



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 02:00 PM EDT

PDB ID : 8EV2
Title : Dual Modulators
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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

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 : 1.8.5 (274361), 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

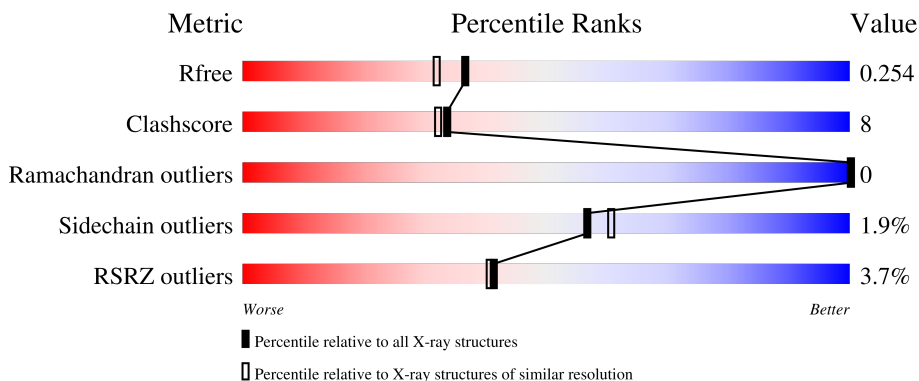
1 Overall quality at a glance i

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 ≥ 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	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
1	B	257	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
2	C	13	<div style="display: flex; align-items: center;"> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: grey;"></div> </div>
2	D	13	<div style="display: flex; align-items: center;"> <div style="width: 23%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: grey;"></div> </div>

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

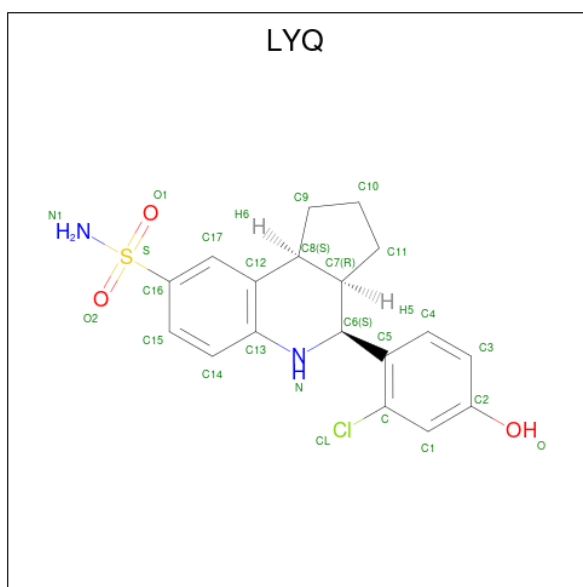
There are 2 discrepancies between the modelled and reference sequences:

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.

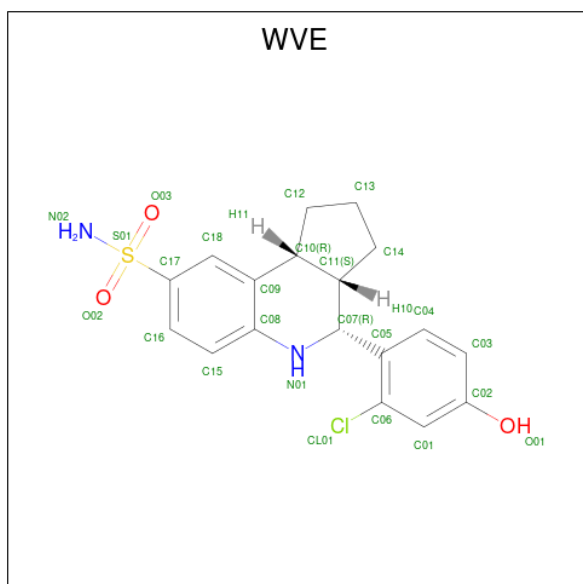
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	9	76	50	16	10	0	0	0
2	D	6	53	36	11	6	0	0	0

- 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 (three-letter code: LYQ) (formula: C₁₈H₁₉ClN₂O₃S) (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 (three-letter code: WVE) (formula: C₁₈H₁₉ClN₂O₃S) (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		

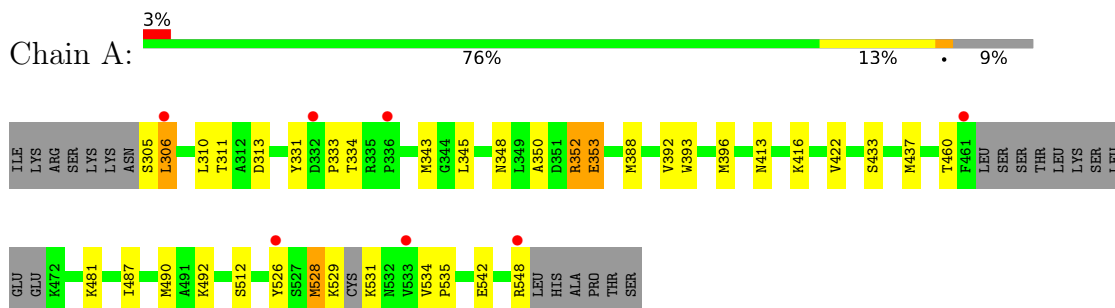
- Molecule 5 is water.

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		

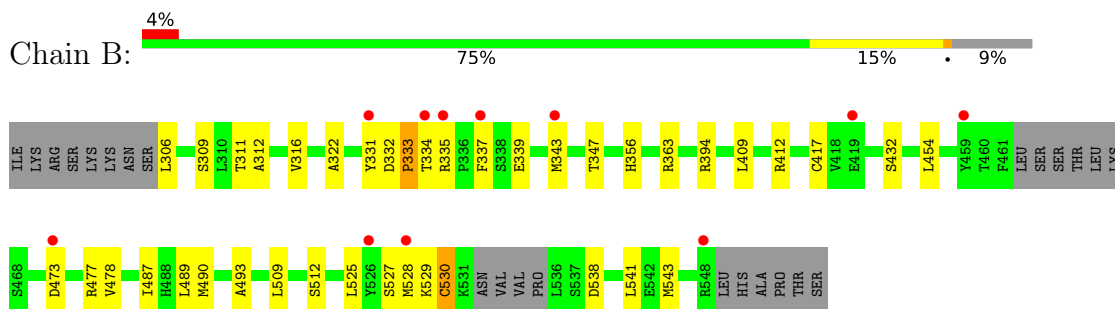
3 Residue-property plots [i](#)

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



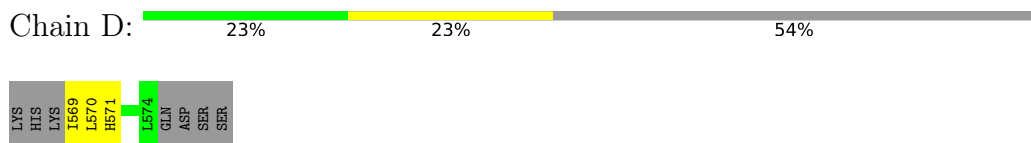
- Molecule 1: Estrogen receptor



- 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, α , β , γ	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) 70.6 (54.65-2.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.193 , 0.248 0.200 , 0.254	Depositor DCC
R_{free} test set	1132 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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: LYQ, WVE

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	0.74	1/1889 (0.1%)	0.78	2/2553 (0.1%)
1	B	0.70	0/1862	0.76	1/2515 (0.0%)
2	C	0.62	0/76	0.69	0/100
2	D	0.66	0/53	0.77	0/70
All	All	0.71	1/3880 (0.0%)	0.77	3/5238 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	GLU	CD-OE1	-8.32	1.16	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	A	352	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	394	ARG	CG-CD-NE	5.13	122.58	111.80

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	31	1
1	B	1830	0	1844	25	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	9	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	67	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 (67) 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
4:A:604[C]:WVE:C15	4:A:604[C]:WVE:CL01	2.54	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:343:MET:CE	1:A:528:MET:HE2	2.04	0.88
1:A:343:MET:HA	4:A:604[C]:WVE:N02	1.88	0.88
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:A:343:MET:CE	1:A:528:MET:CE	2.61	0.77
1:B:409:LEU:HD23	1:B:409:LEU:O	1.85	0.77
4:B:604[C]:WVE:CL01	4:B:604[C]:WVE:N01	2.58	0.73
1:A:343:MET:HA	4:A:603[A]:WVE:N02	2.04	0.73
1:A:343:MET:HE1	1:A:528:MET:HE2	1.71	0.72
1:A:343:MET:HE3	1:A:528:MET:HE2	1.73	0.69
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:A:343:MET:HE1	1:A:528:MET:CE	2.23	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
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
1:A:487:ILE:HA	1:A:490:MET:HE3	1.85	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:B:487:ILE:HA	1:B:490:MET:HE3	1.89	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:343:MET:HA	4:A:603[A]:WVE:O02	2.09	0.52
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:A:542:GLU:OE2	2:C:569:ILE:N	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD23	1:B:409:LEU:C	2.35	0.46
2:D:571:HIS:HB3	5:D:601:HOH:O	2.16	0.45
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:A:343:MET:HE1	1:A:528:MET:HE3	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:529:LYS:CE	1:B:541:LEU:HD22	2.49	0.42
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:A:343:MET:CA	4:A:603[A]:WVE:O02	2.69	0.40
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%)	202 (98%)	5 (2%)	49	51
1	B	200/232 (86%)	196 (98%)	4 (2%)	55	58
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%)	412 (98%)	9 (2%)	57	57

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	SER
1	A	306	LEU
1	A	460	THR
1	A	512[A]	SER
1	A	512[B]	SER
1	B	412	ARG
1	B	432	SER
1	B	512	SER
1	B	525	LEU

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	ASN
1	A	524	HIS
1	B	356	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 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	$\# Z > 2$
3	LYQ	A	602[D]	-	28,28,28	2.71	15 (53%)	41,43,43	3.98	14 (34%)
4	WVE	A	603[A]	-	28,28,28	2.65	16 (57%)	41,43,43	3.91	13 (31%)
4	WVE	B	603[A]	-	28,28,28	2.68	16 (57%)	41,43,43	3.86	13 (31%)
4	WVE	B	604[C]	-	28,28,28	2.68	15 (53%)	41,43,43	3.82	14 (34%)
3	LYQ	B	601[B]	-	28,28,28	2.63	14 (50%)	41,43,43	4.15	15 (36%)
3	LYQ	B	602[D]	-	28,28,28	2.72	15 (53%)	41,43,43	3.89	14 (34%)
4	WVE	A	604[C]	-	28,28,28	2.68	16 (57%)	41,43,43	3.89	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LYQ	A	601[B]	-	28,28,28	2.60	14 (50%)	41,43,43	4.27	16 (39%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	WVE	B	603[A]	-	-	0/10/32/32	0/4/4/4
4	WVE	B	604[C]	-	-	2/10/32/32	0/4/4/4
3	LYQ	B	601[B]	-	-	7/10/32/32	0/4/4/4
3	LYQ	B	602[D]	-	-	10/10/32/32	0/4/4/4
4	WVE	A	604[C]	-	-	2/10/32/32	0/4/4/4
3	LYQ	A	601[B]	-	-	10/10/32/32	0/4/4/4

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602[D]	LYQ	C13-N	-6.72	1.26	1.39
3	A	602[D]	LYQ	C13-N	-6.57	1.26	1.39
3	B	601[B]	LYQ	C13-N	-6.55	1.26	1.39
4	B	604[C]	WVE	C08-N01	-6.34	1.27	1.39
4	A	604[C]	WVE	C08-N01	-6.33	1.27	1.39
4	B	603[A]	WVE	C08-N01	-6.33	1.27	1.39
4	A	603[A]	WVE	C08-N01	-6.24	1.27	1.39
3	A	601[B]	LYQ	C13-N	-6.15	1.27	1.39
3	A	601[B]	LYQ	S-N1	5.26	1.70	1.60
3	A	602[D]	LYQ	S-N1	5.05	1.70	1.60
4	A	604[C]	WVE	S01-N02	5.00	1.70	1.60
3	B	602[D]	LYQ	S-N1	4.99	1.70	1.60
4	B	604[C]	WVE	S01-N02	4.97	1.70	1.60
4	A	603[A]	WVE	S01-N02	4.93	1.70	1.60
4	B	603[A]	WVE	S01-N02	4.89	1.70	1.60
4	B	603[A]	WVE	C08-C09	-4.86	1.34	1.40
4	A	603[A]	WVE	C08-C09	-4.74	1.34	1.40
3	B	601[B]	LYQ	S-N1	4.73	1.69	1.60
4	B	604[C]	WVE	C08-C09	-4.67	1.34	1.40
4	A	604[C]	WVE	C08-C09	-4.64	1.34	1.40
3	B	602[D]	LYQ	C13-C12	-4.41	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601[B]	LYQ	C13-C12	-4.36	1.35	1.40
3	B	602[D]	LYQ	C10-C9	-4.33	1.33	1.51
3	B	601[B]	LYQ	C10-C9	-4.30	1.33	1.51
3	A	602[D]	LYQ	C10-C9	-4.26	1.34	1.51
3	A	602[D]	LYQ	C13-C12	-4.21	1.35	1.40
4	B	604[C]	WVE	C13-C12	-4.21	1.34	1.51
3	A	601[B]	LYQ	C10-C9	-4.20	1.34	1.51
4	B	603[A]	WVE	C13-C12	-4.19	1.34	1.51
4	A	604[C]	WVE	C13-C12	-4.18	1.34	1.51
4	A	603[A]	WVE	C13-C12	-4.17	1.34	1.51
3	A	601[B]	LYQ	C13-C12	-4.08	1.35	1.40
4	A	603[A]	WVE	C04-C05	-3.62	1.35	1.39
4	A	604[C]	WVE	C06-C05	-3.62	1.35	1.39
4	B	604[C]	WVE	C04-C05	-3.56	1.35	1.39
4	B	603[A]	WVE	C04-C05	-3.56	1.35	1.39
4	A	604[C]	WVE	C04-C05	-3.54	1.35	1.39
3	A	602[D]	LYQ	C-C5	-3.46	1.35	1.39
3	A	602[D]	LYQ	C1-C2	-3.43	1.34	1.39
3	B	601[B]	LYQ	C-C5	-3.41	1.35	1.39
3	A	602[D]	LYQ	C4-C5	-3.40	1.35	1.39
3	B	602[D]	LYQ	C1-C2	-3.38	1.34	1.39
4	B	604[C]	WVE	C06-C05	-3.37	1.35	1.39
3	B	602[D]	LYQ	C4-C5	-3.35	1.35	1.39
3	B	602[D]	LYQ	C-C5	-3.29	1.35	1.39
3	B	601[B]	LYQ	C4-C5	-3.17	1.35	1.39
4	B	603[A]	WVE	C01-C02	-3.17	1.34	1.39
3	A	601[B]	LYQ	C4-C5	-3.10	1.35	1.39
4	B	603[A]	WVE	C06-C05	-3.08	1.35	1.39
3	A	601[B]	LYQ	C1-C2	-3.07	1.34	1.39
4	B	604[C]	WVE	C01-C02	-3.06	1.34	1.39
4	A	604[C]	WVE	C01-C02	-3.01	1.34	1.39
4	A	603[A]	WVE	C01-C02	-2.98	1.34	1.39
3	B	601[B]	LYQ	C1-C2	-2.93	1.34	1.39
3	A	602[D]	LYQ	C17-C12	-2.91	1.34	1.39
3	B	602[D]	LYQ	C14-C13	-2.91	1.34	1.39
3	A	601[B]	LYQ	C17-C12	-2.88	1.34	1.39
4	B	604[C]	WVE	C15-C08	-2.88	1.34	1.39
4	A	603[A]	WVE	C15-C08	-2.88	1.34	1.39
4	A	604[C]	WVE	C15-C08	-2.86	1.34	1.39
3	A	602[D]	LYQ	C14-C13	-2.86	1.34	1.39
4	B	603[A]	WVE	C15-C08	-2.83	1.34	1.39
4	B	604[C]	WVE	C18-C09	-2.82	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603[A]	WVE	C06-C05	-2.82	1.36	1.39
3	A	602[D]	LYQ	C1-C	-2.81	1.34	1.38
3	B	601[B]	LYQ	C17-C12	-2.80	1.35	1.39
3	B	602[D]	LYQ	C1-C	-2.76	1.34	1.38
4	B	603[A]	WVE	C18-C09	-2.74	1.35	1.39
3	B	602[D]	LYQ	C17-C12	-2.69	1.35	1.39
4	A	604[C]	WVE	C18-C09	-2.66	1.35	1.39
3	B	602[D]	LYQ	C15-C16	-2.64	1.34	1.38
4	B	604[C]	WVE	C16-C17	-2.64	1.34	1.38
3	A	601[B]	LYQ	C14-C13	-2.62	1.35	1.39
3	B	601[B]	LYQ	C14-C13	-2.59	1.35	1.39
4	A	603[A]	WVE	C18-C09	-2.58	1.35	1.39
4	A	604[C]	WVE	C16-C17	-2.56	1.34	1.38
4	B	603[A]	WVE	C16-C17	-2.53	1.34	1.38
3	A	602[D]	LYQ	C15-C16	-2.52	1.34	1.38
4	A	603[A]	WVE	C03-C02	-2.50	1.34	1.38
3	A	601[B]	LYQ	C-C5	-2.50	1.36	1.39
3	A	601[B]	LYQ	C3-C2	-2.48	1.34	1.38
3	B	601[B]	LYQ	C3-C2	-2.46	1.34	1.38
4	A	603[A]	WVE	C04-C03	-2.43	1.34	1.38
4	A	603[A]	WVE	C16-C17	-2.42	1.35	1.38
3	A	601[B]	LYQ	C1-C	-2.39	1.34	1.38
4	B	603[A]	WVE	C03-C02	-2.39	1.34	1.38
3	A	601[B]	LYQ	C15-C16	-2.37	1.35	1.38
4	B	603[A]	WVE	C01-C06	-2.36	1.34	1.38
3	B	602[D]	LYQ	C15-C14	-2.35	1.34	1.38
4	A	604[C]	WVE	C01-C06	-2.34	1.34	1.38
3	A	601[B]	LYQ	C3-C4	-2.33	1.34	1.38
4	B	604[C]	WVE	C01-C06	-2.32	1.34	1.38
3	A	602[D]	LYQ	C17-C16	-2.32	1.34	1.39
3	A	601[B]	LYQ	C17-C16	-2.30	1.34	1.39
3	B	601[B]	LYQ	C3-C4	-2.28	1.34	1.38
4	B	604[C]	WVE	C18-C17	-2.28	1.35	1.39
3	B	601[B]	LYQ	C15-C16	-2.28	1.35	1.38
4	A	603[A]	WVE	C07-N01	2.28	1.48	1.46
4	B	603[A]	WVE	C04-C03	-2.26	1.34	1.38
4	B	604[C]	WVE	C15-C16	-2.24	1.34	1.38
4	B	604[C]	WVE	C03-C02	-2.24	1.34	1.38
4	B	604[C]	WVE	C04-C03	-2.24	1.34	1.38
4	B	603[A]	WVE	C18-C17	-2.22	1.35	1.39
4	A	604[C]	WVE	C03-C02	-2.21	1.34	1.38
4	A	603[A]	WVE	C18-C17	-2.21	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604[C]	WVE	C18-C17	-2.21	1.35	1.39
3	B	602[D]	LYQ	C3-C2	-2.20	1.34	1.38
4	A	603[A]	WVE	C01-C06	-2.18	1.35	1.38
3	A	602[D]	LYQ	C15-C14	-2.17	1.34	1.38
4	A	604[C]	WVE	C15-C16	-2.16	1.34	1.38
4	A	604[C]	WVE	C04-C03	-2.16	1.34	1.38
4	A	604[C]	WVE	C07-N01	2.15	1.48	1.46
3	B	602[D]	LYQ	C3-C4	-2.15	1.34	1.38
3	B	602[D]	LYQ	C17-C16	-2.14	1.35	1.39
4	B	603[A]	WVE	C07-N01	2.13	1.48	1.46
4	B	603[A]	WVE	C15-C16	-2.09	1.35	1.38
3	A	602[D]	LYQ	C3-C4	-2.08	1.35	1.38
4	A	603[A]	WVE	C15-C16	-2.08	1.35	1.38
3	B	601[B]	LYQ	C1-C	-2.08	1.35	1.38
3	B	601[B]	LYQ	C17-C16	-2.07	1.35	1.39
3	A	602[D]	LYQ	C3-C2	-2.03	1.35	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	LYQ	O1-S-N1	-14.42	85.99	107.36
4	A	603[A]	WVE	O03-S01-N02	-13.47	87.40	107.36
4	B	603[A]	WVE	O03-S01-N02	-13.37	87.53	107.36
3	A	601[B]	LYQ	O1-S-N1	-13.28	87.67	107.36
4	A	604[C]	WVE	O02-S01-N02	-13.11	87.92	107.36
4	B	603[A]	WVE	O02-S01-N02	-13.08	87.97	107.36
4	B	604[C]	WVE	O03-S01-N02	-13.02	88.06	107.36
3	A	601[B]	LYQ	O2-S-N1	-13.01	88.07	107.36
3	A	602[D]	LYQ	O2-S-N1	-13.01	88.08	107.36
4	A	604[C]	WVE	O03-S01-N02	-12.99	88.11	107.36
3	B	601[B]	LYQ	O2-S-N1	-12.97	88.13	107.36
4	B	604[C]	WVE	O02-S01-N02	-12.90	88.24	107.36
3	B	602[D]	LYQ	O2-S-N1	-12.86	88.29	107.36
3	A	602[D]	LYQ	O1-S-N1	-12.84	88.32	107.36
3	B	602[D]	LYQ	O1-S-N1	-12.77	88.43	107.36
4	A	603[A]	WVE	O02-S01-N02	-12.76	88.45	107.36
3	A	601[B]	LYQ	O2-S-C16	10.77	119.37	107.35
3	B	601[B]	LYQ	O2-S-C16	10.55	119.12	107.35
3	A	602[D]	LYQ	O2-S-C16	9.63	118.09	107.35
4	B	604[C]	WVE	O02-S01-C17	9.24	117.66	107.35
3	B	602[D]	LYQ	O2-S-C16	9.20	117.61	107.35
4	B	603[A]	WVE	O02-S01-C17	8.98	117.37	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604[C]	WVE	O03-S01-C17	8.80	117.17	107.35
4	A	603[A]	WVE	O02-S01-C17	8.67	117.02	107.35
4	A	603[A]	WVE	O03-S01-C17	8.54	116.88	107.35
4	A	604[C]	WVE	O02-S01-C17	8.53	116.87	107.35
3	B	602[D]	LYQ	O1-S-C16	8.38	116.70	107.35
3	A	602[D]	LYQ	O1-S-C16	8.08	116.37	107.35
4	B	603[A]	WVE	O03-S01-C17	8.00	116.28	107.35
4	B	604[C]	WVE	O03-S01-C17	7.78	116.03	107.35
3	B	601[B]	LYQ	O1-S-C16	7.61	115.84	107.35
3	A	601[B]	LYQ	O1-S-C16	7.30	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	5.79	126.41	120.41
3	B	601[B]	LYQ	C5-C6-C7	5.67	121.36	112.53
3	A	601[B]	LYQ	C-C5-C6	5.32	129.21	121.60
3	A	601[B]	LYQ	C5-C6-C7	5.27	120.73	112.53
4	A	604[C]	WVE	C17-S01-N02	5.27	115.84	108.38
4	B	603[A]	WVE	C17-S01-N02	5.24	115.80	108.38
4	A	603[A]	WVE	C17-S01-N02	5.10	115.60	108.38
3	A	602[D]	LYQ	C10-C9-C8	5.04	112.21	104.28
4	A	604[C]	WVE	C13-C12-C10	4.89	111.97	104.28
4	B	604[C]	WVE	C13-C12-C10	4.82	111.87	104.28
4	A	603[A]	WVE	C13-C12-C10	4.66	111.61	104.28
3	A	601[B]	LYQ	C10-C9-C8	4.65	111.58	104.28
4	B	603[A]	WVE	C13-C12-C10	4.63	111.55	104.28
4	B	604[C]	WVE	C17-S01-N02	4.59	114.88	108.38
4	A	604[C]	WVE	C11-C07-N01	4.52	113.22	108.59
3	B	601[B]	LYQ	C10-C9-C8	4.52	111.39	104.28
4	B	604[C]	WVE	C11-C07-N01	4.33	113.02	108.59
3	A	602[D]	LYQ	C16-S-N1	4.18	114.30	108.38
4	A	603[A]	WVE	C11-C07-N01	3.98	112.67	108.59
3	A	601[B]	LYQ	C16-S-N1	3.98	114.01	108.38
3	A	601[B]	LYQ	C4-C5-C6	-3.95	114.79	120.91
3	B	602[D]	LYQ	C10-C9-C8	3.91	110.43	104.28
3	B	602[D]	LYQ	C16-S-N1	3.85	113.83	108.38
4	B	603[A]	WVE	C11-C07-N01	3.70	112.38	108.59
3	B	601[B]	LYQ	C-C5-C6	3.69	126.88	121.60
3	A	601[B]	LYQ	C5-C6-N	3.65	116.35	110.77
3	B	601[B]	LYQ	C16-S-N1	3.64	113.53	108.38
3	A	601[B]	LYQ	C2-C1-C	3.46	123.08	118.90
3	A	601[B]	LYQ	C7-C6-N	3.28	111.95	108.59
3	B	602[D]	LYQ	C5-C-CL	3.27	123.80	120.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	LYQ	C5-C6-N	3.27	115.77	110.77
3	A	602[D]	LYQ	C3-C2-C1	-3.20	116.66	120.17
3	A	601[B]	LYQ	C1-C-CL	-3.14	113.42	118.49
4	A	603[A]	WVE	C13-C14-C11	-3.13	98.73	104.87
3	A	602[D]	LYQ	C5-C-CL	3.12	123.64	120.41
4	A	604[C]	WVE	C13-C14-C11	-3.07	98.83	104.87
3	B	601[B]	LYQ	C3-C2-C1	-3.03	116.86	120.17
3	B	602[D]	LYQ	C3-C2-C1	-2.90	117.00	120.17
3	B	602[D]	LYQ	C2-C1-C	2.84	122.33	118.90
3	A	602[D]	LYQ	C7-C6-N	2.84	111.49	108.59
3	B	601[B]	LYQ	C2-C1-C	2.82	122.31	118.90
3	A	601[B]	LYQ	C3-C2-C1	-2.80	117.11	120.17
4	A	604[C]	WVE	C03-C02-C01	-2.72	117.19	120.17
4	B	604[C]	WVE	C03-C02-C01	-2.69	117.22	120.17
3	A	602[D]	LYQ	C2-C1-C	2.60	122.05	118.90
3	A	602[D]	LYQ	C1-C-CL	-2.56	114.36	118.49
4	B	603[A]	WVE	C03-C02-C01	-2.54	117.39	120.17
3	A	602[D]	LYQ	C11-C10-C9	2.54	112.50	105.79
4	A	603[A]	WVE	C05-C06-CL01	2.53	123.03	120.41
4	A	603[A]	WVE	C02-C01-C06	2.52	121.95	118.90
4	B	604[C]	WVE	C13-C14-C11	-2.51	99.94	104.87
4	A	603[A]	WVE	C03-C02-C01	-2.50	117.43	120.17
4	B	604[C]	WVE	C12-C10-C11	-2.49	99.62	103.60
3	B	601[B]	LYQ	C11-C7-C8	2.46	106.98	104.05
4	B	603[A]	WVE	C12-C10-C11	-2.44	99.70	103.60
4	B	604[C]	WVE	C02-C01-C06	2.30	121.68	118.90
3	B	601[B]	LYQ	C4-C5-C6	-2.28	117.37	120.91
3	B	602[D]	LYQ	C11-C7-C8	2.28	106.76	104.05
4	B	603[A]	WVE	C02-C01-C06	2.27	121.65	118.90
3	B	601[B]	LYQ	C11-C10-C9	2.26	111.77	105.79
4	B	603[A]	WVE	C13-C14-C11	-2.26	100.43	104.87
3	B	602[D]	LYQ	C7-C6-N	2.25	110.89	108.59
3	A	602[D]	LYQ	C11-C7-C8	2.25	106.72	104.05
3	B	602[D]	LYQ	C1-C-CL	-2.21	114.92	118.49
4	A	603[A]	WVE	C10-C11-C07	2.19	113.61	110.65
4	A	604[C]	WVE	C12-C10-C11	-2.18	100.11	103.60
4	B	604[C]	WVE	C08-N01-C07	2.12	125.08	119.20
4	A	603[A]	WVE	C06-C05-C07	2.12	124.63	121.60
3	B	602[D]	LYQ	C11-C10-C9	2.09	111.32	105.79
4	A	604[C]	WVE	C02-C01-C06	2.06	121.40	118.90
4	B	603[A]	WVE	C12-C13-C14	2.06	111.23	105.79
4	B	604[C]	WVE	O03-S01-O02	2.05	122.13	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	LYQ	O1-S-O2	2.05	122.12	118.76
4	B	603[A]	WVE	O03-S01-O02	2.05	122.12	118.76
4	B	604[C]	WVE	C12-C13-C14	2.01	111.10	105.79
3	A	601[B]	LYQ	C13-C12-C8	2.00	122.26	118.96

There are no chirality outliers.

All (41) 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	C04-C05-C07-N01
4	A	604[C]	WVE	C06-C05-C07-N01
4	B	604[C]	WVE	C04-C05-C07-N01
4	B	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
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
3	A	602[D]	LYQ	C17-C16-S-O1
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	B	601[B]	LYQ	C17-C16-S-N1
3	A	601[B]	LYQ	C17-C16-S-O2
3	A	601[B]	LYQ	C17-C16-S-O1
3	B	602[D]	LYQ	C15-C16-S-O2
3	A	602[D]	LYQ	C4-C5-C6-N

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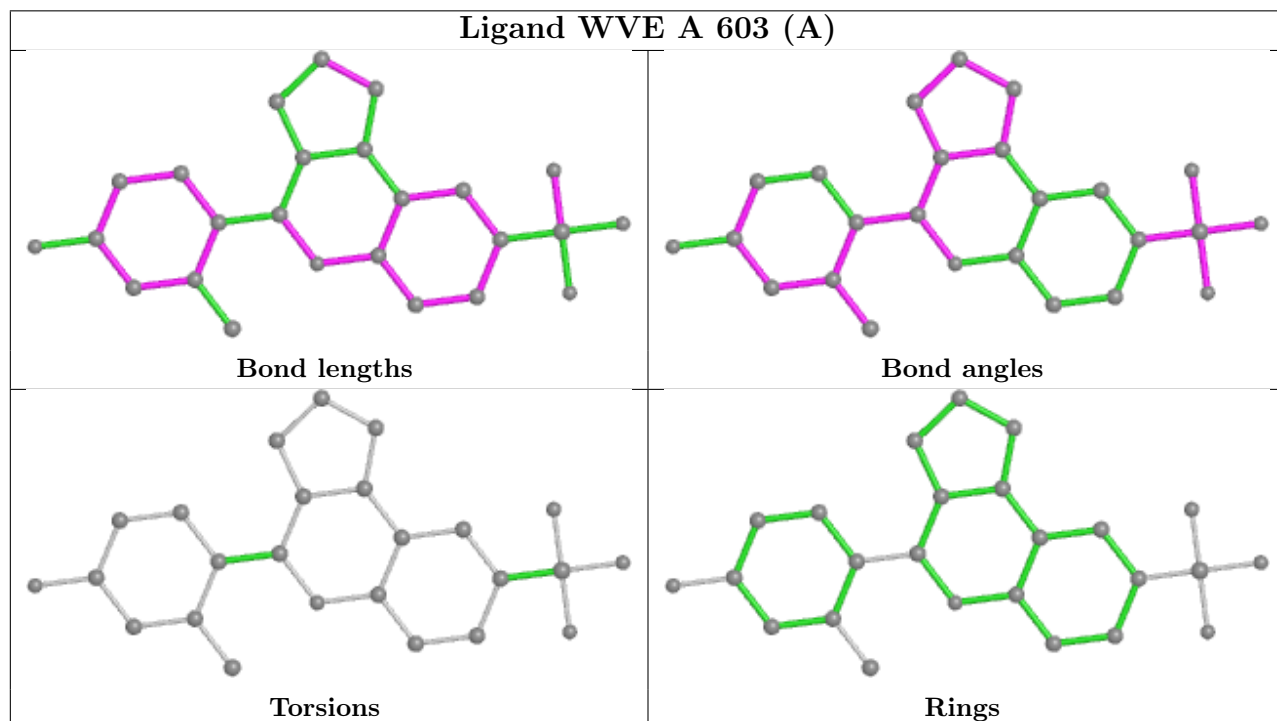
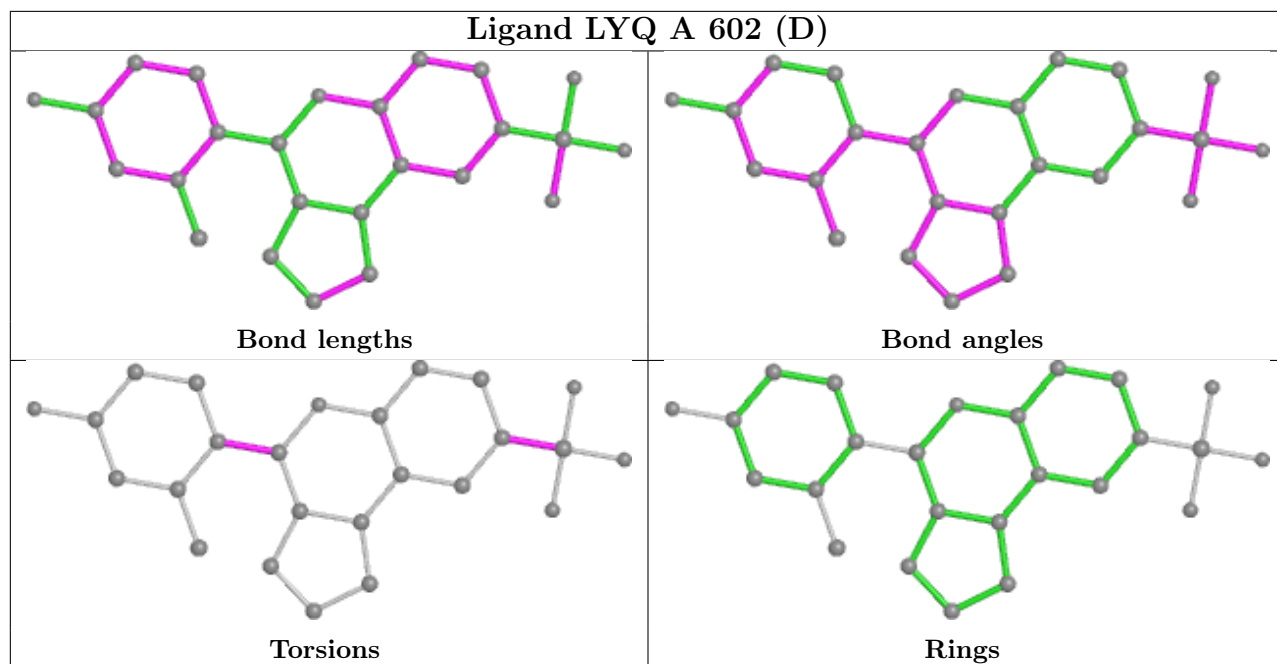
Mol	Chain	Res	Type	Atoms
3	B	602[D]	LYQ	C4-C5-C6-N
3	B	602[D]	LYQ	C17-C16-S-O2
3	B	601[B]	LYQ	C15-C16-S-N1
3	A	602[D]	LYQ	C15-C16-S-O2
3	A	602[D]	LYQ	C17-C16-S-O2
3	A	602[D]	LYQ	C-C5-C6-N
3	B	602[D]	LYQ	C-C5-C6-N
3	B	601[B]	LYQ	C15-C16-S-O1

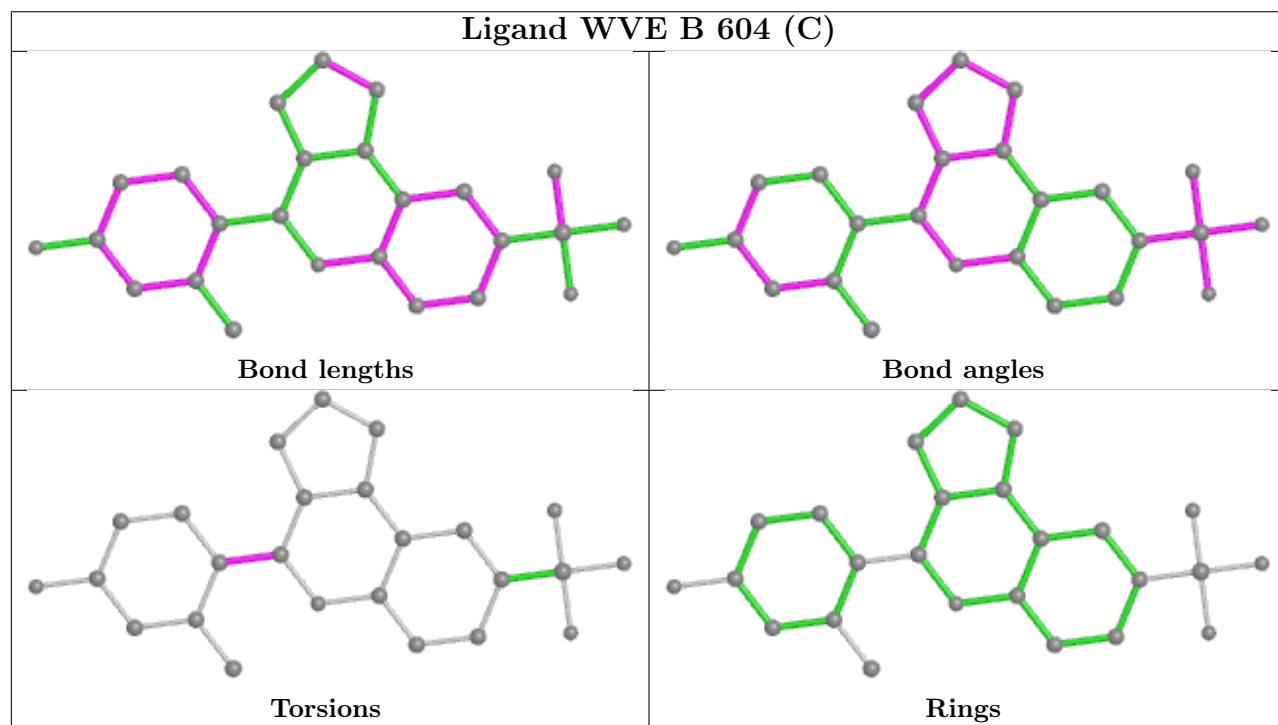
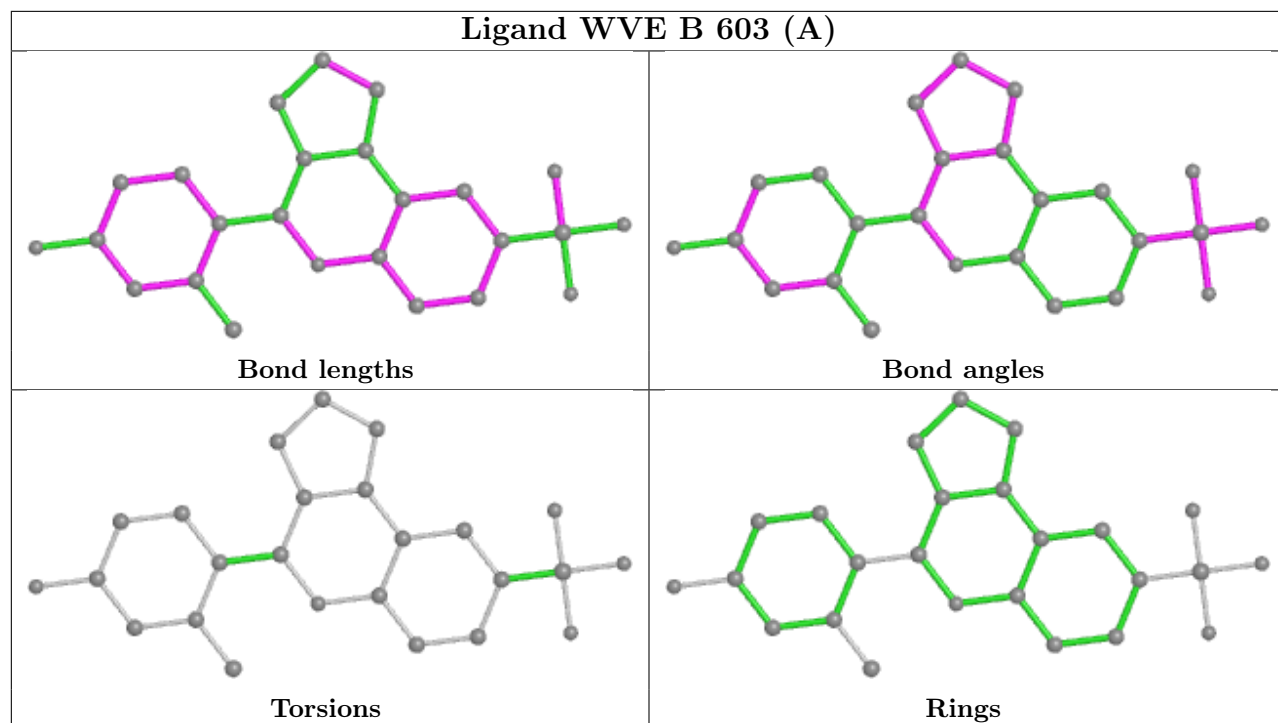
There are no ring outliers.

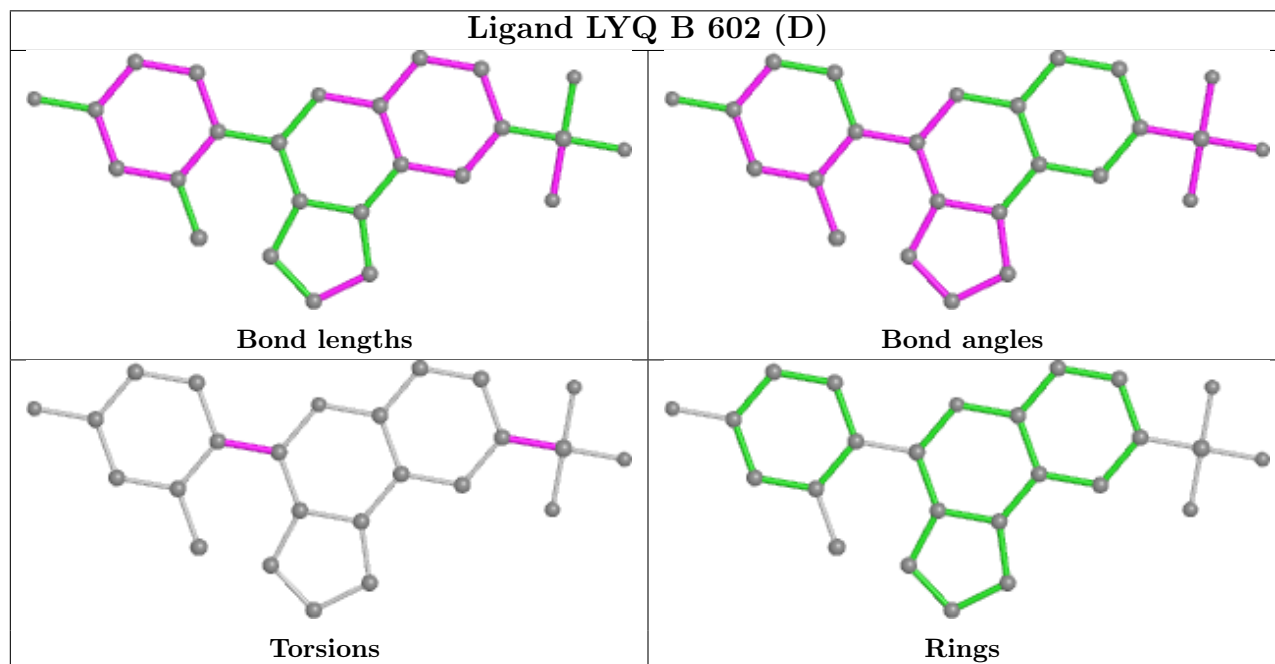
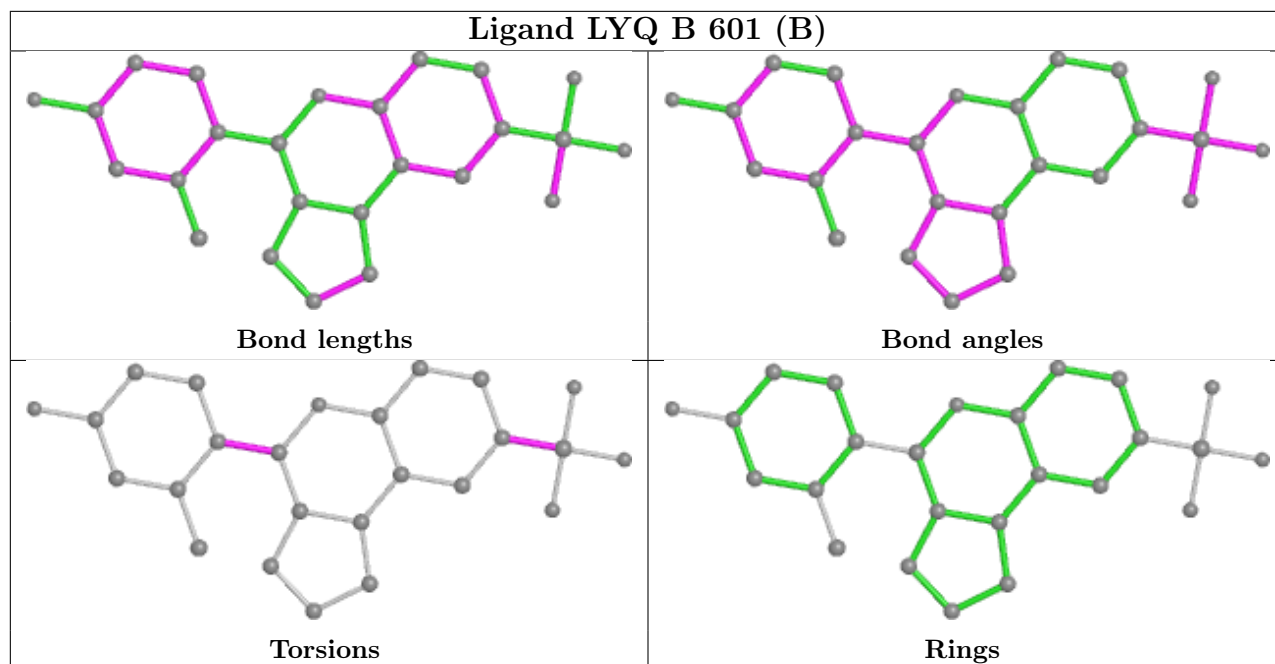
5 monomers are involved in 17 short contacts:

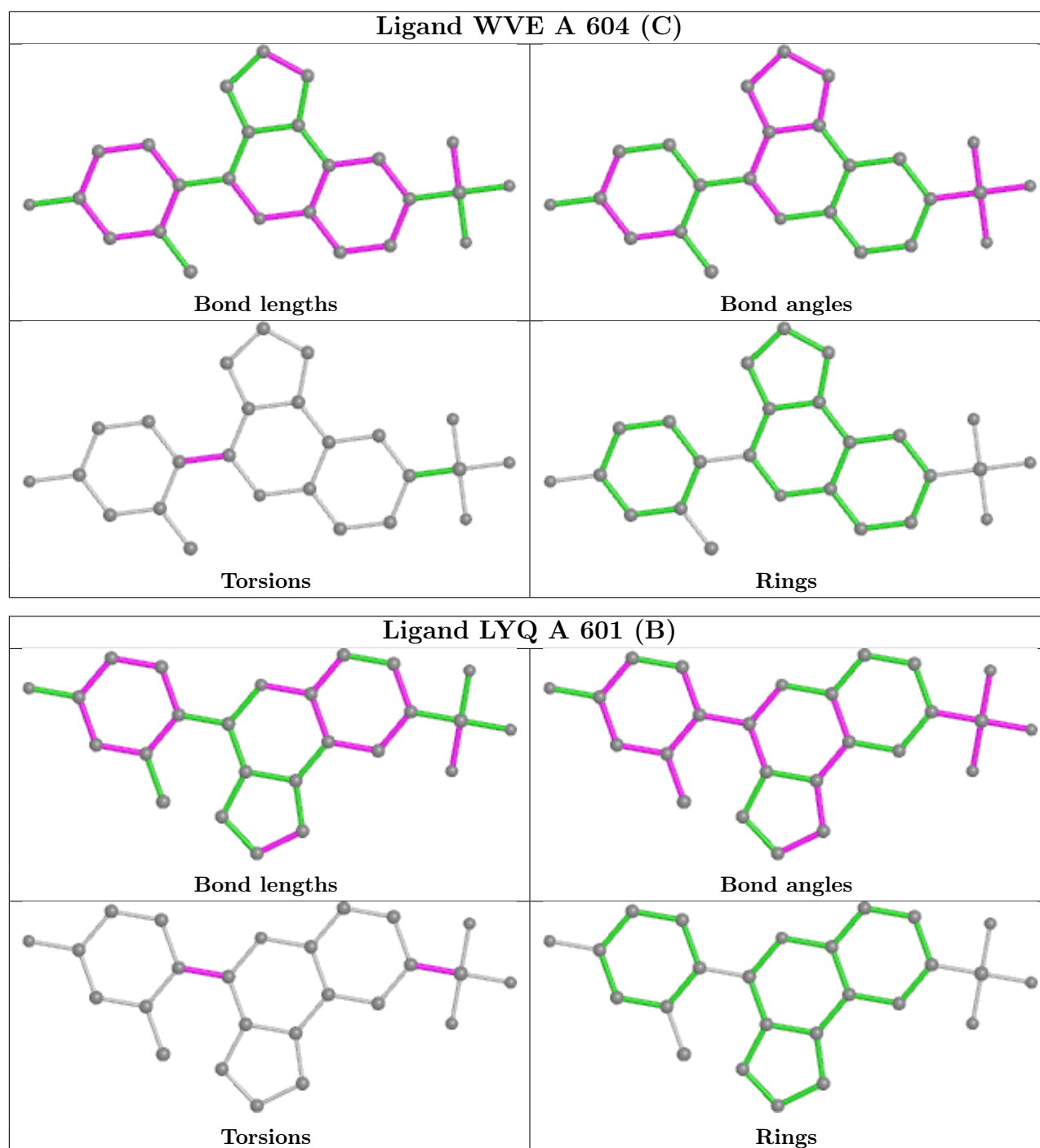
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603[A]	WVE	4	0
4	B	604[C]	WVE	3	0
3	B	601[B]	LYQ	3	0
4	A	604[C]	WVE	5	0
3	A	601[B]	LYQ	2	0

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	233/257 (90%)	-0.12	7 (3%) 50 49	19, 42, 83, 114	1 (0%)
1	B	233/257 (90%)	0.07	11 (4%) 31 30	26, 52, 104, 132	0
2	C	9/13 (69%)	-0.22	0 100 100	39, 43, 63, 75	0
2	D	6/13 (46%)	0.38	0 100 100	57, 60, 82, 83	0
All	All	481/540 (89%)	-0.02	18 (3%) 41 41	19, 47, 99, 132	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	VAL	4.4
1	B	337	PHE	4.3
1	B	548	ARG	3.5
1	B	334	THR	3.1
1	A	332	ASP	3.0
1	A	461	PHE	2.9
1	A	548	ARG	2.8
1	A	336	PRO	2.6
1	B	528	MET	2.6
1	B	419	GLU	2.6
1	B	331	TYR	2.3
1	A	526	TYR	2.2
1	B	343	MET	2.2
1	B	526	TYR	2.1
1	B	459	TYR	2.1
1	B	335	ARG	2.1
1	B	473	ASP	2.1
1	A	306	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 [i](#)

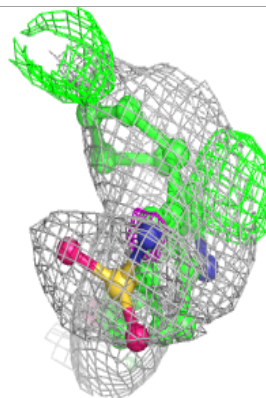
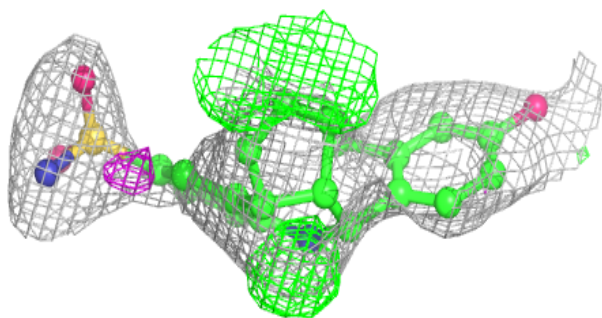
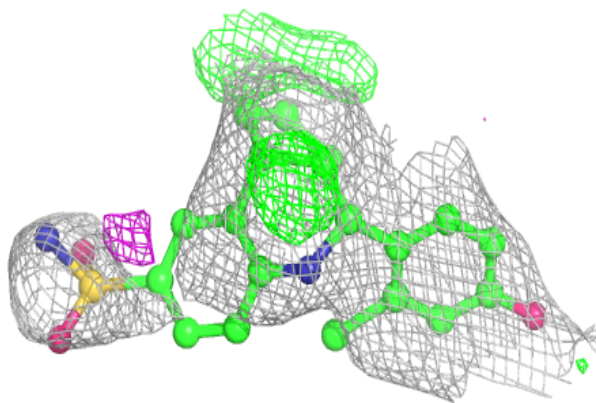
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	WVE	B	604[C]	25/25	0.81	0.19	73,81,85,86	25
3	LYQ	B	601[B]	25/25	0.82	0.18	34,49,57,58	25
4	WVE	B	603[A]	25/25	0.83	0.20	25,28,29,29	25
3	LYQ	B	602[D]	25/25	0.86	0.18	107,152,224,228	25
3	LYQ	A	601[B]	25/25	0.87	0.13	25,36,38,41	25
3	LYQ	A	602[D]	25/25	0.88	0.14	51,91,130,133	25
4	WVE	A	604[C]	25/25	0.89	0.14	39,49,52,52	25
4	WVE	A	603[A]	25/25	0.90	0.14	18,22,25,25	25

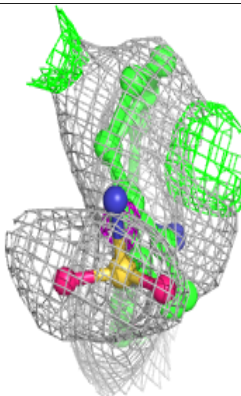
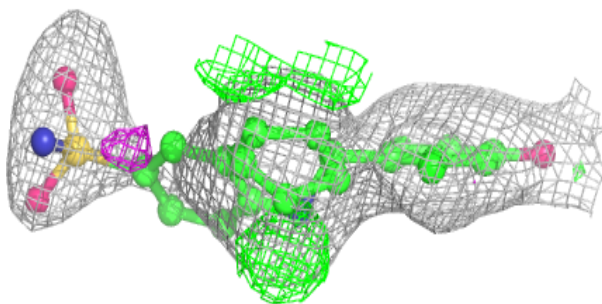
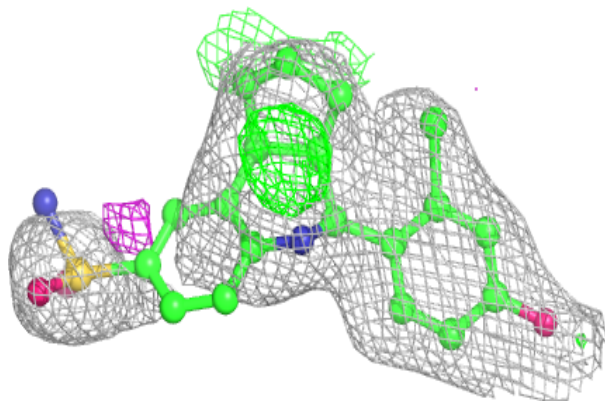
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

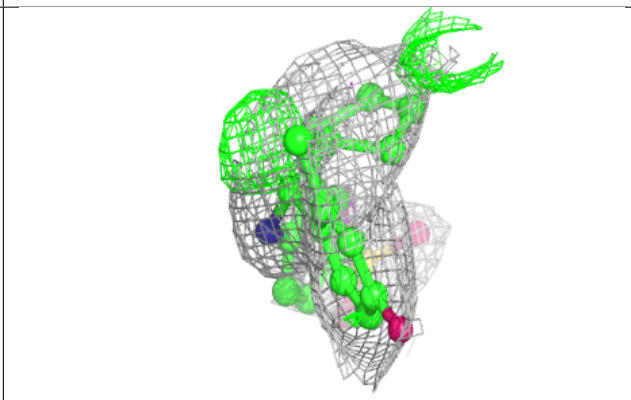
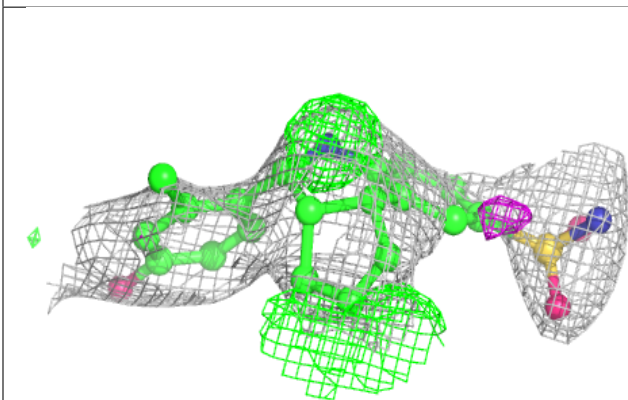
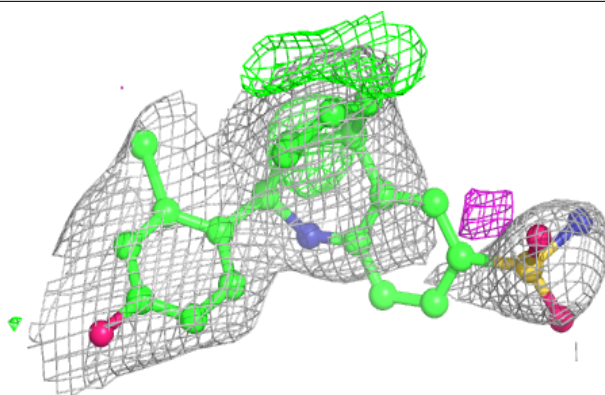
**Electron density around LYQ B 601 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

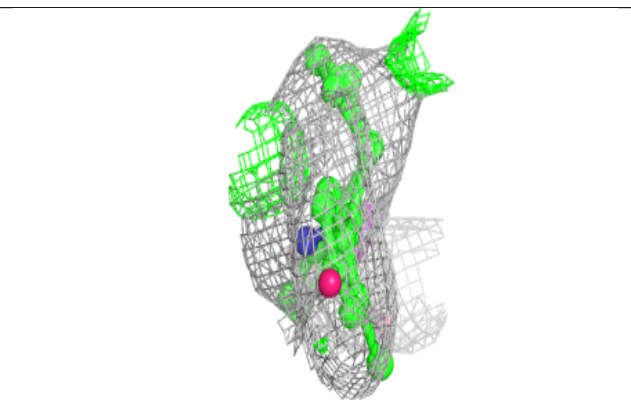
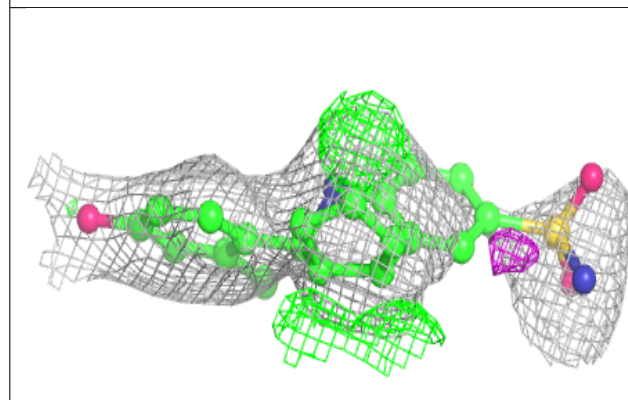
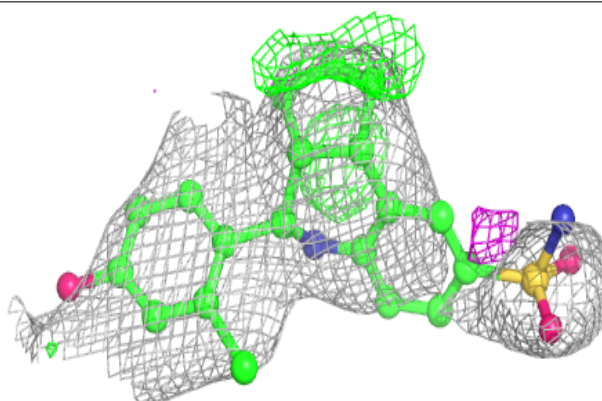


Electron density around WVE B 603 (A):

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

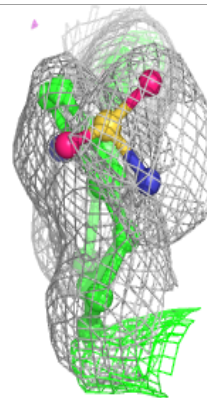
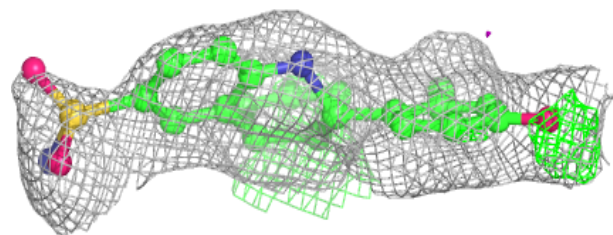
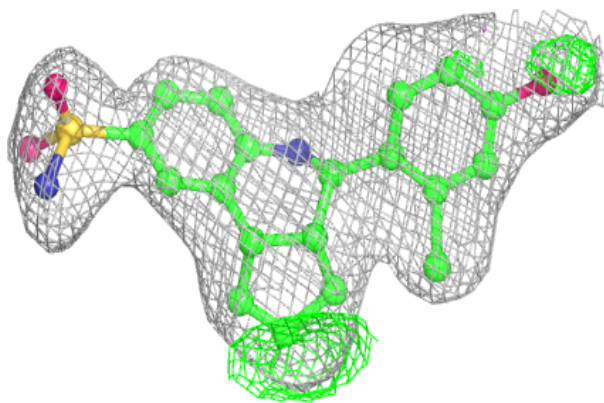
**Electron density around LYQ B 602 (D):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

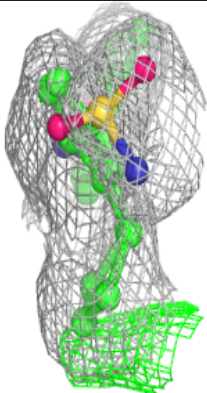
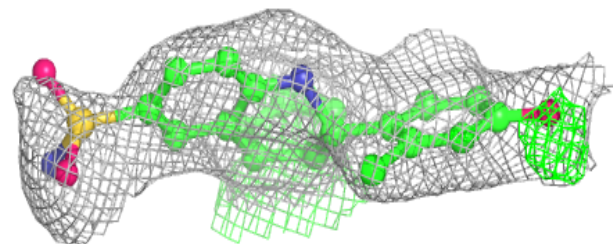
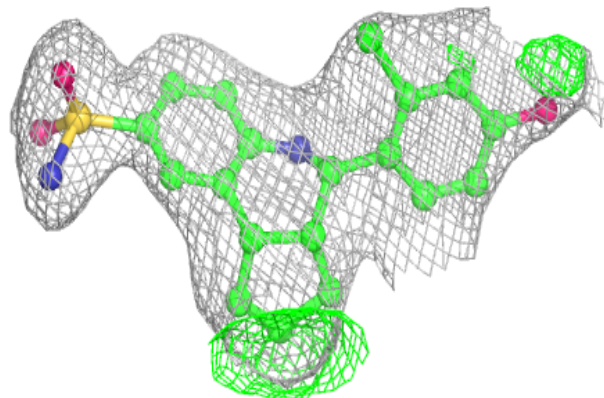


Electron density around LYQ A 601 (B):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

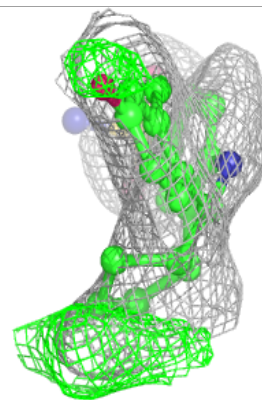
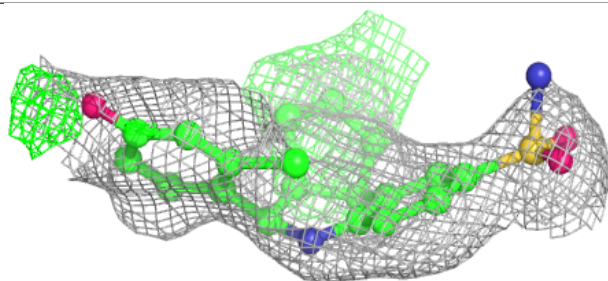
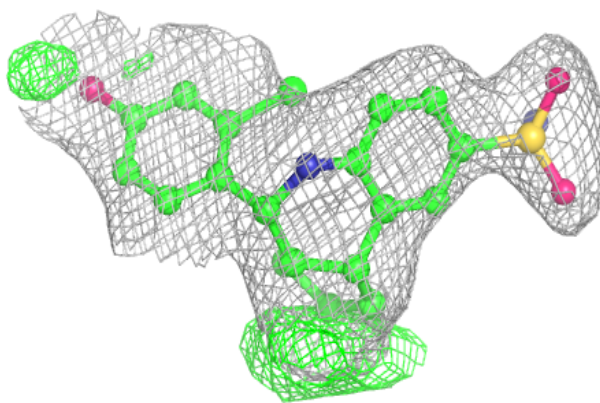
**Electron density around LYQ A 602 (D):**

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and green (positive)

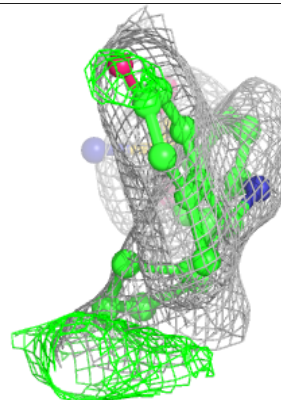
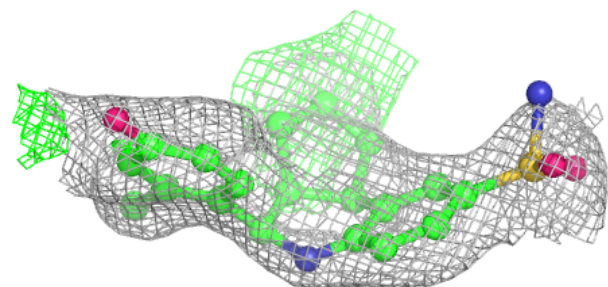
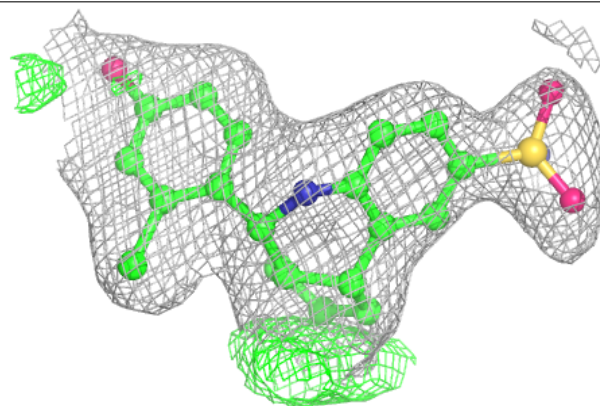


Electron density around WVE A 604 (C):

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

**Electron density around WVE 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.