



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:37 PM UTC

PDB ID : 8EV2 / pdb\_00008ev2  
Title : Dual Modulators  
Authors : Tinivella, A.; Nwachukwu, J.C.; Angeli, A.; Foschi, F.; Benatti, A.L.; Pinzi, L.; Izard, T.; Ferraroni, M.; Rangarajan, E.S.; Christodoulou, M.; Passarella, D.; Supuran, C.; Nettles, K.W.; Rastelli, G.  
Deposited on : 2022-10-19  
Resolution : 2.01 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

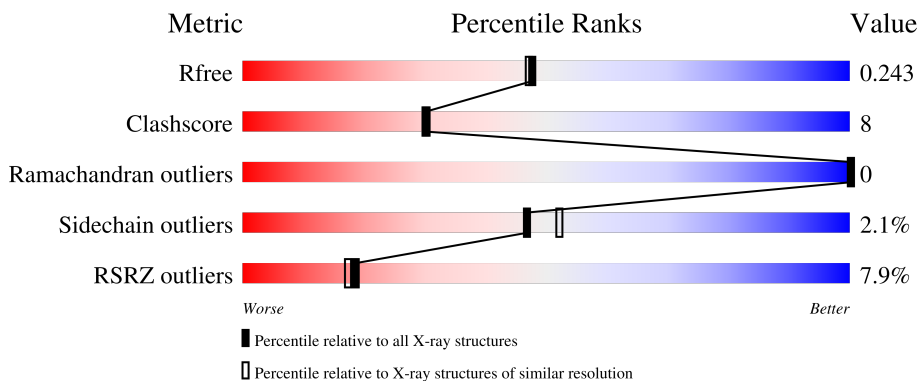
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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  $\geq 3$ , 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	257	 5% 74% 15% 9%
1	B	257	 9% 74% 16% 9%
2	C	13	 62% 8% 31%
2	D	13	 23% 23% 54%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	LYQ	A	601[B]	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4087 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1855	1188	318	331	18	0	1	0
1	B	233	1830	1169	315	327	19	0	0	0

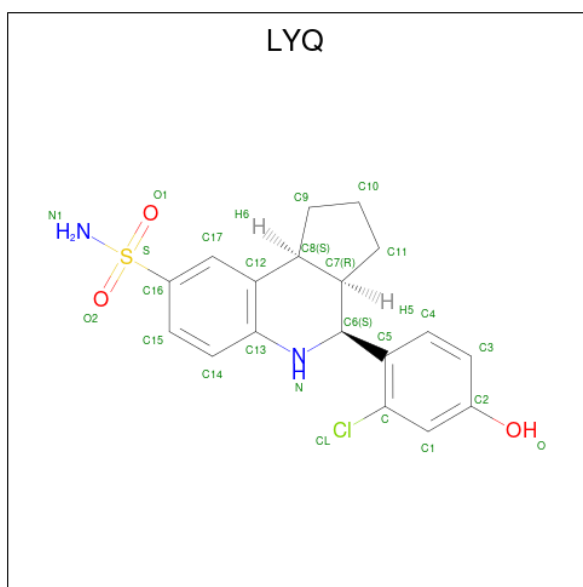
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	SER	TYR	engineered mutation	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

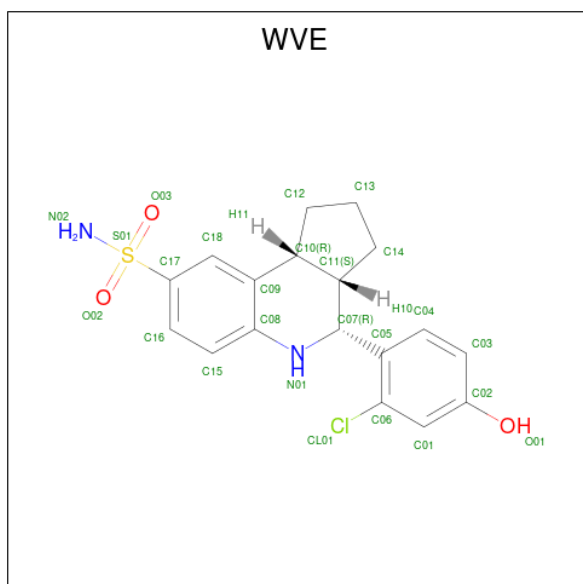
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	9	76	50	16	10	0	0	0
2	D	6	53	36	11	6	0	0	0

- Molecule 3 is (3 {a} {R},4 {S},9 {b} {S})-4-(2-chloranyl-4-oxidanyl-phenyl)-2,3,3 {a},4,5,9 {b}-hexahydro-1 {H}-cyclopenta[c]quinoline-8-sulfonamide (CCD ID: LYQ) (formula: C<sub>18</sub>H<sub>19</sub>ClN<sub>2</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
3	A	1	Total	C	Cl	N	O	S	0	1
			25	18	1	2	3	1		
3	A	1	Total	C	Cl	N	O	S	0	1
			25	18	1	2	3	1		
3	B	1	Total	C	Cl	N	O	S	0	1
			25	18	1	2	3	1		
3	B	1	Total	C	Cl	N	O	S	0	1
			25	18	1	2	3	1		

- Molecule 4 is (3a*S*,4*R*,9*bR*)-4-(2-chloro-4-hydroxyphenyl)-2,3,3*a*,4,5,9*b*-hexahydro-1*H*-cyclopenta[*c*]quinoline-8-sulfonamide (CCD ID: WVE) (formula: C<sub>18</sub>H<sub>19</sub>ClN<sub>2</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	Cl	N	O	S	0	1
			25	18	1	2	3	1		
4	A	1	Total	C	Cl	N	O	S	0	1
			25	18	1	2	3	1		
4	B	1	Total	C	Cl	N	O	S	0	1
			25	18	1	2	3	1		
4	B	1	Total	C	Cl	N	O	S	0	1
			25	18	1	2	3	1		

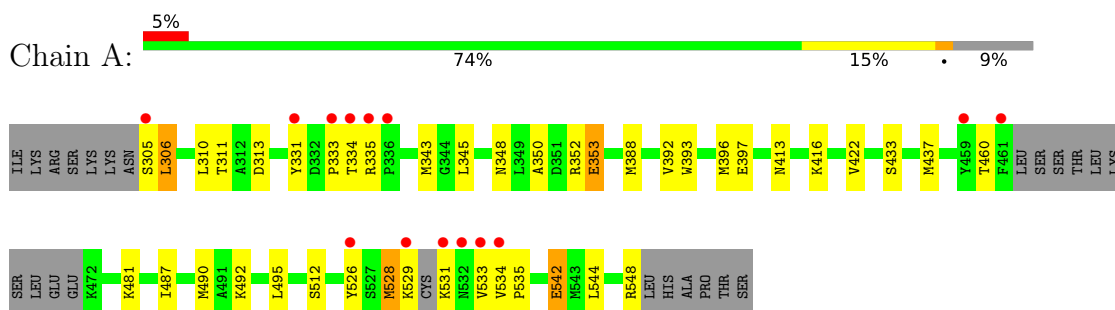
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	45	Total	O	0	0
			45	45		
5	B	24	Total	O	0	0
			24	24		
5	C	2	Total	O	0	0
			2	2		
5	D	2	Total	O	0	0
			2	2		

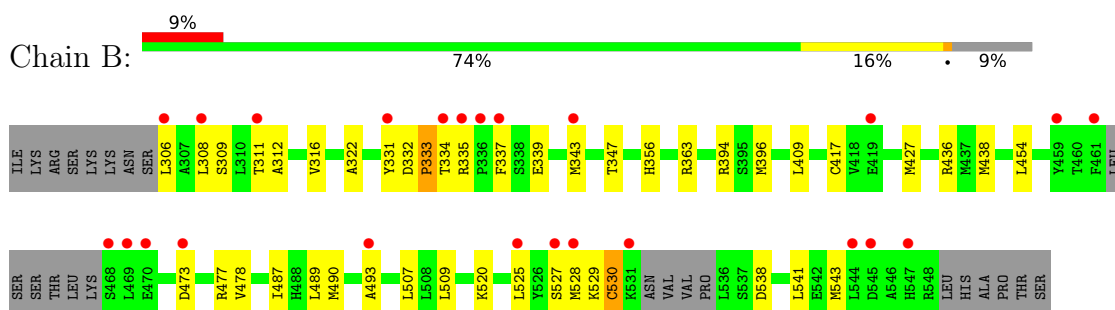
### 3 Residue-property plots [i](#)

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: Estrogen receptor



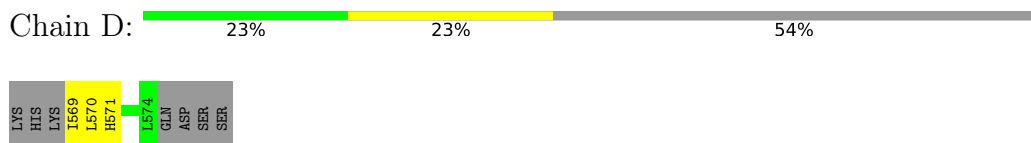
- Molecule 1: Estrogen receptor



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.96Å 81.77Å 58.55Å 90.00° 111.04° 90.00°	Depositor
Resolution (Å)	54.65 – 2.01 54.65 – 2.01	Depositor EDS
% Data completeness (in resolution range)	70.6 (54.65-2.01) 70.8 (54.65-2.01)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.193 , 0.248 (Not available) , 0.243	Depositor DCC
$R_{free}$ test set	35122 reflections (62.26%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.06	2/1889 (0.1%)	1.46	1/2553 (0.0%)
1	B	1.05	1/1862 (0.1%)	1.47	0/2515
2	C	0.91	0/76	1.36	0/100
2	D	0.97	0/53	1.37	0/70
All	All	1.05	3/3880 (0.1%)	1.46	1/5238 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	0	4
All	All	1	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	394	ARG	C-O	-6.09	1.16	1.24
1	A	353	GLU	C-O	-5.68	1.17	1.24
1	A	495	LEU	C-O	5.21	1.30	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	VAL	CB-CA-C	-5.66	104.72	111.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	305	SER	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	528	MET	Peptide
1	B	333	PRO	Peptide
1	B	335	ARG	Peptide
1	B	493	ALA	Peptide
1	B	530	CYS	Peptide

## 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	1855	0	1888	27	1
1	B	1830	0	1844	28	1
2	C	76	0	86	1	0
2	D	53	0	63	5	0
3	A	50	0	0	2	0
3	B	50	0	0	3	0
4	A	50	0	0	5	0
4	B	50	0	0	3	0
5	A	45	0	0	0	0
5	B	24	0	0	2	0
5	C	2	0	0	0	0
5	D	2	0	0	2	0
All	All	4087	0	3881	66	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (66) 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)
3:B:601[B]:LYQ:CL	3:B:601[B]:LYQ:C11	2.44	1.03
1:A:343:MET:HE3	1:A:528:MET:CE	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:HE3	1:A:528:MET:HE3	1.45	0.95
4:A:604[C]:WVE:C15	4:A:604[C]:WVE:CL01	2.54	0.93
1:A:343:MET:CE	1:A:528:MET:HE3	1.98	0.93
4:A:604[C]:WVE:CL01	4:A:604[C]:WVE:C08	2.56	0.91
1:A:416:LYS:HG3	1:A:422:VAL:HG11	1.52	0.89
4:A:604[C]:WVE:CL01	4:A:604[C]:WVE:N01	2.45	0.86
3:A:601[B]:LYQ:CL	3:A:601[B]:LYQ:C11	2.61	0.86
1:B:527:SER:O	1:B:530:CYS:O	2.00	0.79
1:B:339:GLU:HB2	1:B:417:CYS:O	1.84	0.78
1:B:409:LEU:HD23	1:B:409:LEU:O	1.85	0.77
1:A:343:MET:CE	1:A:528:MET:CE	2.61	0.73
4:B:604[C]:WVE:CL01	4:B:604[C]:WVE:N01	2.58	0.73
4:B:604[C]:WVE:CL01	4:B:604[C]:WVE:C08	2.79	0.67
1:B:454:LEU:HD13	1:B:478:VAL:HG23	1.77	0.67
1:A:353:GLU:OE2	4:A:603[A]:WVE:O01	2.12	0.67
1:B:311:THR:HG22	1:B:312:ALA:N	2.11	0.66
1:B:306:LEU:O	1:B:309:SER:OG	2.13	0.66
1:A:492:LYS:N	1:A:492:LYS:HD3	2.12	0.64
1:A:343:MET:HE3	1:A:528:MET:HE2	1.80	0.63
4:B:604[C]:WVE:CL01	4:B:604[C]:WVE:C15	2.86	0.60
1:A:393:TRP:O	1:A:396:MET:HG2	2.02	0.59
2:D:569:ILE:N	5:D:601:HOH:O	2.38	0.57
1:B:528:MET:HG3	3:B:601[B]:LYQ:N1	2.20	0.57
1:B:332:ASP:OD1	1:B:334:THR:CB	2.55	0.55
1:A:353:GLU:OE2	3:A:601[B]:LYQ:O	2.26	0.54
1:A:529:LYS:O	1:A:531:LYS:N	2.41	0.54
1:B:337:PHE:CB	5:B:723:HOH:O	2.55	0.54
1:B:538:ASP:HB3	2:D:569:ILE:HD11	1.90	0.54
1:A:487:ILE:HA	1:A:490:MET:HE3	1.90	0.53
1:A:311:THR:HG22	1:A:313:ASP:H	1.74	0.52
1:B:529:LYS:HE2	1:B:541:LEU:HD22	1.91	0.52
1:B:343:MET:O	1:B:347:THR:HG22	2.10	0.51
1:A:416:LYS:HG3	1:A:422:VAL:CG1	2.31	0.50
1:B:409:LEU:HD23	1:B:409:LEU:C	2.35	0.50
1:A:542:GLU:OE2	2:C:569:ILE:N	2.38	0.49
1:A:526:TYR:OH	1:A:544:LEU:O	2.29	0.49
1:B:487:ILE:HA	1:B:490:MET:HE3	1.95	0.49
1:B:473:ASP:O	1:B:477:ARG:HG3	2.14	0.47
3:B:601[B]:LYQ:CL	3:B:601[B]:LYQ:C7	2.99	0.47
1:B:311:THR:CG2	1:B:312:ALA:N	2.78	0.46
2:D:571:HIS:HB3	5:D:601:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:O	1:A:481:LYS:CE	2.65	0.45
1:B:356:HIS:HD2	5:B:721:HOH:O	1.99	0.45
1:A:343:MET:SD	1:A:528:MET:CE	3.05	0.44
1:A:534:VAL:HG22	1:A:535:PRO:HD2	2.00	0.44
1:B:454:LEU:HD13	1:B:478:VAL:CG2	2.46	0.44
1:A:433:SER:O	1:A:437:MET:HG2	2.18	0.44
1:B:538:ASP:HB3	2:D:569:ILE:CD1	2.47	0.44
1:A:306:LEU:O	1:A:306:LEU:HD22	2.18	0.43
1:A:333:PRO:HD2	1:A:345:LEU:HD21	2.00	0.42
1:B:331:TYR:CE2	1:B:333:PRO:HB3	2.54	0.42
1:B:316:VAL:HG21	1:B:489:LEU:HD21	2.01	0.42
1:B:438:MET:HE1	1:B:507:LEU:HD23	2.00	0.42
1:B:529:LYS:CE	1:B:541:LEU:HD22	2.49	0.42
1:B:396:MET:HE3	1:B:436:ARG:HA	2.03	0.41
1:A:348:ASN:OD1	1:A:352:ARG:NH1	2.53	0.41
1:B:509:LEU:HD23	1:B:509:LEU:HA	1.89	0.41
1:A:526:TYR:OH	1:A:548:ARG:HB2	2.20	0.41
1:A:388:MET:O	1:A:392:VAL:HG23	2.20	0.41
1:B:543:MET:SD	2:D:570:LEU:HD22	2.61	0.41
1:A:350:ALA:HB2	4:A:604[C]:WVE:CL01	2.58	0.41
1:B:427:MET:HE1	1:B:520:LYS:HG3	2.03	0.41
1:B:322:ALA:HA	1:B:363:ARG:HE	1.87	0.40
1:A:331:TYR:O	1:A:334:THR:HB	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ASN:ND2	1:B:333:PRO:O[2_545]	1.88	0.32

## 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	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
1	B	227/257 (88%)	223 (98%)	4 (2%)	0	100	100
2	C	7/13 (54%)	7 (100%)	0	0	100	100
2	D	4/13 (31%)	2 (50%)	2 (50%)	0	100	100
All	All	466/540 (86%)	457 (98%)	9 (2%)	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	207/232 (89%)	199 (96%)	8 (4%)	28	28
1	B	200/232 (86%)	198 (99%)	2 (1%)	68	75
2	C	8/13 (62%)	8 (100%)	0	100	100
2	D	6/13 (46%)	6 (100%)	0	100	100
All	All	421/490 (86%)	411 (98%)	10 (2%)	47	47

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

Mol	Chain	Res	Type
1	A	305	SER
1	A	306	LEU
1	A	335	ARG
1	A	397	GLU
1	A	460	THR
1	A	512[A]	SER
1	A	512[B]	SER
1	A	542	GLU
1	B	308	LEU
1	B	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	519	ASN
1	A	547	HIS
1	B	356	HIS
1	B	516	HIS
1	B	519	ASN
2	C	575	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 oligosaccharides 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
4	WVE	A	604[C]	-	28,28,28	2.77	15 (53%)	41,43,43	3.93	12 (29%)
4	WVE	B	604[C]	-	28,28,28	2.77	15 (53%)	41,43,43	3.86	14 (34%)
3	LYQ	B	602[D]	-	28,28,28	2.81	17 (60%)	41,43,43	3.94	13 (31%)
3	LYQ	A	601[B]	-	28,28,28	2.69	16 (57%)	41,43,43	4.31	20 (48%)
3	LYQ	A	602[D]	-	28,28,28	2.80	15 (53%)	41,43,43	4.02	16 (39%)
4	WVE	A	603[A]	-	28,28,28	2.74	16 (57%)	41,43,43	3.95	13 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LYQ	B	601[B]	-	28,28,28	2.72	15 (53%)	41,43,43	4.20	15 (36%)
4	WVE	B	603[A]	-	28,28,28	2.77	15 (53%)	41,43,43	3.90	13 (31%)

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
4	WVE	A	604[C]	-	-	2/10/32/32	0/4/4/4
4	WVE	B	604[C]	-	-	2/10/32/32	0/4/4/4
3	LYQ	B	602[D]	-	-	10/10/32/32	0/4/4/4
3	LYQ	A	601[B]	-	-	10/10/32/32	0/4/4/4
3	LYQ	A	602[D]	-	-	10/10/32/32	0/4/4/4
4	WVE	A	603[A]	-	-	0/10/32/32	0/4/4/4
3	LYQ	B	601[B]	-	-	8/10/32/32	0/4/4/4
4	WVE	B	603[A]	-	-	0/10/32/32	0/4/4/4

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602[D]	LYQ	C13-N	-6.84	1.26	1.39
3	A	602[D]	LYQ	C13-N	-6.70	1.26	1.39
3	B	601[B]	LYQ	C13-N	-6.67	1.26	1.39
4	B	604[C]	WVE	C08-N01	-6.46	1.27	1.39
4	A	604[C]	WVE	C08-N01	-6.45	1.27	1.39
4	B	603[A]	WVE	C08-N01	-6.45	1.27	1.39
4	A	603[A]	WVE	C08-N01	-6.36	1.27	1.39
3	A	601[B]	LYQ	C13-N	-6.26	1.27	1.39
3	A	601[B]	LYQ	S-N1	5.32	1.70	1.60
4	B	603[A]	WVE	C08-C09	-5.10	1.34	1.40
3	A	602[D]	LYQ	S-N1	5.10	1.70	1.60
4	A	604[C]	WVE	S01-N02	5.05	1.70	1.60
3	B	602[D]	LYQ	S-N1	5.04	1.70	1.60
4	B	604[C]	WVE	S01-N02	5.02	1.70	1.60
4	A	603[A]	WVE	S01-N02	4.99	1.70	1.60
4	A	603[A]	WVE	C08-C09	-4.97	1.34	1.40
4	B	603[A]	WVE	S01-N02	4.94	1.70	1.60
4	B	604[C]	WVE	C08-C09	-4.90	1.34	1.40
4	A	604[C]	WVE	C08-C09	-4.87	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601[B]	LYQ	S-N1	4.78	1.69	1.60
3	B	602[D]	LYQ	C13-C12	-4.63	1.35	1.40
3	B	601[B]	LYQ	C13-C12	-4.57	1.35	1.40
3	B	602[D]	LYQ	C10-C9	-4.46	1.33	1.51
3	B	601[B]	LYQ	C10-C9	-4.44	1.33	1.51
3	A	602[D]	LYQ	C13-C12	-4.42	1.35	1.40
3	A	602[D]	LYQ	C10-C9	-4.39	1.34	1.51
4	B	604[C]	WVE	C13-C12	-4.34	1.34	1.51
3	A	601[B]	LYQ	C10-C9	-4.32	1.34	1.51
4	B	603[A]	WVE	C13-C12	-4.32	1.34	1.51
4	A	604[C]	WVE	C13-C12	-4.31	1.34	1.51
4	A	603[A]	WVE	C13-C12	-4.30	1.34	1.51
3	A	601[B]	LYQ	C13-C12	-4.28	1.35	1.40
4	A	603[A]	WVE	C04-C05	-3.95	1.35	1.39
4	B	604[C]	WVE	C04-C05	-3.89	1.35	1.39
4	B	603[A]	WVE	C04-C05	-3.88	1.35	1.39
4	A	604[C]	WVE	C04-C05	-3.86	1.35	1.39
3	A	602[D]	LYQ	C4-C5	-3.71	1.35	1.39
4	A	604[C]	WVE	C06-C05	-3.71	1.35	1.39
3	B	602[D]	LYQ	C4-C5	-3.66	1.35	1.39
3	A	602[D]	LYQ	C-C5	-3.55	1.35	1.39
3	B	601[B]	LYQ	C-C5	-3.49	1.35	1.39
3	B	601[B]	LYQ	C4-C5	-3.47	1.35	1.39
4	B	604[C]	WVE	C06-C05	-3.46	1.35	1.39
3	A	602[D]	LYQ	C1-C2	-3.42	1.34	1.39
3	A	601[B]	LYQ	C4-C5	-3.39	1.35	1.39
3	B	602[D]	LYQ	C-C5	-3.38	1.35	1.39
3	B	602[D]	LYQ	C1-C2	-3.38	1.34	1.39
4	B	603[A]	WVE	C01-C02	-3.16	1.34	1.39
4	B	603[A]	WVE	C06-C05	-3.16	1.35	1.39
3	A	601[B]	LYQ	C1-C2	-3.06	1.34	1.39
4	B	604[C]	WVE	C01-C02	-3.06	1.34	1.39
3	B	602[D]	LYQ	C14-C13	-3.05	1.34	1.39
4	B	604[C]	WVE	C15-C08	-3.02	1.34	1.39
4	A	603[A]	WVE	C15-C08	-3.02	1.34	1.39
4	A	604[C]	WVE	C01-C02	-3.00	1.34	1.39
3	A	602[D]	LYQ	C17-C12	-3.00	1.34	1.39
4	A	604[C]	WVE	C15-C08	-3.00	1.34	1.39
3	A	602[D]	LYQ	C14-C13	-3.00	1.34	1.39
3	A	601[B]	LYQ	C17-C12	-2.98	1.34	1.39
4	A	603[A]	WVE	C01-C02	-2.97	1.34	1.39
4	B	603[A]	WVE	C15-C08	-2.97	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601[B]	LYQ	C1-C2	-2.93	1.34	1.39
4	B	604[C]	WVE	C18-C09	-2.92	1.35	1.39
4	A	603[A]	WVE	C06-C05	-2.89	1.36	1.39
3	B	601[B]	LYQ	C17-C12	-2.89	1.35	1.39
4	B	603[A]	WVE	C18-C09	-2.83	1.35	1.39
3	A	602[D]	LYQ	C1-C	-2.83	1.34	1.38
3	B	602[D]	LYQ	C17-C12	-2.78	1.35	1.39
3	B	602[D]	LYQ	C1-C	-2.77	1.34	1.38
4	A	603[A]	WVE	C04-C03	-2.77	1.34	1.38
3	A	601[B]	LYQ	C14-C13	-2.75	1.35	1.39
4	A	604[C]	WVE	C18-C09	-2.75	1.35	1.39
3	B	602[D]	LYQ	C15-C16	-2.72	1.34	1.38
3	B	601[B]	LYQ	C14-C13	-2.72	1.35	1.39
4	B	604[C]	WVE	C16-C17	-2.72	1.34	1.38
3	B	602[D]	LYQ	C15-C14	-2.68	1.34	1.38
4	A	603[A]	WVE	C18-C09	-2.66	1.35	1.39
3	A	601[B]	LYQ	C3-C4	-2.65	1.34	1.38
4	A	604[C]	WVE	C16-C17	-2.63	1.34	1.38
4	B	603[A]	WVE	C16-C17	-2.61	1.34	1.38
3	B	601[B]	LYQ	C3-C4	-2.61	1.34	1.38
3	A	602[D]	LYQ	C15-C16	-2.60	1.34	1.38
4	A	603[A]	WVE	C03-C02	-2.57	1.34	1.39
4	B	603[A]	WVE	C04-C03	-2.57	1.34	1.38
3	A	601[B]	LYQ	C-C5	-2.56	1.36	1.39
4	B	604[C]	WVE	C15-C16	-2.56	1.34	1.38
3	A	601[B]	LYQ	C3-C2	-2.55	1.34	1.39
4	B	604[C]	WVE	C04-C03	-2.55	1.34	1.38
3	B	601[B]	LYQ	C3-C2	-2.54	1.34	1.39
4	A	603[A]	WVE	C16-C17	-2.50	1.35	1.38
3	A	602[D]	LYQ	C15-C14	-2.48	1.34	1.38
4	A	604[C]	WVE	C15-C16	-2.47	1.34	1.38
4	A	604[C]	WVE	C04-C03	-2.46	1.34	1.38
4	B	603[A]	WVE	C03-C02	-2.46	1.34	1.39
3	B	602[D]	LYQ	C3-C4	-2.45	1.34	1.38
3	A	601[B]	LYQ	C15-C16	-2.45	1.35	1.38
3	A	601[B]	LYQ	C1-C	-2.41	1.34	1.38
3	A	602[D]	LYQ	C17-C16	-2.39	1.34	1.39
4	B	603[A]	WVE	C15-C16	-2.38	1.35	1.38
3	A	602[D]	LYQ	C3-C4	-2.38	1.35	1.38
4	A	603[A]	WVE	C15-C16	-2.38	1.35	1.38
3	A	601[B]	LYQ	C17-C16	-2.37	1.34	1.39
4	B	603[A]	WVE	C01-C06	-2.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601[B]	LYQ	C15-C16	-2.36	1.35	1.38
4	B	604[C]	WVE	C18-C17	-2.35	1.35	1.39
4	A	604[C]	WVE	C01-C06	-2.35	1.34	1.38
4	B	604[C]	WVE	C01-C06	-2.34	1.34	1.38
4	B	604[C]	WVE	C03-C02	-2.31	1.34	1.39
4	B	603[A]	WVE	C18-C17	-2.28	1.35	1.39
4	A	604[C]	WVE	C03-C02	-2.28	1.34	1.39
4	A	603[A]	WVE	C18-C17	-2.28	1.35	1.39
4	A	604[C]	WVE	C18-C17	-2.28	1.35	1.39
3	B	602[D]	LYQ	C3-C2	-2.27	1.34	1.39
3	B	602[D]	LYQ	C17-C16	-2.20	1.35	1.39
4	A	603[A]	WVE	C01-C06	-2.19	1.35	1.38
3	B	601[B]	LYQ	C15-C14	-2.14	1.35	1.38
3	B	601[B]	LYQ	C17-C16	-2.13	1.35	1.39
3	A	602[D]	LYQ	C3-C2	-2.09	1.35	1.39
3	B	601[B]	LYQ	C1-C	-2.09	1.35	1.38
3	A	601[B]	LYQ	O2-S	2.07	1.47	1.43
3	B	602[D]	LYQ	C9-C8	-2.05	1.50	1.54
3	A	601[B]	LYQ	C15-C14	-2.04	1.35	1.38
4	A	603[A]	WVE	C07-N01	2.03	1.48	1.46
3	B	602[D]	LYQ	O1-S	2.00	1.47	1.43

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	LYQ	O1-S-N1	-14.82	85.99	107.35
4	A	603[A]	WVE	O03-S01-N02	-13.84	87.40	107.35
4	B	603[A]	WVE	O03-S01-N02	-13.75	87.53	107.35
3	A	601[B]	LYQ	O1-S-N1	-13.65	87.67	107.35
4	A	604[C]	WVE	O02-S01-N02	-13.48	87.92	107.35
4	B	603[A]	WVE	O02-S01-N02	-13.45	87.97	107.35
4	B	604[C]	WVE	O03-S01-N02	-13.38	88.06	107.35
3	A	601[B]	LYQ	O2-S-N1	-13.38	88.07	107.35
3	A	602[D]	LYQ	O2-S-N1	-13.37	88.08	107.35
4	A	604[C]	WVE	O03-S01-N02	-13.35	88.11	107.35
3	B	601[B]	LYQ	O2-S-N1	-13.33	88.13	107.35
4	B	604[C]	WVE	O02-S01-N02	-13.26	88.24	107.35
3	B	602[D]	LYQ	O2-S-N1	-13.22	88.29	107.35
3	A	602[D]	LYQ	O1-S-N1	-13.20	88.32	107.35
3	B	602[D]	LYQ	O1-S-N1	-13.12	88.43	107.35
4	A	603[A]	WVE	O02-S01-N02	-13.11	88.45	107.35
3	A	601[B]	LYQ	O2-S-C16	10.64	119.37	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	LYQ	O2-S-C16	10.41	119.12	107.35
3	A	602[D]	LYQ	O2-S-C16	9.51	118.09	107.35
4	B	604[C]	WVE	O02-S01-C17	9.12	117.66	107.35
3	B	602[D]	LYQ	O2-S-C16	9.08	117.61	107.35
4	B	603[A]	WVE	O02-S01-C17	8.87	117.37	107.35
4	A	604[C]	WVE	O03-S01-C17	8.69	117.17	107.35
4	A	603[A]	WVE	O02-S01-C17	8.56	117.02	107.35
4	A	603[A]	WVE	O03-S01-C17	8.43	116.88	107.35
4	A	604[C]	WVE	O02-S01-C17	8.42	116.87	107.35
3	B	602[D]	LYQ	O1-S-C16	8.28	116.70	107.35
3	A	602[D]	LYQ	O1-S-C16	7.98	116.37	107.35
4	B	603[A]	WVE	O03-S01-C17	7.90	116.28	107.35
4	B	604[C]	WVE	O03-S01-C17	7.68	116.03	107.35
3	B	601[B]	LYQ	O1-S-C16	7.52	115.84	107.35
3	A	601[B]	LYQ	O1-S-C16	7.21	115.50	107.35
3	B	602[D]	LYQ	C5-C6-C7	6.19	122.16	112.53
3	A	602[D]	LYQ	C5-C6-C7	6.04	121.92	112.53
3	A	601[B]	LYQ	C5-C-CL	5.86	126.41	120.41
3	B	601[B]	LYQ	C5-C6-C7	5.67	121.36	112.53
4	A	604[C]	WVE	C17-S01-N02	5.34	115.84	108.40
4	B	603[A]	WVE	C17-S01-N02	5.31	115.80	108.40
3	A	601[B]	LYQ	C5-C6-C7	5.27	120.73	112.53
4	A	603[A]	WVE	C17-S01-N02	5.17	115.60	108.40
3	A	601[B]	LYQ	C-C5-C6	4.99	129.21	121.75
3	A	602[D]	LYQ	C10-C9-C8	4.74	112.21	104.32
4	B	604[C]	WVE	C17-S01-N02	4.65	114.88	108.40
4	A	604[C]	WVE	C13-C12-C10	4.60	111.97	104.32
4	B	604[C]	WVE	C13-C12-C10	4.54	111.87	104.32
4	A	603[A]	WVE	C13-C12-C10	4.38	111.61	104.32
3	A	601[B]	LYQ	C10-C9-C8	4.37	111.58	104.32
4	B	603[A]	WVE	C13-C12-C10	4.35	111.55	104.32
3	B	601[B]	LYQ	C10-C9-C8	4.25	111.39	104.32
3	A	602[D]	LYQ	C16-S-N1	4.23	114.30	108.40
3	A	601[B]	LYQ	C5-C6-N	4.17	116.35	110.78
4	A	604[C]	WVE	C11-C07-N01	4.09	113.22	108.69
3	A	601[B]	LYQ	C16-S-N1	4.03	114.01	108.40
4	B	604[C]	WVE	C11-C07-N01	3.91	113.02	108.69
3	B	602[D]	LYQ	C16-S-N1	3.89	113.83	108.40
3	A	601[B]	LYQ	C4-C5-C6	-3.83	114.79	120.78
3	B	601[B]	LYQ	C5-C6-N	3.73	115.77	110.78
3	B	601[B]	LYQ	C16-S-N1	3.68	113.53	108.40
3	B	602[D]	LYQ	C10-C9-C8	3.67	110.43	104.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603[A]	WVE	C11-C07-N01	3.59	112.67	108.69
3	A	601[B]	LYQ	C2-C1-C	3.47	123.08	118.92
3	B	601[B]	LYQ	C-C5-C6	3.43	126.88	121.75
4	B	603[A]	WVE	C11-C07-N01	3.33	112.38	108.69
3	B	602[D]	LYQ	C5-C-CL	3.31	123.80	120.41
3	A	602[D]	LYQ	C3-C2-C1	-3.21	116.66	120.19
3	A	602[D]	LYQ	C5-C-CL	3.16	123.64	120.41
4	A	603[A]	WVE	C13-C14-C11	-3.15	98.73	104.85
4	A	604[C]	WVE	C13-C14-C11	-3.10	98.83	104.85
3	A	601[B]	LYQ	C1-C-CL	-3.07	113.42	118.45
3	B	601[B]	LYQ	C3-C2-C1	-3.03	116.86	120.19
3	A	601[B]	LYQ	C7-C6-N	2.94	111.95	108.69
3	B	602[D]	LYQ	C3-C2-C1	-2.91	117.00	120.19
3	B	602[D]	LYQ	C2-C1-C	2.84	122.33	118.92
3	B	601[B]	LYQ	C2-C1-C	2.83	122.31	118.92
3	A	601[B]	LYQ	C3-C2-C1	-2.80	117.11	120.19
4	A	604[C]	WVE	C03-C02-C01	-2.73	117.19	120.19
4	B	604[C]	WVE	C03-C02-C01	-2.70	117.22	120.19
3	A	602[D]	LYQ	C11-C10-C9	2.68	112.50	105.59
3	A	602[D]	LYQ	C2-C1-C	2.61	122.05	118.92
3	B	601[B]	LYQ	C11-C7-C8	2.59	106.98	103.97
4	A	603[A]	WVE	C05-C06-CL01	2.56	123.03	120.41
4	B	603[A]	WVE	C03-C02-C01	-2.55	117.39	120.19
4	B	604[C]	WVE	C12-C10-C11	-2.54	99.62	103.63
3	A	602[D]	LYQ	C7-C6-N	2.53	111.49	108.69
4	A	603[A]	WVE	C02-C01-C06	2.53	121.95	118.92
4	B	604[C]	WVE	C13-C14-C11	-2.53	99.94	104.85
4	A	603[A]	WVE	C03-C02-C01	-2.51	117.43	120.19
3	A	602[D]	LYQ	C1-C-CL	-2.50	114.36	118.45
4	B	603[A]	WVE	C12-C10-C11	-2.49	99.70	103.63
3	B	602[D]	LYQ	C11-C7-C8	2.40	106.76	103.97
3	B	601[B]	LYQ	C11-C10-C9	2.39	111.77	105.59
3	A	602[D]	LYQ	C11-C7-C8	2.37	106.72	103.97
4	B	604[C]	WVE	C02-C01-C06	2.30	121.68	118.92
4	B	603[A]	WVE	C13-C14-C11	-2.28	100.43	104.85
4	B	603[A]	WVE	C02-C01-C06	2.27	121.65	118.92
4	A	604[C]	WVE	C12-C10-C11	-2.23	100.11	103.63
3	B	602[D]	LYQ	C11-C10-C9	2.22	111.32	105.59
4	B	604[C]	WVE	C08-N01-C07	2.21	125.08	118.91
4	A	603[A]	WVE	C10-C11-C07	2.19	113.61	110.65
4	B	603[A]	WVE	C12-C13-C14	2.19	111.23	105.59
3	B	601[B]	LYQ	C4-C5-C6	-2.18	117.37	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602[D]	LYQ	C5-C6-N	2.18	113.69	110.78
3	A	601[B]	LYQ	C13-C12-C8	2.17	122.26	118.74
4	B	604[C]	WVE	O03-S01-O02	2.17	122.13	118.80
3	B	601[B]	LYQ	O1-S-O2	2.16	122.12	118.80
4	B	603[A]	WVE	O03-S01-O02	2.16	122.12	118.80
3	B	602[D]	LYQ	C1-C-CL	-2.15	114.92	118.45
4	B	604[C]	WVE	C12-C13-C14	2.14	111.10	105.59
3	A	601[B]	LYQ	C1-C-C5	-2.12	120.17	122.46
3	A	601[B]	LYQ	C11-C7-C8	2.08	106.39	103.97
4	A	604[C]	WVE	C08-N01-C07	2.08	124.70	118.91
4	A	604[C]	WVE	C02-C01-C06	2.06	121.40	118.92
3	A	602[D]	LYQ	C13-C12-C8	2.06	122.08	118.74
3	A	601[B]	LYQ	C11-C10-C9	2.04	110.87	105.59
3	A	601[B]	LYQ	C15-C16-S	2.02	122.47	119.72
4	A	603[A]	WVE	C12-C10-C11	-2.00	100.47	103.63

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601[B]	LYQ	C4-C5-C6-C7
3	A	601[B]	LYQ	C-C5-C6-C7
3	A	601[B]	LYQ	C-C5-C6-N
3	A	602[D]	LYQ	C4-C5-C6-C7
3	A	602[D]	LYQ	C-C5-C6-C7
3	B	601[B]	LYQ	C4-C5-C6-C7
3	B	601[B]	LYQ	C-C5-C6-C7
3	B	602[D]	LYQ	C4-C5-C6-C7
3	B	602[D]	LYQ	C-C5-C6-C7
4	A	604[C]	WVE	C06-C05-C07-N01
3	A	601[B]	LYQ	C17-C16-S-N1
3	A	601[B]	LYQ	C4-C5-C6-N
3	B	601[B]	LYQ	C4-C5-C6-N
3	A	601[B]	LYQ	C15-C16-S-N1
3	B	602[D]	LYQ	C17-C16-S-N1
3	B	601[B]	LYQ	C-C5-C6-N
4	B	604[C]	WVE	C06-C05-C07-N01
3	B	602[D]	LYQ	C15-C16-S-N1
3	A	602[D]	LYQ	C15-C16-S-N1
3	A	602[D]	LYQ	C17-C16-S-N1
3	A	602[D]	LYQ	C15-C16-S-O1
3	A	601[B]	LYQ	C15-C16-S-O1

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Mol	Chain	Res	Type	Atoms
3	A	602[D]	LYQ	C17-C16-S-O1
4	A	604[C]	WVE	C04-C05-C07-N01
3	B	602[D]	LYQ	C15-C16-S-O1
3	A	601[B]	LYQ	C15-C16-S-O2
3	B	602[D]	LYQ	C17-C16-S-O1
3	A	601[B]	LYQ	C17-C16-S-O1
3	A	601[B]	LYQ	C17-C16-S-O2
3	B	601[B]	LYQ	C17-C16-S-N1
3	A	602[D]	LYQ	C4-C5-C6-N
3	B	602[D]	LYQ	C4-C5-C6-N
3	B	602[D]	LYQ	C15-C16-S-O2
3	B	602[D]	LYQ	C17-C16-S-O2
3	B	601[B]	LYQ	C15-C16-S-N1
3	A	602[D]	LYQ	C-C5-C6-N
3	B	602[D]	LYQ	C-C5-C6-N
3	A	602[D]	LYQ	C15-C16-S-O2
3	A	602[D]	LYQ	C17-C16-S-O2
3	B	601[B]	LYQ	C15-C16-S-O1
4	B	604[C]	WVE	C04-C05-C07-N01
3	B	601[B]	LYQ	C17-C16-S-O1

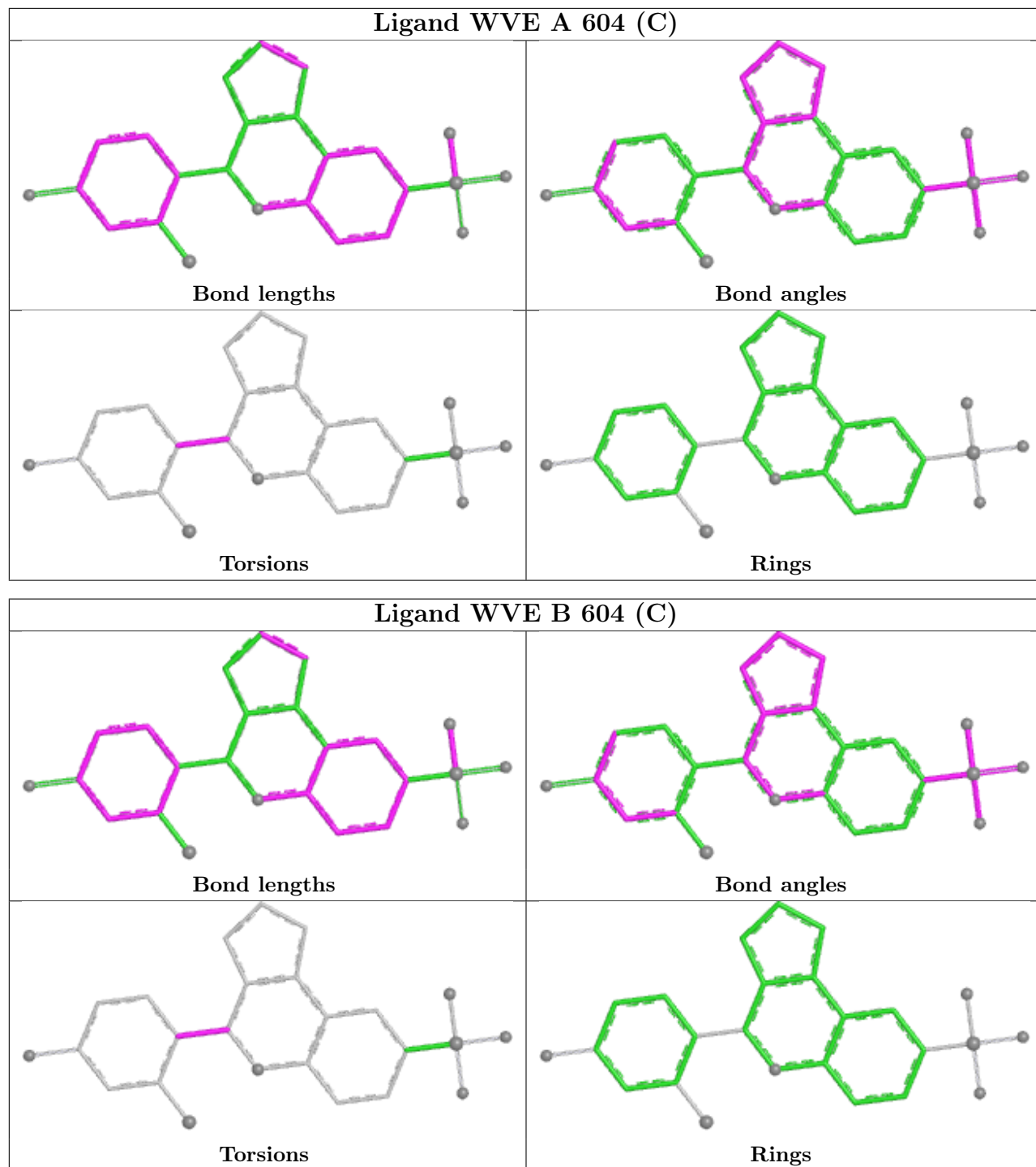
There are no ring outliers.

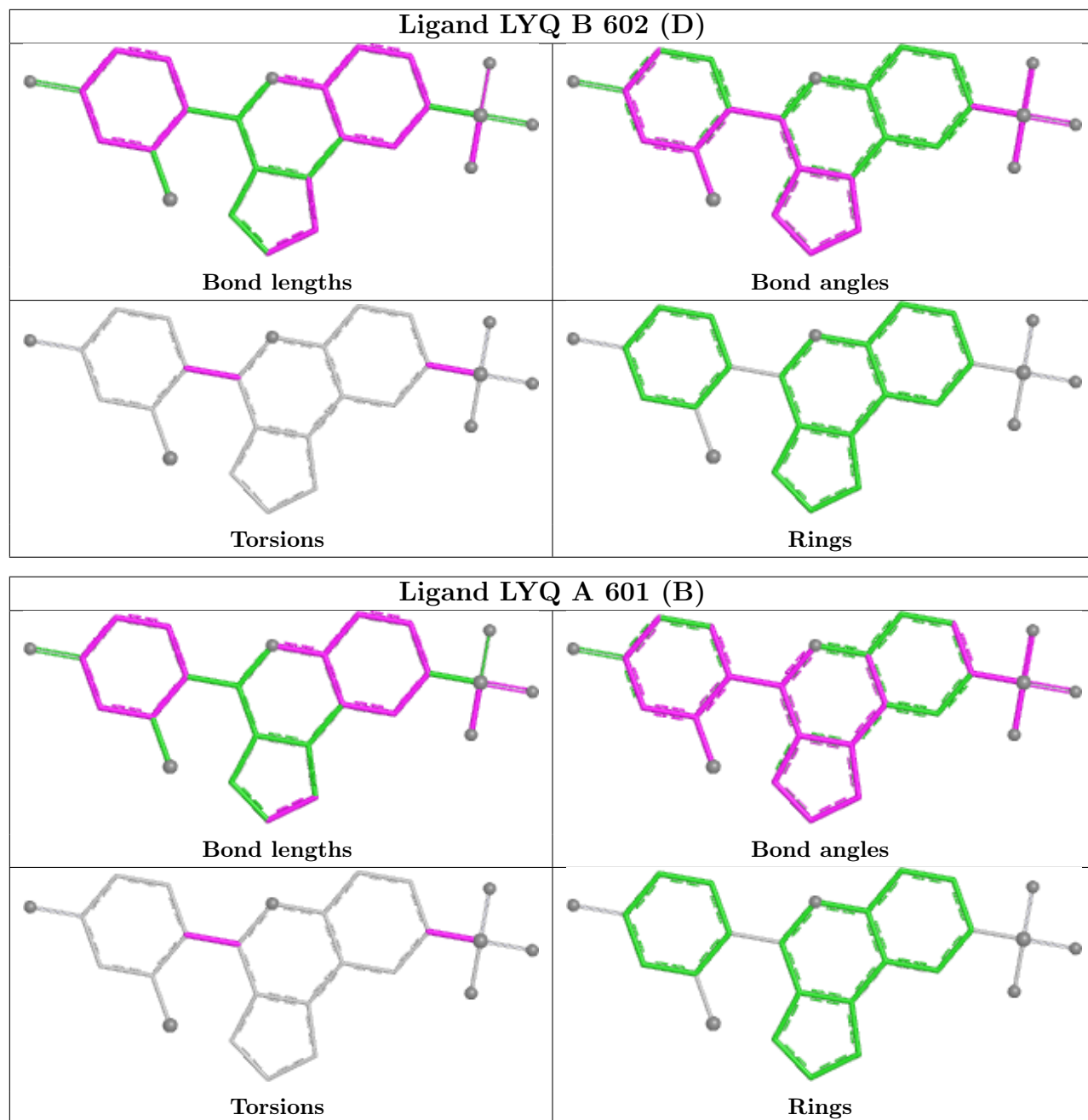
5 monomers are involved in 13 short contacts:

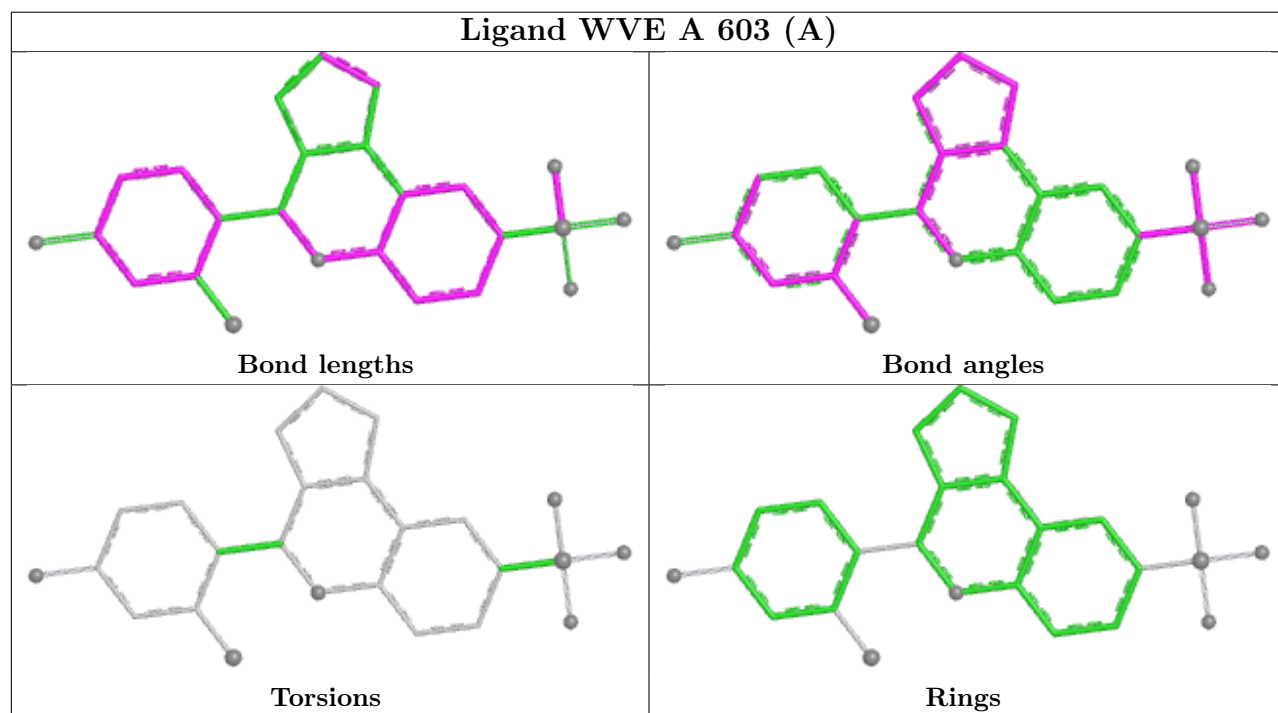
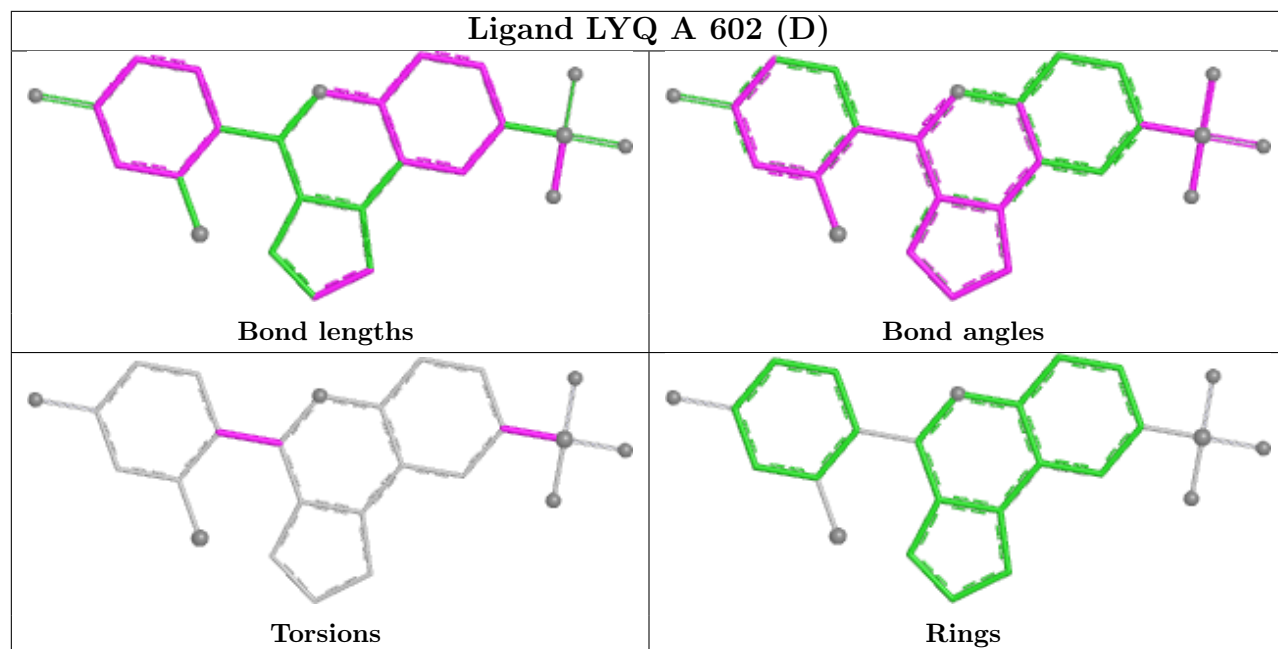
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604[C]	WVE	4	0
4	B	604[C]	WVE	3	0
3	A	601[B]	LYQ	2	0
4	A	603[A]	WVE	1	0
3	B	601[B]	LYQ	3	0

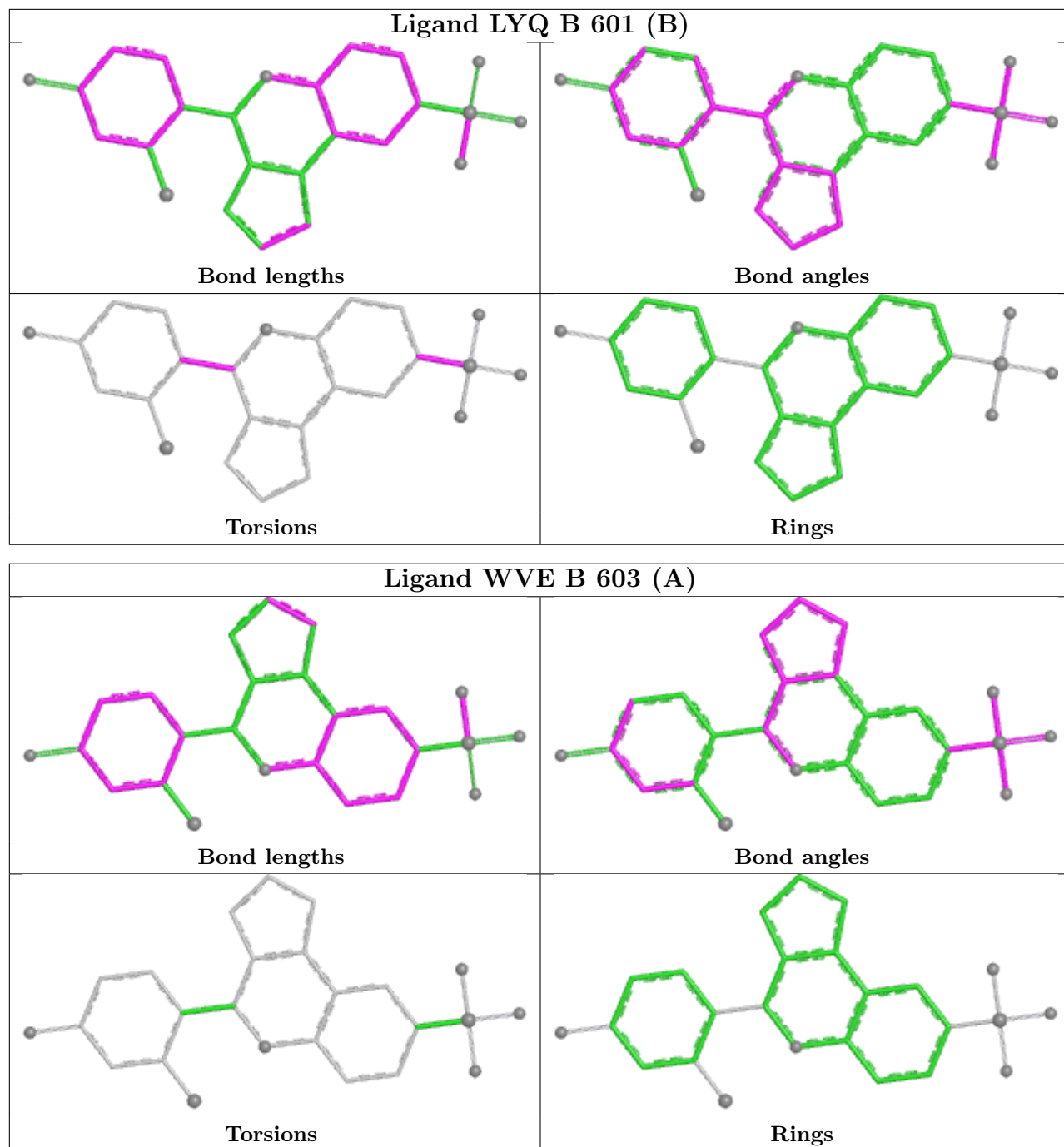
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	233/257 (90%)	0.29	14 (6%) 27 26	12, 41, 83, 114	2 (0%)
1	B	233/257 (90%)	0.68	24 (10%) 12 11	26, 52, 104, 132	0
2	C	9/13 (69%)	0.64	0 100 100	39, 43, 63, 75	0
2	D	6/13 (46%)	1.17	0 100 100	57, 60, 82, 83	0
All	All	481/540 (89%)	0.50	38 (7%) 18 17	12, 47, 99, 132	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	PHE	5.6
1	B	468	SER	5.3
1	A	336	PRO	4.9
1	B	461	PHE	4.6
1	B	336	PRO	4.4
1	A	533	VAL	3.9
1	A	459	TYR	3.9
1	B	459	TYR	3.5
1	B	335	ARG	3.4
1	A	526	TYR	3.4
1	B	531	LYS	3.4
1	B	469	LEU	3.3
1	B	306	LEU	3.2
1	B	493	ALA	3.1
1	A	305	SER	3.0
1	A	532	ASN	2.9
1	B	470	GLU	2.8
1	B	334	THR	2.8
1	A	531	LYS	2.7
1	A	529	LYS	2.6
1	A	461	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	334	THR	2.5
1	A	534	VAL	2.5
1	A	333	PRO	2.5
1	B	308	LEU	2.5
1	B	473	ASP	2.3
1	B	343	MET	2.3
1	B	527	SER	2.2
1	A	335	ARG	2.2
1	B	545	ASP	2.1
1	B	525	LEU	2.1
1	B	544	LEU	2.1
1	B	331	TYR	2.1
1	B	528	MET	2.0
1	B	311	THR	2.0
1	A	331	TYR	2.0
1	B	419	GLU	2.0
1	B	547	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

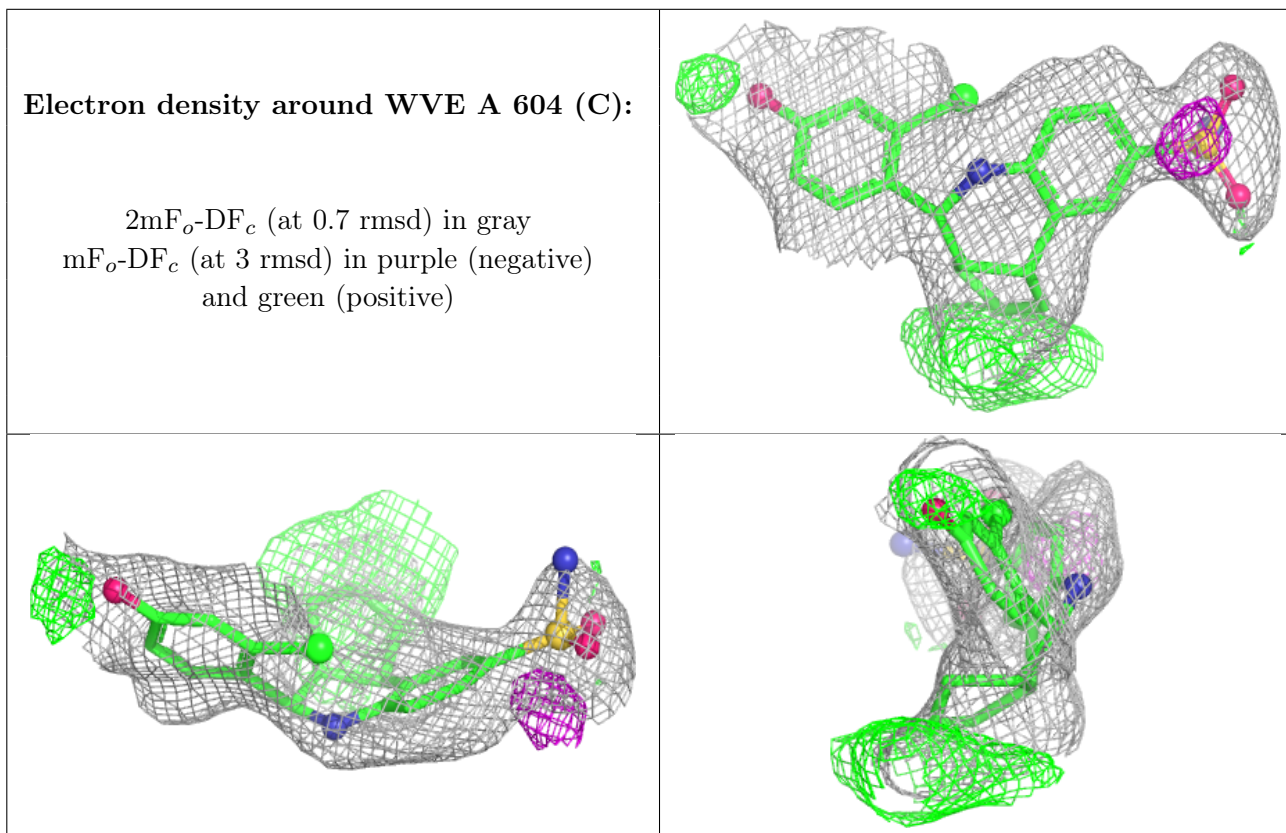
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	WVE	A	604[C]	25/25	0.59	0.22	39,49,52,52	25
4	WVE	B	604[C]	25/25	0.66	0.29	73,81,85,86	25
4	WVE	B	603[A]	25/25	0.76	0.15	25,28,29,29	25
3	LYQ	B	601[B]	25/25	0.82	0.14	34,49,57,58	25
3	LYQ	A	601[B]	25/25	0.82	0.12	25,36,38,41	25
4	WVE	A	603[A]	25/25	0.85	0.10	18,22,25,25	25

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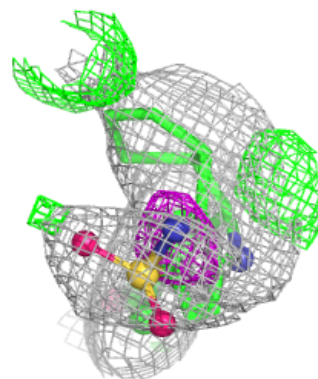
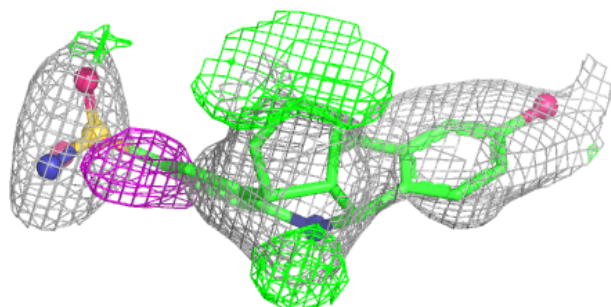
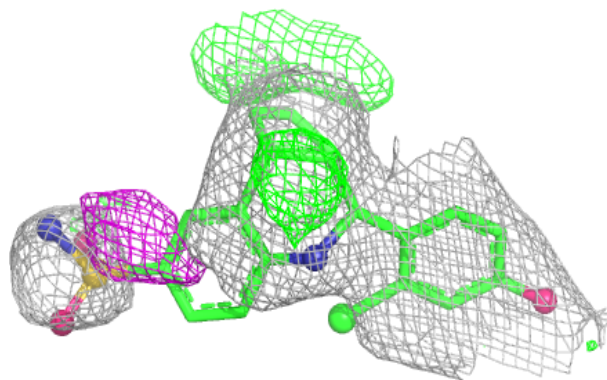
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LYQ	A	602[D]	25/25	0.87	0.27	51,91,130,133	25
3	LYQ	B	602[D]	25/25	0.91	0.33	107,152,224,228	25

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.

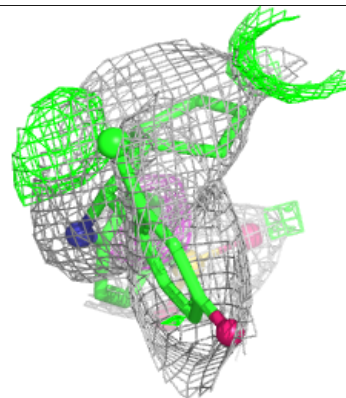
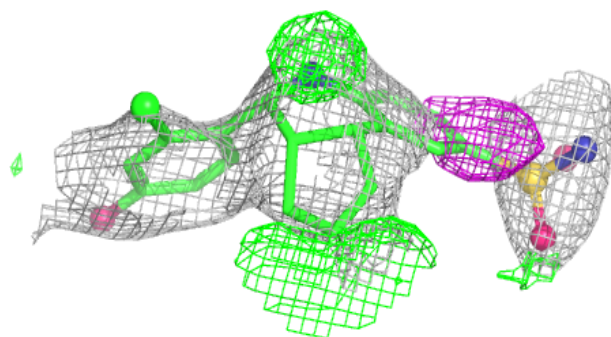
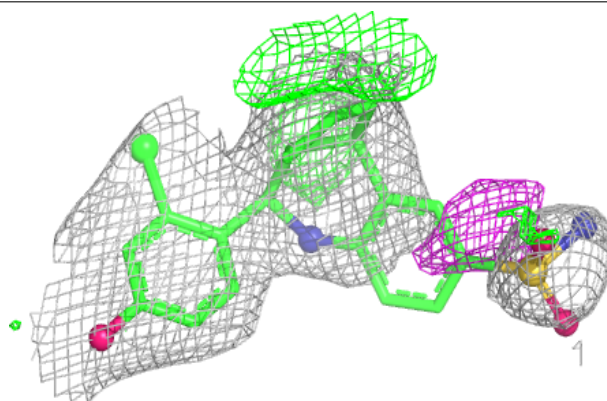


**Electron density around WVE B 604 (C):**

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

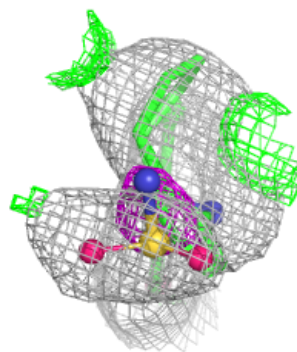
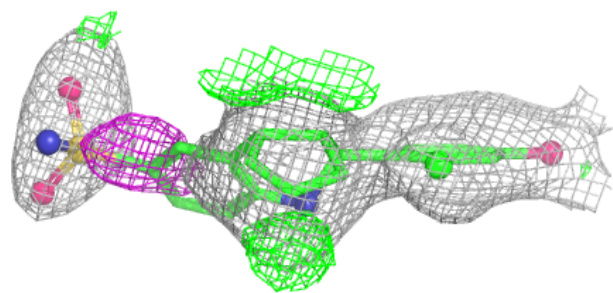
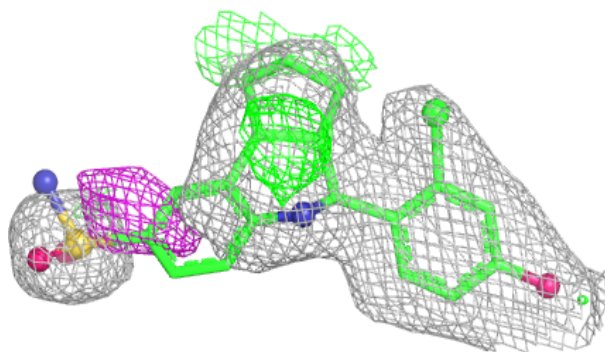
**Electron density around WVE B 603 (A):**

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

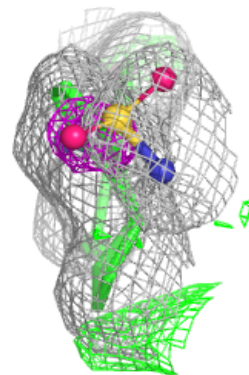
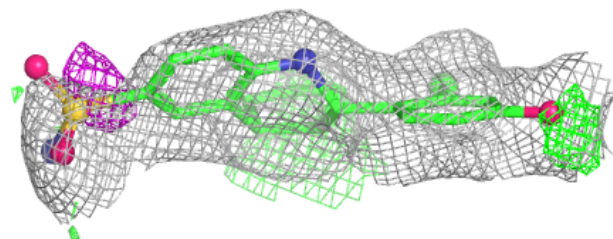
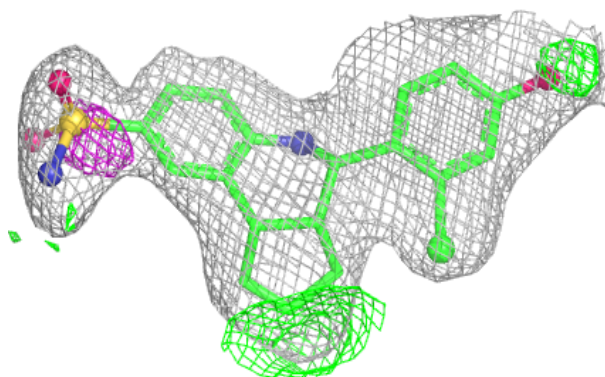


**Electron density around LYQ B 601 (B):**

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

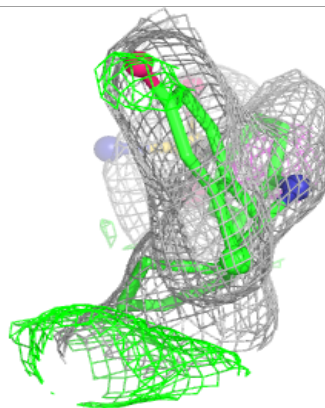
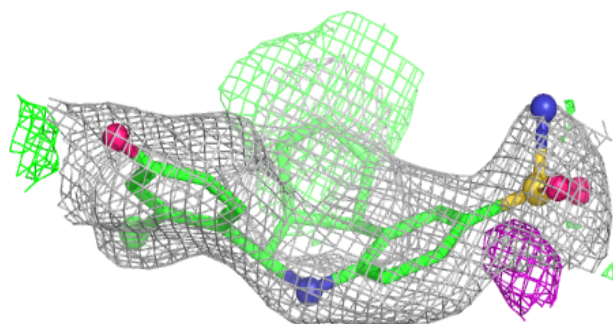
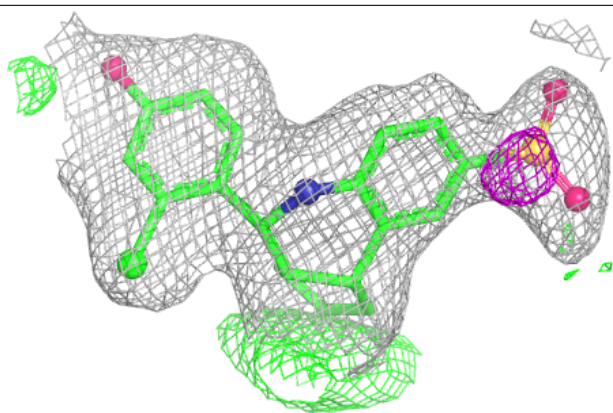
**Electron density around LYQ A 601 (B):**

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

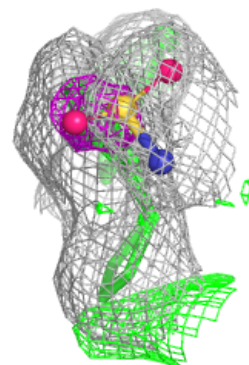
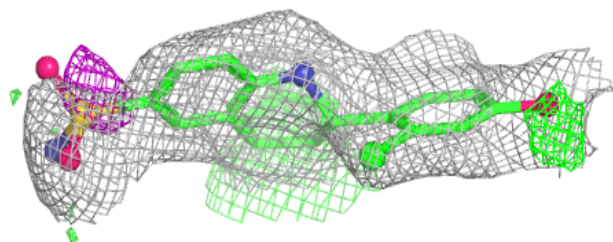
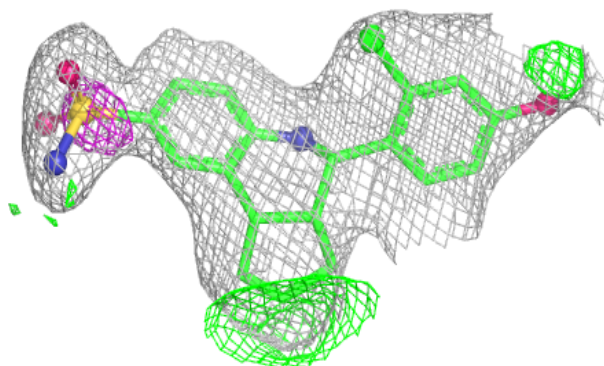


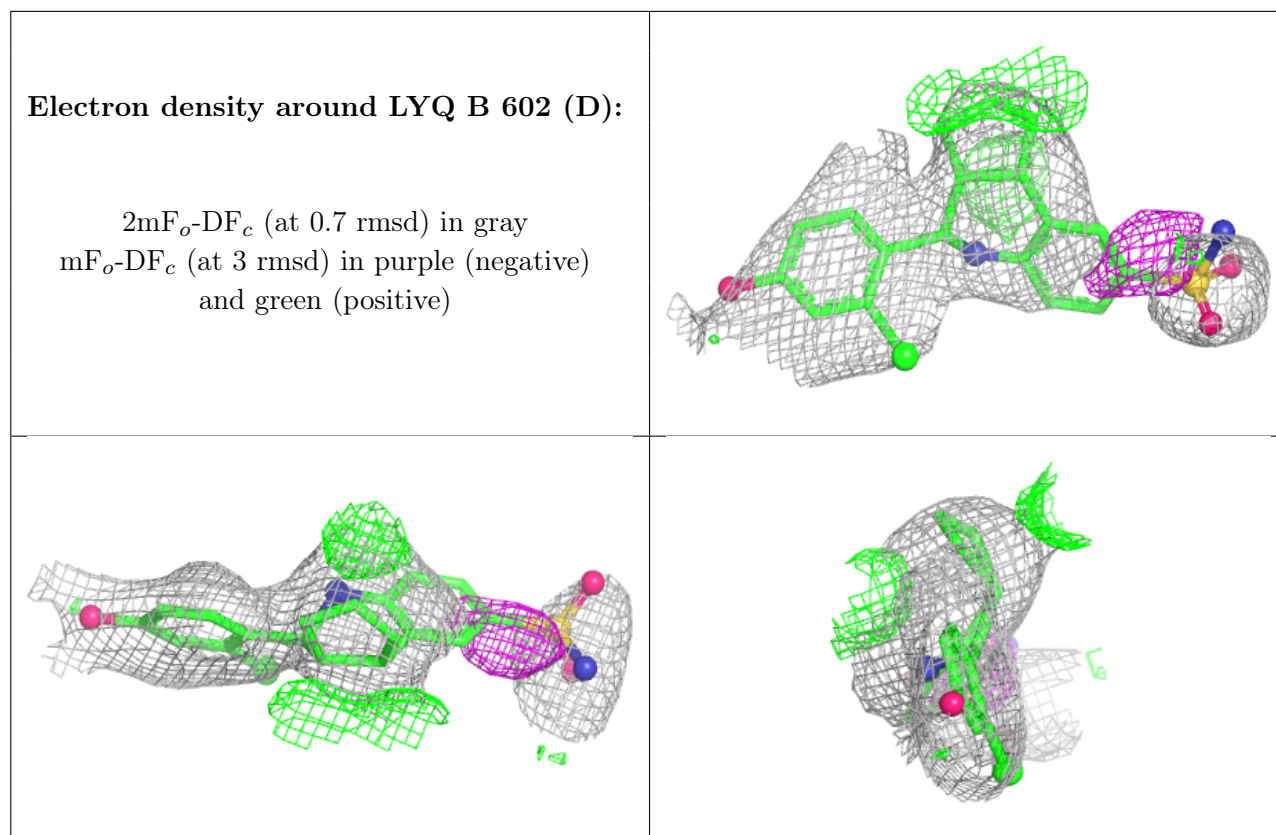
**Electron density around WVE A 603 (A):**

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

**Electron density around LYQ A 602 (D):**

$2mF_o-DF_c$  (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.