



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2025 – 06:25 pm GMT

PDB ID : 9GU6 / pdb_00009gu6
Title : NCS-1 bound to FDA ligand 3
Authors : Munoz-Reyes, D.; Sanchez-Barrena, M.J.
Deposited on : 2024-09-19
Resolution : 1.93 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 : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

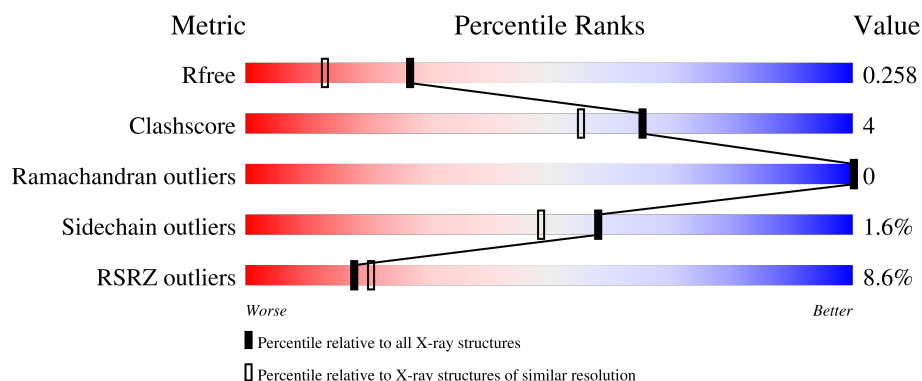
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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 $\leq 5\%$. 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	B	190	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div> </div>
1	D	190	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>..</div> </div> </div>
1	F	190	<div> <div>12%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>7%</div> </div> </div>
1	H	190	<div> <div>12%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12937 atoms, of which 6043 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.

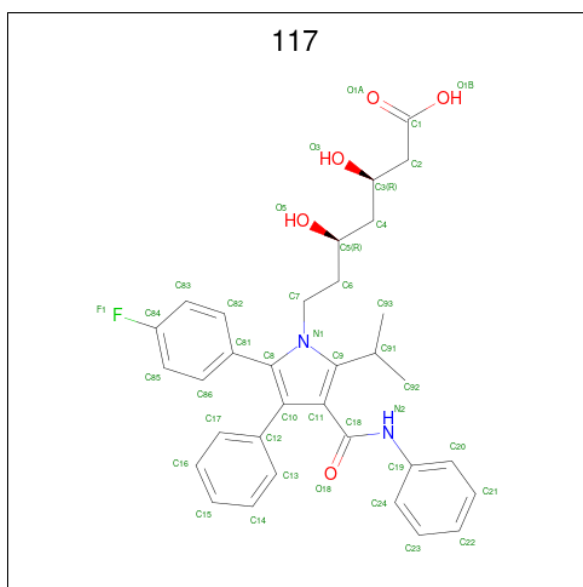
- Molecule 1 is a protein called Neuronal calcium sensor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	184	Total	C	H	N	O	S	0	1	0
			2968	965	1462	241	294	6			
1	D	185	Total	C	H	N	O	S	0	1	0
			2984	970	1471	242	295	6			
1	F	176	Total	C	H	N	O	S	0	1	0
			2858	930	1411	234	278	5			
1	H	179	Total	C	H	N	O	S	0	0	0
			2886	941	1423	234	283	5			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	D	3	Total	Ca	0	0
			3	3		
2	F	3	Total	Ca	0	0
			3	3		
2	H	3	Total	Ca	0	0
			3	3		

- Molecule 3 is 7-[2-(4-FLUORO-PHENYL)-5-ISOPROPYL-3-PHENYL-4-PHENYLCARBAMOYL-PYRROL-1-YL]- 3,5-DIHYDROXY-HEPTANOIC ACID (CCD ID: 117) (formula: C₃₃H₃₅FN₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 75	C 33	F 1	H 34	N 2	O 5	0	0
3	B	1	Total 75	C 33	F 1	H 34	N 2	O 5	0	0
3	D	1	Total 75	C 33	F 1	H 34	N 2	O 5	0	0
3	D	1	Total 75	C 33	F 1	H 34	N 2	O 5	0	0
3	F	1	Total 75	C 33	F 1	H 34	N 2	O 5	0	0
3	H	1	Total 75	C 33	F 1	H 34	N 2	O 5	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		
4	D	2	Total	Na	0	0
			2	2		
4	F	2	Total	Na	0	0
			2	2		
4	H	2	Total	Na	0	0
			2	2		

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



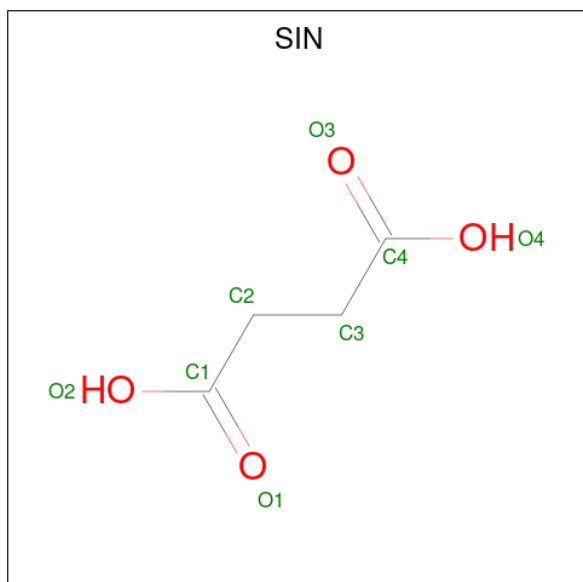
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			9	3	2	4		
5	B	1	Total	C	H	O	0	0
			9	3	2	4		
5	B	1	Total	C	H	O	0	0
			9	3	2	4		
5	D	1	Total	C	H	O	0	0
			9	3	2	4		
5	D	1	Total	C	H	O	0	0
			9	3	2	4		
5	F	1	Total	C	H	O	0	0
			9	3	2	4		
5	F	1	Total	C	H	O	0	0
			9	3	2	4		
5	H	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



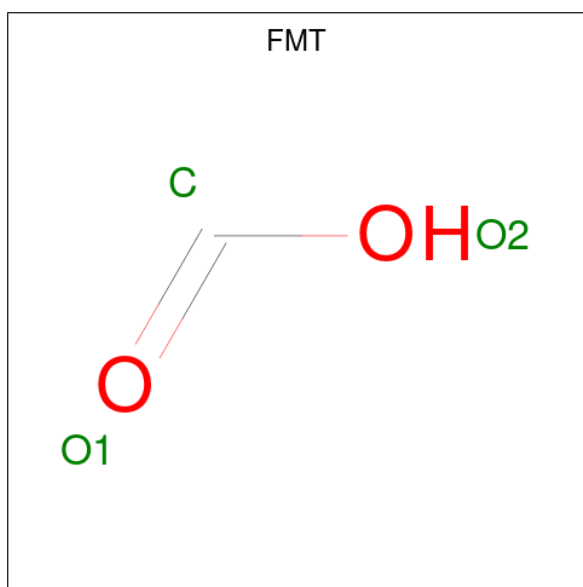
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			7	2	3	2		
6	B	1	Total	C	H	O	0	0
			7	2	3	2		
6	D	1	Total	C	H	O	0	0
			7	2	3	2		
6	D	1	Total	C	H	O	0	0
			7	2	3	2		
6	H	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 7 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			12	4	4	4		
7	B	1	Total	C	H	O	0	0
			12	4	4	4		
7	D	1	Total	C	H	O	0	0
			12	4	4	4		
7	D	1	Total	C	H	O	0	0
			12	4	4	4		
7	F	1	Total	C	H	O	0	0
			12	4	4	4		
7	F	1	Total	C	H	O	0	0
			12	4	4	4		
7	H	1	Total	C	H	O	0	0
			12	4	4	4		
7	H	1	Total	C	H	O	0	0
			12	4	4	4		
7	H	1	Total	C	H	O	0	0
			12	4	4	4		
7	H	1	Total	C	H	O	0	0
			12	4	4	4		

- Molecule 8 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			4	1	1	2		

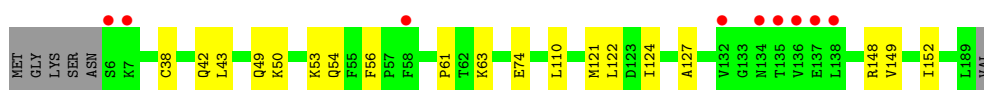
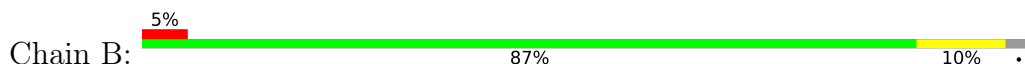
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	156	Total 156	O 156	0	0
9	D	154	Total 154	O 154	0	0
9	F	111	Total 111	O 111	0	0
9	H	119	Total 119	O 119	0	0

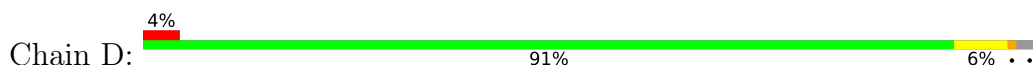
3 Residue-property plots [i](#)

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.

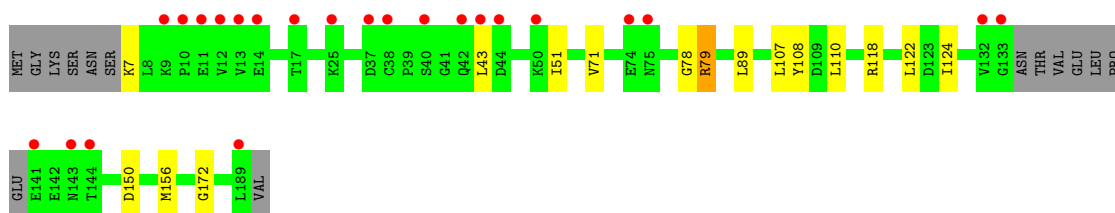
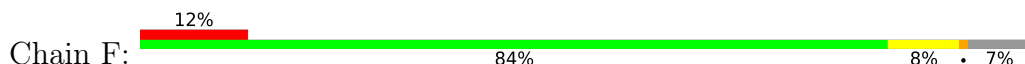
- Molecule 1: Neuronal calcium sensor 1



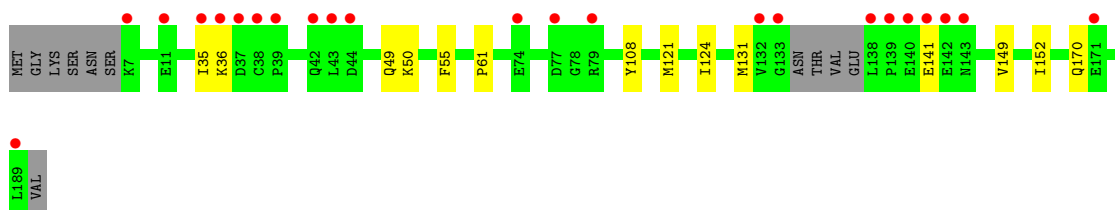
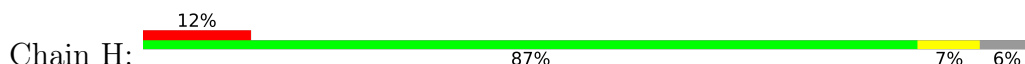
- Molecule 1: Neuronal calcium sensor 1



- Molecule 1: Neuronal calcium sensor 1



- Molecule 1: Neuronal calcium sensor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.29Å 59.62Å 65.45Å 87.36° 89.96° 85.06°	Depositor
Resolution (Å)	24.70 – 1.93 24.70 – 1.93	Depositor EDS
% Data completeness (in resolution range)	66.6 (24.70-1.93) 66.9 (24.70-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.21.1-5286	Depositor
R, R_{free}	0.219 , 0.256 0.220 , 0.258	Depositor DCC
R_{free} test set	2095 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	8.4	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12937	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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: CA, FMT, ACY, NA, SIN, MLI, 117

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	B	0.18	0/1538	0.26	0/2074
1	D	0.18	0/1545	0.29	0/2084
1	F	0.18	0/1480	0.26	0/1990
1	H	0.17	0/1494	0.27	0/2011
All	All	0.18	0/6057	0.27	0/8159

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	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	79	ARG	Sidechain

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	B	1506	1462	1462	13	0
1	D	1513	1471	1471	7	0
1	F	1447	1411	1412	12	0
1	H	1463	1423	1423	8	0
2	B	3	0	0	0	0
2	D	3	0	0	0	0
2	F	3	0	0	0	0
2	H	3	0	0	0	0
3	B	82	68	68	2	0
3	D	82	68	68	2	0
3	F	41	34	34	4	0
3	H	41	34	34	3	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	H	2	0	0	0	0
5	B	21	6	6	0	0
5	D	14	4	4	0	0
5	F	14	4	4	0	0
5	H	7	2	2	0	0
6	B	8	6	6	0	0
6	D	8	6	6	0	0
6	H	4	3	3	0	0
7	B	16	8	8	1	0
7	D	16	8	8	0	0
7	F	16	8	8	0	0
7	H	32	16	16	0	0
8	B	3	1	1	0	0
9	B	156	0	0	1	0
9	D	154	0	0	0	0
9	F	111	0	0	1	0
9	H	119	0	0	2	0
All	All	6894	6043	6044	46	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 4.

All (46) 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:F:78:GLY:O	1:F:79:ARG:HD3	1.84	0.78
1:F:110:LEU:HD21	1:F:124:ILE:HD11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:GLU:OE1	9:H:301:HOH:O	2.02	0.76
1:F:89:LEU:HD11	3:F:204:117:H16	1.77	0.65
1:D:68:VAL:HG22	3:D:205:117:H16	1.81	0.63
1:H:108:TYR:CE1	1:H:124:ILE:HG21	2.37	0.60
1:F:108:TYR:CE1	1:F:124:ILE:HG21	2.40	0.57
1:F:118[A]:ARG:NH2	1:F:150:ASP:OD1	2.40	0.55
1:B:121:MET:SD	9:B:452:HOH:O	2.58	0.55
1:B:38[B]:CYS:SG	1:B:43:LEU:HD13	2.48	0.54
1:B:121:MET:HE1	1:B:152:ILE:HG13	1.89	0.53
1:F:71:VAL:HG21	1:F:107:LEU:HA	1.91	0.53
1:D:122:LEU:O	1:D:122:LEU:HD13	2.10	0.52
1:B:42:GLN:HG3	1:D:62:THR:HG21	1.92	0.52
3:F:204:117:HN2	3:F:204:117:H933	1.76	0.51
1:D:189:LEU:O	1:D:190:VAL:HB	2.11	0.49
3:F:204:117:H922	3:F:204:117:N2	2.28	0.49
1:B:121:MET:HE1	1:B:152:ILE:HG21	1.94	0.49
1:H:121:MET:HG2	1:H:149:VAL:HG22	1.93	0.48
1:B:121:MET:HG2	1:B:149:VAL:HG22	1.95	0.48
1:F:43:LEU:HD21	1:F:51:ILE:HD12	1.97	0.47
1:H:55:PHE:CE2	3:H:204:117:H13	2.49	0.47
1:D:132:VAL:HG11	1:D:136:VAL:HB	1.97	0.47
3:F:204:117:H61	3:F:204:117:H932	1.97	0.46
1:F:122:LEU:HD13	1:F:122:LEU:O	2.16	0.46
1:F:118[B]:ARG:HD3	9:F:326:HOH:O	2.15	0.45
1:B:63:LYS:HD3	1:B:127:ALA:HB2	2.00	0.44
3:B:205:117:H922	3:B:205:117:C18	2.48	0.43
3:D:205:117:C18	3:D:205:117:H922	2.48	0.43
1:D:189:LEU:O	1:D:190:VAL:CB	2.67	0.43
1:B:53:LYS:HA	1:B:61:PRO:HG2	2.01	0.42
1:F:156:MET:HG2	1:F:172:GLY:HA3	2.00	0.42
1:B:122:LEU:C	1:B:122:LEU:HD13	2.44	0.42
1:H:170:GLN:NE2	9:H:311:HOH:O	2.52	0.42
1:H:121:MET:SD	1:H:152:ILE:HG21	2.60	0.42
1:H:61:PRO:HB3	1:H:131:MET:HG3	2.02	0.41
1:F:7:LYS:O	1:F:7:LYS:HG2	2.20	0.41
1:B:50:LYS:O	1:B:54:GLN:HG3	2.20	0.41
1:B:148:ARG:HE	7:B:210:SIN:H32	1.85	0.41
1:H:36:LYS:HB2	3:H:204:117:H22A	2.02	0.41
3:B:204:117:H933	3:B:204:117:C18	2.51	0.41
1:D:68:VAL:O	1:D:71:VAL:HG12	2.20	0.41
1:B:110:LEU:HD21	1:B:124:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:PHE:HB2	1:B:61:PRO:HG3	2.03	0.40
1:F:110:LEU:HD21	1:F:124:ILE:CD1	2.44	0.40
3:H:204:117:O18	3:H:204:117:H922	2.21	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	B	183/190 (96%)	180 (98%)	3 (2%)	0	100	100
1	D	184/190 (97%)	184 (100%)	0	0	100	100
1	F	173/190 (91%)	170 (98%)	3 (2%)	0	100	100
1	H	175/190 (92%)	174 (99%)	1 (1%)	0	100	100
All	All	715/760 (94%)	708 (99%)	7 (1%)	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	B	164/168 (98%)	162 (99%)	2 (1%)	67	61
1	D	165/168 (98%)	159 (96%)	6 (4%)	30	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	156/168 (93%)	156 (100%)	0	100	100
1	H	158/168 (94%)	155 (98%)	3 (2%)	52	41
All	All	643/672 (96%)	632 (98%)	11 (2%)	58	45

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	GLN
1	B	74	GLU
1	D	38[A]	CYS
1	D	38[B]	CYS
1	D	52	TYR
1	D	71	VAL
1	D	137	GLU
1	D	138	LEU
1	H	35	ILE
1	H	49	GLN
1	H	50	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	134	ASN
1	D	167	GLN
1	H	49	GLN
1	H	130	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 20 are monoatomic - leaving 30 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	117	D	204	-	38,44,44	0.70	0	44,61,61	0.87	2 (4%)
7	SIN	H	207	-	7,7,7	1.04	0	8,8,8	1.66	1 (12%)
7	SIN	F	208	-	7,7,7	0.97	0	8,8,8	1.71	2 (25%)
7	SIN	B	211	-	7,7,7	1.07	0	8,8,8	1.62	1 (12%)
7	SIN	F	207	-	7,7,7	1.26	0	8,8,8	1.34	0
6	ACY	H	211	-	3,3,3	0.91	0	3,3,3	1.60	1 (33%)
7	SIN	H	209	-	7,7,7	1.02	0	8,8,8	1.56	1 (12%)
5	MLI	B	214	-	6,6,6	1.59	1 (16%)	7,7,7	1.17	0
5	MLI	B	208	-	6,6,6	1.57	1 (16%)	7,7,7	1.10	0
5	MLI	F	209	-	6,6,6	1.62	1 (16%)	7,7,7	1.17	0
7	SIN	D	209	-	7,7,7	0.89	0	8,8,8	1.72	2 (25%)
3	117	D	205	-	38,44,44	0.95	2 (5%)	44,61,61	0.80	2 (4%)
3	117	B	205	-	38,44,44	0.95	2 (5%)	44,61,61	0.81	1 (2%)
5	MLI	B	215	-	6,6,6	1.59	1 (16%)	7,7,7	1.10	0
6	ACY	D	208	-	3,3,3	0.96	0	3,3,3	1.62	0
7	SIN	H	208	-	7,7,7	1.03	0	8,8,8	1.63	1 (12%)
7	SIN	H	210	-	7,7,7	1.06	0	8,8,8	1.68	2 (25%)
3	117	B	204	-	38,44,44	0.72	1 (2%)	44,61,61	0.97	5 (11%)
5	MLI	F	210	-	6,6,6	1.53	1 (16%)	7,7,7	1.16	0
5	MLI	H	212	-	6,6,6	1.71	1 (16%)	7,7,7	1.26	1 (14%)
7	SIN	D	210	-	7,7,7	1.06	0	8,8,8	1.74	3 (37%)
3	117	H	204	-	38,44,44	0.86	2 (5%)	44,61,61	0.64	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MLI	D	212	-	6,6,6	1.60	1 (16%)	7,7,7	1.20	1 (14%)
3	117	F	204	-	38,44,44	0.72	1 (2%)	44,61,61	0.79	1 (2%)
6	ACY	B	213	-	3,3,3	0.96	0	3,3,3	1.47	1 (33%)
6	ACY	B	209	-	3,3,3	0.93	0	3,3,3	1.40	0
8	FMT	B	212	-	2,2,2	0.71	0	1,1,1	0.47	0
7	SIN	B	210	-	7,7,7	0.98	0	8,8,8	1.67	2 (25%)
5	MLI	D	213	-	6,6,6	1.64	1 (16%)	7,7,7	1.09	0
6	ACY	D	211	-	3,3,3	0.98	0	3,3,3	1.40	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	117	D	204	-	-	8/21/33/33	0/4/4/4
7	SIN	H	207	-	-	0/5/5/5	-
7	SIN	F	208	-	-	3/5/5/5	-
7	SIN	B	211	-	-	5/5/5/5	-
7	SIN	F	207	-	-	5/5/5/5	-
7	SIN	H	209	-	-	5/5/5/5	-
5	MLI	B	214	-	-	2/4/4/4	-
5	MLI	B	208	-	-	0/4/4/4	-
5	MLI	F	209	-	-	4/4/4/4	-
7	SIN	D	209	-	-	3/5/5/5	-
3	117	D	205	-	-	5/21/33/33	0/4/4/4
3	117	B	205	-	-	4/21/33/33	0/4/4/4
5	MLI	B	215	-	-	0/4/4/4	-
7	SIN	H	208	-	-	2/5/5/5	-
7	SIN	H	210	-	-	4/5/5/5	-
3	117	B	204	-	-	6/21/33/33	0/4/4/4
5	MLI	F	210	-	-	4/4/4/4	-
5	MLI	H	212	-	-	0/4/4/4	-
7	SIN	D	210	-	-	3/5/5/5	-
3	117	H	204	-	-	8/21/33/33	0/4/4/4
5	MLI	D	212	-	-	2/4/4/4	-
3	117	F	204	-	-	6/21/33/33	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SIN	B	210	-	-	5/5/5/5	-
5	MLI	D	213	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	205	117	C11-C18	-3.48	1.46	1.51
3	H	204	117	C10-C8	-3.45	1.38	1.42
3	D	205	117	C11-C18	-3.34	1.46	1.51
3	D	205	117	C10-C8	-3.09	1.38	1.42
3	B	205	117	C10-C8	-3.02	1.38	1.42
5	H	212	MLI	C1-C3	2.80	1.55	1.51
5	D	212	MLI	C1-C3	2.72	1.55	1.51
5	D	213	MLI	C1-C3	2.69	1.55	1.51
5	B	208	MLI	C1-C3	2.69	1.55	1.51
5	B	215	MLI	C1-C3	2.67	1.55	1.51
5	F	209	MLI	C1-C3	2.62	1.55	1.51
5	B	214	MLI	C1-C3	2.59	1.55	1.51
5	F	210	MLI	C1-C3	2.48	1.54	1.51
3	B	204	117	C11-C18	-2.20	1.48	1.51
3	F	204	117	C11-C18	-2.04	1.48	1.51
3	H	204	117	C11-C18	-2.04	1.48	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	205	117	C4-C5-C6	-3.41	105.19	112.51
3	D	205	117	C5-C4-C3	2.81	118.46	114.18
3	B	204	117	C4-C5-C6	2.74	118.38	112.51
3	D	204	117	C4-C3-C2	2.57	118.32	113.19
3	H	204	117	C5-C4-C3	2.48	117.96	114.18
3	D	205	117	C4-C5-C6	-2.42	107.31	112.51
3	B	204	117	C11-C18-N2	2.42	118.08	114.81
7	B	210	SIN	C3-C2-C1	-2.39	108.45	113.60
7	D	210	SIN	O2-C1-O1	-2.35	117.45	123.30
7	D	210	SIN	O2-C1-C2	2.31	121.46	114.03
7	H	207	SIN	C2-C3-C4	-2.26	108.74	113.60
7	D	209	SIN	O2-C1-C2	2.24	121.22	114.03
5	H	212	MLI	O6-C2-C1	-2.19	115.68	122.08
3	B	204	117	O1B-C1-C2	2.13	120.89	114.07
7	D	210	SIN	O4-C4-O3	-2.12	118.03	123.30
7	D	209	SIN	O4-C4-C3	2.11	120.81	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	204	117	C93-C91-C9	2.10	116.68	112.14
7	H	210	SIN	O4-C4-C3	2.09	120.75	114.03
7	B	211	SIN	C3-C2-C1	-2.09	109.11	113.60
7	H	208	SIN	O2-C1-C2	2.08	120.72	114.03
7	F	208	SIN	C2-C3-C4	-2.08	109.12	113.60
3	F	204	117	C5-C4-C3	2.08	117.35	114.18
6	B	213	ACY	OXT-C-O	2.08	129.71	122.05
7	F	208	SIN	O4-C4-C3	2.07	120.69	114.03
3	B	204	117	O1A-C1-C2	-2.07	116.16	122.80
5	D	212	MLI	O6-C2-C1	-2.07	116.04	122.08
7	H	209	SIN	O2-C1-C2	2.06	120.66	114.03
7	B	210	SIN	O4-C4-C3	2.03	120.56	114.03
3	D	204	117	C11-C18-N2	2.03	117.56	114.81
6	H	211	ACY	OXT-C-O	2.02	129.49	122.05
7	H	210	SIN	O2-C1-C2	2.00	120.47	114.03

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	204	117	C3-C4-C5-O5
3	B	204	117	C11-C9-C91-C93
3	B	205	117	C1-C2-C3-O3
3	B	205	117	C1-C2-C3-C4
3	D	204	117	C3-C4-C5-O5
3	D	205	117	C1-C2-C3-O3
3	D	205	117	C1-C2-C3-C4
3	F	204	117	C1-C2-C3-O3
3	F	204	117	C1-C2-C3-C4
3	H	204	117	O3-C3-C4-C5
3	H	204	117	C2-C3-C4-C5
3	H	204	117	C3-C4-C5-O5
3	H	204	117	C11-C18-N2-C19
3	H	204	117	O18-C18-N2-C19
7	B	211	SIN	C1-C2-C3-C4
7	B	210	SIN	C1-C2-C3-C4
7	F	207	SIN	C1-C2-C3-C4
7	F	208	SIN	C1-C2-C3-C4
7	H	209	SIN	C1-C2-C3-C4
3	D	204	117	C3-C4-C5-C6
7	D	210	SIN	C1-C2-C3-C4
5	F	210	MLI	C3-C1-C2-O7

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Mol	Chain	Res	Type	Atoms
7	D	209	SIN	C1-C2-C3-C4
5	F	209	MLI	C2-C1-C3-O9
3	B	205	117	N1-C9-C91-C92
3	F	204	117	N1-C9-C91-C92
5	D	212	MLI	C3-C1-C2-O6
5	F	210	MLI	C3-C1-C2-O6
5	F	210	MLI	C2-C1-C3-O8
5	B	214	MLI	C2-C1-C3-O8
5	F	209	MLI	C2-C1-C3-O8
5	F	210	MLI	C2-C1-C3-O9
5	B	214	MLI	C2-C1-C3-O9
5	D	212	MLI	C3-C1-C2-O7
5	F	209	MLI	C3-C1-C2-O7
5	F	209	MLI	C3-C1-C2-O6
3	D	204	117	O1B-C1-C2-C3
7	H	210	SIN	C2-C3-C4-O4
7	F	207	SIN	C2-C3-C4-O3
3	B	204	117	C3-C4-C5-C6
7	B	211	SIN	C2-C3-C4-O3
7	F	208	SIN	C2-C3-C4-O3
7	H	210	SIN	C2-C3-C4-O3
3	B	205	117	C11-C9-C91-C92
3	B	204	117	O1B-C1-C2-C3
3	D	204	117	O1A-C1-C2-C3
3	F	204	117	O1B-C1-C2-C3
7	D	210	SIN	O1-C1-C2-C3
7	F	207	SIN	C2-C3-C4-O4
7	H	209	SIN	C2-C3-C4-O3
3	D	204	117	N1-C9-C91-C93
3	D	204	117	N1-C9-C91-C92
3	D	205	117	N1-C9-C91-C93
3	D	205	117	N1-C9-C91-C92
3	F	204	117	N1-C9-C91-C93
3	H	204	117	N1-C9-C91-C93
3	H	204	117	N1-C9-C91-C92
7	B	211	SIN	C2-C3-C4-O4
7	F	207	SIN	O2-C1-C2-C3
7	F	207	SIN	O1-C1-C2-C3
7	F	208	SIN	C2-C3-C4-O4
7	B	210	SIN	C2-C3-C4-O4
7	B	210	SIN	C2-C3-C4-O3
7	D	210	SIN	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	B	211	SIN	O1-C1-C2-C3
7	D	209	SIN	O2-C1-C2-C3
7	D	209	SIN	O1-C1-C2-C3
7	H	209	SIN	O2-C1-C2-C3
7	B	210	SIN	O2-C1-C2-C3
3	B	204	117	C20-C19-N2-C18
7	H	209	SIN	C2-C3-C4-O4
3	B	204	117	O1A-C1-C2-C3
3	D	204	117	C1-C2-C3-C4
7	H	208	SIN	C2-C3-C4-O3
7	B	210	SIN	O1-C1-C2-C3
7	H	208	SIN	C2-C3-C4-O4
3	D	205	117	O5-C5-C6-C7
3	H	204	117	O5-C5-C6-C7
7	B	211	SIN	O2-C1-C2-C3
7	H	209	SIN	O1-C1-C2-C3
3	D	204	117	C5-C6-C7-N1
3	F	204	117	O1A-C1-C2-C3
7	H	210	SIN	O2-C1-C2-C3
7	H	210	SIN	O1-C1-C2-C3

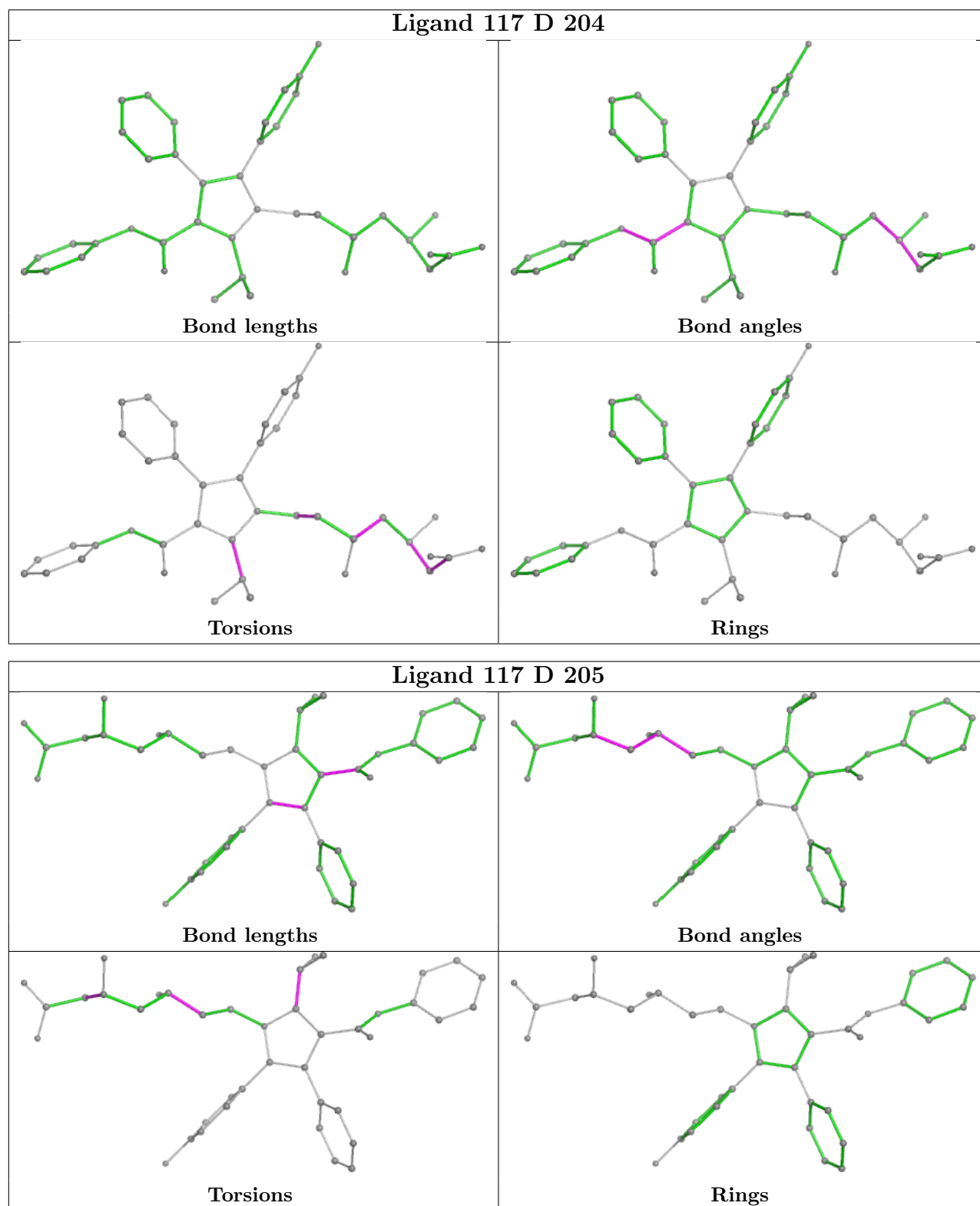
There are no ring outliers.

6 monomers are involved in 12 short contacts:

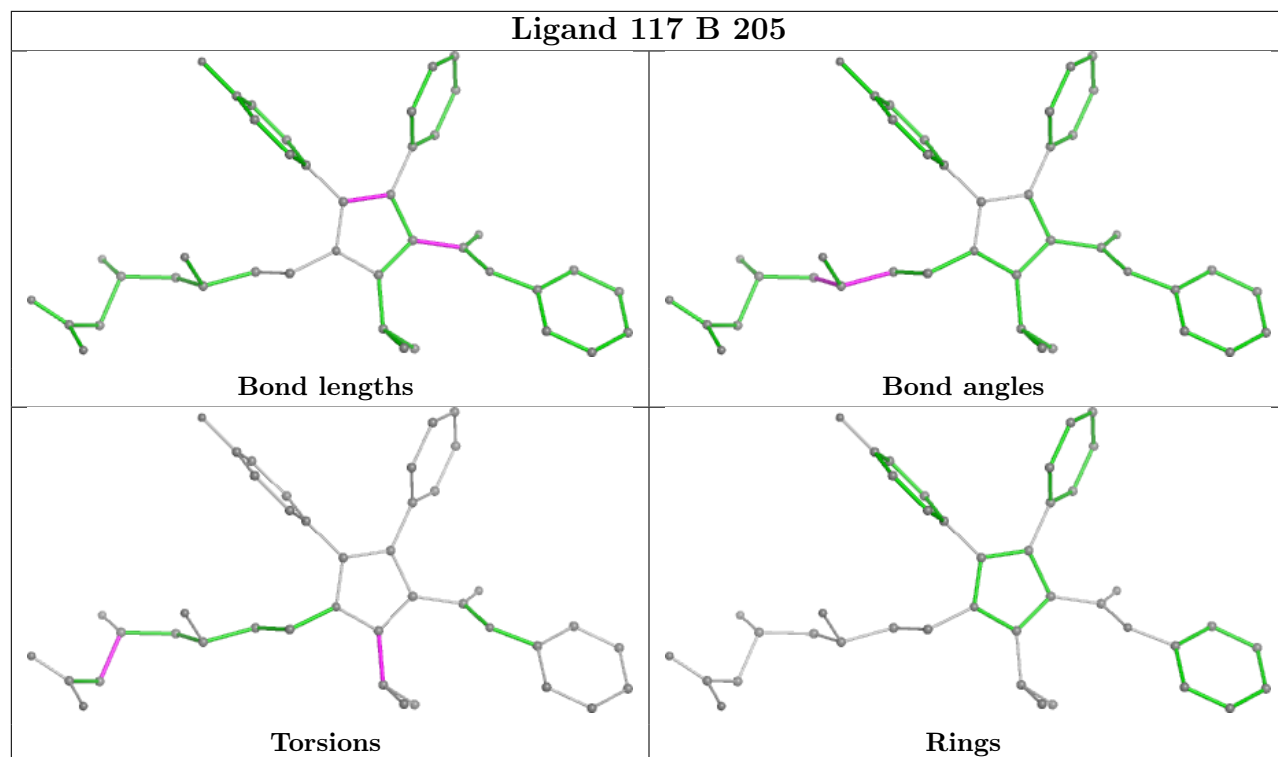
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	205	117	2	0
3	B	205	117	1	0
3	B	204	117	1	0
3	H	204	117	3	0
3	F	204	117	4	0
7	B	210	SIN	1	0

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 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.

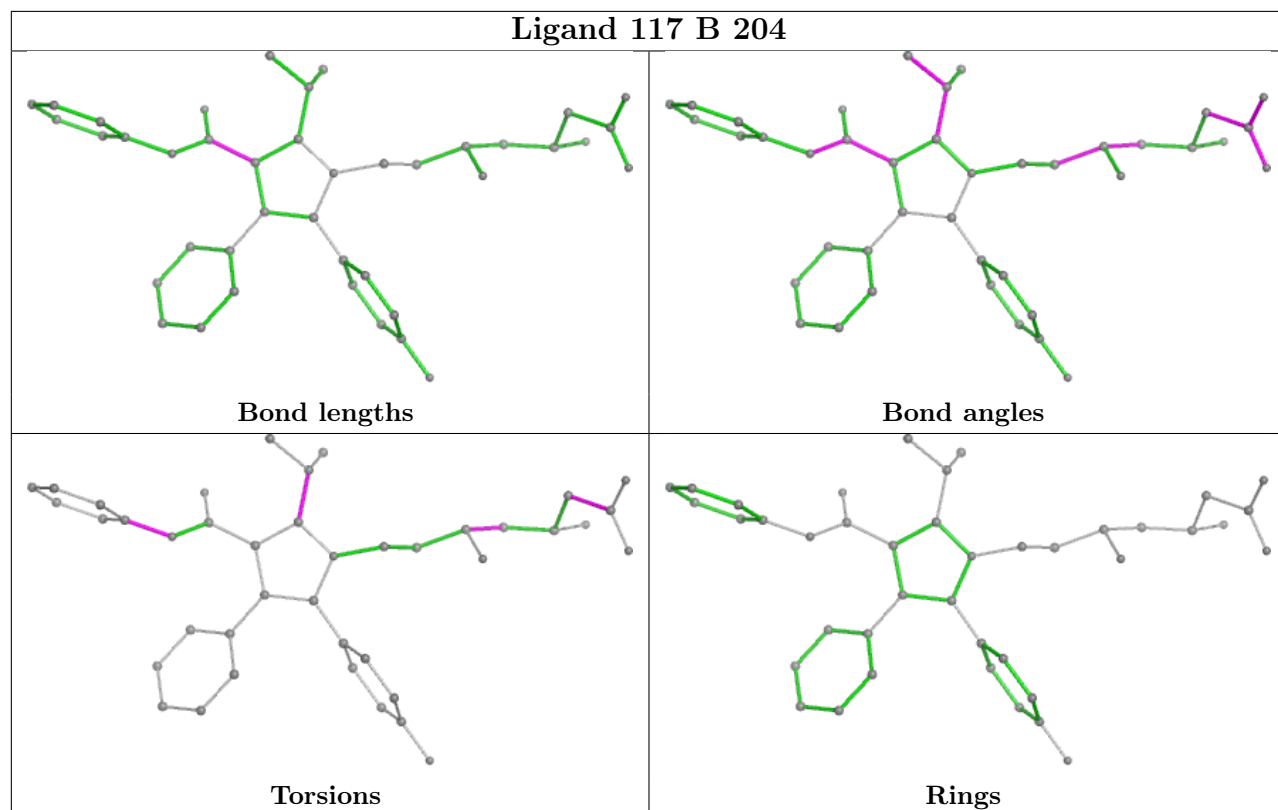
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

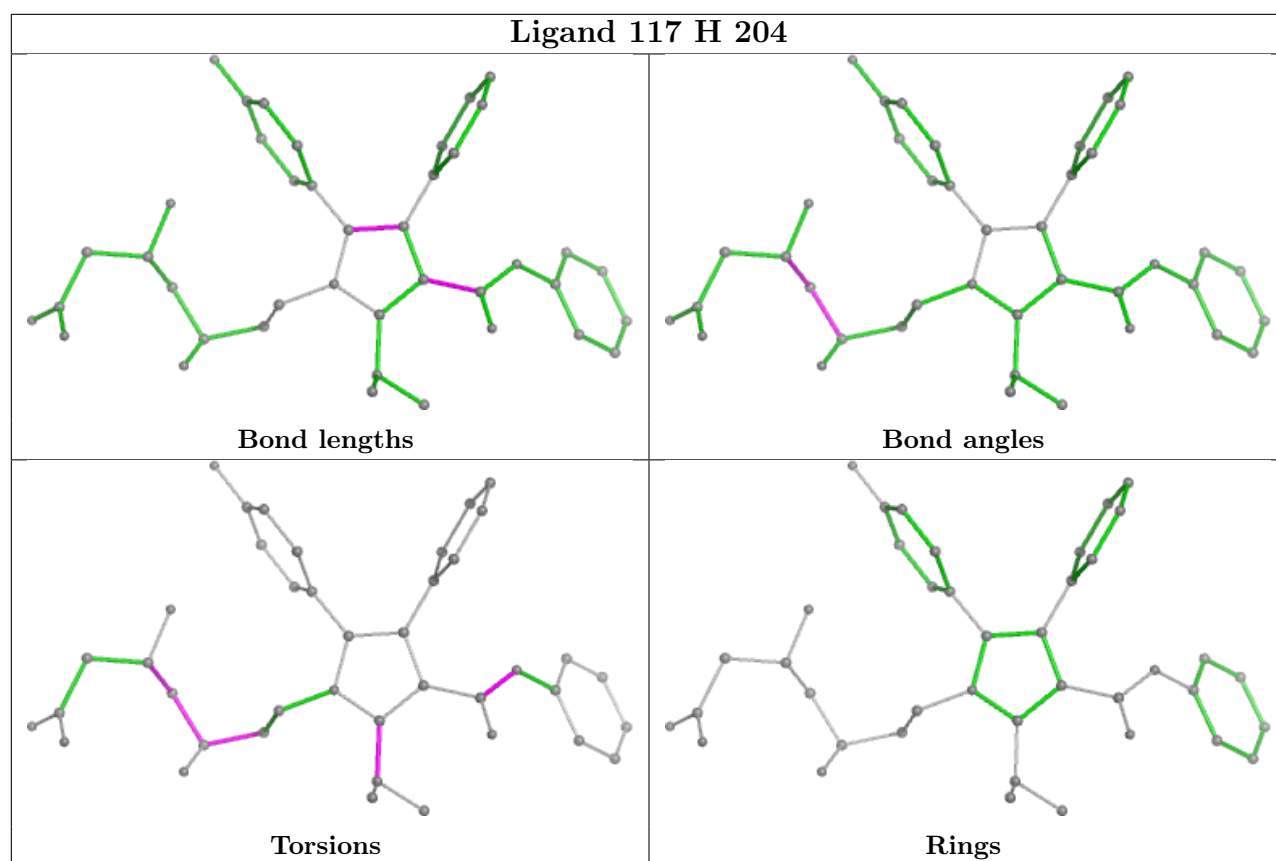


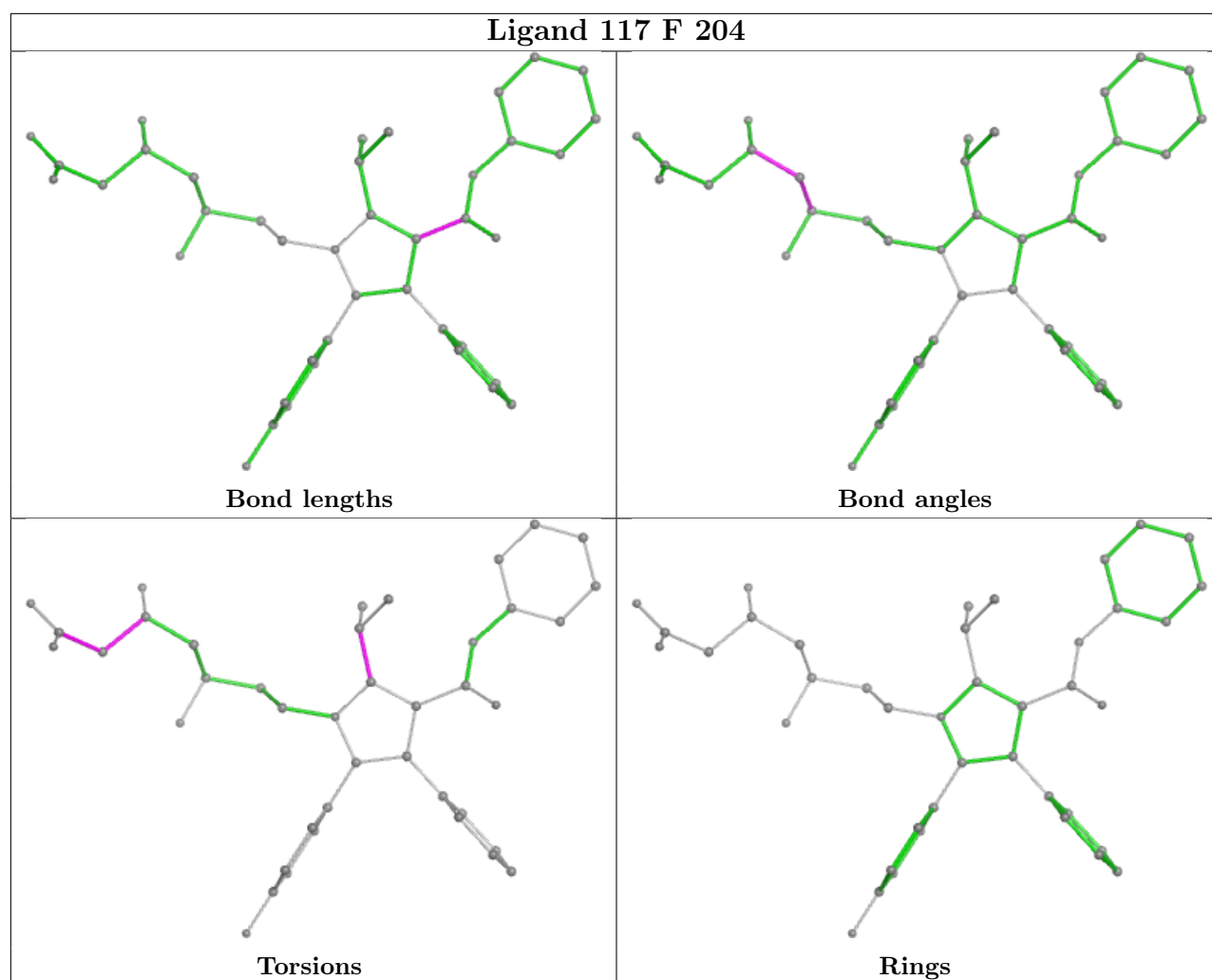
Ligand 117 B 205



Ligand 117 B 204







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	B	184/190 (96%)	0.24	9 (4%)	36	40	3, 16, 41, 67	1 (0%)
1	D	185/190 (97%)	0.22	7 (3%)	44	49	4, 16, 43, 73	1 (0%)
1	F	176/190 (92%)	0.74	23 (13%)	8	10	9, 27, 60, 74	1 (0%)
1	H	179/190 (94%)	0.72	23 (12%)	9	11	7, 24, 60, 80	0
All	All	724/760 (95%)	0.48	62 (8%)	18	21	3, 21, 56, 80	3 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	139	PRO	4.7
1	D	190	VAL	3.8
1	D	134	ASN	3.7
1	H	7	LYS	3.5
1	F	11	GLU	3.4
1	H	140	GLU	3.4
1	F	12	VAL	3.3
1	H	133	GLY	3.3
1	H	189	LEU	3.2
1	H	43	LEU	3.2
1	F	38	CYS	3.2
1	H	132	VAL	3.1
1	H	79	ARG	3.0
1	B	136	VAL	3.0
1	F	37	ASP	3.0
1	H	142	GLU	3.0
1	D	137	GLU	2.9
1	B	135	THR	2.9
1	H	138	LEU	2.9
1	H	37	ASP	2.8
1	B	137	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	9	LYS	2.8
1	H	141	GLU	2.8
1	H	39	PRO	2.8
1	F	42	GLN	2.7
1	H	38	CYS	2.7
1	B	138	LEU	2.7
1	H	36	LYS	2.7
1	H	143	ASN	2.6
1	D	38[A]	CYS	2.6
1	H	42	GLN	2.6
1	F	189	LEU	2.6
1	D	136	VAL	2.6
1	F	10	PRO	2.6
1	F	74	GLU	2.5
1	F	133	GLY	2.5
1	H	77	ASP	2.5
1	F	144	THR	2.5
1	F	14	GLU	2.4
1	H	11	GLU	2.4
1	B	7	LYS	2.4
1	D	135	THR	2.4
1	B	134	ASN	2.3
1	F	132	VAL	2.3
1	F	43	LEU	2.3
1	B	6	SER	2.3
1	H	171	GLU	2.3
1	H	35	ILE	2.2
1	H	74	GLU	2.2
1	F	40	SER	2.2
1	F	17	THR	2.2
1	F	25	LYS	2.1
1	F	50	LYS	2.1
1	F	141	GLU	2.1
1	F	44	ASP	2.1
1	D	138	LEU	2.1
1	H	44	ASP	2.1
1	B	132	VAL	2.1
1	F	13	VAL	2.0
1	B	58	PHE	2.0
1	F	75	ASN	2.0
1	F	143	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	117	F	204	41/41	0.63	0.22	26,60,91,100	0
5	MLI	H	212	7/7	0.76	0.18	31,42,60,66	0
3	117	H	204	41/41	0.77	0.20	24,48,72,77	0
6	ACY	D	211	4/4	0.78	0.17	33,34,40,45	0
7	SIN	F	208	8/8	0.78	0.18	29,35,43,49	0
5	MLI	F	210	7/7	0.79	0.14	29,36,39,41	0
7	SIN	H	209	8/8	0.81	0.13	29,40,43,44	0
4	NA	F	205	1/1	0.82	0.07	17,17,17,17	0
7	SIN	D	209	8/8	0.82	0.16	15,21,36,40	0
6	ACY	B	209	4/4	0.83	0.12	22,23,27,27	0
7	SIN	H	210	8/8	0.83	0.13	24,30,38,39	0
5	MLI	D	212	7/7	0.84	0.15	21,29,39,46	0
5	MLI	D	213	7/7	0.84	0.14	19,31,35,41	0
3	117	B	204	41/41	0.84	0.15	18,39,86,104	0
7	SIN	B	211	8/8	0.84	0.17	20,26,42,42	0
7	SIN	B	210	8/8	0.85	0.16	16,22,36,51	0
7	SIN	F	207	8/8	0.86	0.13	25,32,49,52	0
3	117	D	204	41/41	0.86	0.14	18,36,74,86	0
6	ACY	D	208	4/4	0.87	0.11	22,28,39,39	0
7	SIN	H	208	8/8	0.87	0.12	14,26,34,44	0
5	MLI	F	209	7/7	0.87	0.11	26,41,44,48	0
6	ACY	B	213	4/4	0.87	0.10	22,26,32,32	0
4	NA	H	206	1/1	0.88	0.07	17,17,17,17	0
8	FMT	B	212	3/3	0.88	0.11	29,33,35,37	0
6	ACY	H	211	4/4	0.89	0.12	19,28,29,29	0
3	117	B	205	41/41	0.89	0.11	10,21,62,75	0
3	117	D	205	41/41	0.90	0.12	5,20,56,67	0

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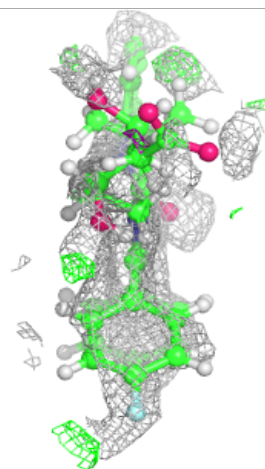
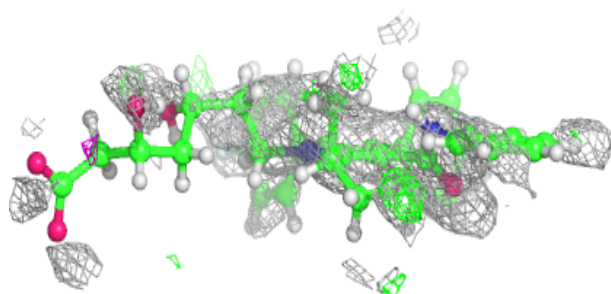
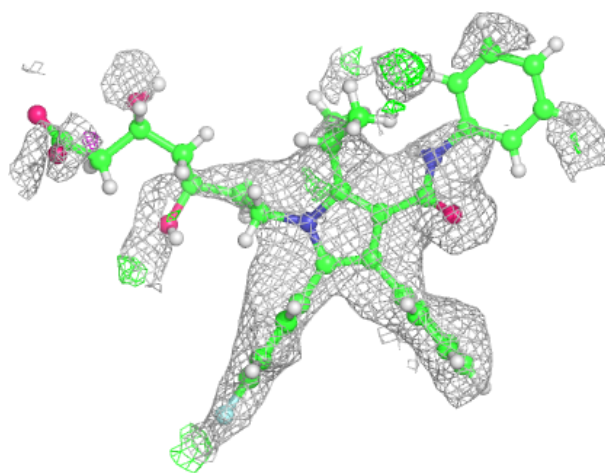
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MLI	B	208	7/7	0.90	0.12	19,32,44,47	0
5	MLI	B	214	7/7	0.90	0.13	17,31,32,40	0
7	SIN	H	207	8/8	0.90	0.09	18,23,34,41	0
2	CA	F	201	1/1	0.92	0.06	29,29,29,29	0
7	SIN	D	210	8/8	0.92	0.12	7,20,29,32	0
5	MLI	B	215	7/7	0.92	0.10	21,26,38,40	0
4	NA	H	205	1/1	0.93	0.05	14,14,14,14	0
4	NA	F	206	1/1	0.93	0.06	19,19,19,19	0
2	CA	B	203	1/1	0.94	0.03	10,10,10,10	0
4	NA	D	207	1/1	0.94	0.04	7,7,7,7	0
4	NA	D	206	1/1	0.95	0.03	4,4,4,4	0
2	CA	F	202	1/1	0.95	0.04	9,9,9,9	0
4	NA	B	207	1/1	0.95	0.04	13,13,13,13	0
2	CA	H	201	1/1	0.96	0.04	22,22,22,22	0
2	CA	F	203	1/1	0.96	0.03	12,12,12,12	0
4	NA	B	206	1/1	0.97	0.04	2,2,2,2	0
2	CA	B	201	1/1	0.97	0.04	11,11,11,11	0
2	CA	D	202	1/1	0.97	0.03	3,3,3,3	0
2	CA	H	203	1/1	0.97	0.02	9,9,9,9	0
2	CA	B	202	1/1	0.98	0.04	11,11,11,11	0
2	CA	D	201	1/1	0.98	0.03	9,9,9,9	0
2	CA	H	202	1/1	0.99	0.05	11,11,11,11	0
2	CA	D	203	1/1	0.99	0.01	6,6,6,6	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.

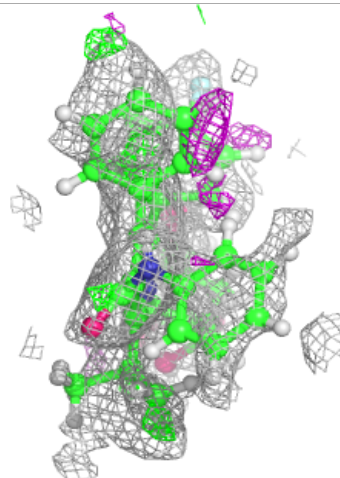
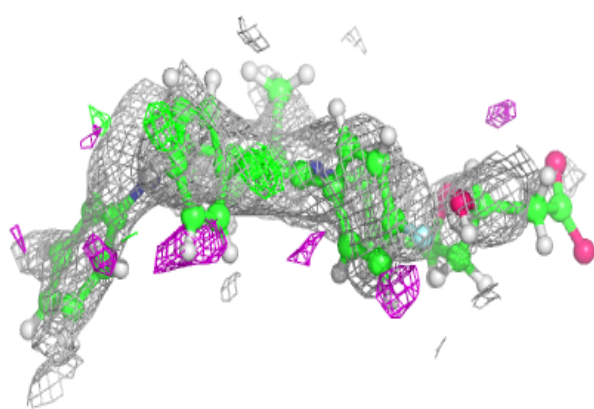
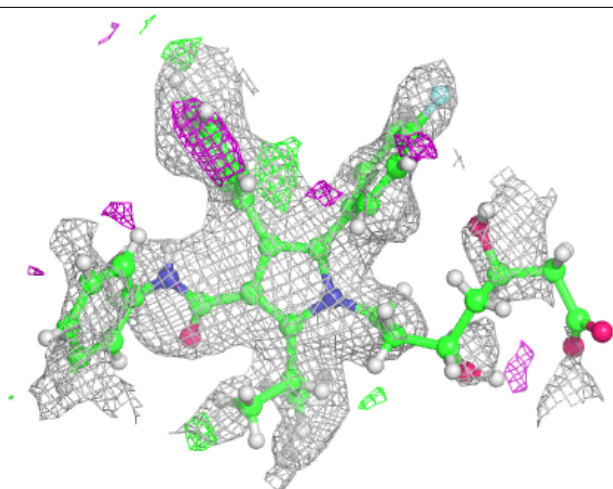
Electron density around 117 F 204:

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



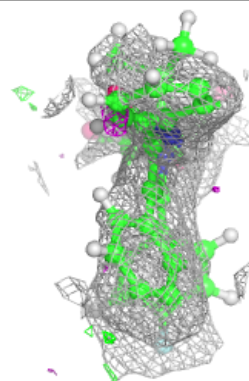
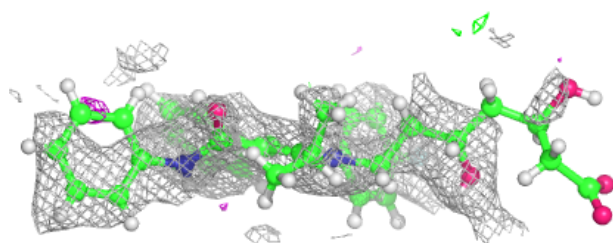
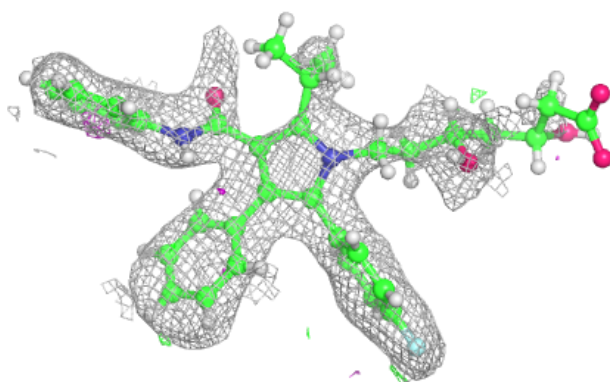
Electron density around 117 H 204:

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

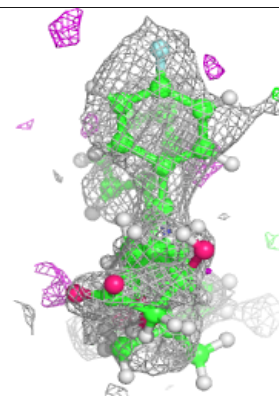
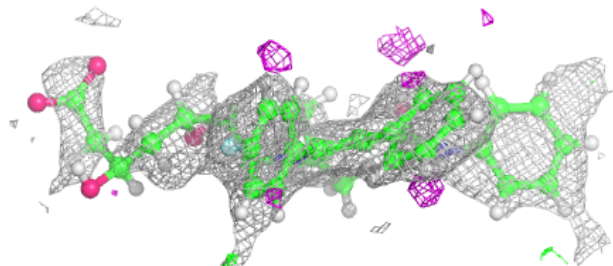
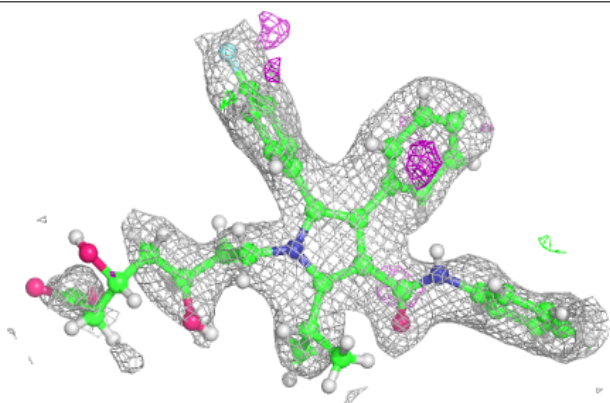


Electron density around 117 B 204:

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

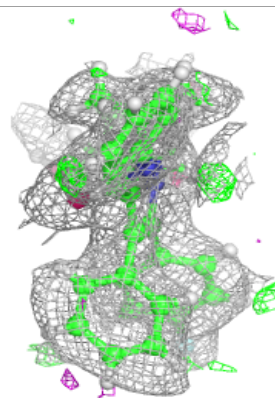
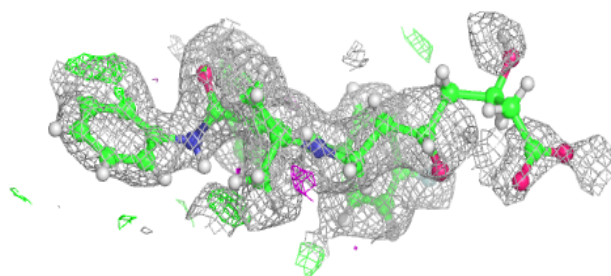
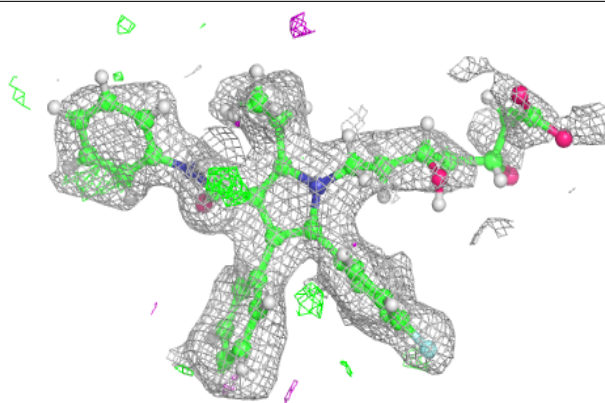
**Electron density around 117 D 204:**

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

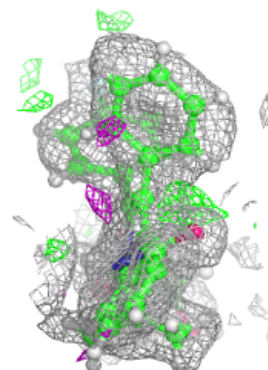
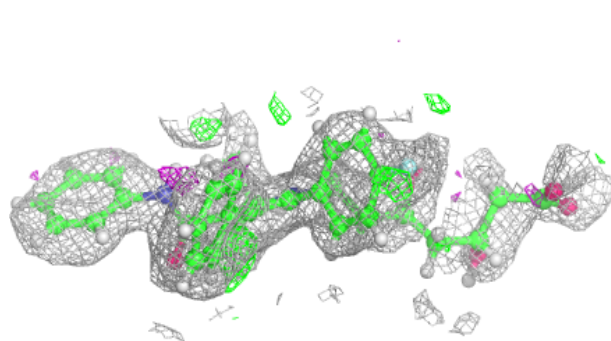
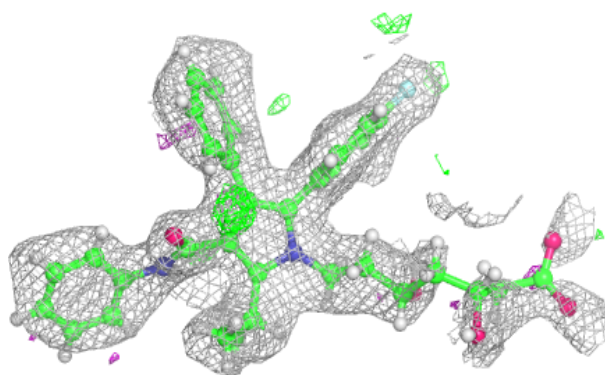


Electron density around 117 B 205:

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

**Electron density around 117 D 205:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.