



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2020 – 12:27 PM JST

PDB ID : 6L37
Title : X-ray structure of human PPARalpha ligand binding domain-GW9662-ciprofibrate co-crystals obtained by delipidation and co-crystallization
Authors : Kamata, S.; Saito, K.; Honda, A.; Ishikawa, R.; Oyama, T.; Ishii, I.
Deposited on : 2019-10-09
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

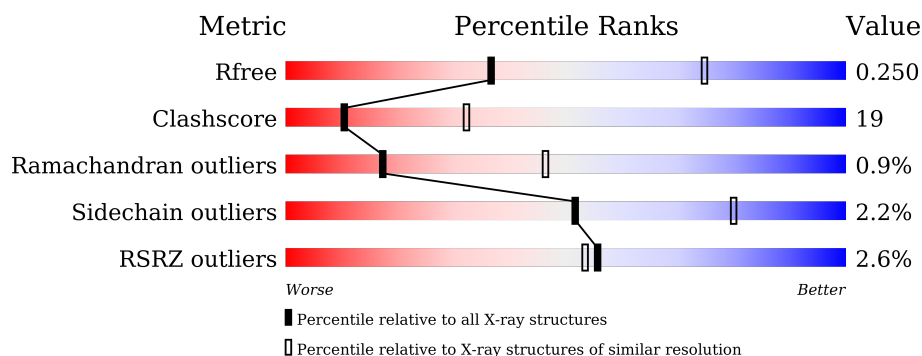
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	273	<div> <div>4%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
1	B	273	<div> <div>%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4471 atoms, of which 80 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.

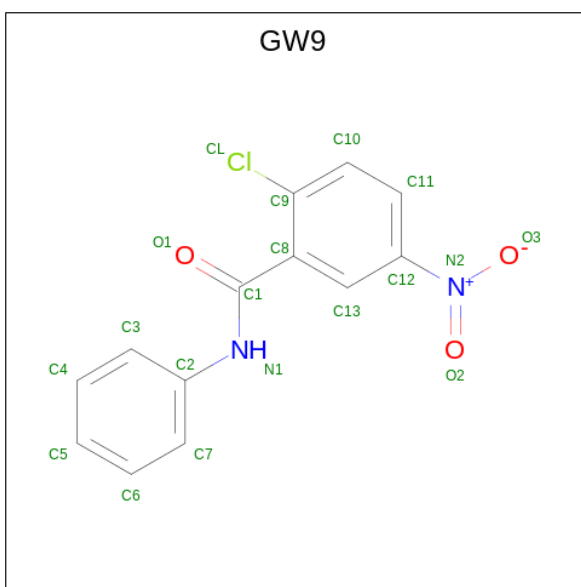
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2125	1364	357	386	18			
1	B	269	Total	C	N	O	S	0	0	0
			2122	1360	355	389	18			

There are 8 discrepancies between the modelled and reference sequences:

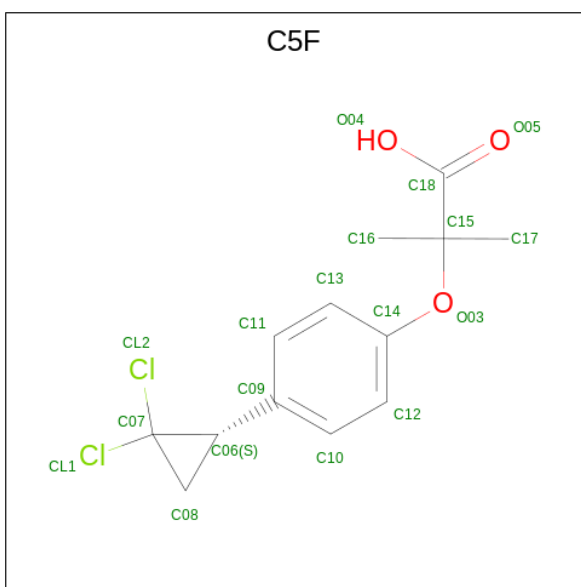
Chain	Residue	Modelled	Actual	Comment	Reference
A	196	GLY	-	expression tag	UNP Q07869
A	197	SER	-	expression tag	UNP Q07869
A	198	HIS	-	expression tag	UNP Q07869
A	199	MET	-	expression tag	UNP Q07869
B	196	GLY	-	expression tag	UNP Q07869
B	197	SER	-	expression tag	UNP Q07869
B	198	HIS	-	expression tag	UNP Q07869
B	199	MET	-	expression tag	UNP Q07869

- Molecule 2 is 2-chloro-5-nitro-N-phenylbenzamide (three-letter code: GW9) (formula: C₁₃H₉ClN₂O₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	13	9	2	3		
2	A	1	Total	C	H	N	O	0	0
			27	13	9	2	3		
2	A	1	Total	C	H	N	O	0	0
			27	13	9	2	3		
2	B	1	Total	C	H	N	O	0	0
			27	13	9	2	3		
2	B	1	Total	C	H	N	O	0	0
			27	13	9	2	3		
2	B	1	Total	C	H	N	O	0	0
			27	13	9	2	3		

- Molecule 3 is 2-{4-[(1S)-2,2-dichlorocyclopropyl]phenoxy}-2-methylpropanoic acid (three-letter code: C5F) (formula: C₁₃H₁₄Cl₂O₃) (labeled as "Ligand of Interest" by author).

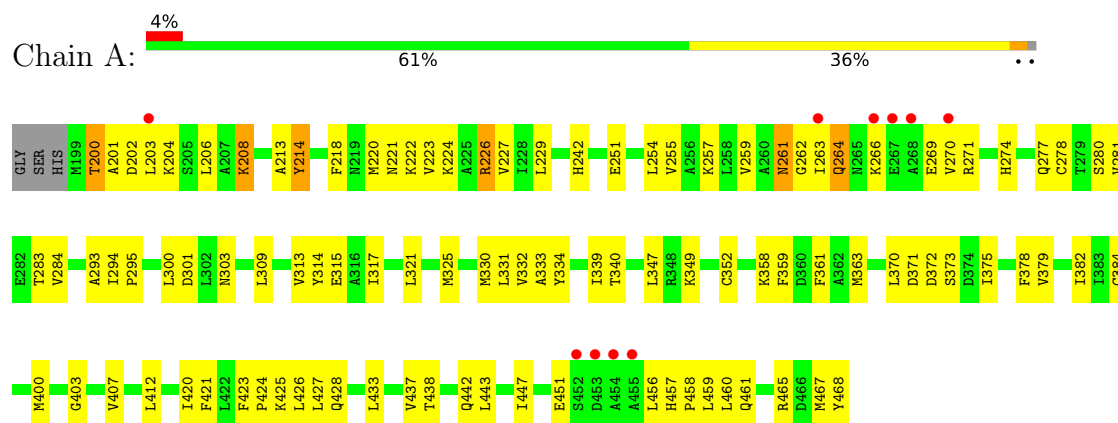


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	O	0	0
			31	13	2	13	3		
3	B	1	Total	C	Cl	H	O	0	0
			31	13	2	13	3		

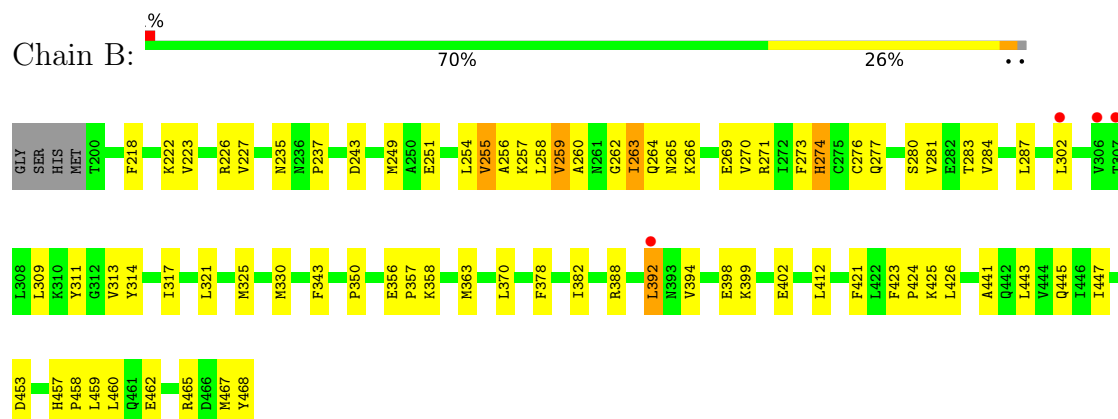
3 Residue-property plots

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: Peroxisome proliferator-activated receptor alpha



- Molecule 1: Peroxisome proliferator-activated receptor alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.01Å 103.26Å 61.13Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	36.48 – 2.91 39.16 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.2 (36.48-2.91) 99.0 (39.16-2.91)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575-000	Depositor
R, R_{free}	0.189 , 0.248 0.191 , 0.250	Depositor DCC
R_{free} test set	824 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4471	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C5F, GW9

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	0.24	0/2163	0.36	0/2918
1	B	0.24	0/2160	0.38	0/2915
All	All	0.24	0/4323	0.37	0/5833

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

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	2125	0	2157	82	0
1	B	2122	0	2148	81	0
2	A	54	27	27	6	0
2	B	54	27	27	2	0
3	A	18	13	0	1	0
3	B	18	13	0	0	0
All	All	4391	80	4359	163	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 19.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:VAL:HG13	1:B:459:LEU:HD23	1.48	0.94
1:B:399:LYS:HE2	1:B:399:LYS:HA	1.50	0.91
1:B:263:ILE:HG23	1:B:266:LYS:HB2	1.54	0.90
1:B:258:LEU:HD13	1:B:264:GLN:HG2	1.53	0.90
1:B:263:ILE:HG21	1:B:271:ARG:HG2	1.54	0.90
1:A:412:LEU:HD11	1:A:426:LEU:HD12	1.58	0.86
1:B:258:LEU:H	1:B:259:VAL:HB	1.41	0.85
1:B:311:TYR:HB2	1:B:388:ARG:HD3	1.58	0.85
1:A:213:ALA:O	1:A:214:TYR:HB3	1.82	0.78
1:B:258:LEU:N	1:B:259:VAL:HB	1.99	0.78
1:B:263:ILE:CG2	1:B:271:ARG:HG2	2.18	0.73
1:A:263:ILE:HA	1:A:266:LYS:HG3	1.71	0.73
1:B:255:VAL:O	1:B:258:LEU:HB2	1.89	0.72
1:A:333:ALA:HA	2:A:502:GW9:H3	1.71	0.71
1:B:258:LEU:HB3	1:B:259:VAL:HG23	1.74	0.70
1:A:270:VAL:O	1:A:274:HIS:HB2	1.91	0.69
1:A:281:VAL:HG13	1:A:459:LEU:HD23	1.75	0.69
1:B:412:LEU:HD11	1:B:426:LEU:HD12	1.75	0.69
1:B:270:VAL:O	1:B:274:HIS:HB2	1.93	0.69
1:A:224:LYS:O	1:A:227:VAL:HG12	1.92	0.68
1:A:206:LEU:HD13	1:A:295:PRO:HG2	1.77	0.67
1:B:263:ILE:HG22	1:B:264:GLN:H	1.60	0.66
1:B:266:LYS:HD2	1:B:453:ASP:HB3	1.78	0.66
1:B:325:MET:HG2	1:B:330:MET:HB3	1.78	0.64
1:B:262:GLY:O	1:B:263:ILE:HD13	1.99	0.63
1:A:277:GLN:OE1	1:A:456:LEU:HD12	1.99	0.62
1:A:339:ILE:HD11	2:A:501:GW9:C7	2.30	0.62
1:B:277:GLN:O	1:B:281:VAL:HG23	2.00	0.62
1:B:280:SER:O	1:B:284:VAL:HG23	2.00	0.61
1:A:277:GLN:HG3	1:A:460:LEU:HD12	1.82	0.60
1:A:467:MET:HG2	1:A:468:TYR:CD2	2.37	0.60
1:B:263:ILE:CG2	1:B:266:LYS:HB2	2.30	0.60
1:B:258:LEU:H	1:B:260:ALA:H	1.50	0.60
1:A:229:LEU:HD21	1:A:331:LEU:HG	1.83	0.60
1:B:378:PHE:CE2	1:B:382:ILE:HD11	2.36	0.60
1:B:273:PHE:O	1:B:277:GLN:HG3	2.02	0.59
1:B:309:LEU:O	1:B:313:VAL:HG13	2.02	0.59
1:A:200:THR:OG1	1:A:201:ALA:N	2.36	0.59
1:B:412:LEU:CD1	1:B:426:LEU:HD12	2.32	0.59
1:A:325:MET:HG2	1:A:330:MET:HB3	1.85	0.58
1:A:456:LEU:HD12	1:A:457:HIS:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:PHE:HB3	1:B:424:PRO:HD3	1.86	0.58
1:B:255:VAL:HG13	1:B:256:ALA:H	1.69	0.58
1:B:218:PHE:HZ	1:B:287:LEU:HD23	1.69	0.58
1:B:370:LEU:HD11	1:B:426:LEU:HD21	1.86	0.57
1:B:314:TYR:OH	1:B:460:LEU:HD22	2.04	0.57
1:A:254:LEU:HD11	1:A:257:LYS:HB2	1.86	0.57
1:A:378:PHE:CE2	1:A:382:ILE:HD11	2.40	0.56
1:B:467:MET:HG2	1:B:468:TYR:CD2	2.39	0.56
1:A:359:PHE:O	1:A:363:MET:HG2	2.05	0.56
1:A:332:VAL:HB	2:A:501:GW9:HN1	1.70	0.56
1:A:280:SER:O	1:A:284:VAL:HG23	2.05	0.56
1:A:317:ILE:O	1:A:321:LEU:HB2	2.06	0.56
1:A:421:PHE:C	1:A:424:PRO:HD2	2.27	0.56
1:A:309:LEU:O	1:A:313:VAL:HG13	2.06	0.55
1:A:421:PHE:O	1:A:425:LYS:HG3	2.06	0.55
1:A:251:GLU:OE1	1:A:271:ARG:NH1	2.39	0.55
1:A:313:VAL:O	1:A:317:ILE:HG13	2.06	0.55
1:B:313:VAL:O	1:B:317:ILE:HG13	2.06	0.55
1:B:251:GLU:HA	2:B:502:GW9:O2	2.07	0.55
1:A:257:LYS:O	1:A:261:ASN:HB2	2.07	0.55
1:A:203:LEU:HD22	1:A:407:VAL:HG22	1.88	0.55
1:B:254:LEU:O	1:B:255:VAL:HB	2.08	0.54
1:A:223:VAL:HG23	1:A:372:ASP:OD2	2.08	0.54
1:B:258:LEU:O	1:B:263:ILE:HG12	2.07	0.53
1:A:214:TYR:HA	1:A:218:PHE:CD2	2.43	0.53
1:A:315:GLU:HG2	1:A:437:VAL:HG21	1.91	0.53
1:A:213:ALA:O	1:A:214:TYR:CB	2.55	0.53
1:B:257:LYS:HG2	1:B:257:LYS:O	2.07	0.53
1:B:257:LYS:HA	1:B:260:ALA:HB3	1.89	0.53
1:A:204:LYS:O	1:A:208:LYS:HD2	2.08	0.53
1:B:421:PHE:O	1:B:425:LYS:HG3	2.08	0.53
1:A:349:LYS:HG2	1:A:352:CYS:SG	2.49	0.53
1:A:254:LEU:CD1	1:A:257:LYS:HB2	2.40	0.52
1:A:294:ILE:HG21	1:A:384:CYS:SG	2.50	0.52
1:A:447:ILE:HG23	1:A:451:GLU:HG3	1.90	0.52
1:A:300:LEU:HD11	1:A:400:MET:HE2	1.92	0.52
1:A:255:VAL:O	1:A:259:VAL:HG23	2.10	0.52
1:A:371:ASP:OD1	1:A:373:SER:HB3	2.10	0.52
1:A:465:ARG:HB3	1:A:465:ARG:NH2	2.25	0.52
1:B:273:PHE:HA	1:B:276:CYS:HB2	1.91	0.52
1:B:399:LYS:CA	1:B:399:LYS:HE2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:TYR:OH	1:A:460:LEU:HD22	2.10	0.51
1:B:255:VAL:HG13	1:B:256:ALA:N	2.25	0.51
1:A:221:ASN:HD21	1:A:224:LYS:HE3	1.74	0.51
1:B:394:VAL:O	1:B:398:GLU:HG3	2.10	0.51
1:A:262:GLY:O	1:A:263:ILE:HD13	2.09	0.51
1:A:412:LEU:CD1	1:A:426:LEU:HD12	2.37	0.51
1:B:363:MET:HA	1:B:363:MET:CE	2.41	0.51
1:B:378:PHE:O	1:B:382:ILE:HG13	2.12	0.50
1:B:457:HIS:CG	1:B:458:PRO:HD2	2.47	0.50
1:B:258:LEU:O	1:B:263:ILE:N	2.45	0.49
1:A:263:ILE:CA	1:A:266:LYS:HG3	2.42	0.49
1:A:315:GLU:CG	1:A:437:VAL:HG21	2.43	0.49
1:B:263:ILE:HG22	1:B:264:GLN:N	2.26	0.49
1:B:443:LEU:O	1:B:447:ILE:HG13	2.13	0.49
1:A:370:LEU:HD11	1:A:426:LEU:HD21	1.93	0.49
1:A:423:PHE:HB3	1:A:424:PRO:HD3	1.94	0.49
1:B:269:GLU:N	1:B:269:GLU:OE1	2.38	0.49
1:A:263:ILE:HG23	1:A:266:LYS:HG3	1.94	0.49
1:A:403:GLY:O	1:A:407:VAL:HG23	2.13	0.49
2:B:501:GW9:O1	2:B:501:GW9:H3	2.11	0.48
1:A:438:THR:O	1:A:442:GLN:HG3	2.13	0.48
1:B:392:LEU:H	1:B:392:LEU:HD23	1.78	0.48
1:B:263:ILE:O	1:B:264:GLN:HB2	2.12	0.48
1:B:358:LYS:N	1:B:358:LYS:HD2	2.28	0.48
1:A:457:HIS:CG	1:A:458:PRO:HD2	2.48	0.48
1:B:223:VAL:O	1:B:227:VAL:HG23	2.13	0.47
1:B:258:LEU:CB	1:B:259:VAL:HG23	2.43	0.47
1:B:259:VAL:H	1:B:263:ILE:H	1.61	0.47
1:B:350:PRO:HG2	1:B:447:ILE:HG12	1.95	0.47
1:B:259:VAL:HG12	1:B:260:ALA:N	2.29	0.47
1:B:421:PHE:C	1:B:424:PRO:HD2	2.35	0.47
1:A:254:LEU:HB2	2:A:502:GW9:O2	2.15	0.47
1:A:363:MET:HE2	1:A:363:MET:HA	1.97	0.47
1:A:358:LYS:HD2	1:A:358:LYS:N	2.29	0.46
1:B:311:TYR:HB3	1:B:388:ARG:NH1	2.30	0.46
1:B:283:THR:HG21	1:B:317:ILE:HG12	1.98	0.46
1:A:293:ALA:O	1:A:295:PRO:HD3	2.16	0.46
1:B:356:GLU:HB3	1:B:357:PRO:HD3	1.98	0.46
1:A:242:HIS:HB3	1:A:340:THR:HG21	1.98	0.46
1:A:427:LEU:HB2	1:B:249:MET:HE3	1.97	0.45
1:B:258:LEU:H	1:B:260:ALA:N	2.12	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LEU:N	1:B:392:LEU:HD23	2.31	0.45
1:A:263:ILE:HG22	1:A:263:ILE:O	2.16	0.45
1:A:206:LEU:CD1	1:A:295:PRO:HG2	2.45	0.45
1:A:269:GLU:HG3	1:A:347:LEU:HB3	1.99	0.45
1:B:255:VAL:O	1:B:259:VAL:HG21	2.17	0.45
1:B:311:TYR:CB	1:B:388:ARG:HD3	2.40	0.45
1:B:235:ASN:O	1:B:237:PRO:HD3	2.17	0.45
2:A:501:GW9:O1	2:A:501:GW9:H7	2.17	0.44
1:B:243:ASP:HA	1:B:343:PHE:CD1	2.52	0.44
1:A:263:ILE:CG2	1:A:266:LYS:HG3	2.48	0.44
1:B:258:LEU:CA	1:B:259:VAL:HB	2.47	0.44
1:B:222:LYS:O	1:B:226:ARG:HG2	2.18	0.44
1:A:465:ARG:HB3	1:A:465:ARG:HH21	1.83	0.44
1:B:259:VAL:N	1:B:263:ILE:H	2.16	0.44
1:A:222:LYS:O	1:A:226:ARG:HB2	2.17	0.43
1:B:255:VAL:HA	1:B:258:LEU:HD12	2.01	0.43
1:A:301:ASP:OD2	1:A:303:ASN:HB2	2.19	0.42
1:A:259:VAL:HA	1:A:264:GLN:CG	2.49	0.42
1:B:462:GLU:OE2	1:B:465:ARG:NH1	2.52	0.42
1:A:375:ILE:O	1:A:379:VAL:HG23	2.20	0.42
1:A:277:GLN:HA	3:A:504:C5F:O05	2.18	0.42
1:B:321:LEU:HG	1:B:325:MET:CE	2.49	0.42
1:A:220:MET:HE3	1:A:334:TYR:HA	2.01	0.42
1:B:321:LEU:HG	1:B:325:MET:HE3	2.01	0.42
1:A:229:LEU:HD21	1:A:331:LEU:CG	2.47	0.42
1:B:441:ALA:O	1:B:445:GLN:HG2	2.20	0.42
1:A:443:LEU:O	1:A:447:ILE:HG13	2.20	0.41
1:A:456:LEU:HD21	1:A:461:GLN:HA	2.02	0.41
1:B:258:LEU:H	1:B:259:VAL:CB	2.21	0.41
1:A:251:GLU:HA	2:A:502:GW9:O3	2.20	0.41
1:A:420:ILE:HG22	1:A:421:PHE:CD1	2.55	0.41
1:A:262:GLY:HA2	1:A:264:GLN:NE2	2.36	0.41
1:A:208:LYS:HE2	1:A:208:LYS:HA	2.02	0.41
1:A:283:THR:HG21	1:A:317:ILE:HG12	2.03	0.41
1:B:254:LEU:O	1:B:255:VAL:CB	2.69	0.41
1:A:264:GLN:CD	1:A:264:GLN:H	2.22	0.41
1:A:361:PHE:CZ	1:A:433:LEU:HD21	2.56	0.41
1:A:428:GLN:N	1:B:249:MET:HE1	2.36	0.41
1:B:218:PHE:CZ	1:B:287:LEU:HD23	2.52	0.41
1:B:263:ILE:C	1:B:265:ASN:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/273 (98%)	255 (95%)	11 (4%)	2 (1%)	22	53
1	B	267/273 (98%)	253 (95%)	11 (4%)	3 (1%)	14	41
All	All	535/546 (98%)	508 (95%)	22 (4%)	5 (1%)	17	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	THR
1	B	255	VAL
1	B	259	VAL
1	A	214	TYR
1	B	263	ILE

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	232/238 (98%)	226 (97%)	6 (3%)	46	76
1	B	233/238 (98%)	229 (98%)	4 (2%)	60	84
All	All	465/476 (98%)	455 (98%)	10 (2%)	52	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ASP

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Mol	Chain	Res	Type
1	A	208	LYS
1	A	226	ARG
1	A	261	ASN
1	A	264	GLN
1	A	278	CYS
1	B	274	HIS
1	B	302	LEU
1	B	392	LEU
1	B	402	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
2	GW9	A	502	1	18,19,20	1.40	4 (22%)	23,25,27	0.77	1 (4%)
2	GW9	B	503	1	18,19,20	1.41	4 (22%)	23,25,27	0.74	0
3	C5F	A	504	-	16,19,19	5.26	8 (50%)	25,30,30	2.37	5 (20%)
2	GW9	A	503	1	18,19,20	1.40	4 (22%)	23,25,27	0.90	1 (4%)
3	C5F	B	504	-	16,19,19	5.23	8 (50%)	25,30,30	2.38	5 (20%)
2	GW9	B	502	1	18,19,20	1.44	4 (22%)	23,25,27	0.72	0
2	GW9	B	501	1	18,19,20	1.45	4 (22%)	23,25,27	0.66	0
2	GW9	A	501	1	18,19,20	1.44	4 (22%)	23,25,27	0.66	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
2	GW9	A	502	1	-	2/10/12/12	0/2/2/2
2	GW9	B	503	1	-	6/10/12/12	0/2/2/2
3	C5F	A	504	-	-	0/9/23/23	0/2/2/2
2	GW9	A	503	1	-	4/10/12/12	0/2/2/2
3	C5F	B	504	-	-	0/9/23/23	0/2/2/2
2	GW9	B	502	1	-	2/10/12/12	0/2/2/2
2	GW9	B	501	1	-	2/10/12/12	0/2/2/2
2	GW9	A	501	1	-	2/10/12/12	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	C5F	C10-C09	9.07	1.53	1.39
3	B	504	C5F	C11-C09	9.07	1.53	1.39
3	A	504	C5F	C11-C09	9.02	1.53	1.39
3	B	504	C5F	C10-C09	8.97	1.53	1.39
3	A	504	C5F	C13-C11	8.19	1.53	1.38
3	A	504	C5F	C12-C10	8.15	1.53	1.38
3	B	504	C5F	C12-C10	8.13	1.53	1.38
3	B	504	C5F	C13-C11	8.11	1.53	1.38
3	A	504	C5F	C13-C14	7.60	1.53	1.38
3	B	504	C5F	C12-C14	7.52	1.53	1.38
3	B	504	C5F	C13-C14	7.50	1.53	1.38
3	A	504	C5F	C12-C14	7.50	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	GW9	C1-N1	4.01	1.46	1.35
2	B	502	GW9	C1-N1	3.99	1.46	1.35
2	A	501	GW9	C1-N1	3.97	1.46	1.35
2	B	503	GW9	C1-N1	3.90	1.46	1.35
2	A	502	GW9	C1-N1	3.87	1.46	1.35
2	A	503	GW9	C1-N1	3.85	1.46	1.35
3	A	504	C5F	C07-C06	3.63	1.53	1.51
3	B	504	C5F	C07-C06	3.47	1.53	1.51
2	A	501	GW9	O2-N2	-2.92	1.17	1.22
2	B	502	GW9	O2-N2	-2.91	1.17	1.22
2	B	501	GW9	O2-N2	-2.90	1.17	1.22
2	A	502	GW9	O2-N2	-2.86	1.18	1.22
2	B	503	GW9	O2-N2	-2.86	1.18	1.22
3	A	504	C5F	C08-C07	2.81	1.53	1.48
2	A	503	GW9	O2-N2	-2.76	1.18	1.22
3	B	504	C5F	C08-C07	2.76	1.53	1.48
2	B	501	GW9	C2-N1	2.42	1.46	1.41
2	A	501	GW9	C2-N1	2.33	1.46	1.41
2	A	503	GW9	O1-C1	-2.31	1.18	1.23
2	B	502	GW9	C2-N1	2.26	1.46	1.41
2	A	502	GW9	O1-C1	-2.26	1.18	1.23
2	B	503	GW9	C2-N1	2.26	1.46	1.41
2	B	501	GW9	O1-C1	-2.23	1.18	1.23
2	B	502	GW9	O1-C1	-2.23	1.18	1.23
2	B	503	GW9	O1-C1	-2.22	1.18	1.23
2	A	501	GW9	O1-C1	-2.19	1.18	1.23
2	A	503	GW9	C2-N1	2.12	1.46	1.41
2	A	502	GW9	C2-N1	2.09	1.45	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	C5F	CL2-C07-CL1	8.32	120.27	110.09
3	A	504	C5F	CL2-C07-CL1	8.26	120.20	110.09
3	A	504	C5F	C08-C06-C09	5.25	131.72	123.45
3	B	504	C5F	C08-C06-C09	5.19	131.63	123.45
3	A	504	C5F	C15-O03-C14	-3.16	115.69	121.04
3	B	504	C5F	C15-O03-C14	-2.97	116.00	121.04
3	A	504	C5F	C08-C07-CL2	-2.70	115.52	118.85
3	B	504	C5F	C08-C07-CL1	-2.65	115.57	118.85
3	B	504	C5F	C08-C07-CL2	-2.62	115.61	118.85
3	A	504	C5F	C08-C07-CL1	-2.55	115.70	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	GW9	C2-N1-C1	-2.48	120.14	126.58
2	A	502	GW9	C2-N1-C1	-2.10	121.14	126.58

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	503	GW9	C11-C12-N2-O2
2	B	503	GW9	C13-C12-N2-O2
2	A	503	GW9	C11-C12-N2-O2
2	A	503	GW9	C13-C12-N2-O2
2	B	502	GW9	C11-C12-N2-O2
2	B	502	GW9	C13-C12-N2-O2
2	B	501	GW9	C11-C12-N2-O2
2	B	501	GW9	C13-C12-N2-O2
2	A	501	GW9	C11-C12-N2-O2
2	A	501	GW9	C13-C12-N2-O2
2	B	503	GW9	O1-C1-C8-C9
2	B	503	GW9	N1-C1-C8-C9
2	B	503	GW9	O1-C1-C8-C13
2	B	503	GW9	N1-C1-C8-C13
2	A	502	GW9	C7-C2-N1-C1
2	A	503	GW9	C7-C2-N1-C1
2	A	502	GW9	C3-C2-N1-C1
2	A	503	GW9	C3-C2-N1-C1

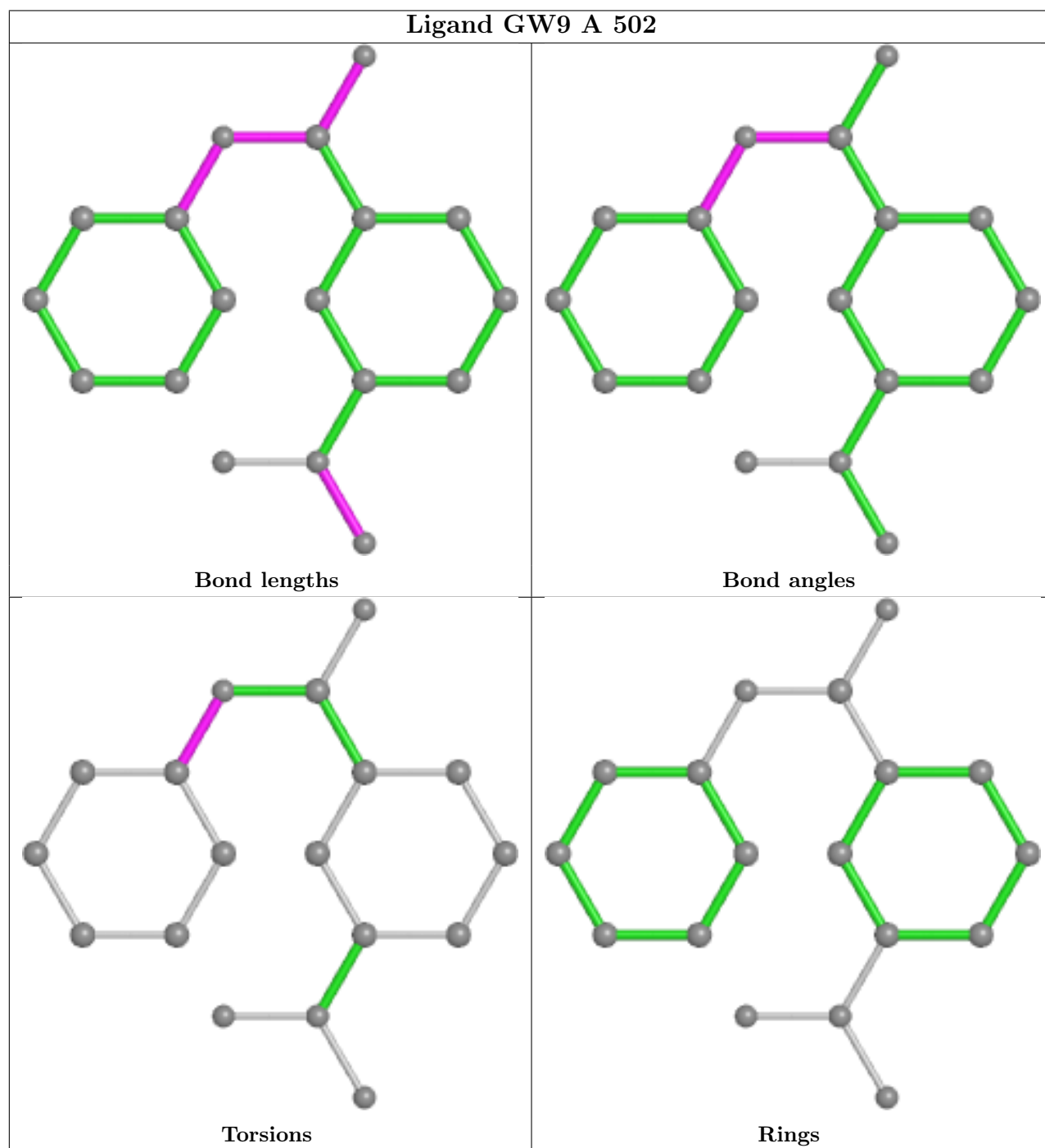
There are no ring outliers.

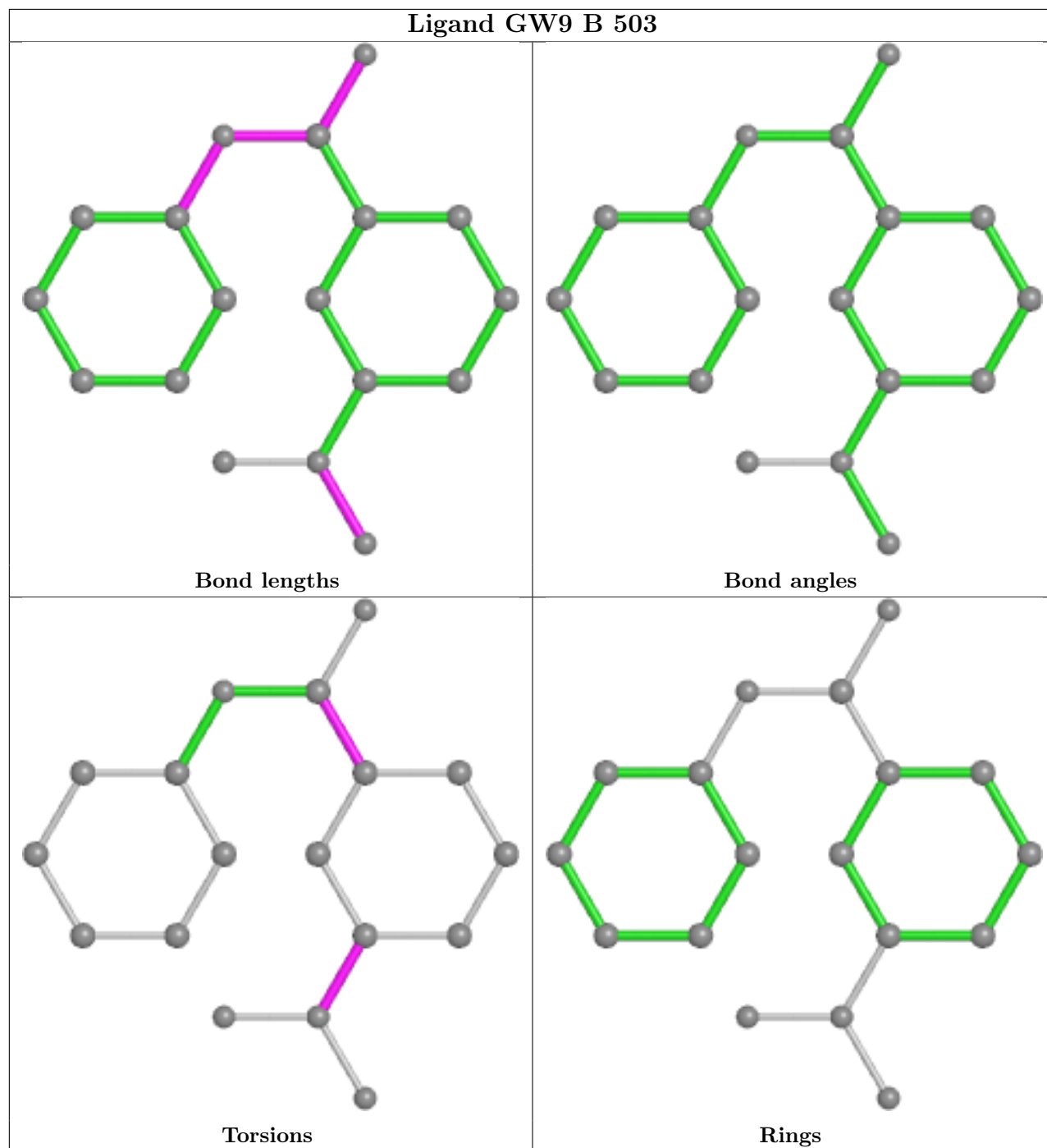
5 monomers are involved in 9 short contacts:

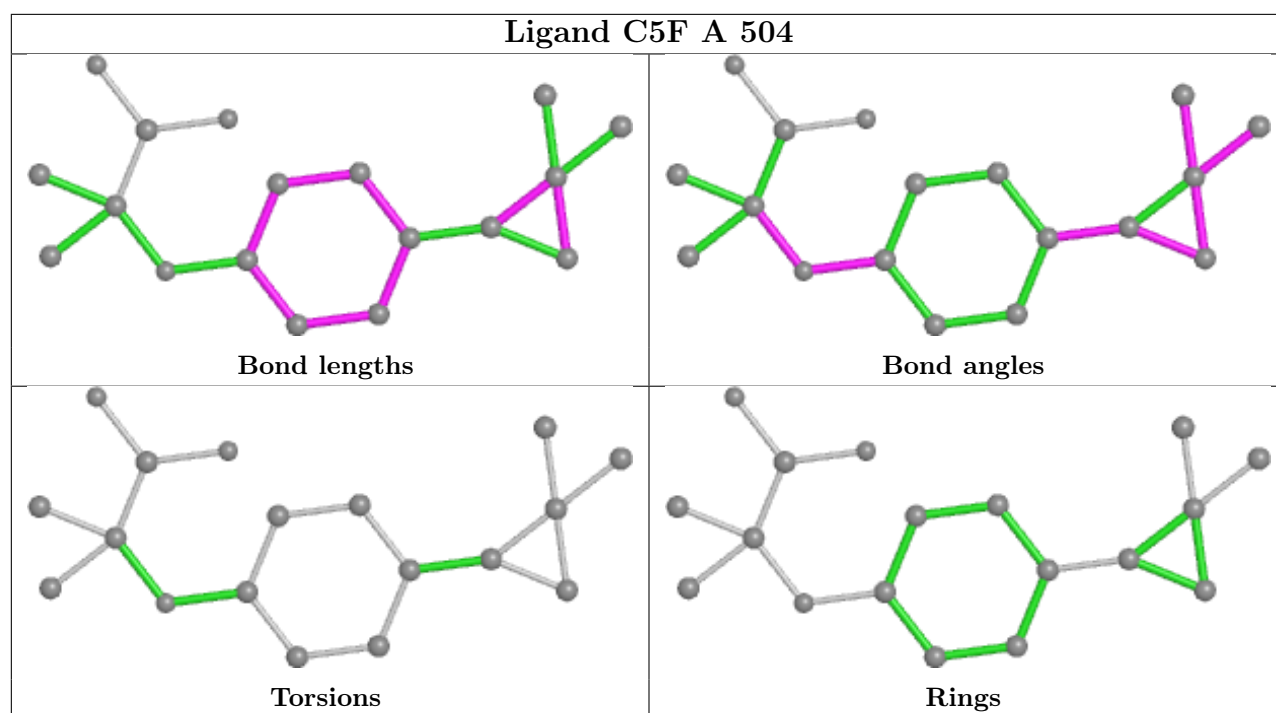
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	GW9	3	0
3	A	504	C5F	1	0
2	B	502	GW9	1	0
2	B	501	GW9	1	0
2	A	501	GW9	3	0

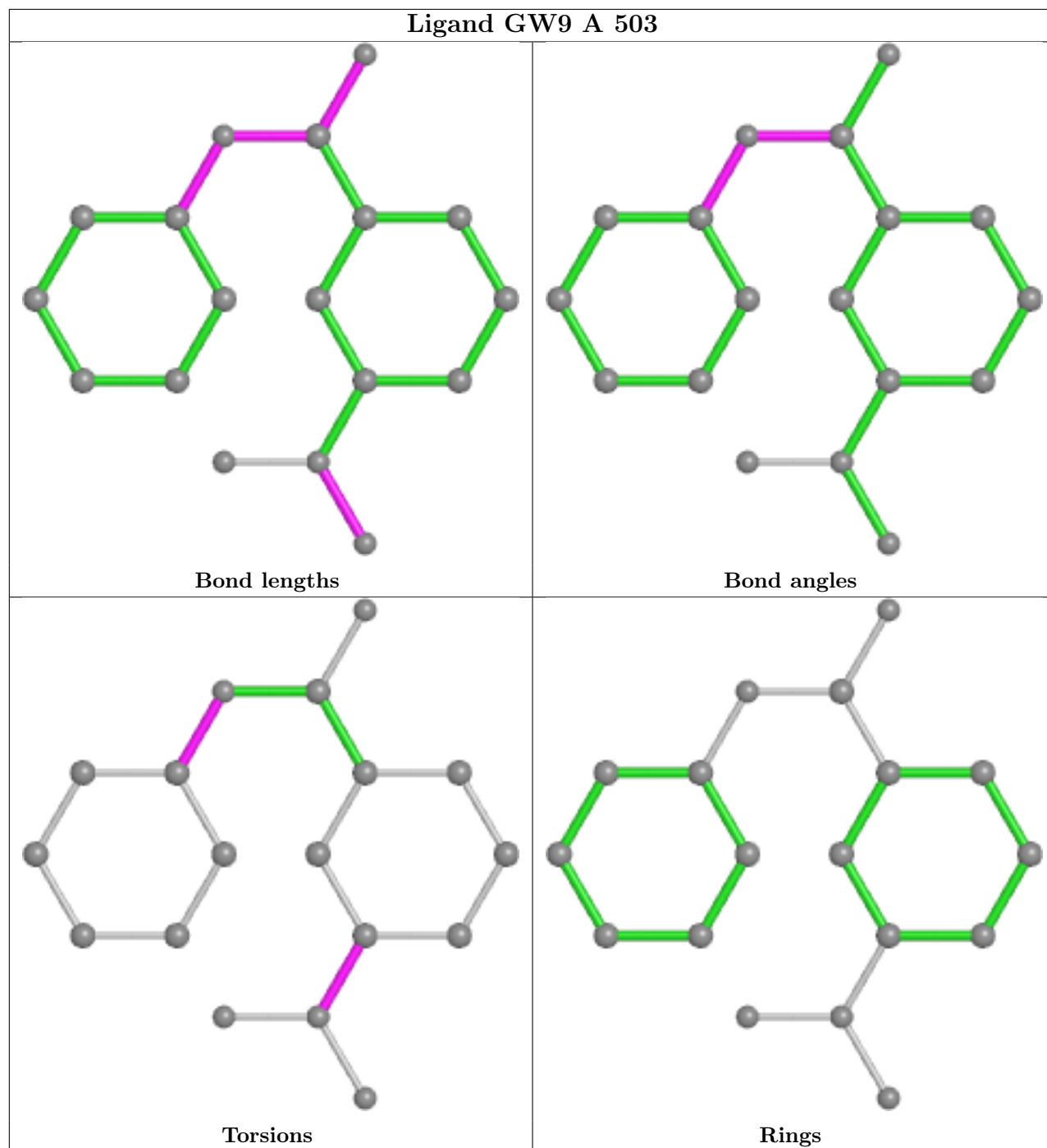
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

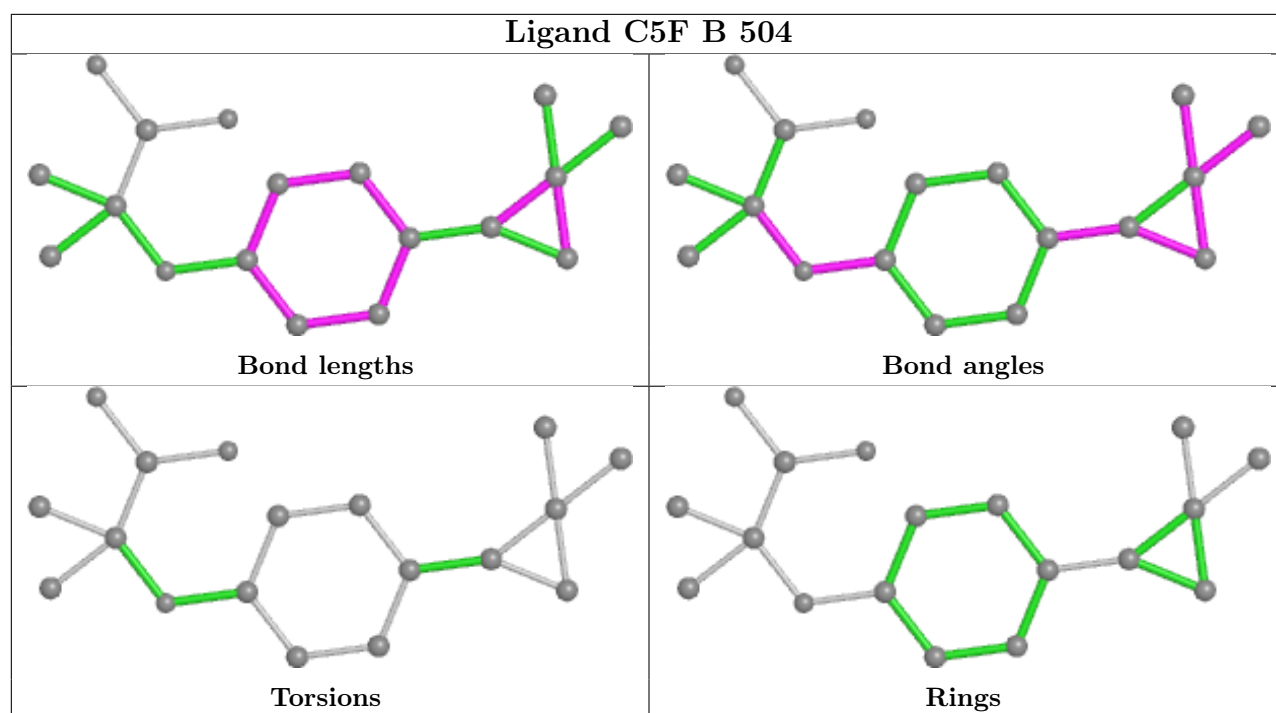
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

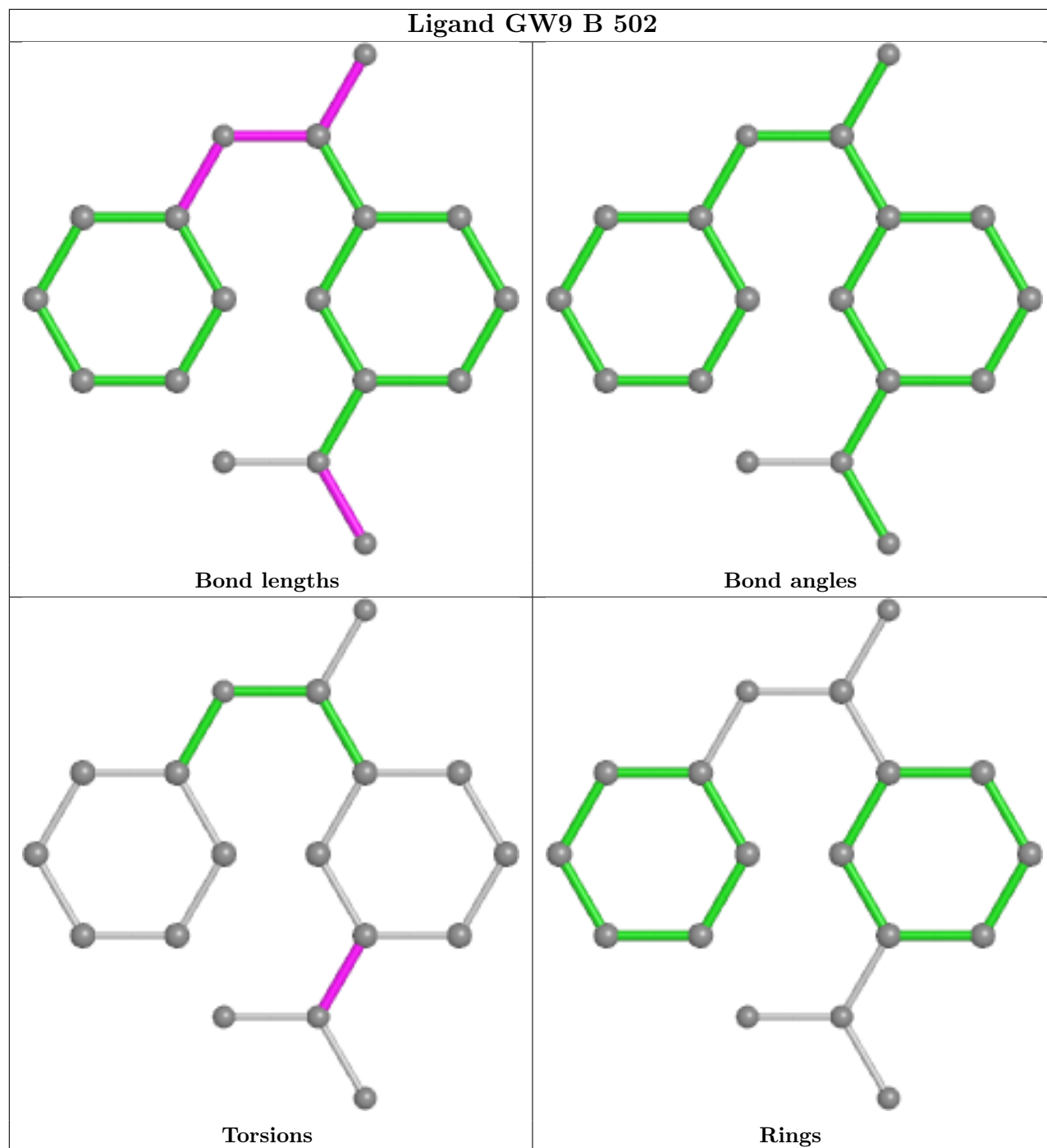


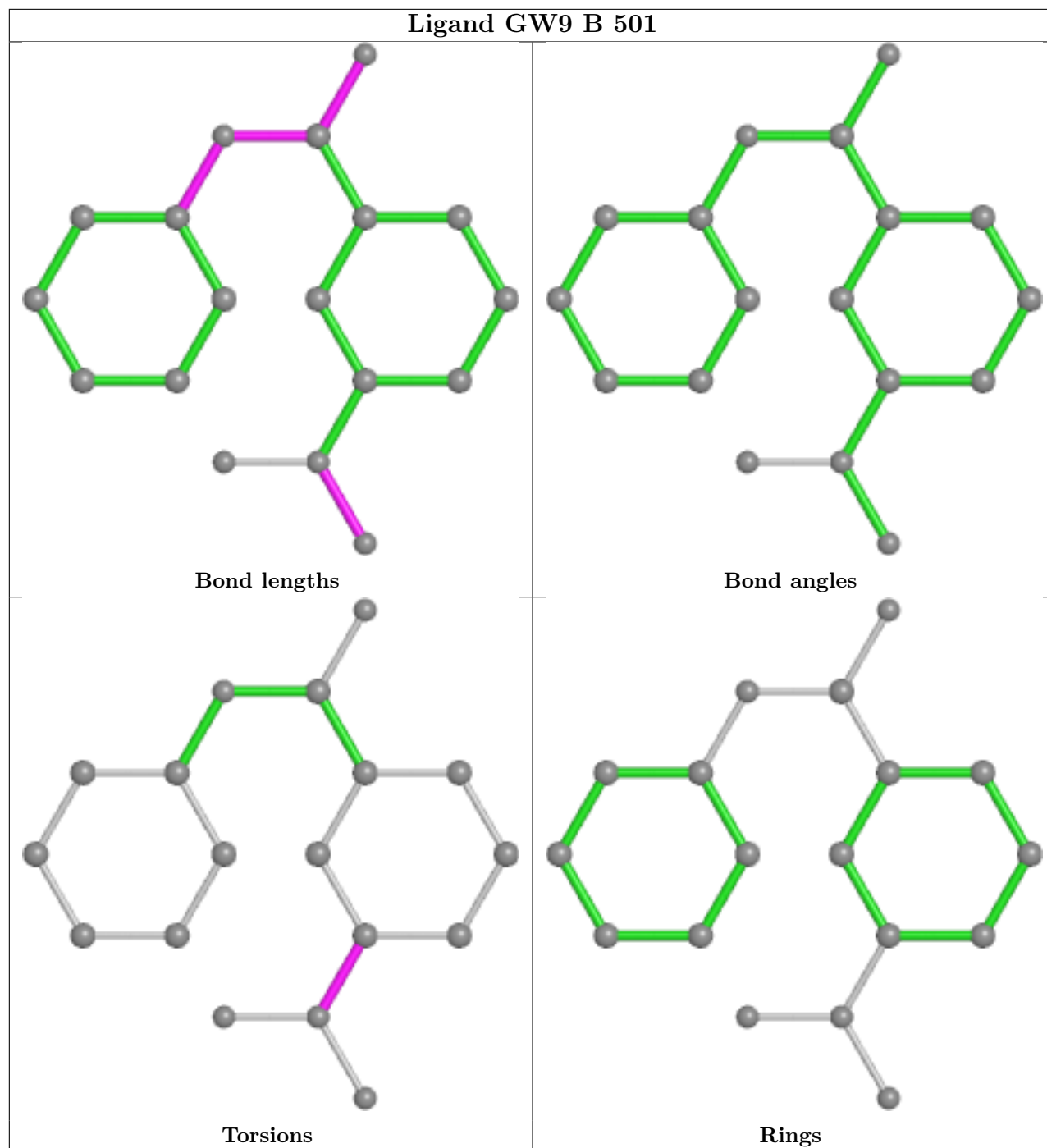


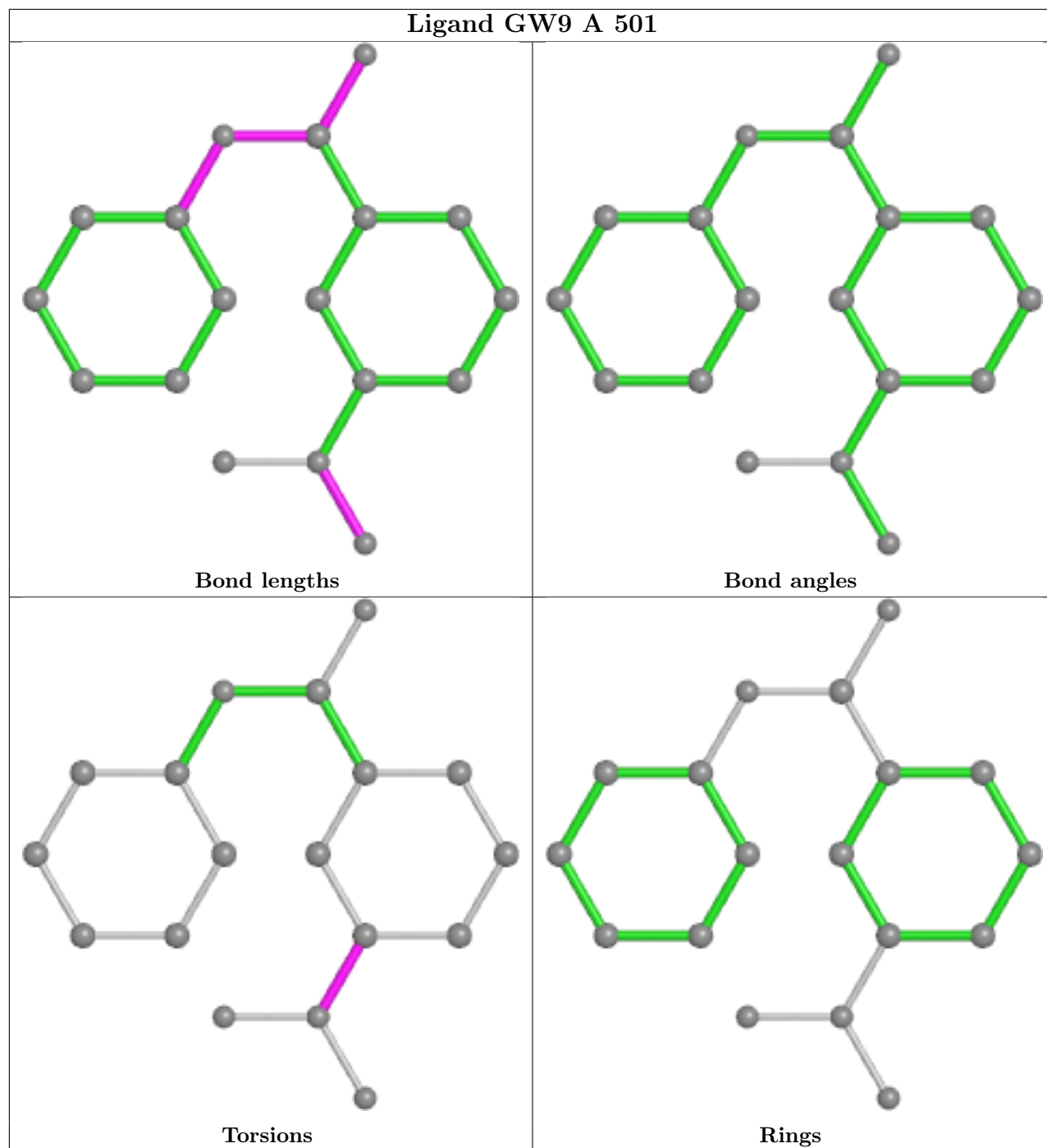












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	270/273 (98%)	0.19	10 (3%) 41 38	54, 80, 116, 150	0
1	B	269/273 (98%)	0.05	4 (1%) 73 73	55, 80, 116, 132	0
All	All	539/546 (98%)	0.12	14 (2%) 56 53	54, 80, 117, 150	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	ALA	4.3
1	A	454	ALA	4.0
1	A	203	LEU	3.4
1	A	453	ASP	3.2
1	B	302	LEU	3.0
1	B	306	VAL	2.8
1	A	263	ILE	2.7
1	A	270	VAL	2.6
1	A	266	LYS	2.3
1	A	452	SER	2.1
1	A	267	GLU	2.0
1	B	307	THR	2.0
1	A	268	ALA	2.0
1	B	392	LEU	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](#)

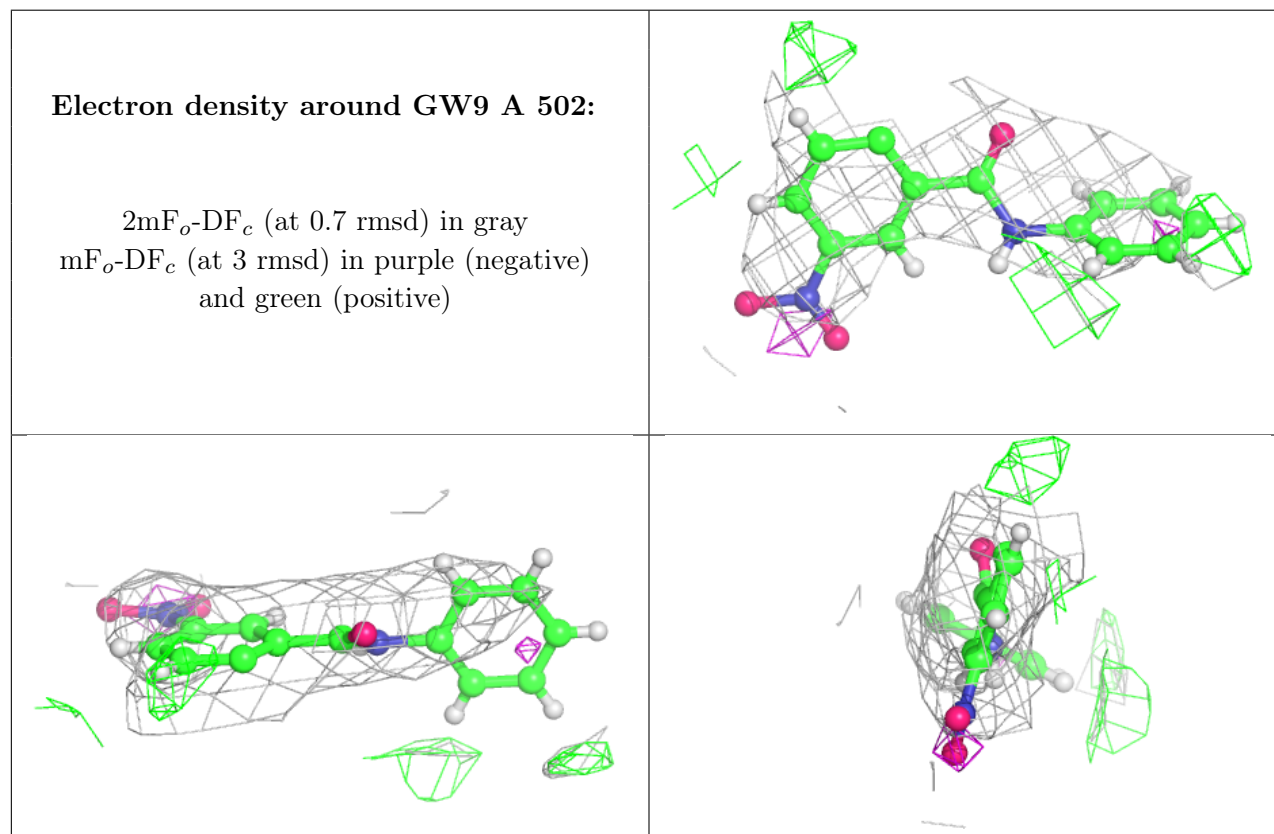
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

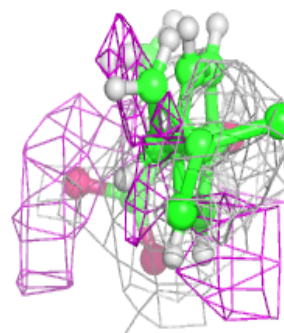
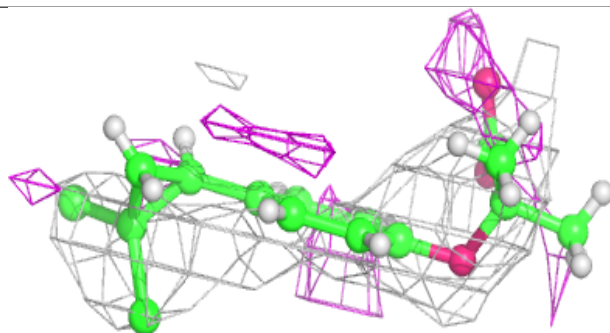
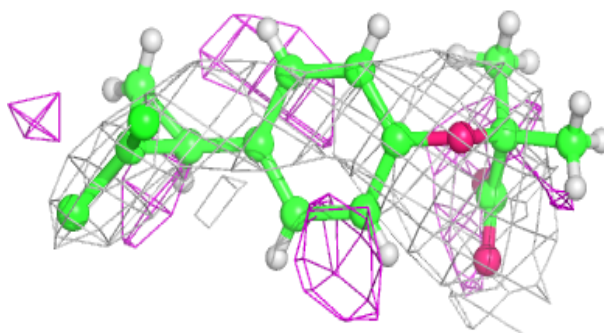
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GW9	A	502	18/19	0.82	0.32	97,116,162,183	0
3	C5F	A	504	18/18	0.83	0.66	97,124,161,175	0
2	GW9	A	503	18/19	0.85	0.32	111,121,145,146	0
2	GW9	A	501	18/19	0.87	0.40	70,111,137,139	0
3	C5F	B	504	18/18	0.88	0.45	83,104,135,160	0
2	GW9	B	503	18/19	0.91	0.29	95,108,125,133	0
2	GW9	B	501	18/19	0.92	0.33	64,91,111,130	0
2	GW9	B	502	18/19	0.93	0.25	78,105,142,150	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.

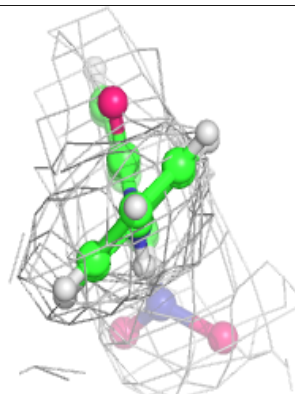
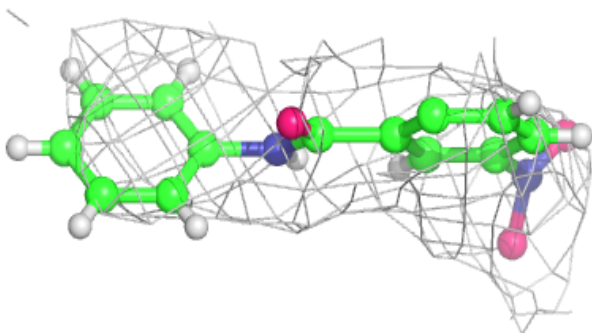
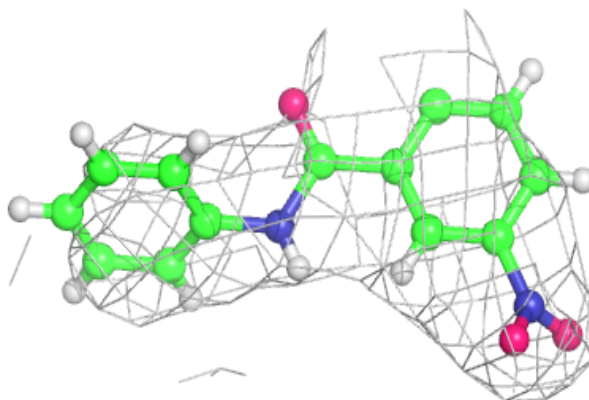


Electron density around C5F A 504:

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

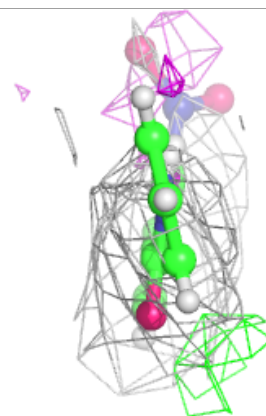
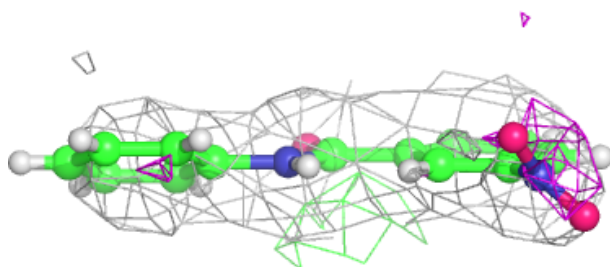
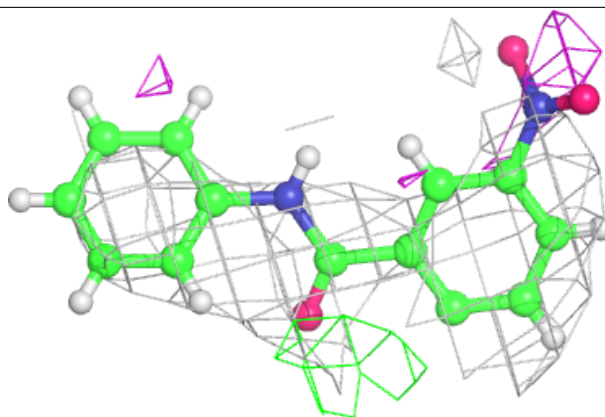
**Electron density around GW9 A 503:**

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

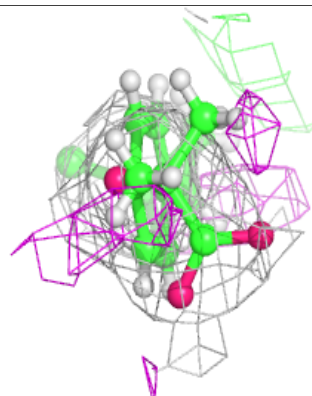
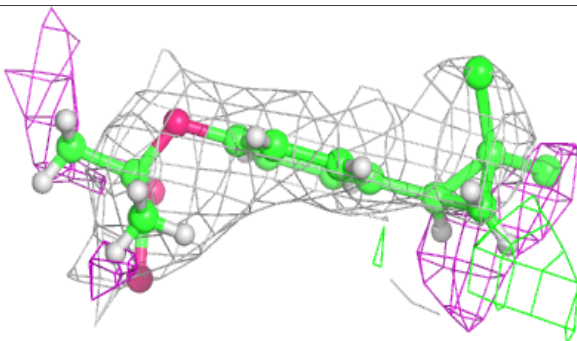
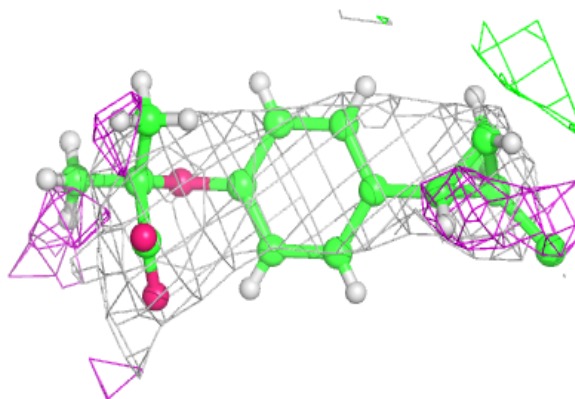


Electron density around GW9 A 501:

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

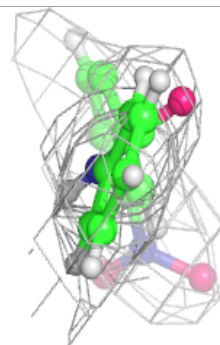
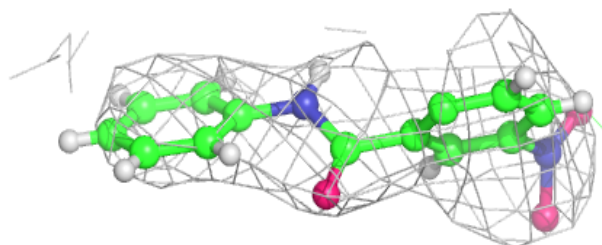
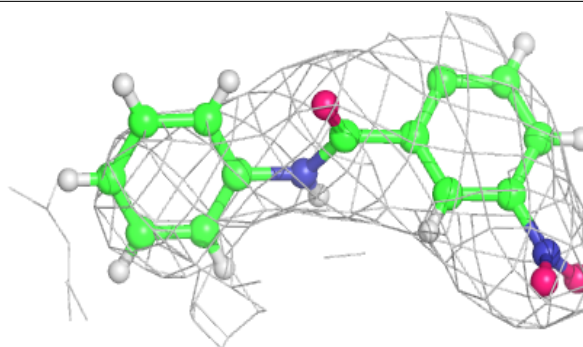
**Electron density around C5F B 504:**

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

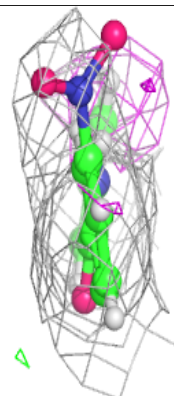
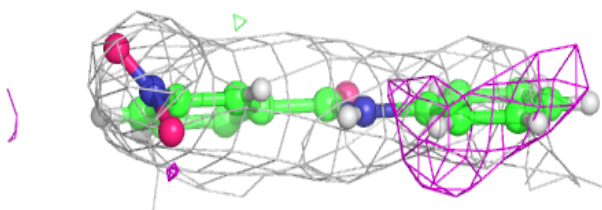
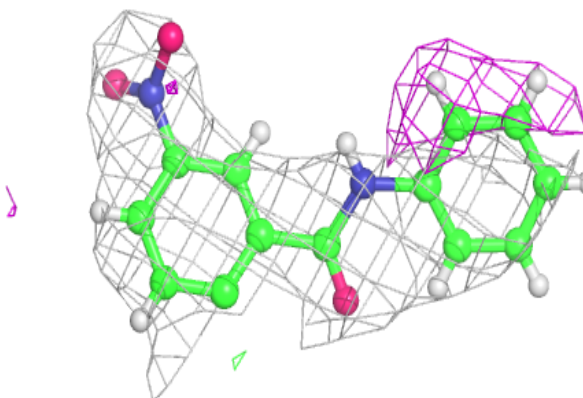


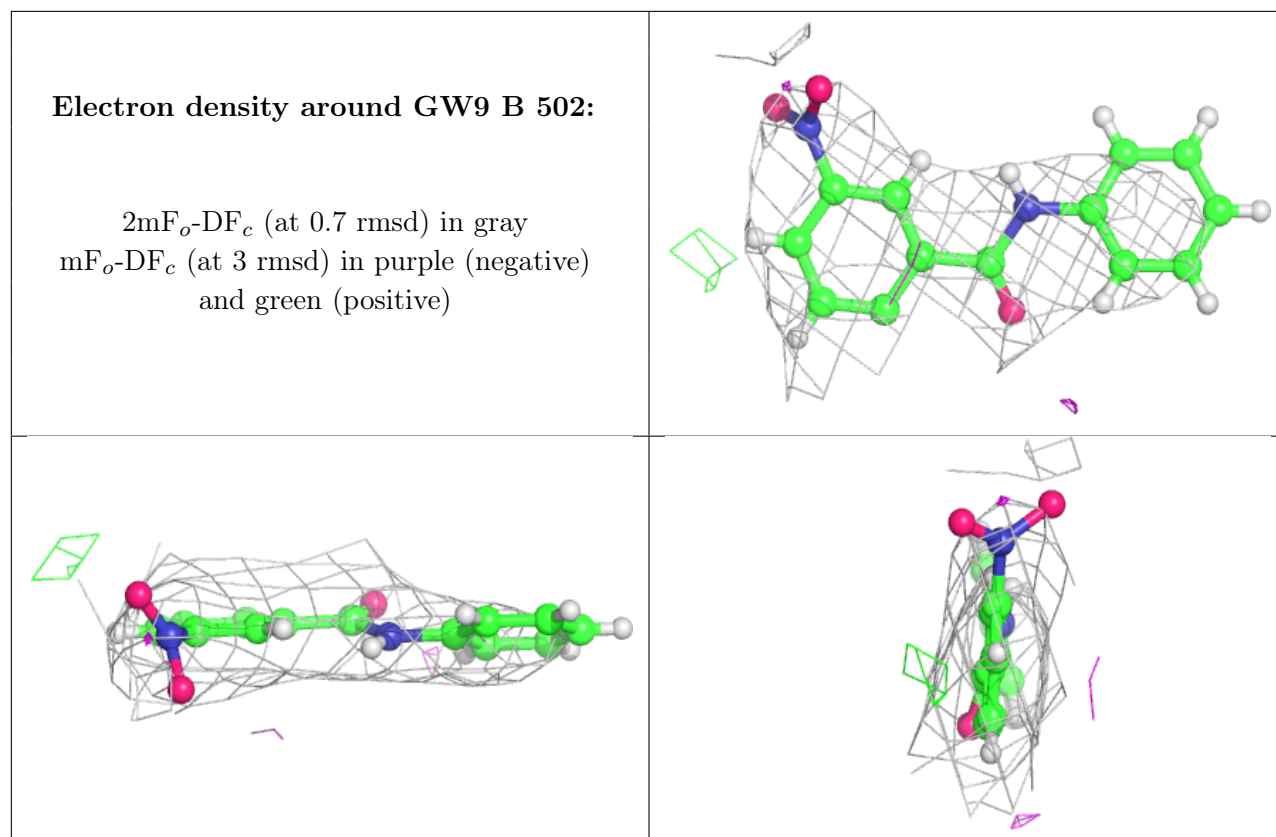
Electron density around GW9 B 503:

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

**Electron density around GW9 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.