Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 05:42 PM JST

PDB ID	:	5GMZ
Title	:	Hepatitis B virus core protein Y132A mutant in complex with 4-methyl heteroaryldihydropyrimidine
Authors	:	Xu, Z.H.; Zhou, Z.
Deposited on	:	2016-07-18
Resolution	:	1.70 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:

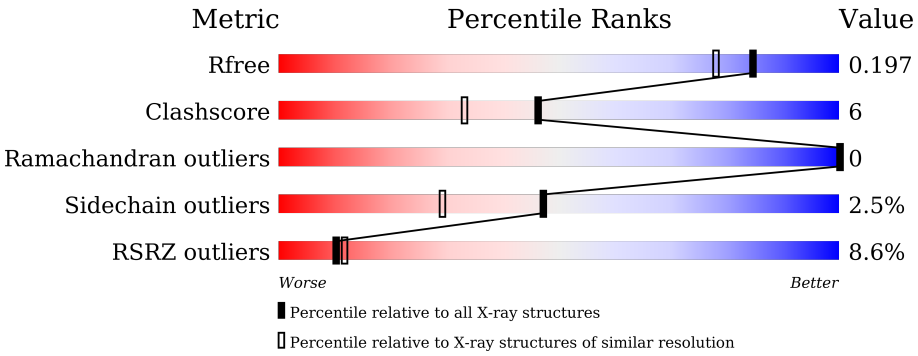
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	155	82% 10% 8%
1	B	155	3% 84% 11% 5%
1	C	155	5% 78% 13% 8%
1	D	155	6% 88% 8%
1	E	155	14% 77% 14% 8%
1	F	155	21% 80% 13%

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
2	IPA	E	203	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8136 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 Core protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	2	0
			1147	744	189	209	5			
1	B	148	Total	C	N	O	S	0	3	0
			1204	780	200	219	5			
1	C	143	Total	C	N	O	S	0	4	0
			1161	753	191	212	5			
1	D	150	Total	C	N	O	S	0	4	0
			1227	797	203	222	5			
1	E	143	Total	C	N	O	S	0	2	0
			1147	744	189	209	5			
1	F	150	Total	C	N	O	S	0	2	0
			1211	787	198	221	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ALA	TYR	engineered mutation	UNP L7R9I1
A	150	GLU	-	expression tag	UNP L7R9I1
A	151	ASN	-	expression tag	UNP L7R9I1
A	152	LEU	-	expression tag	UNP L7R9I1
A	153	TYR	-	expression tag	UNP L7R9I1
A	154	PHE	-	expression tag	UNP L7R9I1
A	155	GLN	-	expression tag	UNP L7R9I1
B	132	ALA	TYR	engineered mutation	UNP L7R9I1
B	150	GLU	-	expression tag	UNP L7R9I1
B	151	ASN	-	expression tag	UNP L7R9I1
B	152	LEU	-	expression tag	UNP L7R9I1
B	153	TYR	-	expression tag	UNP L7R9I1
B	154	PHE	-	expression tag	UNP L7R9I1
B	155	GLN	-	expression tag	UNP L7R9I1
C	132	ALA	TYR	engineered mutation	UNP L7R9I1
C	150	GLU	-	expression tag	UNP L7R9I1
C	151	ASN	-	expression tag	UNP L7R9I1

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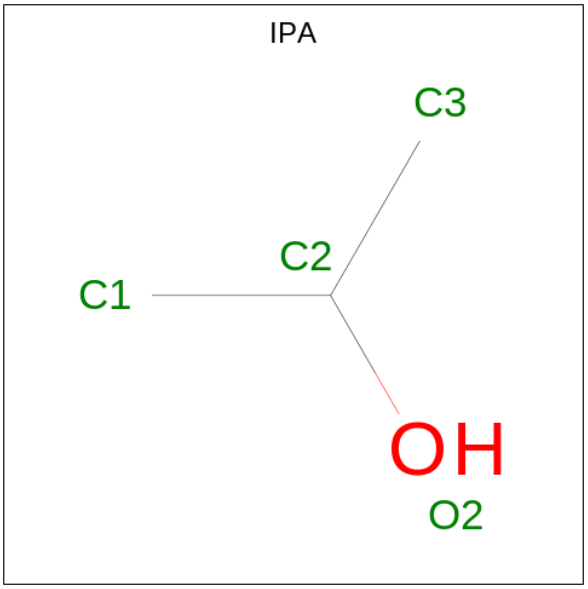
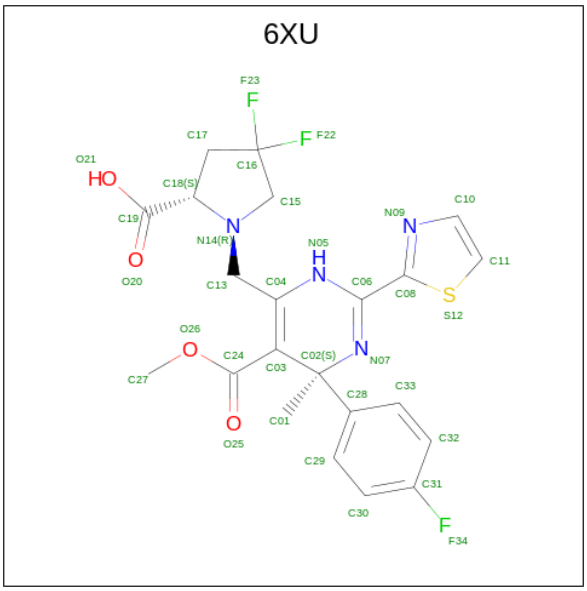
Chain	Residue	Modelled	Actual	Comment	Reference
C	152	LEU	-	expression tag	UNP L7R9I1
C	153	TYR	-	expression tag	UNP L7R9I1
C	154	PHE	-	expression tag	UNP L7R9I1
C	155	GLN	-	expression tag	UNP L7R9I1
D	132	ALA	TYR	engineered mutation	UNP L7R9I1
D	150	GLU	-	expression tag	UNP L7R9I1
D	151	ASN	-	expression tag	UNP L7R9I1
D	152	LEU	-	expression tag	UNP L7R9I1
D	153	TYR	-	expression tag	UNP L7R9I1
D	154	PHE	-	expression tag	UNP L7R9I1
D	155	GLN	-	expression tag	UNP L7R9I1
E	132	ALA	TYR	engineered mutation	UNP L7R9I1
E	150	GLU	-	expression tag	UNP L7R9I1
E	151	ASN	-	expression tag	UNP L7R9I1
E	152	LEU	-	expression tag	UNP L7R9I1
E	153	TYR	-	expression tag	UNP L7R9I1
E	154	PHE	-	expression tag	UNP L7R9I1
E	155	GLN	-	expression tag	UNP L7R9I1
F	132	ALA	TYR	engineered mutation	UNP L7R9I1
F	150	GLU	-	expression tag	UNP L7R9I1
F	151	ASN	-	expression tag	UNP L7R9I1
F	152	LEU	-	expression tag	UNP L7R9I1
F	153	TYR	-	expression tag	UNP L7R9I1
F	154	PHE	-	expression tag	UNP L7R9I1
F	155	GLN	-	expression tag	UNP L7R9I1

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



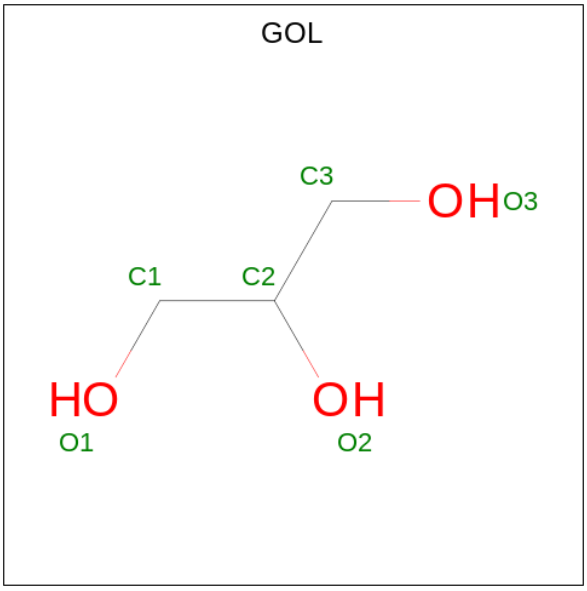
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 3 1	0	0
2	A	1	Total C O 4 3 1	0	0
2	A	1	Total C O 4 3 1	0	0
2	A	1	Total C O 4 3 1	0	0
2	C	1	Total C O 4 3 1	0	0
2	D	1	Total C O 4 3 1	0	0
2	D	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0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

- Molecule 3 is (2S)-4,4-difluoro-1-[[(4S)-4-(4-fluorophenyl)-5-methoxycarbonyl-4-methyl-2-(1,3-thiazol-2-yl)-1H-pyrimidin-6-yl]methyl]pyrrolidine-2-carboxylic acid (three-letter code: 6XU) (formula: $C_{22}H_{21}F_3N_4O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	A	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	B	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	C	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	D	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	E	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		
3	F	1	Total	C	F	N	O	S	0	0
			34	22	3	4	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

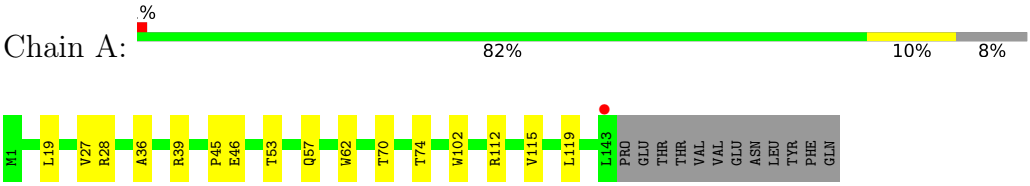
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	129	Total O 129 129	0	0
6	B	153	Total O 153 153	0	0
6	C	125	Total O 125 125	0	0
6	D	139	Total O 139 139	0	0
6	E	96	Total O 96 96	0	0
6	F	102	Total O 102 102	0	0

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.

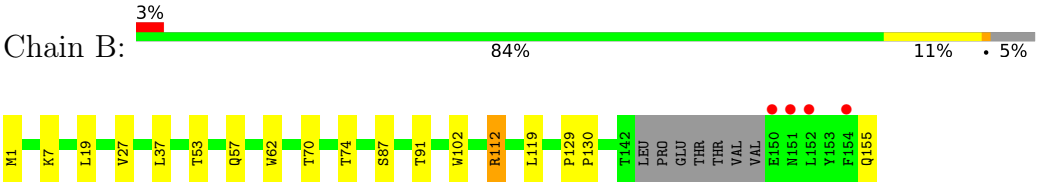
• Molecule 1: Core protein

Chain A:



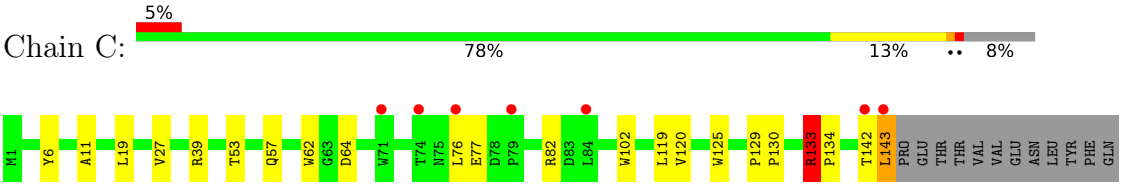
• Molecule 1: Core protein

Chain B:



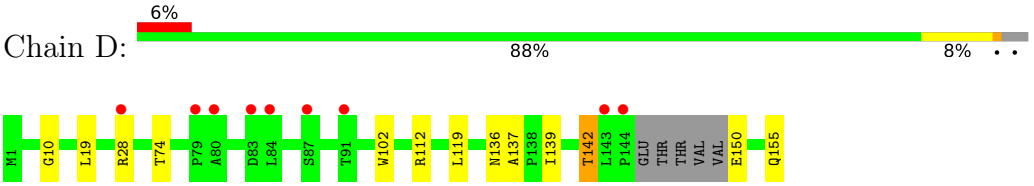
• Molecule 1: Core protein

Chain C:



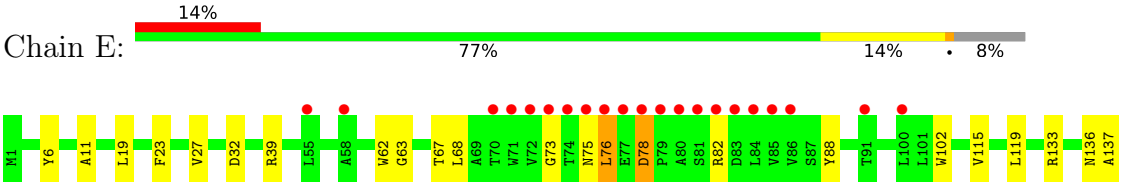
• Molecule 1: Core protein

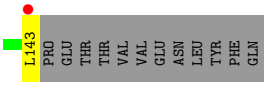
Chain D:



• Molecule 1: Core protein

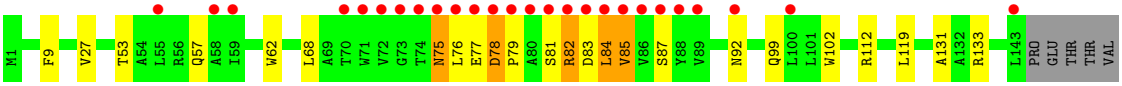
Chain E:

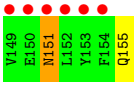




• Molecule 1: Core protein

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.02Å 67.22Å 87.67Å 68.10° 68.43° 83.07°	Depositor
Resolution (Å)	33.31 – 1.70 33.31 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (33.31-1.70) 87.3 (33.31-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.174 , 0.196 0.174 , 0.197	Depositor DCC
R_{free} test set	3335 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8136	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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: 6XU, IPA, CL, 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	A	0.35	0/1181	0.50	0/1620
1	B	0.36	0/1239	0.51	0/1694
1	C	0.37	0/1195	0.56	1/1639 (0.1%)
1	D	0.36	0/1263	0.52	0/1729
1	E	0.34	0/1181	0.50	0/1619
1	F	0.34	0/1246	0.51	0/1706
All	All	0.35	0/7305	0.52	1/10007 (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	C	133	ARG	NE-CZ-NH2	5.74	123.17	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	1147	0	1131	12	0
1	B	1204	0	1175	13	0
1	C	1161	0	1145	20	0
1	D	1227	0	1204	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1147	0	1130	21	0
1	F	1211	0	1185	22	0
2	A	16	0	32	0	0
2	C	4	0	8	0	0
2	D	8	0	16	0	0
2	E	16	0	32	7	0
3	A	68	0	0	0	0
3	B	34	0	0	0	0
3	C	34	0	0	0	0
3	D	34	0	0	0	0
3	E	34	0	0	0	0
3	F	34	0	0	0	0
4	B	6	0	8	0	0
4	F	6	0	8	2	0
5	D	1	0	0	0	0
6	A	129	0	0	1	0
6	B	153	0	0	1	0
6	C	125	0	0	3	0
6	D	139	0	0	2	0
6	E	96	0	0	2	0
6	F	102	0	0	2	0
All	All	8136	0	7074	91	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 6.

All (91) 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:A:19[B]:LEU:HD11	1:A:119:LEU:HD22	1.53	0.90
1:C:19[A]:LEU:HD11	1:C:119[A]:LEU:HD22	1.62	0.79
1:E:136:ASN:HA	2:E:204:IPA:H2	1.69	0.74
1:E:32:ASP:OD2	6:E:301:HOH:O	2.07	0.72
1:E:137:ALA:H	2:E:204:IPA:H33	1.57	0.69
1:A:19[B]:LEU:HD11	1:A:119:LEU:CD2	2.25	0.67
1:E:19:LEU:HD11	1:E:119[A]:LEU:HD22	1.78	0.66
1:D:150:GLU:N	6:D:303:HOH:O	2.28	0.65
1:F:151:ASN:N	1:F:151:ASN:OD1	2.31	0.64
1:D:28:ARG:NH1	6:D:302:HOH:O	2.30	0.64
1:B:112[B]:ARG:NH1	6:B:301:HOH:O	2.31	0.63
1:D:137:ALA:H	2:E:203:IPA:H32	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:PRO:HA	1:F:82:ARG:HG3	1.81	0.61
1:C:64:ASP:OD1	6:C:301:HOH:O	2.16	0.61
1:E:102:TRP:CZ3	1:E:119[A]:LEU:HD21	2.36	0.60
1:C:142:THR:O	1:C:143:LEU:HB2	2.02	0.59
1:F:77:GLU:HG3	1:F:78:ASP:H	1.67	0.59
1:C:19[B]:LEU:HD21	1:C:119[B]:LEU:HG	1.85	0.59
1:A:36:ALA:O	6:A:301:HOH:O	2.17	0.57
1:C:19[B]:LEU:CD2	1:C:119[B]:LEU:HG	2.35	0.57
1:B:37:LEU:HD21	1:C:120:VAL:HG11	1.87	0.56
1:A:102:TRP:CZ3	1:A:119:LEU:HD21	2.41	0.56
1:B:19:LEU:HD21	1:B:119[B]:LEU:HG	1.88	0.56
1:B:70:THR:O	1:B:74:THR:HG23	2.06	0.56
1:E:115:VAL:O	1:E:119[A]:LEU:HG	2.06	0.55
1:E:73:GLY:O	1:E:82:ARG:NE	2.26	0.55
1:F:77:GLU:HG3	1:F:78:ASP:N	2.22	0.55
1:F:131:ALA:O	4:F:201:GOL:H32	2.07	0.54
1:A:70:THR:O	1:A:74:THR:HG23	2.07	0.54
1:F:102:TRP:CZ3	1:F:119[A]:LEU:HD21	2.43	0.53
1:A:39:ARG:HG3	1:B:1:MET:HG2	1.90	0.53
1:E:143:LEU:O	6:E:302:HOH:O	2.19	0.53
1:D:19:LEU:CD2	1:D:119[A]:LEU:HG	2.39	0.53
1:F:155:GLN:HG3	6:F:329:HOH:O	2.08	0.52
1:D:19:LEU:HD21	1:D:119[A]:LEU:HG	1.91	0.52
1:F:79:PRO:HA	1:F:82:ARG:CG	2.40	0.52
1:E:19:LEU:HD11	1:E:119[A]:LEU:CD2	2.40	0.52
1:A:45:PRO:HG3	1:B:7:LYS:HE2	1.92	0.52
1:E:102:TRP:HZ3	1:E:119[A]:LEU:HD21	1.76	0.51
1:B:19:LEU:CD2	1:B:119[B]:LEU:HG	2.40	0.50
1:D:139:ILE:O	1:D:142:THR:HG22	2.10	0.50
1:E:75:ASN:OD1	1:E:76:LEU:N	2.45	0.50
1:E:133:ARG:O	2:E:203:IPA:H33	2.11	0.50
1:C:102:TRP:CZ3	1:C:119[A]:LEU:HD21	2.47	0.50
1:F:82:ARG:HE	1:F:83:ASP:HB2	1.77	0.49
1:D:136:ASN:HA	2:E:203:IPA:H32	1.94	0.49
1:F:75:ASN:N	1:F:75:ASN:OD1	2.46	0.49
1:E:78:ASP:OD1	1:E:78:ASP:N	2.46	0.48
1:C:39:ARG:NH2	6:C:307:HOH:O	2.46	0.48
1:D:10:GLY:HA3	1:D:112:ARG:HE	1.79	0.48
1:B:102:TRP:CZ3	1:B:119[A]:LEU:HD21	2.49	0.48
1:F:112:ARG:HH21	1:F:112:ARG:HB3	1.79	0.48
1:A:46:GLU:HB3	1:B:155:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:TRP:CD1	1:C:133:ARG:HG3	2.49	0.47
1:E:27:VAL:HG11	1:E:62:TRP:CE2	2.48	0.47
1:F:81:SER:O	1:F:85:VAL:HG12	2.14	0.47
1:C:76:LEU:O	1:C:82:ARG:NH1	2.48	0.47
1:C:133:ARG:HD3	6:C:372:HOH:O	2.15	0.46
1:C:53:THR:O	1:C:57:GLN:HG2	2.15	0.46
1:C:102:TRP:HZ3	1:C:119[A]:LEU:HD21	1.79	0.46
1:B:53:THR:O	1:B:57:GLN:HG2	2.16	0.45
1:F:84:LEU:O	1:F:87:SER:OG	2.34	0.45
1:D:102:TRP:CZ3	1:D:119[B]:LEU:HD21	2.52	0.45
1:C:19[A]:LEU:HD11	1:C:119[A]:LEU:CD2	2.41	0.45
1:B:87:SER:O	1:B:91:THR:HG23	2.17	0.45
1:D:137:ALA:H	2:E:203:IPA:C3	2.30	0.44
1:C:133:ARG:HG2	1:C:134:PRO:O	2.18	0.43
1:A:102:TRP:HZ3	1:A:119:LEU:HD21	1.83	0.43
1:E:19:LEU:HD13	1:E:23:PHE:CE1	2.53	0.43
1:B:27:VAL:HG11	1:B:62:TRP:CE2	2.55	0.42
1:C:125:TRP:NE1	1:C:133:ARG:HG3	2.33	0.42
1:E:63:GLY:O	1:E:67:THR:HG23	2.19	0.42
1:F:53:THR:O	1:F:57:GLN:HG2	2.20	0.42
1:E:68:LEU:CD2	1:F:68:LEU:HD12	2.49	0.42
1:E:88:TYR:HE2	1:F:68:LEU:HD23	1.84	0.42
1:F:99:GLN:NE2	6:F:301:HOH:O	2.28	0.42
1:C:27:VAL:HG11	1:C:62:TRP:CE2	2.55	0.42
1:C:133:ARG:HG2	1:C:134:PRO:N	2.31	0.42
1:F:133:ARG:O	4:F:201:GOL:H31	2.20	0.42
1:C:129:PRO:HA	1:C:130:PRO:HD3	1.96	0.42
1:E:39:ARG:HB3	2:E:201:IPA:H11	2.01	0.42
1:E:88:TYR:CE2	1:F:68:LEU:HD23	2.55	0.41
1:F:112:ARG:HB3	1:F:112:ARG:NH2	2.35	0.41
1:A:115:VAL:O	1:A:119:LEU:HG	2.19	0.41
1:B:129:PRO:HA	1:B:130:PRO:HD3	1.99	0.41
1:A:27:VAL:HG11	1:A:62:TRP:CE2	2.56	0.41
1:E:6:TYR:HB3	1:E:11:ALA:HB3	2.02	0.41
1:F:9:PHE:O	1:F:112:ARG:HD2	2.21	0.41
1:C:6:TYR:HB3	1:C:11:ALA:HB3	2.04	0.40
1:A:53:THR:O	1:A:57:GLN:HG2	2.22	0.40
1:F:27:VAL:HG11	1:F:62:TRP:CE2	2.57	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	143/155 (92%)	141 (99%)	2 (1%)	0	100	100
1	B	147/155 (95%)	144 (98%)	3 (2%)	0	100	100
1	C	145/155 (94%)	143 (99%)	2 (1%)	0	100	100
1	D	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
1	E	143/155 (92%)	141 (99%)	2 (1%)	0	100	100
1	F	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
All	All	876/930 (94%)	860 (98%)	16 (2%)	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	127/137 (93%)	125 (98%)	2 (2%)	62	48
1	B	132/137 (96%)	130 (98%)	2 (2%)	65	51
1	C	129/137 (94%)	126 (98%)	3 (2%)	50	33
1	D	135/137 (98%)	132 (98%)	3 (2%)	52	34
1	E	127/137 (93%)	125 (98%)	2 (2%)	62	48
1	F	133/137 (97%)	125 (94%)	8 (6%)	19	6
All	All	783/822 (95%)	763 (97%)	20 (3%)	47	28

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	112	ARG
1	B	112[A]	ARG
1	B	112[B]	ARG
1	C	77	GLU
1	C	133	ARG
1	C	143	LEU
1	D	74	THR
1	D	142	THR
1	D	155	GLN
1	E	76	LEU
1	E	78	ASP
1	F	75	ASN
1	F	76	LEU
1	F	78	ASP
1	F	82	ARG
1	F	84	LEU
1	F	85	VAL
1	F	92	ASN
1	F	151	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\#\|Z\| > 2$
2	IPA	A	203	-	3,3,3	0.60	0	3,3,3	0.41	0
3	6XU	A	205	-	32,37,37	1.80	8 (25%)	33,56,56	1.74	8 (24%)
3	6XU	B	202	-	32,37,37	1.81	7 (21%)	33,56,56	1.78	8 (24%)
4	GOL	F	201	-	5,5,5	0.30	0	5,5,5	0.67	0
2	IPA	A	202	-	3,3,3	0.58	0	3,3,3	0.18	0
3	6XU	A	206	-	32,37,37	3.43	12 (37%)	33,56,56	2.31	11 (33%)
3	6XU	D	204	-	32,37,37	1.73	9 (28%)	33,56,56	1.78	8 (24%)
4	GOL	B	201	-	5,5,5	0.37	0	5,5,5	0.51	0
3	6XU	F	202	-	32,37,37	1.74	9 (28%)	33,56,56	1.95	10 (30%)
2	IPA	A	204	-	3,3,3	0.55	0	3,3,3	0.29	0
2	IPA	E	203	-	3,3,3	0.55	0	3,3,3	0.37	0
2	IPA	D	202	-	3,3,3	0.55	0	3,3,3	0.27	0
2	IPA	E	204	-	3,3,3	0.60	0	3,3,3	0.10	0
2	IPA	E	202	-	3,3,3	0.53	0	3,3,3	0.31	0
3	6XU	C	202	-	32,37,37	1.59	6 (18%)	33,56,56	1.81	8 (24%)
2	IPA	A	201	-	3,3,3	0.58	0	3,3,3	0.19	0
2	IPA	C	201	-	3,3,3	0.53	0	3,3,3	0.26	0
3	6XU	E	205	-	32,37,37	1.60	5 (15%)	33,56,56	1.91	7 (21%)
2	IPA	D	201	-	3,3,3	0.52	0	3,3,3	0.32	0
2	IPA	E	201	-	3,3,3	0.50	0	3,3,3	0.29	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
3	6XU	A	206	-	-	4/18/57/57	0/4/4/4
3	6XU	A	205	-	-	0/18/57/57	0/4/4/4
3	6XU	D	204	-	-	0/18/57/57	0/4/4/4
4	GOL	B	201	-	-	3/4/4/4	-
3	6XU	E	205	-	-	0/18/57/57	0/4/4/4
3	6XU	B	202	-	-	0/18/57/57	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	F	201	-	-	3/4/4/4	-
3	6XU	F	202	-	-	0/18/57/57	0/4/4/4
3	6XU	C	202	-	-	0/18/57/57	0/4/4/4

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	206	6XU	C08-C06	10.37	1.62	1.48
3	A	206	6XU	C08-S12	8.28	1.85	1.73
3	A	206	6XU	C13-C04	5.48	1.58	1.50
3	A	206	6XU	C18-C19	5.09	1.61	1.52
3	B	202	6XU	C08-S12	4.77	1.80	1.73
3	A	206	6XU	C02-C28	4.52	1.60	1.53
3	A	206	6XU	C24-C03	4.46	1.57	1.48
3	F	202	6XU	C08-S12	4.42	1.79	1.73
3	A	205	6XU	C08-S12	4.41	1.79	1.73
3	A	206	6XU	C04-C03	4.40	1.42	1.37
3	E	205	6XU	C08-S12	4.02	1.79	1.73
3	A	205	6XU	C08-C06	-3.87	1.43	1.48
3	D	204	6XU	C08-S12	3.80	1.78	1.73
3	A	205	6XU	F23-C16	-3.79	1.31	1.38
3	C	202	6XU	C08-S12	3.65	1.78	1.73
3	A	206	6XU	O26-C24	3.44	1.41	1.33
3	A	206	6XU	C18-N14	3.32	1.55	1.47
3	A	206	6XU	F23-C16	-3.27	1.32	1.38
3	C	202	6XU	C18-C19	3.24	1.58	1.52
3	E	205	6XU	F23-C16	-3.24	1.32	1.38
3	F	202	6XU	C18-C19	3.20	1.58	1.52
3	A	206	6XU	C04-N05	3.19	1.42	1.37
3	C	202	6XU	F23-C16	-3.14	1.32	1.38
3	D	204	6XU	C18-C19	3.01	1.58	1.52
3	A	205	6XU	C18-C19	3.00	1.58	1.52
3	E	205	6XU	C18-C19	2.95	1.57	1.52
3	B	202	6XU	F22-C16	-2.94	1.33	1.38
3	B	202	6XU	C13-N14	-2.85	1.40	1.47
3	B	202	6XU	C18-C19	2.83	1.57	1.52
3	B	202	6XU	C08-C06	-2.82	1.44	1.48
3	F	202	6XU	F23-C16	-2.81	1.33	1.38
3	D	204	6XU	C02-C28	2.81	1.57	1.53
3	D	204	6XU	C32-C31	2.77	1.42	1.37
3	F	202	6XU	C02-C28	2.67	1.57	1.53
3	C	202	6XU	C08-C06	-2.64	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	204	6XU	F23-C16	-2.61	1.33	1.38
3	D	204	6XU	F22-C16	-2.58	1.33	1.38
3	B	202	6XU	F23-C16	-2.51	1.33	1.38
3	A	205	6XU	F34-C31	-2.35	1.30	1.36
3	F	202	6XU	C30-C31	2.29	1.41	1.37
3	E	205	6XU	C08-C06	-2.26	1.45	1.48
3	D	204	6XU	C08-C06	-2.26	1.45	1.48
3	E	205	6XU	C02-C28	2.25	1.56	1.53
3	F	202	6XU	C13-C04	2.24	1.53	1.50
3	F	202	6XU	C32-C31	2.22	1.41	1.37
3	D	204	6XU	O26-C24	2.19	1.38	1.33
3	F	202	6XU	O26-C24	2.18	1.38	1.33
3	A	206	6XU	C30-C31	2.17	1.41	1.37
3	C	202	6XU	O26-C24	2.13	1.38	1.33
3	C	202	6XU	C32-C31	2.12	1.41	1.37
3	B	202	6XU	C02-C28	2.08	1.56	1.53
3	F	202	6XU	C29-C28	2.07	1.42	1.39
3	A	205	6XU	F22-C16	-2.07	1.34	1.38
3	D	204	6XU	C33-C28	2.05	1.42	1.39
3	A	205	6XU	C32-C31	2.03	1.41	1.37
3	A	205	6XU	C30-C31	2.01	1.41	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	206	6XU	O26-C24-C03	6.61	122.11	111.96
3	E	205	6XU	O26-C24-C03	5.68	120.69	111.96
3	A	206	6XU	O26-C24-O25	-5.67	112.61	123.53
3	F	202	6XU	O26-C24-C03	5.66	120.65	111.96
3	D	204	6XU	O26-C24-C03	4.95	119.56	111.96
3	B	202	6XU	O26-C24-C03	4.89	119.47	111.96
3	A	205	6XU	O26-C24-C03	4.89	119.47	111.96
3	C	202	6XU	O26-C24-C03	4.68	119.15	111.96
3	E	205	6XU	O26-C24-O25	-4.59	114.70	123.53
3	A	206	6XU	C10-N09-C08	4.52	116.06	104.39
3	F	202	6XU	O26-C24-O25	-4.23	115.38	123.53
3	A	205	6XU	O26-C24-O25	-4.05	115.73	123.53
3	B	202	6XU	O26-C24-O25	-3.83	116.15	123.53
3	D	204	6XU	C10-N09-C08	3.83	114.28	104.39
3	D	204	6XU	O26-C24-O25	-3.72	116.37	123.53
3	C	202	6XU	O26-C24-O25	-3.71	116.38	123.53
3	E	205	6XU	C10-N09-C08	3.71	113.97	104.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	205	6XU	C10-N09-C08	3.67	113.85	104.39
3	F	202	6XU	C10-N09-C08	3.62	113.74	104.39
3	C	202	6XU	C10-N09-C08	3.57	113.61	104.39
3	B	202	6XU	C10-N09-C08	3.40	113.17	104.39
3	A	206	6XU	N05-C06-N07	-3.15	119.72	123.96
3	A	206	6XU	C08-C06-N05	3.13	118.13	115.18
3	C	202	6XU	C29-C30-C31	3.00	121.47	118.36
3	C	202	6XU	C32-C31-C30	-2.94	118.91	122.83
3	A	205	6XU	C27-O26-C24	2.90	121.34	115.86
3	F	202	6XU	C32-C31-C30	-2.88	119.00	122.83
3	F	202	6XU	C32-C33-C28	2.84	125.01	121.22
3	E	205	6XU	C32-C31-C30	-2.82	119.08	122.83
3	E	205	6XU	C29-C30-C31	2.77	121.23	118.36
3	B	202	6XU	C08-C06-N05	2.74	117.76	115.18
3	C	202	6XU	C27-O26-C24	2.73	121.02	115.86
3	B	202	6XU	C32-C31-C30	-2.70	119.23	122.83
3	F	202	6XU	C29-C30-C31	2.60	121.05	118.36
3	D	204	6XU	C32-C31-C30	-2.60	119.37	122.83
3	E	205	6XU	C08-C06-N05	2.56	117.59	115.18
3	A	206	6XU	C27-O26-C24	2.55	120.69	115.86
3	A	206	6XU	C32-C31-C30	-2.54	119.45	122.83
3	B	202	6XU	C29-C30-C31	2.53	120.98	118.36
3	F	202	6XU	C29-C28-C02	2.50	124.79	120.61
3	C	202	6XU	C01-C02-N07	2.48	111.26	108.81
3	E	205	6XU	C32-C33-C28	2.44	124.47	121.22
3	A	206	6XU	C32-C33-C28	2.37	124.39	121.22
3	B	202	6XU	C32-C33-C28	2.36	124.38	121.22
3	A	206	6XU	C17-C18-N14	2.32	107.43	102.68
3	D	204	6XU	C01-C02-N07	2.28	111.07	108.81
3	A	205	6XU	C32-C33-C28	2.24	124.21	121.22
3	F	202	6XU	C01-C02-N07	2.24	111.03	108.81
3	D	204	6XU	C29-C30-C31	2.21	120.65	118.36
3	D	204	6XU	C27-O26-C24	2.20	120.02	115.86
3	A	206	6XU	C33-C28-C29	-2.14	114.78	117.97
3	C	202	6XU	C32-C33-C28	2.09	124.02	121.22
3	F	202	6XU	O20-C19-C18	-2.07	115.95	122.48
3	A	206	6XU	C13-N14-C15	-2.07	110.40	113.29
3	D	204	6XU	C08-C06-N05	2.06	117.11	115.18
3	A	205	6XU	C32-C31-C30	-2.05	120.09	122.83
3	B	202	6XU	O20-C19-C18	-2.03	116.09	122.48
3	A	205	6XU	O20-C19-C18	-2.02	116.13	122.48
3	F	202	6XU	C33-C28-C29	-2.01	114.98	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	205	6XU	C29-C28-C02	2.00	123.95	120.61

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	206	6XU	N07-C02-C28-C29
4	F	201	GOL	O1-C1-C2-O2
4	B	201	GOL	C1-C2-C3-O3
4	F	201	GOL	O1-C1-C2-C3
4	F	201	GOL	C1-C2-C3-O3
4	B	201	GOL	O2-C2-C3-O3
3	A	206	6XU	C17-C18-C19-O21
4	B	201	GOL	O1-C1-C2-C3
3	A	206	6XU	C17-C18-C19-O20
3	A	206	6XU	N07-C02-C28-C33

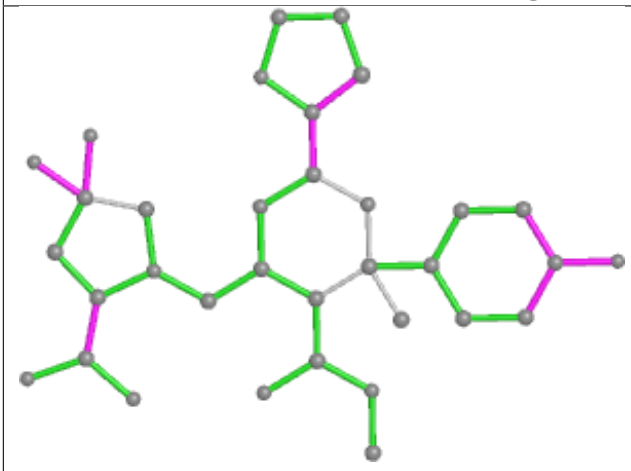
There are no ring outliers.

4 monomers are involved in 9 short contacts:

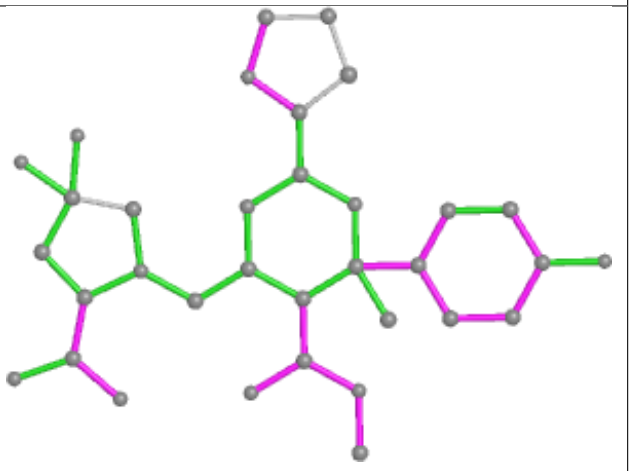
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	201	GOL	2	0
2	E	203	IPA	4	0
2	E	204	IPA	2	0
2	E	201	IPA	1	0

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.

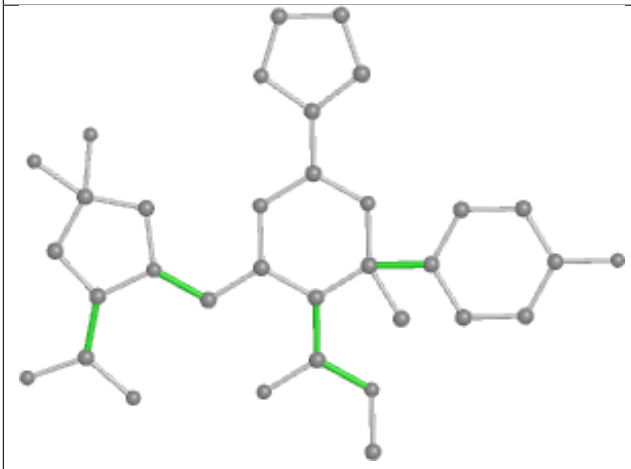
Ligand 6XU A 205



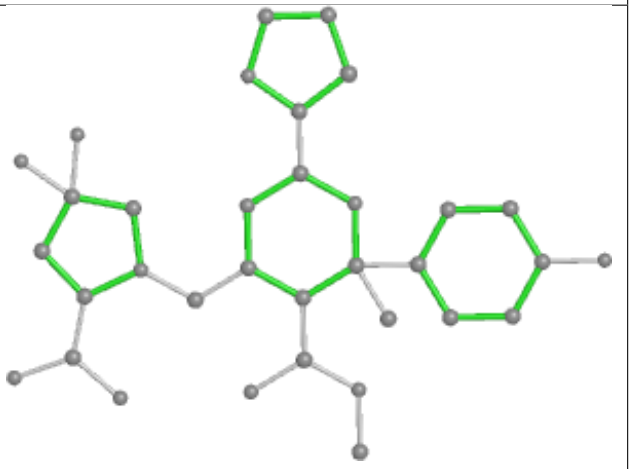
Bond lengths



Bond angles

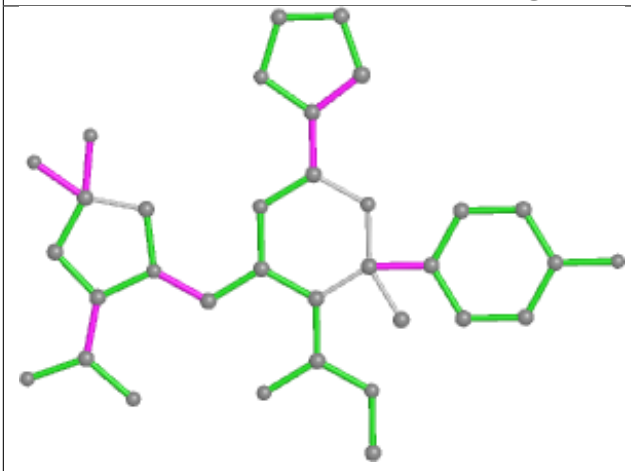


Torsions

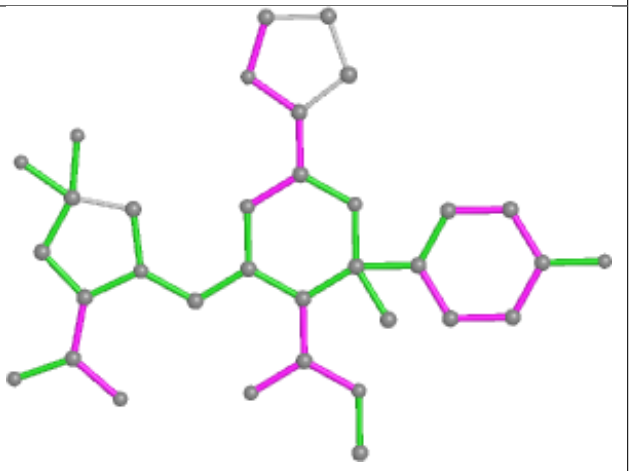


Rings

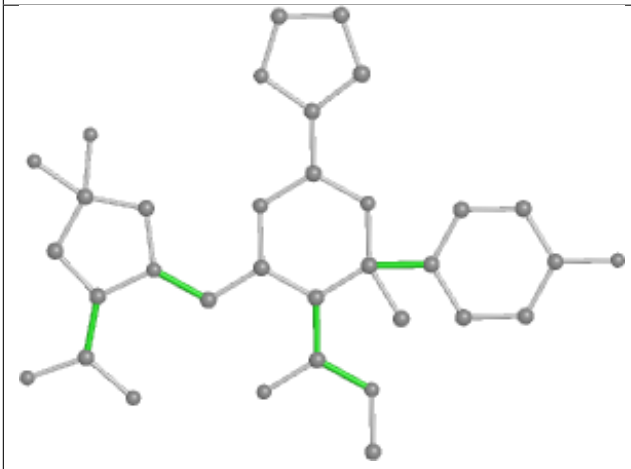
Ligand 6XU B 202



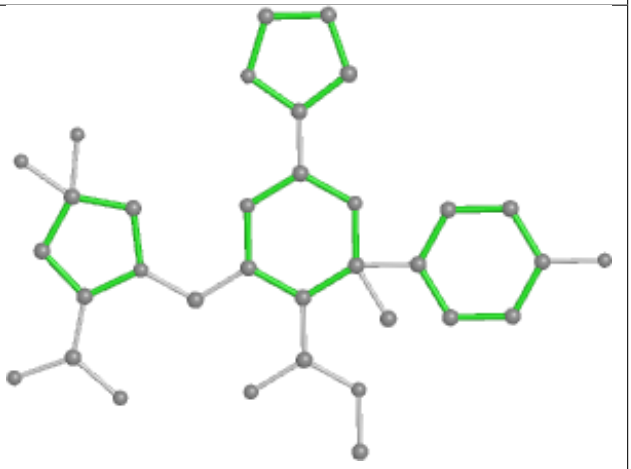
Bond lengths



Bond angles

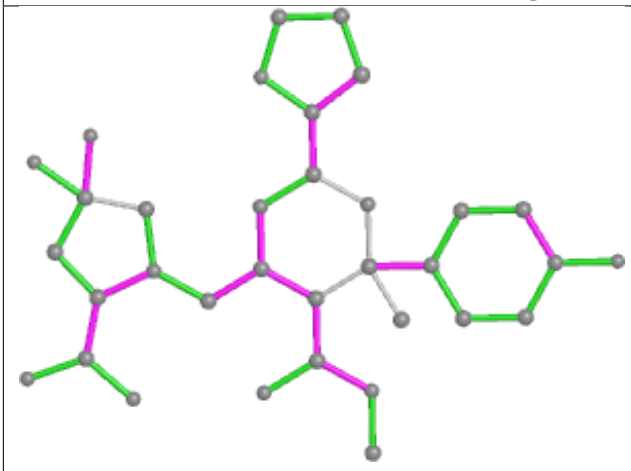


Torsions

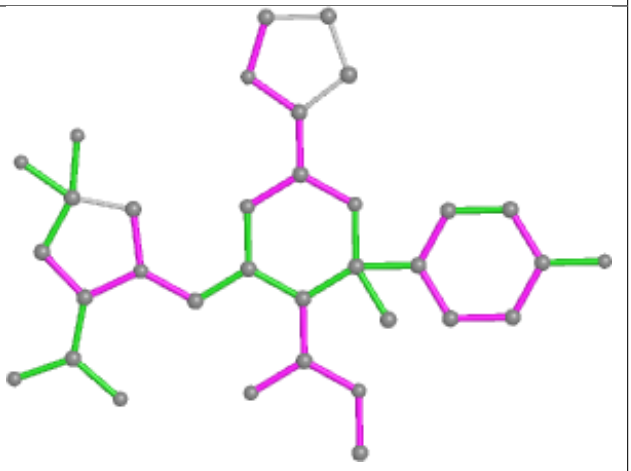


Rings

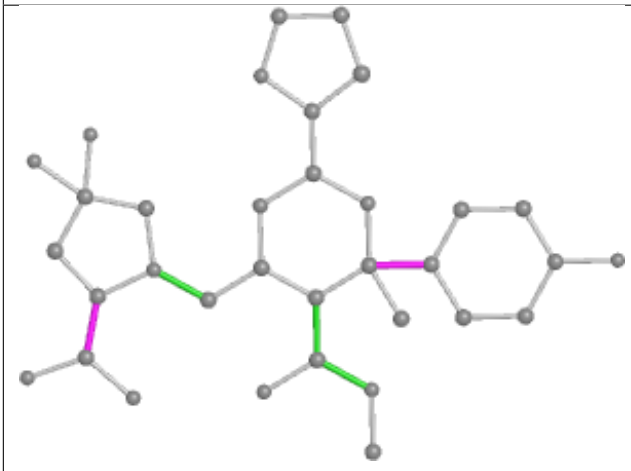
Ligand 6XU A 206



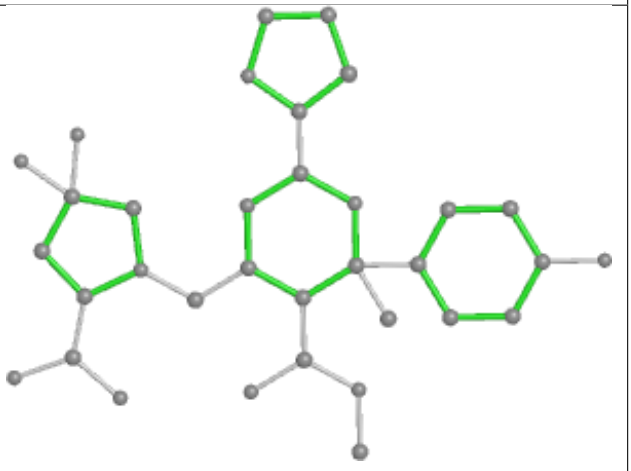
Bond lengths



Bond angles

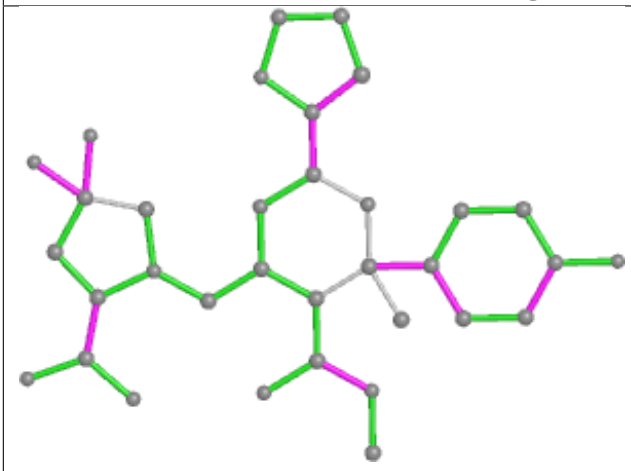


Torsions

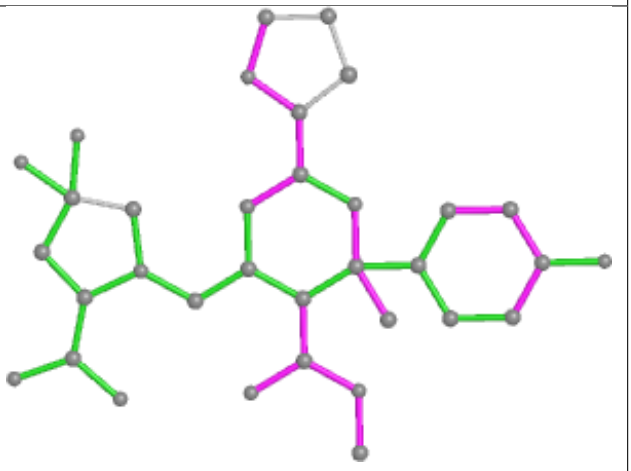


Rings

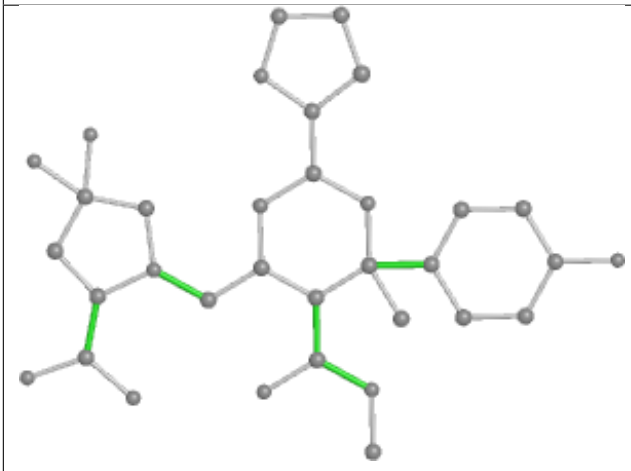
Ligand 6XU D 204



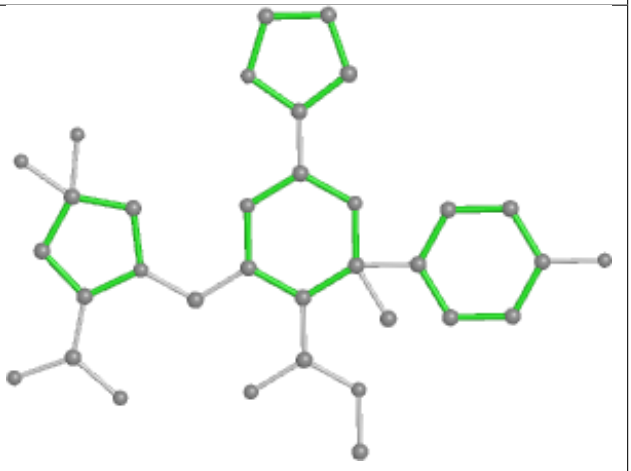
Bond lengths



Bond angles

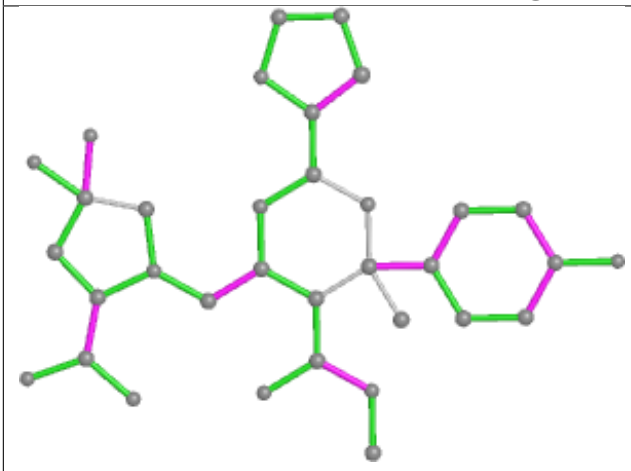


Torsions

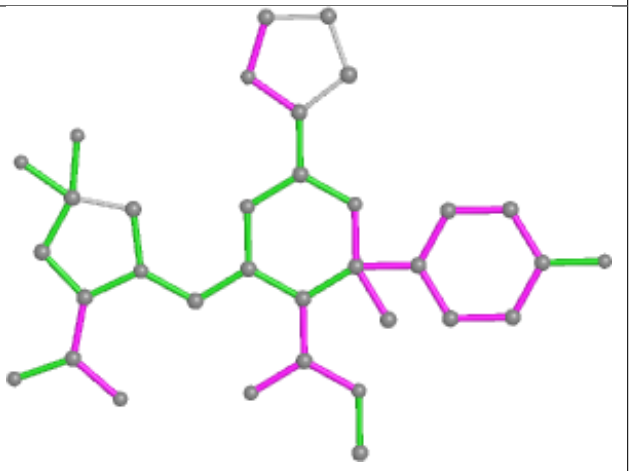


Rings

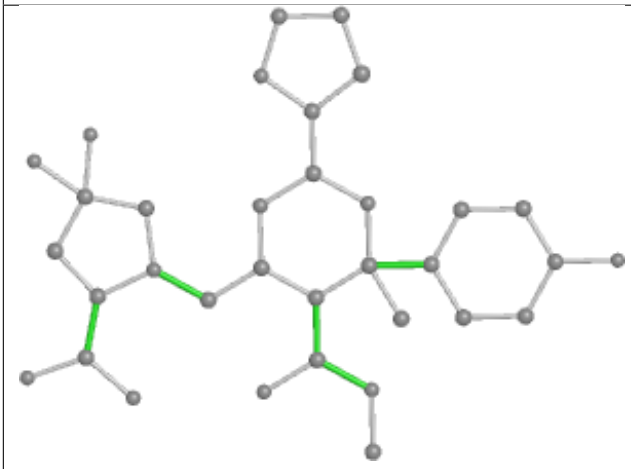
Ligand 6XU F 202



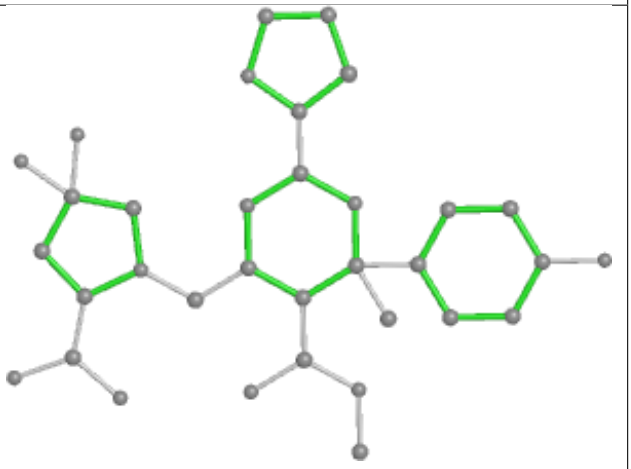
Bond lengths



Bond angles

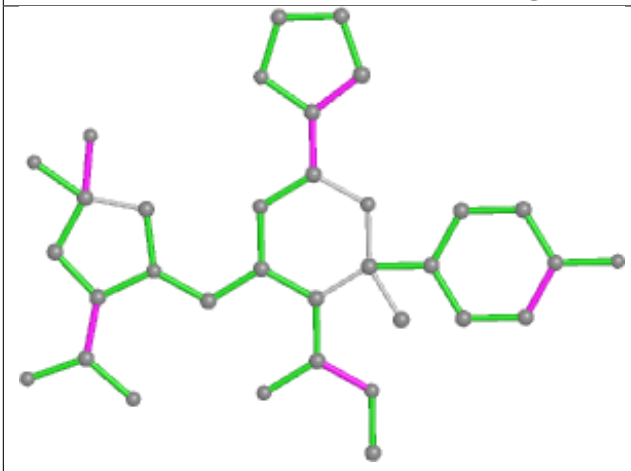


Torsions

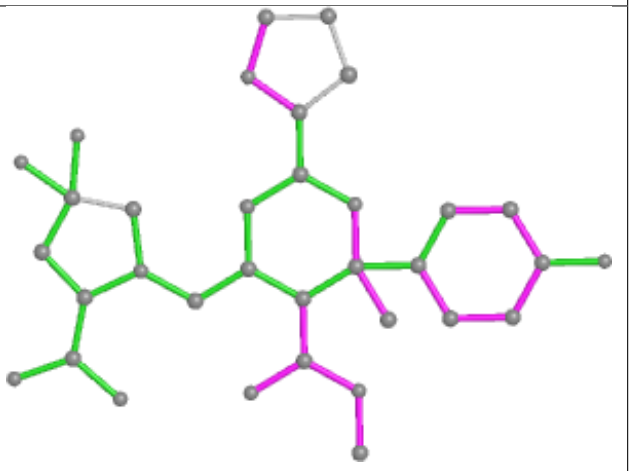


Rings

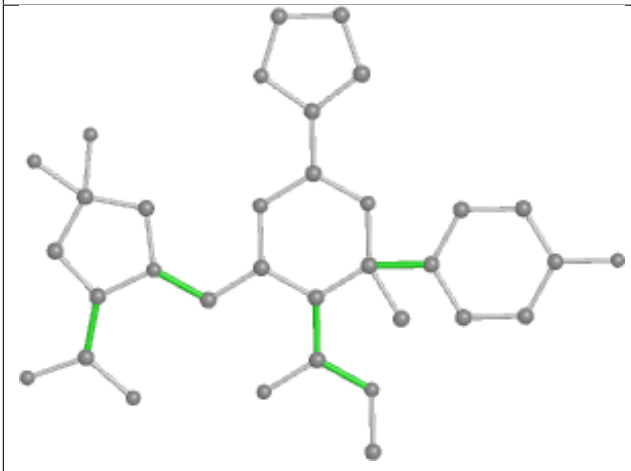
Ligand 6XU C 202



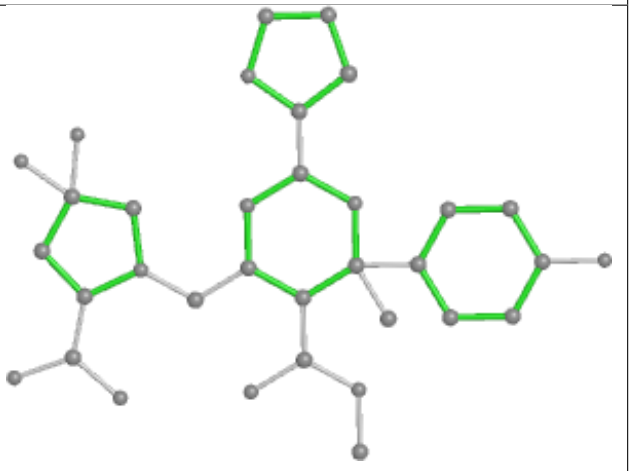
Bond lengths



Bond angles

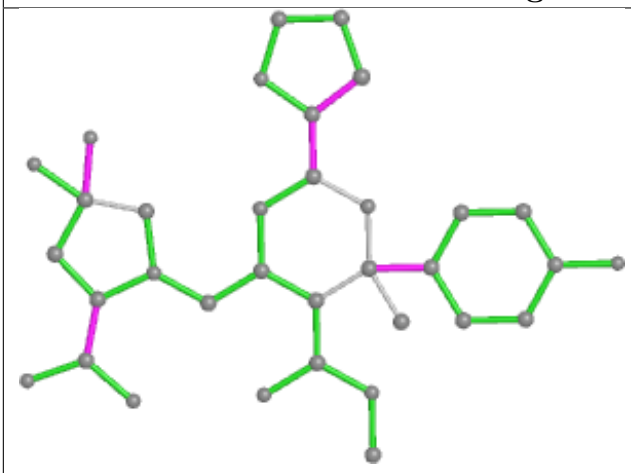


Torsions

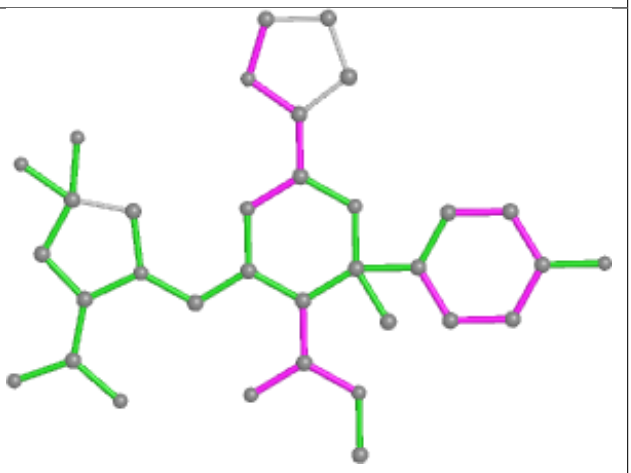


Rings

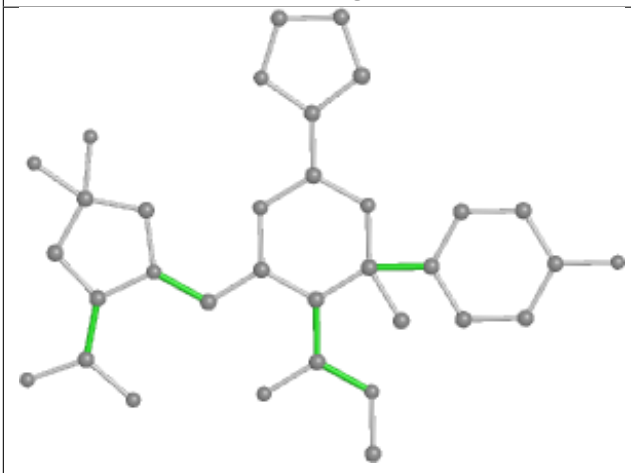
Ligand 6XU E 205



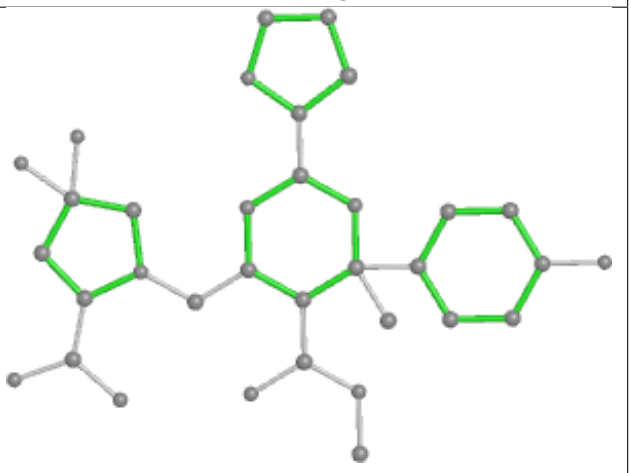
Bond lengths



Bond angles



Torsions



Rings

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	143/155 (92%)	-0.22	1 (0%)	87	90	21, 33, 51, 87	0
1	B	148/155 (95%)	-0.14	4 (2%)	54	58	22, 31, 52, 110	0
1	C	143/155 (92%)	0.13	7 (4%)	29	33	22, 30, 78, 101	0
1	D	150/155 (96%)	-0.03	9 (6%)	21	24	22, 31, 66, 87	0
1	E	143/155 (92%)	0.74	22 (15%)	2	2	27, 37, 114, 141	0
1	F	150/155 (96%)	1.09	32 (21%)	0	0	26, 39, 137, 163	0
All	All	877/930 (94%)	0.26	75 (8%)	10	12	21, 33, 87, 163	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	84	LEU	14.7
1	E	76	LEU	12.7
1	F	79	PRO	11.6
1	F	80	ALA	11.2
1	F	85	VAL	10.8
1	F	77	GLU	9.2
1	F	76	LEU	8.7
1	F	81	SER	8.4
1	C	143	LEU	8.3
1	F	82	ARG	7.7
1	F	86	VAL	7.5
1	E	77	GLU	7.2
1	E	79	PRO	6.9
1	E	143	LEU	6.6
1	E	71	TRP	6.6
1	E	74	THR	6.5
1	F	143	LEU	6.3
1	E	84	LEU	6.3
1	E	80	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	81	SER	5.9
1	F	154	PHE	5.9
1	F	78	ASP	5.6
1	E	72	VAL	5.6
1	F	74	THR	5.2
1	F	83	ASP	5.1
1	F	71	TRP	4.7
1	E	73	GLY	4.7
1	F	149	VAL	4.6
1	F	153	TYR	4.3
1	E	82	ARG	4.3
1	F	73	GLY	4.3
1	E	78	ASP	4.2
1	E	75	ASN	4.2
1	D	143	LEU	4.1
1	F	88	TYR	4.1
1	F	152	LEU	4.1
1	F	72	VAL	3.9
1	F	151	ASN	3.9
1	E	85	VAL	3.8
1	C	79	PRO	3.8
1	D	84	LEU	3.8
1	A	143	LEU	3.6
1	B	150	GLU	3.5
1	E	83	ASP	3.4
1	C	71	TRP	3.3
1	F	150	GLU	3.3
1	D	87	SER	3.1
1	E	70	THR	3.0
1	B	152	LEU	3.0
1	E	86	VAL	3.0
1	F	58	ALA	2.9
1	F	87	SER	2.9
1	F	92	ASN	2.9
1	D	80	ALA	2.9
1	D	79	PRO	2.8
1	B	151	ASN	2.8
1	F	75	ASN	2.8
1	C	84	LEU	2.7
1	B	154	PHE	2.7
1	D	91	THR	2.7
1	C	76	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	83	ASP	2.6
1	D	144	PRO	2.6
1	E	58	ALA	2.6
1	F	89	VAL	2.6
1	F	55	LEU	2.6
1	E	91	THR	2.5
1	E	55	LEU	2.5
1	F	70	THR	2.4
1	D	28	ARG	2.4
1	C	142	THR	2.4
1	C	74	THR	2.4
1	E	100	LEU	2.3
1	F	100	LEU	2.0
1	F	59	ILE	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
2	IPA	A	203	4/4	0.63	0.27	41,42,43,53	0
2	IPA	E	201	4/4	0.71	0.17	55,58,58,71	0
2	IPA	E	203	4/4	0.76	0.25	28,45,46,48	0
2	IPA	A	201	4/4	0.77	0.24	34,34,45,49	0
2	IPA	E	204	4/4	0.77	0.17	26,35,52,53	0
3	6XU	A	206	34/34	0.81	0.21	60,69,88,93	0
2	IPA	D	202	4/4	0.82	0.14	44,50,54,60	0
2	IPA	C	201	4/4	0.87	0.21	32,34,44,46	0
2	IPA	A	204	4/4	0.88	0.15	52,62,64,65	0

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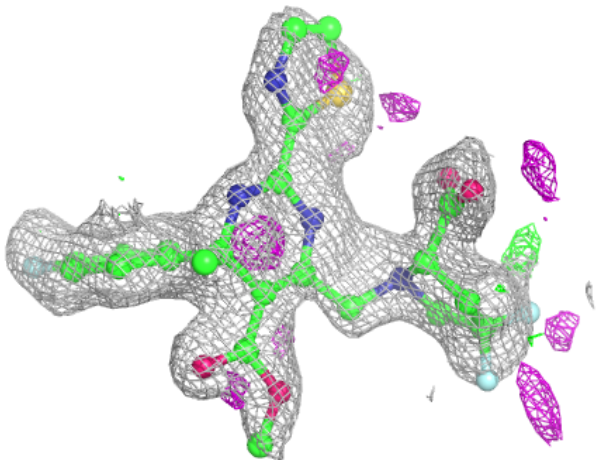
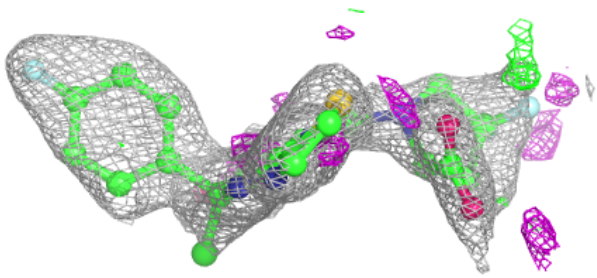
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	D	203	1/1	0.89	0.28	87,87,87,87	0
2	IPA	E	202	4/4	0.92	0.28	36,41,41,47	0
4	GOL	F	201	6/6	0.93	0.24	38,49,51,55	0
4	GOL	B	201	6/6	0.93	0.14	36,43,54,60	0
2	IPA	D	201	4/4	0.94	0.18	32,32,34,36	0
2	IPA	A	202	4/4	0.95	0.18	31,32,35,41	0
3	6XU	F	202	34/34	0.96	0.07	22,28,33,33	0
3	6XU	A	205	34/34	0.97	0.07	22,26,31,32	0
3	6XU	D	204	34/34	0.97	0.06	21,25,30,33	0
3	6XU	B	202	34/34	0.98	0.06	19,25,32,33	0
3	6XU	E	205	34/34	0.98	0.05	20,27,32,38	0
3	6XU	C	202	34/34	0.98	0.06	21,25,29,33	0

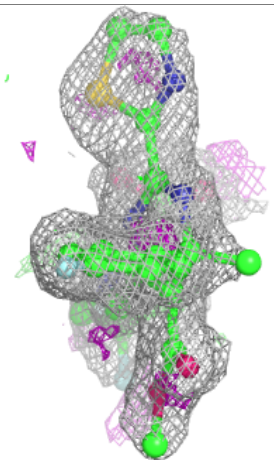
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6XU A 206:

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

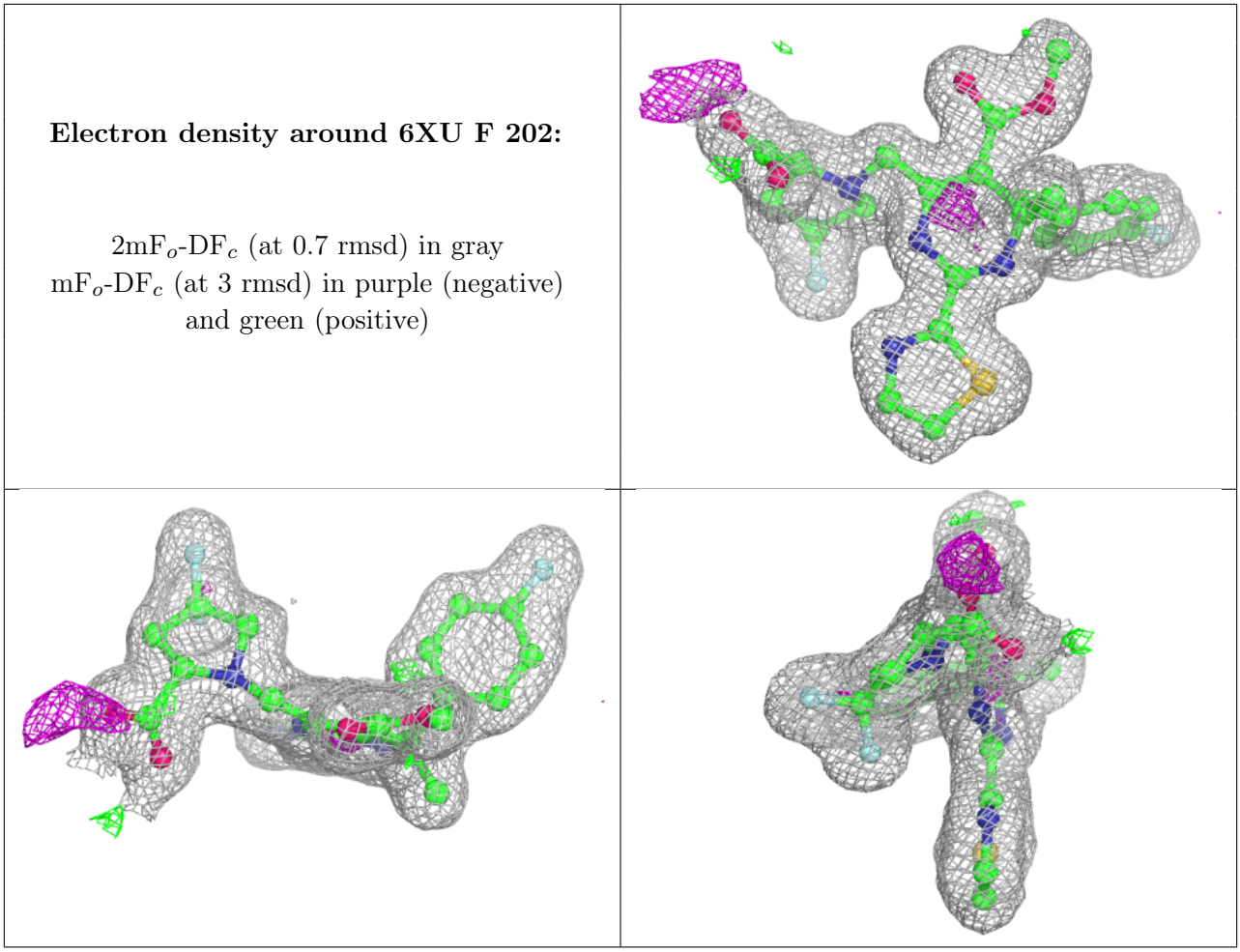






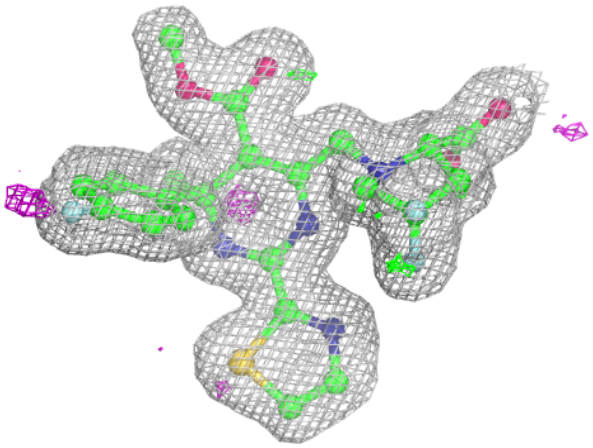
Electron density around 6XU F 202:

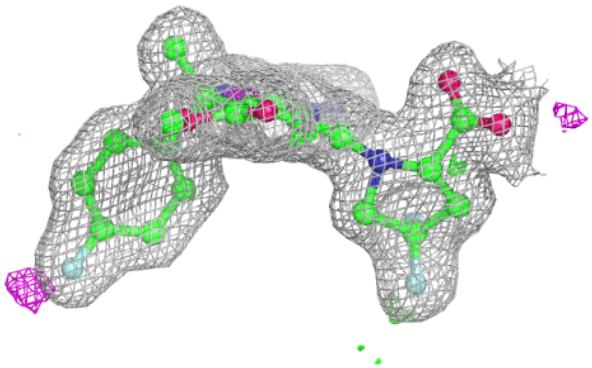
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

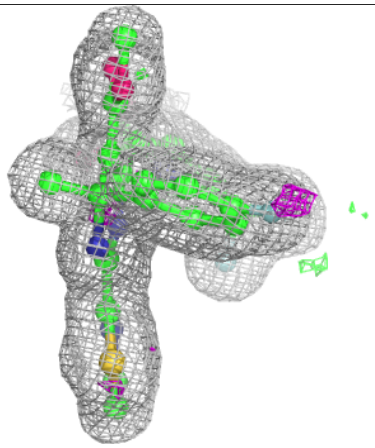


Electron density around 6XU A 205:

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

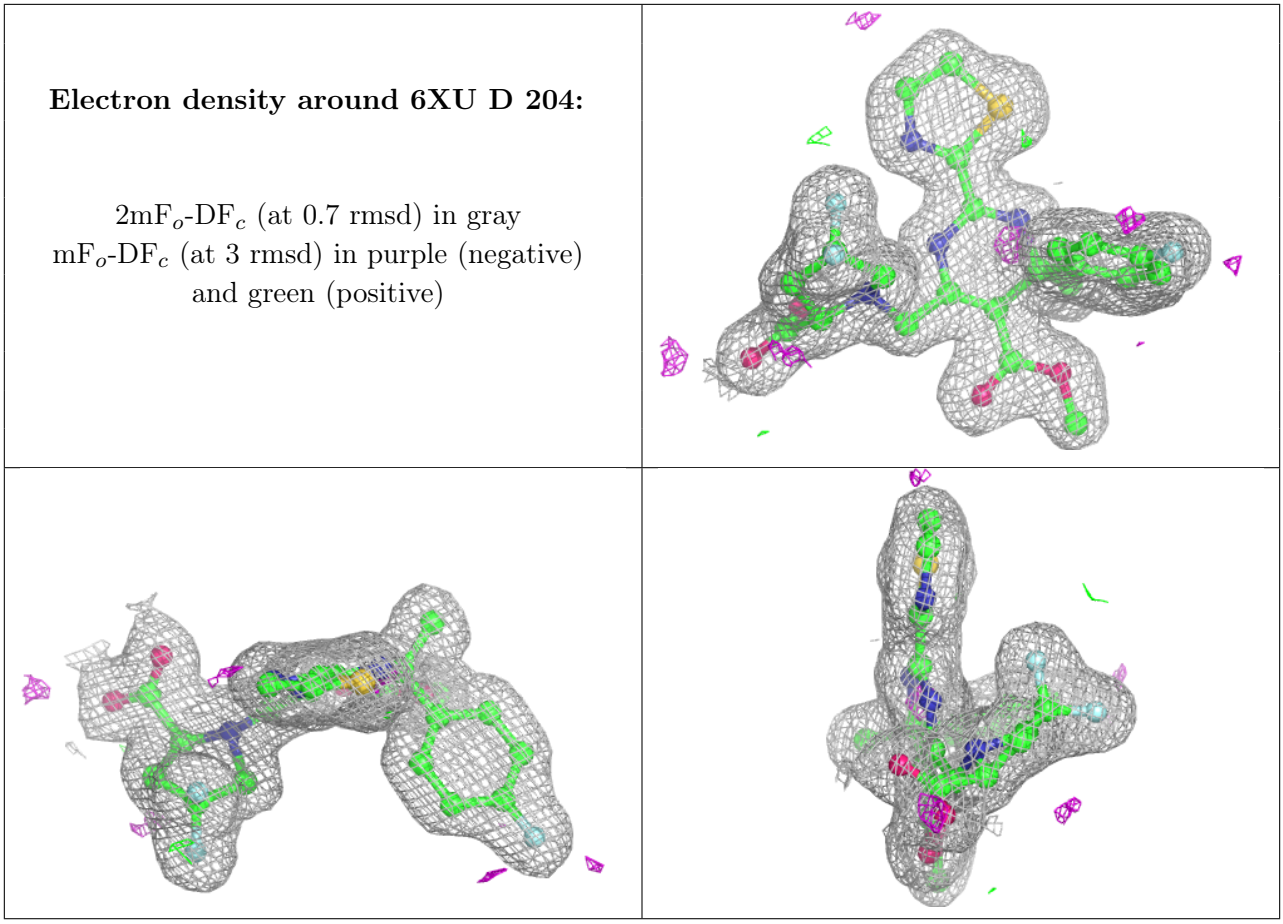






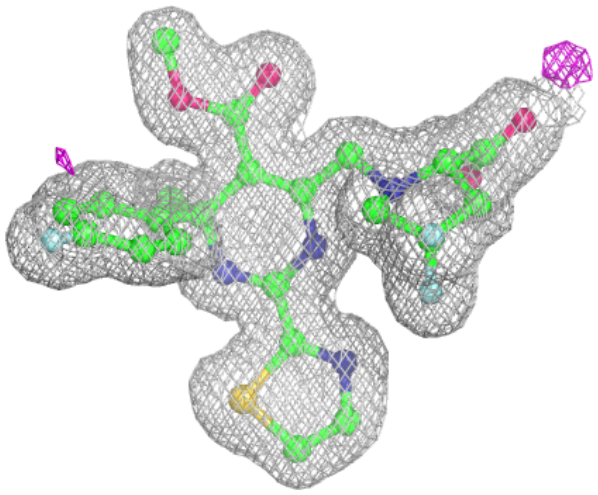
Electron density around 6XU D 204:

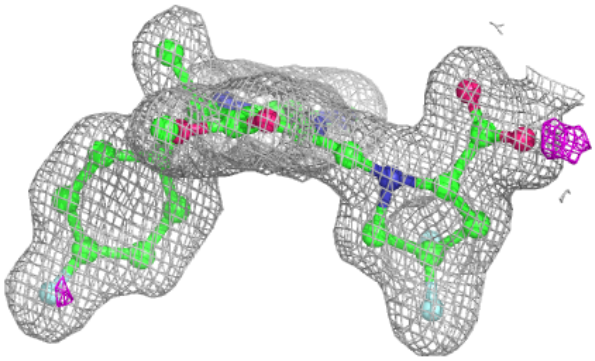
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

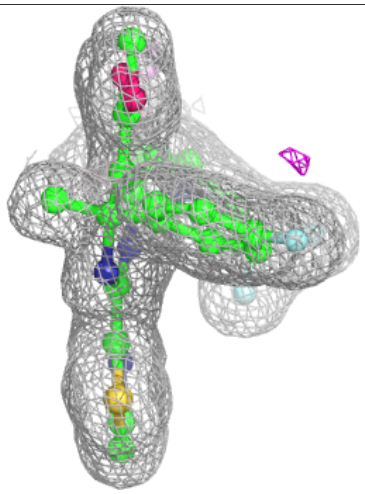


Electron density around 6XU B 202:

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

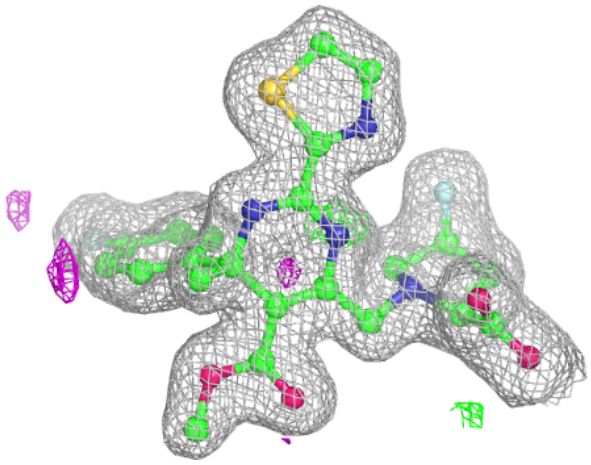


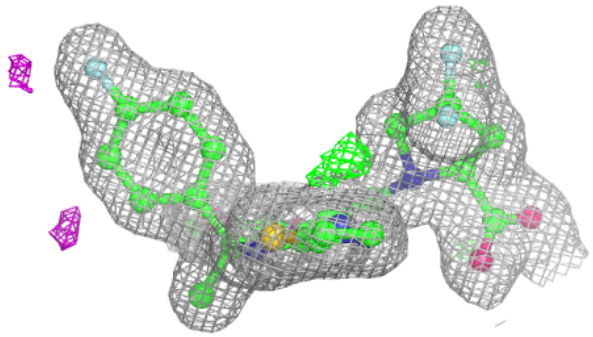


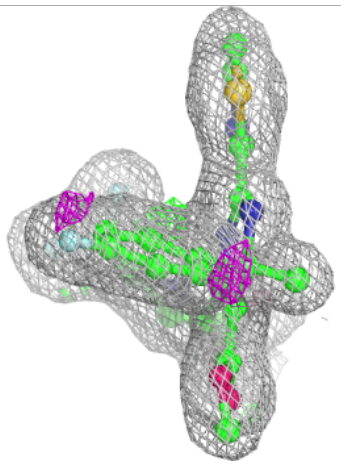


Electron density around 6XU E 205:

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

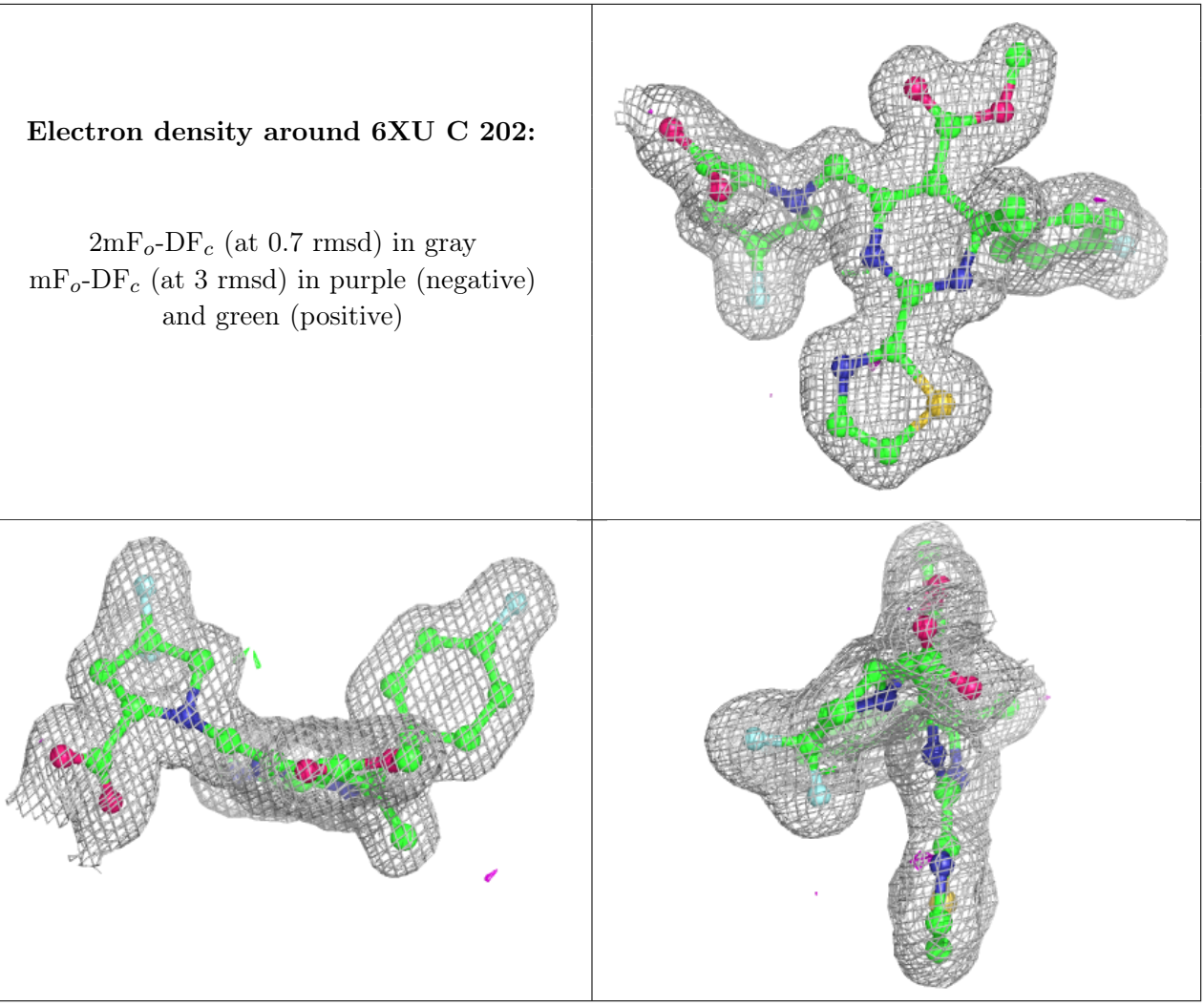






Electron density around 6XU C 202:

$2mF_o$-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.