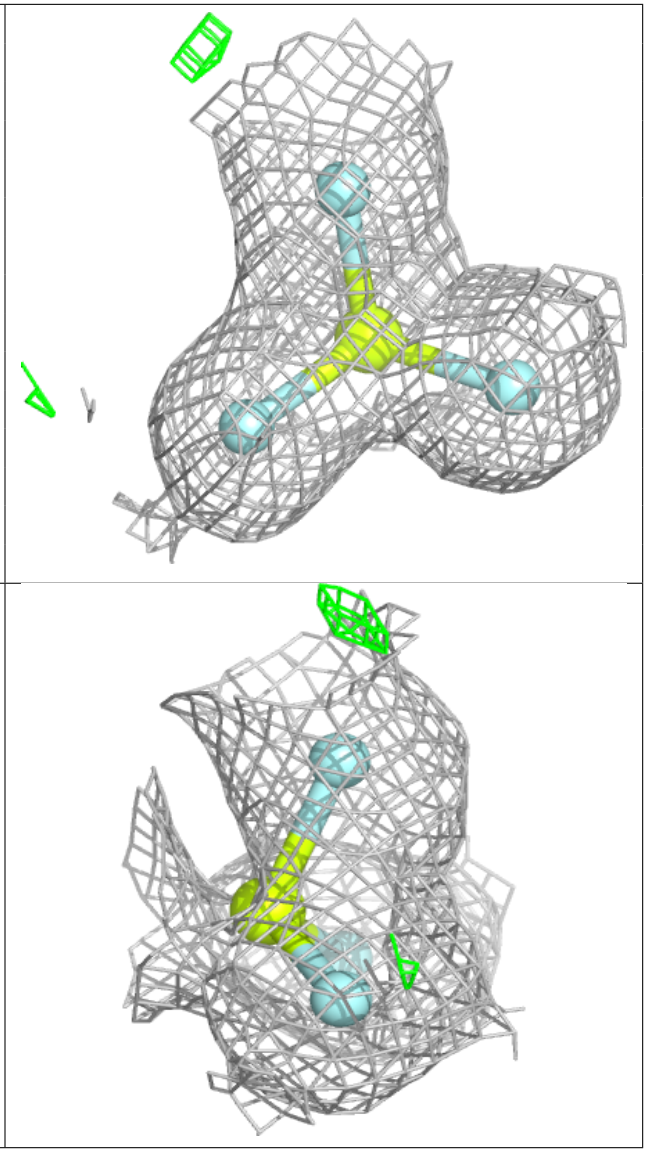






Electron density around BEF D1 403:

$2mF_o$-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.