Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 02:07 PM JST

PDB ID	:	7V1W
Title	:	Difructose dianhydride I synthase/hydrolase (alphaFFase1) from Bifidobacterium dentium in complex with beta-D-arabinofuranose
Authors	:	Kashima, T.; Arakawa, T.; Yamada, C.; Fujita, K.; Fushinobu, S.
Deposited on	:	2021-08-06
Resolution	:	1.86 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:

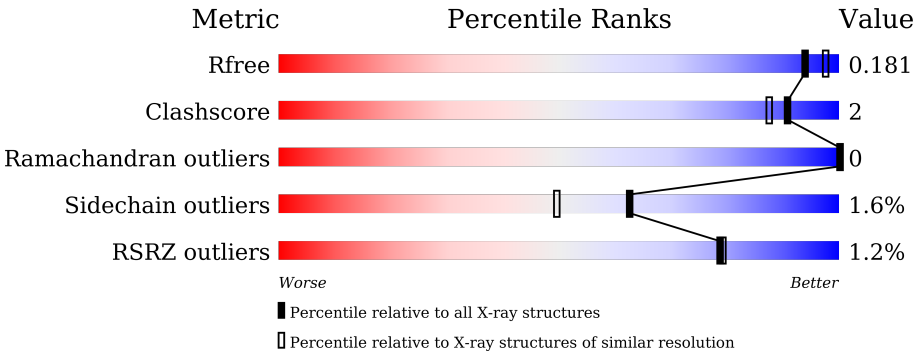
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	460	92% 5%
1	B	460	90% 7%
1	C	460	90% 7%
1	D	460	91% 6%
1	E	460	90% 6%
1	F	460	94%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23582 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 Difructose dianhydride I synthase/hydrolase (alphaFFase1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3628	2321	611	682	14			
1	B	447	Total	C	N	O	S	0	0	0
			3628	2321	611	682	14			
1	C	447	Total	C	N	O	S	0	0	0
			3628	2321	611	682	14			
1	D	447	Total	C	N	O	S	0	0	0
			3628	2321	611	682	14			
1	E	447	Total	C	N	O	S	0	0	0
			3628	2321	611	682	14			
1	F	447	Total	C	N	O	S	0	0	0
			3628	2321	611	682	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	LEU	-	expression tag	UNP A0A6L9SN29
A	454	GLU	-	expression tag	UNP A0A6L9SN29
A	455	HIS	-	expression tag	UNP A0A6L9SN29
A	456	HIS	-	expression tag	UNP A0A6L9SN29
A	457	HIS	-	expression tag	UNP A0A6L9SN29
A	458	HIS	-	expression tag	UNP A0A6L9SN29
A	459	HIS	-	expression tag	UNP A0A6L9SN29
A	460	HIS	-	expression tag	UNP A0A6L9SN29
B	453	LEU	-	expression tag	UNP A0A6L9SN29
B	454	GLU	-	expression tag	UNP A0A6L9SN29
B	455	HIS	-	expression tag	UNP A0A6L9SN29
B	456	HIS	-	expression tag	UNP A0A6L9SN29
B	457	HIS	-	expression tag	UNP A0A6L9SN29
B	458	HIS	-	expression tag	UNP A0A6L9SN29
B	459	HIS	-	expression tag	UNP A0A6L9SN29
B	460	HIS	-	expression tag	UNP A0A6L9SN29
C	453	LEU	-	expression tag	UNP A0A6L9SN29

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Chain	Residue	Modelled	Actual	Comment	Reference
C	454	GLU	-	expression tag	UNP A0A6L9SN29
C	455	HIS	-	expression tag	UNP A0A6L9SN29
C	456	HIS	-	expression tag	UNP A0A6L9SN29
C	457	HIS	-	expression tag	UNP A0A6L9SN29
C	458	HIS	-	expression tag	UNP A0A6L9SN29
C	459	HIS	-	expression tag	UNP A0A6L9SN29
C	460	HIS	-	expression tag	UNP A0A6L9SN29
D	453	LEU	-	expression tag	UNP A0A6L9SN29
D	454	GLU	-	expression tag	UNP A0A6L9SN29
D	455	HIS	-	expression tag	UNP A0A6L9SN29
D	456	HIS	-	expression tag	UNP A0A6L9SN29
D	457	HIS	-	expression tag	UNP A0A6L9SN29
D	458	HIS	-	expression tag	UNP A0A6L9SN29
D	459	HIS	-	expression tag	UNP A0A6L9SN29
D	460	HIS	-	expression tag	UNP A0A6L9SN29
E	453	LEU	-	expression tag	UNP A0A6L9SN29
E	454	GLU	-	expression tag	UNP A0A6L9SN29
E	455	HIS	-	expression tag	UNP A0A6L9SN29
E	456	HIS	-	expression tag	UNP A0A6L9SN29
E	457	HIS	-	expression tag	UNP A0A6L9SN29
E	458	HIS	-	expression tag	UNP A0A6L9SN29
E	459	HIS	-	expression tag	UNP A0A6L9SN29
E	460	HIS	-	expression tag	UNP A0A6L9SN29
F	453	LEU	-	expression tag	UNP A0A6L9SN29
F	454	GLU	-	expression tag	UNP A0A6L9SN29
F	455	HIS	-	expression tag	UNP A0A6L9SN29
F	456	HIS	-	expression tag	UNP A0A6L9SN29
F	457	HIS	-	expression tag	UNP A0A6L9SN29
F	458	HIS	-	expression tag	UNP A0A6L9SN29
F	459	HIS	-	expression tag	UNP A0A6L9SN29
F	460	HIS	-	expression tag	UNP A0A6L9SN29

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	2	Total Ca 2 2	0	0

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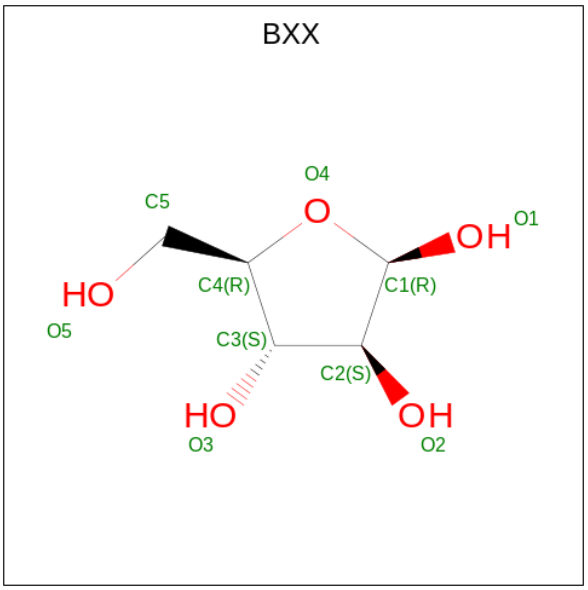
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Ca 1 1	0	0

- Molecule 3 is beta-D-arabinofuranose (three-letter code: BXX) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0
3	E	1	Total C O 10 5 5	0	0
3	F	1	Total C O 10 5 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	290	Total O 290 290	0	0
4	B	329	Total O 329 329	0	0

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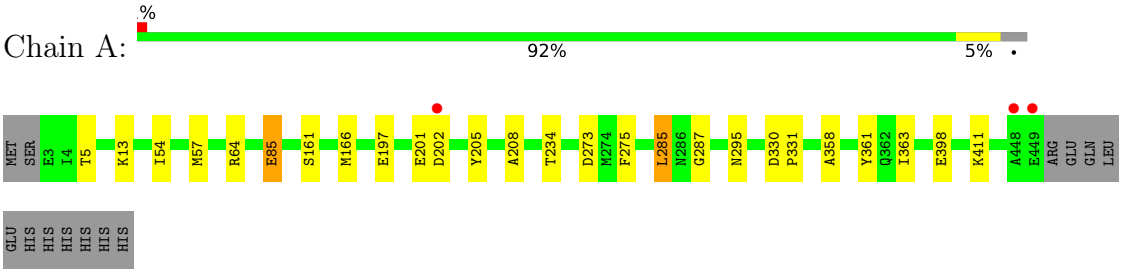
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	267	Total O 267 267	0	0
4	D	305	Total O 305 305	0	0
4	E	287	Total O 287 287	0	0
4	F	270	Total O 270 270	0	0

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.

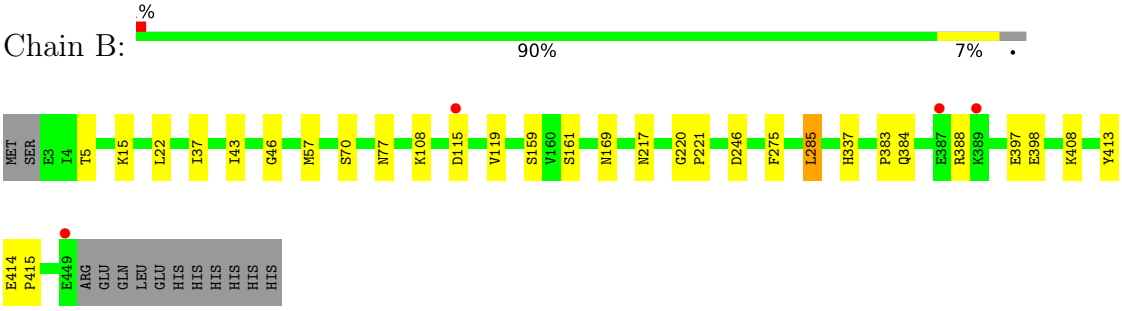
• Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)

Chain A:



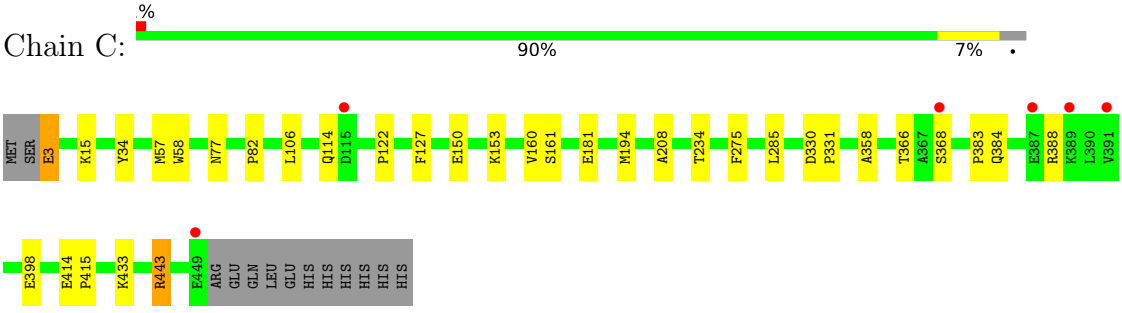
• Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)

Chain B:



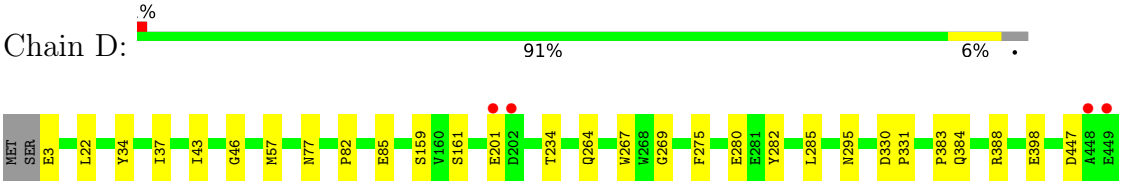
• Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)

Chain C:

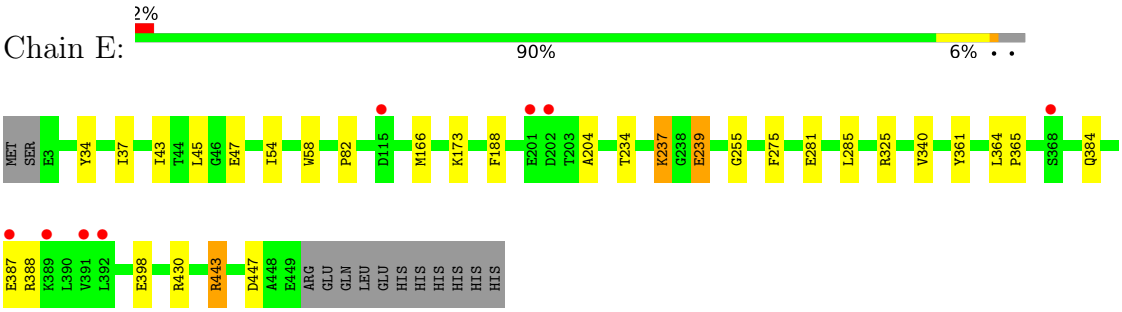


• Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)

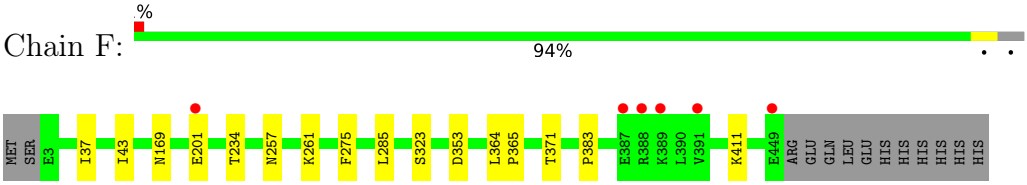
Chain D:



• Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



• Molecule 1: Difructose dianhydride I synthase/hydrolase (alphaFFase1)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.45Å 156.71Å 100.85Å 90.00° 110.66° 90.00°	Depositor
Resolution (Å)	48.77 – 1.86 48.72 – 1.86	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.77-1.86) 100.0 (48.72-1.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.203 0.178 , 0.181	Depositor DCC
R_{free} test set	11986 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.074 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23582	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: CA, BXX

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	0.70	0/3744	0.87	0/5098
1	B	0.71	1/3744 (0.0%)	0.87	0/5098
1	C	0.70	0/3744	0.85	0/5098
1	D	0.70	0/3744	0.86	0/5098
1	E	0.70	0/3744	0.86	4/5098 (0.1%)
1	F	0.71	0/3744	0.84	0/5098
All	All	0.70	1/22464 (0.0%)	0.86	4/30588 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	397	GLU	CD-OE2	5.86	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	443	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	E	443	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	E	430	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	430	ARG	NE-CZ-NH1	5.31	122.95	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	3422	13	0
1	B	3628	0	3422	16	0
1	C	3628	0	3422	18	0
1	D	3628	0	3422	13	0
1	E	3628	0	3422	17	0
1	F	3628	0	3422	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	10	0	10	0	0
3	B	10	0	10	0	0
3	C	10	0	10	0	0
3	D	10	0	10	0	0
3	E	10	0	10	0	0
3	F	10	0	10	0	0
4	A	290	0	0	1	0
4	B	329	0	0	2	0
4	C	267	0	0	1	0
4	D	305	0	0	1	0
4	E	287	0	0	0	0
4	F	270	0	0	1	0
All	All	23582	0	20592	74	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.

All (74) 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:D:275:PHE:HB2	1:D:285:LEU:HB2	1.75	0.69
1:E:443:ARG:HD2	1:E:447:ASP:OD2	1.93	0.69
1:A:275:PHE:HB2	1:A:285:LEU:HB2	1.76	0.67
1:B:398:GLU:OE1	1:F:234:THR:HG23	1.95	0.65
1:C:275:PHE:HB2	1:C:285:LEU:HB2	1.79	0.65
1:F:275:PHE:HB2	1:F:285:LEU:HB2	1.80	0.63
1:E:37:ILE:HD12	1:E:43:ILE:HG21	1.82	0.60
1:E:275:PHE:HB2	1:E:285:LEU:HB2	1.83	0.60
1:D:37:ILE:HD12	1:D:43:ILE:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PHE:HB2	1:B:285:LEU:HB2	1.85	0.58
1:C:3:GLU:N	1:C:3:GLU:OE1	2.38	0.56
1:C:234:THR:HG23	1:D:398:GLU:OE2	2.06	0.55
1:F:37:ILE:HD12	1:F:43:ILE:HG21	1.88	0.55
1:E:237:LYS:HE2	1:E:281:GLU:OE1	2.06	0.54
1:B:37:ILE:HD12	1:B:43:ILE:HG21	1.90	0.53
1:C:194:MET:SD	1:C:443:ARG:HG2	2.50	0.51
1:A:234:THR:HG23	1:E:398:GLU:OE1	2.10	0.50
1:D:280:GLU:HG3	1:D:282:TYR:O	2.11	0.50
1:E:275:PHE:CE2	1:E:340:VAL:HG13	2.46	0.50
1:F:364:LEU:HB3	1:F:365:PRO:HA	1.94	0.50
1:C:383:PRO:HB2	1:D:383:PRO:HB2	1.93	0.49
1:C:330:ASP:N	1:C:331:PRO:CD	2.75	0.49
1:C:208:ALA:HA	1:C:358:ALA:O	2.12	0.49
1:B:115:ASP:OD2	4:B:701:HOH:O	2.20	0.48
1:B:246:ASP:OD1	1:B:337:HIS:CE1	2.66	0.48
1:B:217:ASN:CG	1:B:217:ASN:O	2.52	0.47
1:A:202:ASP:O	1:A:363:ILE:HG22	2.13	0.47
1:B:22:LEU:HD13	1:B:46:GLY:HA3	1.96	0.46
1:A:398:GLU:OE2	1:E:234:THR:HG23	2.15	0.46
1:C:414:GLU:HB3	1:C:415:PRO:HD3	1.98	0.46
1:A:205:TYR:O	1:A:361:TYR:HA	2.16	0.46
1:E:47:GLU:HG2	1:E:173:LYS:HG3	1.97	0.46
1:B:115:ASP:HB2	4:B:970:HOH:O	2.16	0.45
1:B:383:PRO:HB2	1:F:383:PRO:HB2	1.98	0.45
1:C:150:GLU:OE1	1:C:153:LYS:NZ	2.42	0.45
1:B:108:LYS:HA	1:B:119:VAL:O	2.17	0.45
1:A:85:GLU:HG3	4:A:973:HOH:O	2.15	0.45
1:A:54:ILE:HB	1:A:166:MET:HB2	1.99	0.45
1:A:208:ALA:HA	1:A:358:ALA:O	2.16	0.45
1:A:295:ASN:HA	1:C:58:TRP:CD1	2.52	0.45
1:B:70:SER:HB3	1:B:413:TYR:CZ	2.52	0.45
1:D:22:LEU:HD13	1:D:46:GLY:HA3	1.98	0.45
1:C:398:GLU:OE1	1:D:234:THR:HG23	2.17	0.44
1:D:34:TYR:CE2	1:D:82:PRO:HB3	2.52	0.44
1:C:106:LEU:HD23	1:C:122:PRO:HA	1.99	0.44
1:E:204:ALA:HB1	1:E:361:TYR:HB3	2.00	0.44
1:C:127:PHE:HB3	1:C:160:VAL:HB	1.99	0.44
1:B:5:THR:HG23	1:C:15:LYS:HE2	1.98	0.44
1:E:364:LEU:HB3	1:E:365:PRO:HA	2.00	0.43
1:C:34:TYR:CE2	1:C:82:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:MET:O	1:C:161:SER:HA	2.18	0.43
1:F:371:THR:HA	4:F:767:HOH:O	2.18	0.43
1:E:54:ILE:HB	1:E:166:MET:HB2	2.00	0.43
1:A:57:MET:O	1:A:161:SER:HA	2.18	0.43
1:B:414:GLU:HB3	1:B:415:PRO:HD3	2.01	0.43
1:A:5:THR:HG23	1:B:15:LYS:HE2	2.02	0.42
1:B:57:MET:O	1:B:161:SER:HA	2.18	0.42
1:E:239:GLU:H	1:E:239:GLU:HG2	1.49	0.42
1:C:366:THR:HG22	1:C:368:SER:O	2.20	0.42
1:D:57:MET:O	1:D:161:SER:HA	2.20	0.42
1:D:267:TRP:CZ2	1:D:269:GLY:HA3	2.54	0.42
1:C:181:GLU:HG3	4:C:730:HOH:O	2.19	0.41
1:B:220:GLY:N	1:B:221:PRO:CD	2.83	0.41
1:E:34:TYR:CE1	1:E:82:PRO:HB3	2.55	0.41
1:E:443:ARG:O	1:E:443:ARG:HD3	2.21	0.41
1:D:447:ASP:OD2	4:D:701:HOH:O	2.22	0.41
1:A:330:ASP:N	1:A:331:PRO:CD	2.84	0.41
1:E:45:LEU:HD22	1:E:188:PHE:CE1	2.56	0.41
1:F:257:ASN:HA	1:F:323:SER:O	2.21	0.41
1:F:261:LYS:HB3	1:F:353:ASP:HB3	2.03	0.41
1:D:295:ASN:HA	1:E:58:TRP:CD1	2.56	0.40
1:E:255:GLY:HA3	1:E:325:ARG:O	2.21	0.40
1:A:273:ASP:OD1	1:A:287:GLY:HA3	2.21	0.40
1:D:330:ASP:N	1:D:331:PRO:CD	2.85	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	445/460 (97%)	432 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	445/460 (97%)	431 (97%)	14 (3%)	0	100	100
1	C	445/460 (97%)	429 (96%)	16 (4%)	0	100	100
1	D	445/460 (97%)	432 (97%)	13 (3%)	0	100	100
1	E	445/460 (97%)	430 (97%)	15 (3%)	0	100	100
1	F	445/460 (97%)	433 (97%)	12 (3%)	0	100	100
All	All	2670/2760 (97%)	2587 (97%)	83 (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	388/401 (97%)	381 (98%)	7 (2%)	59	45
1	B	388/401 (97%)	381 (98%)	7 (2%)	59	45
1	C	388/401 (97%)	381 (98%)	7 (2%)	59	45
1	D	388/401 (97%)	380 (98%)	8 (2%)	53	38
1	E	388/401 (97%)	383 (99%)	5 (1%)	69	58
1	F	388/401 (97%)	385 (99%)	3 (1%)	81	76
All	All	2328/2406 (97%)	2291 (98%)	37 (2%)	62	49

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	64	ARG
1	A	85	GLU
1	A	197	GLU
1	A	201	GLU
1	A	285	LEU
1	A	411	LYS
1	B	77	ASN

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Mol	Chain	Res	Type
1	B	159	SER
1	B	169	ASN
1	B	285	LEU
1	B	384	GLN
1	B	388	ARG
1	B	408	LYS
1	C	3	GLU
1	C	77	ASN
1	C	114	GLN
1	C	384	GLN
1	C	388	ARG
1	C	433	LYS
1	C	443	ARG
1	D	3	GLU
1	D	77	ASN
1	D	85	GLU
1	D	159	SER
1	D	201	GLU
1	D	264	GLN
1	D	384	GLN
1	D	388	ARG
1	E	237	LYS
1	E	239	GLU
1	E	384	GLN
1	E	387	GLU
1	E	388	ARG
1	F	169	ASN
1	F	201	GLU
1	F	411	LYS

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

Mol	Chain	Res	Type
1	C	27	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)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	BXX	C	602	-	10,10,10	1.38	2 (20%)	13,14,14	1.13	1 (7%)
3	BXX	A	602	-	10,10,10	1.27	1 (10%)	13,14,14	1.29	2 (15%)
3	BXX	E	602	-	10,10,10	1.22	2 (20%)	13,14,14	1.08	1 (7%)
3	BXX	D	602	-	10,10,10	1.42	1 (10%)	13,14,14	1.07	0
3	BXX	B	602	-	10,10,10	1.59	3 (30%)	13,14,14	1.41	2 (15%)
3	BXX	F	501	-	10,10,10	1.21	2 (20%)	13,14,14	1.07	2 (15%)

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	BXX	C	602	-	-	0/2/18/18	0/1/1/1
3	BXX	A	602	-	-	0/2/18/18	0/1/1/1
3	BXX	E	602	-	-	0/2/18/18	0/1/1/1
3	BXX	D	602	-	-	0/2/18/18	0/1/1/1
3	BXX	B	602	-	-	0/2/18/18	0/1/1/1
3	BXX	F	501	-	-	0/2/18/18	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	BXX	C1-C2	3.19	1.56	1.52
3	C	602	BXX	O4-C1	2.97	1.46	1.43
3	B	602	BXX	O4-C1	2.76	1.46	1.43
3	F	501	BXX	O4-C1	2.70	1.46	1.43
3	E	602	BXX	O4-C1	2.52	1.46	1.43
3	B	602	BXX	O1-C1	2.34	1.47	1.39
3	C	602	BXX	O1-C1	2.28	1.46	1.39
3	B	602	BXX	C1-C2	2.26	1.55	1.52
3	E	602	BXX	O1-C1	2.03	1.46	1.39
3	F	501	BXX	O1-C1	2.03	1.46	1.39
3	A	602	BXX	O4-C1	2.02	1.45	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	BXX	O2-C2-C1	2.99	120.08	111.82
3	A	602	BXX	O4-C1-C2	2.87	107.99	104.46
3	E	602	BXX	C1-C2-C3	2.67	105.64	102.30
3	C	602	BXX	O1-C1-O4	-2.64	107.75	111.13
3	B	602	BXX	O4-C1-C2	2.33	107.33	104.46
3	A	602	BXX	O2-C2-C1	2.12	117.69	111.82
3	F	501	BXX	O2-C2-C1	2.10	117.61	111.82
3	F	501	BXX	O4-C1-C2	2.08	107.02	104.46

There are no chirality outliers.

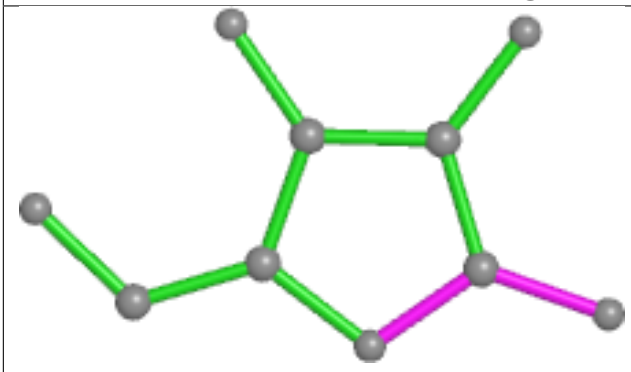
There are no torsion outliers.

There are no ring outliers.

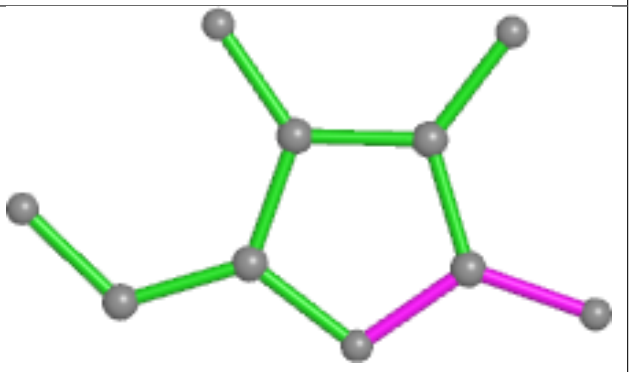
No monomer is involved in short contacts.

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

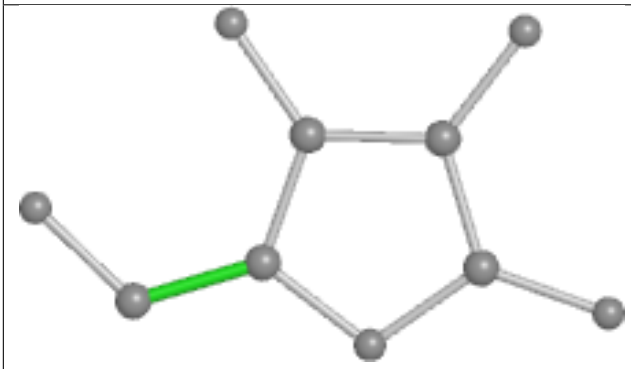
Ligand BXX C 602



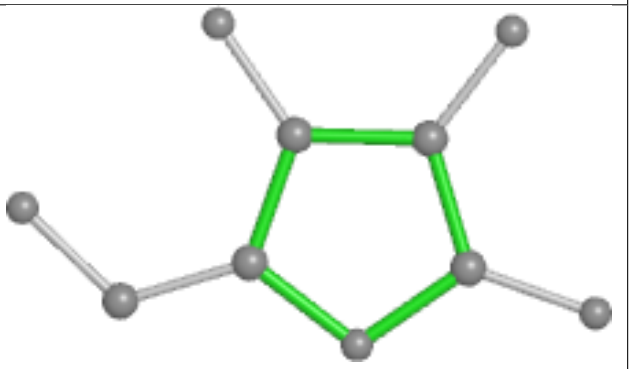
Bond lengths



Bond angles

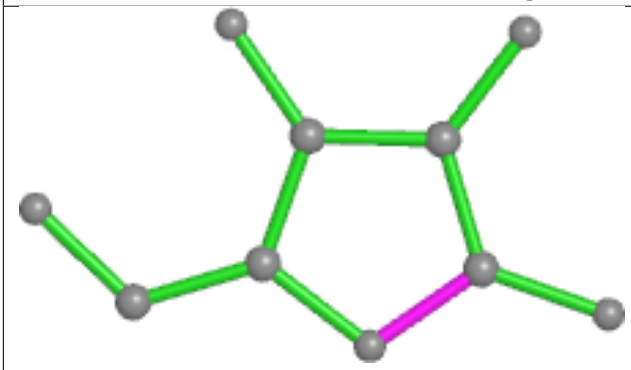


Torsions

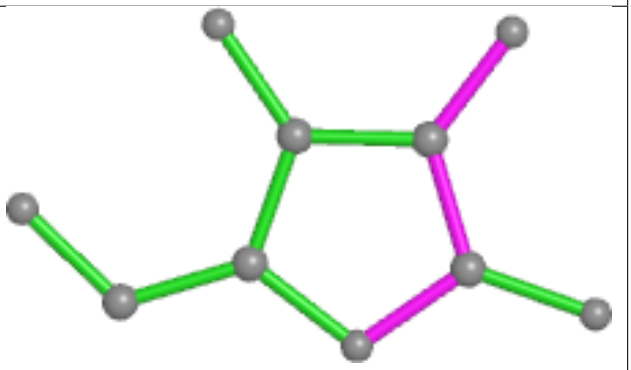


Rings

Ligand BXX A 602



Bond lengths



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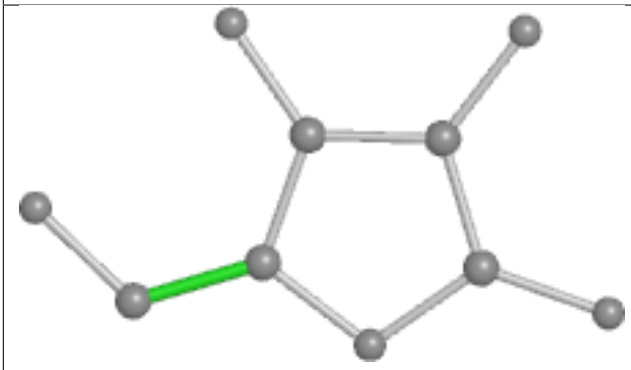
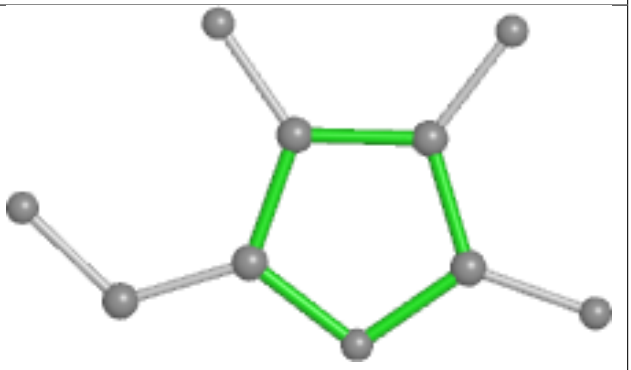
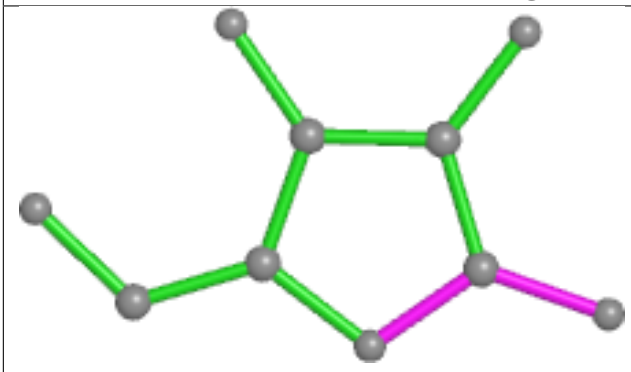


Torsions

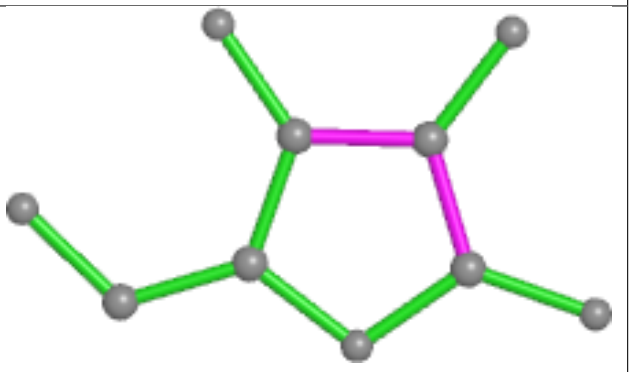


Rings

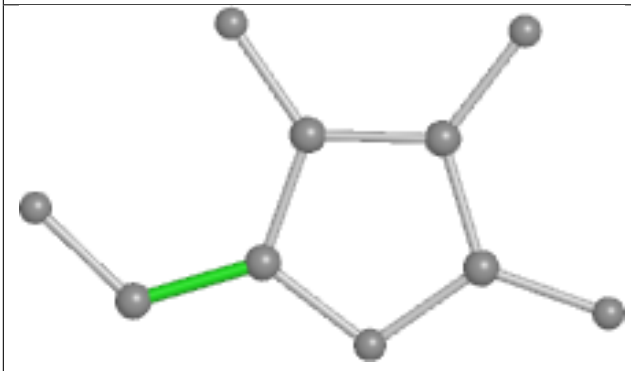
Ligand BXX E 602



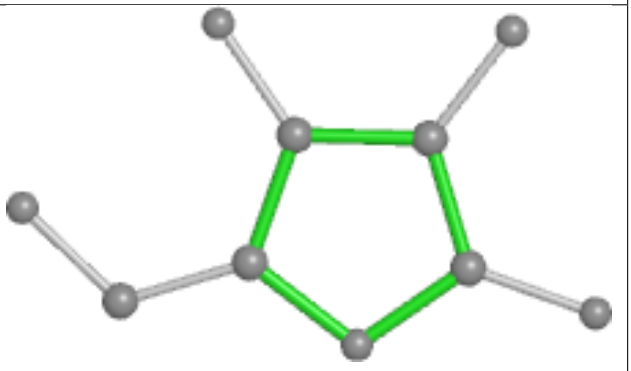
Bond lengths



Bond angles

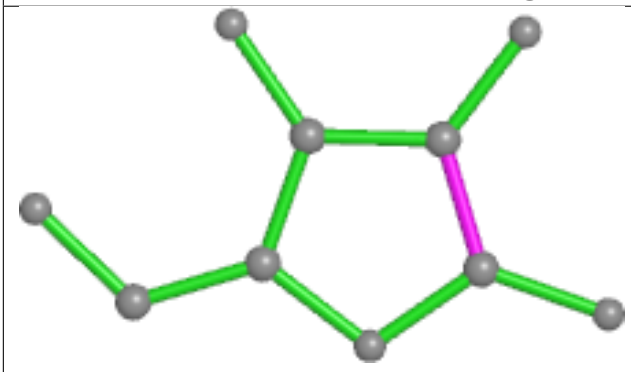


Torsions

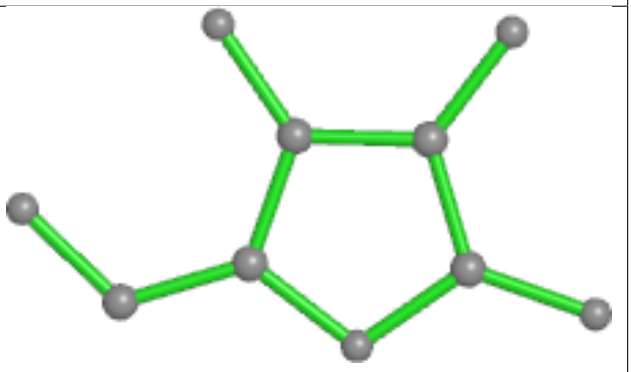


Rings

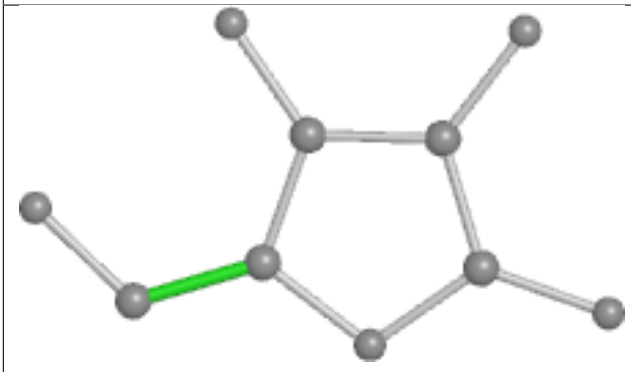
Ligand BXX D 602



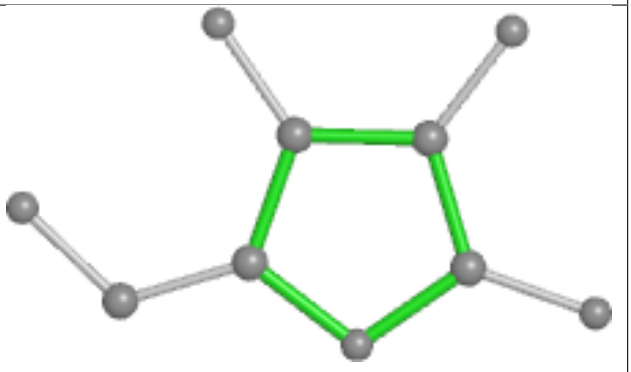
Bond lengths



Bond angles

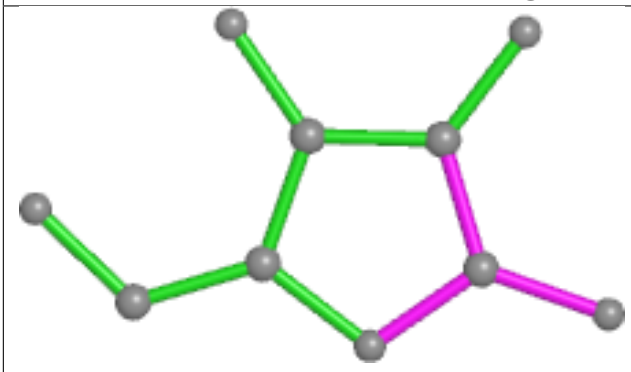


Torsions

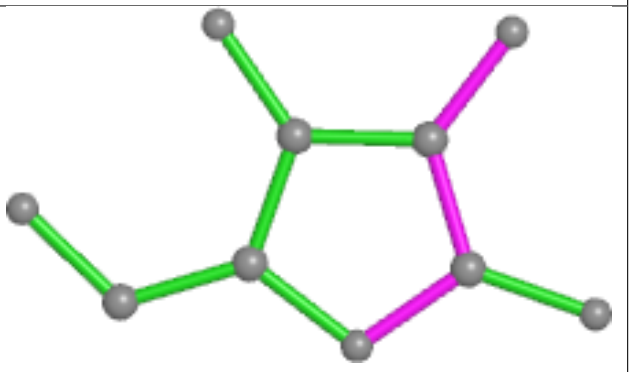


Rings

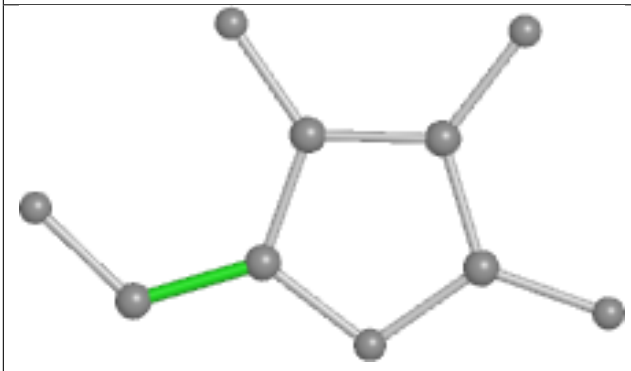
Ligand BXX B 602



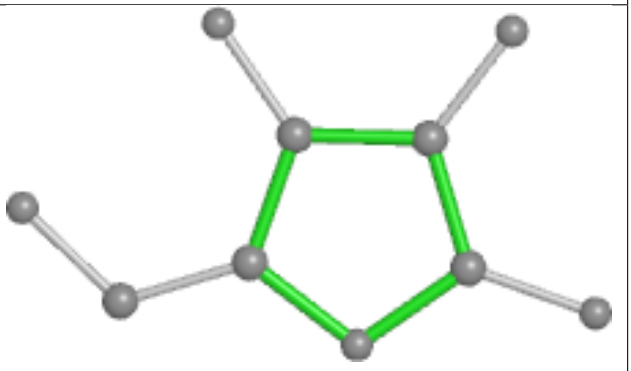
Bond lengths



Bond angles

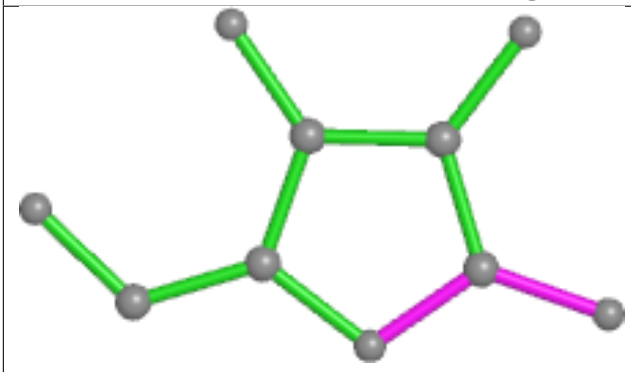


Torsions

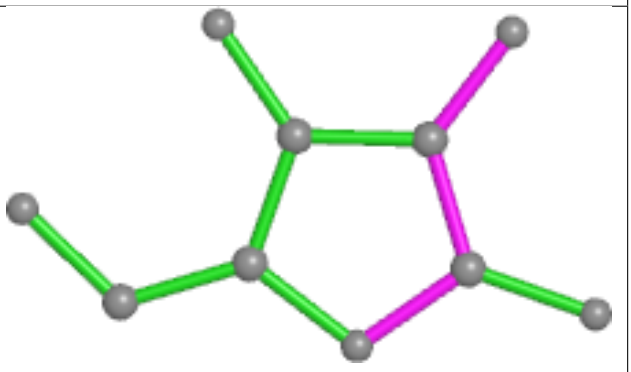


Rings

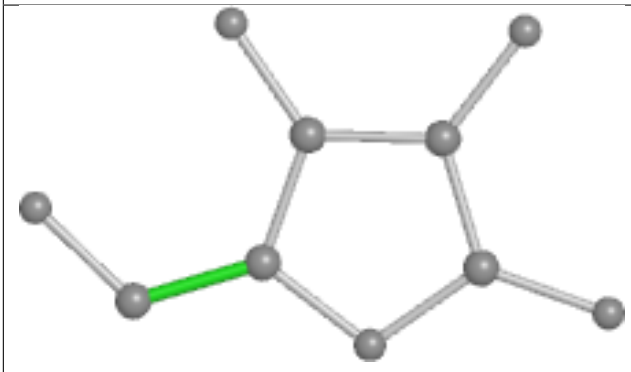
Ligand BXX F 501



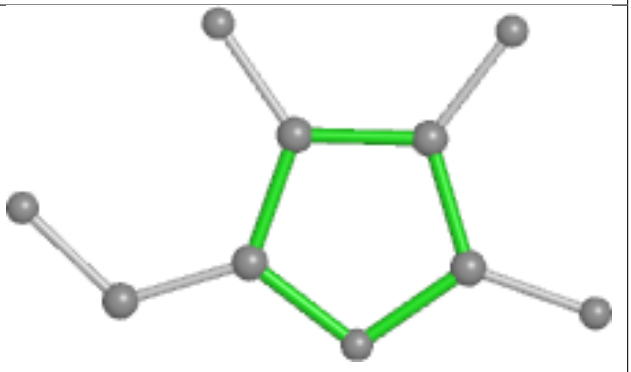
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	447/460 (97%)	-0.43	3 (0%)	87	88	18, 25, 42, 70	0
1	B	447/460 (97%)	-0.49	4 (0%)	84	84	17, 25, 43, 82	0
1	C	447/460 (97%)	-0.38	6 (1%)	77	78	19, 27, 46, 82	0
1	D	447/460 (97%)	-0.47	4 (0%)	84	84	19, 26, 40, 77	0
1	E	447/460 (97%)	-0.42	8 (1%)	68	68	19, 26, 45, 81	0
1	F	447/460 (97%)	-0.40	6 (1%)	77	78	19, 27, 44, 81	0
All	All	2682/2760 (97%)	-0.43	31 (1%)	79	79	17, 26, 44, 82	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	389	LYS	4.9
1	F	389	LYS	4.6
1	E	391	VAL	4.3
1	E	387	GLU	3.9
1	E	389	LYS	3.5
1	B	387	GLU	3.4
1	D	201	GLU	3.4
1	C	391	VAL	3.4
1	C	389	LYS	3.2
1	C	387	GLU	3.2
1	E	201	GLU	3.0
1	C	115	ASP	3.0
1	B	115	ASP	2.9
1	F	387	GLU	2.8
1	E	115	ASP	2.7
1	A	448	ALA	2.5
1	C	449	GLU	2.4
1	E	368	SER	2.4
1	E	202	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	202	ASP	2.3
1	F	201	GLU	2.3
1	F	449	GLU	2.3
1	D	202	ASP	2.3
1	A	449	GLU	2.2
1	C	368	SER	2.2
1	E	392	LEU	2.1
1	D	449	GLU	2.1
1	F	391	VAL	2.1
1	B	449	GLU	2.1
1	D	448	ALA	2.1
1	F	388	ARG	2.1

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
3	BXX	A	602	10/10	0.93	0.09	24,28,30,32	0
3	BXX	D	602	10/10	0.93	0.10	22,26,28,30	0
3	BXX	B	602	10/10	0.95	0.09	22,25,27,28	0
3	BXX	F	501	10/10	0.95	0.07	21,25,27,28	0
3	BXX	E	602	10/10	0.96	0.08	25,28,31,31	0
3	BXX	C	602	10/10	0.96	0.06	22,25,26,28	0
2	CA	A	601	1/1	0.99	0.04	25,25,25,25	0
2	CA	C	601	1/1	1.00	0.04	22,22,22,22	0
2	CA	D	601	1/1	1.00	0.07	21,21,21,21	0
2	CA	D	603	1/1	1.00	0.06	22,22,22,22	0
2	CA	E	601	1/1	1.00	0.06	22,22,22,22	0

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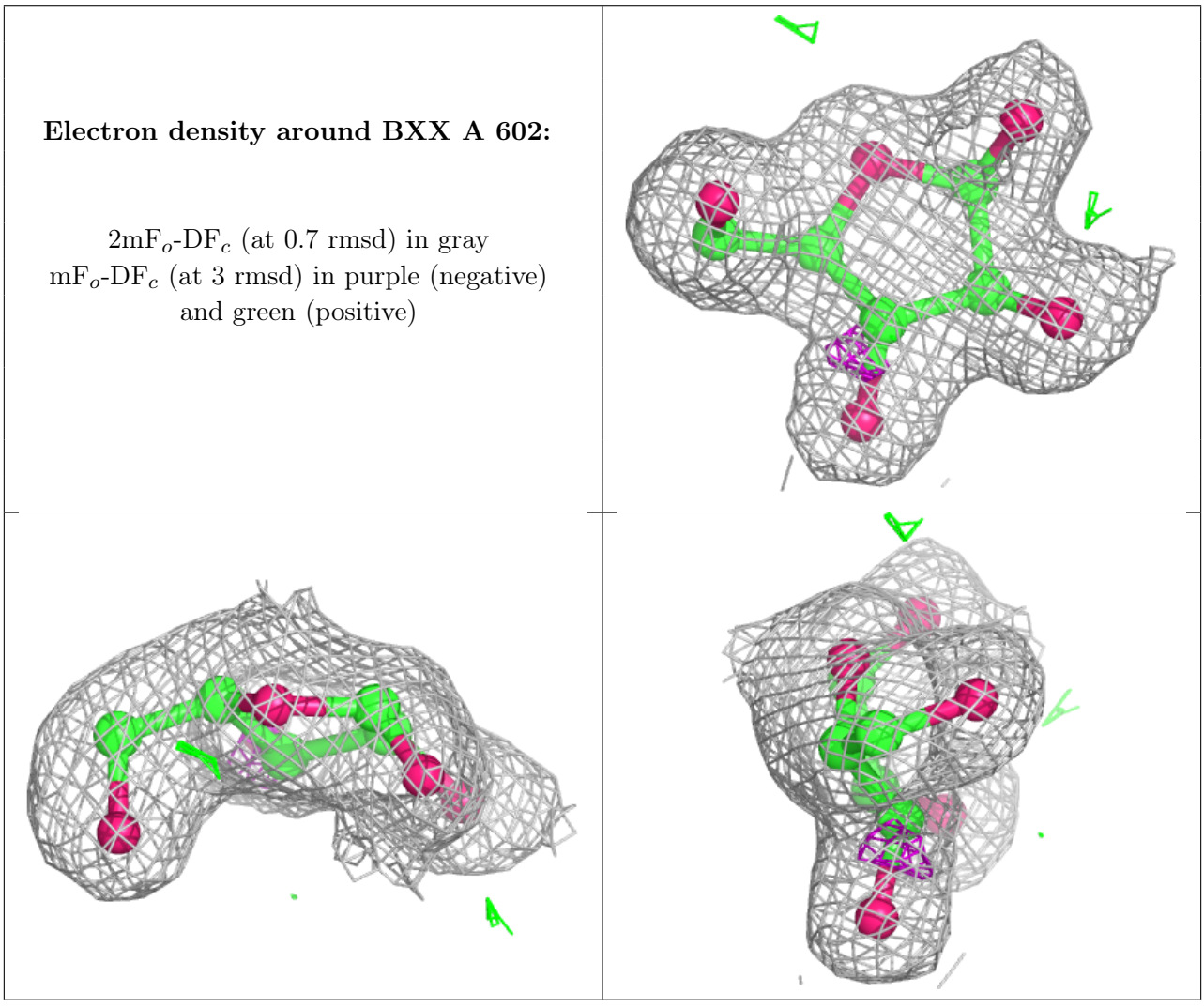
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	B	601	1/1	1.00	0.06	20,20,20,20	0

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.

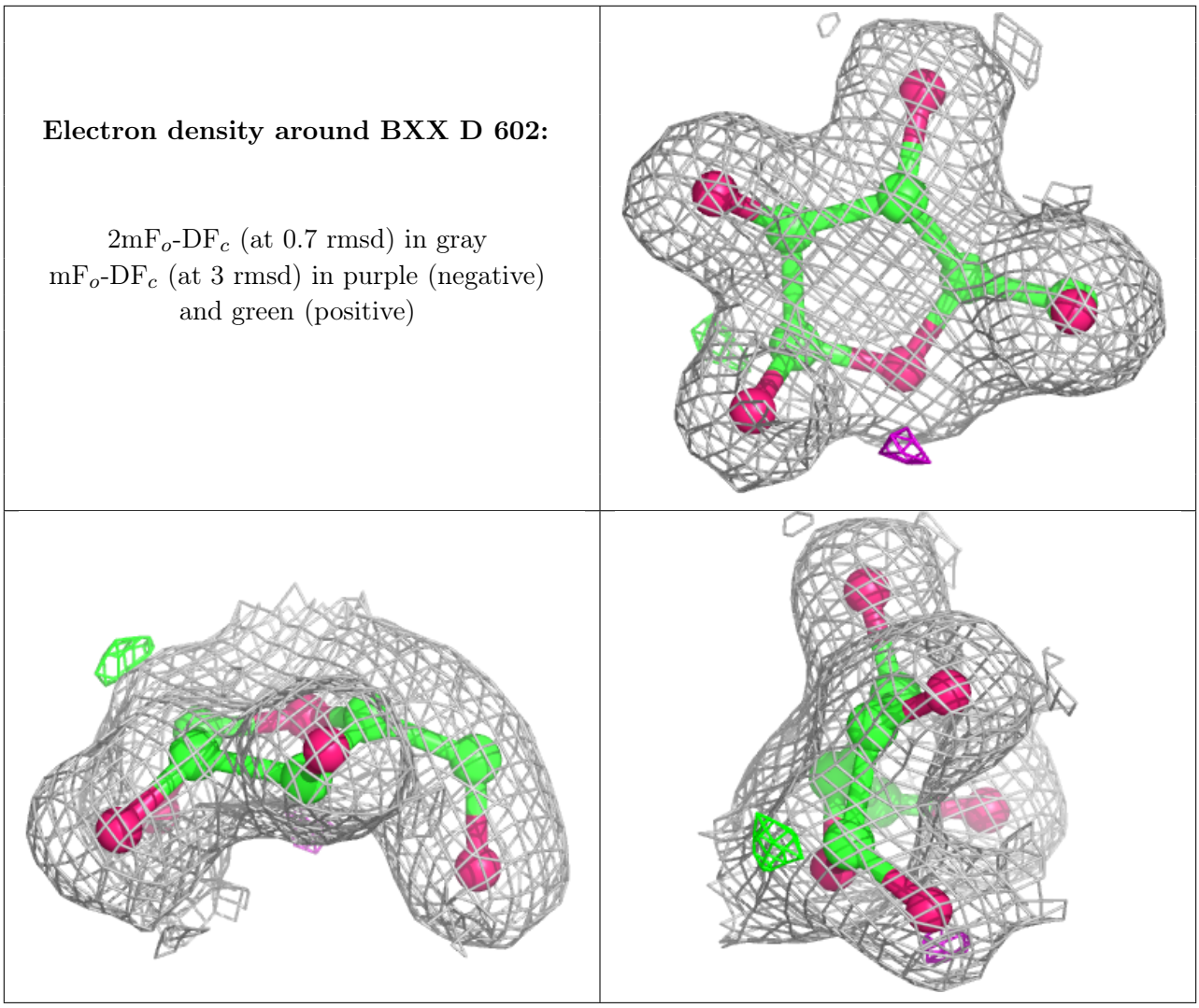
Electron density around BXX A 602:

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



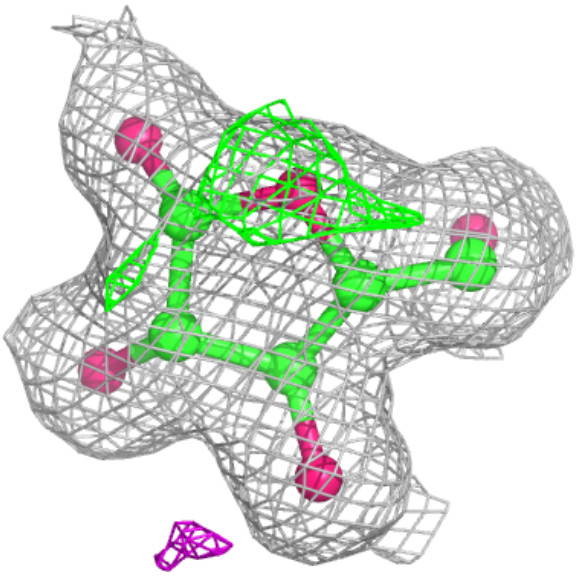
Electron density around BXX D 602:

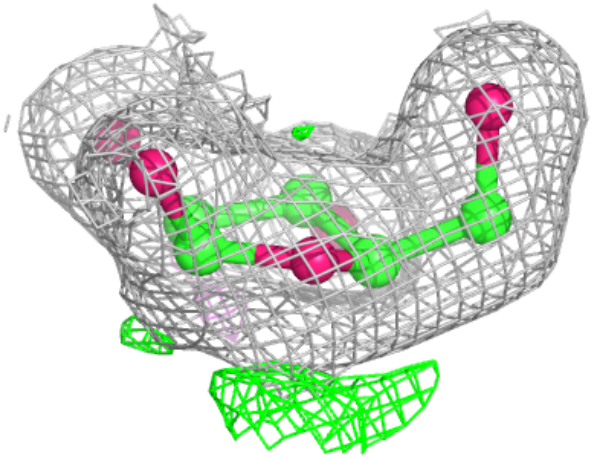
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

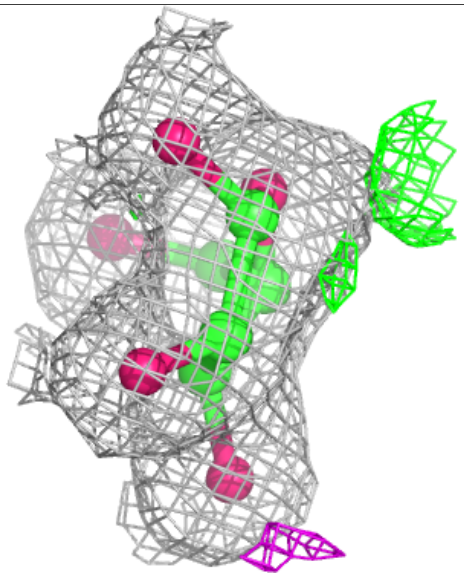


Electron density around BXX B 602:

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

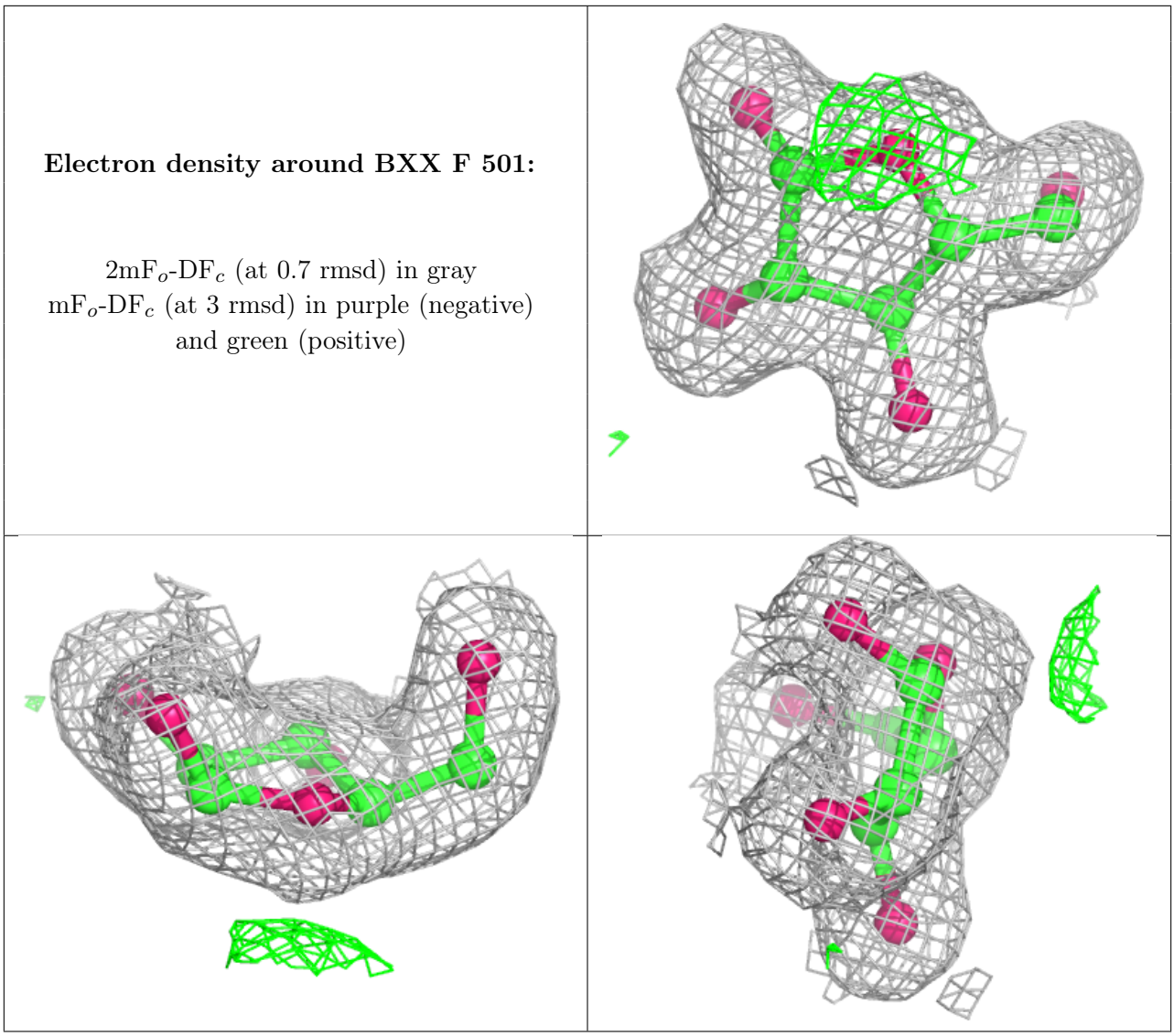






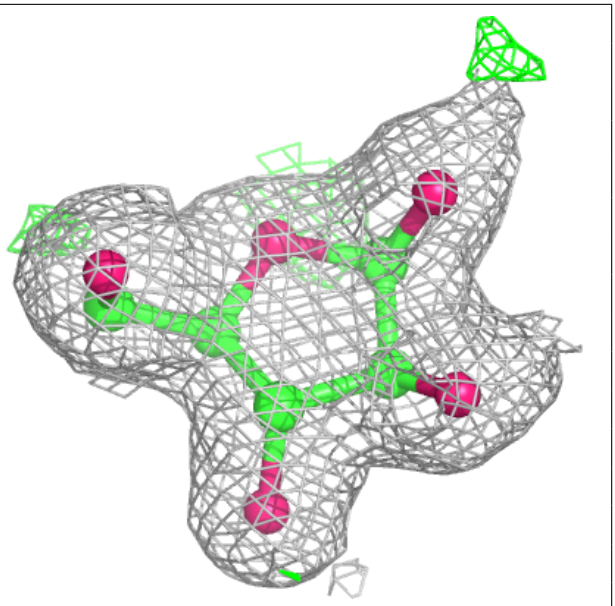
Electron density around BXX F 501:

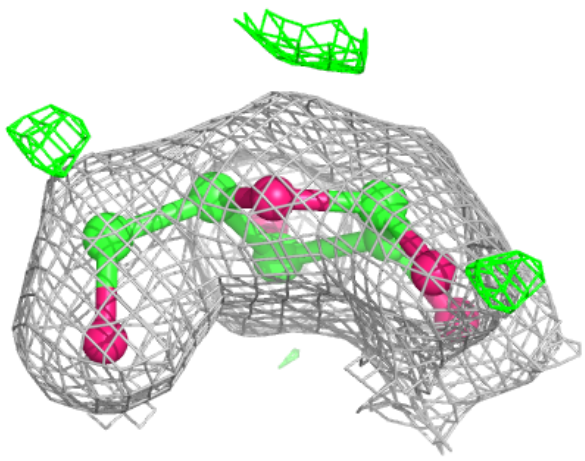
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

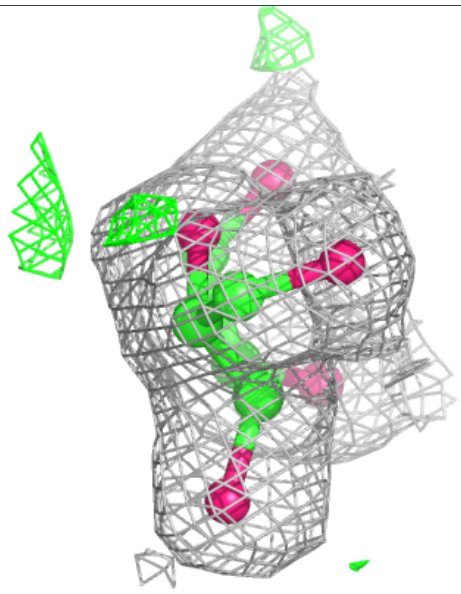


Electron density around BXX E 602:

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

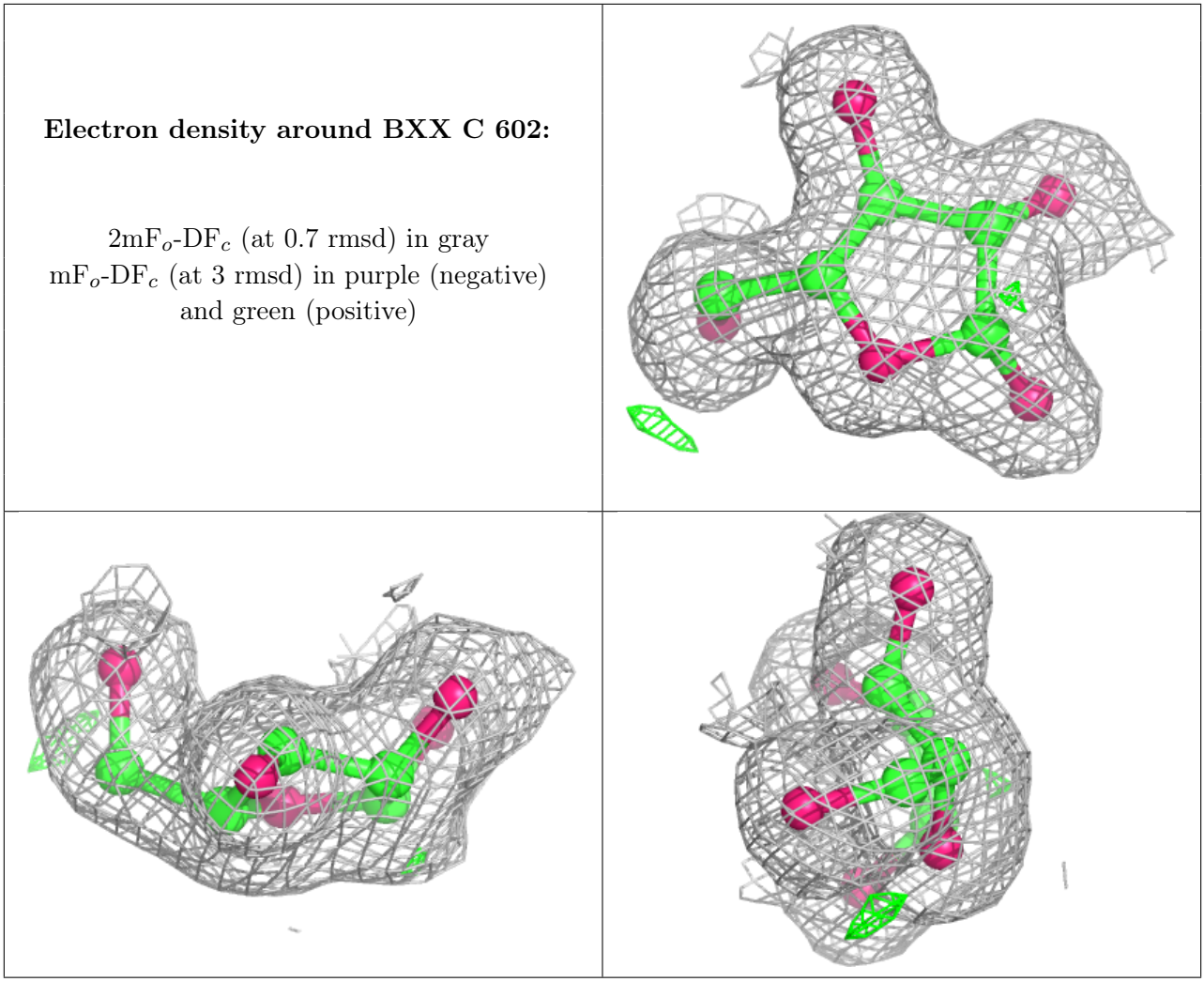






Electron density around BXX C 602:

$2mF_o$-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.