



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2024 – 01:12 pm BST

PDB ID : 8P0M
Title : Crystal structure of TEAD3 in complex with IAG933
Authors : Scheufler, C.; Villard, F.; Chau, S.
Deposited on : 2023-05-10
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

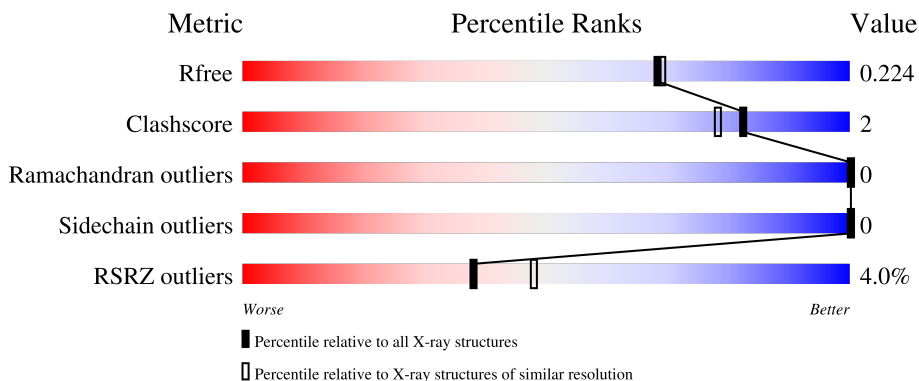
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


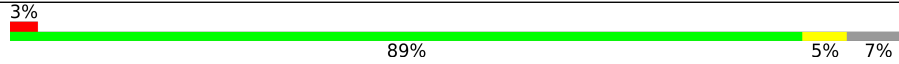
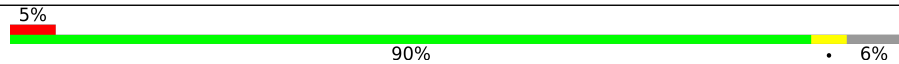
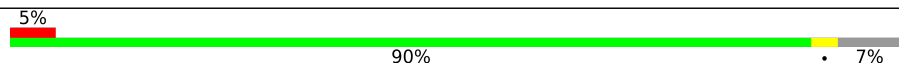
The reported resolution of this entry is 1.96 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	A	222	 2% 88% 5% 6%
1	B	222	 3% 89% 5% 7%
2	C	222	 5% 90% 5% 6%
2	D	222	 5% 90% 5% 7%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7363 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 Transcriptional enhancer factor TEF-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	Total	C	N	O	S	0	6	0
			1702	1093	281	320	8			
1	B	207	Total	C	N	O	S	0	4	0
			1699	1091	286	314	8			

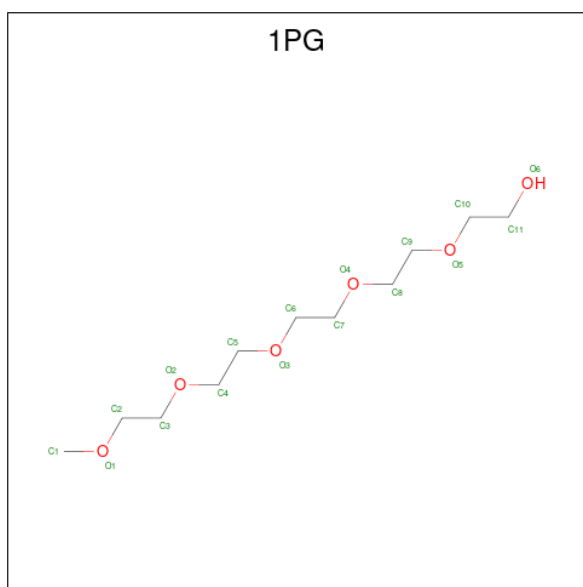
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	GLY	-	expression tag	UNP Q99594
A	216	PRO	-	expression tag	UNP Q99594
A	217	GLY	-	expression tag	UNP Q99594
A	436	GLY	-	expression tag	UNP Q99594
B	215	GLY	-	expression tag	UNP Q99594
B	216	PRO	-	expression tag	UNP Q99594
B	217	GLY	-	expression tag	UNP Q99594
B	436	GLY	-	expression tag	UNP Q99594

- Molecule 2 is a protein called Transcriptional enhancer factor TEF-5.

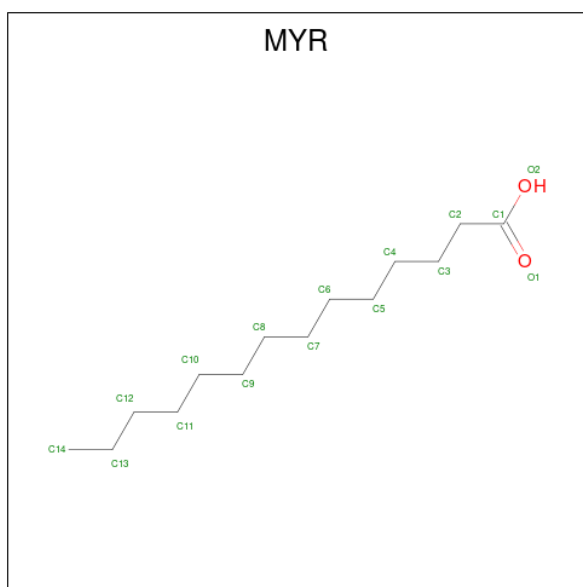
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	208	Total	C	N	O	S	0	1	0
			1691	1091	280	312	8			
2	D	207	Total	C	N	O	S	0	2	0
			1682	1089	277	308	8			

- Molecule 3 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: C₁₁H₂₄O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			17	11 6		
3	B	1	Total	C O	0	0
			17	11 6		
3	D	1	Total	C O	0	0
			17	11 6		

- Molecule 4 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



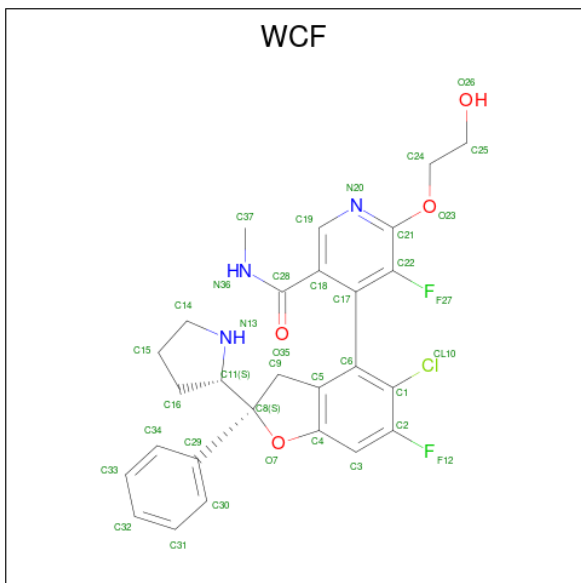
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			15	14 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	15	14	1	0	0

- Molecule 5 is 4-[(2 {S})-5-chloranyl-6-fluoranyl-2-phenyl-2-[(2 {S})-pyrrolidin-2-yl]-3 {H}-1-benzofuran-4-yl]-5-fluoranyl-6-(2-hydroxyethoxy)- {N}-methyl-pyridine-3-carboxamide (three-letter code: WCF) (formula: C₂₇H₂₆ClF₂N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
5	A	1	37	27	1	2	3	4	0	0
5	B	1	37	27	1	2	3	4	0	0
5	C	1	37	27	1	2	3	4	0	0
5	D	1	37	27	1	2	3	4	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

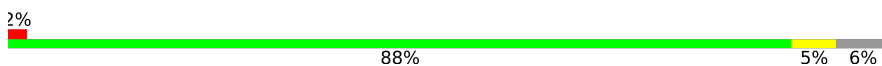
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	94	Total	O	0	0
			94	94		
7	C	87	Total	O	0	0
			87	87		
7	D	88	Total	O	0	0
			88	88		

3 Residue-property plots [i](#)

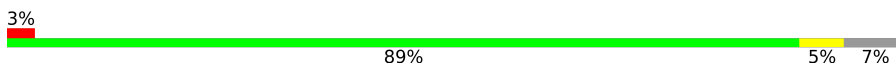
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

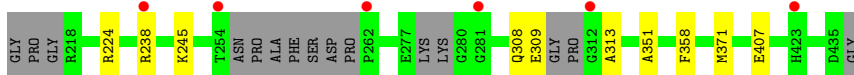
- Molecule 1: Transcriptional enhancer factor TEF-5

Chain A: 

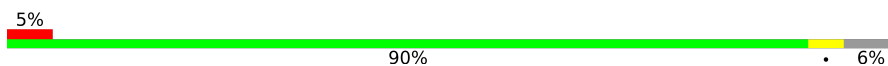


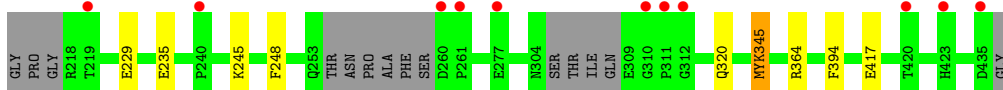
- Molecule 1: Transcriptional enhancer factor TEF-5

Chain B: 

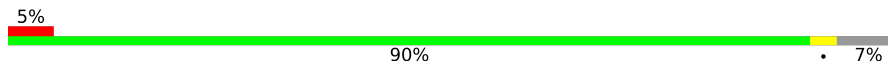


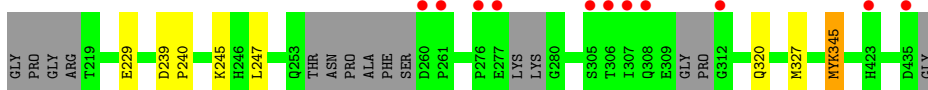
- Molecule 2: Transcriptional enhancer factor TEF-5

Chain C: 



- Molecule 2: Transcriptional enhancer factor TEF-5

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.50Å 127.24Å 155.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.48 – 1.96 98.48 – 1.96	Depositor EDS
% Data completeness (in resolution range)	84.0 (98.48-1.96) 84.0 (98.48-1.96)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.97Å)	Xtrriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.214 , 0.228 0.207 , 0.224	Depositor DCC
R_{free} test set	3974 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7363	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: MYK, WCF, DMS, 1PG, MYR

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	0.43	0/1739	0.59	0/2348
1	B	0.42	0/1740	0.59	0/2346
2	C	0.43	0/1705	0.61	0/2302
2	D	0.41	0/1695	0.59	0/2289
All	All	0.42	0/6879	0.60	0/9285

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1702	0	1640	14	0
1	B	1699	0	1667	6	0
2	C	1691	0	1650	7	0
2	D	1682	0	1646	7	0
3	A	17	0	24	8	0
3	B	17	0	24	1	0
3	D	17	0	24	4	0
4	A	15	0	27	1	0
4	B	15	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	37	0	0	0	0
5	B	37	0	0	0	0
5	C	37	0	0	1	0
5	D	37	0	0	0	0
6	C	4	0	6	0	0
6	D	4	0	6	0	0
7	A	83	0	0	0	0
7	B	94	0	0	0	0
7	C	87	0	0	0	0
7	D	88	0	0	1	0
All	All	7363	0	6741	34	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 2.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:NZ	3:A:501:1PG:H61	1.86	0.90
1:A:245:LYS:HZ1	3:A:501:1PG:H61	1.38	0.87
2:D:245:LYS:HE3	3:D:501:1PG:H102	1.70	0.72
2:C:235:GLU:CD	2:C:364:ARG:HH12	1.99	0.65
1:B:245:LYS:HE2	3:B:501:1PG:H111	1.81	0.62
1:B:224:ARG:NH1	1:B:407:GLU:OE2	2.35	0.60
2:C:235:GLU:OE2	2:C:364:ARG:NH1	2.35	0.60
2:D:245:LYS:HZ1	3:D:501:1PG:C8	2.17	0.58
2:D:247:LEU:HD21	3:D:501:1PG:H42	1.90	0.54
1:A:246:HIS:HB2	1:A:307:ILE:HD12	1.92	0.52
2:C:417:GLU:OE2	5:C:502:WCF:N13	2.44	0.50
1:A:245:LYS:NZ	3:A:501:1PG:H22	2.26	0.50
2:C:245:LYS:HB2	3:D:501:1PG:H111	1.94	0.49
1:A:245:LYS:HD3	3:A:501:1PG:H22	1.95	0.49
1:A:320:GLN:HG2	1:A:361:ARG:HG2	1.96	0.48
1:A:275:PHE:CZ	1:A:413:ALA:HB1	2.49	0.47
1:A:245:LYS:HE2	3:A:501:1PG:H12	1.98	0.46
1:A:233:PHE:CZ	3:A:501:1PG:H13	2.51	0.45
1:A:233:PHE:CD2	3:A:501:1PG:H21	2.52	0.45
1:A:245:LYS:HZ2	3:A:501:1PG:H61	1.74	0.45
2:D:239:ASP:HB2	2:D:240:PRO:CD	2.48	0.43
1:A:351:ALA:HB2	1:A:360:TYR:CE2	2.53	0.43
1:A:371:MET:HG3	4:A:502:MYR:H51	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:248:PHE:HB3	2:C:345:MYK:HUA	2.00	0.43
1:B:351:ALA:HB1	1:B:358:PHE:HB3	1.99	0.42
2:D:327:MET:HB2	7:D:651:HOH:O	2.19	0.42
1:B:371:MET:HG3	4:B:502:MYR:H51	2.00	0.42
2:D:229:GLU:OE1	2:D:320:GLN:NE2	2.52	0.42
2:C:229:GLU:OE1	2:C:320:GLN:NE2	2.53	0.42
2:C:345:MYK:HV	2:C:394:PHE:CE2	2.54	0.42
1:A:351:ALA:HB1	1:A:358:PHE:HB3	2.02	0.42
2:D:345:MYK:HQA	2:D:345:MYK:HVA	1.58	0.42
1:B:238:ARG:HH11	1:B:308:GLN:H	1.69	0.40
1:B:309:GLU:HG3	1:B:313:ALA:HB2	2.02	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	208/222 (94%)	207 (100%)	1 (0%)	0	100	100
1	B	203/222 (91%)	203 (100%)	0	0	100	100
2	C	202/222 (91%)	200 (99%)	2 (1%)	0	100	100
2	D	200/222 (90%)	200 (100%)	0	0	100	100
All	All	813/888 (92%)	810 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/198 (93%)	185 (100%)	0	100	100
1	B	189/198 (96%)	189 (100%)	0	100	100
2	C	182/197 (92%)	182 (100%)	0	100	100
2	D	181/197 (92%)	181 (100%)	0	100	100
All	All	737/790 (93%)	737 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	HIS
2	C	320	GLN
2	D	320	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	MYK	C	345	2	22,23,24	0.90	1 (4%)	19,24,26	0.93	1 (5%)
2	MYK	D	345	2	22,23,24	0.86	1 (4%)	19,24,26	0.97	1 (5%)

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
2	MYK	C	345	2	-	9/22/23/25	-
2	MYK	D	345	2	-	9/22/23/25	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	345	MYK	CB-CA	2.62	1.57	1.53
2	D	345	MYK	CB-CA	2.51	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	345	MYK	CE-NZ-CX	-2.32	118.53	122.84
2	C	345	MYK	CE-NZ-CX	-2.22	118.72	122.84

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	345	MYK	CI-CK-CL-CM
2	C	345	MYK	CI-CK-CL-CM
2	D	345	MYK	CU-CQ-CS-CW
2	D	345	MYK	CM-CP-CR-CU
2	D	345	MYK	CP-CR-CU-CQ
2	C	345	MYK	CM-CP-CR-CU
2	C	345	MYK	CP-CR-CU-CQ
2	C	345	MYK	CU-CQ-CS-CW
2	D	345	MYK	CK-CL-CM-CP
2	C	345	MYK	CK-CL-CM-CP
2	C	345	MYK	CQ-CS-CW-CV
2	D	345	MYK	CQ-CS-CW-CV
2	C	345	MYK	CL-CM-CP-CR
2	C	345	MYK	CE-CD-CG-CB
2	D	345	MYK	CE-CD-CG-CB
2	D	345	MYK	CL-CM-CP-CR
2	C	345	MYK	CS-CQ-CU-CR
2	D	345	MYK	CS-CQ-CU-CR

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	345	MYK	2	0
2	D	345	MYK	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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	1PG	D	501	-	16,16,16	0.83	0	15,15,15	0.30	0
6	DMS	C	501	-	3,3,3	0.95	0	3,3,3	0.31	0
6	DMS	D	502	-	3,3,3	0.87	0	3,3,3	0.33	0
4	MYR	B	502	1	14,14,15	0.73	0	13,13,15	0.51	0
4	MYR	A	502	1	14,14,15	0.68	0	13,13,15	0.58	0
3	1PG	A	501	-	16,16,16	0.82	0	15,15,15	0.45	0
5	WCF	B	503	-	39,41,41	1.11	3 (7%)	43,60,60	1.51	7 (16%)
3	1PG	B	501	-	16,16,16	0.86	0	15,15,15	0.37	0
5	WCF	C	502	-	39,41,41	1.08	2 (5%)	43,60,60	1.43	8 (18%)
5	WCF	A	503	-	39,41,41	1.00	2 (5%)	43,60,60	1.50	8 (18%)
5	WCF	D	503	-	39,41,41	1.05	3 (7%)	43,60,60	1.38	7 (16%)

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	1PG	D	501	-	-	7/14/14/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MYR	B	502	1	-	7/11/12/13	-
4	MYR	A	502	1	-	7/11/12/13	-
3	1PG	A	501	-	-	10/14/14/14	-
5	WCF	B	503	-	-	0/23/43/43	0/5/5/5
3	1PG	B	501	-	-	7/14/14/14	-
5	WCF	C	502	-	-	0/23/43/43	0/5/5/5
5	WCF	A	503	-	-	0/23/43/43	0/5/5/5
5	WCF	D	503	-	-	3/23/43/43	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	WCF	O23-C21	3.05	1.39	1.35
5	D	503	WCF	O23-C21	2.85	1.39	1.35
5	B	503	WCF	O23-C21	2.84	1.39	1.35
5	C	502	WCF	C9-C8	2.63	1.58	1.54
5	B	503	WCF	C28-N36	2.58	1.36	1.33
5	A	503	WCF	O23-C21	2.55	1.39	1.35
5	B	503	WCF	C9-C8	2.30	1.57	1.54
5	D	503	WCF	C28-N36	2.25	1.36	1.33
5	A	503	WCF	C28-N36	2.16	1.36	1.33
5	D	503	WCF	C9-C8	2.15	1.57	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	WCF	O7-C4-C5	4.22	116.35	113.12
5	A	503	WCF	O7-C4-C5	4.18	116.31	113.12
5	B	503	WCF	C8-O7-C4	-4.15	104.54	107.54
5	B	503	WCF	C15-C16-C11	-4.12	99.62	105.28
5	A	503	WCF	C8-O7-C4	-3.87	104.74	107.54
5	D	503	WCF	O7-C4-C5	3.70	115.95	113.12
5	C	502	WCF	O7-C4-C5	3.62	115.89	113.12
5	D	503	WCF	C15-C16-C11	-3.61	100.31	105.28
5	C	502	WCF	C8-O7-C4	-3.49	105.02	107.54
5	C	502	WCF	C8-C9-C5	-3.37	99.69	103.05
5	D	503	WCF	C8-O7-C4	-3.28	105.17	107.54
5	C	502	WCF	C15-C16-C11	-3.09	101.03	105.28
5	C	502	WCF	C18-C19-N20	-2.77	120.10	124.28
5	A	503	WCF	C15-C16-C11	-2.77	101.47	105.28
5	C	502	WCF	C9-C5-C6	2.64	130.44	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	WCF	C37-N36-C28	-2.60	118.94	121.89
5	A	503	WCF	C18-C19-N20	-2.58	120.39	124.28
5	C	502	WCF	O7-C8-C29	2.42	111.52	108.52
5	B	503	WCF	C9-C5-C6	2.40	130.22	127.88
5	A	503	WCF	C9-C5-C6	2.39	130.21	127.88
5	A	503	WCF	C8-C9-C5	-2.27	100.79	103.05
5	A	503	WCF	O23-C21-N20	2.25	122.58	119.23
5	D	503	WCF	C8-C9-C5	-2.21	100.85	103.05
5	C	502	WCF	C19-N20-C21	2.18	121.86	116.27
5	B	503	WCF	C16-C11-C8	2.14	117.14	114.00
5	B	503	WCF	C8-C9-C5	-2.14	100.92	103.05
5	D	503	WCF	C22-C21-N20	-2.13	120.20	122.35
5	B	503	WCF	C22-C21-N20	-2.09	120.24	122.35
5	D	503	WCF	C37-N36-C28	-2.03	119.59	121.89
5	D	503	WCF	C9-C5-C6	2.01	129.83	127.88

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	1PG	O1-C2-C3-O2
3	A	501	1PG	O1-C2-C3-O2
3	A	501	1PG	O3-C6-C7-O4
3	A	501	1PG	O5-C10-C11-O6
4	B	502	MYR	C11-C10-C9-C8
4	A	502	MYR	C11-C10-C9-C8
4	A	502	MYR	C5-C6-C7-C8
4	B	502	MYR	C5-C6-C7-C8
3	A	501	1PG	O4-C8-C9-O5
3	A	501	1PG	O2-C4-C5-O3
3	B	501	1PG	O5-C10-C11-O6
4	A	502	MYR	C7-C8-C9-C10
4	B	502	MYR	C7-C8-C9-C10
4	A	502	MYR	C11-C12-C13-C14
4	B	502	MYR	C11-C12-C13-C14
4	A	502	MYR	C9-C10-C11-C12
4	B	502	MYR	C9-C10-C11-C12
3	D	501	1PG	O2-C4-C5-O3
3	A	501	1PG	C11-C10-O5-C9
3	D	501	1PG	C2-C3-O2-C4
3	B	501	1PG	C8-C9-O5-C10
3	A	501	1PG	C4-C5-O3-C6

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Mol	Chain	Res	Type	Atoms
5	D	503	WCF	O23-C24-C25-O26
3	A	501	1PG	C9-C8-O4-C7
3	D	501	1PG	C11-C10-O5-C9
4	A	502	MYR	C6-C7-C8-C9
3	B	501	1PG	C5-C4-O2-C3
5	D	503	WCF	C30-C29-C8-C11
4	B	502	MYR	C6-C7-C8-C9
3	B	501	1PG	O2-C4-C5-O3
4	B	502	MYR	C10-C11-C12-C13
3	A	501	1PG	C6-C7-O4-C8
3	A	501	1PG	C7-C6-O3-C5
4	A	502	MYR	C10-C11-C12-C13
3	D	501	1PG	C4-C5-O3-C6
3	D	501	1PG	C6-C7-O4-C8
3	B	501	1PG	C6-C7-O4-C8
3	B	501	1PG	O1-C2-C3-O2
3	B	501	1PG	C3-C2-O1-C1
5	D	503	WCF	C34-C29-C8-C11
3	D	501	1PG	O4-C8-C9-O5

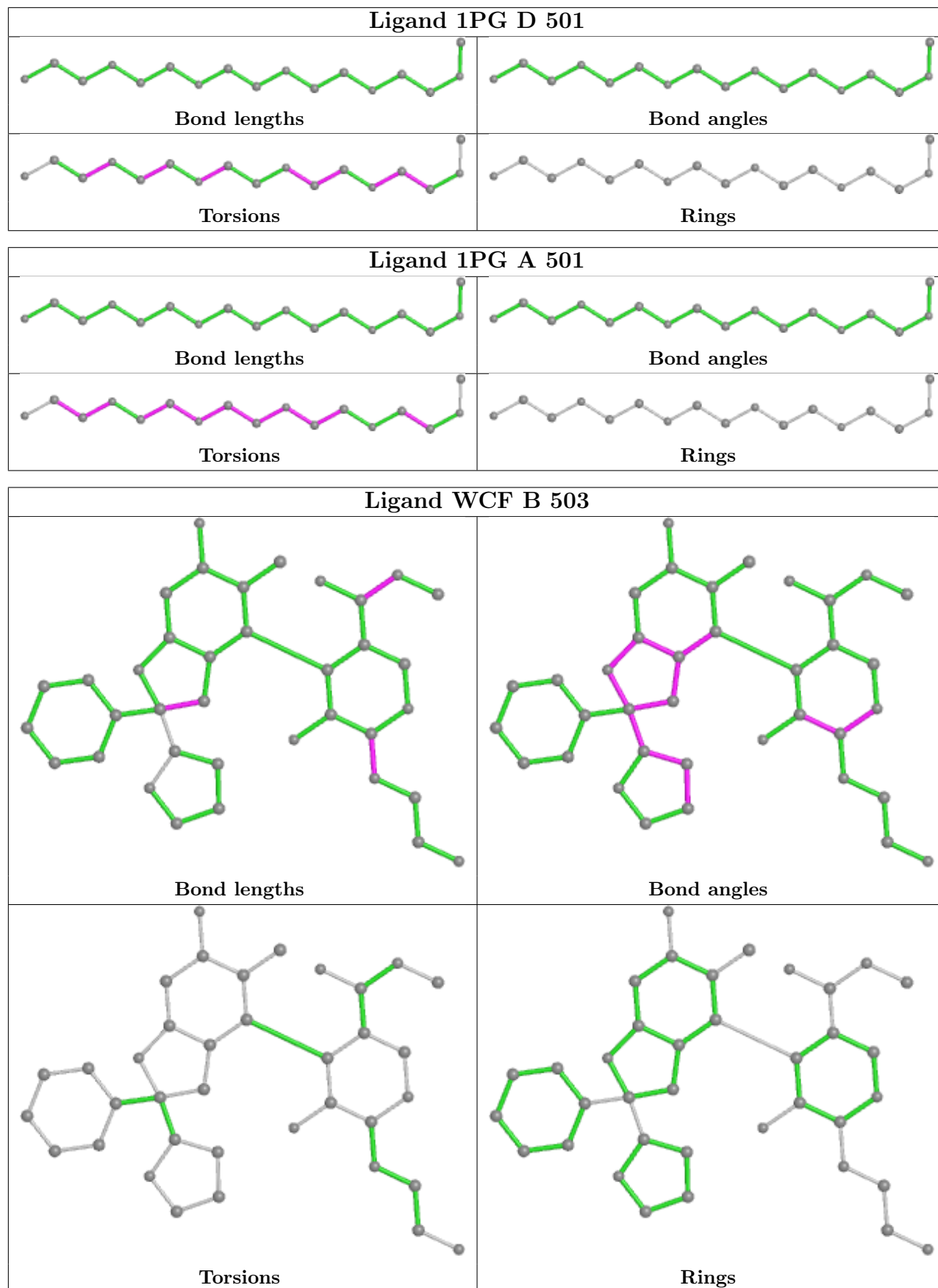
There are no ring outliers.

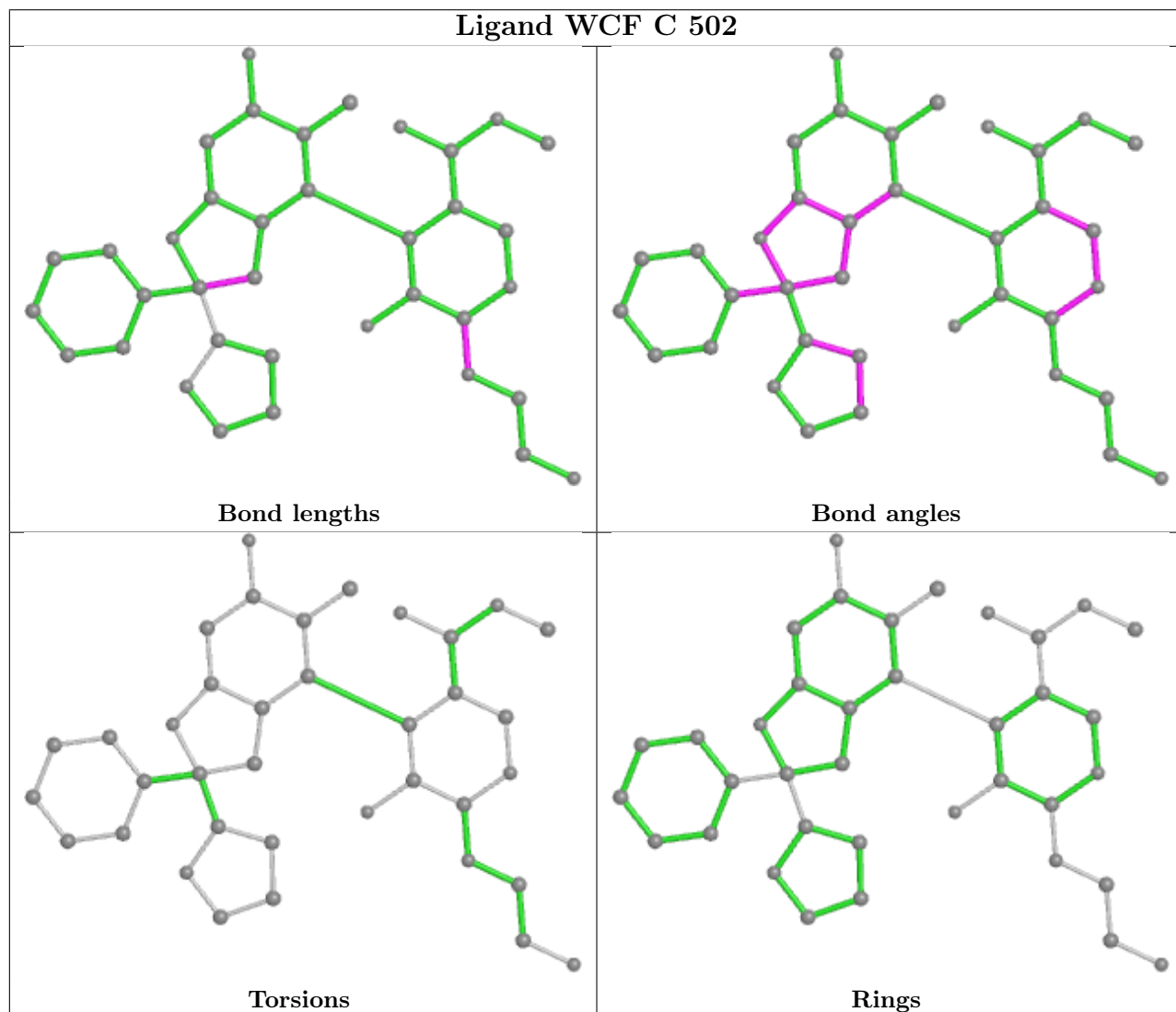
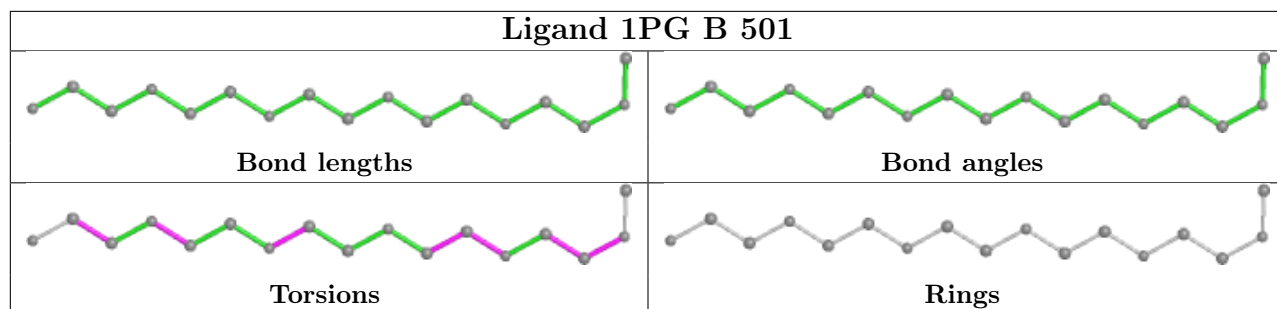
6 monomers are involved in 16 short contacts:

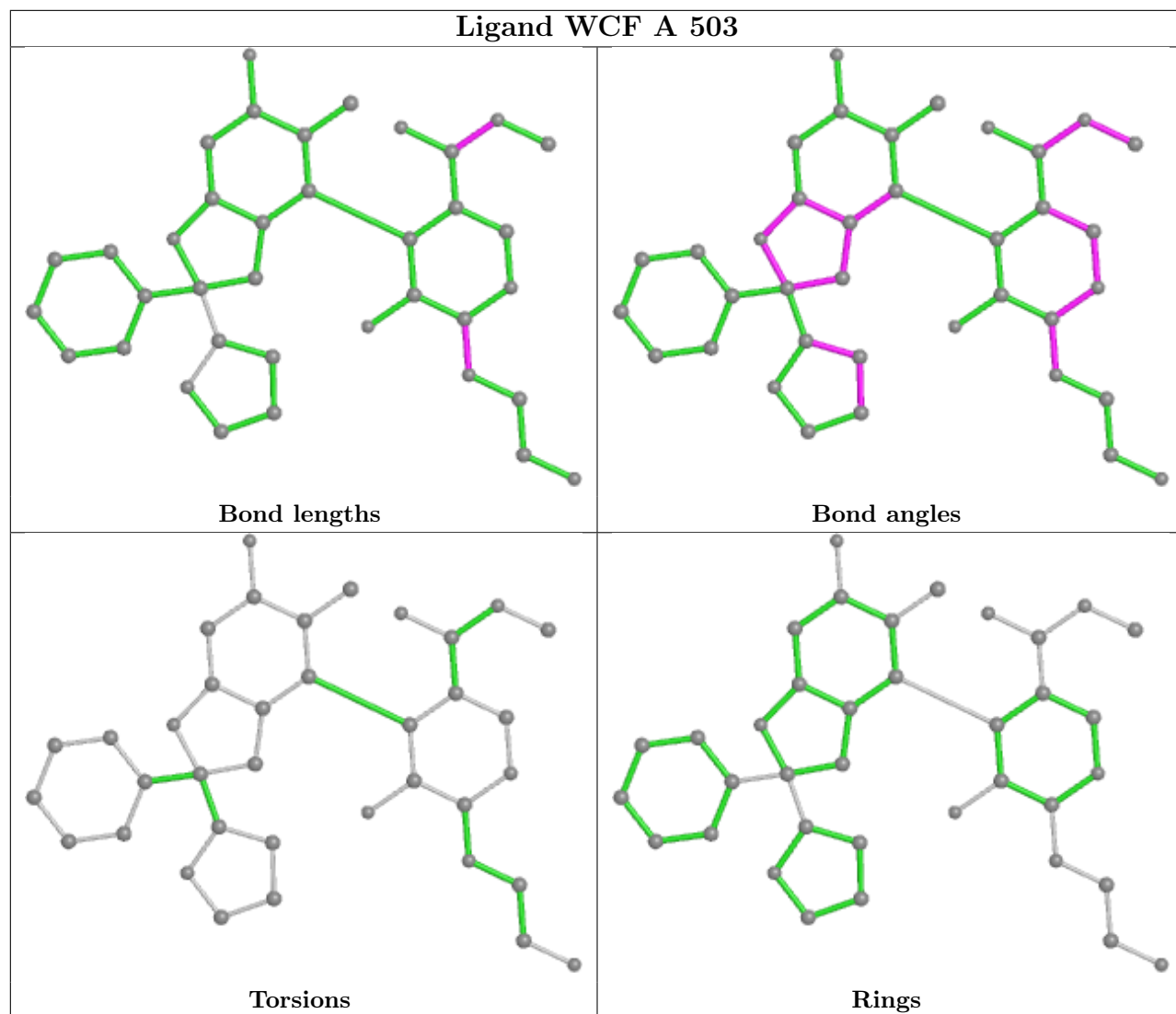
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	1PG	4	0
4	B	502	MYR	1	0
4	A	502	MYR	1	0
3	A	501	1PG	8	0
3	B	501	1PG	1	0
5	C	502	WCF	1	0

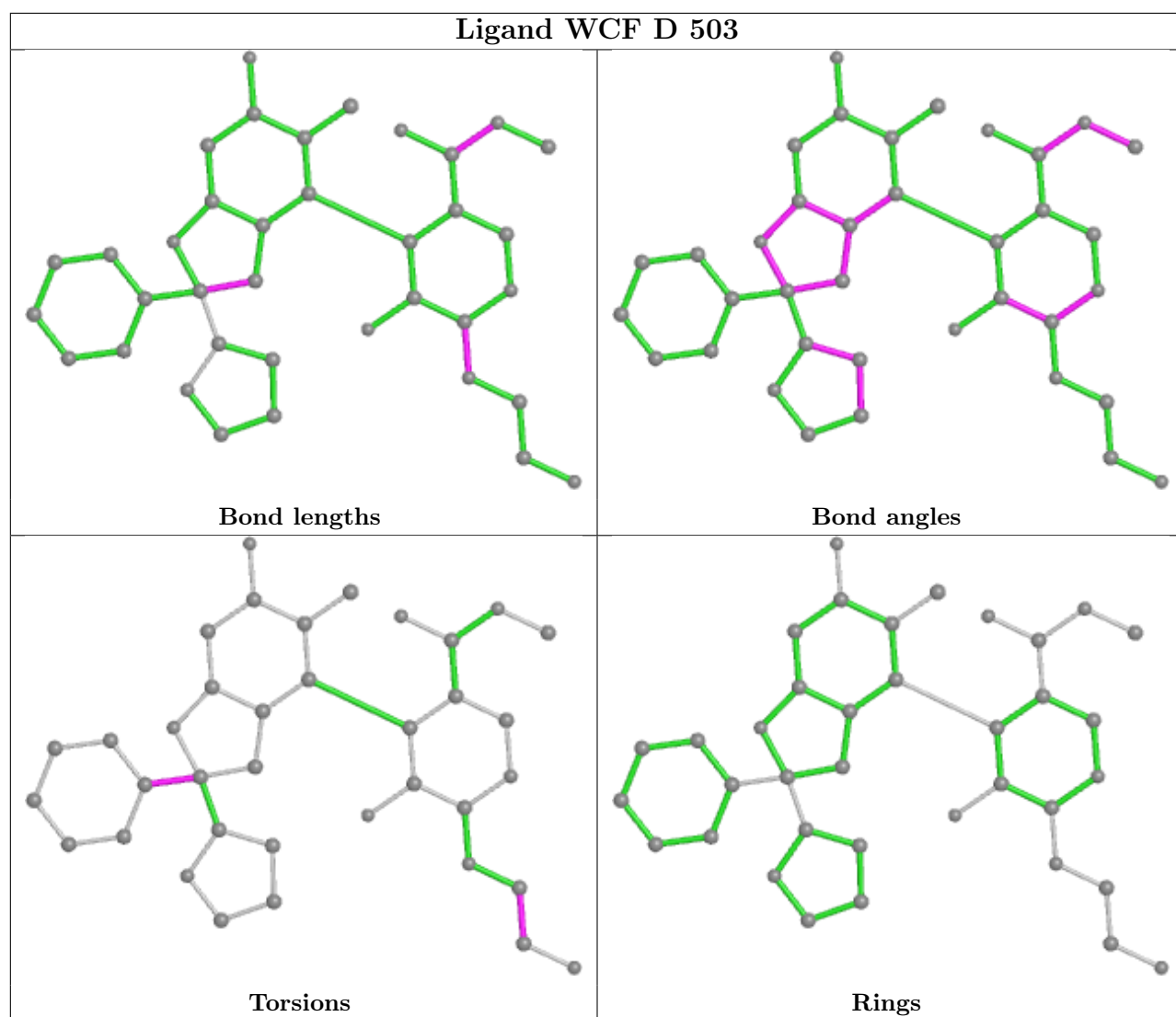
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	208/222 (93%)	0.53	5 (2%) 59 68	22, 35, 55, 77	0
1	B	207/222 (93%)	0.57	6 (2%) 51 60	22, 34, 54, 70	0
2	C	207/222 (93%)	0.65	11 (5%) 26 35	24, 35, 58, 75	0
2	D	206/222 (92%)	0.60	11 (5%) 26 35	23, 35, 57, 78	0
All	All	828/888 (93%)	0.59	33 (3%) 38 48	22, 35, 57, 78	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	312	GLY	4.6
2	D	305	SER	4.3
2	C	261	PRO	4.1
2	D	261	PRO	4.0
2	C	310	GLY	3.9
1	A	312	GLY	3.9
2	D	260	ASP	3.8
2	C	260	ASP	3.8
2	C	311	PRO	3.8
1	B	262	PRO	3.6
1	B	423	HIS	3.5
1	B	254	THR	3.3
2	D	312	GLY	3.2
2	C	277	GLU	3.2
1	A	380	HIS	3.1
2	D	277	GLU	2.9
2	D	308	GLN	2.8
2	D	307	ILE	2.7
2	C	219	THR	2.6
2	D	276	PRO	2.6
2	C	423	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	306	THR	2.5
1	B	312	GLY	2.5
2	C	435	ASP	2.4
1	B	238	ARG	2.4
2	D	435	ASP	2.4
2	C	420	THR	2.3
2	D	306	THR	2.3
1	A	278	LYS	2.2
2	D	423	HIS	2.1
1	B	281	GLY	2.1
1	A	352	ARG	2.1
2	C	240	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	MYK	C	345	24/25	0.88	0.20	23,37,47,48	0
2	MYK	D	345	24/25	0.92	0.17	25,39,46,46	0

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.

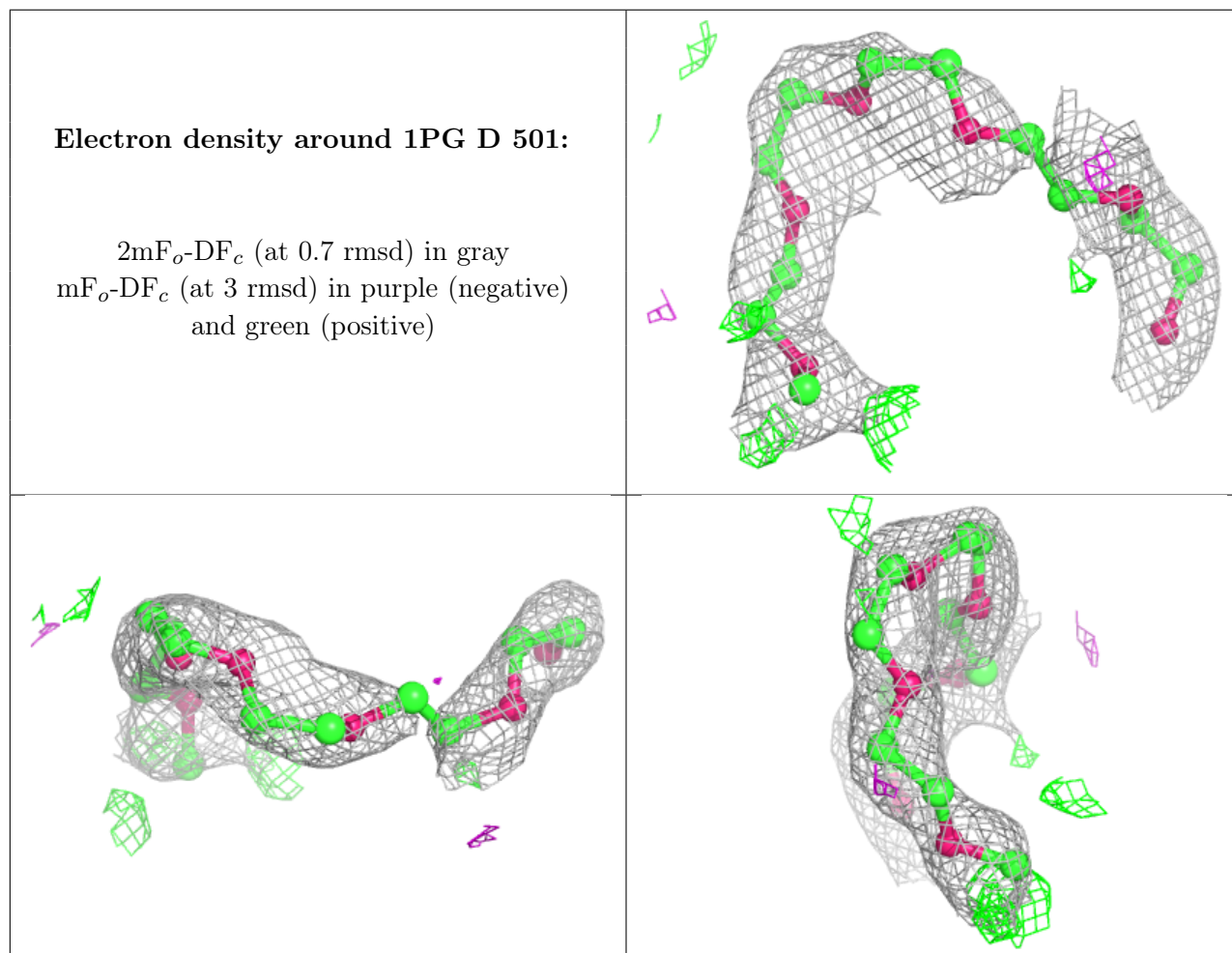
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MYR	A	502	15/16	0.73	0.23	47,48,50,50	0
4	MYR	B	502	15/16	0.74	0.21	44,45,48,49	0
3	1PG	D	501	17/17	0.76	0.26	67,71,71,71	0
3	1PG	B	501	17/17	0.80	0.18	58,60,62,62	0

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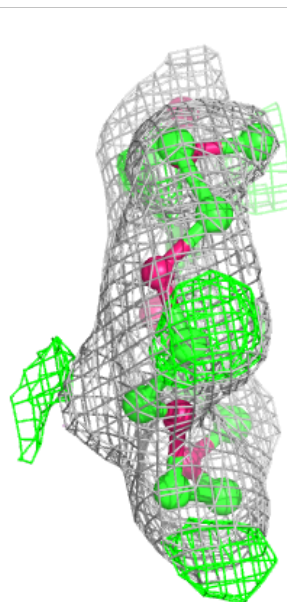
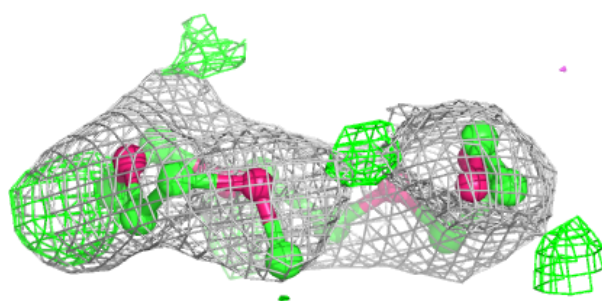
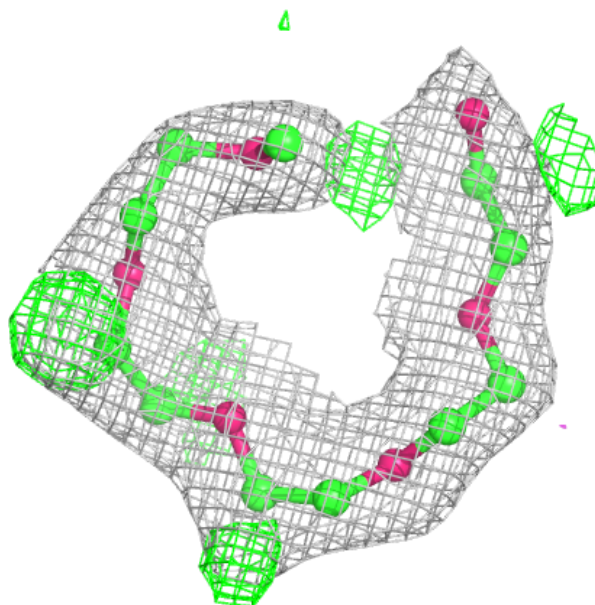
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	1PG	A	501	17/17	0.84	0.22	66,66,68,68	0
5	WCF	A	503	37/37	0.96	0.12	28,32,35,37	0
5	WCF	B	503	37/37	0.96	0.12	28,33,36,36	0
5	WCF	C	502	37/37	0.96	0.11	30,33,37,38	0
5	WCF	D	503	37/37	0.96	0.13	28,32,36,37	0
6	DMS	D	502	4/4	0.98	0.12	26,27,27,28	0
6	DMS	C	501	4/4	0.99	0.13	28,29,29,29	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.



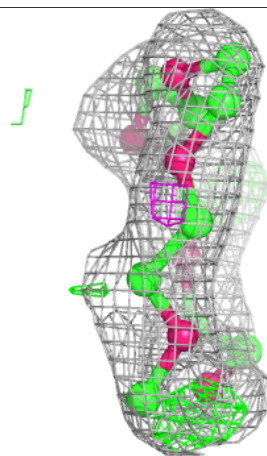
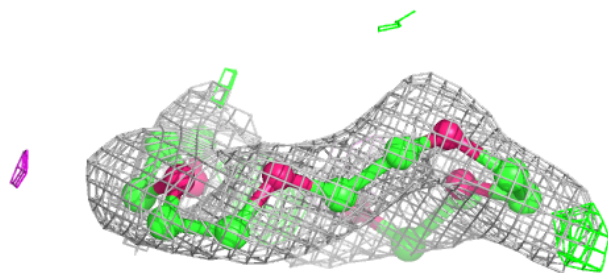
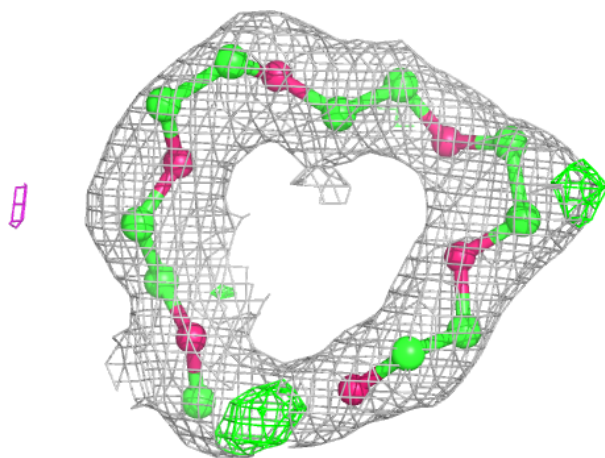
Electron density around 1PG B 501:

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



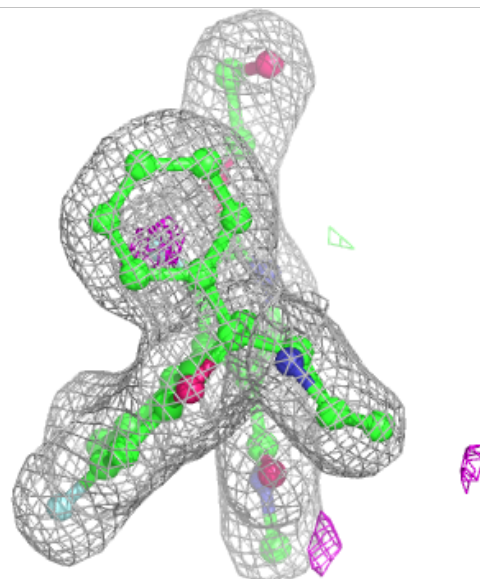
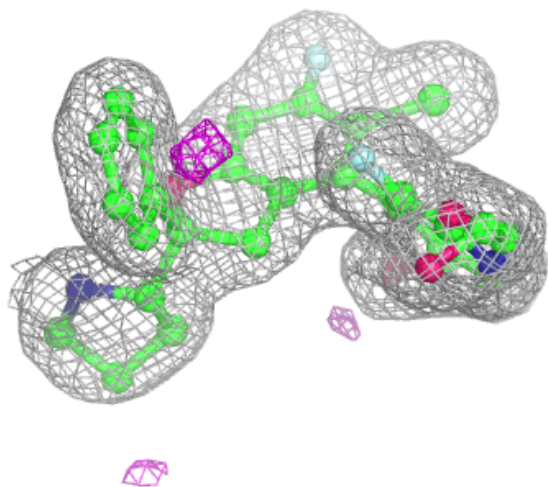
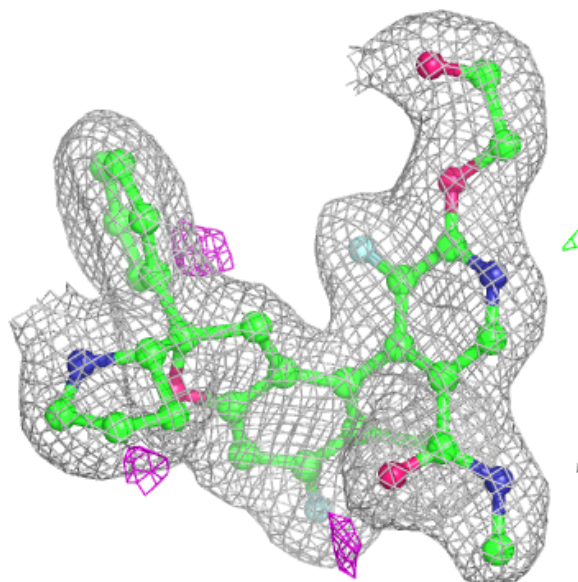
Electron density around 1PG A 501:

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



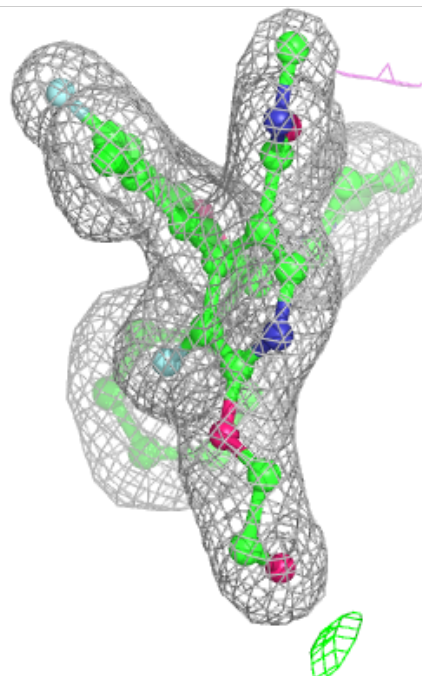
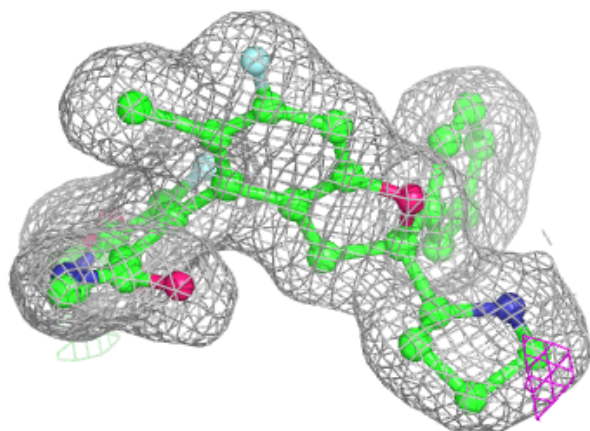
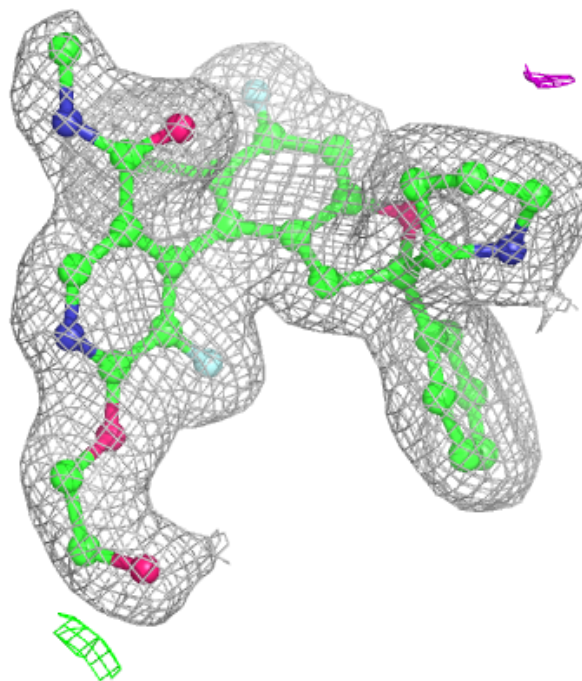
Electron density around WCF A 503:

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



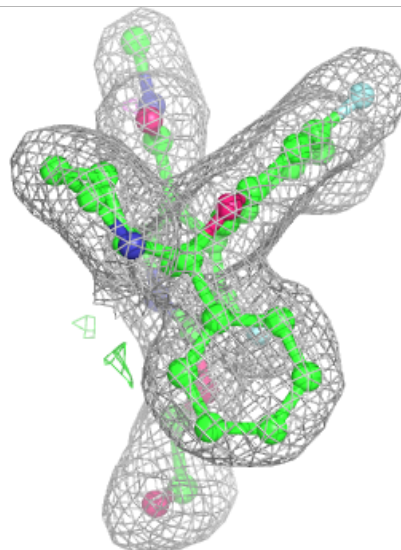
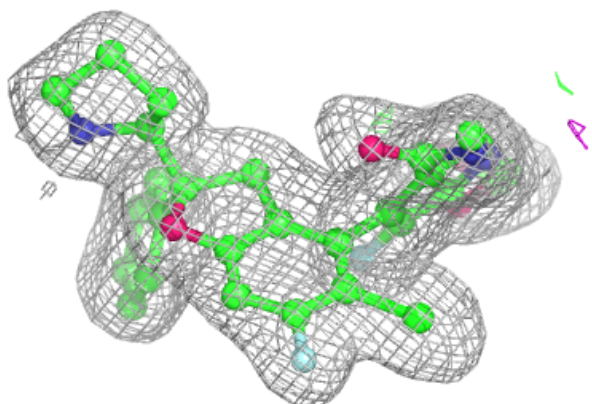
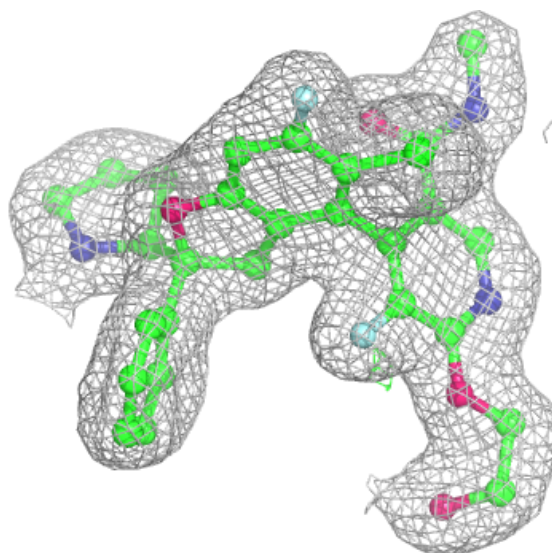
Electron density around WCF B 503:

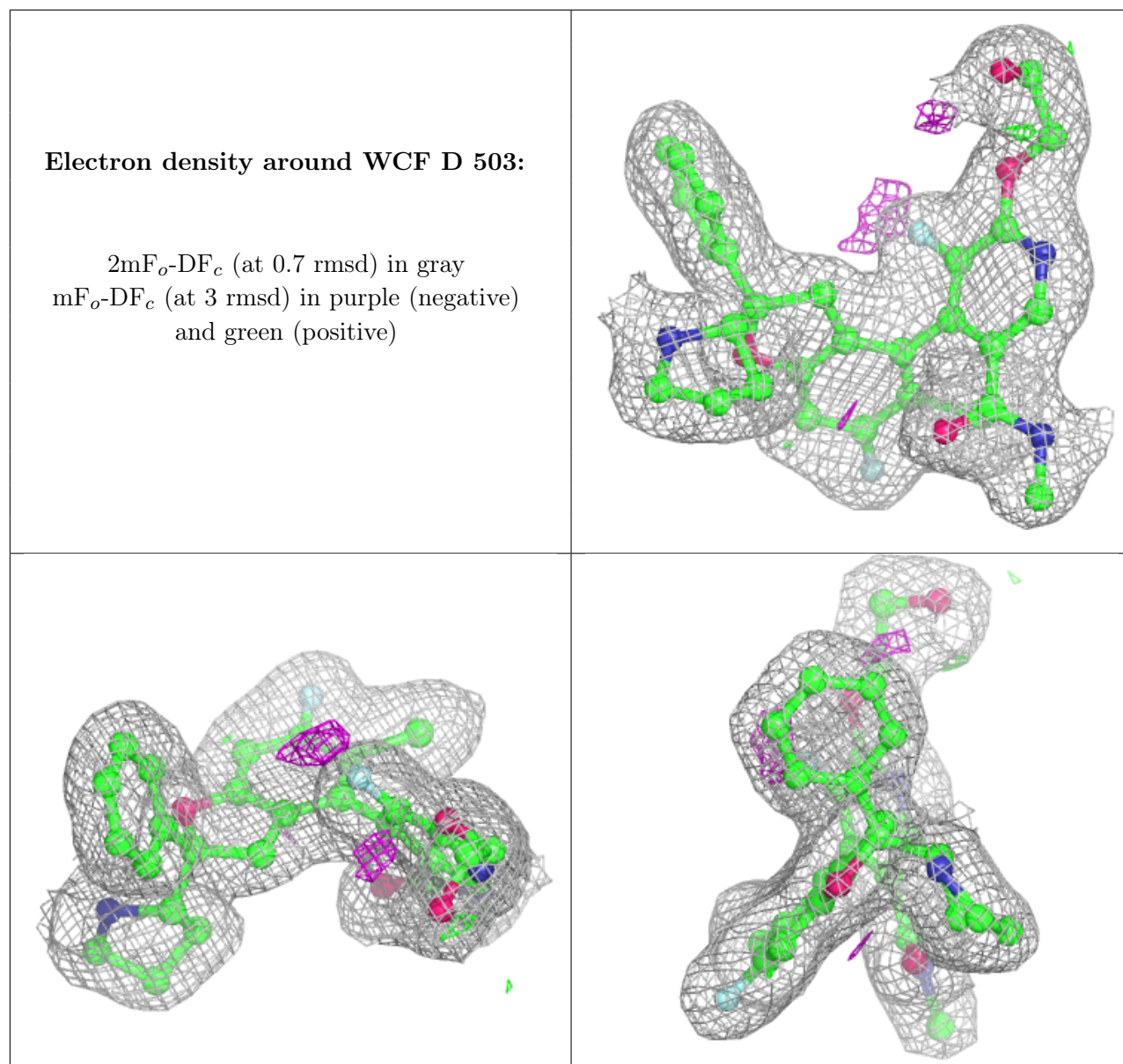
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around WCF C 502:

$2mF_o-DF_c$ (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.