



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:51 am BST

PDB ID : 2XH1
Title : Crystal structure of human KAT II-inhibitor complex
Authors : Rossi, F.; Casazza, V.; Garavaglia, S.; Sathyaikumar, K.V.; Schwarcz, R.;
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Deposited on : 2010-06-08
Resolution : 2.10 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 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 : 2.11
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) : 2.11

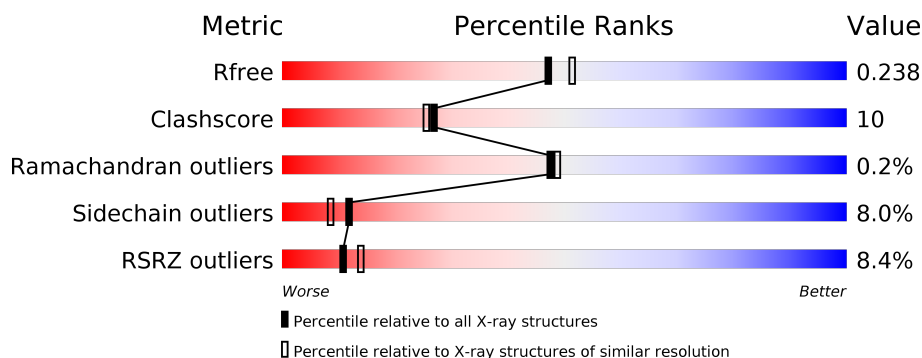
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	425	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	425	<div> <div>10%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6972 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.

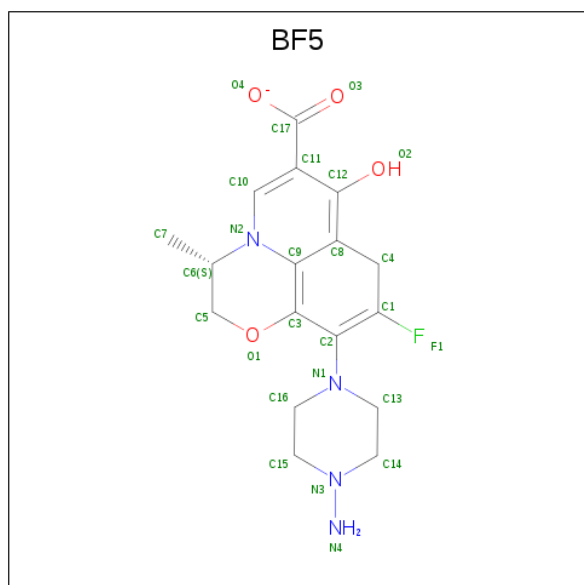
- Molecule 1 is a protein called KYNURENINE/ α -AMINOADIPATE AMINOTRANSFERASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3233	2079	539	599	16			
1	B	412	Total	C	N	O	S	0	0	0
			3234	2079	539	600	16			

There are 2 discrepancies between the modelled and reference sequences:

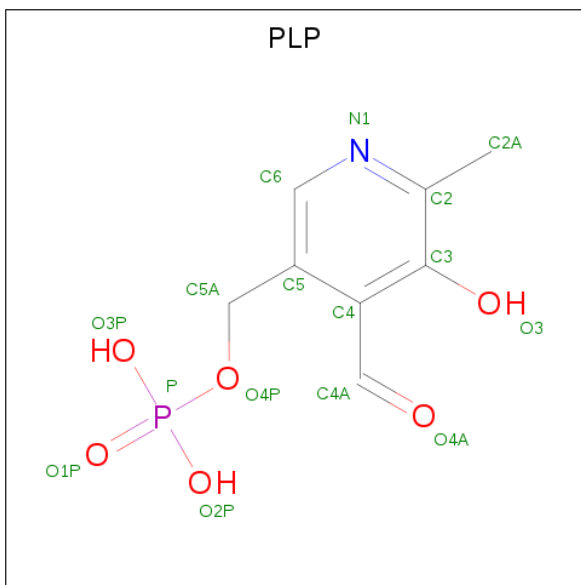
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	MET	engineered mutation	UNP Q8N5Z0
B	-1	GLU	MET	engineered mutation	UNP Q8N5Z0

- Molecule 2 is (3S)-10-(4-AMINOPIPERAZIN-1-YL)-9-FLUORO-7-HYDROXY-3-METHYL-2,3-DIHYDRO-8H-[1,4]OXAZINO[2,3,4-IJ]QUINOLINE-6-CARBOXYLATE (three-letter code: BF5) (formula: C₁₇H₁₉FN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	B	1	Total 26	C 17	F 1	N 4	O 4	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $\text{C}_8\text{H}_{10}\text{NO}_6\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total I 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	241	Total	O	0	0
			241	241		
6	B	175	Total	O	0	0
			175	175		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.32Å 152.86Å 60.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.04 – 2.10 30.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.04-2.10) 99.9 (30.73-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.241 0.191 , 0.238	Depositor DCC
R_{free} test set	1111 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6972	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IOD, BF5, PLP

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	0.91	1/3313 (0.0%)	0.84	4/4498 (0.1%)
1	B	0.84	2/3314 (0.1%)	0.87	7/4498 (0.2%)
All	All	0.87	3/6627 (0.0%)	0.85	11/8996 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	GLU	CD-OE1	6.42	1.32	1.25
1	B	107	GLY	N-CA	5.76	1.54	1.46
1	A	225	PHE	CE1-CZ	5.43	1.47	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH1	10.15	125.37	120.30
1	B	106	GLN	C-N-CA	-9.45	102.46	122.30
1	B	283	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	B	137	LEU	CA-CB-CG	7.89	133.46	115.30
1	A	380	LEU	CA-CB-CG	6.74	130.80	115.30
1	A	270	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	169	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	A	301	LEU	CB-CG-CD1	5.35	120.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	121	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	106	GLN	O-C-N	-5.09	114.55	123.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3233	0	3241	67	1
1	B	3234	0	3241	71	0
2	A	26	0	17	4	0
2	B	26	0	17	1	0
3	A	15	0	6	0	0
3	B	15	0	7	0	0
4	A	1	0	0	0	0
5	B	6	0	8	0	0
6	A	241	0	0	14	0
6	B	175	0	0	8	0
All	All	6972	0	6537	133	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 10.

All (133) 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:B:89:GLN:HG3	1:B:93:LYS:HE2	1.42	0.99
1:B:112:CYS:HB2	6:B:2076:HOH:O	1.66	0.94
1:A:99:THR:HG21	6:A:2073:HOH:O	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:CYS:SG	6:B:2076:HOH:O	2.36	0.82
1:A:196:THR:HG22	6:A:2170:HOH:O	1.80	0.81
1:A:121:LEU:CD2	1:A:228:ILE:HD11	2.15	0.76
1:A:63:PHE:HD2	1:A:68:MET:HE1	1.48	0.76
1:A:368:GLU:HG3	6:A:2232:HOH:O	1.87	0.74
1:B:121:LEU:CD1	1:B:228:ILE:HD11	2.20	0.72
1:B:112:CYS:CB	6:B:2076:HOH:O	2.28	0.71
1:B:172:ARG:HG2	1:B:219:LEU:HD11	1.71	0.71
1:B:379:VAL:HG11	1:B:413:ALA:HA	1.71	0.71
1:A:264:ILE:O	1:A:318:HIS:HE1	1.75	0.69
1:B:145:THR:HG21	1:B:195:TYR:CZ	2.29	0.67
1:A:5:ARG:HD3	6:A:2004:HOH:O	1.94	0.67
1:B:294:HIS:HD2	1:B:295:PRO:O	1.78	0.66
1:A:63:PHE:HD2	1:A:68:MET:CE	2.09	0.65
1:A:34:ILE:HD13	1:B:409:GLN:HB3	1.79	0.65
1:B:271:ILE:HG13	1:B:303:ILE:HD12	1.78	0.65
1:B:42:ASN:HD22	1:B:44:ASN:H	1.44	0.65
1:B:73:GLN:O	1:B:297:THR:HG21	1.97	0.64
1:A:370:ILE:HD11	1:A:380:LEU:HA	1.78	0.63
1:A:299:ASN:HD21	1:B:299:ASN:HD21	1.46	0.63
1:A:68:MET:HA	1:A:68:MET:CE	2.28	0.63
1:B:121:LEU:HD11	1:B:228:ILE:HD11	1.80	0.62
1:A:80:ILE:CD1	1:A:301:LEU:HD13	2.30	0.62
1:B:344:LEU:HD23	1:B:344:LEU:H	1.65	0.62
1:A:283:ARG:HD3	6:A:2192:HOH:O	1.99	0.61
1:A:174:ILE:O	1:A:177:ARG:HD3	2.01	0.61
1:B:369:LEU:HA	1:B:373:LYS:HG3	1.82	0.61
2:A:1426:BF5:H4	1:B:40:LEU:CD2	2.31	0.61
1:B:84:LEU:HD11	1:B:113:VAL:HG23	1.84	0.60
1:B:89:GLN:CG	1:B:93:LYS:HE2	2.26	0.60
1:B:214:LYS:O	1:B:218:GLU:HG3	2.02	0.59
1:A:99:THR:HG22	1:A:109:MET:HB2	1.83	0.59
1:A:101:HIS:HD2	6:A:2068:HOH:O	1.84	0.59
1:B:304:SER:O	1:B:308:HIS:HD2	1.85	0.58
1:B:195:TYR:OH	1:B:230:ASP:OD2	2.17	0.58
1:A:341:LEU:HD22	1:A:414:PHE:HD2	1.69	0.58
1:B:370:ILE:HG13	1:B:398:LEU:HD21	1.85	0.58
1:A:2:ASN:HA	6:A:2071:HOH:O	2.03	0.58
1:B:185:ASN:HD22	1:B:185:ASN:C	2.07	0.58
1:B:344:LEU:N	1:B:344:LEU:HD23	2.19	0.58
1:A:173:ASP:C	1:A:173:ASP:OD1	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:HB2	1:A:76:PRO:CD	2.33	0.57
1:B:421:ILE:O	1:B:425:LEU:HG	2.04	0.57
1:B:217:TYR:HB2	1:B:249:MET:CE	2.35	0.57
2:A:1426:BF5:H4	1:B:40:LEU:HD21	1.85	0.56
1:A:17:SER:C	1:A:19:ILE:H	2.09	0.56
1:B:84:LEU:CD1	1:B:113:VAL:HG23	2.35	0.55
1:A:89:GLN:HE21	1:A:93:LYS:HG3	1.70	0.55
1:A:68:MET:HA	1:A:68:MET:HE3	1.89	0.55
1:B:42:ASN:ND2	1:B:44:ASN:H	2.04	0.55
1:B:239:ASN:O	1:B:241:PHE:N	2.40	0.54
1:B:218:GLU:CD	6:B:2130:HOH:O	2.46	0.54
1:B:52:VAL:HG22	1:B:62:GLN:NE2	2.21	0.54
2:A:1426:BF5:F1	2:A:1426:BF5:H16A	1.97	0.54
1:A:67:MET:CE	6:A:2201:HOH:O	2.57	0.53
1:B:18:PRO:O	1:B:19:ILE:HB	2.08	0.53
1:B:136:LEU:HD23	1:B:157:ILE:HB	1.91	0.53
1:A:294:HIS:HD2	1:A:295:PRO:O	1.90	0.52
1:A:121:LEU:HD22	1:A:228:ILE:HD11	1.90	0.52
1:B:17:SER:HB2	1:B:18:PRO:O	2.10	0.52
1:A:256:ILE:HD11	1:A:280:LEU:HD13	1.91	0.51
1:A:341:LEU:HD22	1:A:414:PHE:CD2	2.44	0.51
1:A:15:ASN:O	1:B:147:GLN:NE2	2.43	0.51
1:A:369:LEU:HA	1:A:373:LYS:HE2	1.92	0.51
1:A:293:LEU:HD21	1:B:118:GLN:HE21	1.75	0.50
1:A:283:ARG:CD	6:A:2192:HOH:O	2.56	0.50
1:A:80:ILE:HD13	1:A:301:LEU:HD13	1.93	0.50
1:B:367:LYS:HE3	1:B:371:GLU:OE1	2.12	0.50
1:A:63:PHE:CD2	1:A:68:MET:CE	2.93	0.50
1:A:173:ASP:OD1	1:A:174:ILE:N	2.45	0.49
1:B:145:THR:HG21	1:B:195:TYR:OH	2.12	0.49
1:B:121:LEU:HD12	1:B:228:ILE:HD11	1.93	0.49
1:B:2:ASN:ND2	6:B:2173:HOH:O	2.45	0.49
1:A:121:LEU:HD23	1:A:228:ILE:HD11	1.94	0.49
2:A:1426:BF5:F1	2:A:1426:BF5:C16	2.51	0.49
1:B:185:ASN:ND2	1:B:187:GLN:H	2.11	0.48
1:B:121:LEU:HD21	1:B:230:ASP:CG	2.33	0.48
1:B:73:GLN:O	1:B:297:THR:CG2	2.60	0.48
1:B:74:TYR:HA	1:B:294:HIS:CE1	2.48	0.48
1:A:197:VAL:HB	1:A:201:ASN:HD22	1.79	0.48
1:B:337:ALA:O	1:B:341:LEU:HB2	2.14	0.47
1:A:150:HIS:HE1	6:B:2012:HOH:O	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:HD21	1:B:299:ASN:ND2	2.12	0.47
1:B:102:TYR:O	1:B:108:GLN:HB2	2.14	0.47
1:B:264:ILE:HG13	1:B:265:ILE:HG13	1.97	0.46
1:A:42:ASN:OD1	1:A:44:ASN:HB2	2.16	0.46
1:A:99:THR:HG23	1:A:109:MET:N	2.31	0.45
1:A:214:LYS:O	1:A:218:GLU:HG3	2.15	0.45
1:B:2:ASN:N	6:B:2003:HOH:O	2.47	0.45
1:A:95:HIS:HE1	6:A:2185:HOH:O	2.00	0.45
1:B:-1:GLU:O	1:B:105:SER:O	2.34	0.45
1:A:48:PHE:HB2	1:A:72:LEU:HD11	1.99	0.45
1:B:304:SER:O	1:B:308:HIS:CD2	2.69	0.45
1:B:42:ASN:HD21	1:B:44:ASN:HD22	1.65	0.45
1:A:264:ILE:O	1:A:318:HIS:CE1	2.65	0.44
1:A:295:PRO:O	1:A:296:SER:C	2.55	0.44
1:B:77:SER:OG	1:B:289:GLN:HG2	2.17	0.44
1:A:283:ARG:N	1:A:283:ARG:HD2	2.32	0.44
1:A:60:THR:HG22	6:A:2025:HOH:O	2.17	0.44
1:A:270:ARG:HD3	1:B:294:HIS:CE1	2.52	0.44
1:A:313:GLU:CD	1:A:313:GLU:H	2.20	0.44
1:A:68:MET:HE2	1:A:71:ALA:HB3	2.00	0.44
1:A:359:LYS:HB2	1:A:397:TYR:CE2	2.53	0.44
6:A:2007:HOH:O	1:B:150:HIS:HE1	2.01	0.44
1:A:95:HIS:HD2	6:A:2180:HOH:O	2.00	0.43
1:B:75:SER:HB2	1:B:76:PRO:CD	2.48	0.43
1:B:315:PHE:O	1:B:319:VAL:HG12	2.18	0.43
1:A:95:HIS:O	1:A:96:ASN:C	2.57	0.43
1:A:326:TYR:CE1	1:A:354:MET:HE2	2.54	0.43
1:A:33:MET:HG3	1:A:34:ILE:N	2.34	0.42
1:A:49:LYS:HE2	1:B:56:GLU:HB2	2.00	0.42
1:A:339:LYS:HE2	1:A:340:TRP:CZ2	2.54	0.42
1:B:206:ASN:ND2	6:B:2125:HOH:O	2.40	0.42
1:B:294:HIS:NE2	1:B:297:THR:HG22	2.35	0.42
1:B:185:ASN:HD22	1:B:186:PRO:N	2.17	0.41
1:B:65:GLU:HG2	1:B:65:GLU:H	1.60	0.41
1:A:80:ILE:HD12	1:A:301:LEU:HD13	2.01	0.41
1:A:68:MET:HE1	1:A:298:PHE:CE2	2.56	0.41
1:B:366:VAL:HG21	1:B:398:LEU:HG	2.03	0.41
1:B:217:TYR:HB2	1:B:249:MET:HE1	2.02	0.41
1:A:140:PRO:HG2	1:A:204:THR:HG23	2.03	0.41
1:A:368:GLU:CG	6:A:2232:HOH:O	2.59	0.41
1:B:197:VAL:HA	1:B:230:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HD22	1:B:414:PHE:CD2	2.56	0.41
1:A:40:LEU:HD21	2:B:1426:BF5:H4	2.02	0.40
1:B:129:ILE:CG2	1:B:154:CYS:HB3	2.51	0.40
1:A:68:MET:HE2	1:A:68:MET:HA	1.99	0.40
1:A:63:PHE:CD2	1:A:68:MET:HE1	2.40	0.40
1:B:341:LEU:HD22	1:B:414:PHE:HD2	1.85	0.40
1:A:91:GLN:NE2	1:A:91:GLN:HA	2.36	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:A:211:GLU:OE1	1:A:211:GLU:OE1[2_565]	1.73	0.47

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	408/425 (96%)	395 (97%)	13 (3%)	0	100	100
1	B	408/425 (96%)	390 (96%)	16 (4%)	2 (0%)	29	26
All	All	816/850 (96%)	785 (96%)	29 (4%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	LYS
1	B	378	GLY

5.3.2 Protein sidechains ⓘ

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	358/370 (97%)	338 (94%)	20 (6%)	21	18
1	B	358/370 (97%)	321 (90%)	37 (10%)	7	4
All	All	716/740 (97%)	659 (92%)	57 (8%)	12	8

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	33	MET
1	A	60	THR
1	A	68	MET
1	A	99	THR
1	A	177	ARG
1	A	228	ILE
1	A	263	LYS
1	A	283	ARG
1	A	301	LEU
1	A	307	LEU
1	A	313	GLU
1	A	334	LEU
1	A	341	LEU
1	A	370	ILE
1	A	379	VAL
1	A	380	LEU
1	A	407	PRO
1	A	417	LEU
1	A	420	LEU
1	B	17	SER
1	B	42	ASN
1	B	62	GLN
1	B	65	GLU
1	B	121	LEU
1	B	137	LEU
1	B	145	THR

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Mol	Chain	Res	Type
1	B	163	GLU
1	B	178	TRP
1	B	185	ASN
1	B	189	ASN
1	B	219	LEU
1	B	226	LEU
1	B	228	ILE
1	B	241	PHE
1	B	243	VAL
1	B	259	ASP
1	B	280	LEU
1	B	282	GLU
1	B	288	ILE
1	B	297	THR
1	B	307	LEU
1	B	319	VAL
1	B	322	VAL
1	B	334	LEU
1	B	342	THR
1	B	344	LEU
1	B	363	ILE
1	B	368	GLU
1	B	369	LEU
1	B	370	ILE
1	B	373	LYS
1	B	376	LYS
1	B	380	LEU
1	B	381	MET
1	B	417	LEU
1	B	424	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	91	GLN
1	A	95	HIS
1	A	150	HIS
1	A	201	ASN
1	A	237	GLN
1	A	294	HIS
1	A	305	GLN

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Mol	Chain	Res	Type
1	A	318	HIS
1	A	328	ASN
1	B	2	ASN
1	B	42	ASN
1	B	62	GLN
1	B	118	GLN
1	B	150	HIS
1	B	185	ASN
1	B	189	ASN
1	B	201	ASN
1	B	237	GLN
1	B	294	HIS
1	B	299	ASN
1	B	308	HIS
1	B	328	ASN
1	B	348	HIS
1	B	419	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	PLP	B	1427	2	15,15,16	1.00	0	20,22,23	1.53	3 (15%)
5	GOL	B	1428	-	5,5,5	0.26	0	5,5,5	0.91	0
2	BF5	B	1426	3	21,29,29	3.14	8 (38%)	17,44,44	1.77	2 (11%)
3	PLP	A	1427	2	15,15,16	0.89	0	20,22,23	1.65	1 (5%)
2	BF5	A	1426	3	21,29,29	3.27	7 (33%)	17,44,44	2.12	5 (29%)

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	PLP	B	1427	2	-	3/6/6/8	0/1/1/1
5	GOL	B	1428	-	-	2/4/4/4	-
2	BF5	B	1426	3	-	1/4/43/43	0/3/4/4
3	PLP	A	1427	2	-	3/6/6/8	0/1/1/1
2	BF5	A	1426	3	-	2/4/43/43	0/3/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1426	BF5	C12-C8	10.24	1.50	1.38
2	B	1426	BF5	C12-C8	8.87	1.49	1.38
2	A	1426	BF5	C4-C8	-5.46	1.37	1.51
2	B	1426	BF5	O2-C12	-4.95	1.25	1.37
2	B	1426	BF5	C4-C8	-4.85	1.39	1.51
2	A	1426	BF5	C11-C12	4.72	1.48	1.40
2	B	1426	BF5	C11-C17	4.71	1.52	1.47
2	B	1426	BF5	C11-C12	4.71	1.48	1.40
2	A	1426	BF5	O2-C12	-4.30	1.27	1.37
2	A	1426	BF5	C11-C17	3.97	1.51	1.47
2	B	1426	BF5	C2-C1	3.96	1.40	1.36
2	A	1426	BF5	C2-C1	3.26	1.39	1.36
2	A	1426	BF5	F1-C1	-2.84	1.33	1.36
2	B	1426	BF5	C9-N2	2.63	1.43	1.40
2	B	1426	BF5	O1-C3	2.01	1.38	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1426	BF5	C11-C12-C8	-5.62	117.21	121.69
3	A	1427	PLP	O4P-C5A-C5	5.06	118.99	109.35
2	B	1426	BF5	C11-C12-C8	-4.46	118.14	121.69
2	B	1426	BF5	C13-N1-C2	-3.96	108.41	121.09
2	A	1426	BF5	C13-N1-C2	-3.92	108.55	121.09
3	B	1427	PLP	O4P-C5A-C5	2.97	115.01	109.35
2	A	1426	BF5	C14-C13-N1	2.84	116.53	110.44
3	B	1427	PLP	C3-C4-C5	2.82	121.78	118.74
2	A	1426	BF5	C16-N1-C2	-2.45	113.26	121.09
3	B	1427	PLP	C6-C5-C4	-2.27	116.37	118.16
2	A	1426	BF5	O2-C12-C8	2.17	121.00	118.68

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1427	PLP	C5A-O4P-P-O1P
3	B	1427	PLP	C5A-O4P-P-O2P
3	B	1427	PLP	C5A-O4P-P-O3P
5	B	1428	GOL	O1-C1-C2-C3
3	A	1427	PLP	C4-C5-C5A-O4P
3	A	1427	PLP	C6-C5-C5A-O4P
3	A	1427	PLP	C5A-O4P-P-O2P
2	A	1426	BF5	C3-C2-N1-C16
5	B	1428	GOL	O1-C1-C2-O2
2	B	1426	BF5	C3-C2-N1-C16
2	A	1426	BF5	C1-C2-N1-C16

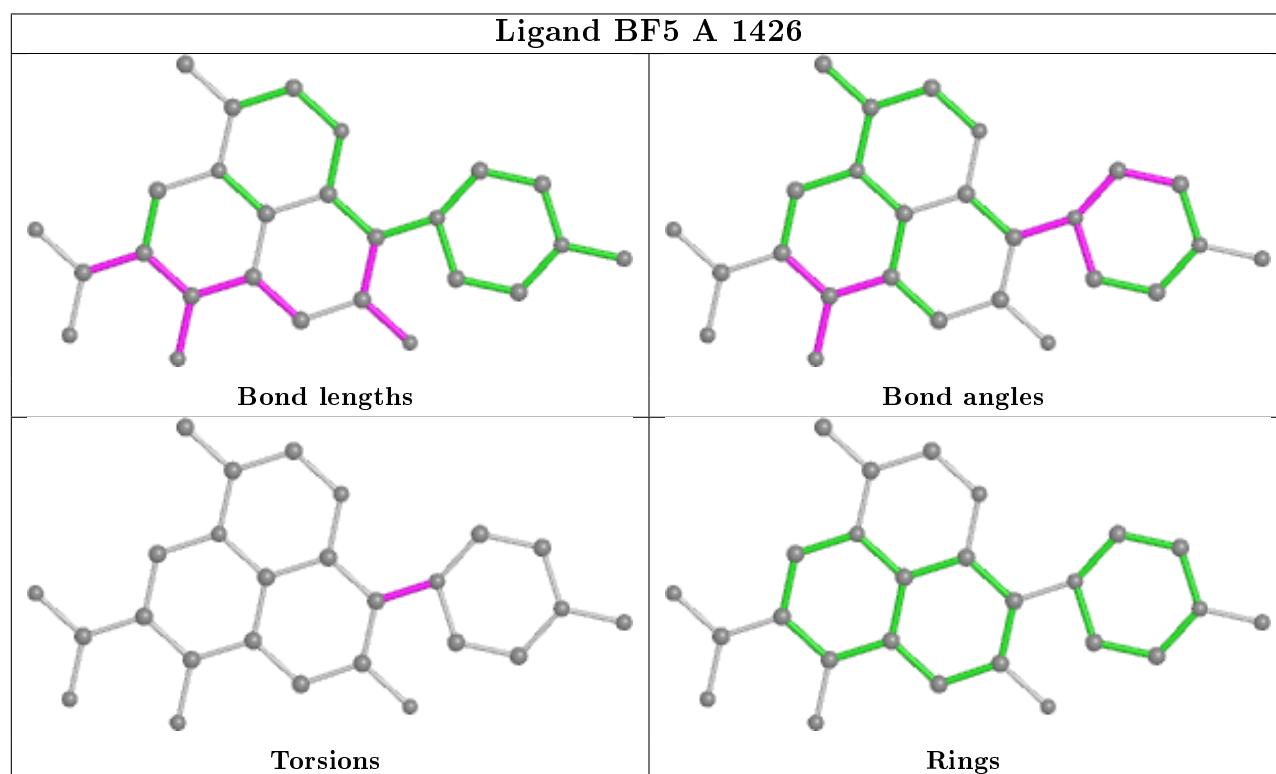
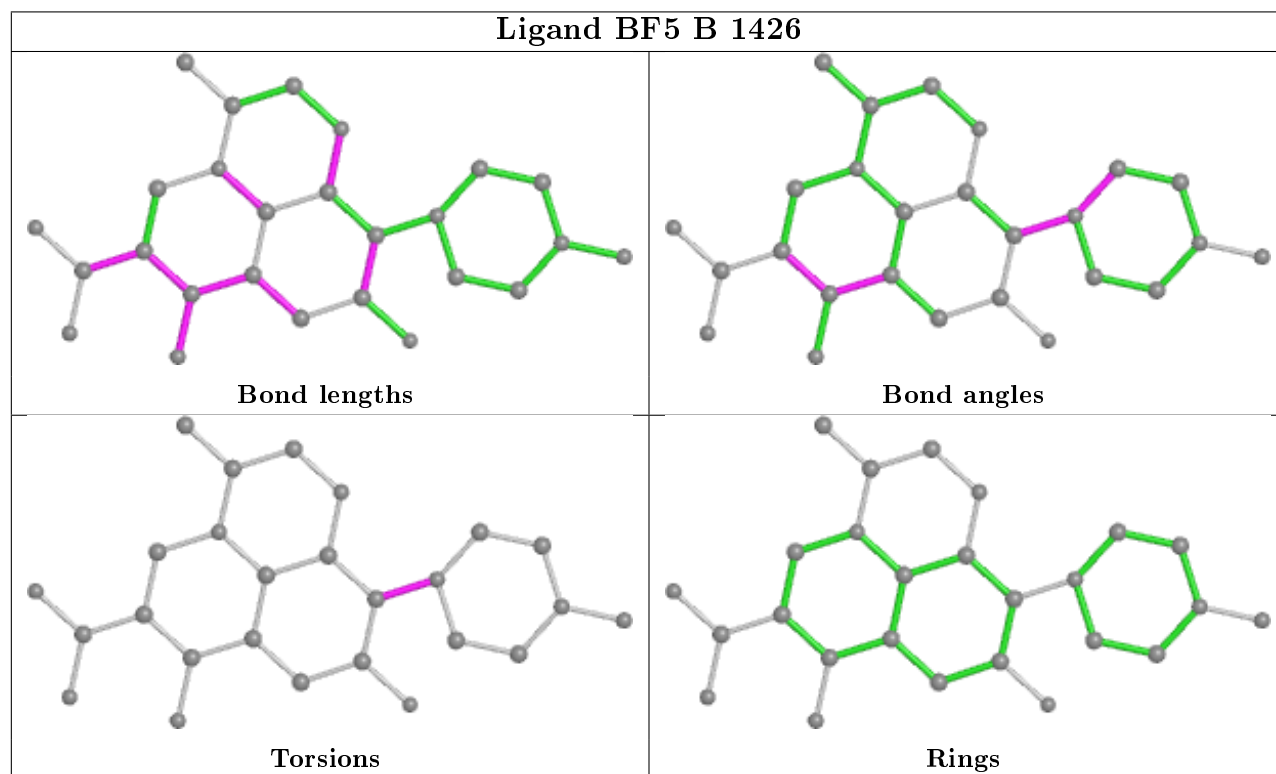
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1426	BF5	1	0
2	A	1426	BF5	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	412/425 (96%)	0.21	26 (6%) 20 24	11, 22, 52, 69	0
1	B	412/425 (96%)	0.57	43 (10%) 6 8	13, 27, 73, 91	0
All	All	824/850 (96%)	0.39	69 (8%) 11 14	11, 24, 64, 91	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	LEU	9.4
1	A	33	MET	6.4
1	B	375	VAL	6.3
1	B	372	GLU	6.2
1	B	377	MET	5.7
1	B	394	PRO	5.6
1	B	365	ASP	5.2
1	A	376	LYS	5.2
1	B	379	VAL	5.1
1	B	374	ALA	5.1
1	A	425	LEU	5.0
1	A	379	VAL	4.9
1	B	369	LEU	4.6
1	B	376	LYS	4.5
1	B	363	ILE	4.4
1	B	371	GLU	4.4
1	B	241	PHE	4.3
1	B	57	ASN	4.2
1	B	424	SER	3.9
1	A	392	SER	3.9
1	A	373	LYS	3.9
1	B	370	ILE	3.9
1	B	392	SER	3.8
1	B	378	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	370	ILE	3.7
1	A	371	GLU	3.6
1	A	372	GLU	3.6
1	B	373	LYS	3.6
1	B	33	MET	3.6
1	B	411	ASP	3.5
1	A	34	ILE	3.5
1	B	408	GLU	3.4
1	A	35	SER	3.3
1	B	420	LEU	3.2
1	A	380	LEU	3.2
1	B	239	ASN	3.2
1	B	368	GLU	3.1
1	A	393	ALA	3.1
1	B	-1	GLU	3.0
1	B	228	ILE	2.9
1	A	173	ASP	2.9
1	A	374	ALA	2.8
1	B	407	PRO	2.8
1	A	377	MET	2.8
1	A	368	GLU	2.8
1	B	393	ALA	2.7
1	A	375	VAL	2.7
1	A	367	LYS	2.6
1	B	258	ALA	2.6
1	B	367	LYS	2.5
1	A	228	ILE	2.5
1	B	423	GLU	2.5
1	A	57	ASN	2.4
1	B	412	VAL	2.4
1	B	364	ASN	2.4
1	B	34	ILE	2.4
1	A	40	LEU	2.3
1	A	369	LEU	2.3
1	B	19	ILE	2.3
1	A	424	SER	2.3
1	B	406	SER	2.3
1	B	59	LYS	2.2
1	A	419	GLN	2.2
1	B	311	GLY	2.2
1	B	195	TYR	2.2
1	A	38	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	340	TRP	2.1
1	B	226	LEU	2.1
1	B	419	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

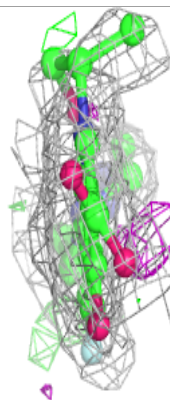
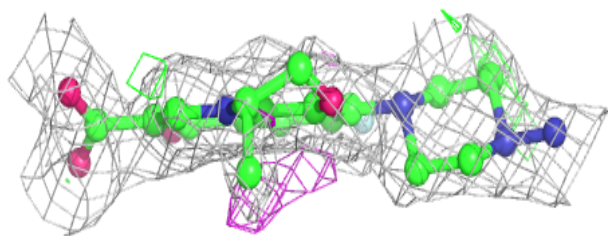
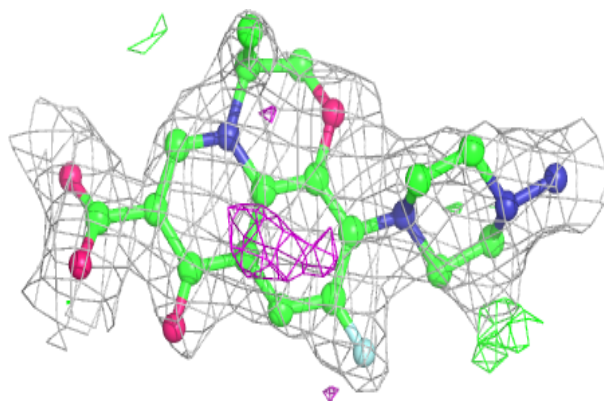
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BF5	B	1426	26/26	0.76	0.22	40,51,52,52	0
5	GOL	B	1428	6/6	0.80	0.20	47,49,50,52	0
2	BF5	A	1426	26/26	0.85	0.20	35,40,41,43	0
3	PLP	B	1427	15/16	0.97	0.17	20,31,34,34	0
3	PLP	A	1427	15/16	0.98	0.16	18,26,29,29	0
4	IOD	A	1428	1/1	1.00	0.05	20,20,20,20	0

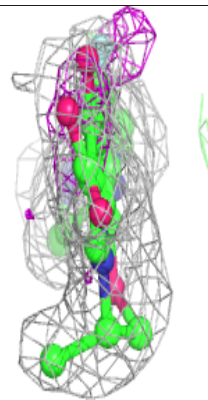
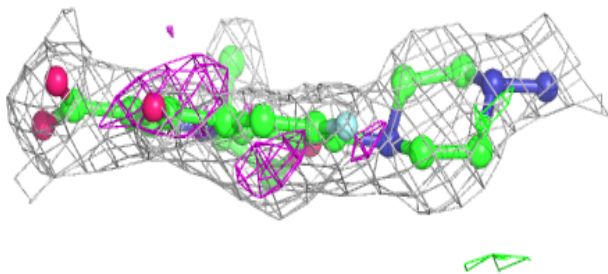
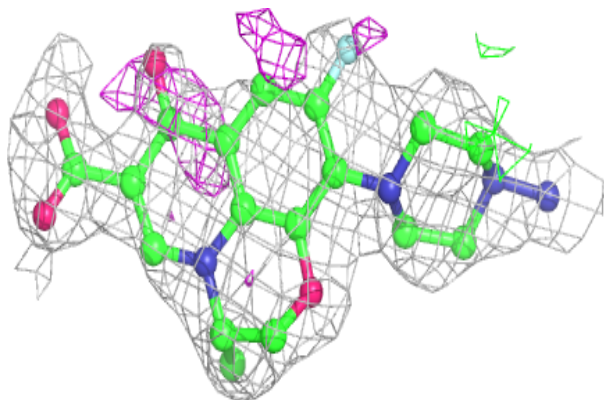
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BF5 B 1426:

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

**Electron density around BF5 A 1426:**

$2mF_o-DF_c$ (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.