



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 09:38 AM EST

PDB ID : 7HIH
Title : Group deposition for combi-soaks of Chikungunya virus nsP3 macrodomain – Crystal structure of Chikungunya virus nsP3 macrodomain in complex with Z1741976468, Z3219959731 and Z4628744292 (CHIKV_MacB-x1689)
Authors : Aschenbrenner, J.C.; Fairhead, M.; Godoy, A.S.; Balcomb, B.H.; Capkin, E.; Chandran, A.V.; Golding, M.; Koekemoer, L.; Lithgo, R.M.; Marples, P.G.; Ni, X.; Thompson, W.; Tomlinson, C.W.E.; Wild, C.; Winokan, M.; Xavier, M.-A.E.; Fearon, D.; von Delft, F.
Deposited on : 2024-10-02
Resolution : 1.46 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11

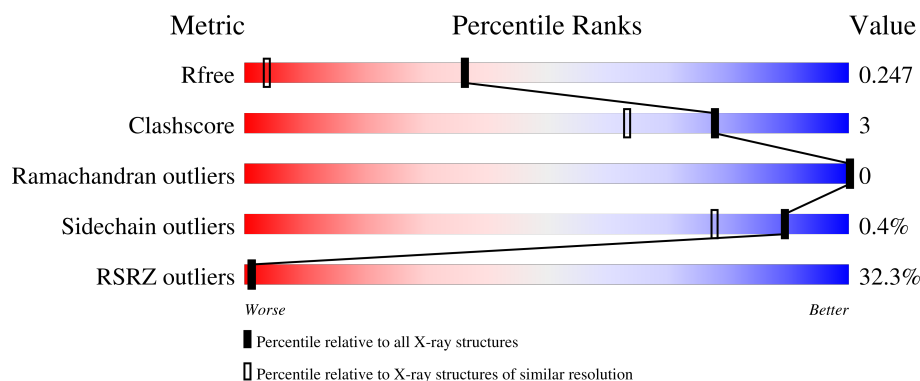
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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	1556 (1.46-1.46)
Clashscore	180529	1653 (1.46-1.46)
Ramachandran outliers	177936	1635 (1.46-1.46)
Sidechain outliers	177891	1635 (1.46-1.46)
RSRZ outliers	164620	1556 (1.46-1.46)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	163	<div> <div>24%</div> <div>98%</div> <div>.</div> </div>
1	B	163	<div> <div>39%</div> <div>94%</div> <div>6%</div> </div>
1	C	163	<div> <div>32%</div> <div>91%</div> <div>9%</div> </div>

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.40

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Mol	Chain	Length	Quality of chain
1	D	163	<div><div></div><div>33%</div><div></div><div>96%</div><div></div><div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5817 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	2	0
			1262	787	220	245	10			
1	B	163	Total	C	N	O	S	0	3	0
			1271	791	221	250	9			
1	C	163	Total	C	N	O	S	0	4	0
			1282	799	226	247	10			
1	D	159	Total	C	N	O	S	0	2	0
			1238	772	216	242	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8JUX6
A	-1	ALA	-	expression tag	UNP Q8JUX6
A	0	MET	-	expression tag	UNP Q8JUX6
A	77	THR	SER	conflict	UNP Q8JUX6
B	-2	GLY	-	expression tag	UNP Q8JUX6
B	-1	ALA	-	expression tag	UNP Q8JUX6
B	0	MET	-	expression tag	UNP Q8JUX6
B	77	THR	SER	conflict	UNP Q8JUX6
C	-2	GLY	-	expression tag	UNP Q8JUX6
C	-1	ALA	-	expression tag	UNP Q8JUX6
C	0	MET	-	expression tag	UNP Q8JUX6
C	77	THR	SER	conflict	UNP Q8JUX6
D	-2	GLY	-	expression tag	UNP Q8JUX6
D	-1	ALA	-	expression tag	UNP Q8JUX6
D	0	MET	-	expression tag	UNP Q8JUX6
D	77	THR	SER	conflict	UNP Q8JUX6

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

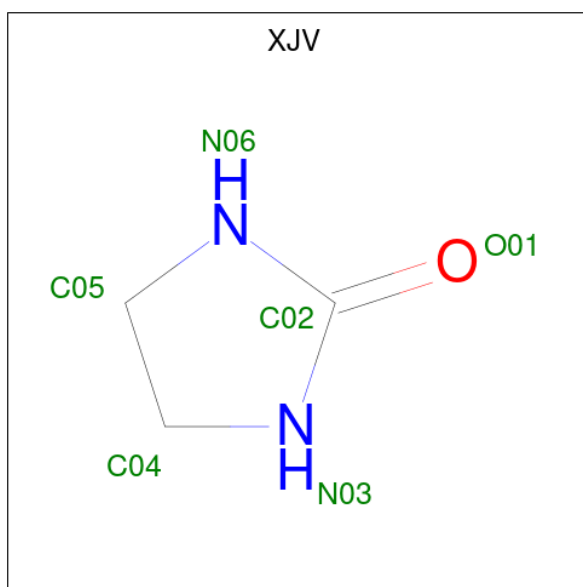


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

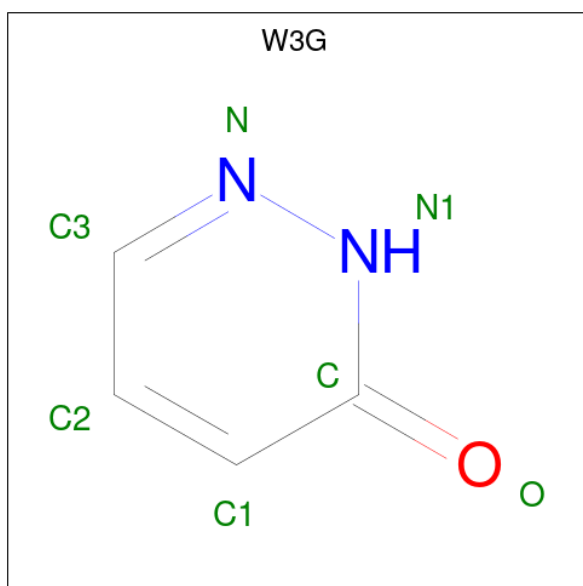
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is imidazolidin-2-one (three-letter code: XJV) (formula: C₃H₆N₂O) (labeled as "Ligand of Interest" by depositor).



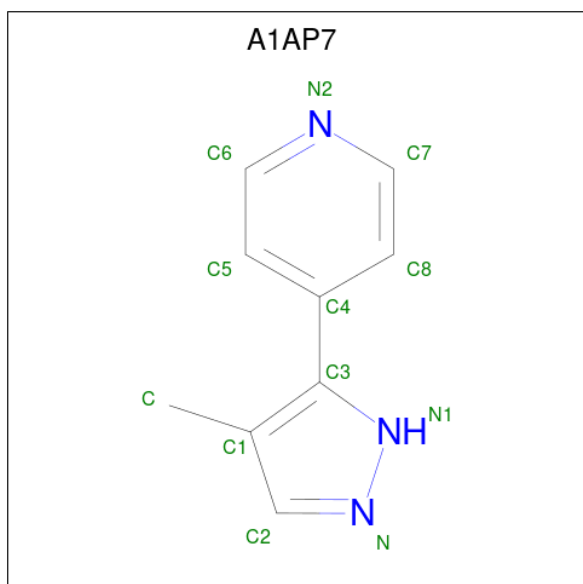
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			6	3	2	1		
5	B	1	Total	C	N	O	0	0
			6	3	2	1		
5	D	1	Total	C	N	O	0	0
			6	3	2	1		

- Molecule 6 is pyridazin-3(2H)-one (three-letter code: W3G) (formula: $C_4H_4N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			7	4	2	1		
6	A	1	Total	C	N	O	0	0
			7	4	2	1		
6	B	1	Total	C	N	O	0	0
			7	4	2	1		
6	C	1	Total	C	N	O	0	0
			7	4	2	1		
6	D	1	Total	C	N	O	0	0
			7	4	2	1		
6	D	1	Total	C	N	O	0	0
			7	4	2	1		

- Molecule 7 is 4-(4-methyl-1H-pyrazol-5-yl)pyridine (three-letter code: A1AP7) (formula: C₉H₉N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			12	9	3		
7	B	1	Total	C	N	0	0
			12	9	3		
7	C	1	Total	C	N	0	0
			12	9	3		
7	D	1	Total	C	N	0	0
			12	9	3		

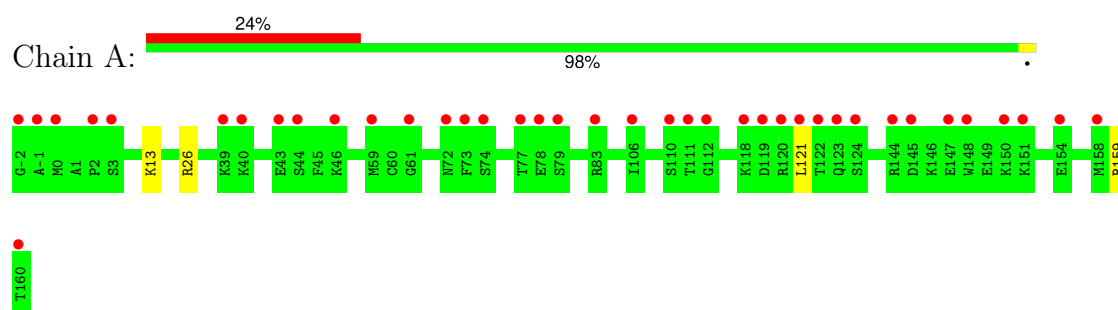
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	189	Total 189	O 189	0	0
8	B	111	Total 111	O 111	0	0
8	C	145	Total 145	O 145	0	0
8	D	141	Total 141	O 141	0	0

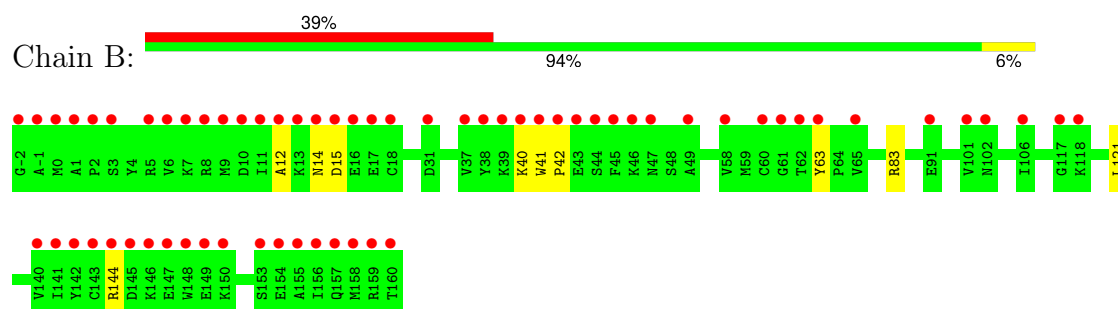
3 Residue-property plots [i](#)

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. 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. 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.

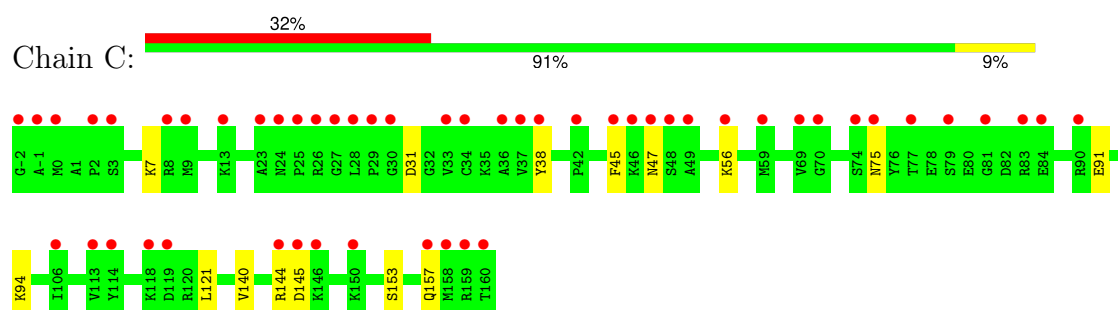
- Molecule 1: Non-structural protein 3



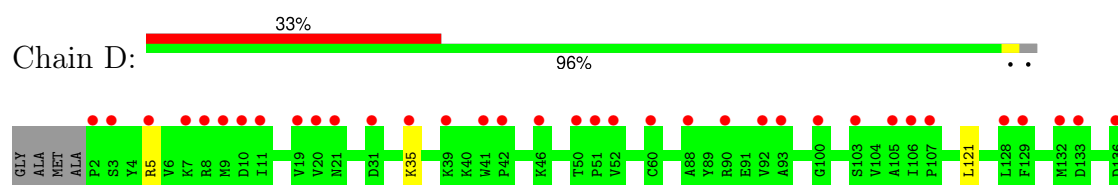
- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3



A137	D138	V139	V140	I141	Y142	C143	R144	D145	K146	E147	W148	E149	K150	S153	E154	A155	I156	Q157	M158	R159	T160
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	87.28Å 87.28Å 85.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.91 – 1.46 38.91 – 1.46	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.91-1.46) 97.0 (38.91-1.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.224 0.224 , 0.247	Depositor DCC
R_{free} test set	6312 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.028 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5817	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9015e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W3G, XJV, A1AP7, DMS, TRS, CL

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	0.79	0/1285	0.86	2/1739 (0.1%)
1	B	0.82	0/1294	0.88	0/1752
1	C	0.77	1/1305 (0.1%)	0.83	0/1764
1	D	0.76	0/1261	0.83	0/1707
All	All	0.79	1/5145 (0.0%)	0.85	2/6962 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	91	GLU	CD-OE1	5.56	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	26	ARG	NE-CZ-NH2	-5.17	117.71	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	1262	0	1256	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1271	0	1256	12	0
1	C	1282	0	1280	10	0
1	D	1238	0	1228	3	0
2	A	8	0	12	2	0
2	B	4	0	6	0	0
2	C	20	0	30	1	0
2	D	8	0	12	0	0
3	A	8	0	12	0	0
3	B	8	0	12	1	0
3	D	8	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	D	6	0	0	0	0
6	A	14	0	0	0	0
6	B	7	0	0	0	0
6	C	7	0	0	0	0
6	D	14	0	0	0	0
7	A	12	0	0	0	0
7	B	12	0	0	1	0
7	C	12	0	0	0	0
7	D	12	0	0	0	0
8	A	189	0	0	2	0
8	B	111	0	0	0	0
8	C	145	0	0	2	0
8	D	141	0	0	3	0
All	All	5817	0	5116	28	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 3.

All (28) 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:C:47:ASN:O	1:C:56:LYS:NZ	1.99	0.95
1:B:14:ASN:OD1	1:B:63:TYR:OH	1.98	0.81
1:D:35:LYS:NZ	8:D:301:HOH:O	2.20	0.74
1:B:12:ALA:HB1	1:B:40:LYS:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ALA:HA	1:B:41:TRP:CZ3	2.37	0.59
2:A:201:DMS:H12	8:A:449:HOH:O	2.03	0.58
1:C:144:ARG:HD2	1:C:145:ASP:OD2	2.05	0.56
1:C:31:ASP:H	2:C:204:DMS:H13	1.71	0.55
1:C:121:LEU:C	1:C:121:LEU:HD23	2.26	0.55
1:A:13:LYS:CD	1:B:42:PRO:HG3	2.37	0.54
1:B:83:ARG:HD3	3:B:205:TRS:H22	1.91	0.53
1:B:144:ARG:HG2	7:B:206:A1AP7:C8	2.42	0.50
1:C:94:LYS:NZ	8:C:304:HOH:O	2.45	0.49
1:A:13:LYS:HD3	1:B:42:PRO:HG3	1.96	0.48
1:D:121:LEU:C	1:D:121:LEU:HD23	2.34	0.48
2:A:203:DMS:H11	8:A:420:HOH:O	2.14	0.48
1:B:14:ASN:CG	1:B:63:TYR:OH	2.54	0.46
1:C:7:LYS:HD3	1:C:140:VAL:HG11	1.97	0.46
1:B:12:ALA:HA	1:B:41:TRP:CH2	2.50	0.45
1:A:13:LYS:HD2	1:B:42:PRO:HG3	1.97	0.45
1:B:14:ASN:ND2	1:B:63:TYR:OH	2.49	0.45
1:C:38:TYR:HA	1:C:45:PHE:CE1	2.52	0.45
1:A:121:LEU:C	1:A:121:LEU:HD23	2.39	0.43
1:C:153:SER:O	1:C:157:GLN:HG2	2.18	0.43
1:C:56:LYS:NZ	8:C:307:HOH:O	2.53	0.42
1:D:5:ARG:HD3	8:D:307:HOH:O	2.20	0.42
1:B:121:LEU:C	1:B:121:LEU:HD23	2.42	0.40
1:C:94:LYS:HD2	8:D:391:HOH:O	2.20	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	163/163 (100%)	162 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	164/163 (101%)	161 (98%)	3 (2%)	0	100	100
1	C	165/163 (101%)	163 (99%)	2 (1%)	0	100	100
1	D	159/163 (98%)	159 (100%)	0	0	100	100
All	All	651/652 (100%)	645 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	136/134 (102%)	136 (100%)	0	100	100
1	B	137/134 (102%)	136 (99%)	1 (1%)	81	62
1	C	138/134 (103%)	137 (99%)	1 (1%)	81	62
1	D	135/134 (101%)	135 (100%)	0	100	100
All	All	546/536 (102%)	544 (100%)	2 (0%)	89	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	ASP
1	C	75	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 [i](#)

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 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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	DMS	C	208	-	3,3,3	0.21	0	3,3,3	0.06	0
6	W3G	A	207	-	7,7,7	0.63	0	8,8,8	0.81	0
2	DMS	C	204	-	3,3,3	0.18	0	3,3,3	0.06	0
6	W3G	A	209	-	7,7,7	0.77	0	8,8,8	0.72	0
3	TRS	B	205	-	7,7,7	0.19	0	9,9,9	0.60	0
2	DMS	C	203	-	3,3,3	0.31	0	3,3,3	0.23	0
6	W3G	D	206	-	7,7,7	0.57	0	8,8,8	0.69	0
6	W3G	D	208	-	7,7,7	0.57	0	8,8,8	0.67	0
6	W3G	C	206	-	7,7,7	0.58	0	8,8,8	0.75	0
3	TRS	A	202	-	7,7,7	0.38	0	9,9,9	0.57	0
2	DMS	C	205	-	3,3,3	0.25	0	3,3,3	0.12	0
2	DMS	A	201	-	3,3,3	0.26	0	3,3,3	0.09	0
2	DMS	D	203	-	3,3,3	0.33	0	3,3,3	0.06	0
2	DMS	D	202	-	3,3,3	0.57	0	3,3,3	0.23	0
2	DMS	A	203	-	3,3,3	0.22	0	3,3,3	0.27	0
7	A1AP7	C	207	-	12,13,13	0.51	0	12,17,17	0.34	0
3	TRS	D	201	-	7,7,7	0.22	0	9,9,9	0.36	0
2	DMS	C	201	-	3,3,3	0.22	0	3,3,3	0.16	0
7	A1AP7	B	206	-	12,13,13	0.53	0	12,17,17	0.35	0
7	A1AP7	D	207	-	12,13,13	0.55	0	12,17,17	0.38	0
5	XJV	A	206	-	6,6,6	0.18	0	7,7,7	0.29	0
2	DMS	B	201	-	3,3,3	0.15	0	3,3,3	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	W3G	B	204	-	7,7,7	0.52	0	8,8,8	0.64	0
5	XJV	D	205	-	6,6,6	0.15	0	7,7,7	0.29	0
7	A1AP7	A	208	-	12,13,13	0.60	0	12,17,17	0.44	0
5	XJV	B	203	-	6,6,6	0.15	0	7,7,7	0.28	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
6	W3G	A	209	-	-	-	0/1/1/1
3	TRS	B	205	-	-	8/9/9/9	-
6	W3G	C	206	-	-	-	0/1/1/1
3	TRS	A	202	-	-	3/9/9/9	-
6	W3G	D	206	-	-	-	0/1/1/1
6	W3G	D	208	-	-	-	0/1/1/1
7	A1AP7	B	206	-	-	2/4/4/4	0/2/2/2
7	A1AP7	D	207	-	-	2/4/4/4	0/2/2/2
6	W3G	A	207	-	-	-	0/1/1/1
5	XJV	A	206	-	-	-	0/1/1/1
7	A1AP7	C	207	-	-	0/4/4/4	0/2/2/2
6	W3G	B	204	-	-	-	0/1/1/1
5	XJV	D	205	-	-	-	0/1/1/1
3	TRS	D	201	-	-	4/9/9/9	-
7	A1AP7	A	208	-	-	2/4/4/4	0/2/2/2
5	XJV	B	203	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	205	TRS	C1-C-C2-O2
3	B	205	TRS	C3-C-C2-O2
3	B	205	TRS	N-C-C2-O2
3	B	205	TRS	C1-C-C3-O3
3	B	205	TRS	C2-C-C3-O3

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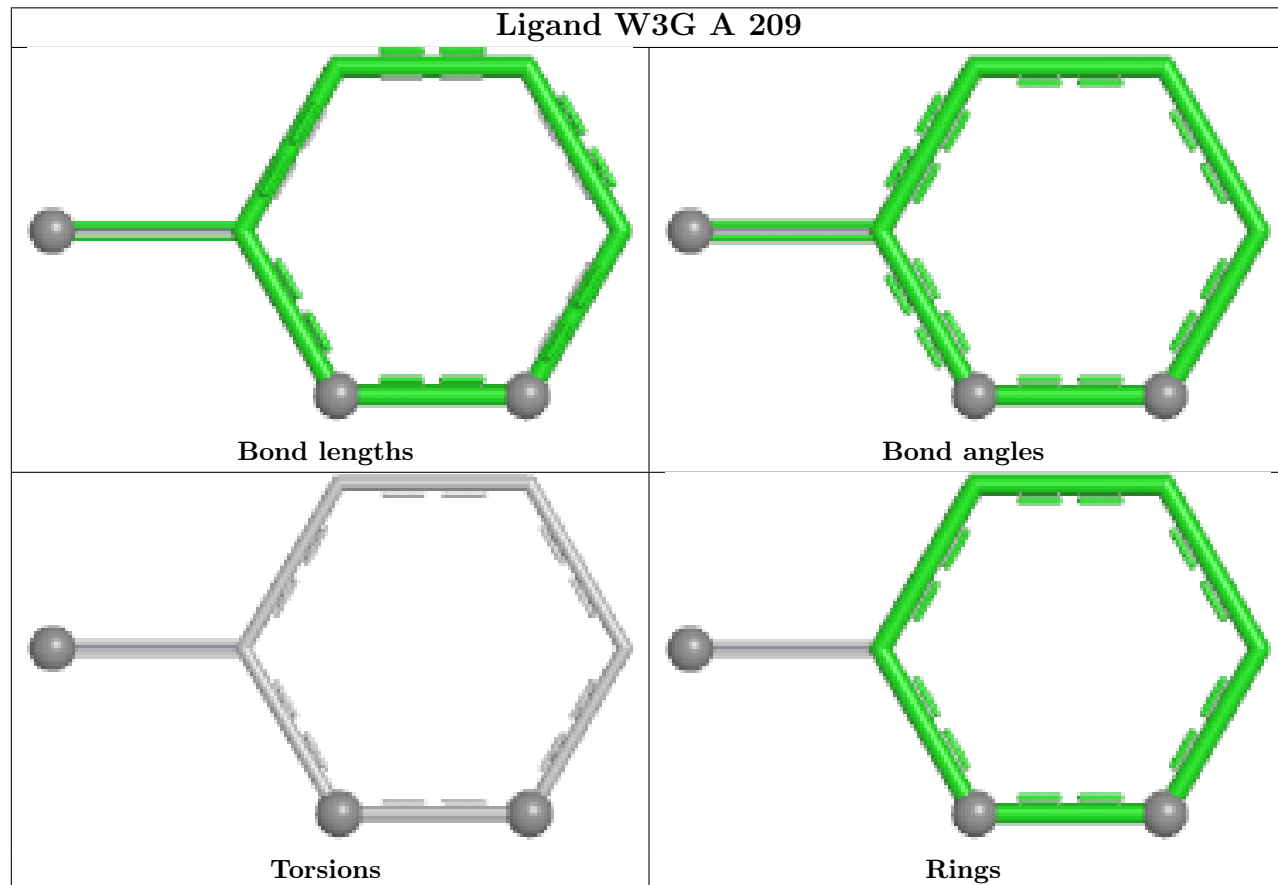
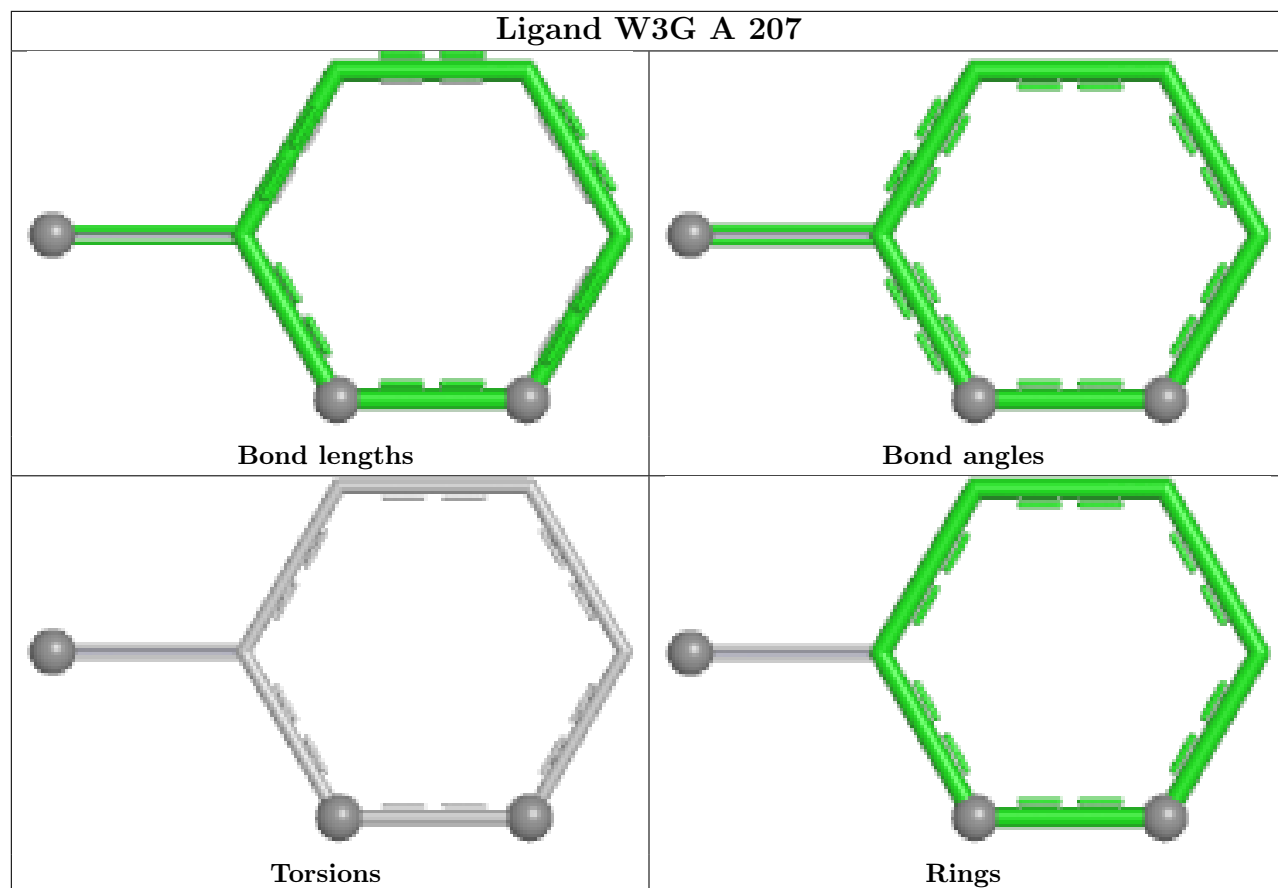
Mol	Chain	Res	Type	Atoms
3	B	205	TRS	N-C-C3-O3
7	B	206	A1AP7	C1-C3-C4-C5
7	B	206	A1AP7	C1-C3-C4-C8
7	D	207	A1AP7	C1-C3-C4-C5
3	D	201	TRS	C1-C-C3-O3
7	A	208	A1AP7	C1-C3-C4-C5
7	A	208	A1AP7	C1-C3-C4-C8
7	D	207	A1AP7	C1-C3-C4-C8
3	A	202	TRS	N-C-C3-O3
3	D	201	TRS	N-C-C3-O3
3	A	202	TRS	C1-C-C3-O3
3	D	201	TRS	C2-C-C3-O3
3	A	202	TRS	C2-C-C3-O3
3	B	205	TRS	C3-C-C1-O1
3	D	201	TRS	C3-C-C1-O1
3	B	205	TRS	N-C-C1-O1

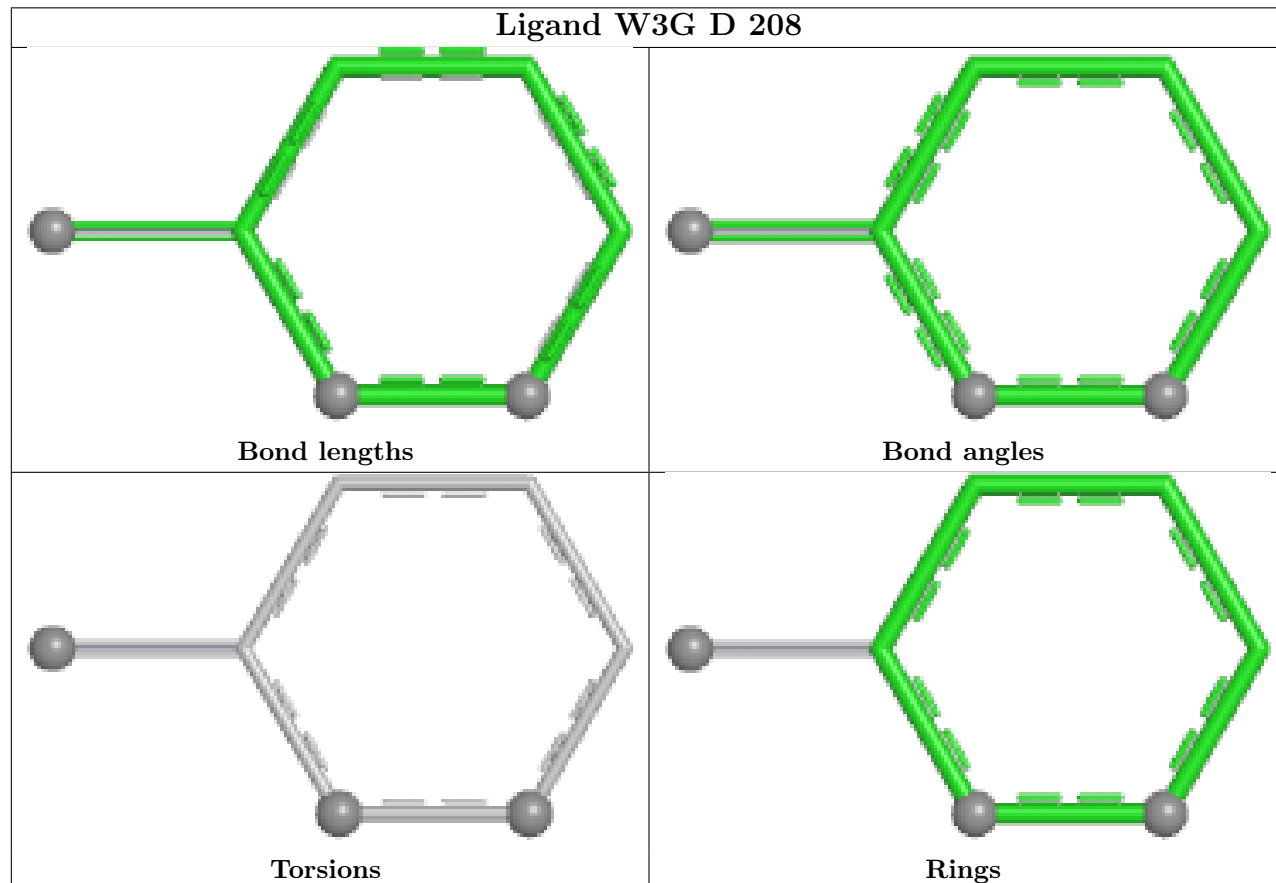
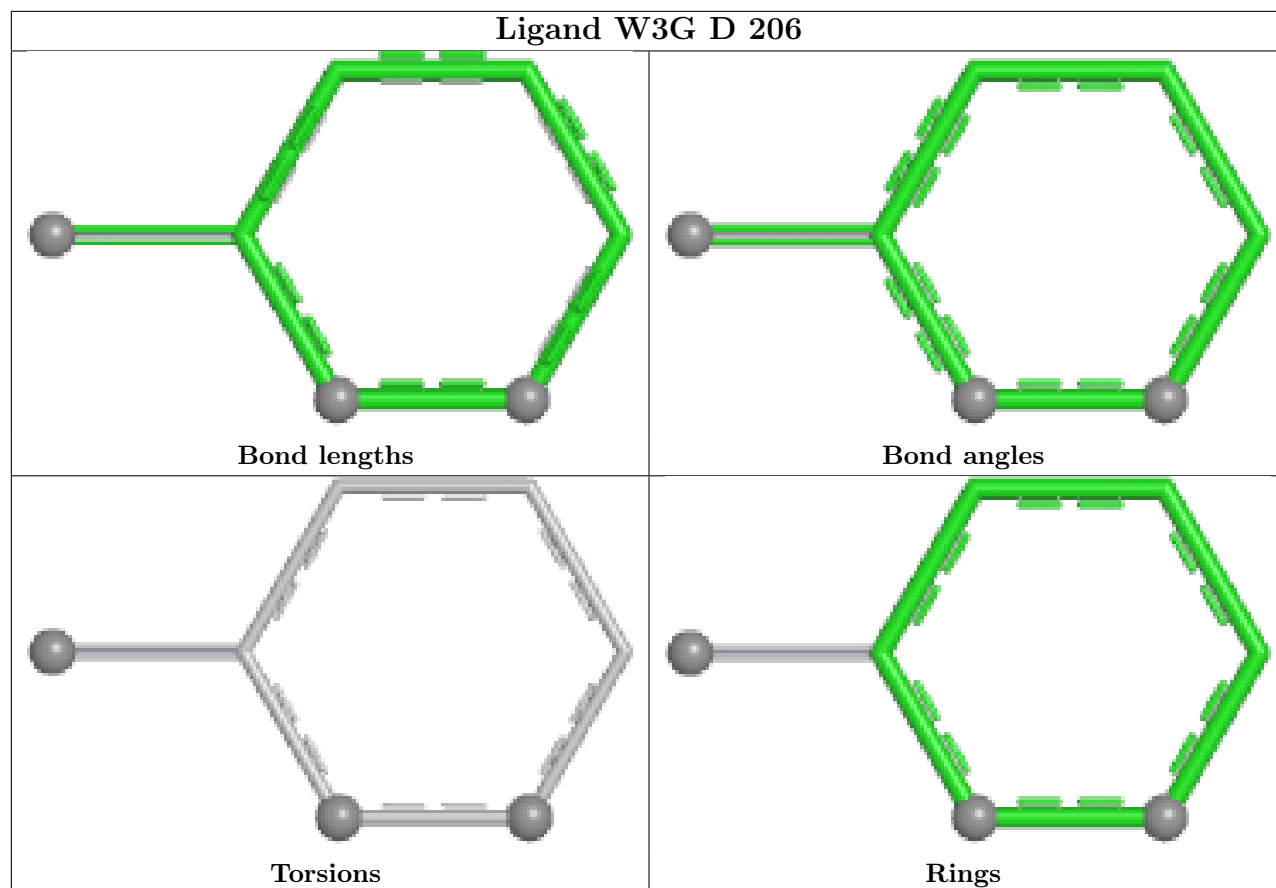
There are no ring outliers.

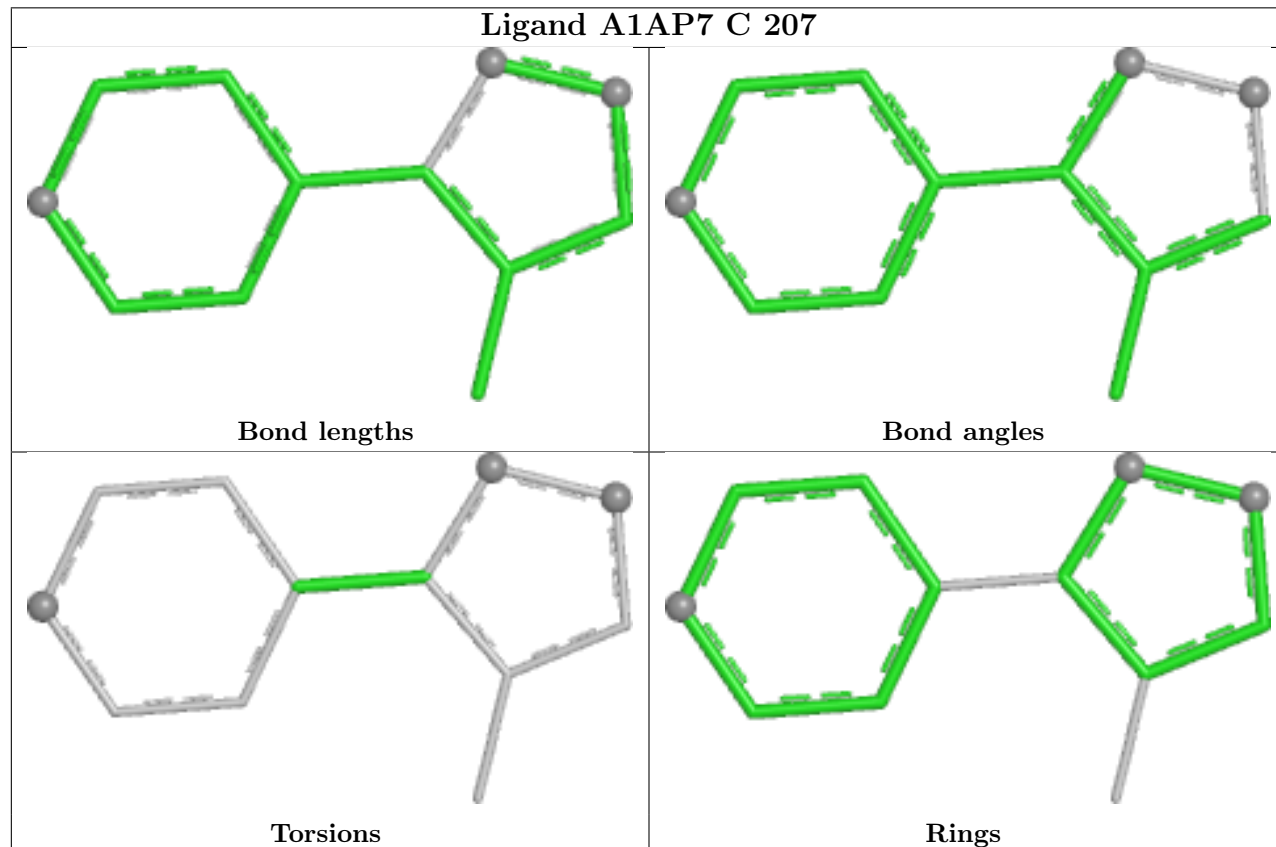
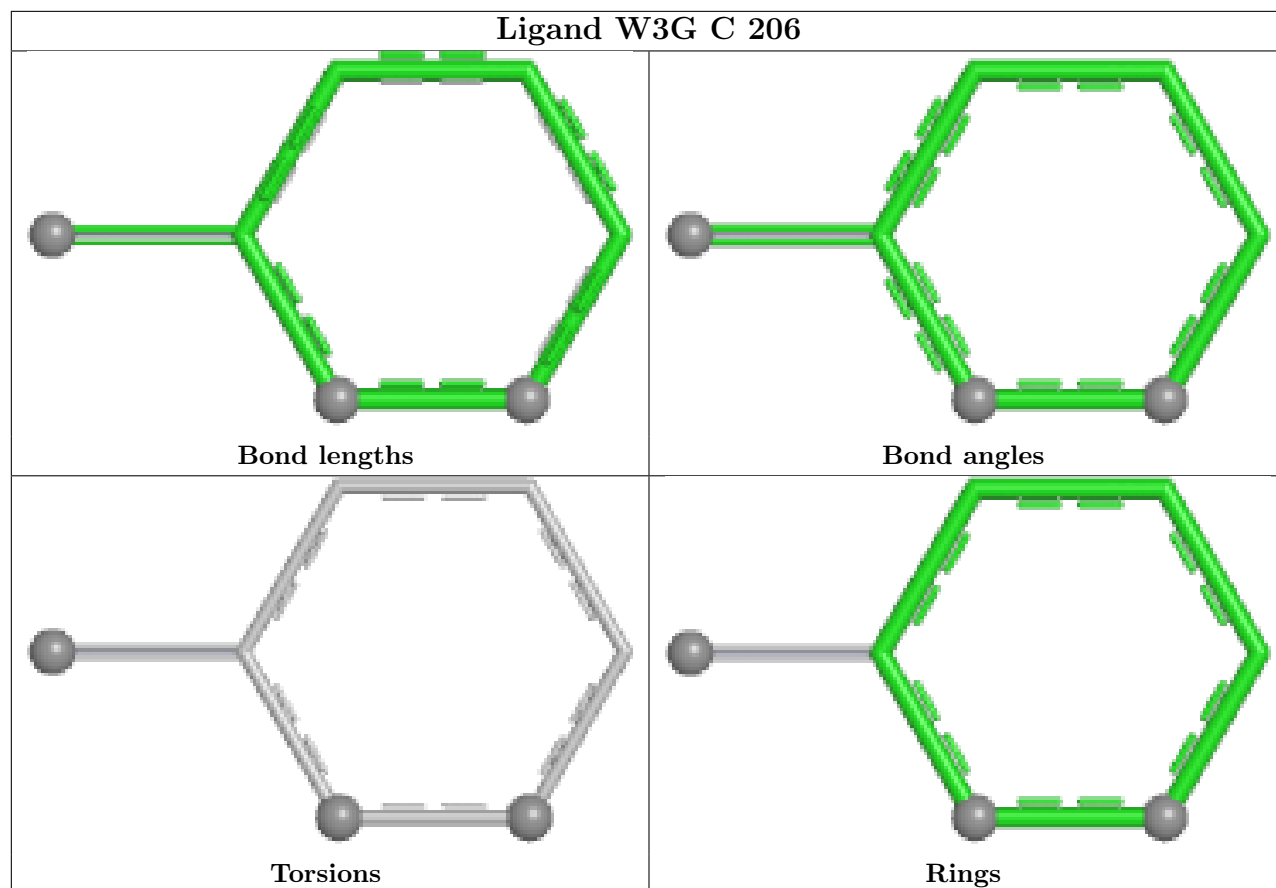
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	204	DMS	1	0
3	B	205	TRS	1	0
2	A	201	DMS	1	0
2	A	203	DMS	1	0
7	B	206	A1AP7	1	0

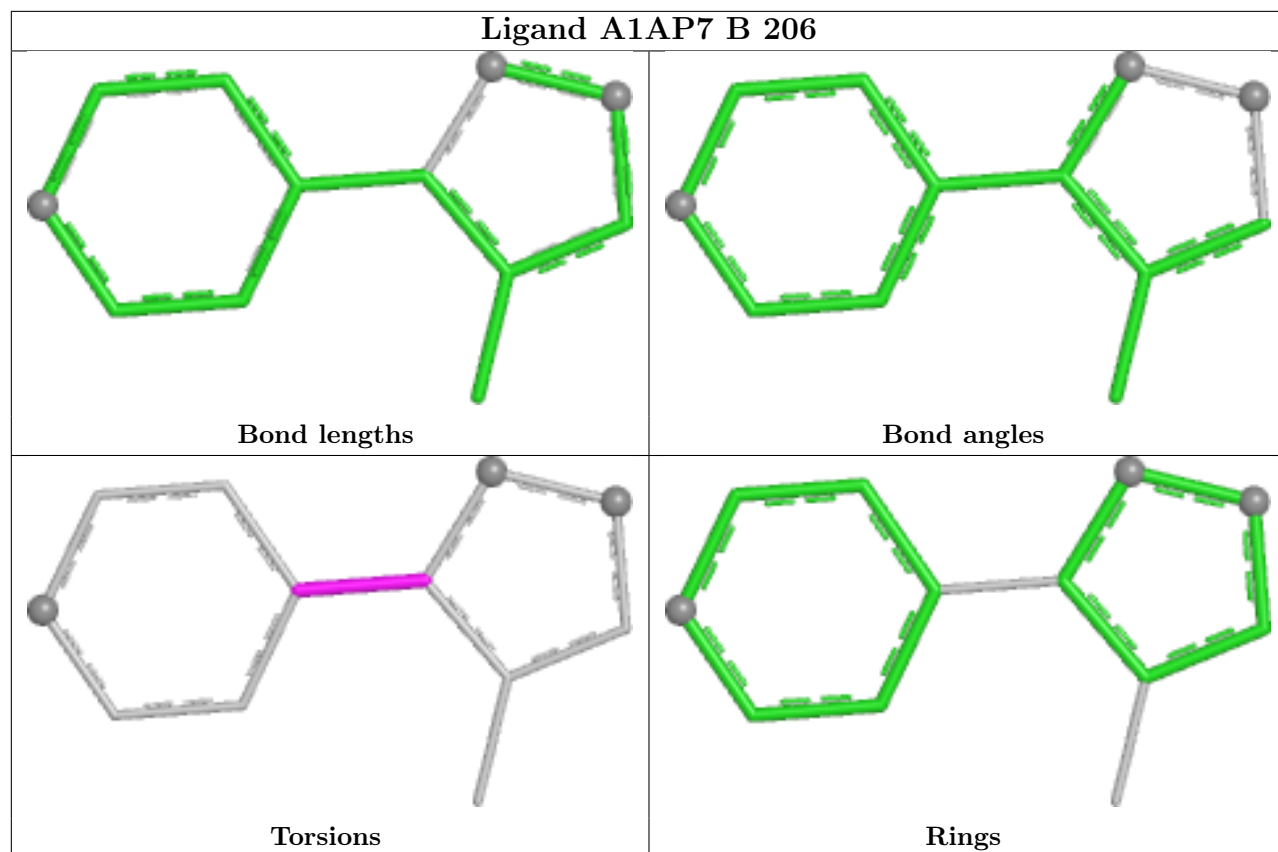
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



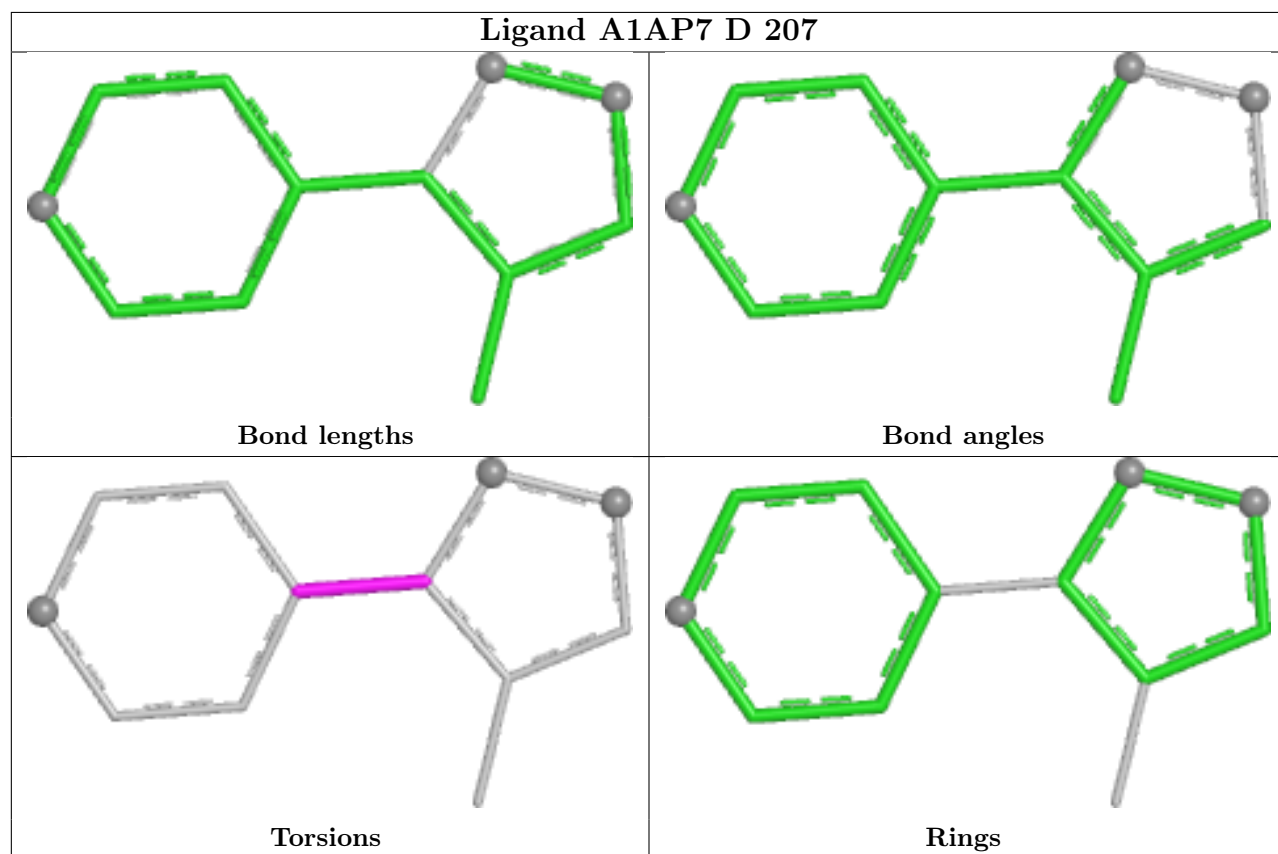




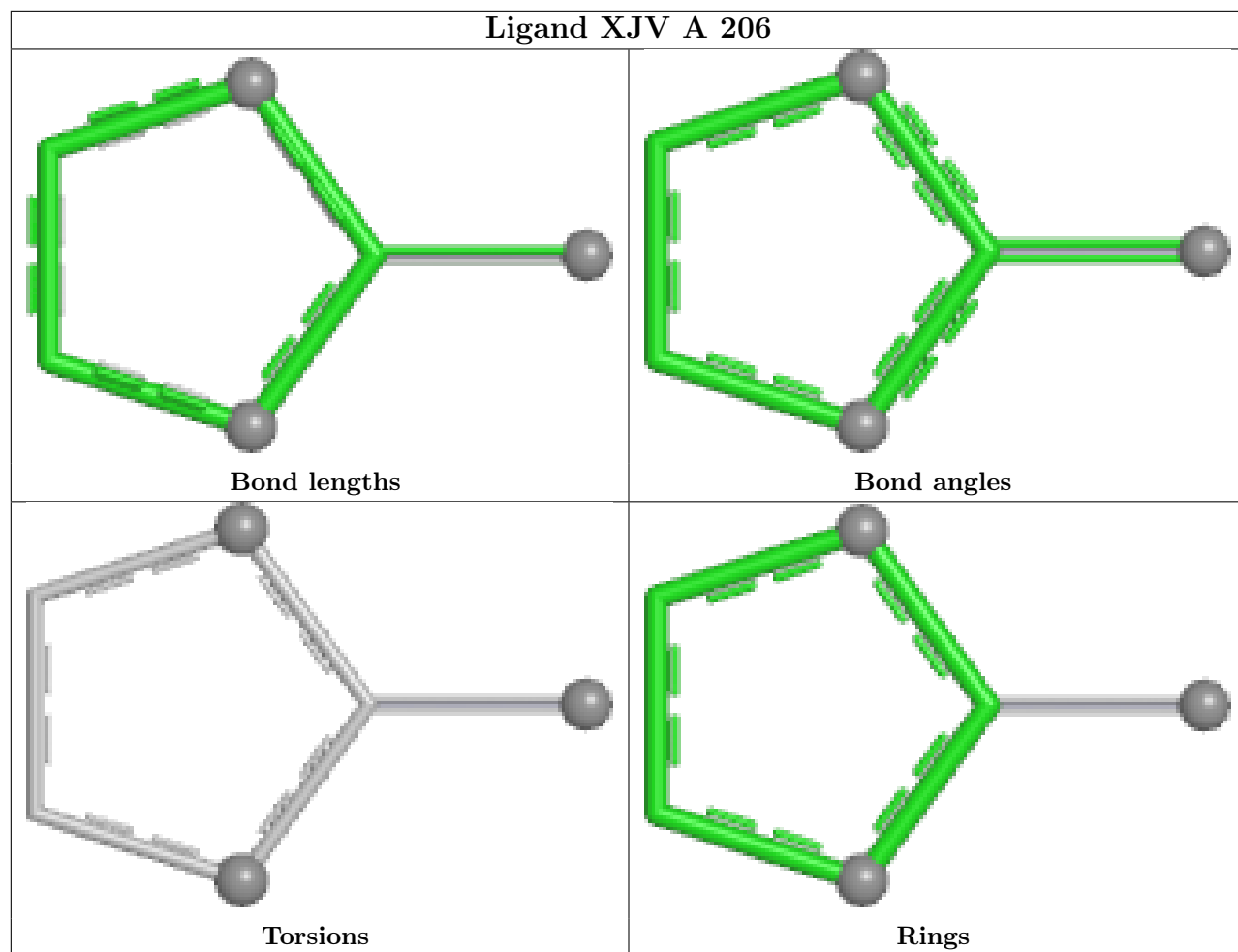
Ligand A1AP7 B 206

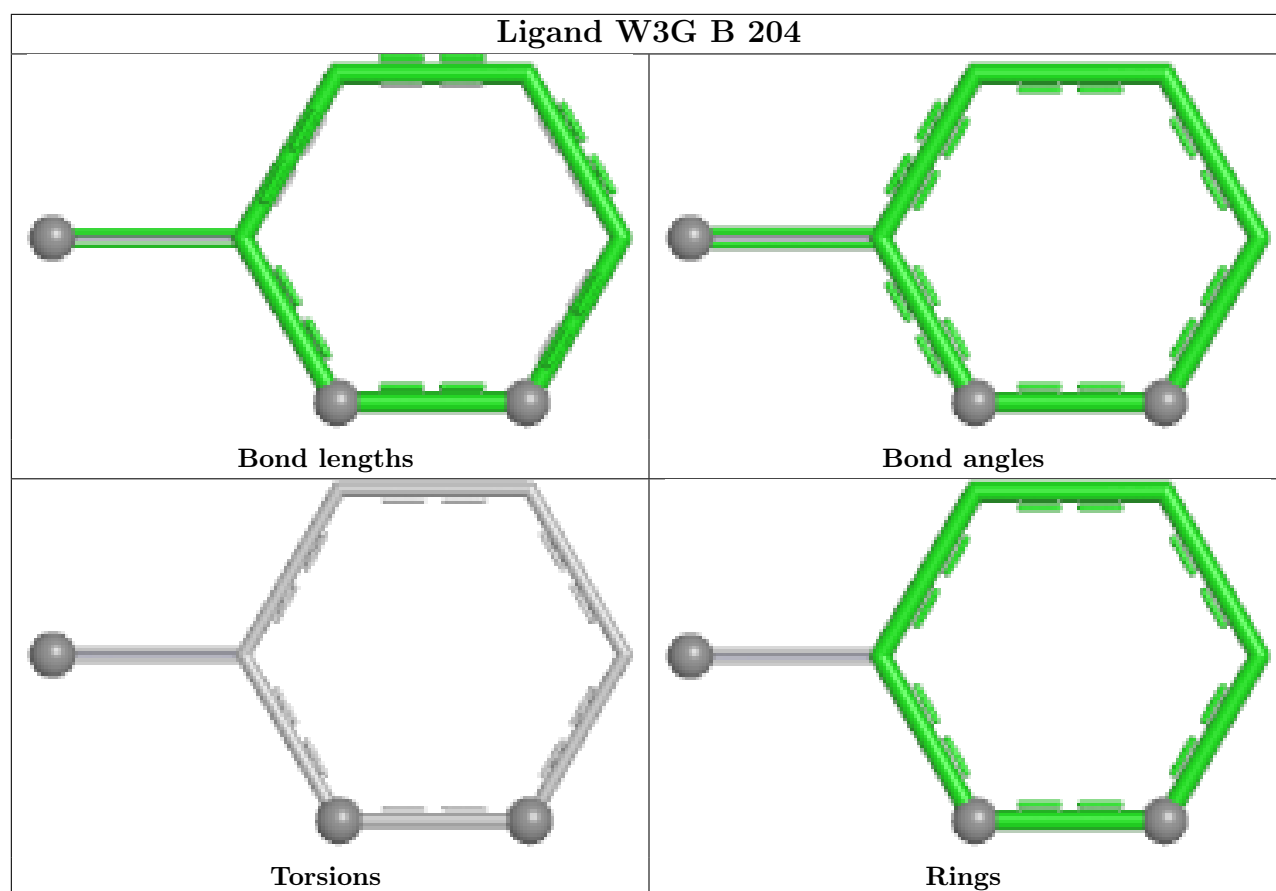


Ligand A1AP7 D 207

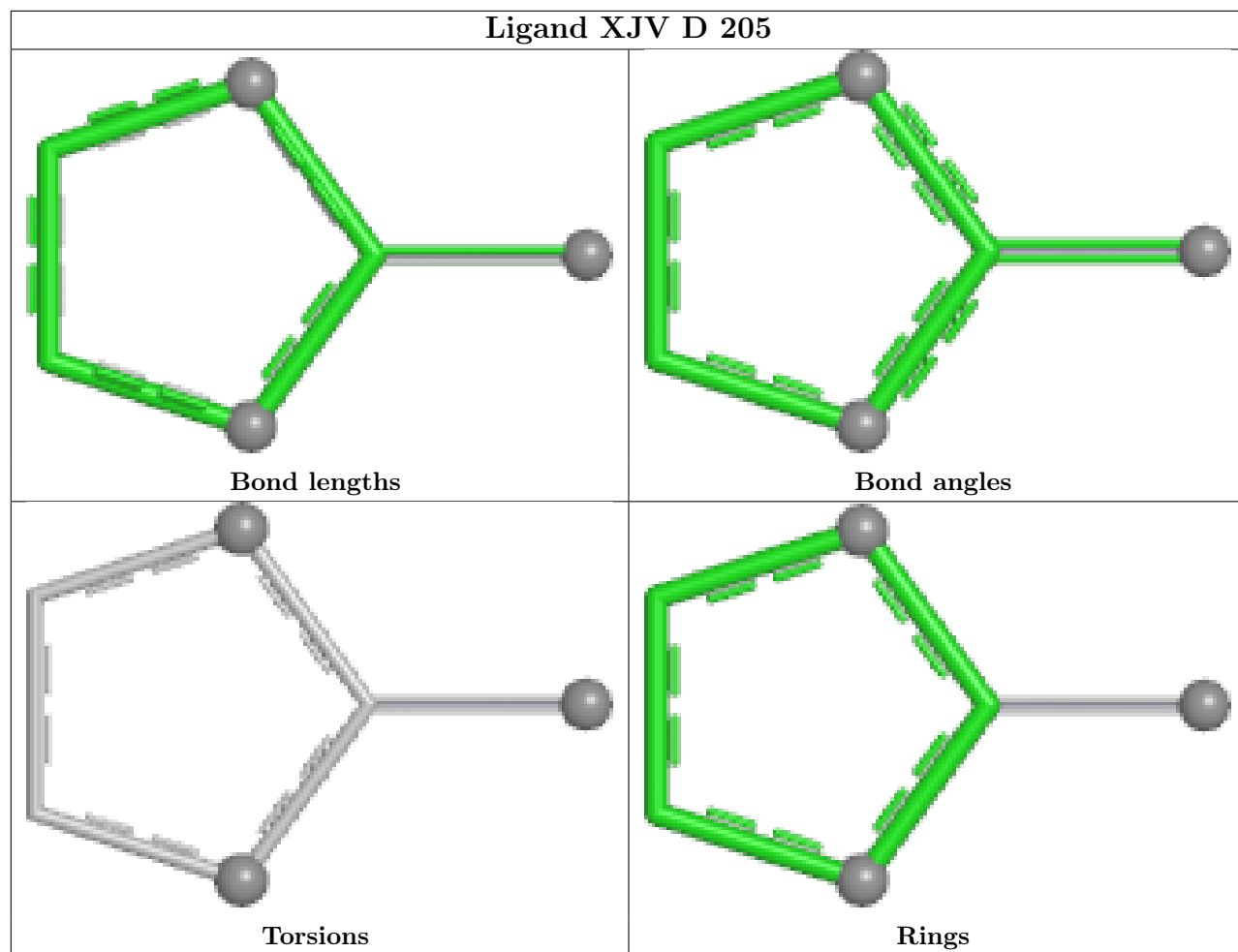


Ligand XJV A 206

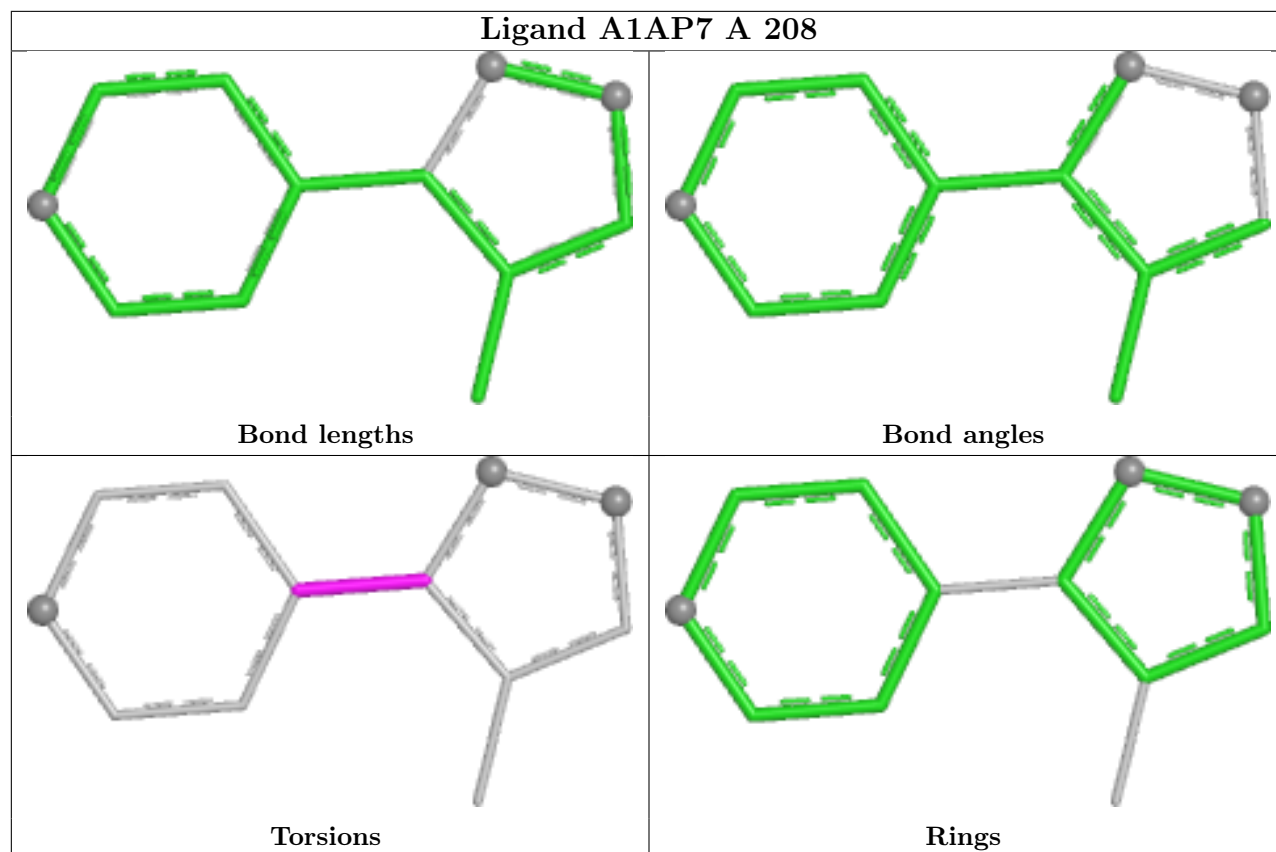


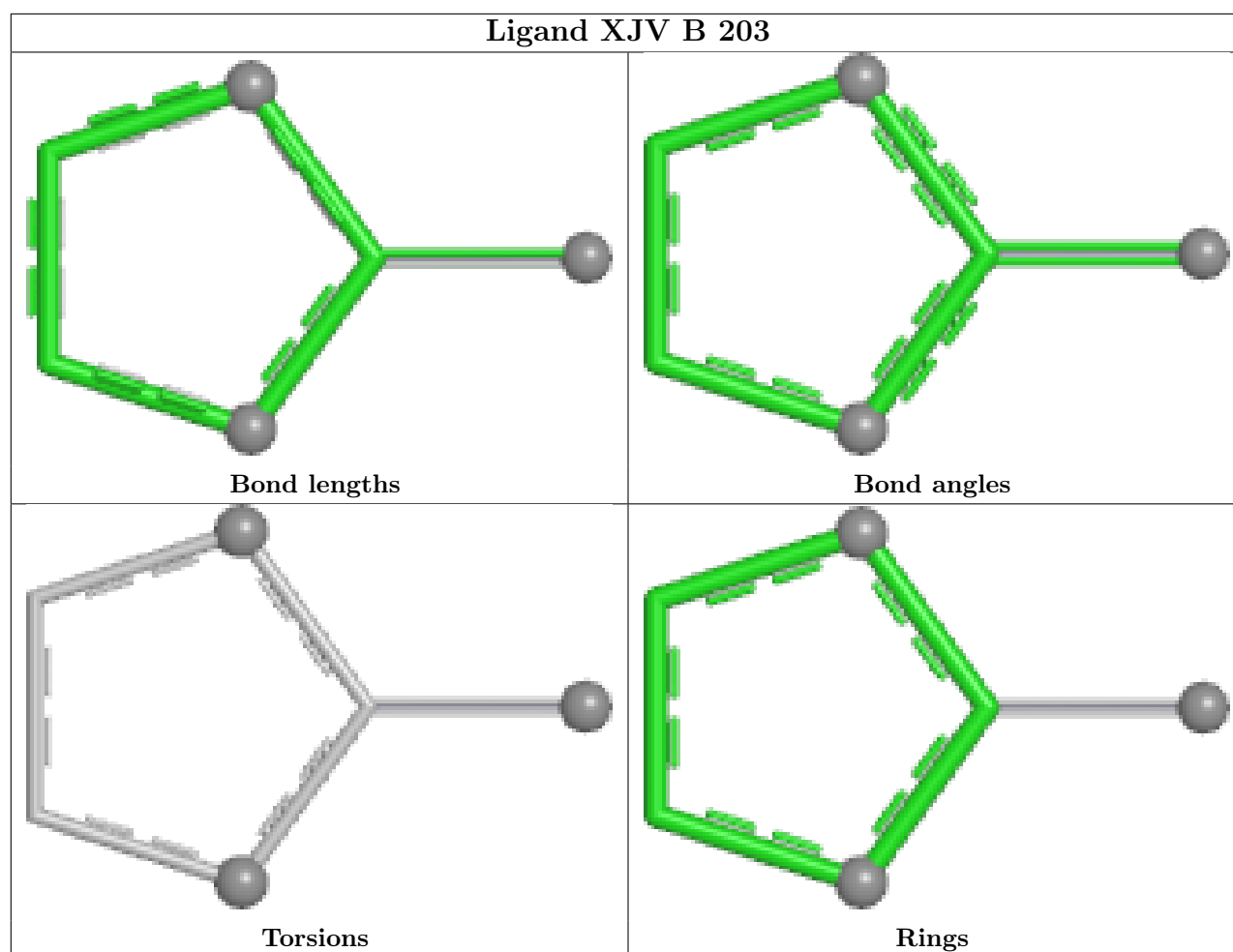


Ligand XJV D 205



Ligand A1AP7 A 208





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 ⓘ

Warning: The R factor obtained from EDS is 0.2473, which does not match the depositor's R factor of 0.18952. Please interpret the results in this section carefully.

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	163/163 (100%)	1.05	39 (23%)	2 2	4, 19, 31, 69	37 (22%)
1	B	163/163 (100%)	2.01	64 (39%)	1 1	7, 25, 37, 53	50 (30%)
1	C	163/163 (100%)	1.50	52 (31%)	1 1	5, 23, 40, 59	43 (26%)
1	D	159/163 (97%)	1.71	54 (33%)	1 1	7, 24, 38, 56	45 (28%)
All	All	648/652 (99%)	1.57	209 (32%)	1 1	4, 23, 38, 69	175 (27%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106[A]	ILE	9.7
1	C	106[A]	ILE	9.7
1	B	6	VAL	8.2
1	C	-1	ALA	8.1
1	B	145[A]	ASP	8.0
1	B	11	ILE	7.5
1	B	142	TYR	7.3
1	D	128	LEU	7.1
1	B	12	ALA	6.8
1	B	106[A]	ILE	6.8
1	B	60	CYS	6.4
1	D	92	VAL	6.4
1	C	28	LEU	6.3
1	B	-1	ALA	6.2
1	D	142	TYR	6.2
1	C	113	VAL	6.1
1	A	121	LEU	6.1
1	B	148	TRP	6.0
1	D	106[A]	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	13[A]	LYS	5.9
1	B	14	ASN	5.9
1	C	-2	GLY	5.8
1	B	41	TRP	5.8
1	B	156	ILE	5.5
1	D	139	VAL	5.5
1	A	79	SER	5.5
1	A	112	GLY	5.5
1	D	93	ALA	5.5
1	D	11	ILE	5.4
1	A	148	TRP	5.4
1	C	9	MET	5.3
1	D	143	CYS	5.3
1	A	0	MET	5.3
1	B	143	CYS	5.3
1	A	77	THR	5.2
1	D	88	ALA	5.2
1	A	111	THR	5.2
1	D	3[A]	SER	5.2
1	B	15	ASP	5.2
1	D	141	ILE	5.1
1	D	155	ALA	5.1
1	A	61	GLY	5.1
1	B	155	ALA	5.0
1	B	9	MET	5.0
1	D	20	VAL	5.0
1	B	0	MET	5.0
1	C	29	PRO	4.9
1	B	38	TYR	4.8
1	B	158	MET	4.8
1	C	25	PRO	4.8
1	A	122	THR	4.7
1	B	10	ASP	4.7
1	D	52	VAL	4.7
1	B	3	SER	4.7
1	D	9	MET	4.7
1	A	3	SER	4.7
1	B	160	THR	4.6
1	C	59[A]	MET	4.6
1	B	118	LYS	4.6
1	D	129	PHE	4.6
1	C	49	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	160	THR	4.5
1	C	160	THR	4.5
1	B	146	LYS	4.5
1	B	147	GLU	4.5
1	A	74	SER	4.5
1	C	27	GLY	4.5
1	C	75	ASN	4.4
1	C	0	MET	4.4
1	B	5	ARG	4.4
1	A	83	ARG	4.3
1	B	141	ILE	4.3
1	D	153	SER	4.3
1	A	73	PHE	4.2
1	D	19	VAL	4.2
1	D	158	MET	4.2
1	B	153	SER	4.2
1	D	107	PRO	4.2
1	B	1	ALA	4.2
1	D	156	ILE	4.2
1	B	18	CYS	4.1
1	B	7	LYS	4.1
1	B	13	LYS	4.1
1	D	7	LYS	4.1
1	D	144	ARG	4.1
1	B	42	PRO	4.1
1	D	157	GLN	4.0
1	D	51	PRO	4.0
1	B	150	LYS	4.0
1	A	144	ARG	3.9
1	A	151	LYS	3.9
1	D	103	SER	3.9
1	A	150	LYS	3.9
1	C	146	LYS	3.9
1	B	154	GLU	3.9
1	C	2	PRO	3.9
1	D	39	LYS	3.8
1	B	2	PRO	3.8
1	C	47	ASN	3.8
1	B	16	GLU	3.8
1	B	44	SER	3.7
1	C	81	GLY	3.7
1	D	150	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	114	TYR	3.7
1	C	90[A]	ARG	3.7
1	A	2	PRO	3.7
1	A	124	SER	3.7
1	C	8	ARG	3.7
1	A	46	LYS	3.7
1	D	5	ARG	3.6
1	D	35	LYS	3.6
1	B	31	ASP	3.5
1	D	138	ASP	3.5
1	C	38	TYR	3.5
1	C	33	VAL	3.5
1	A	147	GLU	3.5
1	A	59[A]	MET	3.4
1	B	144	ARG	3.4
1	A	160	THR	3.4
1	B	91[A]	GLU	3.4
1	C	23	ALA	3.4
1	C	36	ALA	3.4
1	C	26	ARG	3.4
1	C	42	PRO	3.4
1	C	3	SER	3.3
1	A	72	ASN	3.3
1	A	123	GLN	3.3
1	B	39	LYS	3.3
1	C	74	SER	3.3
1	D	148	TRP	3.3
1	D	50	THR	3.3
1	D	8	ARG	3.2
1	D	21	ASN	3.2
1	D	145	ASP	3.2
1	A	-2	GLY	3.2
1	A	118	LYS	3.2
1	B	8	ARG	3.2
1	C	30	GLY	3.2
1	C	83	ARG	3.1
1	D	2	PRO	3.1
1	C	24	ASN	3.1
1	B	46	LYS	3.1
1	D	10	ASP	3.1
1	B	140	VAL	3.1
1	B	149	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	158	MET	3.0
1	A	110	SER	3.0
1	C	48	SER	3.0
1	C	79	SER	3.0
1	C	145	ASP	2.9
1	B	-2	GLY	2.9
1	C	119	ASP	2.9
1	B	43	GLU	2.9
1	C	56	LYS	2.9
1	D	31	ASP	2.9
1	B	159	ARG	2.9
1	A	44	SER	2.9
1	A	145	ASP	2.8
1	D	159	ARG	2.8
1	A	-1	ALA	2.8
1	B	62	THR	2.8
1	B	101	VAL	2.8
1	B	157	GLN	2.8
1	D	133	ASP	2.7
1	A	120	ARG	2.7
1	D	90	ARG	2.7
1	A	39	LYS	2.7
1	C	150	LYS	2.7
1	C	157	GLN	2.7
1	A	40	LYS	2.7
1	D	46	LYS	2.7
1	C	144	ARG	2.7
1	D	154	GLU	2.7
1	D	105	ALA	2.7
1	B	65	VAL	2.7
1	B	49	ALA	2.6
1	C	159	ARG	2.6
1	A	43	GLU	2.6
1	C	46	LYS	2.6
1	D	147	GLU	2.6
1	A	78	GLU	2.5
1	A	119	ASP	2.5
1	B	40	LYS	2.5
1	D	132	MET	2.5
1	B	37	VAL	2.4
1	C	37	VAL	2.4
1	B	17	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	61	GLY	2.4
1	C	77	THR	2.4
1	D	136	ASP	2.3
1	C	34	CYS	2.3
1	B	45	PHE	2.3
1	C	70	GLY	2.3
1	B	47	ASN	2.3
1	B	117	GLY	2.3
1	C	158	MET	2.2
1	B	63	TYR	2.2
1	D	146	LYS	2.2
1	C	45	PHE	2.2
1	D	41	TRP	2.1
1	C	84	GLU	2.1
1	D	100	GLY	2.1
1	C	118	LYS	2.1
1	C	69	VAL	2.1
1	D	60	CYS	2.1
1	B	102	ASN	2.1
1	B	58	VAL	2.0
1	D	42	PRO	2.0
1	A	154	GLU	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, 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	DMS	C	203	4/4	0.50	0.28	61,72,73,79	0

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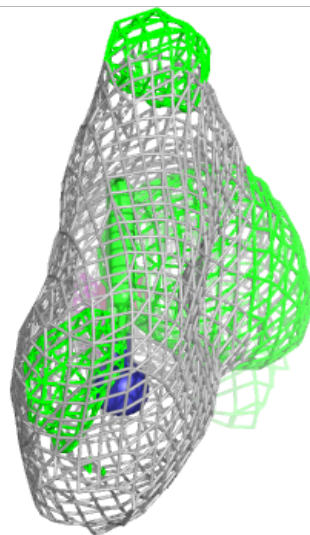
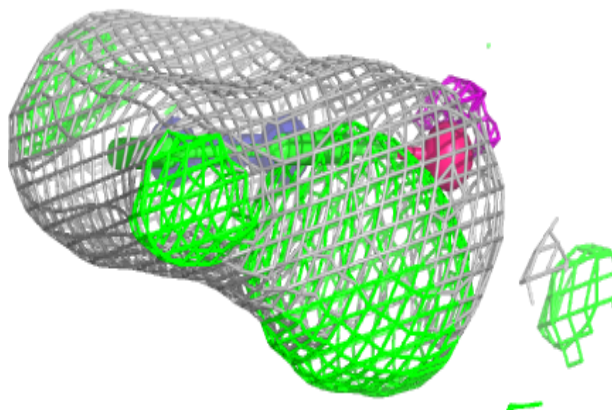
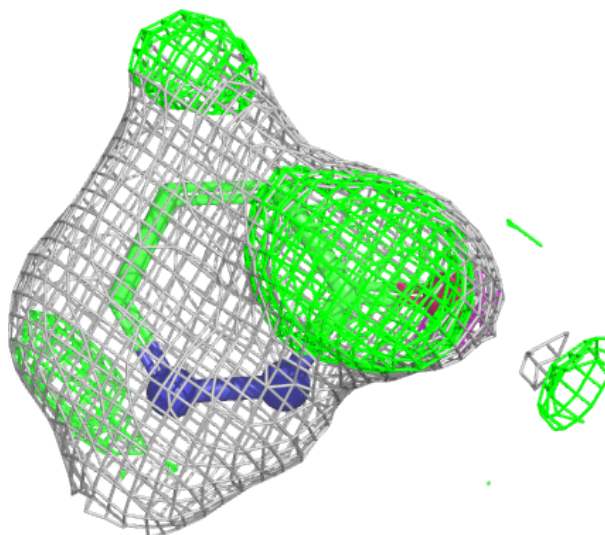
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	W3G	A	207	7/7	0.50	0.26	23,25,26,27	7
2	DMS	D	203	4/4	0.64	0.24	51,69,81,86	0
7	A1AP7	A	208	12/12	0.65	0.26	35,37,38,39	12
6	W3G	C	206	7/7	0.67	0.20	23,25,26,28	7
7	A1AP7	C	207	12/12	0.69	0.22	44,45,48,48	12
7	A1AP7	D	207	12/12	0.70	0.21	33,36,38,38	12
5	XJV	A	206	6/6	0.71	0.18	22,23,23,23	6
7	A1AP7	B	206	12/12	0.71	0.33	49,51,56,58	12
3	TRS	D	201	8/8	0.74	0.22	42,45,47,48	8
6	W3G	D	206	7/7	0.78	0.17	27,27,29,29	7
2	DMS	C	201	4/4	0.79	0.20	60,69,70,82	0
2	DMS	C	204	4/4	0.81	0.30	65,69,71,73	4
2	DMS	C	205	4/4	0.82	0.31	55,61,63,65	4
6	W3G	B	204	7/7	0.83	0.18	31,35,36,36	7
6	W3G	D	208	7/7	0.83	0.24	24,32,35,35	7
2	DMS	A	201	4/4	0.83	0.29	51,52,57,59	4
2	DMS	D	202	4/4	0.84	0.16	41,44,44,49	0
3	TRS	B	205	8/8	0.85	0.15	33,36,37,37	8
2	DMS	A	203	4/4	0.85	0.18	53,67,75,76	0
2	DMS	C	208	4/4	0.87	0.19	53,54,57,59	4
5	XJV	B	203	6/6	0.88	0.13	25,27,27,28	6
2	DMS	B	201	4/4	0.88	0.16	28,30,31,33	4
5	XJV	D	205	6/6	0.89	0.10	23,23,25,25	6
6	W3G	A	209	7/7	0.89	0.20	26,30,31,31	7
3	TRS	A	202	8/8	0.91	0.10	31,40,45,45	0
4	CL	B	207	1/1	0.92	0.11	57,57,57,57	0
4	CL	A	205	1/1	0.94	0.22	46,46,46,46	0
4	CL	A	204	1/1	0.99	0.02	18,18,18,18	0
4	CL	C	202	1/1	0.99	0.04	25,25,25,25	0
4	CL	D	204	1/1	0.99	0.03	19,19,19,19	0
4	CL	B	202	1/1	0.99	0.02	18,18,18,18	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.

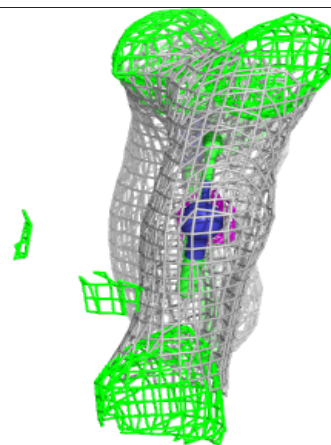
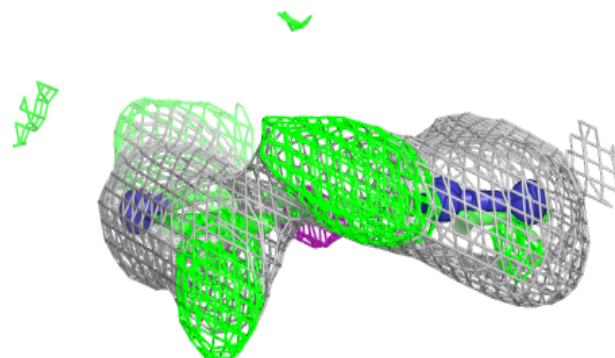
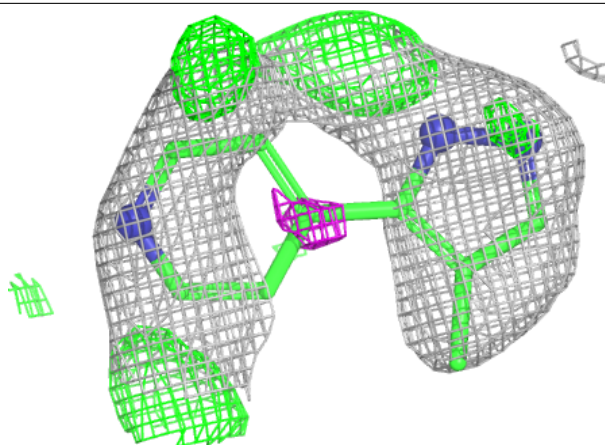
Electron density around W3G A 207:

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



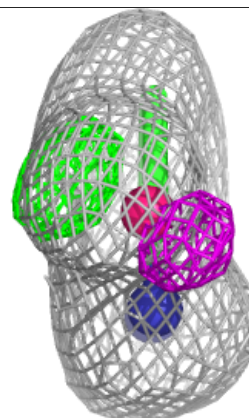
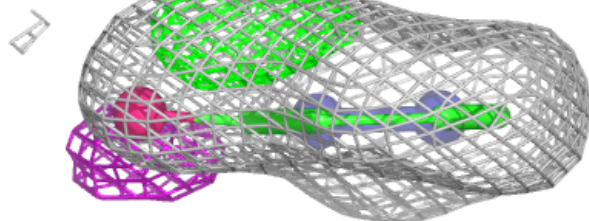
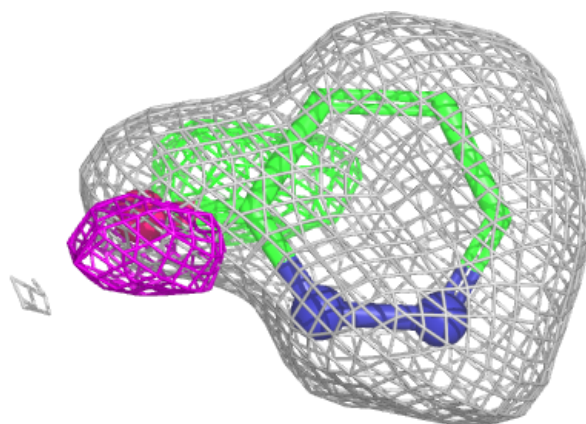
Electron density around A1AP7 A 208:

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

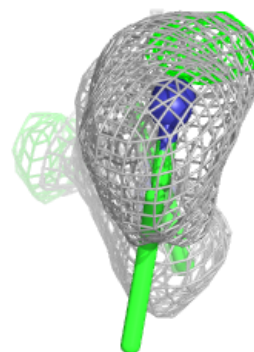
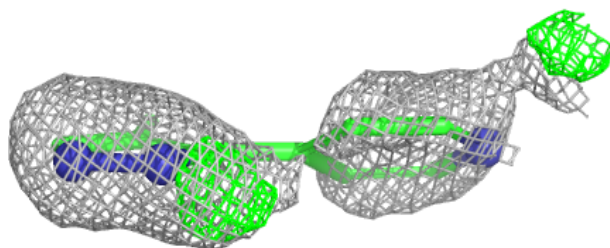
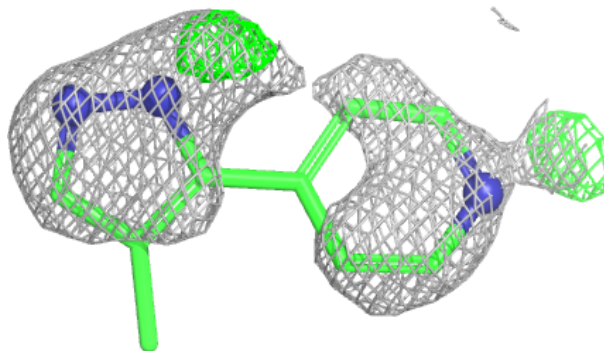


Electron density around W3G C 206:

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

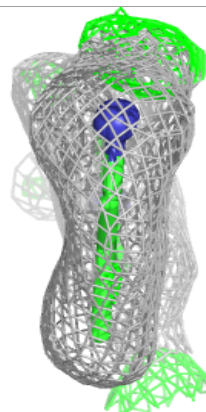
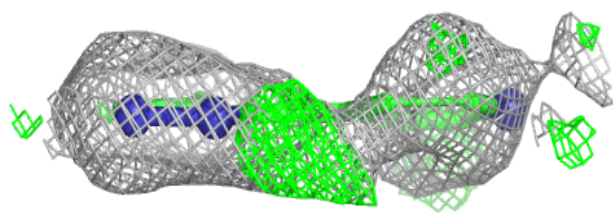
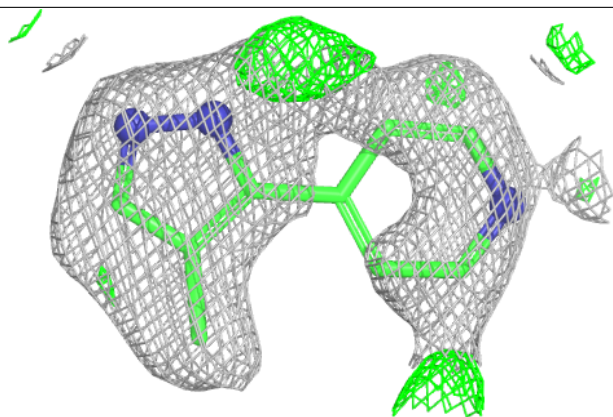
**Electron density around A1AP7 C 207:**

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

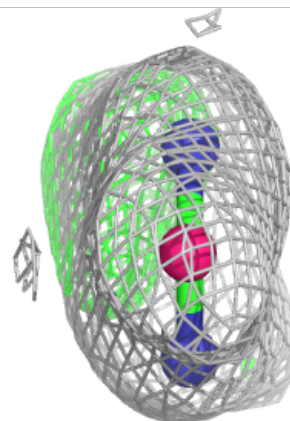
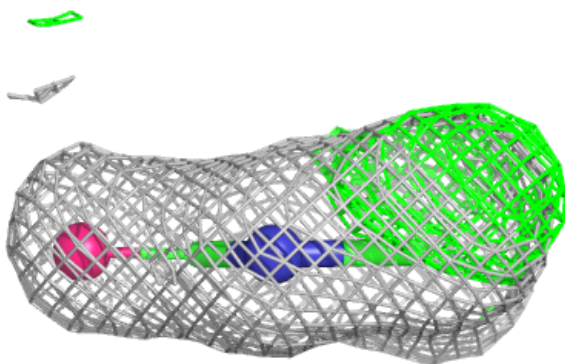
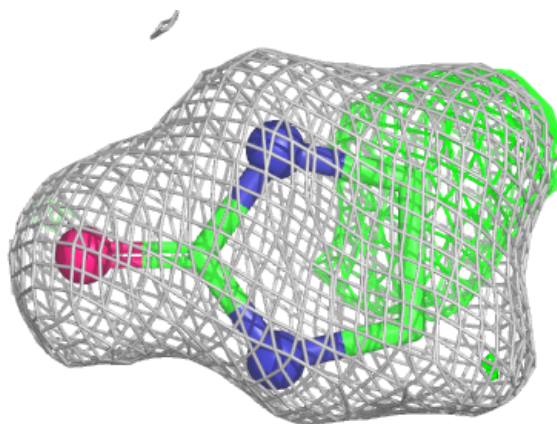


Electron density around A1AP7 D 207:

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

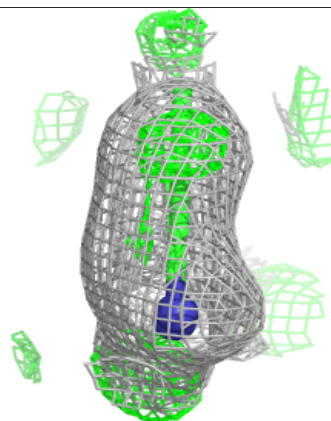
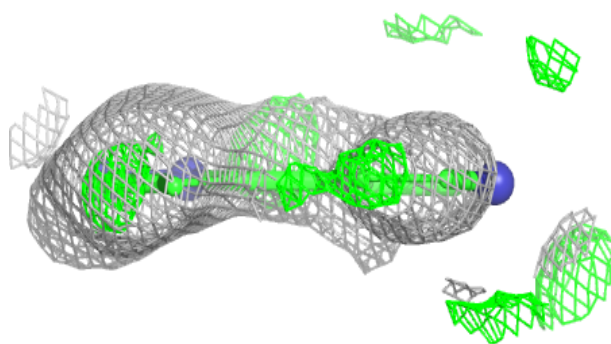
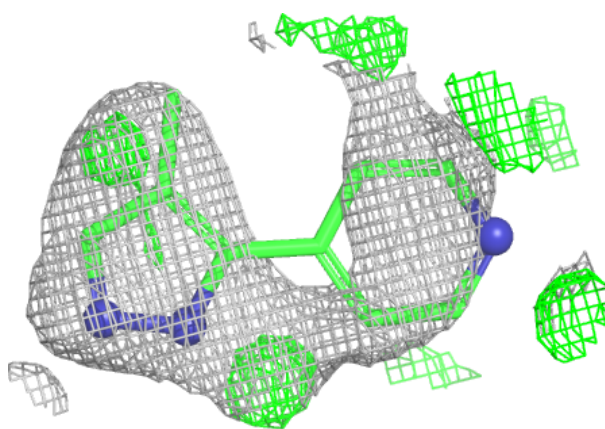
**Electron density around XJV A 206:**

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



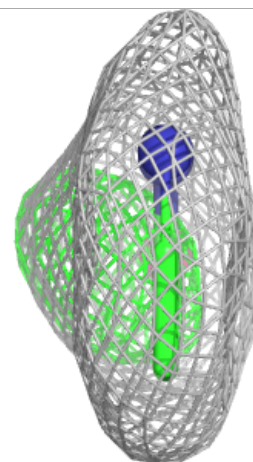
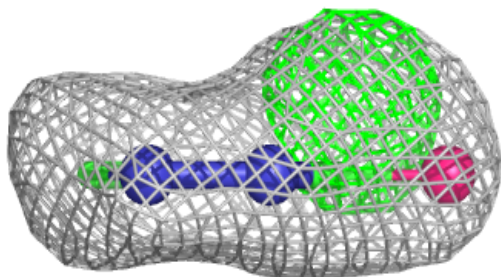
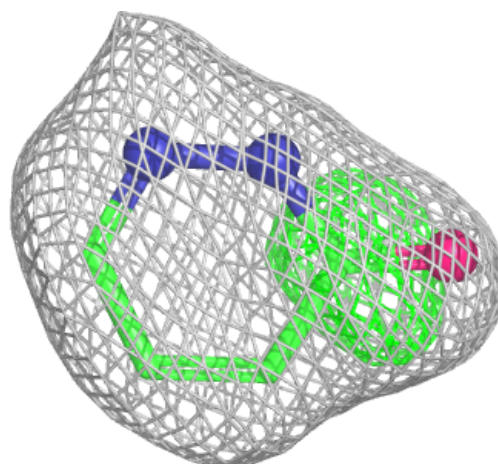
Electron density around A1AP7 B 206:

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



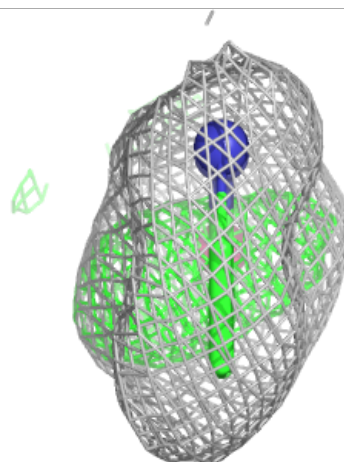
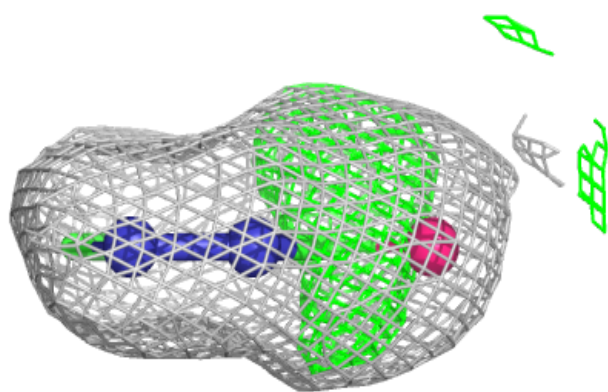
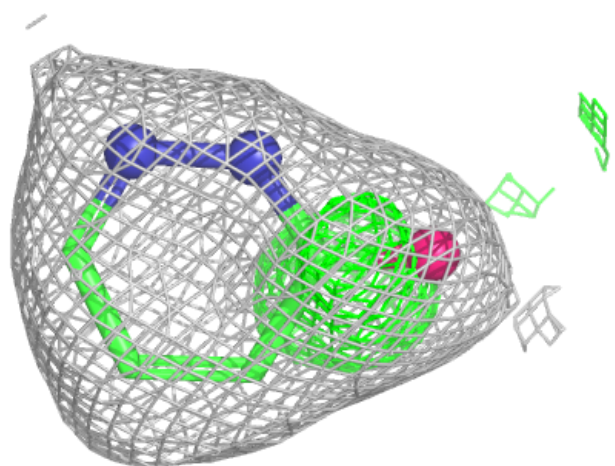
Electron density around W3G D 206:

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



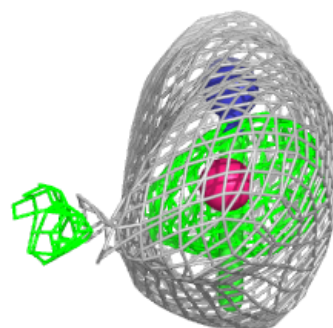
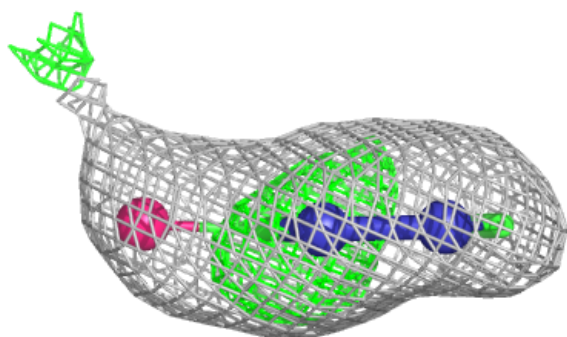
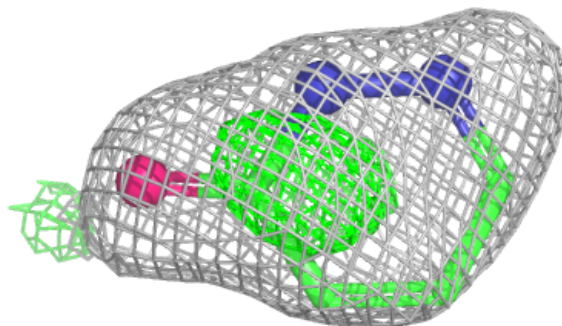
Electron density around W3G B 204:

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



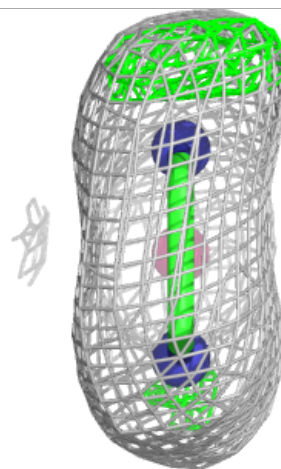
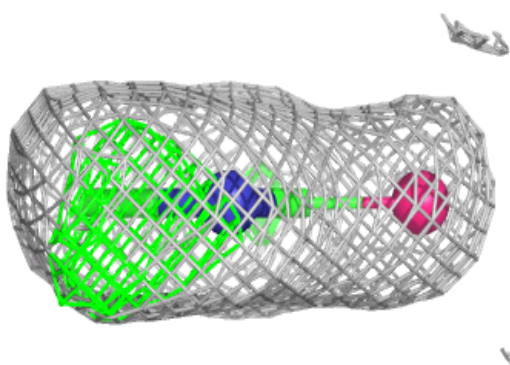
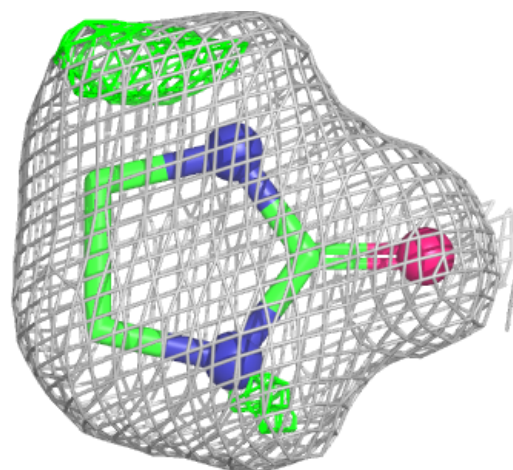
Electron density around W3G D 208:

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



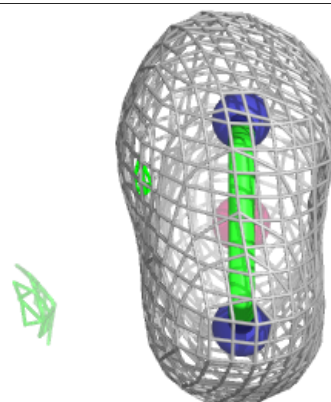
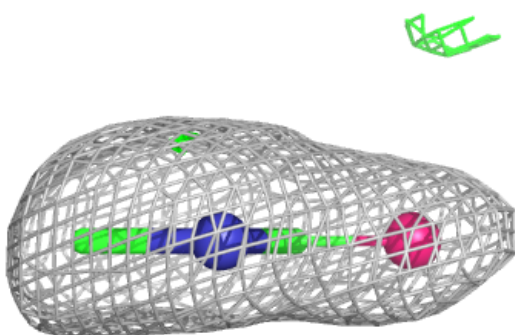
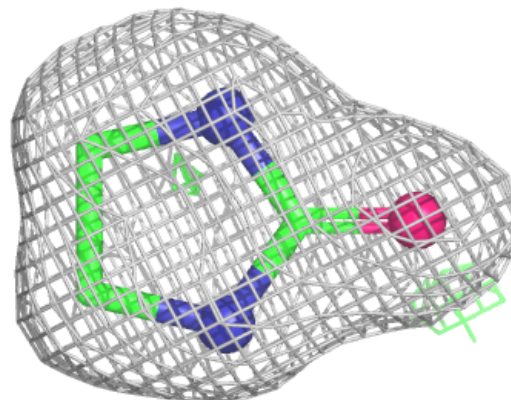
Electron density around XJV B 203:

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

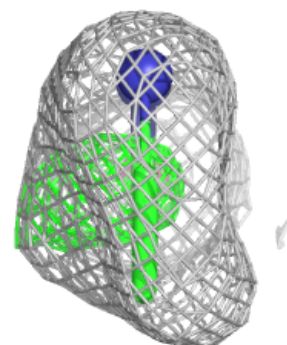
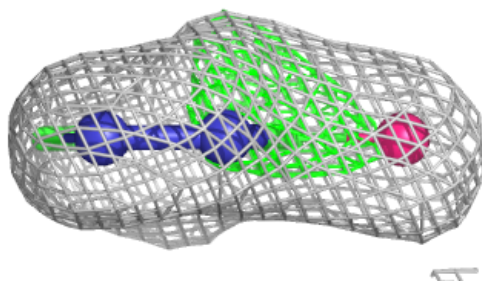
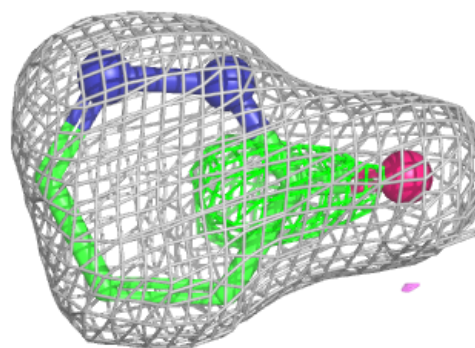


Electron density around XJV D 205:

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

**Electron density around W3G A 209:**

$2mF_o-DF_c$ (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.