Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2025 – 12:36 PM JST

PDB ID	:	8Y4I
Title	:	Metal Beta-Lactamase VIM-2 in Complex with MBL inhibitor B7
Authors	:	Li, G.-B.; Wang, S.-Y.
Deposited on	:	2024-01-30
Resolution	:	1.94 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:

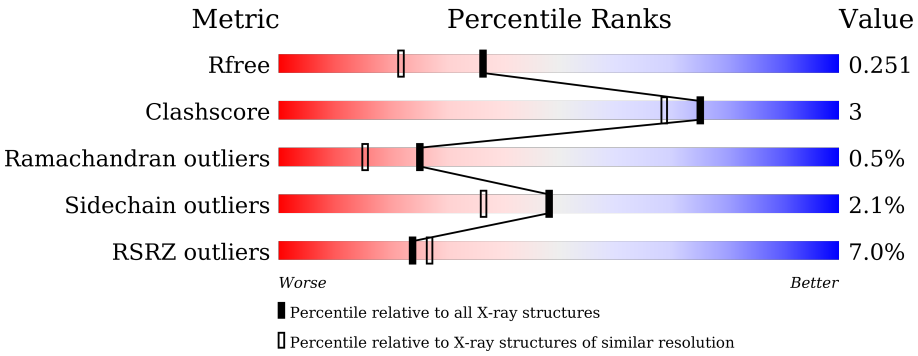
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.94 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}	164625	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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	231	3% 97% .
1	B	231	3% 95% 5%
1	C	231	6% 87% 12% .
1	D	231	5% 88% 10% .
1	E	231	14% 91% 8% .
1	F	231	3% 92% 6% .

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Mol	Chain	Length	Quality of chain
1	G	231	7% 93% 6%
1	H	231	15% 90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	A1LXF	A	303	-	X	-	-
3	A1LXF	B	303	-	X	-	-
3	A1LXF	D	303	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14264 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 Metal Beta-Lactamase VIM-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	B	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	C	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	D	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	E	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	F	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	G	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	H	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

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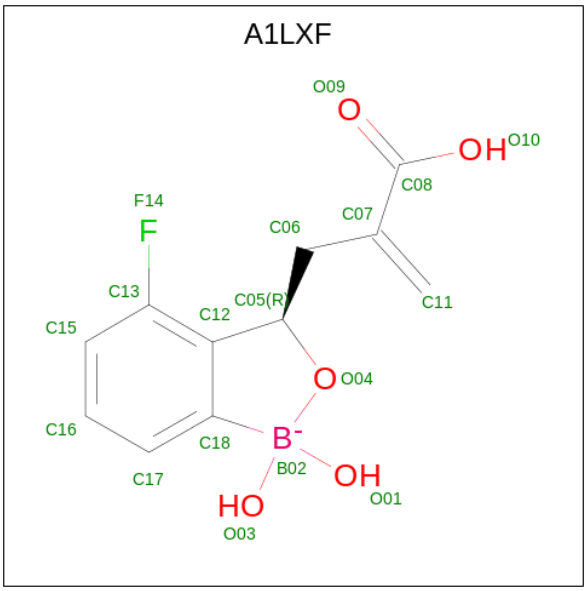
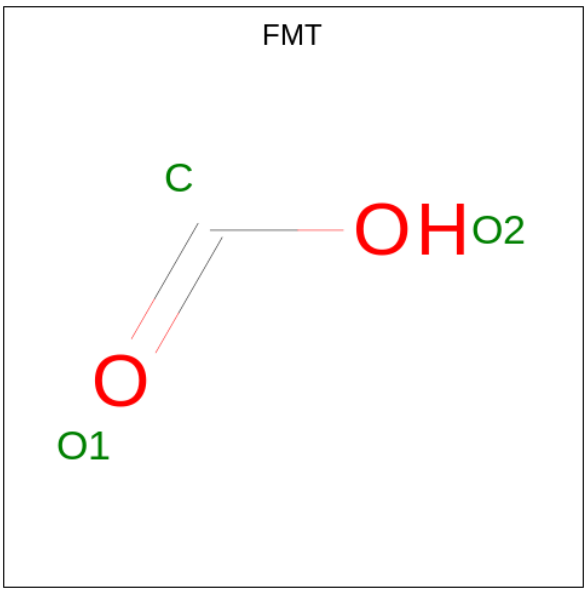
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0

- Molecule 3 is 2-[[(9R)-2-fluoranyl-7,7-bis(oxidanyl)-8-oxa-7-boranuidabicyclo[4.3.0]nona-1,3,5-trien-9-yl]methyl]prop-2-enoic acid (three-letter code: A1LXF) (formula: $C_{11}H_{11}BFO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total B C F O 18 1 11 1 5	0	0
3	B	1	Total B C F O 18 1 11 1 5	0	0
3	C	1	Total B C F O 18 1 11 1 5	0	0
3	D	1	Total B C F O 18 1 11 1 5	0	0
3	E	1	Total B C F O 18 1 11 1 5	0	0
3	F	1	Total B C F O 18 1 11 1 5	0	0
3	G	1	Total B C F O 18 1 11 1 5	0	0
3	H	1	Total B C F O 18 1 11 1 5	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 3 1 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	41	Total O 41 41	0	0
5	B	35	Total O 35 35	0	0
5	C	26	Total O 26 26	0	0
5	D	41	Total O 41 41	0	0
5	E	14	Total O 14 14	0	0
5	F	44	Total O 44 44	0	0
5	G	19	Total O 19 19	0	0
5	H	17	Total O 17 17	0	0

3 Residue-property plots (i)

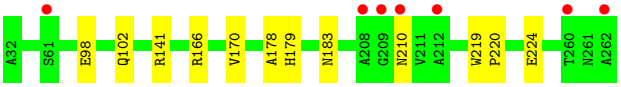
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Metal Beta-Lactamase VIM-2

Chain A:

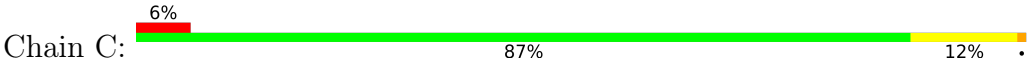
• Molecule 1: Metal Beta-Lactamase VIM-2

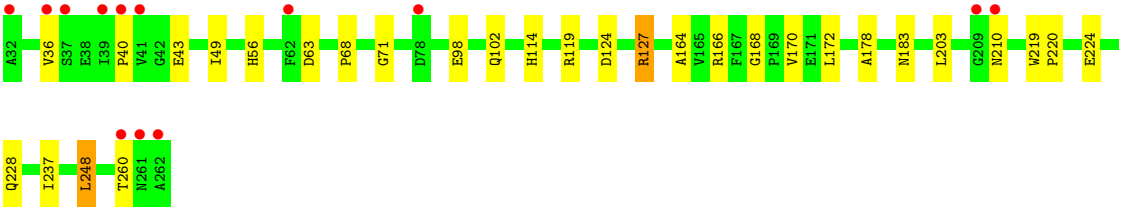
Chain B:



• Molecule 1: Metal Beta-Lactamase VIM-2

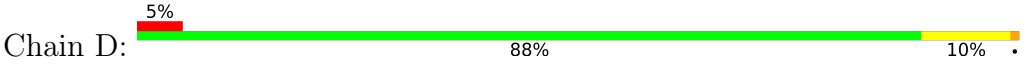
Chain C:

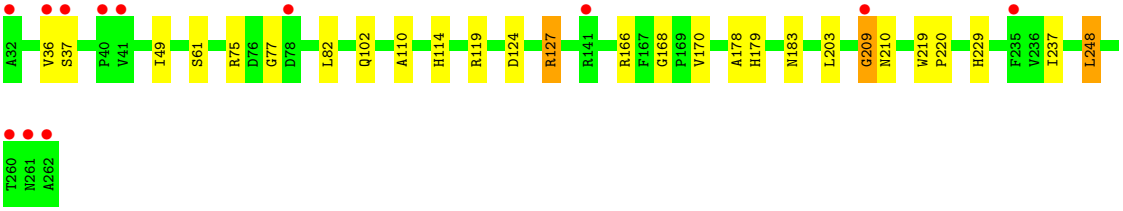




• Molecule 1: Metal Beta-Lactamase VIM-2

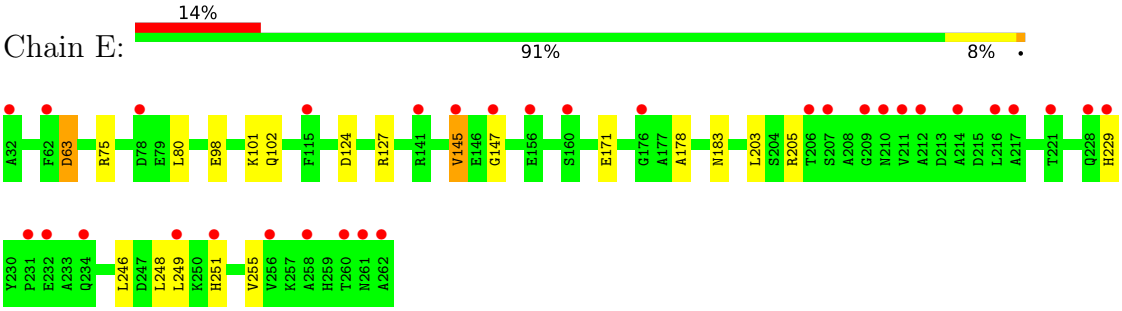
Chain D:





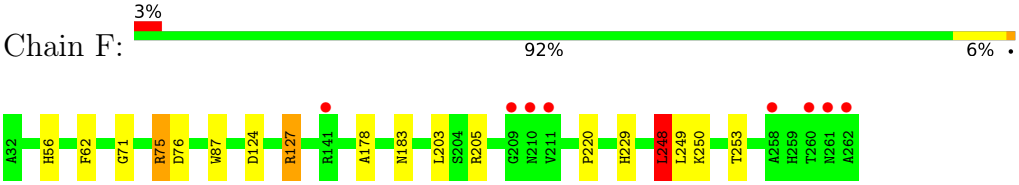
• Molecule 1: Metal Beta-Lactamase VIM-2

Chain E:



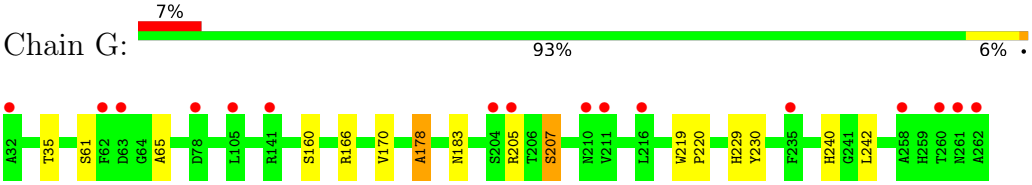
• Molecule 1: Metal Beta-Lactamase VIM-2

Chain F:



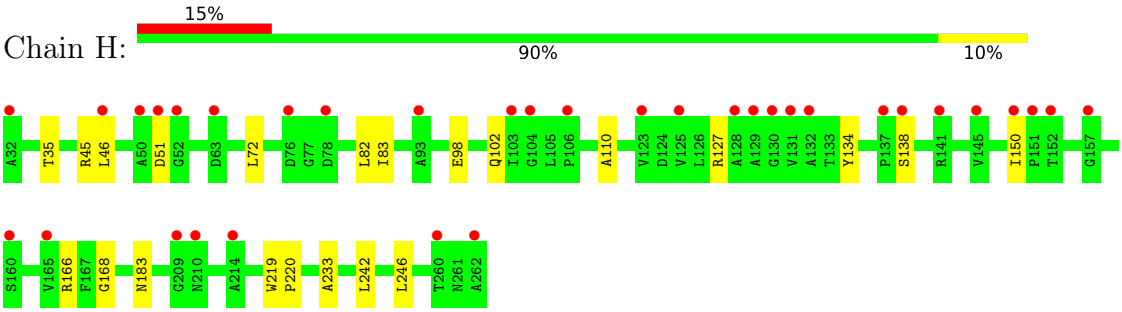
• Molecule 1: Metal Beta-Lactamase VIM-2

Chain G:



• Molecule 1: Metal Beta-Lactamase VIM-2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.15Å 245.80Å 87.97Å 90.00° 93.76° 90.00°	Depositor
Resolution (Å)	43.89 – 1.94 43.89 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.89-1.94) 97.8 (43.89-1.94)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.21-5207	Depositor
R, R_{free}	0.191 , 0.244 0.201 , 0.251	Depositor DCC
R_{free} test set	123982 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 38.3	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	0.94	EDS
Total number of atoms	14264	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8048e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FMT, ZN, A1LXF

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	0.59	0/1774	0.73	0/2429
1	B	0.52	0/1774	0.70	0/2429
1	C	0.57	0/1774	0.69	1/2429 (0.0%)
1	D	0.63	0/1774	0.76	2/2429 (0.1%)
1	E	0.49	0/1774	0.66	0/2429
1	F	0.62	1/1774 (0.1%)	0.74	4/2429 (0.2%)
1	G	0.50	0/1774	0.65	0/2429
1	H	0.46	0/1774	0.60	0/2429
All	All	0.55	1/14192 (0.0%)	0.69	7/19432 (0.0%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	127	ARG	CZ-NH2	-6.01	1.25	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	75	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	D	127	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	D	248	LEU	CA-CB-CG	6.12	129.37	115.30
1	F	248	LEU	CA-CB-CG	5.78	128.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	75	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	F	127	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	127	ARG	NE-CZ-NH2	-5.35	117.63	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	209	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1733	0	1682	2	0
1	B	1733	0	1682	5	0
1	C	1733	0	1682	16	0
1	D	1733	0	1682	12	0
1	E	1733	0	1682	10	1
1	F	1733	0	1682	9	0
1	G	1733	0	1682	8	1
1	H	1733	0	1682	10	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	18	0	0	1	0
3	B	18	0	0	2	0
3	C	18	0	0	3	0
3	D	18	0	0	3	0
3	E	18	0	0	1	0
3	F	18	0	0	4	0
3	G	18	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	18	0	0	1	0
4	C	3	0	1	0	0
5	A	41	0	0	0	0
5	B	35	0	0	0	0
5	C	26	0	0	0	0
5	D	41	0	0	0	0
5	E	14	0	0	0	0
5	F	44	0	0	2	0
5	G	19	0	0	1	0
5	H	17	0	0	0	0
All	All	14264	0	13457	79	1

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 3.

All (79) 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)
3:A:303:A1LXF:C18	3:A:303:A1LXF:C12	1.75	1.62
3:H:303:A1LXF:C12	3:H:303:A1LXF:C18	1.76	1.60
3:B:303:A1LXF:C18	3:B:303:A1LXF:C12	1.75	1.59
3:E:303:A1LXF:C18	3:E:303:A1LXF:C12	1.75	1.59
3:D:303:A1LXF:C12	3:D:303:A1LXF:C18	1.75	1.57
3:C:303:A1LXF:C18	3:C:303:A1LXF:C12	1.74	1.56
3:G:303:A1LXF:C12	3:G:303:A1LXF:C18	1.75	1.56
3:F:303:A1LXF:C18	3:F:303:A1LXF:C12	1.75	1.55
1:G:205:ARG:NH1	5:G:401:HOH:O	1.85	0.97
1:G:205:ARG:HH12	1:G:240:HIS:HB2	1.34	0.90
1:C:124:ASP:OD1	1:C:127:ARG:NH2	2.06	0.88
1:C:98:GLU:OE2	1:C:102:GLN:NE2	2.09	0.86
1:A:75:ARG:NH2	1:E:101:LYS:O	2.09	0.85
1:D:124:ASP:OD1	1:D:127:ARG:NH2	2.11	0.82
1:E:98:GLU:OE2	1:E:102:GLN:NE2	2.17	0.77
1:H:98:GLU:OE2	1:H:102:GLN:NE2	2.24	0.70
1:C:224:GLU:O	1:C:228:GLN:HG2	1.90	0.70
1:F:203:LEU:HG	1:F:248:LEU:HD22	1.80	0.63
1:F:124:ASP:OD1	1:F:127:ARG:NH2	2.34	0.60
1:E:203:LEU:HG	1:E:248:LEU:CD2	2.32	0.60
1:D:203:LEU:HG	1:D:248:LEU:HD22	1.84	0.59
1:E:124:ASP:OD1	1:E:127:ARG:NH2	2.36	0.58
1:D:49:ILE:HD13	1:D:237:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ARG:HD3	1:D:170:VAL:O	2.09	0.53
1:G:61:SER:HA	1:G:65:ALA:O	2.10	0.52
1:D:75:ARG:HD3	1:D:77:GLY:O	2.10	0.51
1:D:166:ARG:HD2	1:D:168:GLY:O	2.11	0.51
1:C:210:ASN:HB3	3:C:303:A1LXF:O09	2.10	0.51
1:C:166:ARG:HD3	1:C:170:VAL:O	2.10	0.50
3:F:303:A1LXF:C18	3:F:303:A1LXF:C13	2.50	0.50
3:G:303:A1LXF:C18	3:G:303:A1LXF:C13	2.51	0.49
1:C:210:ASN:CB	3:C:303:A1LXF:O09	2.61	0.48
1:C:49:ILE:HD13	1:C:237:ILE:HD11	1.95	0.48
1:H:35:THR:HG22	1:H:242:LEU:HD21	1.96	0.48
1:C:203:LEU:HG	1:C:248:LEU:HD22	1.95	0.48
1:D:114:HIS:CE1	1:D:119:ARG:HG3	2.49	0.48
1:B:166:ARG:HD3	1:B:170:VAL:O	2.13	0.48
1:B:219:TRP:HB3	1:B:220:PRO:HD3	1.95	0.48
1:C:114:HIS:CE1	1:C:119:ARG:HG3	2.49	0.47
1:F:250:LYS:NZ	5:F:402:HOH:O	2.46	0.47
1:F:205:ARG:NH1	5:F:404:HOH:O	2.46	0.47
1:E:251:HIS:O	1:E:255:VAL:HG23	2.14	0.47
1:B:166:ARG:HG2	1:E:171:GLU:OE2	2.15	0.47
1:D:229:HIS:NE2	1:H:51:ASP:OD2	2.48	0.47
1:H:82:LEU:O	1:H:110:ALA:HA	2.15	0.47
1:C:219:TRP:HB3	1:C:220:PRO:HD3	1.97	0.46
1:E:246:LEU:CD2	1:E:249:LEU:HD22	2.46	0.46
1:G:166:ARG:HD3	1:G:170:VAL:O	2.16	0.46
1:H:127:ARG:NH1	1:H:150:ILE:O	2.44	0.46
1:D:219:TRP:HB3	1:D:220:PRO:HD3	1.97	0.46
3:G:303:A1LXF:O04	3:G:303:A1LXF:O10	2.34	0.45
1:D:210:ASN:HB2	3:D:303:A1LXF:C11	2.47	0.45
1:H:45:ARG:O	1:H:46:LEU:HD23	2.17	0.45
1:H:166:ARG:HD2	1:H:168:GLY:O	2.17	0.45
1:E:145:VAL:O	1:E:147:GLY:N	2.49	0.44
1:F:75:ARG:HG3	1:F:76:ASP:N	2.33	0.44
1:C:40:PRO:HD2	1:C:43:GLU:OE1	2.17	0.43
1:G:35:THR:HG22	1:G:242:LEU:HD21	2.01	0.43
1:F:87:TRP:CZ2	3:F:303:A1LXF:F14	2.61	0.43
1:C:36:VAL:HB	1:C:68:PRO:CG	2.49	0.43
1:G:229:HIS:HD2	1:G:230:TYR:CZ	2.36	0.43
1:B:98:GLU:OE2	1:B:102:GLN:NE2	2.38	0.43
1:C:164:ALA:HA	1:C:172:LEU:O	2.19	0.42
1:F:220:PRO:HB3	1:F:253:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:O	1:D:110:ALA:HA	2.19	0.42
1:C:166:ARG:HD2	1:C:168:GLY:O	2.20	0.42
1:H:233:ALA:HB3	1:H:246:LEU:HD21	2.01	0.42
1:F:62:PHE:CG	3:F:303:A1LXF:F14	2.63	0.41
1:G:178:ALA:HB1	1:G:219:TRP:CD1	2.55	0.41
1:C:56:HIS:NE2	1:C:71:GLY:HA3	2.35	0.41
1:H:72:LEU:HB3	1:H:83:ILE:HB	2.03	0.41
1:G:219:TRP:HB3	1:G:220:PRO:HD3	2.01	0.41
1:A:101:LYS:O	1:E:75:ARG:NH2	2.42	0.41
1:D:179:HIS:CE1	3:D:303:A1LXF:O01	2.74	0.40
1:E:75:ARG:HA	1:E:80:LEU:HD23	2.03	0.40
1:F:56:HIS:NE2	1:F:71:GLY:HA3	2.36	0.40
1:B:179:HIS:CE1	3:B:303:A1LXF:O01	2.75	0.40
1:C:178:ALA:HB1	1:C:219:TRP:CD1	2.56	0.40
1:H:219:TRP:HB3	1:H:220:PRO:HD3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ASP:OD2	1:G:207:SER:OG[2_756]	2.00	0.20

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	229/231 (99%)	223 (97%)	4 (2%)	2 (1%)	14 6
1	B	229/231 (99%)	225 (98%)	3 (1%)	1 (0%)	30 22
1	C	229/231 (99%)	221 (96%)	8 (4%)	0	100 100
1	D	229/231 (99%)	220 (96%)	7 (3%)	2 (1%)	14 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	229/231 (99%)	217 (95%)	10 (4%)	2 (1%)	14 6
1	F	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	30 22
1	G	229/231 (99%)	221 (96%)	7 (3%)	1 (0%)	30 22
1	H	229/231 (99%)	221 (96%)	8 (4%)	0	100 100
All	All	1832/1848 (99%)	1771 (97%)	52 (3%)	9 (0%)	25 15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	178	ALA
1	B	178	ALA
1	E	145	VAL
1	G	178	ALA
1	A	210	ASN
1	F	178	ALA
1	A	84	ASP
1	D	178	ALA
1	D	209	GLY

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	182/182 (100%)	178 (98%)	4 (2%)	47 35
1	B	182/182 (100%)	178 (98%)	4 (2%)	47 35
1	C	182/182 (100%)	178 (98%)	4 (2%)	47 35
1	D	182/182 (100%)	177 (97%)	5 (3%)	40 26
1	E	182/182 (100%)	178 (98%)	4 (2%)	47 35
1	F	182/182 (100%)	178 (98%)	4 (2%)	47 35
1	G	182/182 (100%)	179 (98%)	3 (2%)	58 49
1	H	182/182 (100%)	179 (98%)	3 (2%)	58 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1456/1456 (100%)	1425 (98%)	31 (2%)	48 36

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	183	ASN
1	A	205	ARG
1	A	210	ASN
1	B	141	ARG
1	B	183	ASN
1	B	210	ASN
1	B	224	GLU
1	C	63	ASP
1	C	183	ASN
1	C	248	LEU
1	C	260	THR
1	D	36	VAL
1	D	37	SER
1	D	61	SER
1	D	102	GLN
1	D	183	ASN
1	E	63	ASP
1	E	183	ASN
1	E	205	ARG
1	E	229	HIS
1	F	183	ASN
1	F	229	HIS
1	F	248	LEU
1	F	249	LEU
1	G	160	SER
1	G	183	ASN
1	G	207	SER
1	H	134	TYR
1	H	138	SER
1	H	183	ASN

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

Mol	Chain	Res	Type
1	D	102	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 25 ligands modelled in this entry, 16 are monoatomic - leaving 9 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	A1LXF	G	303	2	17,19,19	11.85	10 (58%)	19,29,29	7.12	13 (68%)
3	A1LXF	D	303	2	17,19,19	11.67	10 (58%)	19,29,29	6.30	14 (73%)
3	A1LXF	H	303	2	17,19,19	12.06	11 (64%)	19,29,29	6.80	12 (63%)
3	A1LXF	A	303	2	17,19,19	11.88	11 (64%)	19,29,29	6.64	15 (78%)
3	A1LXF	B	303	2	17,19,19	11.79	12 (70%)	19,29,29	6.95	16 (84%)
3	A1LXF	F	303	2	17,19,19	11.91	11 (64%)	19,29,29	7.05	12 (63%)
3	A1LXF	E	303	2	17,19,19	11.90	11 (64%)	19,29,29	6.49	12 (63%)
4	FMT	C	304	-	2,2,2	0.60	0	1,1,1	0.47	0
3	A1LXF	C	303	2	17,19,19	11.52	10 (58%)	19,29,29	6.24	13 (68%)

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	A1LXF	G	303	2	-	3/8/23/23	0/2/2/2
3	A1LXF	D	303	2	-	8/8/23/23	0/2/2/2
3	A1LXF	H	303	2	-	3/8/23/23	0/2/2/2
3	A1LXF	A	303	2	-	5/8/23/23	0/2/2/2
3	A1LXF	B	303	2	-	8/8/23/23	0/2/2/2
3	A1LXF	F	303	2	-	5/8/23/23	0/2/2/2
3	A1LXF	E	303	2	-	5/8/23/23	0/2/2/2
3	A1LXF	C	303	2	-	1/8/23/23	0/2/2/2

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	303	A1LXF	C12-C18	44.51	1.76	1.39
3	A	303	A1LXF	C12-C18	43.84	1.75	1.39
3	E	303	A1LXF	C12-C18	43.61	1.75	1.39
3	B	303	A1LXF	C12-C18	43.55	1.75	1.39
3	F	303	A1LXF	C12-C18	43.49	1.75	1.39
3	G	303	A1LXF	C12-C18	43.36	1.75	1.39
3	D	303	A1LXF	C12-C18	43.18	1.75	1.39
3	C	303	A1LXF	C12-C18	42.86	1.74	1.39
3	D	303	A1LXF	C11-C07	10.72	1.55	1.32
3	H	303	A1LXF	C11-C07	10.54	1.54	1.32
3	B	303	A1LXF	C11-C07	10.37	1.54	1.32
3	F	303	A1LXF	C11-C07	10.27	1.54	1.32
3	A	303	A1LXF	C11-C07	10.24	1.54	1.32
3	F	303	A1LXF	C16-C15	-10.04	1.17	1.38
3	G	303	A1LXF	C11-C07	10.03	1.53	1.32
3	C	303	A1LXF	C11-C07	9.85	1.53	1.32
3	E	303	A1LXF	C11-C07	9.83	1.53	1.32
3	G	303	A1LXF	C16-C15	-9.82	1.18	1.38
3	E	303	A1LXF	C16-C15	-9.73	1.18	1.38
3	H	303	A1LXF	C16-C15	-9.46	1.19	1.38
3	D	303	A1LXF	C16-C15	-9.36	1.19	1.38
3	A	303	A1LXF	C16-C15	-8.87	1.20	1.38
3	B	303	A1LXF	C16-C15	-8.85	1.20	1.38
3	C	303	A1LXF	C16-C15	-8.84	1.20	1.38
3	F	303	A1LXF	C12-C13	8.60	1.47	1.38
3	G	303	A1LXF	C12-C13	8.20	1.47	1.38
3	H	303	A1LXF	C12-C13	8.16	1.47	1.38
3	B	303	A1LXF	C12-C13	7.89	1.46	1.38
3	A	303	A1LXF	C12-C13	7.82	1.46	1.38
3	E	303	A1LXF	C08-C07	7.70	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	303	A1LXF	C16-C17	-7.60	1.22	1.38
3	G	303	A1LXF	C16-C17	-7.29	1.23	1.38
3	H	303	A1LXF	C16-C17	-7.28	1.23	1.38
3	D	303	A1LXF	C12-C13	7.26	1.46	1.38
3	F	303	A1LXF	C08-C07	7.17	1.54	1.49
3	E	303	A1LXF	B02-O01	7.01	1.67	1.47
3	C	303	A1LXF	B02-O01	6.96	1.67	1.47
3	A	303	A1LXF	C08-C07	6.91	1.54	1.49
3	F	303	A1LXF	C16-C17	-6.88	1.24	1.38
3	C	303	A1LXF	C16-C17	-6.83	1.24	1.38
3	D	303	A1LXF	C16-C17	-6.82	1.24	1.38
3	A	303	A1LXF	C16-C17	-6.81	1.24	1.38
3	G	303	A1LXF	B02-O03	6.79	1.66	1.47
3	E	303	A1LXF	C12-C13	6.75	1.45	1.38
3	B	303	A1LXF	C16-C17	-6.68	1.24	1.38
3	G	303	A1LXF	C08-C07	6.56	1.54	1.49
3	F	303	A1LXF	O04-C05	-6.51	1.27	1.43
3	B	303	A1LXF	B02-O01	6.48	1.65	1.47
3	G	303	A1LXF	B02-O01	6.39	1.65	1.47
3	H	303	A1LXF	B02-O03	6.37	1.65	1.47
3	B	303	A1LXF	O04-C05	-6.37	1.27	1.43
3	F	303	A1LXF	B02-O01	6.34	1.65	1.47
3	E	303	A1LXF	B02-O03	6.32	1.65	1.47
3	C	303	A1LXF	O04-C05	-6.32	1.27	1.43
3	A	303	A1LXF	B02-O01	6.25	1.65	1.47
3	E	303	A1LXF	O04-C05	-6.21	1.27	1.43
3	D	303	A1LXF	B02-O01	6.14	1.64	1.47
3	H	303	A1LXF	B02-O01	6.13	1.64	1.47
3	H	303	A1LXF	O04-C05	-6.12	1.28	1.43
3	G	303	A1LXF	O04-C05	-6.10	1.28	1.43
3	A	303	A1LXF	O04-C05	-6.01	1.28	1.43
3	F	303	A1LXF	B02-O03	6.00	1.64	1.47
3	B	303	A1LXF	B02-O03	5.95	1.64	1.47
3	C	303	A1LXF	C12-C13	5.94	1.44	1.38
3	D	303	A1LXF	O04-C05	-5.92	1.28	1.43
3	A	303	A1LXF	B02-O03	5.89	1.64	1.47
3	D	303	A1LXF	B02-O03	5.84	1.64	1.47
3	C	303	A1LXF	B02-O03	5.68	1.63	1.47
3	H	303	A1LXF	C08-C07	5.53	1.53	1.49
3	B	303	A1LXF	C08-C07	5.23	1.53	1.49
3	C	303	A1LXF	C08-C07	5.02	1.52	1.49
3	D	303	A1LXF	C08-C07	4.05	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	303	A1LXF	C15-C13	-3.66	1.30	1.37
3	F	303	A1LXF	C15-C13	-3.42	1.30	1.37
3	G	303	A1LXF	C15-C13	-3.34	1.30	1.37
3	D	303	A1LXF	C15-C13	-3.30	1.31	1.37
3	A	303	A1LXF	C15-C13	-3.19	1.31	1.37
3	H	303	A1LXF	C15-C13	-3.16	1.31	1.37
3	C	303	A1LXF	C15-C13	-3.05	1.31	1.37
3	B	303	A1LXF	C15-C13	-2.97	1.31	1.37
3	A	303	A1LXF	C06-C07	2.89	1.54	1.50
3	H	303	A1LXF	C06-C07	2.62	1.53	1.50
3	B	303	A1LXF	C06-C07	2.39	1.53	1.50
3	F	303	A1LXF	C17-C18	2.17	1.43	1.40
3	B	303	A1LXF	C17-C18	2.14	1.43	1.40
3	E	303	A1LXF	O09-C08	2.07	1.28	1.22

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	303	A1LXF	C13-C12-C18	-23.55	101.73	119.22
3	G	303	A1LXF	C13-C12-C18	-22.61	102.42	119.22
3	H	303	A1LXF	C13-C12-C18	-22.40	102.58	119.22
3	E	303	A1LXF	C13-C12-C18	-21.57	103.20	119.22
3	D	303	A1LXF	C13-C12-C18	-20.19	104.22	119.22
3	B	303	A1LXF	C13-C12-C18	-19.89	104.44	119.22
3	C	303	A1LXF	C13-C12-C18	-19.50	104.73	119.22
3	A	303	A1LXF	C13-C12-C18	-19.28	104.90	119.22
3	G	303	A1LXF	C11-C07-C08	-12.10	109.84	120.61
3	B	303	A1LXF	C11-C07-C08	-12.08	109.85	120.61
3	A	303	A1LXF	C11-C07-C08	-12.00	109.92	120.61
3	H	303	A1LXF	C11-C07-C08	-11.51	110.36	120.61
3	C	303	A1LXF	F14-C13-C12	-11.31	107.05	118.13
3	B	303	A1LXF	F14-C13-C12	-9.34	108.98	118.13
3	D	303	A1LXF	F14-C13-C12	-9.24	109.09	118.13
3	E	303	A1LXF	B02-O04-C05	9.06	126.74	109.58
3	B	303	A1LXF	B02-O04-C05	8.98	126.58	109.58
3	F	303	A1LXF	F14-C13-C12	-8.63	109.68	118.13
3	E	303	A1LXF	F14-C13-C12	-8.45	109.86	118.13
3	A	303	A1LXF	B02-O04-C05	8.40	125.50	109.58
3	A	303	A1LXF	F14-C13-C12	-8.33	109.97	118.13
3	H	303	A1LXF	B02-O04-C05	8.20	125.11	109.58
3	D	303	A1LXF	B02-O04-C05	8.18	125.08	109.58
3	G	303	A1LXF	B02-O04-C05	8.11	124.94	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	303	A1LXF	C17-C18-C12	-7.88	112.51	118.02
3	F	303	A1LXF	B02-O04-C05	7.82	124.39	109.58
3	C	303	A1LXF	C17-C18-C12	-7.72	112.62	118.02
3	F	303	A1LXF	C17-C18-C12	-7.72	112.63	118.02
3	B	303	A1LXF	C17-C18-C12	-7.66	112.67	118.02
3	C	303	A1LXF	B02-O04-C05	7.62	124.00	109.58
3	A	303	A1LXF	C17-C18-C12	-7.55	112.74	118.02
3	E	303	A1LXF	C17-C18-C12	-7.34	112.89	118.02
3	H	303	A1LXF	F14-C13-C12	-6.82	111.45	118.13
3	G	303	A1LXF	F14-C13-C12	-6.80	111.47	118.13
3	F	303	A1LXF	C11-C07-C08	-6.71	114.64	120.61
3	G	303	A1LXF	C17-C18-C12	-6.50	113.48	118.02
3	A	303	A1LXF	C06-C07-C11	-6.32	106.40	122.68
3	G	303	A1LXF	O10-C08-C07	6.31	121.95	115.05
3	G	303	A1LXF	C06-C07-C11	-6.21	106.68	122.68
3	H	303	A1LXF	C17-C18-C12	-5.93	113.87	118.02
3	F	303	A1LXF	C15-C13-C12	5.81	130.12	123.98
3	B	303	A1LXF	O04-C05-C06	5.69	123.46	111.40
3	F	303	A1LXF	O10-C08-C07	5.69	121.27	115.05
3	E	303	A1LXF	O10-C08-C07	5.51	121.08	115.05
3	C	303	A1LXF	O10-C08-C07	5.37	120.92	115.05
3	B	303	A1LXF	C06-C07-C11	-5.30	109.02	122.68
3	D	303	A1LXF	C06-C05-C12	-5.25	92.00	114.72
3	F	303	A1LXF	C06-C07-C11	-5.01	109.76	122.68
3	D	303	A1LXF	O04-C05-C06	4.51	120.96	111.40
3	G	303	A1LXF	C16-C15-C13	4.50	125.84	118.46
3	H	303	A1LXF	C16-C15-C13	4.30	125.51	118.46
3	E	303	A1LXF	C16-C15-C13	4.23	125.40	118.46
3	B	303	A1LXF	C16-C15-C13	4.19	125.33	118.46
3	F	303	A1LXF	C16-C17-C18	4.17	127.21	121.64
3	H	303	A1LXF	C06-C07-C11	-4.08	112.17	122.68
3	A	303	A1LXF	C17-C16-C15	4.05	126.00	120.25
3	A	303	A1LXF	C16-C15-C13	3.98	124.99	118.46
3	E	303	A1LXF	C06-C07-C11	-3.98	112.43	122.68
3	C	303	A1LXF	C16-C15-C13	3.97	124.97	118.46
3	D	303	A1LXF	C16-C15-C13	3.84	124.76	118.46
3	G	303	A1LXF	C15-C13-C12	3.77	127.97	123.98
3	F	303	A1LXF	C16-C15-C13	3.66	124.46	118.46
3	B	303	A1LXF	O10-C08-C07	3.61	119.00	115.05
3	D	303	A1LXF	C17-C16-C15	3.61	125.37	120.25
3	A	303	A1LXF	O04-C05-C06	3.59	119.00	111.40
3	E	303	A1LXF	C15-C13-C12	3.55	127.73	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	303	A1LXF	O10-C08-C07	3.47	118.84	115.05
3	H	303	A1LXF	C15-C13-C12	3.44	127.62	123.98
3	G	303	A1LXF	C16-C17-C18	3.44	126.23	121.64
3	H	303	A1LXF	C17-C16-C15	3.37	125.02	120.25
3	E	303	A1LXF	C17-C16-C15	3.32	124.96	120.25
3	C	303	A1LXF	O09-C08-C07	-3.32	118.51	121.61
3	D	303	A1LXF	C05-C06-C07	3.30	120.04	113.07
3	D	303	A1LXF	C15-C13-C12	3.28	127.45	123.98
3	B	303	A1LXF	C05-C06-C07	3.27	119.98	113.07
3	A	303	A1LXF	O10-C08-C07	3.27	118.62	115.05
3	E	303	A1LXF	C05-C06-C07	-3.27	106.17	113.07
3	C	303	A1LXF	C17-C16-C15	3.24	124.84	120.25
3	F	303	A1LXF	O09-C08-C07	-3.22	118.60	121.61
3	C	303	A1LXF	F14-C13-C15	3.20	125.72	118.59
3	B	303	A1LXF	C17-C16-C15	3.20	124.78	120.25
3	E	303	A1LXF	C16-C17-C18	3.13	125.81	121.64
3	B	303	A1LXF	C16-C17-C18	3.08	125.75	121.64
3	C	303	A1LXF	C15-C13-C12	3.05	127.20	123.98
3	D	303	A1LXF	C16-C17-C18	2.98	125.61	121.64
3	C	303	A1LXF	C16-C17-C18	2.96	125.59	121.64
3	G	303	A1LXF	O09-C08-C07	-2.92	118.88	121.61
3	B	303	A1LXF	C15-C13-C12	2.86	127.01	123.98
3	H	303	A1LXF	C16-C17-C18	2.79	125.37	121.64
3	D	303	A1LXF	O03-B02-O04	2.73	116.54	110.09
3	G	303	A1LXF	C17-C16-C15	2.68	124.05	120.25
3	D	303	A1LXF	C06-C07-C11	-2.66	115.82	122.68
3	H	303	A1LXF	C06-C05-C12	-2.63	103.33	114.72
3	A	303	A1LXF	C06-C05-C12	-2.60	103.45	114.72
3	B	303	A1LXF	C06-C05-C12	-2.55	103.66	114.72
3	A	303	A1LXF	C16-C17-C18	2.54	125.03	121.64
3	F	303	A1LXF	C17-C16-C15	2.52	123.83	120.25
3	B	303	A1LXF	F14-C13-C15	2.43	124.01	118.59
3	C	303	A1LXF	C05-C06-C07	-2.33	108.16	113.07
3	A	303	A1LXF	F14-C13-C15	2.29	123.70	118.59
3	B	303	A1LXF	O03-B02-O04	2.24	115.39	110.09
3	A	303	A1LXF	C15-C13-C12	2.21	126.32	123.98
3	G	303	A1LXF	C06-C05-C12	-2.20	105.19	114.72
3	D	303	A1LXF	F14-C13-C15	2.17	123.43	118.59
3	C	303	A1LXF	C06-C05-C12	-2.17	105.34	114.72
3	E	303	A1LXF	C11-C07-C08	-2.10	118.74	120.61
3	A	303	A1LXF	O10-C08-O09	-2.02	118.98	123.61

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	A1LXF	C05-C06-C07-C11
3	A	303	A1LXF	C11-C07-C08-O09
3	A	303	A1LXF	C11-C07-C08-O10
3	B	303	A1LXF	O04-C05-C06-C07
3	B	303	A1LXF	C12-C05-C06-C07
3	B	303	A1LXF	C05-C06-C07-C08
3	B	303	A1LXF	C05-C06-C07-C11
3	B	303	A1LXF	C11-C07-C08-O09
3	B	303	A1LXF	C11-C07-C08-O10
3	D	303	A1LXF	O04-C05-C06-C07
3	D	303	A1LXF	C12-C05-C06-C07
3	D	303	A1LXF	C05-C06-C07-C08
3	D	303	A1LXF	C06-C07-C08-O09
3	D	303	A1LXF	C06-C07-C08-O10
3	D	303	A1LXF	C11-C07-C08-O09
3	D	303	A1LXF	C11-C07-C08-O10
3	E	303	A1LXF	C05-C06-C07-C11
3	E	303	A1LXF	C06-C07-C08-O09
3	E	303	A1LXF	C06-C07-C08-O10
3	F	303	A1LXF	C06-C07-C08-O09
3	F	303	A1LXF	C06-C07-C08-O10
3	G	303	A1LXF	C05-C06-C07-C11
3	H	303	A1LXF	C05-C06-C07-C11
3	H	303	A1LXF	C06-C07-C08-O09
3	H	303	A1LXF	C06-C07-C08-O10
3	F	303	A1LXF	C11-C07-C08-O09
3	A	303	A1LXF	C06-C07-C08-O10
3	B	303	A1LXF	C06-C07-C08-O09
3	B	303	A1LXF	C06-C07-C08-O10
3	G	303	A1LXF	C06-C07-C08-O09
3	G	303	A1LXF	C06-C07-C08-O10
3	C	303	A1LXF	C05-C06-C07-C08
3	F	303	A1LXF	C05-C06-C07-C08
3	D	303	A1LXF	C05-C06-C07-C11
3	E	303	A1LXF	C11-C07-C08-O09
3	E	303	A1LXF	C11-C07-C08-O10
3	F	303	A1LXF	C11-C07-C08-O10
3	A	303	A1LXF	C06-C07-C08-O09

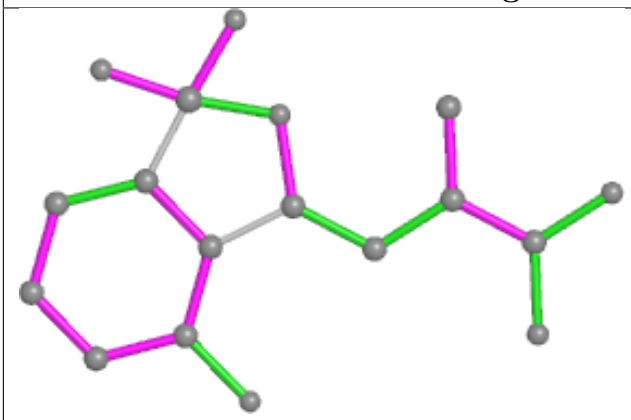
There are no ring outliers.

8 monomers are involved in 18 short contacts:

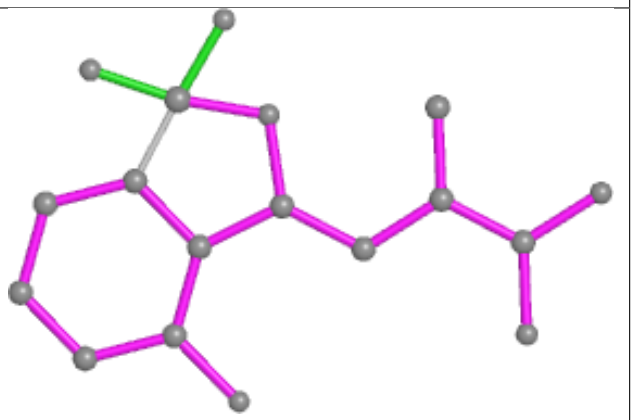
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	303	A1LXF	3	0
3	D	303	A1LXF	3	0
3	H	303	A1LXF	1	0
3	A	303	A1LXF	1	0
3	B	303	A1LXF	2	0
3	F	303	A1LXF	4	0
3	E	303	A1LXF	1	0
3	C	303	A1LXF	3	0

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.

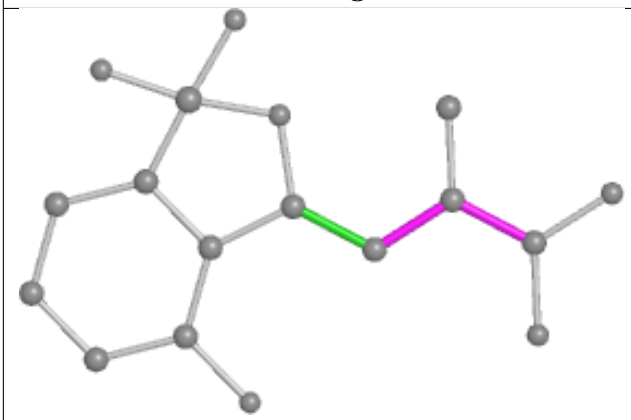
Ligand A1LXF G 303



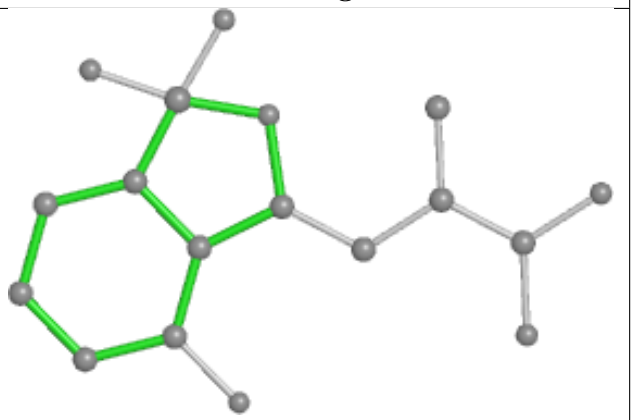
Bond lengths



Bond angles

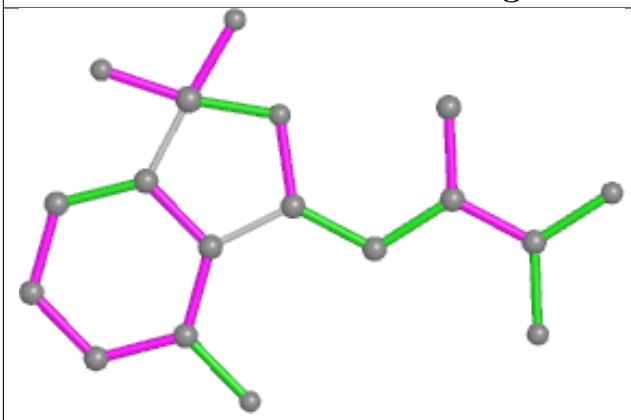


Torsions

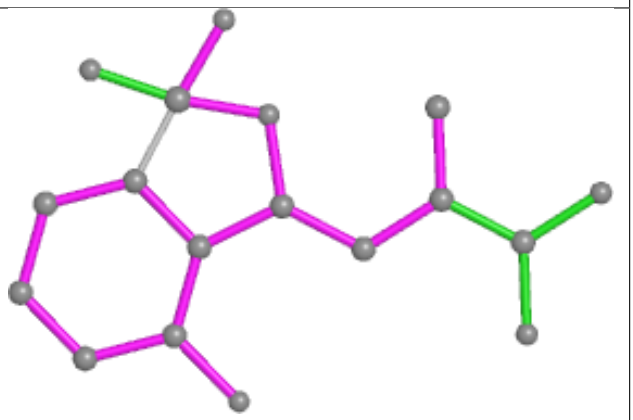


Rings

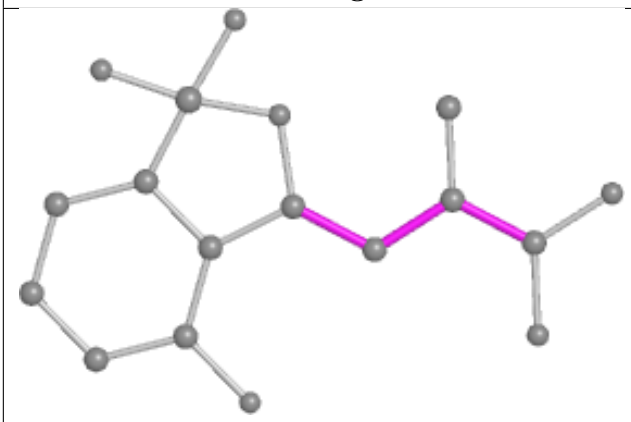
Ligand A1LXF D 303



Bond lengths



Bond angles



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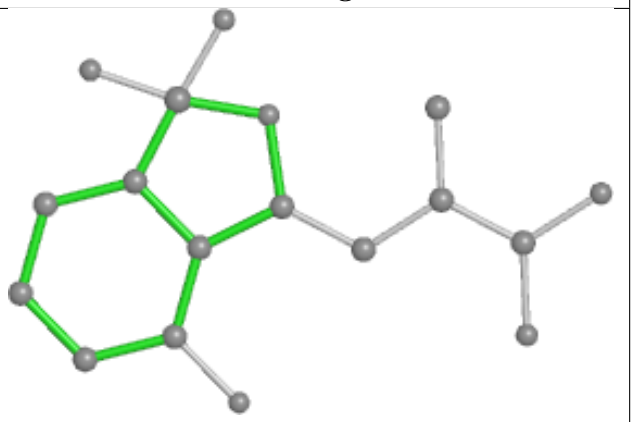
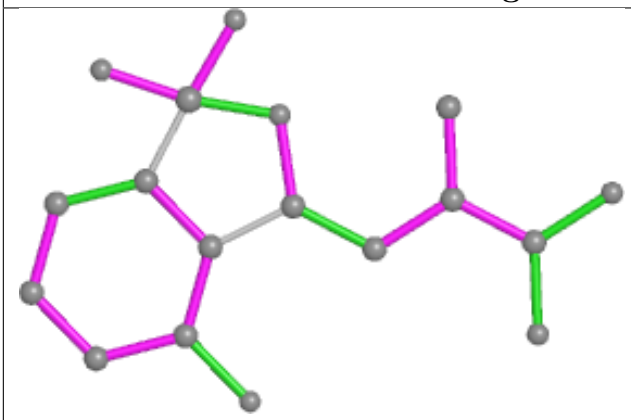
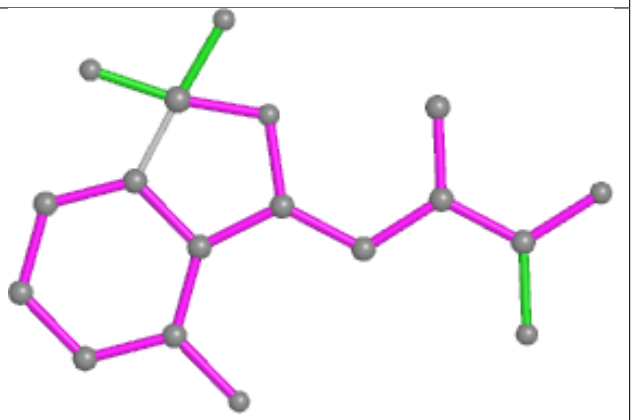


Rings

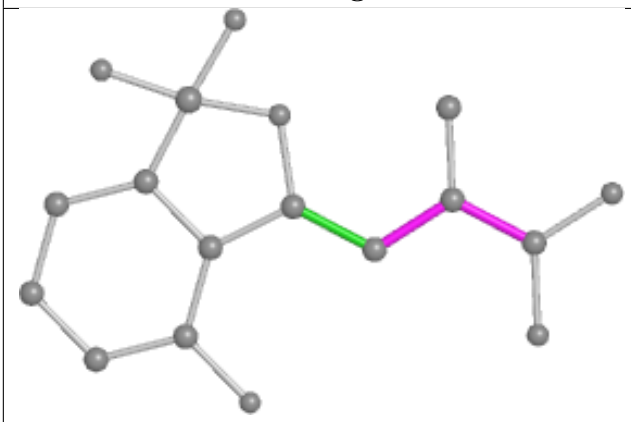
Ligand A1LXF H 303



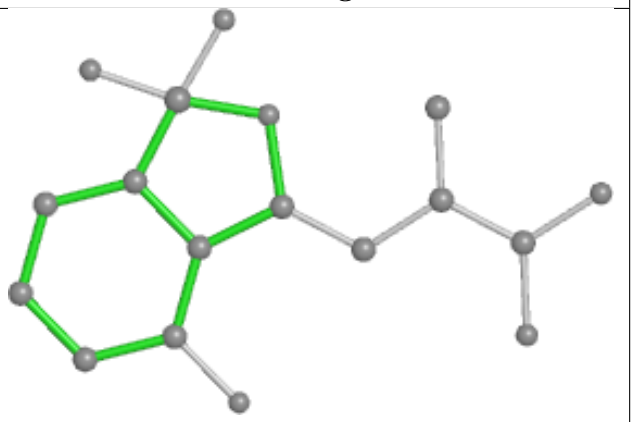
Bond lengths



Bond angles

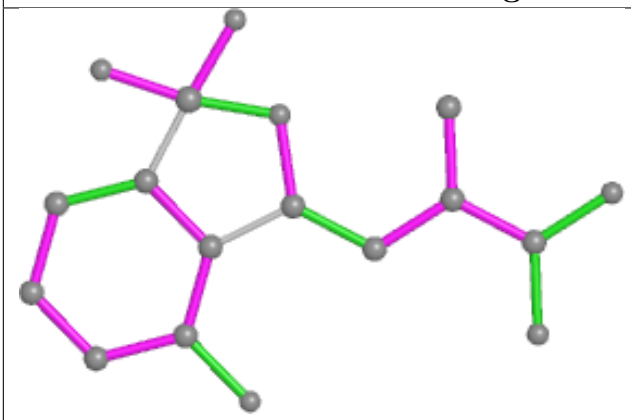


Torsions

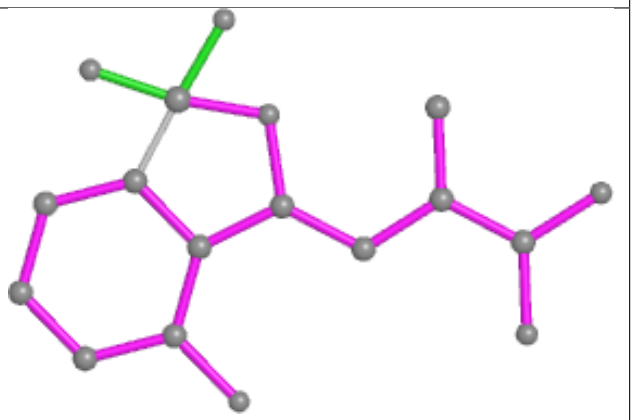


Rings

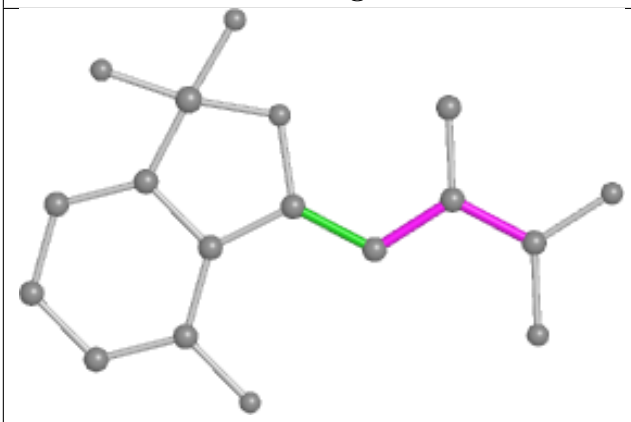
Ligand A1LXF A 303



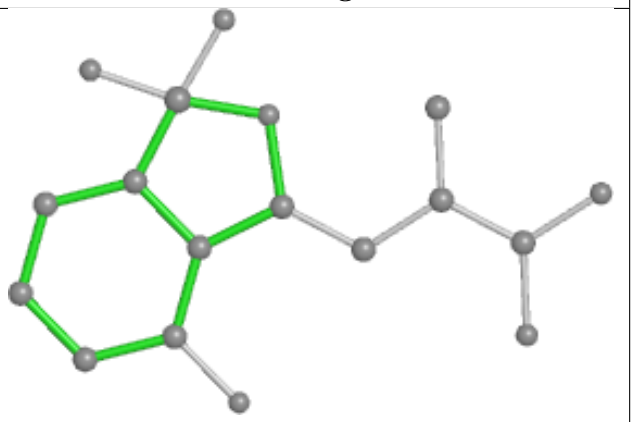
Bond lengths



Bond angles

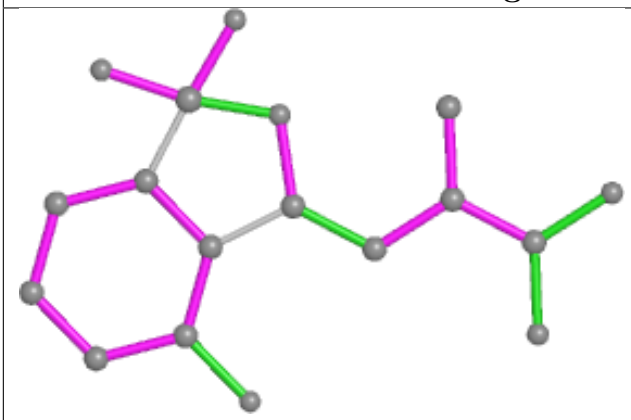


Torsions

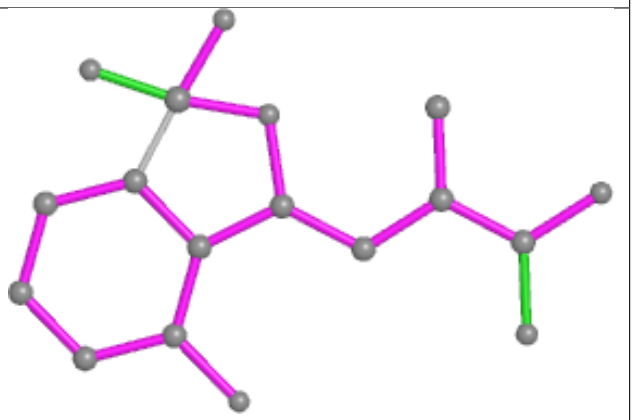


Rings

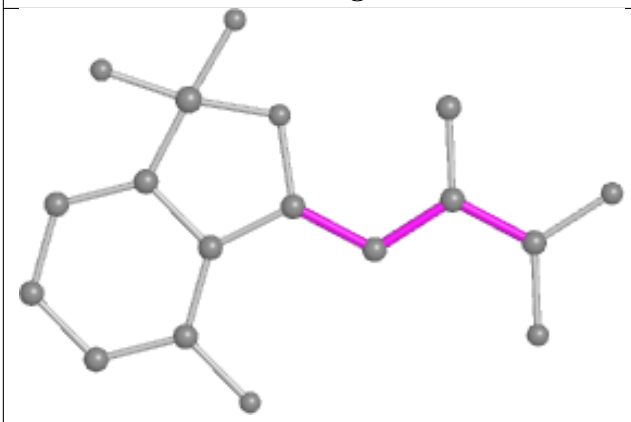
Ligand A1LXF B 303



Bond lengths



Bond angles



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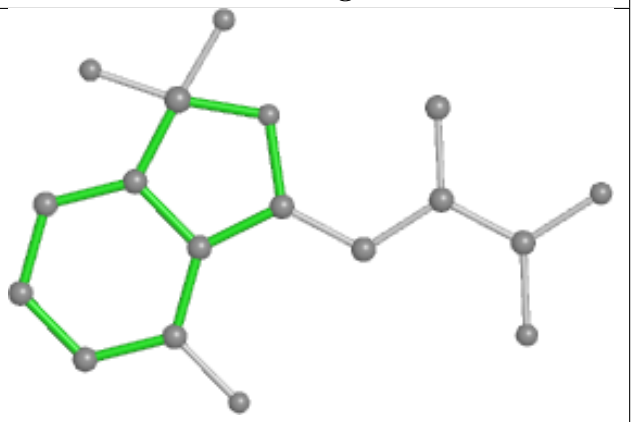
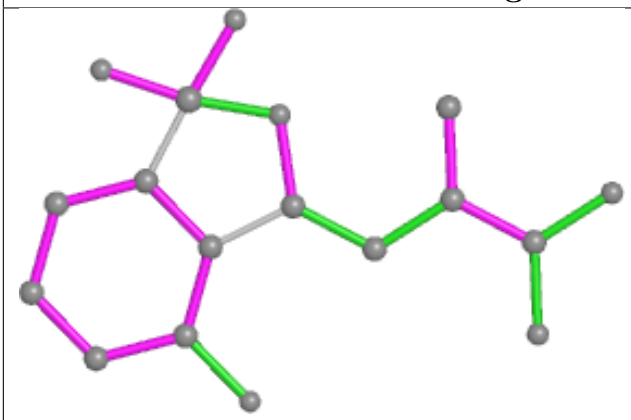
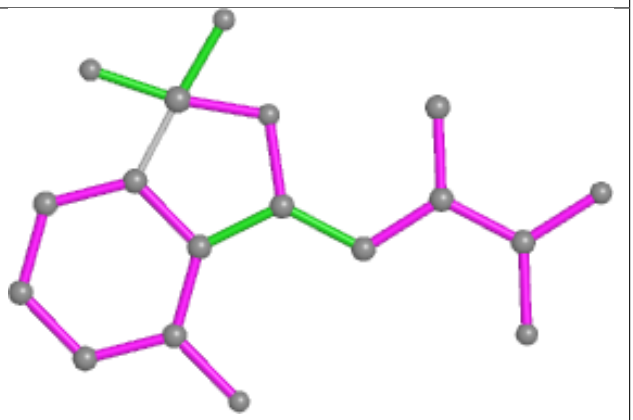


Rings

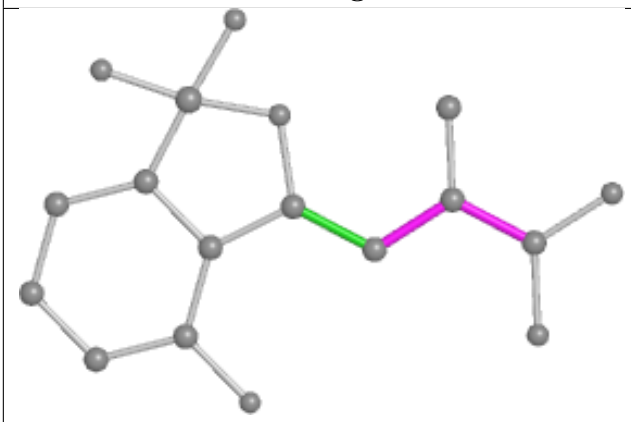
Ligand A1LXF F 303



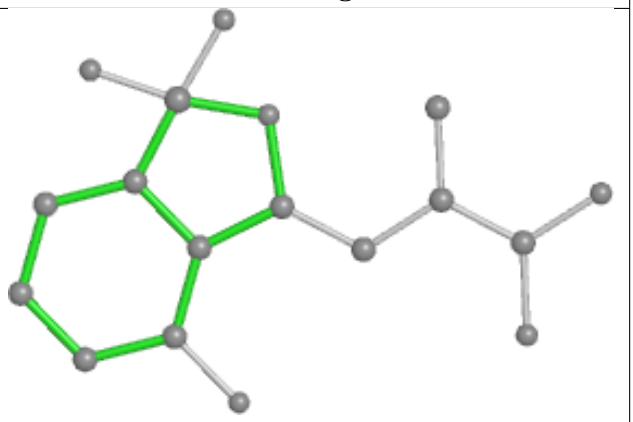
Bond lengths



Bond angles

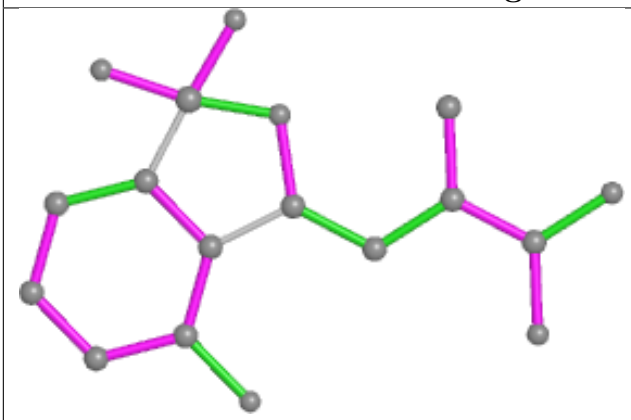


Torsions

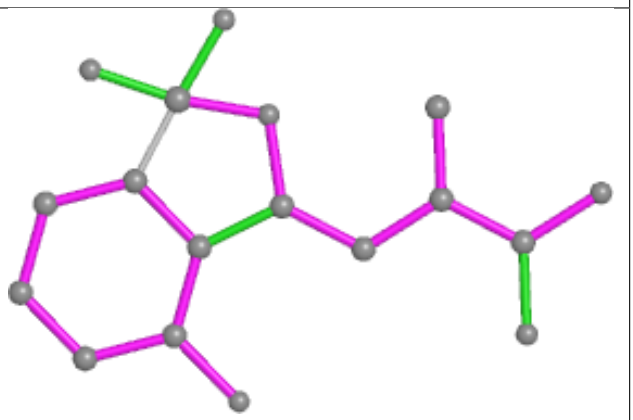


Rings

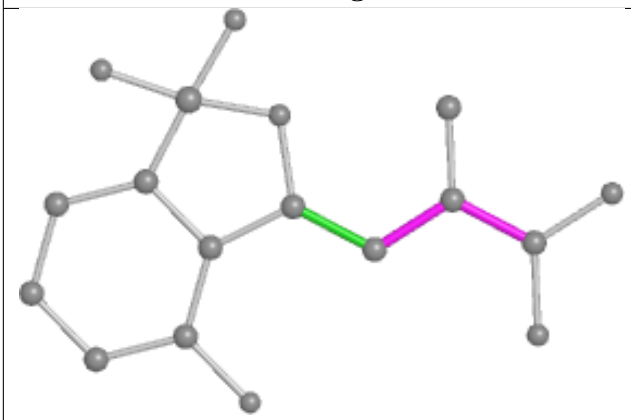
Ligand A1LXF E 303



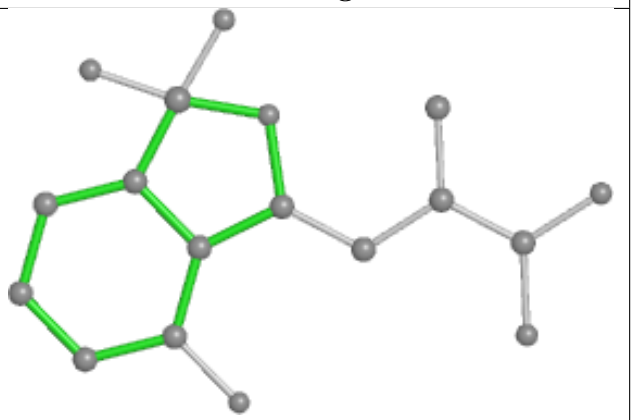
Bond lengths



Bond angles

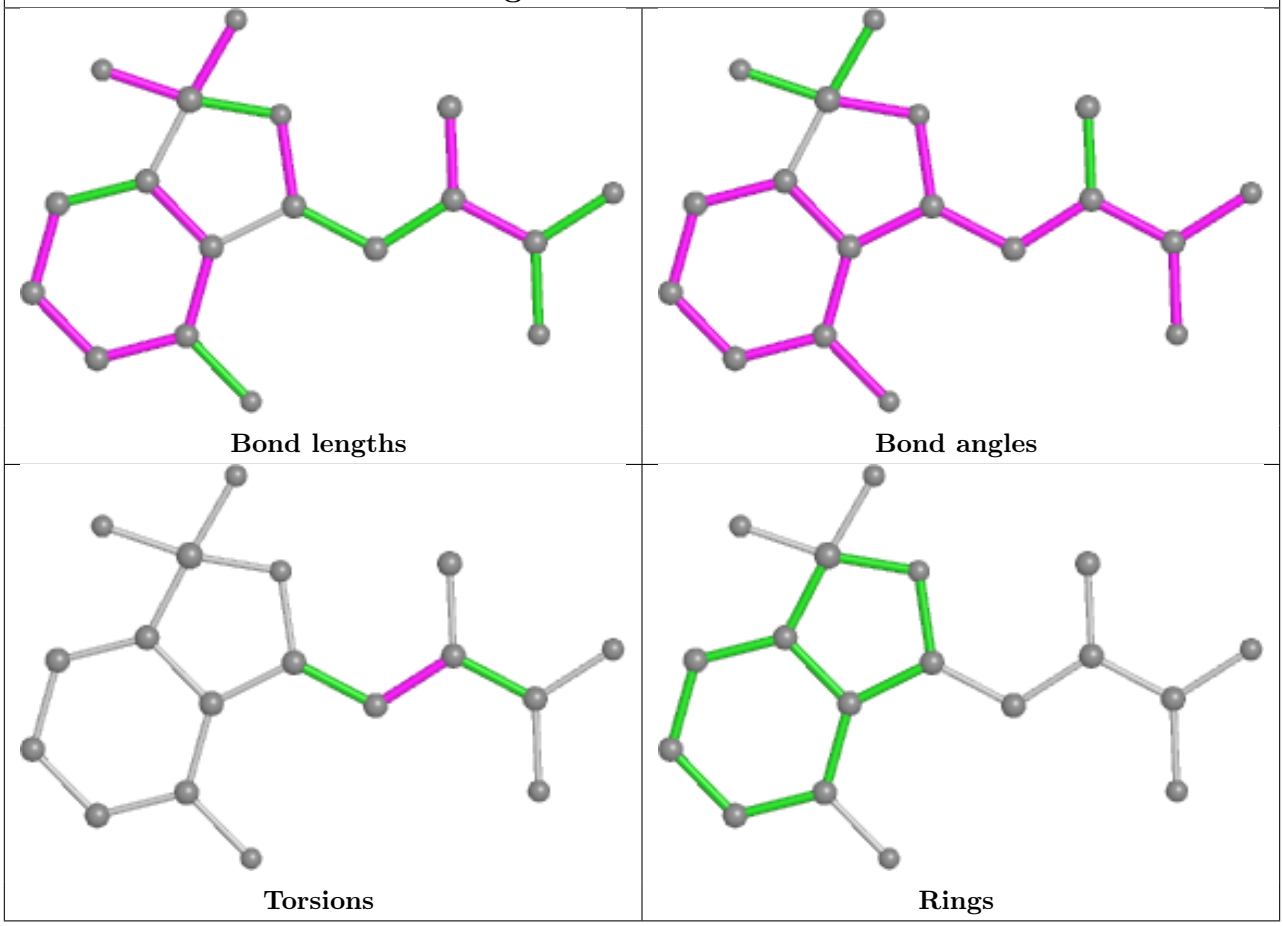


Torsions



Rings

Ligand A1LXF C 303



5.7 Other polymers

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, 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	231/231 (100%)	0.18	8 (3%) 47 52	15, 24, 40, 68	0
1	B	231/231 (100%)	0.39	7 (3%) 52 58	17, 27, 46, 78	0
1	C	231/231 (100%)	0.35	13 (5%) 31 35	16, 25, 46, 64	0
1	D	231/231 (100%)	0.35	12 (5%) 34 37	15, 23, 43, 59	0
1	E	231/231 (100%)	0.89	32 (13%) 7 9	20, 33, 52, 73	0
1	F	231/231 (100%)	0.13	8 (3%) 47 52	14, 21, 38, 69	0
1	G	231/231 (100%)	0.78	16 (6%) 24 27	21, 32, 47, 66	0
1	H	231/231 (100%)	1.04	34 (14%) 7 8	22, 37, 54, 62	0
All	All	1848/1848 (100%)	0.52	130 (7%) 24 27	14, 28, 49, 78	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	ALA	7.6
1	E	262	ALA	6.6
1	A	262	ALA	5.9
1	C	209	GLY	5.6
1	H	209	GLY	5.6
1	D	209	GLY	5.4
1	G	262	ALA	5.3
1	F	262	ALA	5.3
1	F	210	ASN	4.9
1	C	262	ALA	4.9
1	D	36	VAL	4.9
1	D	262	ALA	4.8
1	C	36	VAL	4.0
1	G	210	ASN	3.8
1	E	260	THR	3.8
1	E	207	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	141	ARG	3.6
1	B	260	THR	3.5
1	D	41	VAL	3.5
1	B	209	GLY	3.5
1	D	40	PRO	3.5
1	G	205	ARG	3.5
1	A	260	THR	3.4
1	E	211	VAL	3.3
1	H	129	ALA	3.3
1	H	262	ALA	3.3
1	H	138	SER	3.2
1	E	216	LEU	3.2
1	E	210	ASN	3.2
1	E	256	VAL	3.1
1	E	160	SER	3.1
1	G	78	ASP	3.1
1	C	41	VAL	3.1
1	G	260	THR	3.1
1	A	209	GLY	3.1
1	E	209	GLY	3.1
1	H	210	ASN	3.0
1	D	78	ASP	3.0
1	H	32	ALA	3.0
1	C	260	THR	3.0
1	H	145	VAL	3.0
1	H	78	ASP	3.0
1	E	62	PHE	2.9
1	E	217	ALA	2.9
1	F	209	GLY	2.9
1	H	63	ASP	2.9
1	E	212	ALA	2.9
1	E	145	VAL	2.8
1	E	234	GLN	2.8
1	C	39	ILE	2.8
1	F	141	ARG	2.7
1	B	208	ALA	2.7
1	G	211	VAL	2.7
1	H	93	ALA	2.7
1	H	128	ALA	2.7
1	A	210	ASN	2.7
1	H	151	PRO	2.7
1	H	260	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	32	ALA	2.6
1	D	32	ALA	2.6
1	E	258	ALA	2.6
1	G	32	ALA	2.6
1	H	50	ALA	2.6
1	E	229	HIS	2.6
1	C	210	ASN	2.6
1	D	260	THR	2.6
1	F	260	THR	2.6
1	G	63	ASP	2.6
1	H	76	ASP	2.6
1	H	131	VAL	2.5
1	E	232	GLU	2.5
1	H	165	VAL	2.5
1	B	210	ASN	2.5
1	D	261	ASN	2.5
1	C	40	PRO	2.4
1	H	130	GLY	2.4
1	E	231	PRO	2.4
1	H	137	PRO	2.4
1	H	160	SER	2.4
1	H	103	ILE	2.4
1	E	261	ASN	2.4
1	H	141	ARG	2.4
1	G	62	PHE	2.4
1	H	104	GLY	2.4
1	E	206	THR	2.4
1	E	221	THR	2.4
1	D	37	SER	2.4
1	D	235	PHE	2.4
1	H	150	ILE	2.3
1	F	258	ALA	2.3
1	E	228	GLN	2.3
1	B	212	ALA	2.3
1	C	37	SER	2.3
1	E	32	ALA	2.3
1	E	78	ASP	2.3
1	H	51	ASP	2.3
1	D	141	ARG	2.3
1	G	204	SER	2.3
1	C	32	ALA	2.2
1	G	258	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	235	PHE	2.2
1	A	212	ALA	2.2
1	E	176	GLY	2.2
1	H	106	PRO	2.2
1	E	115	PHE	2.2
1	E	214	ALA	2.2
1	G	105	LEU	2.2
1	H	152	THR	2.1
1	H	125	VAL	2.1
1	G	261	ASN	2.1
1	E	251	HIS	2.1
1	B	61	SER	2.1
1	E	156	GLU	2.1
1	E	147	GLY	2.1
1	H	123	VAL	2.1
1	H	214	ALA	2.1
1	C	62	PHE	2.1
1	H	46	LEU	2.1
1	F	261	ASN	2.1
1	G	141	ARG	2.1
1	C	78	ASP	2.0
1	A	211	VAL	2.0
1	F	211	VAL	2.0
1	H	132	ALA	2.0
1	E	249	LEU	2.0
1	G	216	LEU	2.0
1	H	52	GLY	2.0
1	H	157	GLY	2.0
1	A	100	GLU	2.0
1	C	261	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

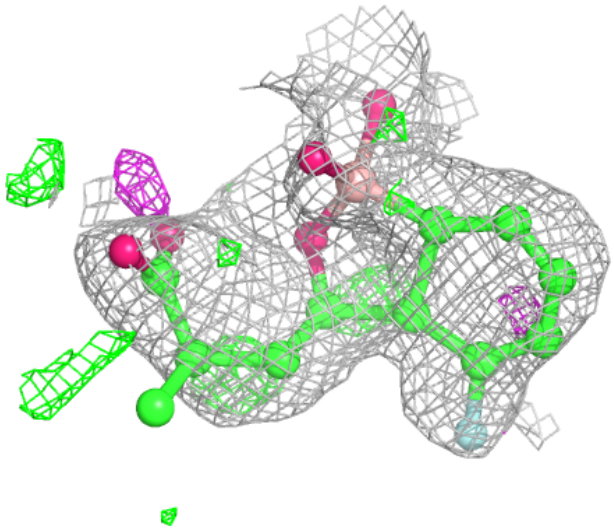
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

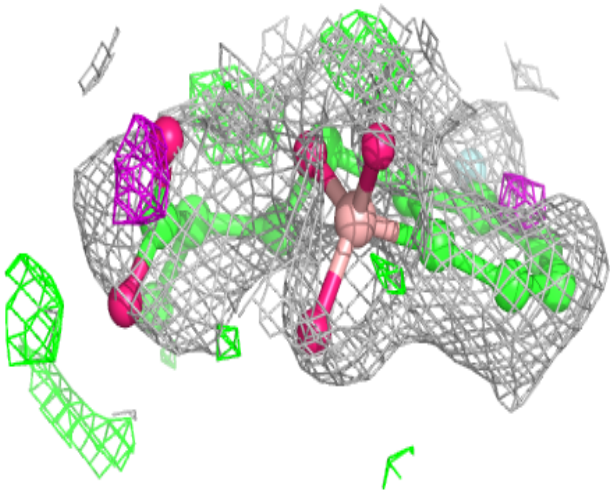
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	C	304	3/3	0.77	0.13	35,35,36,38	0
3	A1LXF	H	303	18/18	0.78	0.19	23,44,57,67	0
3	A1LXF	G	303	18/18	0.78	0.18	28,48,59,65	0
3	A1LXF	F	303	18/18	0.79	0.21	20,46,63,64	0
3	A1LXF	E	303	18/18	0.82	0.17	25,47,51,54	0
3	A1LXF	D	303	18/18	0.83	0.18	22,40,57,60	0
3	A1LXF	B	303	18/18	0.86	0.15	26,37,59,70	0
3	A1LXF	A	303	18/18	0.87	0.15	22,39,52,65	0
3	A1LXF	C	303	18/18	0.90	0.13	22,30,45,46	0
2	ZN	G	301	1/1	0.99	0.03	27,27,27,27	0
2	ZN	G	302	1/1	0.99	0.04	29,29,29,29	0
2	ZN	A	301	1/1	0.99	0.02	22,22,22,22	0
2	ZN	A	302	1/1	0.99	0.03	20,20,20,20	0
2	ZN	B	301	1/1	0.99	0.03	26,26,26,26	0
2	ZN	B	302	1/1	0.99	0.04	23,23,23,23	0
2	ZN	D	301	1/1	0.99	0.04	19,19,19,19	0
2	ZN	D	302	1/1	0.99	0.03	21,21,21,21	0
2	ZN	E	301	1/1	0.99	0.03	31,31,31,31	0
2	ZN	E	302	1/1	0.99	0.03	33,33,33,33	0
2	ZN	F	302	1/1	0.99	0.05	20,20,20,20	0
2	ZN	H	302	1/1	1.00	0.01	28,28,28,28	0
2	ZN	C	301	1/1	1.00	0.03	16,16,16,16	0
2	ZN	C	302	1/1	1.00	0.02	19,19,19,19	0
2	ZN	F	301	1/1	1.00	0.02	19,19,19,19	0
2	ZN	H	301	1/1	1.00	0.01	28,28,28,28	0

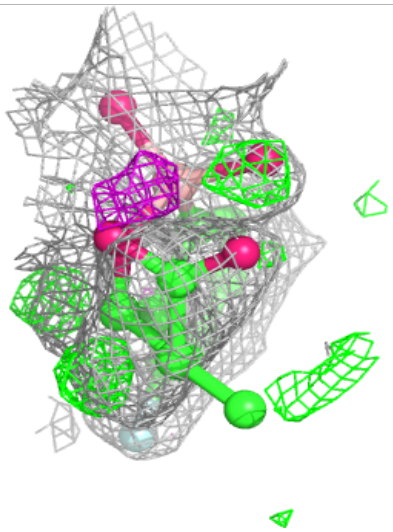
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1LXF H 303:

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

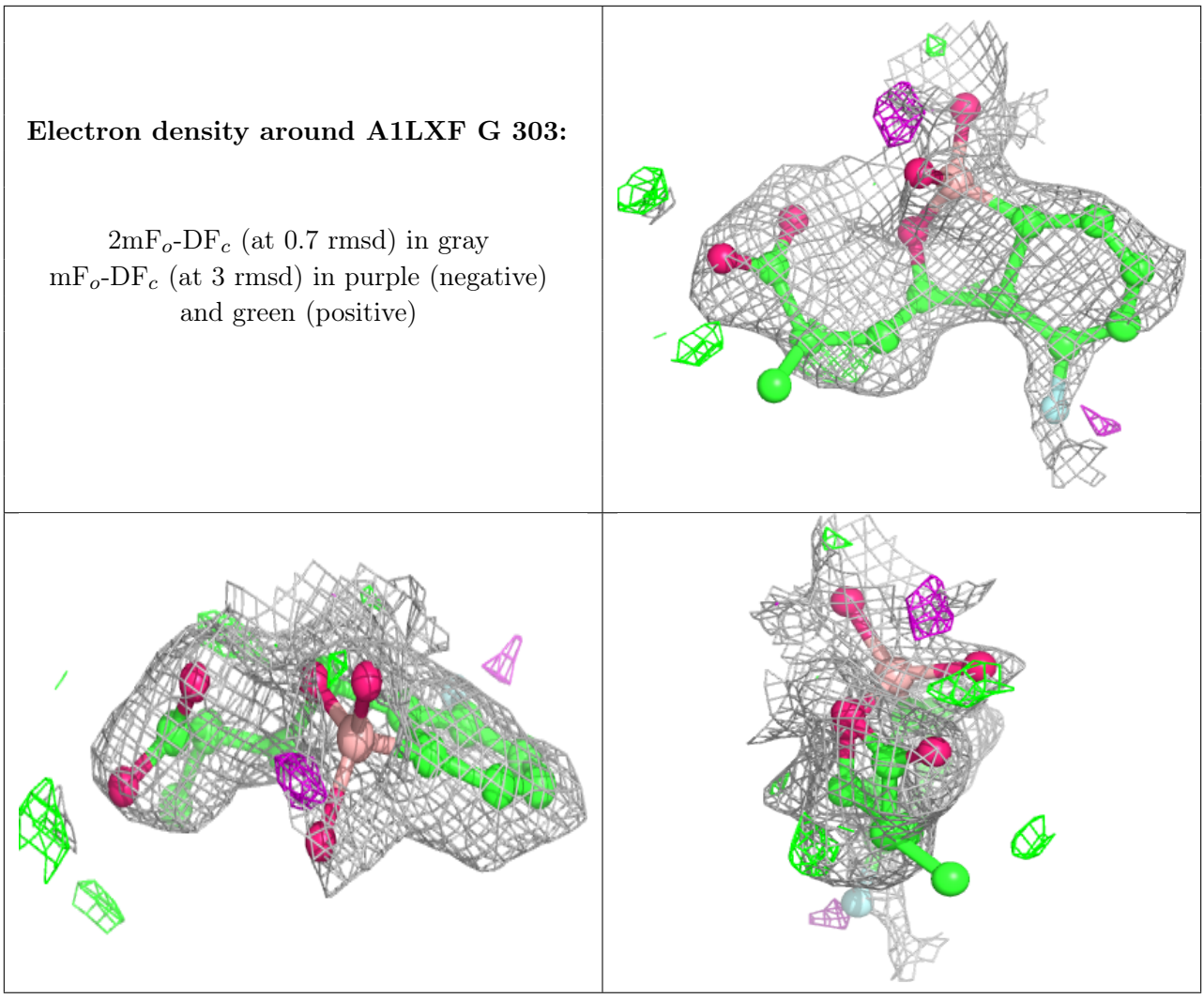






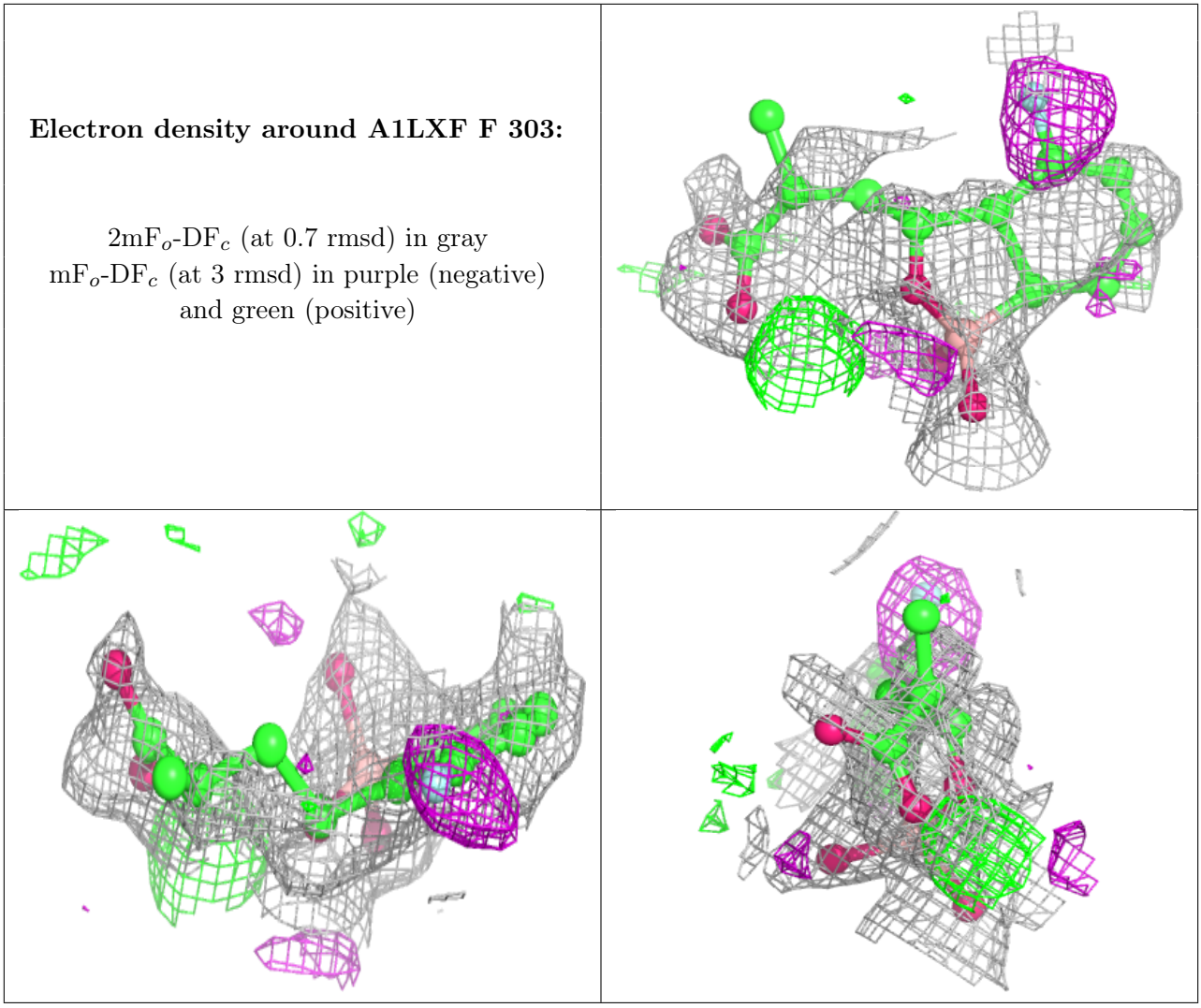
Electron density around A1LXF G 303:

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



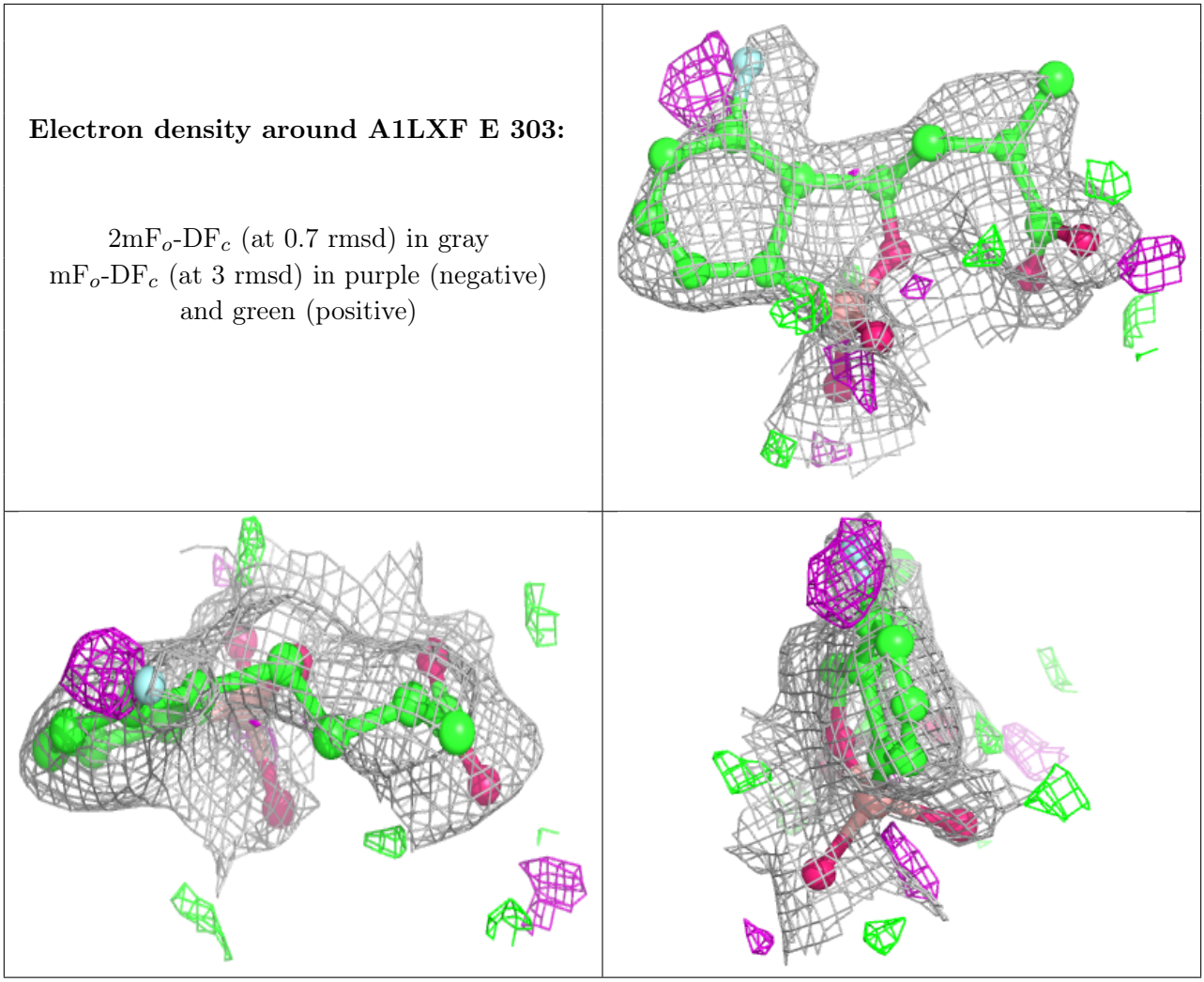
Electron density around A1LXF F 303:

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



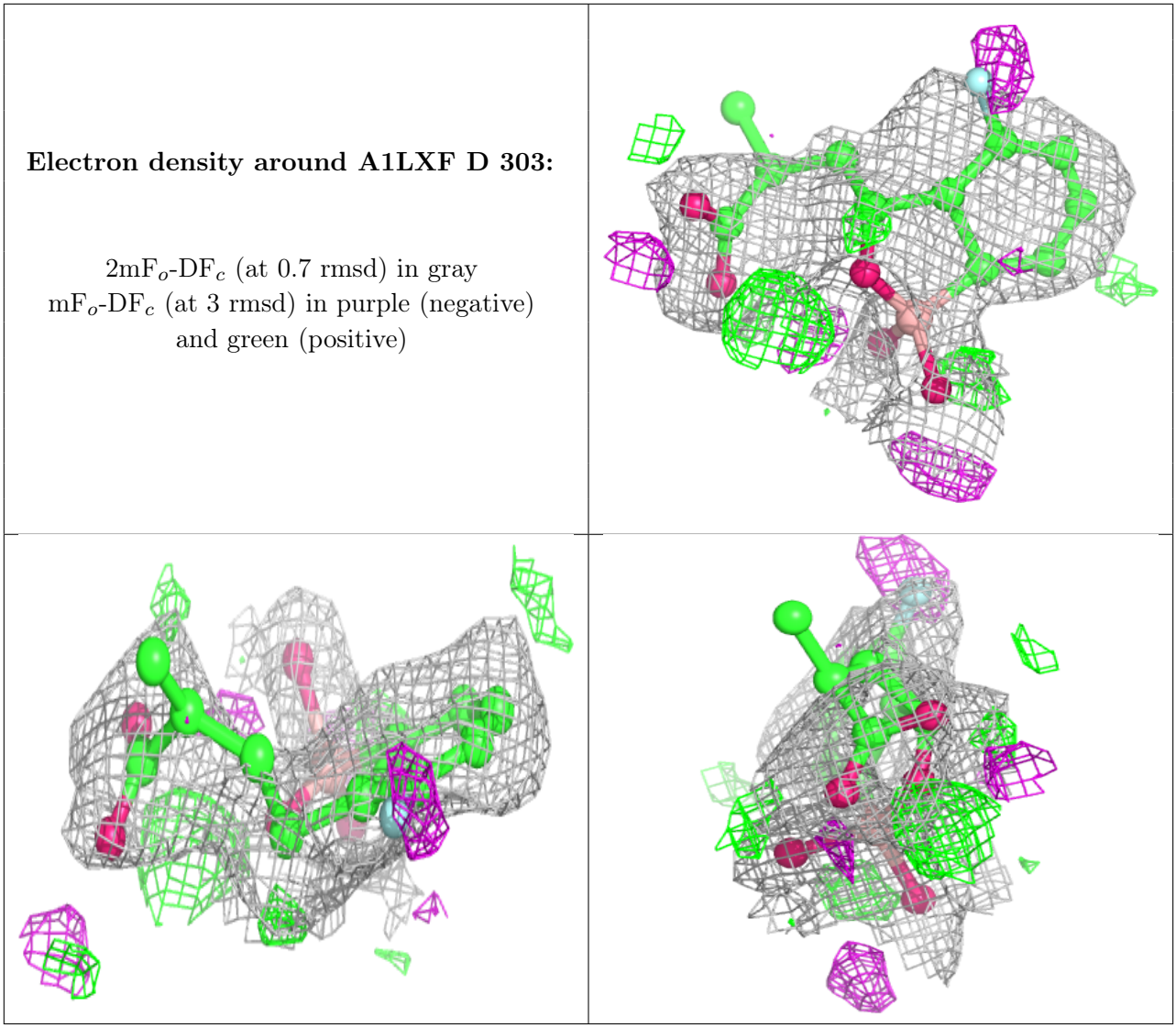
Electron density around A1LXF E 303:

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



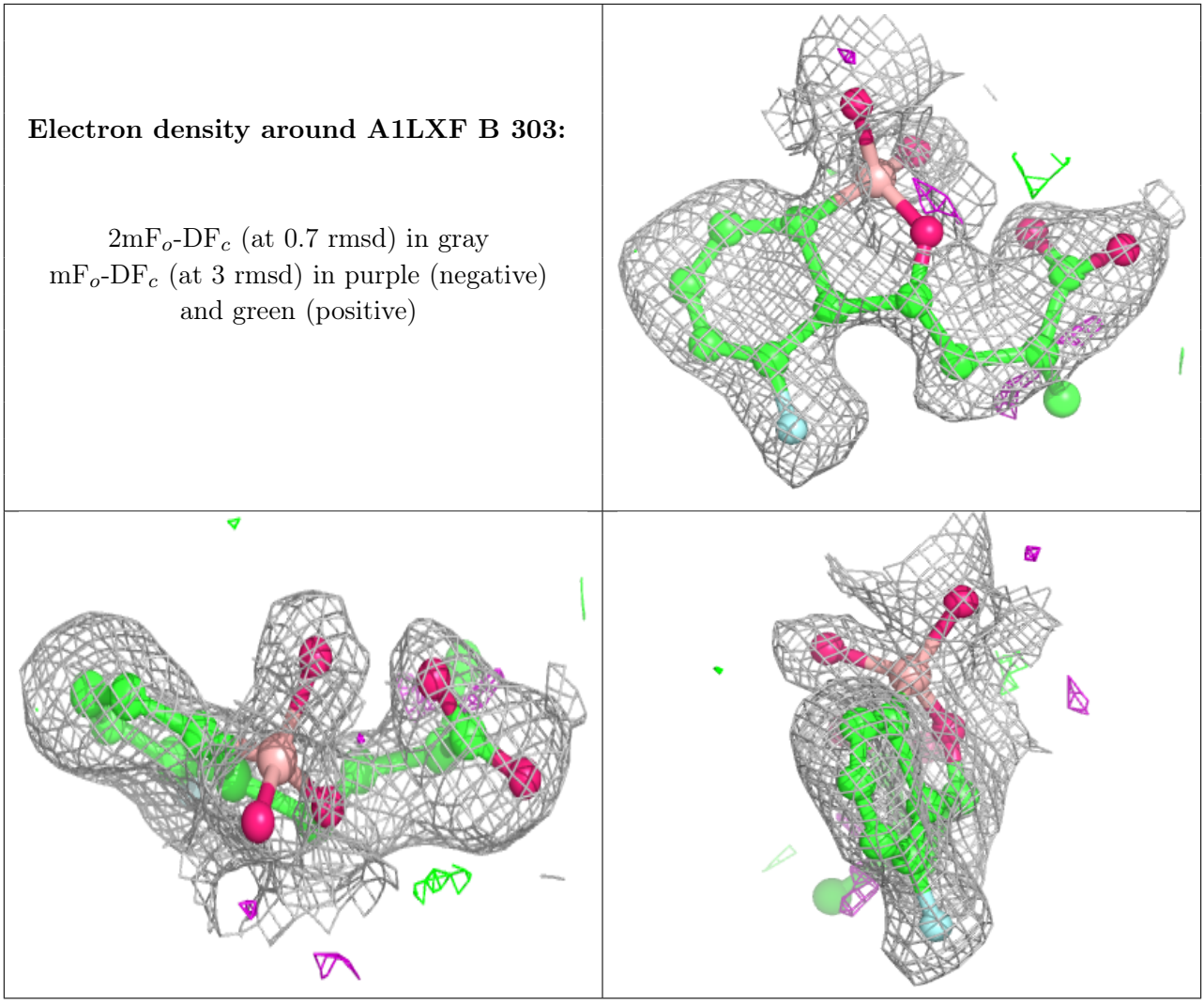
Electron density around A1LXF D 303:

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



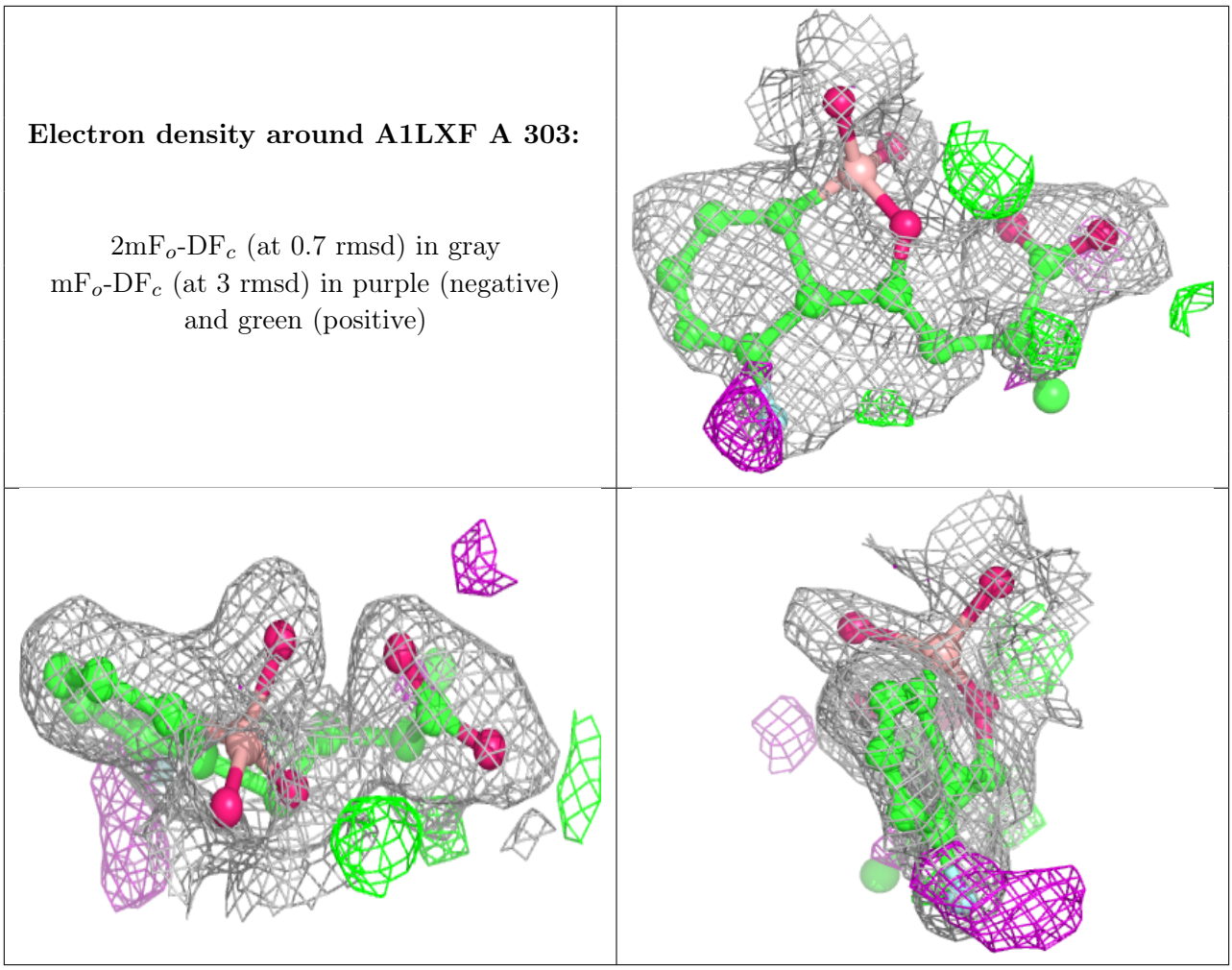
Electron density around A1LXF B 303:

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



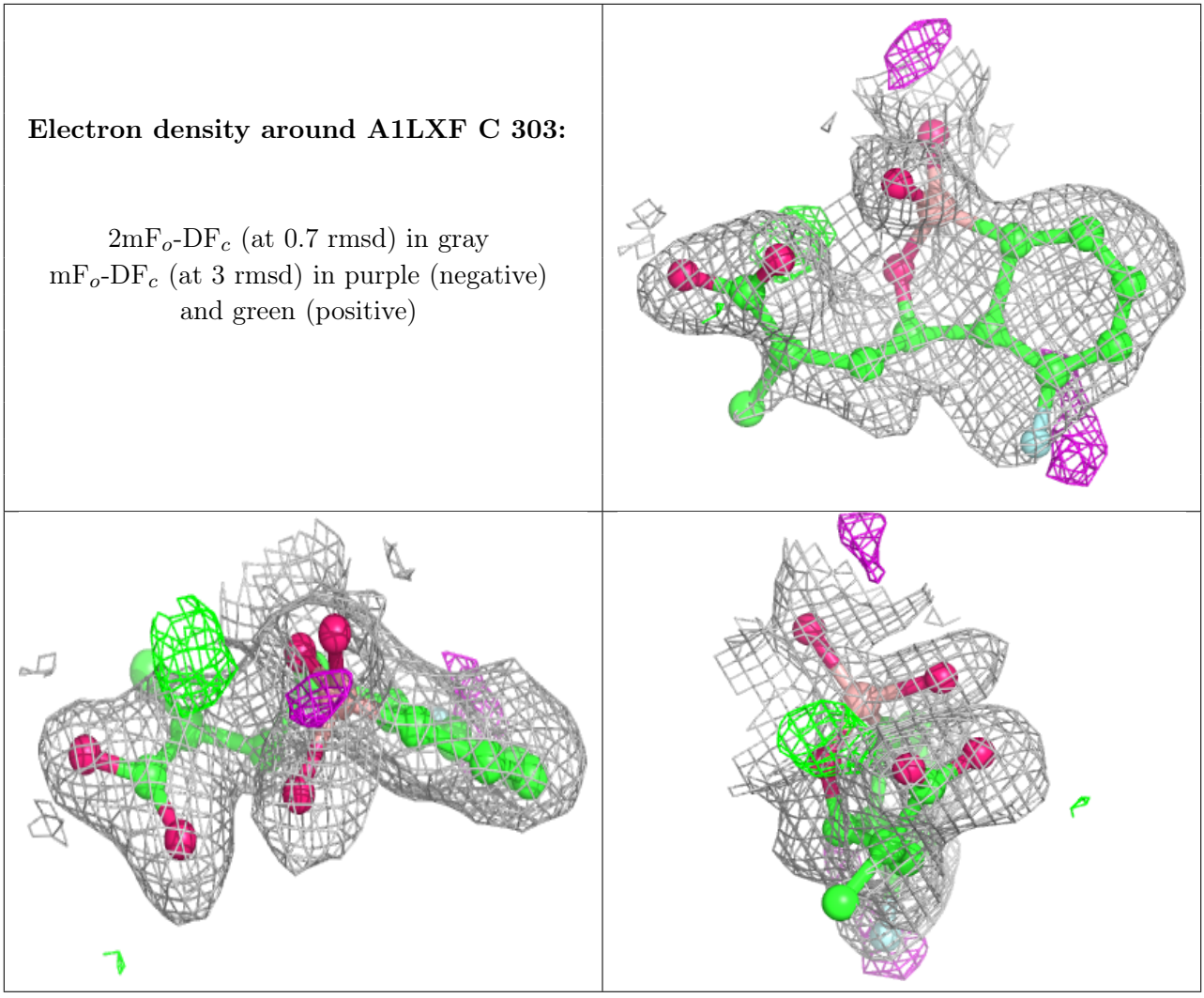
Electron density around A1LXF A 303:

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



Electron density around A1LXF C 303:

$2mF_o$-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.