



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:08 pm BST

PDB ID : 5U2B  
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (Y537S) in Complex with the phenylamino-substituted estrogen, (8R,9S,13S,14S,17S)-13-methyl-17-(phenylamino)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-ol, without a coactivator peptide  
Authors : Nwachukwu, J.C.; Nowak, J.; Carlson, K.E.; Katzenellenbogen, J.A.; Nettles, K.W.  
Deposited on : 2016-11-30  
Resolution : 2.22 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 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 : 2.11  
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) : 2.11

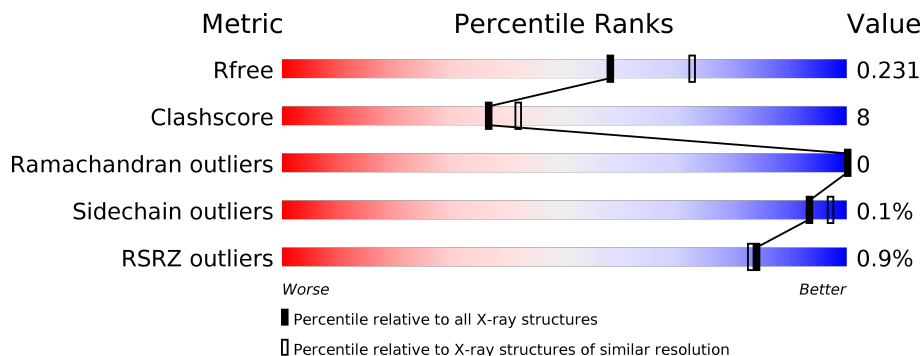
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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  $\geq 3$ , 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	
1	B	257	
1	C	257	
1	D	257	
1	E	257	
1	F	257	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11621 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.

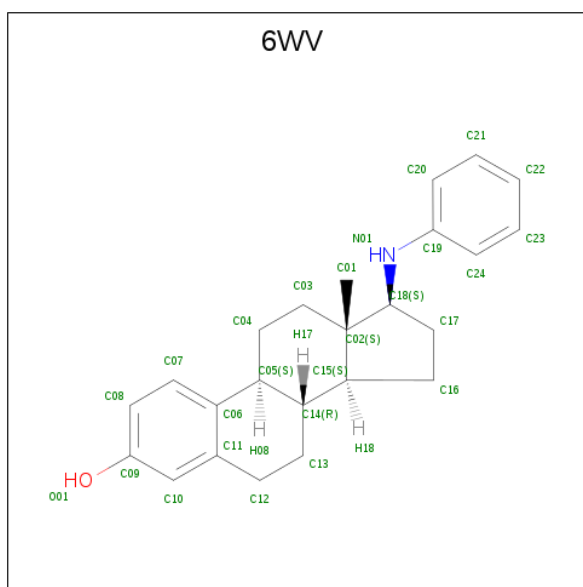
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	Total 1909	C 1220	N 327	O 343	S 19	0	0	0
1	B	228	Total 1789	C 1145	N 312	O 314	S 18	0	1	0
1	C	244	Total 1922	C 1225	N 332	O 347	S 18	0	1	0
1	D	226	Total 1747	C 1113	N 305	O 310	S 19	0	0	0
1	E	221	Total 1701	C 1084	N 295	O 306	S 16	0	0	0
1	F	225	Total 1720	C 1095	N 299	O 311	S 15	0	0	0

There are 6 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
C	537	SER	TYR	engineered mutation	UNP P03372
D	537	SER	TYR	engineered mutation	UNP P03372
E	537	SER	TYR	engineered mutation	UNP P03372
F	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is (8 {R},9 {S},13 {S},14 {S},17 {S})-13-methyl-17-phenylazanyl-6,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-3-ol (three-letter code: 6WV) (formula: C<sub>24</sub>H<sub>29</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	24	1	1		
2	B	1	Total	C	N	O	0	0
			20	18	1	1		
2	C	1	Total	C	N	O	0	0
			26	24	1	1		
2	D	1	Total	C	N	O	0	0
			20	18	1	1		
2	E	1	Total	C	N	O	0	0
			21	19	1	1		
2	F	1	Total	C	N	O	0	0
			20	18	1	1		


- Molecule 3 is water.

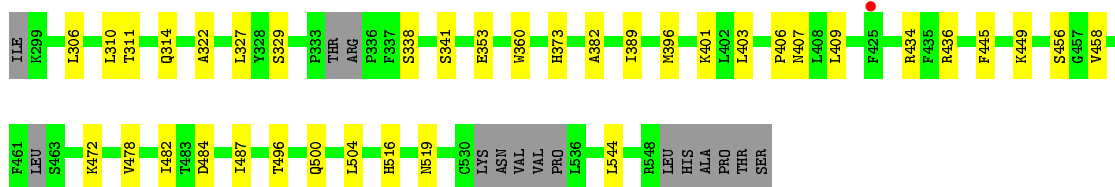
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	146	Total	O	0	0
			146	146		
3	C	147	Total	O	0	0
			147	147		
3	D	115	Total	O	0	0
			115	115		
3	E	69	Total	O	0	0
			69	69		
3	F	78	Total	O	0	0
			78	78		

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

These plots are drawn for all protein, RNA and DNA 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.

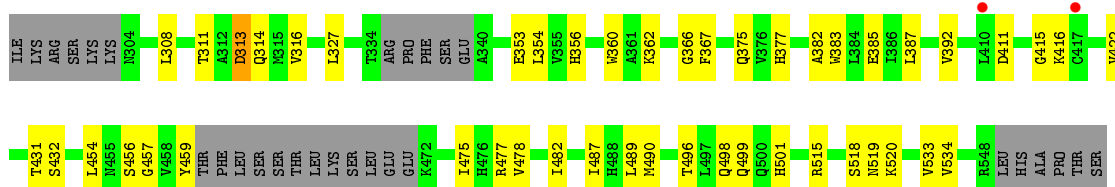
- Molecule 1: Estrogen receptor

Chain A: 




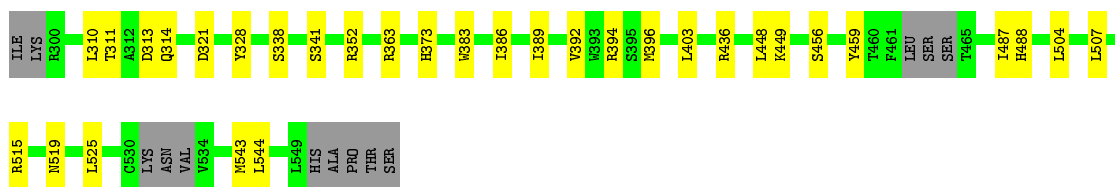
- Molecule 1: Estrogen receptor

Chain B: 




- Molecule 1: Estrogen receptor

Chain C: 



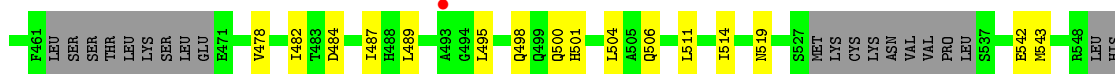
- Molecule 1: Estrogen receptor

Chain D: 

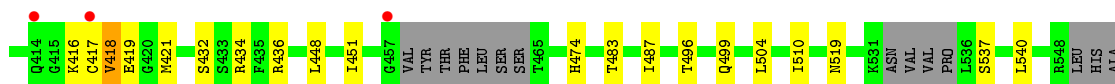
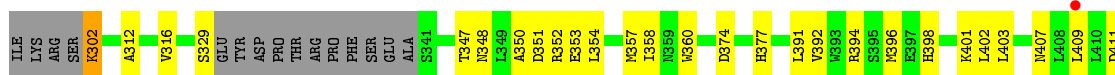




- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.58Å 64.44Å 135.41Å 83.11° 75.20° 61.99°	Depositor
Resolution (Å)	34.63 – 2.22 34.63 – 2.22	Depositor EDS
% Data completeness (in resolution range)	97.8 (34.63-2.22) 92.7 (34.63-2.22)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.201 , 0.229 0.202 , 0.231	Depositor DCC
$R_{free}$ test set	2000 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,h-k,h-l 0.468 for -h,-h+k,-l 0.018 for -h,-k,-h+l	Xtriage
Reported twinning fraction	0.500 for -h,-h+k,-l	Depositor
Outliers	0 of 84041 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: 6WV

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	0.23	0/1941	0.38	0/2616
1	B	0.23	0/1820	0.39	0/2460
1	C	0.23	0/1957	0.38	0/2646
1	D	0.26	0/1774	0.42	1/2395 (0.0%)
1	E	0.23	0/1729	0.37	0/2340
1	F	0.41	2/1746 (0.1%)	0.38	0/2363
All	All	0.27	2/10967 (0.0%)	0.39	1/14820 (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	D	0	2
1	F	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	302	LYS	CD-CE	11.32	1.79	1.51
1	F	302	LYS	CG-CD	8.34	1.80	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	534	VAL	C-N-CD	5.20	139.32	128.40

There are no chirality outliers.



All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	534	VAL	Peptide
1	D	535	PRO	Peptide
1	F	416	LYS	Peptide
1	F	417	CYS	Peptide
1	F	418	VAL	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	1909	0	1944	28	0
1	B	1789	0	1818	37	0
1	C	1922	0	1916	22	0
1	D	1747	0	1759	32	1
1	E	1701	0	1685	25	1
1	F	1720	0	1683	43	0
2	A	26	0	0	1	0
2	B	20	0	0	2	0
2	C	26	0	0	0	0
2	D	20	0	0	0	0
2	E	21	0	0	0	0
2	F	20	0	0	1	0
3	A	145	0	0	1	0
3	B	146	0	0	2	0
3	C	147	0	0	0	0
3	D	115	0	0	2	0
3	E	69	0	0	1	0
3	F	78	0	0	1	0
All	All	11621	0	10805	171	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 (171) 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:F:302:LYS:CD	1:F:302:LYS:CG	1.80	1.56
1:F:302:LYS:CE	1:F:302:LYS:CD	1.79	1.55
1:D:541:LEU:HD22	3:D:787:HOH:O	1.55	1.04
1:F:418:VAL:HG22	1:F:419:GLU:HB2	1.09	1.02
1:F:418:VAL:HG22	1:F:419:GLU:CB	1.99	0.91
1:A:519:ASN:HD22	1:B:519:ASN:HD22	1.19	0.88
1:D:541:LEU:CD2	3:D:787:HOH:O	2.14	0.86
1:F:418:VAL:CG2	1:F:419:GLU:HB2	2.02	0.83
1:B:308:LEU:HD21	1:B:477:ARG:HB3	1.72	0.70
1:B:377:HIS:NE2	1:B:457:GLY:O	2.24	0.70
1:F:418:VAL:CG1	1:F:421:MET:HG2	2.22	0.69
1:C:311:THR:H	1:C:314:GLN:HE21	1.40	0.69
1:C:328:TYR:O	1:C:352:ARG:NH2	2.25	0.69
1:A:403:LEU:HD13	1:A:409:LEU:HD12	1.75	0.69
1:B:353:GLU:OE1	2:B:601:6WV:O01	2.11	0.68
1:A:311:THR:H	1:A:314:GLN:HE21	1.39	0.68
1:B:327:LEU:HD22	1:B:353:GLU:HG2	1.75	0.68
1:A:396:MET:O	1:A:436:ARG:NH1	2.27	0.67
1:F:418:VAL:CG1	1:F:421:MET:CG	2.73	0.67
1:A:338:SER:H	1:A:341:SER:HB3	1.59	0.67
1:E:543:MET:O	3:E:701:HOH:O	2.15	0.64
1:A:329:SER:O	1:A:407:ASN:ND2	2.31	0.63
1:F:348:ASN:OD1	1:F:352:ARG:NH2	2.31	0.63
1:B:416:LYS:HG3	1:B:422:VAL:HG22	1.80	0.62
1:D:534:VAL:HB	1:D:535:PRO:HD3	1.82	0.62
1:F:394:ARG:HB3	1:F:403:LEU:HD23	1.82	0.62
1:B:411:ASP:O	1:B:415:GLY:N	2.24	0.62
1:C:448:LEU:HD11	1:C:507:LEU:HD22	1.82	0.62
1:F:302:LYS:CE	1:F:302:LYS:CG	2.78	0.62
1:B:496:THR:H	1:B:499:GLN:HE21	1.49	0.61
1:A:353:GLU:OE2	2:A:601:6WV:O01	2.18	0.61
1:B:311:THR:OG1	1:B:314:GLN:N	2.29	0.60
1:E:385:GLU:HG2	1:E:514:ILE:HG22	1.85	0.59
1:E:396:MET:O	1:E:436:ARG:NH1	2.36	0.59
1:C:396:MET:O	1:C:436:ARG:NH2	2.33	0.58
1:D:313:ASP:OD2	1:D:488:HIS:NE2	2.36	0.58
1:D:360:TRP:HA	1:D:363:ARG:HD2	1.85	0.58
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.39	0.58
1:E:357:MET:HA	1:E:360:TRP:HB3	1.87	0.57
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.40	0.56
1:E:394:ARG:NH1	1:E:403:LEU:O	2.37	0.56
1:A:544:LEU:O	1:A:544:LEU:HD23	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:HIS:O	1:E:360:TRP:N	2.35	0.56
1:A:327:LEU:HD12	1:A:353:GLU:HG2	1.86	0.56
1:C:515:ARG:HH22	1:D:513:HIS:CE1	2.24	0.55
1:A:401:LYS:HD2	1:A:409:LEU:HD21	1.88	0.55
1:C:519:ASN:HD22	1:D:519:ASN:HD22	1.54	0.55
1:B:356:HIS:O	1:B:360:TRP:N	2.38	0.55
1:F:392:VAL:HG13	1:F:432:SER:HA	1.88	0.54
1:D:370:LEU:HD12	1:D:375:GLN:HG3	1.89	0.54
1:F:357:MET:HA	1:F:360:TRP:HB3	1.89	0.54
1:C:459:TYR:HE1	1:D:434:ARG:HG2	1.73	0.54
1:B:311:THR:OG1	1:B:314:GLN:HG3	2.09	0.54
1:A:516:HIS:HD2	1:B:515:ARG:HD2	1.73	0.53
1:E:433:SER:OG	1:E:436:ARG:NH2	2.42	0.53
1:F:418:VAL:HG12	1:F:421:MET:CG	2.38	0.53
1:F:353:GLU:OE1	2:F:601:6WV:O01	2.26	0.53
1:B:311:THR:OG1	1:B:314:GLN:CB	2.57	0.53
1:B:311:THR:OG1	1:B:314:GLN:HB2	2.09	0.53
1:A:516:HIS:CD2	1:B:515:ARG:HD2	2.45	0.52
1:D:351:ASP:HA	1:D:354:LEU:HD12	1.92	0.52
1:F:302:LYS:CD	1:F:302:LYS:CB	2.78	0.52
1:F:448:LEU:HD23	1:F:451:ILE:HD12	1.91	0.52
1:D:394:ARG:HB3	1:D:403:LEU:HD22	1.92	0.51
1:F:401:LYS:HG2	1:F:411:ASP:HB3	1.91	0.51
1:A:487:ILE:HD11	1:A:504:LEU:HD22	1.93	0.51
1:B:354:LEU:HD21	1:B:383:TRP:HB2	1.93	0.51
1:F:487:ILE:HD11	1:F:504:LEU:HD22	1.91	0.51
1:C:338:SER:H	1:C:341:SER:HB3	1.75	0.51
1:D:358:ILE:HG22	1:D:362:LYS:HZ1	1.75	0.51
1:D:370:LEU:HD12	1:D:370:LEU:C	2.31	0.51
1:E:452:ILE:HD11	1:E:511:LEU:HD22	1.93	0.50
1:A:487:ILE:HG13	1:B:501:HIS:CG	2.47	0.50
1:C:515:ARG:HD2	1:D:516:HIS:HB2	1.93	0.50
1:F:391:LEU:HD11	1:F:402:LEU:HB3	1.92	0.50
1:E:498:GLN:HA	1:E:501:HIS:CE1	2.47	0.50
1:F:401:LYS:HB3	1:F:409:LEU:CD2	2.42	0.50
1:B:367:PHE:N	3:B:718:HOH:O	2.44	0.49
1:F:418:VAL:HG13	1:F:421:MET:HG2	1.94	0.49
1:B:316:VAL:HG21	1:B:489:LEU:HD11	1.95	0.49
1:E:382:ALA:O	1:E:386:ILE:HG12	2.13	0.49
1:E:495:LEU:O	1:E:500:GLN:NE2	2.44	0.49
1:E:393:TRP:HD1	1:E:440:LEU:HD23	1.76	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:LEU:O	1:F:358:ILE:HG12	2.13	0.49
1:C:311:THR:H	1:C:314:GLN:NE2	2.08	0.49
1:C:487:ILE:HD11	1:C:504:LEU:HD22	1.95	0.49
1:D:354:LEU:HD11	1:D:540:LEU:HD13	1.95	0.48
1:F:396:MET:O	1:F:436:ARG:NE	2.46	0.48
1:E:501:HIS:HD2	1:F:483:THR:HG22	1.77	0.48
1:B:487:ILE:HA	1:B:490:MET:HE2	1.94	0.48
1:A:389:ILE:HG12	1:A:445:PHE:HE2	1.77	0.48
1:D:370:LEU:HD11	1:D:375:GLN:HG2	1.96	0.48
1:C:519:ASN:HD22	1:D:519:ASN:ND2	2.11	0.48
1:A:496:THR:O	1:A:500:GLN:N	2.45	0.48
1:A:458:VAL:HG22	1:A:472:LYS:HD3	1.95	0.47
1:A:434:ARG:NE	1:B:459:TYR:OH	2.38	0.47
1:E:320:LEU:HD23	1:E:446:VAL:HG11	1.96	0.47
1:B:392:VAL:HG11	1:B:431:THR:HG22	1.96	0.47
1:C:383:TRP:CE2	1:C:543:MET:HB3	2.50	0.47
1:D:392:VAL:HG13	1:D:432:SER:HA	1.95	0.47
1:F:374:ASP:HA	1:F:377:HIS:HB3	1.94	0.47
1:B:362:LYS:NZ	1:B:375:GLN:HE22	2.13	0.47
1:F:329:SER:H	1:F:407:ASN:HD21	1.63	0.47
1:A:306:LEU:O	1:A:310:LEU:HG	2.15	0.47
1:E:501:HIS:CG	1:F:487:ILE:HG13	2.50	0.47
1:C:525:LEU:HG	1:C:544:LEU:HD12	1.97	0.47
1:F:407:ASN:O	3:F:701:HOH:O	2.20	0.47
1:F:418:VAL:HG12	1:F:421:MET:HG3	1.97	0.47
1:B:533:VAL:HA	1:B:534:VAL:HA	1.70	0.47
1:C:389:ILE:HA	1:C:392:VAL:HG22	1.96	0.47
1:C:321:ASP:O	1:C:363:ARG:NH2	2.48	0.46
1:A:484:ASP:OD2	1:B:501:HIS:NE2	2.35	0.46
1:D:358:ILE:HG22	1:D:362:LYS:NZ	2.31	0.45
1:F:434:ARG:HE	1:F:510:ILE:HD11	1.81	0.45
1:E:389:ILE:HA	1:E:392:VAL:HG22	1.97	0.45
1:D:383:TRP:NE1	1:D:543:MET:HB3	2.31	0.45
1:B:392:VAL:HG13	1:B:432:SER:HA	1.98	0.45
1:E:316:VAL:HG21	1:E:489:LEU:HD21	1.98	0.45
1:E:404:PHE:HB2	1:E:408:LEU:HD23	1.99	0.45
1:E:374:ASP:O	1:E:378:LEU:HG	2.17	0.45
1:D:392:VAL:HG11	1:D:431:THR:HG22	1.98	0.44
1:E:519:ASN:OD1	1:F:519:ASN:ND2	2.36	0.44
1:F:398:HIS:HE1	1:F:403:LEU:HD22	1.83	0.44
1:D:541:LEU:O	1:D:541:LEU:HD23	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:434:ARG:HH21	1:E:506:GLN:HB3	1.83	0.44
1:E:385:GLU:HB3	1:E:452:ILE:HG21	2.01	0.43
1:A:478:VAL:O	1:A:482:ILE:HG12	2.18	0.43
1:C:313:ASP:OD1	1:C:488:HIS:NE2	2.50	0.43
1:B:456:SER:HA	1:B:515:ARG:NH2	2.34	0.43
1:C:456:SER:HA	1:C:515:ARG:HH22	1.84	0.43
1:D:412:ARG:HD2	1:D:426:ASP:OD1	2.19	0.43
1:F:418:VAL:O	1:F:421:MET:HB2	2.19	0.43
1:F:496:THR:H	1:F:499:GLN:NE2	2.17	0.43
1:B:366:GLY:N	3:B:718:HOH:O	2.52	0.43
1:D:456:SER:HA	1:D:515:ARG:NH2	2.34	0.43
1:C:386:ILE:HG23	1:C:449:LYS:HD2	2.01	0.42
1:D:370:LEU:HD12	1:D:375:GLN:CG	2.48	0.42
1:E:478:VAL:O	1:E:482:ILE:HG13	2.19	0.42
1:F:347:THR:HG23	1:F:540:LEU:HD13	2.01	0.42
1:A:360:TRP:CZ2	1:A:449:LYS:HE3	2.54	0.42
1:F:302:LYS:HD2	1:F:474:HIS:HB2	2.01	0.42
1:F:312:ALA:O	1:F:316:VAL:HG23	2.19	0.42
1:F:351:ASP:OD2	1:F:537:SER:OG	2.27	0.42
1:B:382:ALA:HB2	1:B:456:SER:HB2	2.02	0.42
1:D:348:ASN:O	1:D:352:ARG:HG3	2.19	0.42
1:A:373:HIS:HD2	1:C:373:HIS:CD2	2.37	0.42
1:A:382:ALA:HB2	1:A:456:SER:HB2	2.01	0.42
1:A:401:LYS:HD2	1:A:409:LEU:CD2	2.49	0.42
1:C:310:LEU:HD22	1:C:314:GLN:HB3	2.02	0.42
1:C:394:ARG:HB3	1:C:403:LEU:HD12	2.01	0.42
1:D:370:LEU:CD1	1:D:375:GLN:CG	2.97	0.42
1:B:520:LYS:HD3	1:B:520:LYS:HA	1.86	0.42
1:D:539:LEU:O	1:D:543:MET:HG2	2.20	0.41
1:F:418:VAL:O	1:F:418:VAL:HG13	2.19	0.41
1:E:504:LEU:HD23	1:F:504:LEU:HD23	2.02	0.41
1:F:496:THR:HB	1:F:499:GLN:HG3	2.03	0.41
1:B:385:GLU:HG2	1:B:518:SER:HB2	2.02	0.41
1:B:454:LEU:HB3	1:B:475:ILE:HG23	2.02	0.41
1:B:478:VAL:O	1:B:482:ILE:HG13	2.21	0.41
1:F:398:HIS:CE1	1:F:403:LEU:HD22	2.56	0.41
1:A:406:PRO:HG3	3:A:826:HOH:O	2.20	0.41
1:A:472:LYS:HE3	1:A:472:LYS:HB2	1.91	0.41
1:B:313:ASP:N	1:B:313:ASP:OD1	2.52	0.41
1:B:311:THR:OG1	1:B:314:GLN:CG	2.69	0.41
1:B:387:LEU:HB3	2:B:601:6WV:C10	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:SER:O	1:D:437:MET:HG2	2.21	0.41
1:D:370:LEU:CD1	1:D:375:GLN:HG2	2.50	0.40
1:E:484:ASP:HA	1:E:487:ILE:HG22	2.02	0.40
1:F:350:ALA:O	1:F:354:LEU:HG	2.21	0.40
1:A:322:ALA:O	1:A:360:TRP:HD1	2.04	0.40
1:D:322:ALA:O	1:D:360:TRP:HD1	2.04	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:D:371:THR:CG2	1:E:542:GLU:OE1[1_654]	2.07	0.13

## 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	234/257 (91%)	230 (98%)	4 (2%)	0	100	100
1	B	223/257 (87%)	217 (97%)	6 (3%)	0	100	100
1	C	239/257 (93%)	235 (98%)	4 (2%)	0	100	100
1	D	218/257 (85%)	215 (99%)	3 (1%)	0	100	100
1	E	213/257 (83%)	212 (100%)	1 (0%)	0	100	100
1	F	217/257 (84%)	213 (98%)	4 (2%)	0	100	100
All	All	1344/1542 (87%)	1322 (98%)	22 (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	213/232 (92%)	213 (100%)	0	100	100
1	B	195/232 (84%)	194 (100%)	1 (0%)	88	94
1	C	210/232 (90%)	210 (100%)	0	100	100
1	D	189/232 (82%)	189 (100%)	0	100	100
1	E	182/232 (78%)	182 (100%)	0	100	100
1	F	179/232 (77%)	179 (100%)	0	100	100
All	All	1168/1392 (84%)	1167 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	313	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	A	373	HIS
1	A	441	GLN
1	A	498	GLN
1	A	499	GLN
1	A	502	GLN
1	A	506	GLN
1	A	516	HIS
1	B	375	GLN
1	B	398	HIS
1	B	476	HIS
1	B	499	GLN
1	B	500	GLN
1	B	502	GLN
1	B	519	ASN
1	C	314	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	348	ASN
1	C	373	HIS
1	C	414	GLN
1	C	455	ASN
1	C	498	GLN
1	C	499	GLN
1	C	547	HIS
1	D	414	GLN
1	D	502	GLN
1	D	513	HIS
1	D	519	ASN
1	E	375	GLN
1	E	506	GLN
1	F	398	HIS
1	F	439	ASN
1	F	499	GLN
1	F	502	GLN
1	F	506	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	6WV	A	601	-	30,30,30	2.20	5 (16%)	41,45,45	2.00	12 (29%)
2	6WV	D	601	-	22,23,30	2.44	4 (18%)	30,36,45	1.80	9 (30%)
2	6WV	F	601	-	22,23,30	2.48	4 (18%)	30,36,45	1.94	9 (30%)
2	6WV	C	601	-	30,30,30	2.21	5 (16%)	41,45,45	2.03	11 (26%)
2	6WV	E	601	-	23,24,30	2.58	5 (21%)	35,37,45	2.73	13 (37%)
2	6WV	B	601	-	22,23,30	2.44	4 (18%)	30,36,45	1.85	9 (30%)

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	6WV	A	601	-	-	1/4/44/44	0/5/5/5
2	6WV	D	601	-	-	-	0/4/4/5
2	6WV	F	601	-	-	-	0/4/4/5
2	6WV	C	601	-	-	1/4/44/44	0/5/5/5
2	6WV	E	601	-	-	0/0/42/44	0/4/4/5
2	6WV	B	601	-	-	-	0/4/4/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	6WV	C06-C05	-8.14	1.40	1.52
2	C	601	6WV	C06-C05	-8.00	1.40	1.52
2	D	601	6WV	C06-C05	-7.95	1.40	1.52
2	E	601	6WV	C06-C05	-7.89	1.41	1.52
2	B	601	6WV	C06-C05	-7.86	1.41	1.52
2	A	601	6WV	C06-C05	-7.84	1.41	1.52
2	B	601	6WV	C12-C11	-6.22	1.40	1.51
2	A	601	6WV	C12-C11	-6.22	1.40	1.51
2	C	601	6WV	C12-C11	-6.19	1.40	1.51
2	E	601	6WV	C12-C11	-6.17	1.40	1.51
2	D	601	6WV	C12-C11	-6.13	1.40	1.51
2	F	601	6WV	C12-C11	-6.08	1.40	1.51
2	E	601	6WV	C19-N01	-4.66	1.34	1.46
2	F	601	6WV	C02-C18	-3.39	1.50	1.54
2	D	601	6WV	C02-C18	-3.12	1.51	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6WV	C02-C18	-3.09	1.51	1.54
2	E	601	6WV	C02-C18	-3.09	1.51	1.54
2	C	601	6WV	C02-C18	-2.93	1.51	1.54
2	A	601	6WV	C19-N01	-2.79	1.34	1.39
2	A	601	6WV	C02-C18	-2.79	1.51	1.54
2	C	601	6WV	C19-N01	-2.74	1.34	1.39
2	A	601	6WV	C16-C15	-2.49	1.49	1.54
2	E	601	6WV	C16-C15	-2.47	1.49	1.54
2	C	601	6WV	C16-C15	-2.47	1.49	1.54
2	B	601	6WV	C16-C15	-2.39	1.49	1.54
2	F	601	6WV	C16-C15	-2.39	1.49	1.54
2	D	601	6WV	C16-C15	-2.39	1.49	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	6WV	C19-N01-C18	11.78	129.06	114.53
2	C	601	6WV	C17-C18-N01	6.43	119.63	112.07
2	A	601	6WV	C17-C18-N01	5.77	118.85	112.07
2	E	601	6WV	C01-C02-C15	4.63	120.34	111.71
2	B	601	6WV	C01-C02-C15	4.57	120.23	111.71
2	A	601	6WV	C01-C02-C15	4.53	120.17	111.71
2	D	601	6WV	C01-C02-C15	4.51	120.12	111.71
2	F	601	6WV	C01-C02-C15	4.48	120.07	111.71
2	F	601	6WV	C03-C04-C05	-4.42	106.37	112.33
2	E	601	6WV	C17-C18-N01	4.37	120.02	112.34
2	C	601	6WV	C01-C02-C15	4.36	119.85	111.71
2	A	601	6WV	C17-C16-C15	-4.27	96.67	105.13
2	A	601	6WV	C03-C04-C05	-4.13	106.77	112.33
2	C	601	6WV	C17-C16-C15	-4.11	96.99	105.13
2	C	601	6WV	C03-C04-C05	-4.11	106.79	112.33
2	E	601	6WV	C17-C16-C15	-3.90	97.39	105.13
2	B	601	6WV	C17-C16-C15	-3.69	97.82	105.13
2	B	601	6WV	C03-C04-C05	-3.69	107.36	112.33
2	D	601	6WV	C03-C04-C05	-3.57	107.52	112.33
2	F	601	6WV	C17-C16-C15	-3.53	98.14	105.13
2	D	601	6WV	C17-C16-C15	-3.50	98.19	105.13
2	C	601	6WV	C06-C05-C14	3.40	115.72	111.58
2	A	601	6WV	C06-C05-C14	3.28	115.58	111.58
2	F	601	6WV	C16-C15-C02	-3.26	99.91	103.84
2	F	601	6WV	C04-C03-C02	-3.16	107.36	112.78
2	E	601	6WV	C03-C04-C05	-3.03	108.25	112.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	6WV	C06-C05-C14	2.84	115.04	111.58
2	B	601	6WV	C06-C05-C14	2.75	114.93	111.58
2	B	601	6WV	C16-C15-C02	-2.73	100.56	103.84
2	D	601	6WV	C04-C03-C02	-2.68	108.19	112.78
2	D	601	6WV	C06-C05-C14	2.67	114.82	111.58
2	B	601	6WV	C16-C15-C14	-2.65	114.72	119.08
2	B	601	6WV	C04-C05-C06	2.64	117.90	113.84
2	A	601	6WV	C04-C05-C06	2.61	117.86	113.84
2	A	601	6WV	C16-C15-C02	-2.59	100.72	103.84
2	D	601	6WV	C16-C15-C14	-2.59	114.82	119.08
2	E	601	6WV	C16-C15-C14	-2.59	114.82	119.08
2	E	601	6WV	C04-C03-C02	-2.56	108.39	112.78
2	C	601	6WV	C16-C15-C02	-2.56	100.76	103.84
2	A	601	6WV	C16-C15-C14	-2.49	114.98	119.08
2	B	601	6WV	C04-C03-C02	-2.46	108.55	112.78
2	F	601	6WV	C16-C15-C14	-2.44	115.07	119.08
2	D	601	6WV	C16-C15-C02	-2.39	100.96	103.84
2	C	601	6WV	C16-C15-C14	-2.34	115.23	119.08
2	C	601	6WV	C04-C05-C06	2.34	117.44	113.84
2	F	601	6WV	C04-C05-C06	2.31	117.39	113.84
2	E	601	6WV	C06-C05-C14	2.24	114.31	111.58
2	E	601	6WV	C04-C05-C06	2.23	117.27	113.84
2	C	601	6WV	C09-C10-C11	-2.21	118.37	120.83
2	E	601	6WV	C16-C15-C02	-2.18	101.22	103.84
2	C	601	6WV	C20-C19-N01	-2.17	115.92	120.95
2	D	601	6WV	C04-C05-C06	2.17	117.18	113.84
2	F	601	6WV	C09-C10-C11	-2.13	118.47	120.83
2	A	601	6WV	C09-C10-C11	-2.12	118.48	120.83
2	A	601	6WV	C23-C24-C19	2.10	122.23	119.72
2	C	601	6WV	C04-C03-C02	-2.09	109.20	112.78
2	E	601	6WV	C09-C10-C11	-2.08	118.52	120.83
2	D	601	6WV	C09-C10-C11	-2.06	118.55	120.83
2	A	601	6WV	C20-C19-N01	-2.05	116.20	120.95
2	A	601	6WV	C04-C03-C02	-2.05	109.27	112.78
2	E	601	6WV	C17-C18-C02	2.05	105.70	103.67
2	E	601	6WV	C02-C18-N01	2.03	116.49	113.09
2	B	601	6WV	C09-C10-C11	-2.01	118.60	120.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

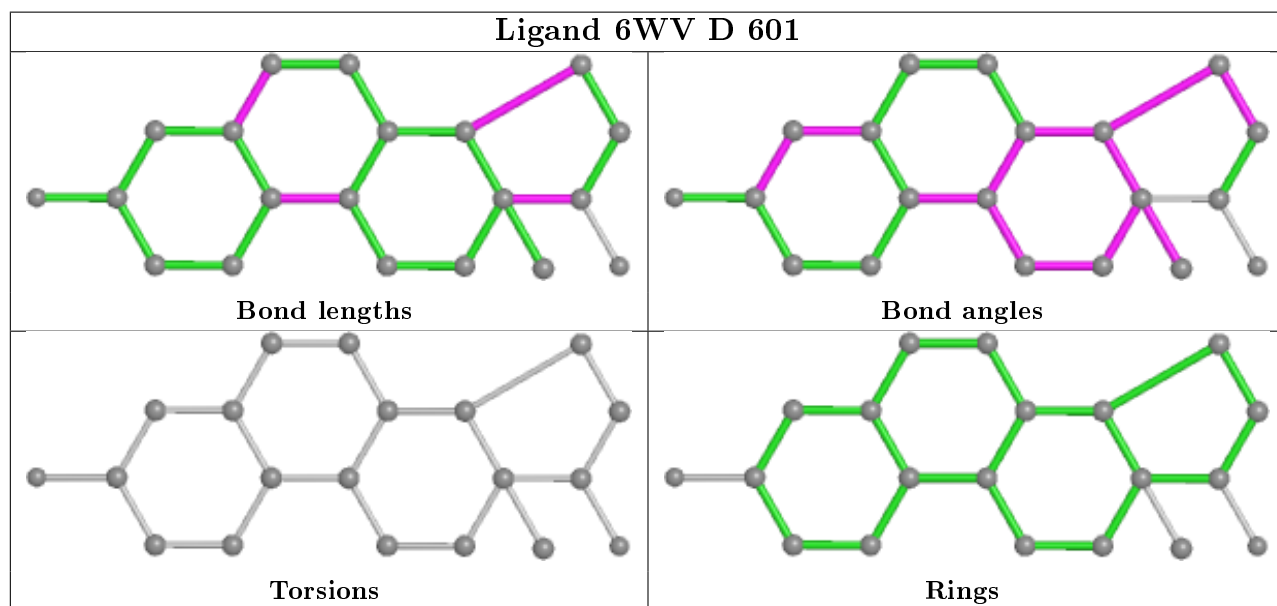
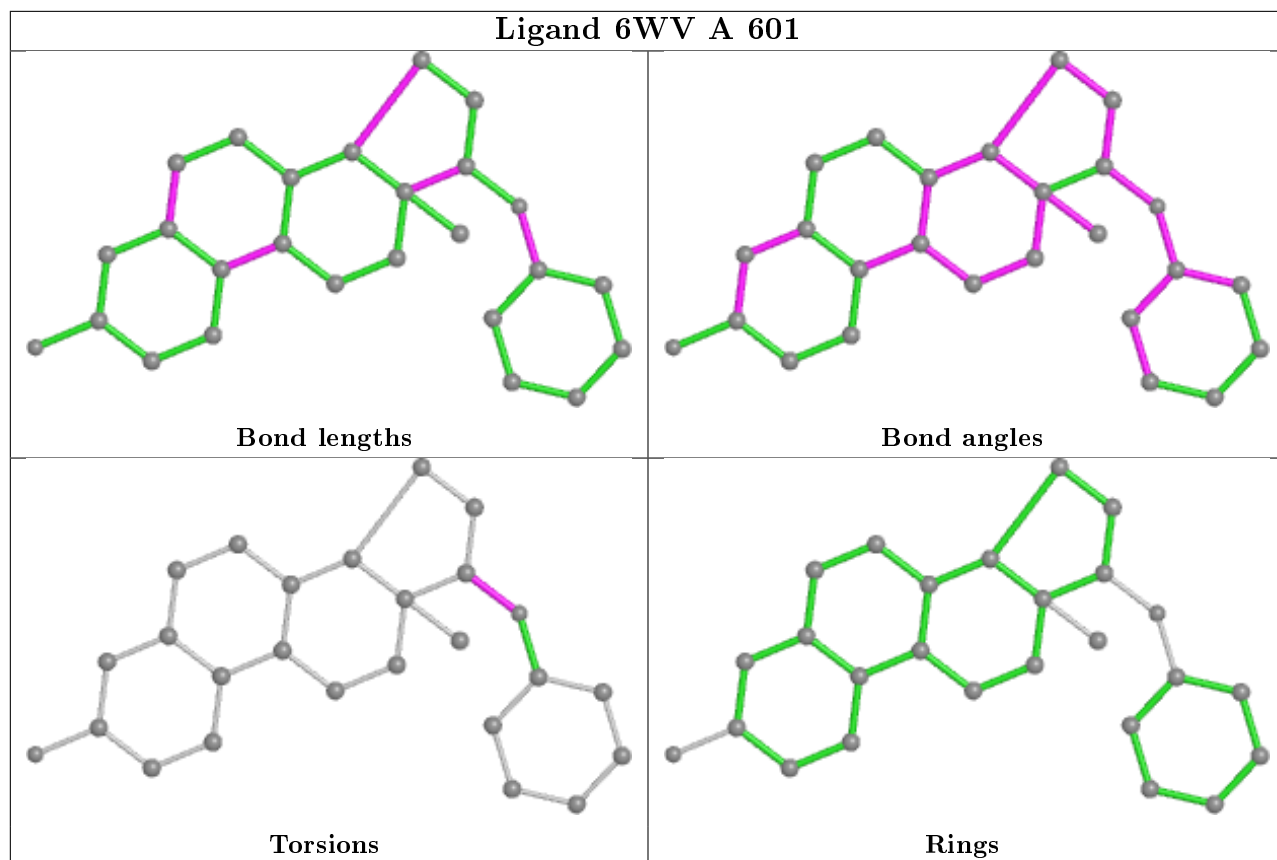
Mol	Chain	Res	Type	Atoms
2	A	601	6WV	C02-C18-N01-C19
2	C	601	6WV	C02-C18-N01-C19

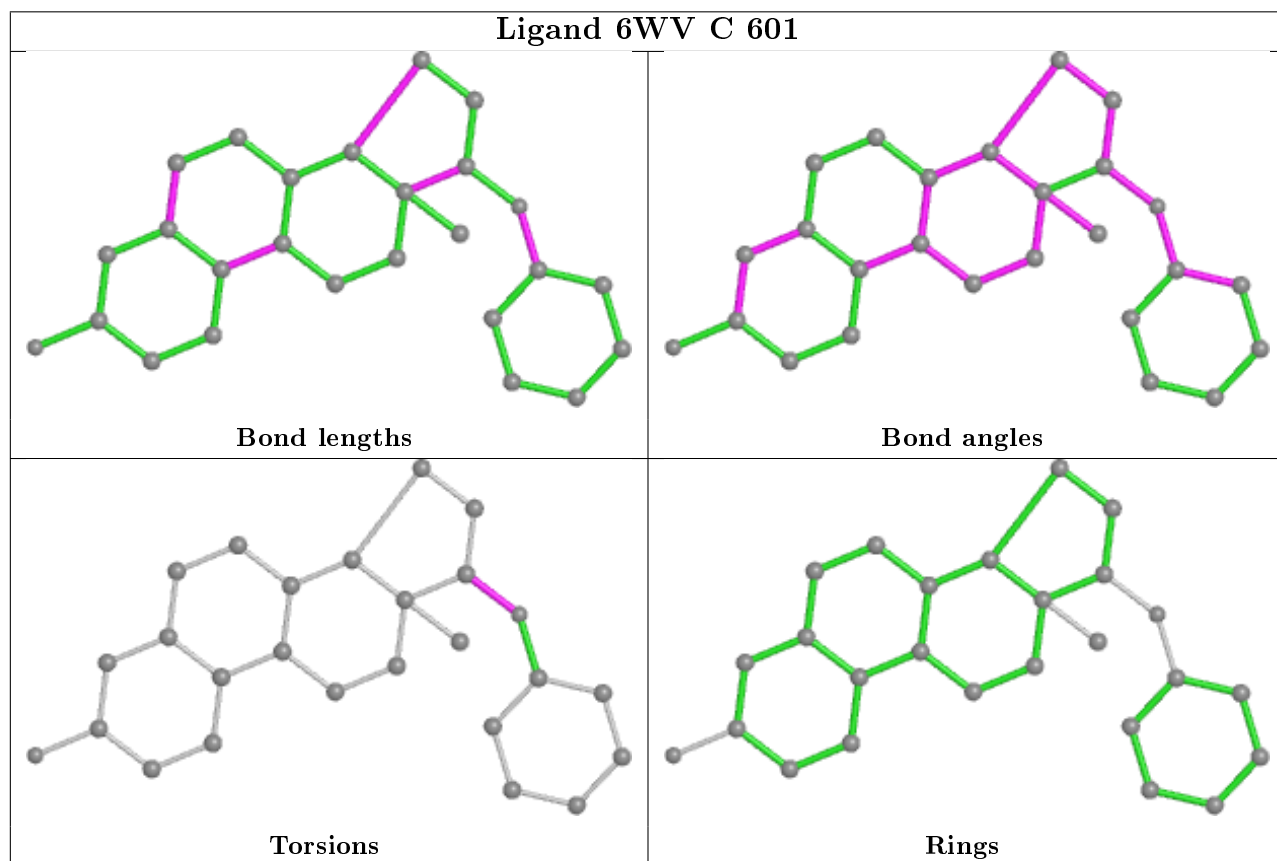
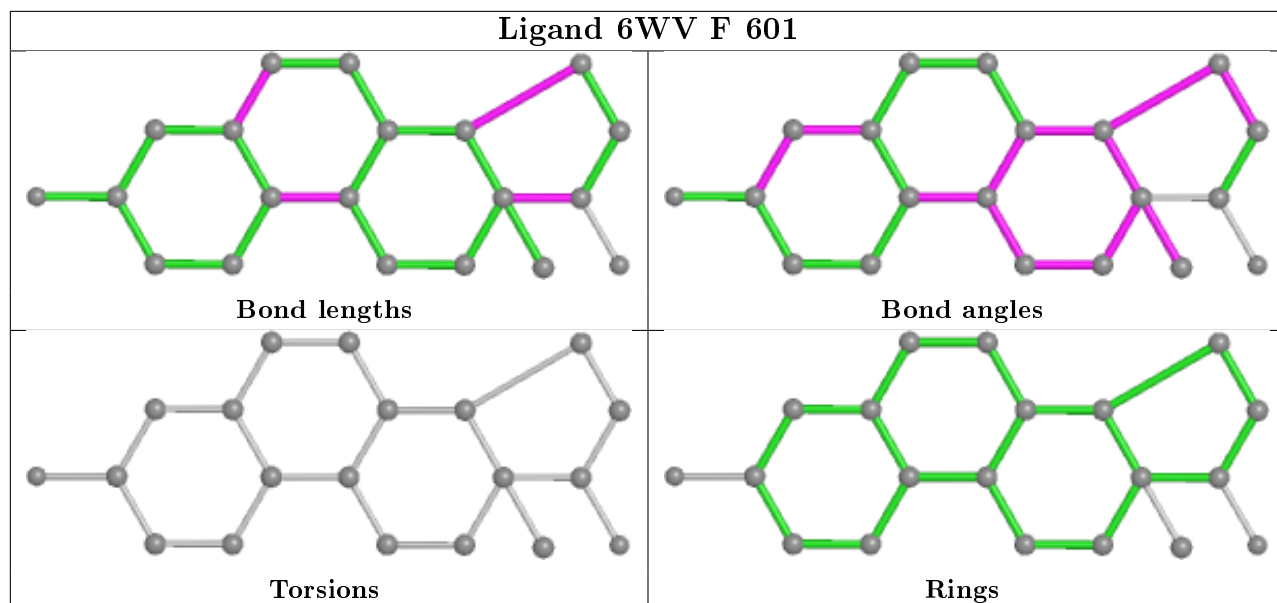
There are no ring outliers.

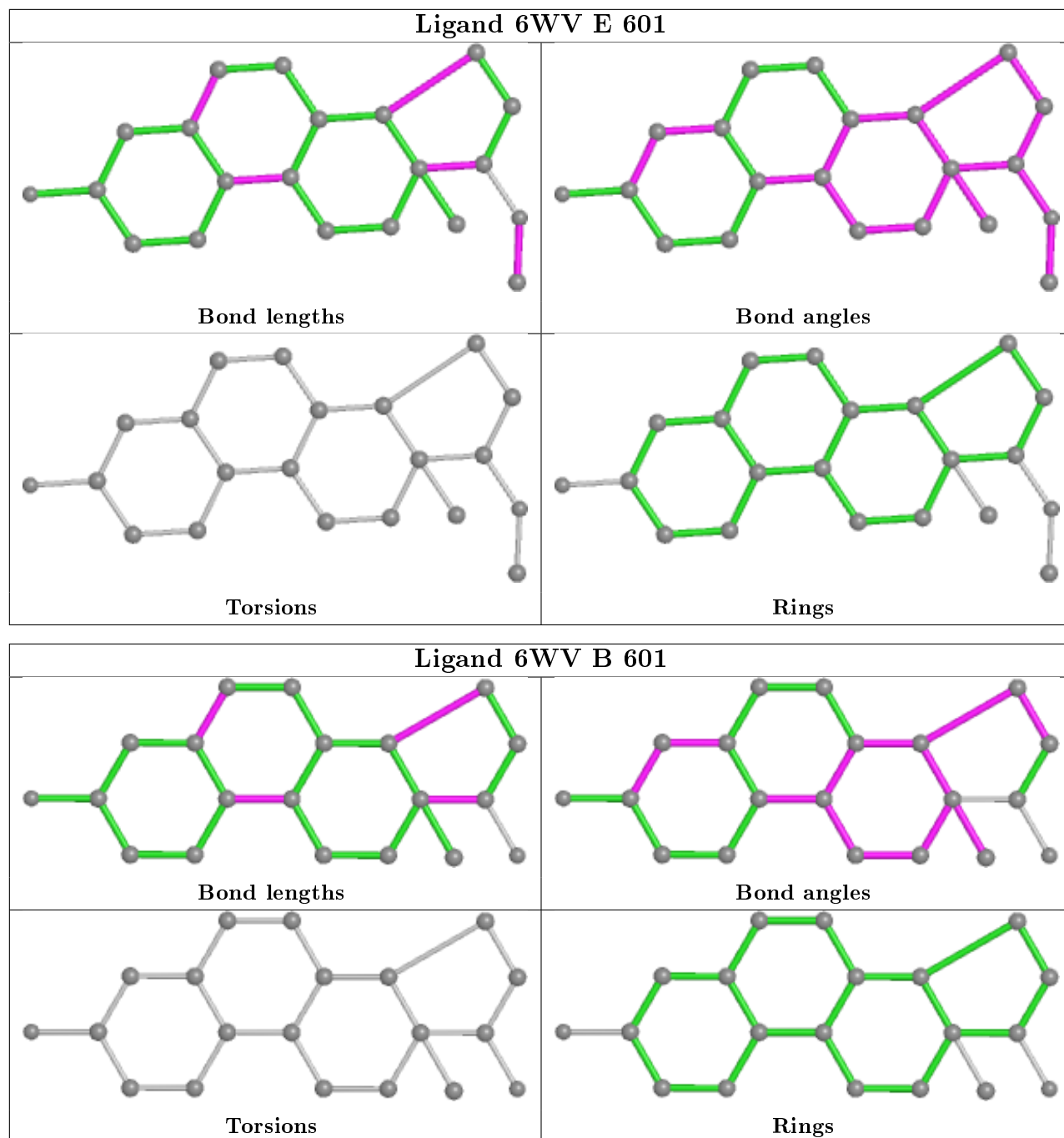
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	6WV	1	0
2	F	601	6WV	1	0
2	B	601	6WV	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 [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, 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	242/257 (94%)	-0.55	1 (0%) 92 92	23, 43, 65, 92	0
1	B	228/257 (88%)	-0.37	2 (0%) 84 83	25, 51, 81, 104	0
1	C	244/257 (94%)	-0.49	0 100 100	23, 46, 70, 84	0
1	D	226/257 (87%)	-0.36	3 (1%) 77 75	26, 51, 78, 101	0
1	E	221/257 (85%)	-0.19	3 (1%) 75 73	39, 59, 90, 108	0
1	F	225/257 (87%)	-0.20	4 (1%) 68 66	35, 62, 84, 97	0
All	All	1386/1542 (89%)	-0.36	13 (0%) 84 83	23, 52, 81, 108	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	LEU	3.8
1	E	306	LEU	3.6
1	E	340	ALA	3.5
1	E	493	ALA	3.2
1	D	538	ASP	2.8
1	F	457	GLY	2.7
1	B	417	CYS	2.5
1	D	539	LEU	2.5
1	F	409	LEU	2.4
1	D	541	LEU	2.4
1	F	417	CYS	2.3
1	A	425	PHE	2.2
1	F	414	GLN	2.1

### 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](#)

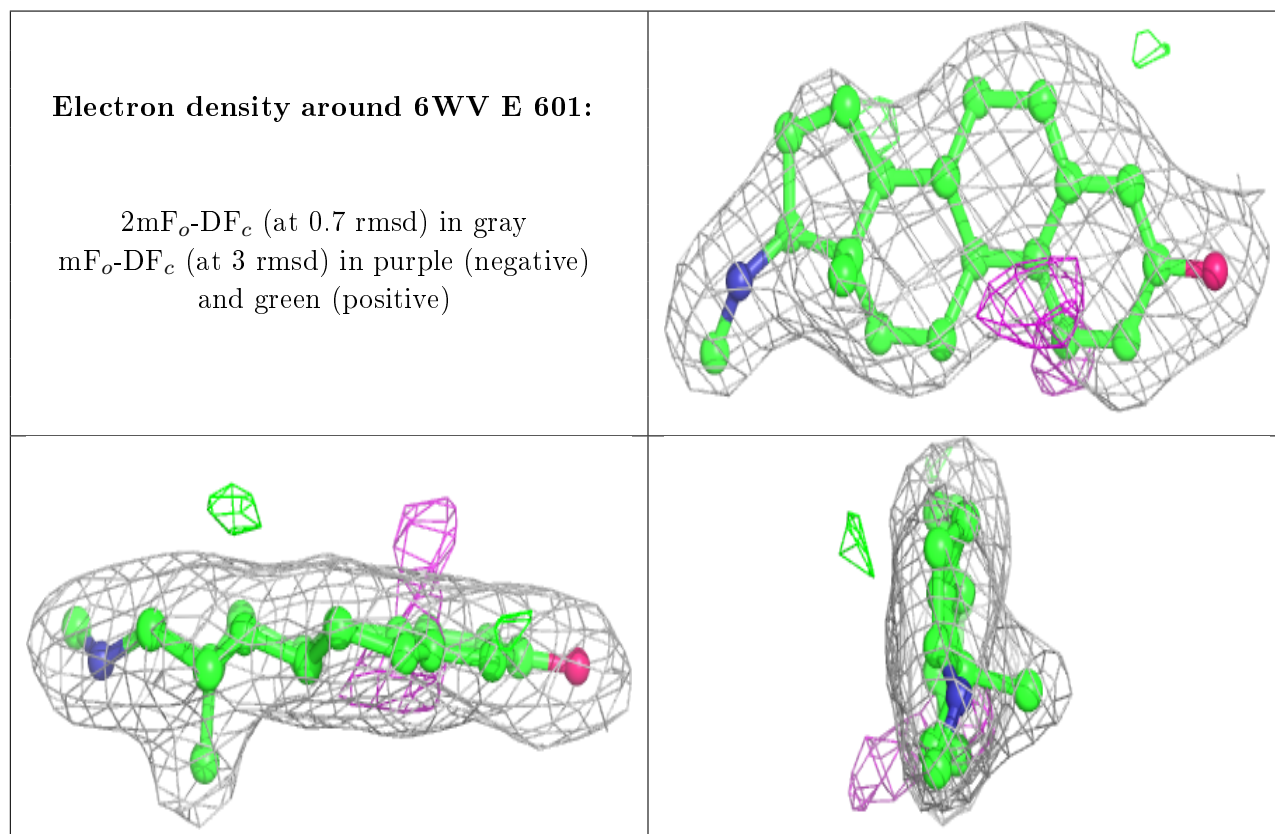
There are no carbohydrates in this entry.

### 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.

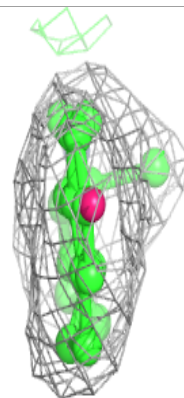
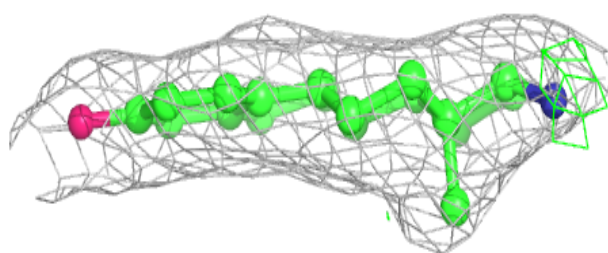
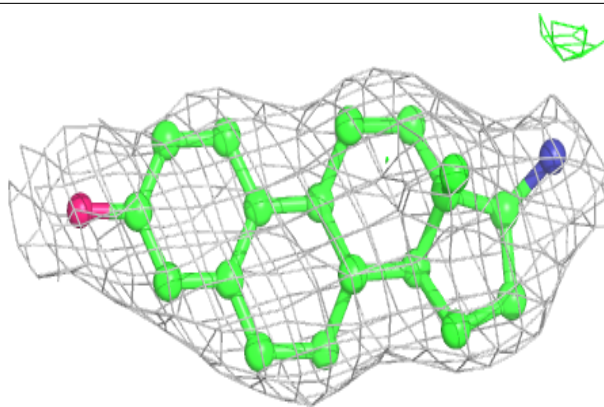
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	6WV	E	601	21/26	0.91	0.13	22,39,47,54	0
2	6WV	D	601	20/26	0.94	0.10	28,42,56,56	0
2	6WV	F	601	20/26	0.95	0.09	26,45,53,55	0
2	6WV	C	601	26/26	0.96	0.10	23,37,47,48	0
2	6WV	A	601	26/26	0.96	0.10	14,38,53,57	0
2	6WV	B	601	20/26	0.96	0.10	21,38,50,57	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.

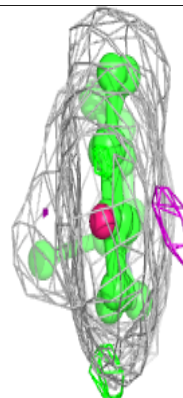
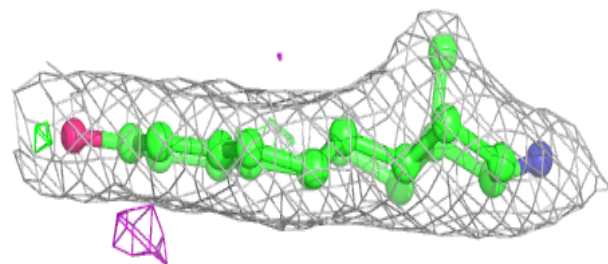
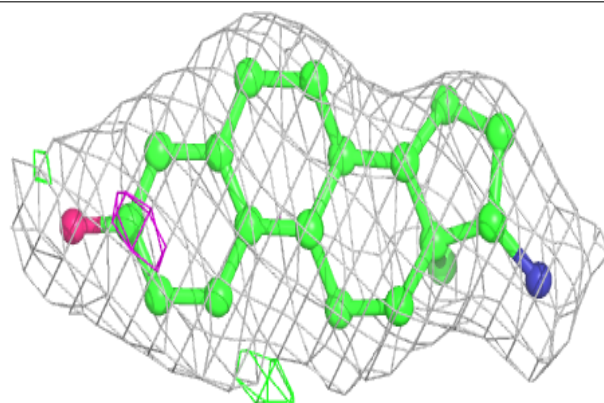


**Electron density around 6WV D 601:**

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

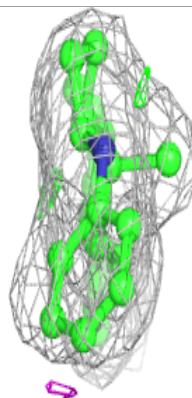
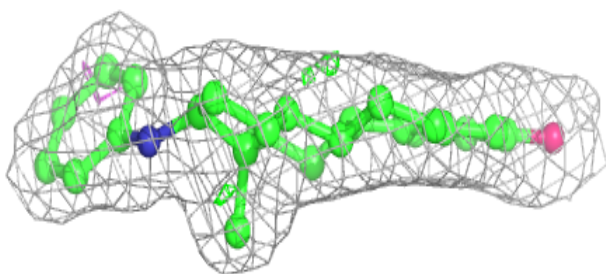
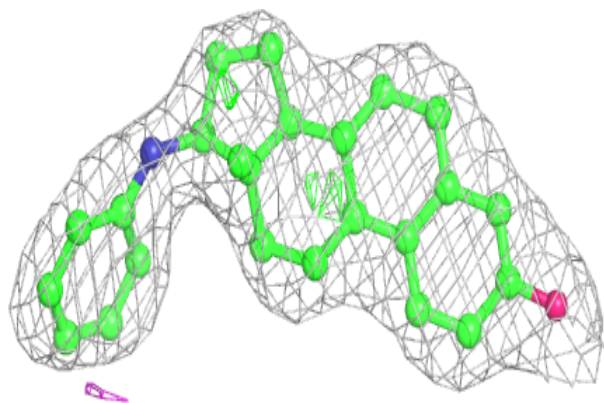
**Electron density around 6WV F 601:**

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

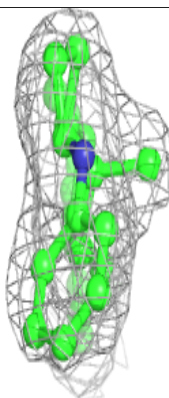
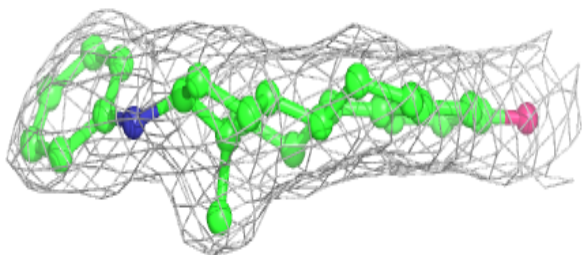
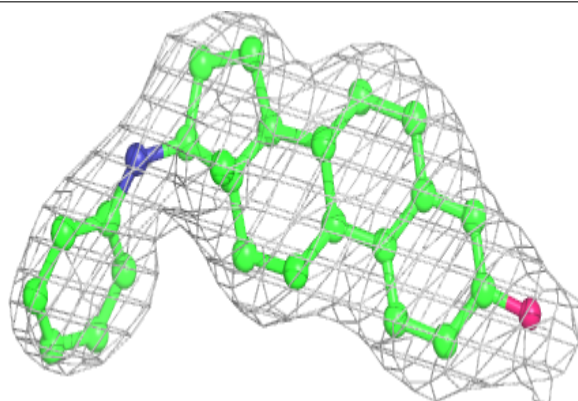


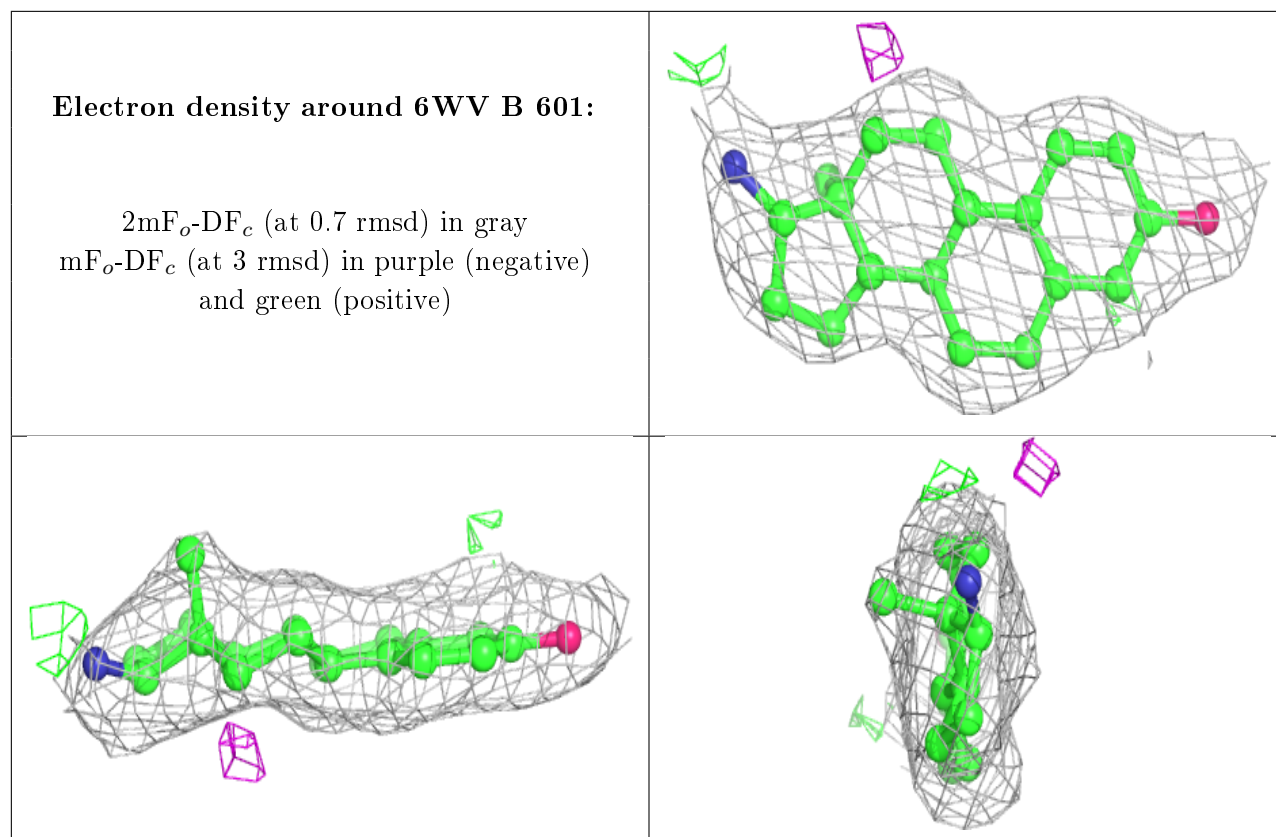
**Electron density around 6WV C 601:**

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

**Electron density around 6WV A 601:**

$2mF_o-DF_c$  (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.