



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:08 AM EDT

PDB ID : 7RS8  
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-16  
Authors : Min, J.; Nwachukwu, J.C.; Min, C.K.; Njeri, J.W.; Srinivasan, S.; Rangarajan, E.S.; Nettles, C.C.; Yan, S.; Houtman, R.; Griffin, P.R.; Izard, T.; Katzenellenbogen, B.S.; Katzenellenbogen, J.A.; Nettles, K.W.  
Deposited on : 2021-08-11  
Resolution : 1.64 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

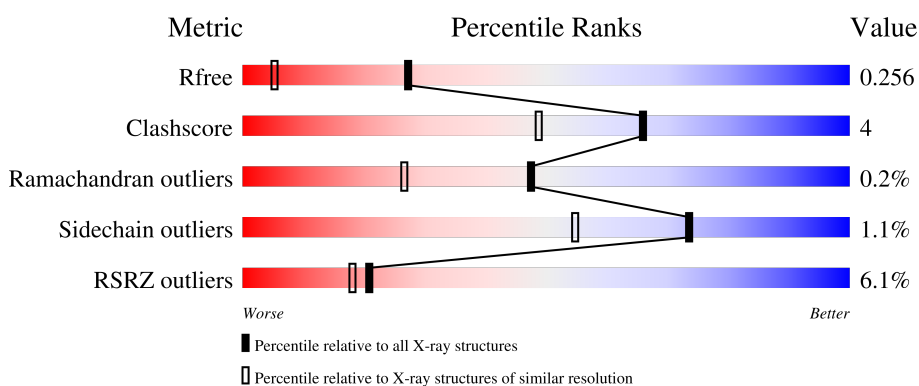
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	
1	B	257	
1	C	257	
2	D	257	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8186 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	228	Total 1836	C 1178	N 310	O 332	S 16	0	1	0
1	B	227	Total 1831	C 1172	N 309	O 334	S 16	0	2	0
1	C	229	Total 1842	C 1181	N 310	O 335	S 16	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is a protein called Estrogen receptor.

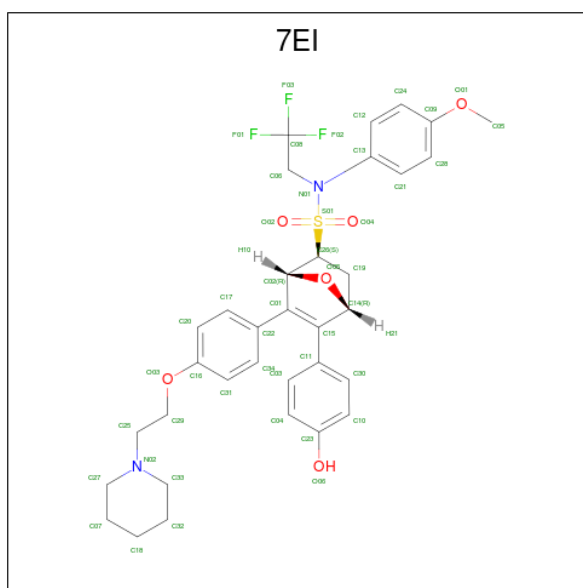
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	217	Total 1738	C 1118	N 291	O 312	S 17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 3 is (1R,2S,4R)-5-(4-hydroxyphenyl)-N-(4-methoxyphenyl)-6-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (three-letter code: 7EI) (formula: C<sub>34</sub>H<sub>37</sub>F<sub>3</sub>N<sub>2</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by

depositor).

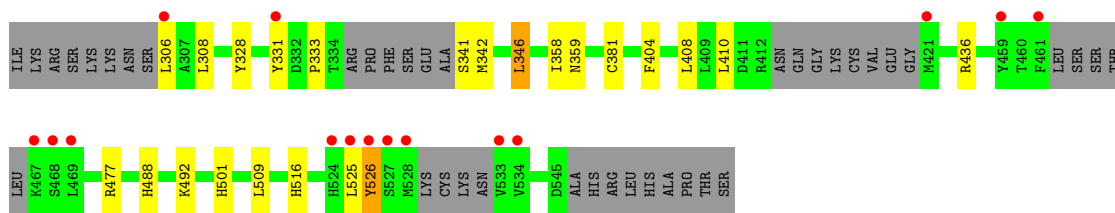


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
3	A	1	46	34	3	2	6	1	0	0
3	B	1	88	67	3	4	12	2	0	1
3	C	1	46	34	3	2	6	1	0	0
3	D	1	46	34	3	2	6	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total	O	0	0
			190	190		
4	B	176	Total	O	0	0
			176	176		
4	C	187	Total	O	0	0
			187	187		
4	D	160	Total	O	0	0
			160	160		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.53Å 58.62Å 93.90Å 86.94° 75.26° 62.85°	Depositor
Resolution (Å)	90.57 – 1.64 90.57 – 1.64	Depositor EDS
% Data completeness (in resolution range)	69.0 (90.57-1.64) 69.0 (90.57-1.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 1.63Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.210 , 0.250 0.220 , 0.256	Depositor DCC
$R_{free}$ test set	4122 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.107 for h,h-k,h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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: 7EI, YCM

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	0.62	0/1858	0.76	1/2508 (0.0%)
1	B	0.62	0/1852	0.81	3/2502 (0.1%)
1	C	0.64	0/1864	0.77	2/2518 (0.1%)
2	D	0.64	0/1768	0.79	2/2386 (0.1%)
All	All	0.63	0/7342	0.78	8/9914 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	A	436	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	436	ARG	NE-CZ-NH2	-8.29	116.16	120.30
2	D	436	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	C	515	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	313	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	352	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	D	359	ASN	CB-CA-C	5.15	120.70	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1836	0	1873	18	1
1	B	1831	0	1863	15	1
1	C	1842	0	1870	13	1
2	D	1738	0	1774	16	1
3	A	46	0	0	0	0
3	B	88	0	0	3	0
3	C	46	0	0	0	0
3	D	46	0	0	0	0
4	A	190	0	0	3	1
4	B	176	0	0	5	0
4	C	187	0	0	4	0
4	D	160	0	0	3	1
All	All	8186	0	7380	60	3

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 4.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.33	1.06
2:D:381:CYS:SG	4:D:850:HOH:O	2.20	0.97
3:B:601[B]:7EI:C12	3:B:601[B]:7EI:O04	2.19	0.85
1:B:525:LEU:HD11	1:B:533:VAL:HG11	1.63	0.80
1:B:381:YCM:NZ2	4:B:701:HOH:O	2.17	0.77
2:D:342:MET:O	2:D:346:LEU:HD23	1.87	0.75
1:C:533:VAL:N	4:C:701:HOH:O	2.20	0.73
1:A:473:ASP:OD2	1:A:477:ARG:CZ	2.38	0.72
1:A:421:MET:HG3	1:A:524:HIS:NE2	2.04	0.72
1:A:467:LYS:NZ	4:A:702:HOH:O	2.26	0.67
1:B:524:HIS:ND1	3:B:601[B]:7EI:C06	2.58	0.67
1:A:489:LEU:O	1:A:492:LYS:HG3	1.94	0.66
1:B:477:ARG:NH2	4:B:703:HOH:O	2.26	0.65
1:A:385:GLU:OE1	4:A:701:HOH:O	2.14	0.64
1:B:341:SER:N	4:B:704:HOH:O	2.30	0.64
1:C:484:ASP:OD1	2:D:501:HIS:HE1	1.80	0.63
1:B:525:LEU:HD21	1:B:533:VAL:HG11	1.84	0.60
2:D:346:LEU:CD2	2:D:408:LEU:HD21	2.33	0.58
1:A:472:LYS:NZ	4:A:705:HOH:O	2.33	0.58
2:D:346:LEU:HD11	2:D:404:PHE:CD2	2.39	0.58
1:B:524:HIS:CE1	3:B:601[B]:7EI:C06	2.89	0.56
2:D:341:SER:N	4:D:703:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:LEU:HD22	2:D:408:LEU:HD21	1.89	0.55
1:A:489:LEU:O	1:A:492:LYS:HE3	2.07	0.54
1:C:460:THR:HG21	4:C:745:HOH:O	2.07	0.54
2:D:308:LEU:HD11	2:D:477:ARG:HE	1.73	0.54
1:A:370:LEU:CD1	1:A:475:ILE:HD11	2.23	0.53
1:C:396:MET:O	1:C:436:ARG:HD3	2.09	0.53
1:C:306:LEU:N	4:C:707:HOH:O	2.42	0.52
1:A:396:MET:O	1:A:436:ARG:HD3	2.11	0.51
2:D:404:PHE:CE1	2:D:410:LEU:HD12	2.46	0.51
1:B:525:LEU:HB3	4:B:837:HOH:O	2.11	0.51
2:D:525:LEU:O	2:D:526:TYR:HB2	2.12	0.49
2:D:328:TYR:OH	4:D:701:HOH:O	2.20	0.48
1:A:473:ASP:OD2	1:A:477:ARG:NH2	2.47	0.48
1:A:421:MET:CG	1:A:524:HIS:NE2	2.77	0.47
1:A:342:MET:CE	1:A:346:LEU:HG	2.44	0.47
1:B:413:ASN:OD1	1:B:413:ASN:C	2.52	0.47
1:C:337:PHE:CD2	1:C:342:MET:CE	2.99	0.45
1:B:335:ARG:CZ	1:B:335:ARG:HB3	2.47	0.45
1:C:337:PHE:CD2	1:C:342:MET:HE2	2.52	0.45
1:A:342:MET:CE	1:A:346:LEU:HD21	2.47	0.44
1:C:306:LEU:CA	4:C:707:HOH:O	2.66	0.44
1:A:404:PHE:CE2	1:A:410:LEU:HD12	2.53	0.44
1:C:404:PHE:CE2	1:C:410:LEU:HD12	2.53	0.44
2:D:346:LEU:CD1	2:D:404:PHE:CD2	3.01	0.43
1:C:519:ASN:HD21	2:D:516:HIS:HA	1.83	0.43
1:A:342:MET:HE3	1:A:346:LEU:HG	2.00	0.43
1:B:473[A]:ASP:OD2	1:B:477:ARG:NH2	2.52	0.42
1:B:469:LEU:HD13	1:C:493:ALA:O	2.20	0.42
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.55	0.42
1:C:376:VAL:HG11	1:C:537:TYR:CD2	2.55	0.42
2:D:488:HIS:NE2	2:D:492:LYS:HD2	2.35	0.41
1:A:398:HIS:CE1	1:A:403:LEU:HD12	2.55	0.41
2:D:509:LEU:HD23	2:D:509:LEU:HA	1.97	0.41
2:D:346:LEU:HD21	2:D:408:LEU:HD21	2.02	0.41
1:A:376:VAL:HG11	1:A:537:TYR:CD2	2.57	0.40
1:B:460:THR:HG23	4:B:781:HOH:O	2.22	0.40
1:B:525:LEU:CD1	1:B:533:VAL:HG11	2.43	0.40
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.40	0.40

All (3) 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:464:SER:OG	2:D:333:PRO:O[1_566]	1.99	0.21
4:A:877:HOH:O	4:D:851:HOH:O[1_566]	2.05	0.15
1:B:335:ARG:O	1:C:464:SER:OG[1_466]	2.17	0.03

### 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	220/257 (86%)	218 (99%)	1 (0%)	1 (0%)	29	11
1	B	220/257 (86%)	216 (98%)	4 (2%)	0	100	100
1	C	221/257 (86%)	220 (100%)	1 (0%)	0	100	100
2	D	207/257 (80%)	203 (98%)	3 (1%)	1 (0%)	29	11
All	All	868/1028 (84%)	857 (99%)	9 (1%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	526	TYR
1	A	415	GLY

#### 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	206/231 (89%)	205 (100%)	1 (0%)	88	80
1	B	207/231 (90%)	204 (99%)	3 (1%)	67	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	206/231 (89%)	205 (100%)	1 (0%)	88	80
2	D	196/232 (84%)	192 (98%)	4 (2%)	55	29
All	All	815/925 (88%)	806 (99%)	9 (1%)	73	55

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

Mol	Chain	Res	Type
1	A	492	LYS
1	B	331	TYR
1	B	358	ILE
1	B	421	MET
1	C	421	MET
2	D	306	LEU
2	D	331	TYR
2	D	346	LEU
2	D	358	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	519	ASN
1	B	398	HIS
1	B	498	GLN
1	B	519	ASN
1	C	519	ASN
2	D	501	HIS
2	D	513	HIS
2	D	519	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	YCM	B	381	1	7,9,10	0.53	0	4,10,12	0.45	0
1	YCM	A	381	1	7,9,10	0.52	0	4,10,12	0.44	0
1	YCM	C	381	1	7,9,10	0.52	0	4,10,12	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	B	381	1	-	1/6/8/10	-
1	YCM	A	381	1	-	2/6/8/10	-
1	YCM	C	381	1	-	2/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381	YCM	CE-CD-SG-CB
1	A	381	YCM	SG-CD-CE-NZ2
1	B	381	YCM	CE-CD-SG-CB
1	C	381	YCM	CE-CD-SG-CB
1	C	381	YCM	SG-CD-CE-NZ2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	381	YCM	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	7EI	D	601	-	48,51,51	2.56	14 (29%)	62,75,75	2.24	20 (32%)
3	7EI	B	601[B]	-	44,47,51	2.20	15 (34%)	55,68,75	3.11	19 (34%)
3	7EI	A	601	-	48,51,51	2.76	16 (33%)	62,75,75	2.12	17 (27%)
3	7EI	C	601	-	48,51,51	2.79	16 (33%)	62,75,75	2.34	18 (29%)
3	7EI	B	601[A]	-	48,51,51	2.67	16 (33%)	62,75,75	2.79	18 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7EI	D	601	-	-	10/35/69/69	0/7/6/6
3	7EI	B	601[B]	-	-	10/30/64/69	0/7/6/6
3	7EI	A	601	-	-	8/35/69/69	0/7/6/6
3	7EI	C	601	-	-	5/35/69/69	0/7/6/6
3	7EI	B	601[A]	-	-	8/35/69/69	0/7/6/6

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601[A]	7EI	C13-N01	-11.30	1.29	1.44
3	D	601	7EI	C13-N01	-11.03	1.29	1.44
3	A	601	7EI	C13-N01	-11.01	1.29	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	7EI	C13-N01	-10.98	1.29	1.44
3	A	601	7EI	C22-C01	-7.04	1.35	1.48
3	C	601	7EI	C22-C01	-6.80	1.35	1.48
3	C	601	7EI	C11-C15	-6.78	1.35	1.48
3	A	601	7EI	C11-C15	-6.75	1.35	1.48
3	B	601[B]	7EI	C11-C15	-6.65	1.35	1.48
3	D	601	7EI	C22-C01	-6.60	1.36	1.48
3	B	601[A]	7EI	C22-C01	-6.18	1.36	1.48
3	B	601[B]	7EI	C22-C01	-6.12	1.36	1.48
3	B	601[A]	7EI	C11-C15	-6.06	1.37	1.48
3	D	601	7EI	C11-C15	-5.57	1.38	1.48
3	A	601	7EI	O04-S01	5.30	1.48	1.43
3	C	601	7EI	O02-S01	4.88	1.47	1.43
3	C	601	7EI	O04-S01	4.46	1.47	1.43
3	B	601[B]	7EI	O02-S01	4.32	1.47	1.43
3	D	601	7EI	O04-S01	4.29	1.47	1.43
3	B	601[A]	7EI	O02-S01	4.06	1.47	1.43
3	B	601[A]	7EI	C02-C01	3.93	1.55	1.50
3	A	601	7EI	O02-S01	3.86	1.46	1.43
3	B	601[A]	7EI	O04-S01	3.34	1.46	1.43
3	A	601	7EI	C02-C01	3.32	1.54	1.50
3	D	601	7EI	S01-N01	3.24	1.74	1.67
3	C	601	7EI	C02-C01	3.19	1.54	1.50
3	B	601[B]	7EI	O04-S01	3.18	1.46	1.43
3	D	601	7EI	C02-C01	2.96	1.53	1.50
3	C	601	7EI	C34-C31	-2.88	1.33	1.38
3	C	601	7EI	C20-C17	-2.80	1.33	1.38
3	C	601	7EI	C04-C23	-2.69	1.33	1.38
3	A	601	7EI	C34-C31	-2.65	1.33	1.38
3	C	601	7EI	C34-C22	-2.65	1.34	1.39
3	C	601	7EI	C04-C03	-2.58	1.34	1.38
3	C	601	7EI	C28-C21	-2.53	1.34	1.38
3	A	601	7EI	C14-C15	2.51	1.55	1.51
3	A	601	7EI	S01-N01	2.48	1.72	1.67
3	A	601	7EI	C34-C22	-2.43	1.35	1.39
3	D	601	7EI	C34-C31	-2.40	1.34	1.38
3	B	601[B]	7EI	C28-C21	-2.39	1.34	1.38
3	B	601[B]	7EI	C04-C23	-2.38	1.34	1.38
3	D	601	7EI	C04-C23	-2.35	1.34	1.38
3	D	601	7EI	O02-S01	2.34	1.45	1.43
3	A	601	7EI	C21-C13	-2.34	1.34	1.39
3	B	601[A]	7EI	C04-C23	-2.33	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	7EI	C04-C03	-2.33	1.34	1.38
3	A	601	7EI	C20-C17	-2.32	1.34	1.38
3	B	601[A]	7EI	S01-N01	2.31	1.72	1.67
3	B	601[B]	7EI	C04-C03	-2.31	1.34	1.38
3	B	601[A]	7EI	C34-C22	-2.31	1.35	1.39
3	A	601	7EI	C28-C21	-2.30	1.34	1.38
3	A	601	7EI	C04-C23	-2.28	1.34	1.38
3	B	601[A]	7EI	C10-C23	-2.26	1.34	1.38
3	B	601[B]	7EI	C12-C24	-2.25	1.34	1.38
3	B	601[A]	7EI	C21-C13	-2.23	1.34	1.39
3	B	601[B]	7EI	C30-C11	-2.22	1.35	1.39
3	D	601	7EI	C14-C15	2.19	1.54	1.51
3	A	601	7EI	C10-C23	-2.18	1.34	1.38
3	B	601[B]	7EI	C10-C23	-2.18	1.34	1.38
3	D	601	7EI	C34-C22	-2.17	1.35	1.39
3	B	601[A]	7EI	C28-C09	-2.15	1.34	1.38
3	B	601[A]	7EI	C28-C21	-2.15	1.34	1.38
3	B	601[A]	7EI	C34-C31	-2.14	1.34	1.38
3	B	601[B]	7EI	C34-C22	-2.13	1.35	1.39
3	B	601[B]	7EI	C12-C13	-2.13	1.35	1.39
3	D	601	7EI	C04-C03	-2.12	1.34	1.38
3	C	601	7EI	C28-C09	-2.12	1.34	1.38
3	B	601[B]	7EI	C03-C11	-2.11	1.35	1.39
3	B	601[A]	7EI	O05-C02	-2.10	1.40	1.43
3	C	601	7EI	C17-C22	-2.10	1.35	1.39
3	C	601	7EI	S01-N01	2.09	1.71	1.67
3	C	601	7EI	C10-C23	-2.08	1.35	1.38
3	D	601	7EI	C20-C17	-2.08	1.35	1.38
3	B	601[B]	7EI	C06-N01	2.07	1.51	1.47
3	D	601	7EI	C10-C23	-2.04	1.35	1.38
3	B	601[A]	7EI	C20-C17	-2.04	1.35	1.38
3	B	601[B]	7EI	C17-C22	-2.00	1.35	1.39

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[A]	7EI	O02-S01-N01	-13.14	91.45	107.56
3	B	601[B]	7EI	O04-S01-N01	-12.95	91.49	107.08
3	B	601[A]	7EI	O04-S01-N01	-10.16	95.11	107.56
3	B	601[B]	7EI	O02-S01-N01	-9.85	95.21	107.08
3	B	601[B]	7EI	O04-S01-O02	9.63	125.40	119.22
3	D	601	7EI	O02-S01-N01	-9.04	96.48	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	7EI	O04-S01-N01	-8.57	97.06	107.56
3	C	601	7EI	O02-S01-N01	-8.25	97.45	107.56
3	A	601	7EI	O02-S01-N01	-7.42	98.46	107.56
3	C	601	7EI	C08-C06-N01	6.09	118.06	112.14
3	A	601	7EI	O04-S01-N01	-5.57	100.74	107.56
3	A	601	7EI	C08-C06-N01	5.53	117.51	112.14
3	B	601[A]	7EI	O04-S01-O02	5.44	122.72	119.22
3	D	601	7EI	O04-S01-N01	-5.43	100.90	107.56
3	B	601[B]	7EI	C21-C13-N01	4.78	127.06	120.02
3	D	601	7EI	O04-S01-O02	4.46	122.08	119.22
3	D	601	7EI	C21-C13-N01	4.12	126.30	120.16
3	B	601[A]	7EI	C21-C13-N01	4.07	126.23	120.16
3	B	601[A]	7EI	C28-C09-C24	-3.76	114.39	120.18
3	B	601[B]	7EI	C31-C16-C20	-3.67	114.53	120.18
3	A	601	7EI	C28-C09-C24	-3.66	114.53	120.18
3	C	601	7EI	C28-C09-C24	-3.65	114.55	120.18
3	B	601[A]	7EI	C21-C28-C09	3.56	124.09	119.73
3	D	601	7EI	C28-C09-C24	-3.55	114.70	120.18
3	A	601	7EI	C22-C01-C02	-3.51	115.50	121.27
3	D	601	7EI	C08-C06-N01	3.45	115.49	112.14
3	C	601	7EI	C22-C01-C15	3.44	137.70	128.81
3	B	601[A]	7EI	C31-C16-C20	-3.41	114.92	120.18
3	D	601	7EI	C33-N02-C27	3.34	116.36	108.83
3	A	601	7EI	C22-C01-C15	3.28	137.30	128.81
3	A	601	7EI	O04-S01-O02	3.19	121.27	119.22
3	B	601[A]	7EI	C30-C11-C03	-3.14	114.11	118.59
3	C	601	7EI	C22-C01-C02	-3.13	116.13	121.27
3	B	601[B]	7EI	C28-C09-C24	-3.03	115.50	120.18
3	B	601[B]	7EI	C22-C01-C02	-3.00	116.33	121.27
3	C	601	7EI	O04-S01-O02	3.00	121.15	119.22
3	B	601[B]	7EI	C17-C20-C16	2.96	123.35	119.73
3	C	601	7EI	C21-C28-C09	2.92	123.30	119.73
3	A	601	7EI	C21-C28-C09	2.91	123.29	119.73
3	B	601[A]	7EI	C34-C22-C17	-2.89	114.47	118.59
3	D	601	7EI	C31-C16-C20	-2.88	115.74	120.18
3	B	601[B]	7EI	C34-C22-C17	-2.85	114.53	118.59
3	D	601	7EI	C30-C11-C03	-2.85	114.53	118.59
3	B	601[B]	7EI	C30-C11-C15	2.83	124.58	120.91
3	B	601[A]	7EI	C30-C11-C15	2.80	124.53	120.91
3	A	601	7EI	C21-C13-N01	2.78	124.31	120.16
3	D	601	7EI	C07-C27-N02	2.78	115.78	111.33
3	A	601	7EI	C30-C11-C03	-2.73	114.70	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	7EI	C21-C28-C09	2.71	123.05	119.73
3	B	601[A]	7EI	C08-C06-N01	2.68	114.74	112.14
3	B	601[B]	7EI	C21-C28-C09	2.64	122.96	119.73
3	A	601	7EI	O05-C14-C15	2.62	105.63	101.99
3	D	601	7EI	C22-C01-C15	2.60	135.54	128.81
3	B	601[A]	7EI	C17-C20-C16	2.56	122.86	119.73
3	B	601[B]	7EI	C22-C01-C15	2.55	135.42	128.81
3	B	601[A]	7EI	C24-C12-C13	2.55	123.68	120.32
3	B	601[A]	7EI	C12-C13-C21	-2.54	113.99	119.16
3	B	601[B]	7EI	C11-C15-C14	-2.53	117.31	121.44
3	C	601	7EI	O05-C14-C15	2.53	105.51	101.99
3	D	601	7EI	C30-C11-C15	2.52	124.17	120.91
3	A	601	7EI	C12-C13-C21	-2.51	114.05	119.16
3	D	601	7EI	C12-C13-C21	-2.47	114.13	119.16
3	C	601	7EI	C12-C13-C21	-2.44	114.19	119.16
3	C	601	7EI	C30-C11-C03	-2.44	115.11	118.59
3	D	601	7EI	C24-C12-C13	2.34	123.41	120.32
3	B	601[B]	7EI	C14-C19-C26	-2.33	98.56	100.61
3	C	601	7EI	C31-C16-C20	-2.31	116.62	120.18
3	D	601	7EI	C17-C20-C16	2.27	122.52	119.73
3	A	601	7EI	C31-C16-C20	-2.25	116.70	120.18
3	A	601	7EI	C14-C15-C01	-2.25	102.25	106.97
3	B	601[B]	7EI	C34-C22-C01	2.23	123.79	120.91
3	C	601	7EI	C33-N02-C27	2.21	113.80	108.83
3	B	601[B]	7EI	C30-C11-C03	-2.20	115.45	118.59
3	C	601	7EI	C21-C13-N01	2.18	123.41	120.16
3	A	601	7EI	C30-C11-C15	2.15	123.69	120.91
3	B	601[B]	7EI	O05-C14-C15	2.15	104.99	101.99
3	C	601	7EI	C12-C24-C09	2.15	122.36	119.73
3	C	601	7EI	C30-C11-C15	2.14	123.68	120.91
3	B	601[A]	7EI	C34-C31-C16	2.14	122.34	119.73
3	B	601[B]	7EI	C34-C31-C16	2.14	122.34	119.73
3	A	601	7EI	C28-C21-C13	2.13	123.12	120.32
3	C	601	7EI	C28-C21-C13	2.10	123.08	120.32
3	B	601[A]	7EI	C14-C15-C01	-2.09	102.59	106.97
3	D	601	7EI	C29-O03-C16	2.09	123.38	117.93
3	D	601	7EI	C03-C04-C23	2.09	122.16	119.88
3	C	601	7EI	C32-C33-N02	2.07	114.64	111.33
3	A	601	7EI	C24-C12-C13	2.06	123.04	120.32
3	B	601[A]	7EI	C04-C23-C10	-2.05	116.32	119.77
3	D	601	7EI	C34-C22-C17	-2.03	115.69	118.59
3	B	601[A]	7EI	C31-C34-C22	2.03	123.14	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	7EI	O05-C14-C19	-2.02	100.66	104.64
3	B	601[B]	7EI	C24-C12-C13	2.01	122.97	120.32

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601[A]	7EI	C06-N01-S01-O02
3	B	601[A]	7EI	C06-N01-S01-O04
3	B	601[B]	7EI	C21-C13-N01-S01
3	B	601[B]	7EI	C12-C13-N01-S01
3	D	601	7EI	C06-N01-S01-O04
3	B	601[B]	7EI	C24-C09-O01-C05
3	B	601[B]	7EI	C28-C09-O01-C05
3	C	601	7EI	C28-C09-O01-C05
3	C	601	7EI	C24-C09-O01-C05
3	B	601[B]	7EI	C29-C25-N02-C33
3	A	601	7EI	C28-C09-O01-C05
3	A	601	7EI	C24-C09-O01-C05
3	B	601[A]	7EI	C03-C11-C15-C01
3	B	601[A]	7EI	C28-C09-O01-C05
3	B	601[A]	7EI	C25-C29-O03-C16
3	D	601	7EI	C25-C29-O03-C16
3	B	601[A]	7EI	C30-C11-C15-C01
3	B	601[A]	7EI	C24-C09-O01-C05
3	A	601	7EI	C29-C25-N02-C27
3	D	601	7EI	C28-C09-O01-C05
3	C	601	7EI	N02-C25-C29-O03
3	A	601	7EI	C02-C01-C22-C34
3	B	601[B]	7EI	C02-C01-C22-C17
3	B	601[B]	7EI	C02-C01-C22-C34
3	B	601[B]	7EI	C06-N01-S01-O04
3	C	601	7EI	C02-C01-C22-C34
3	A	601	7EI	C06-N01-S01-O04
3	D	601	7EI	C06-N01-S01-O02
3	D	601	7EI	C24-C09-O01-C05
3	B	601[B]	7EI	C19-C26-S01-O02
3	B	601[A]	7EI	C06-N01-S01-C26
3	D	601	7EI	C06-N01-S01-C26
3	A	601	7EI	C02-C01-C22-C17
3	C	601	7EI	C02-C01-C22-C17
3	D	601	7EI	C02-C01-C22-C17

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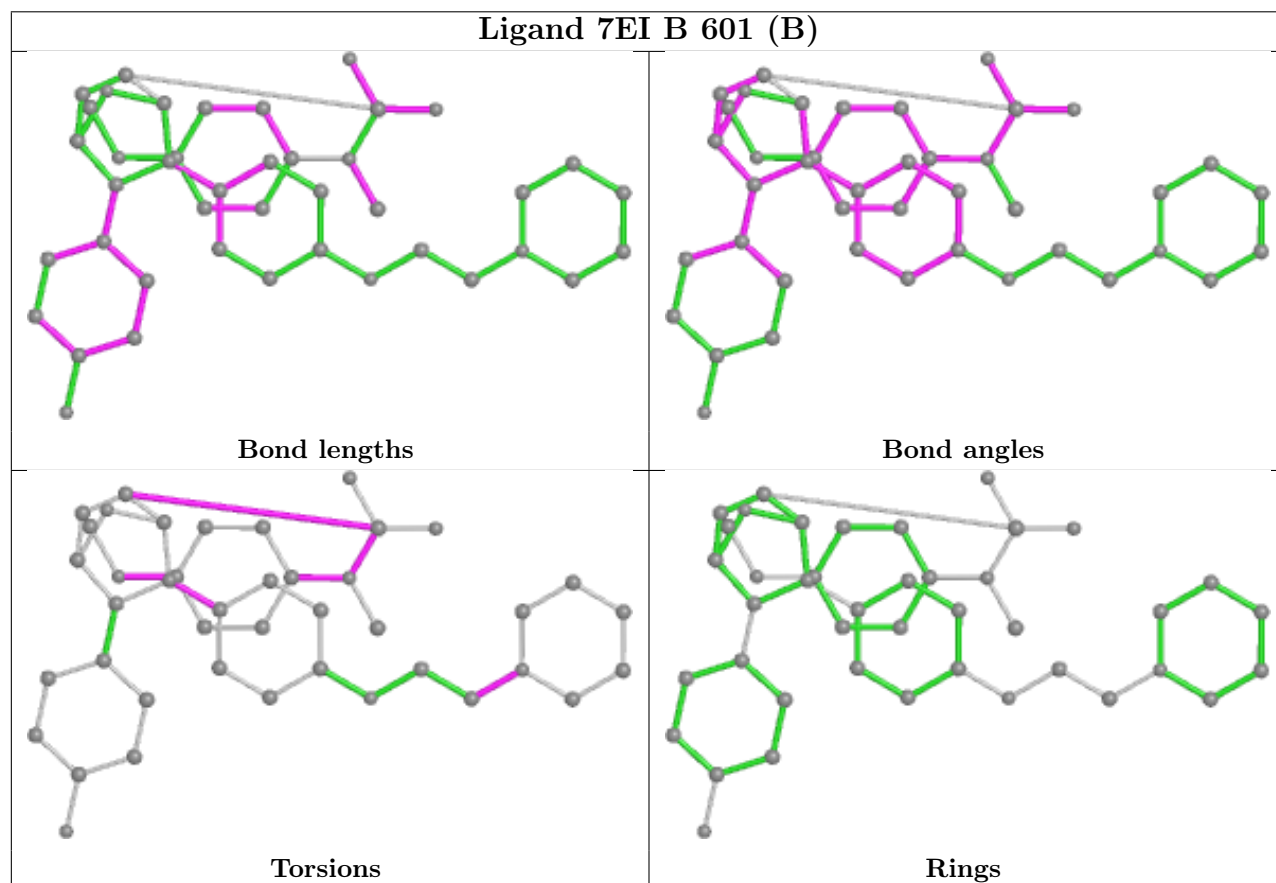
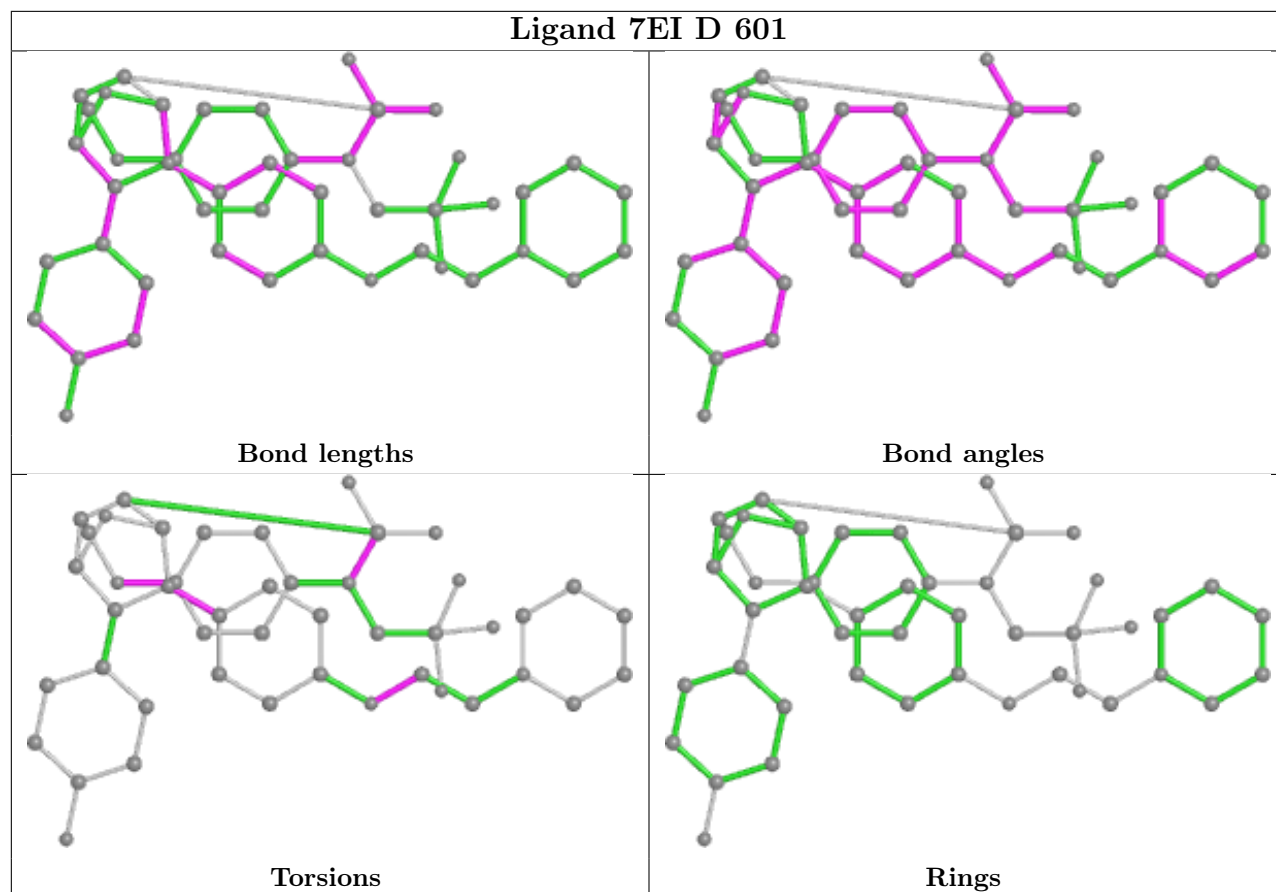
Mol	Chain	Res	Type	Atoms
3	D	601	7EI	C15-C01-C22-C17
3	A	601	7EI	N02-C25-C29-O03
3	B	601[B]	7EI	C06-N01-S01-C26
3	D	601	7EI	C02-C01-C22-C34
3	D	601	7EI	C15-C01-C22-C34
3	A	601	7EI	C06-N01-S01-C26

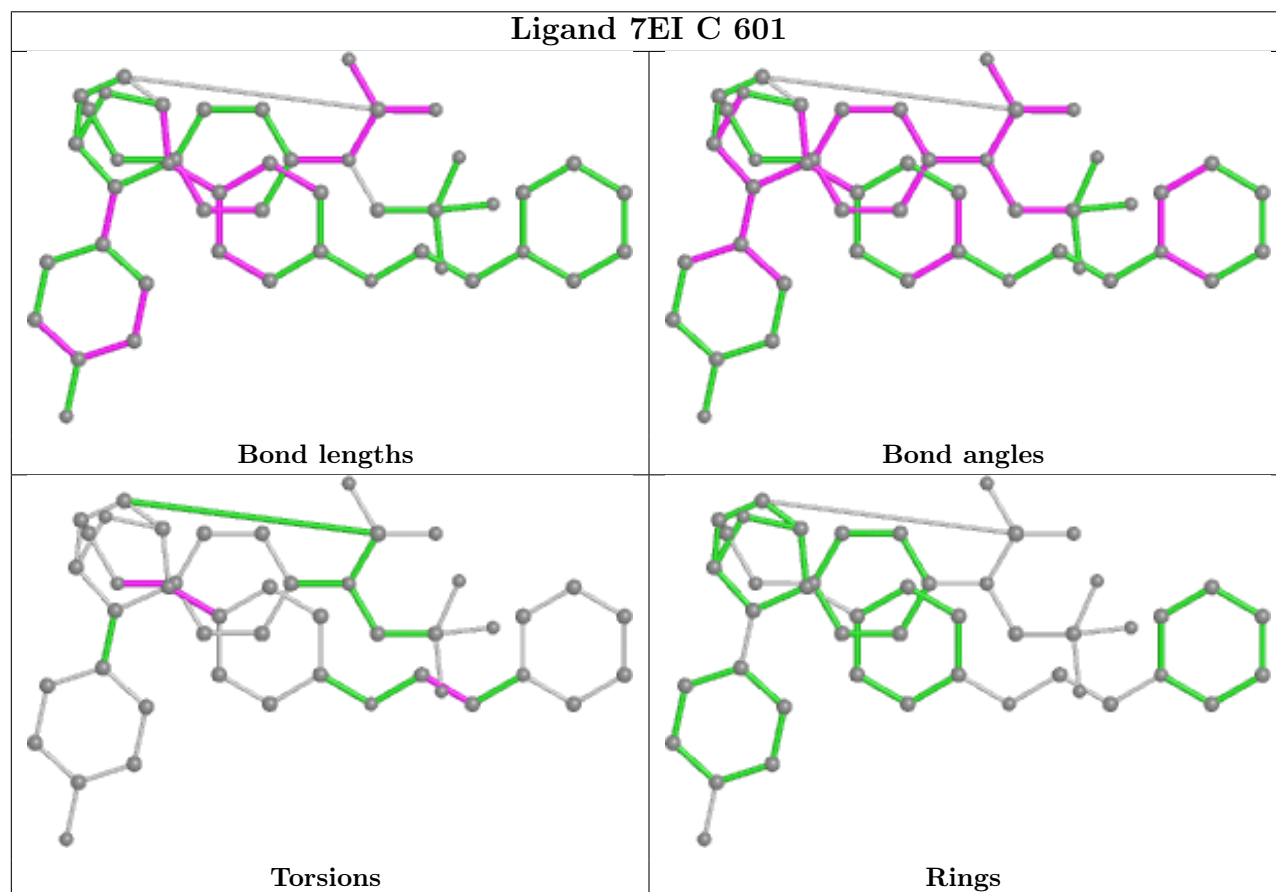
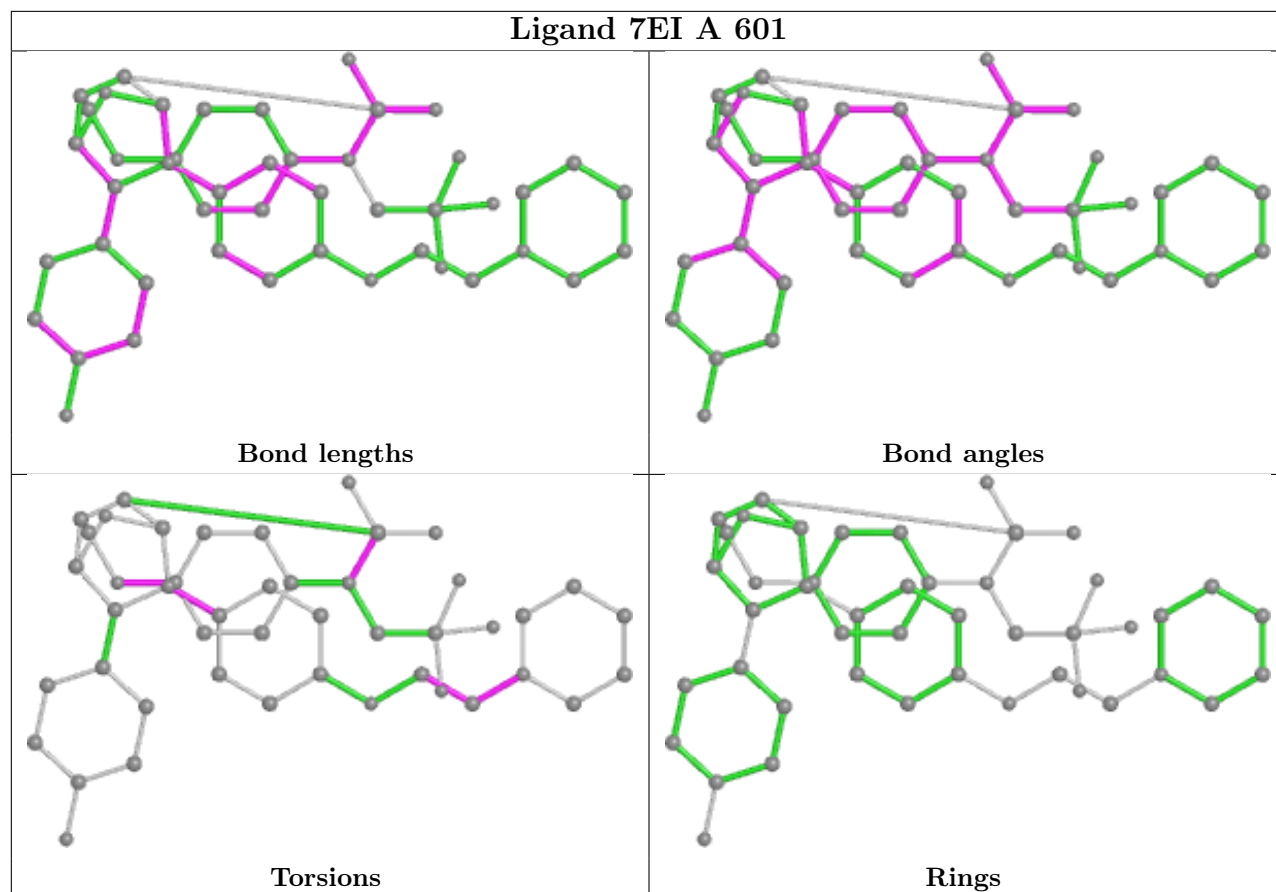
There are no ring outliers.

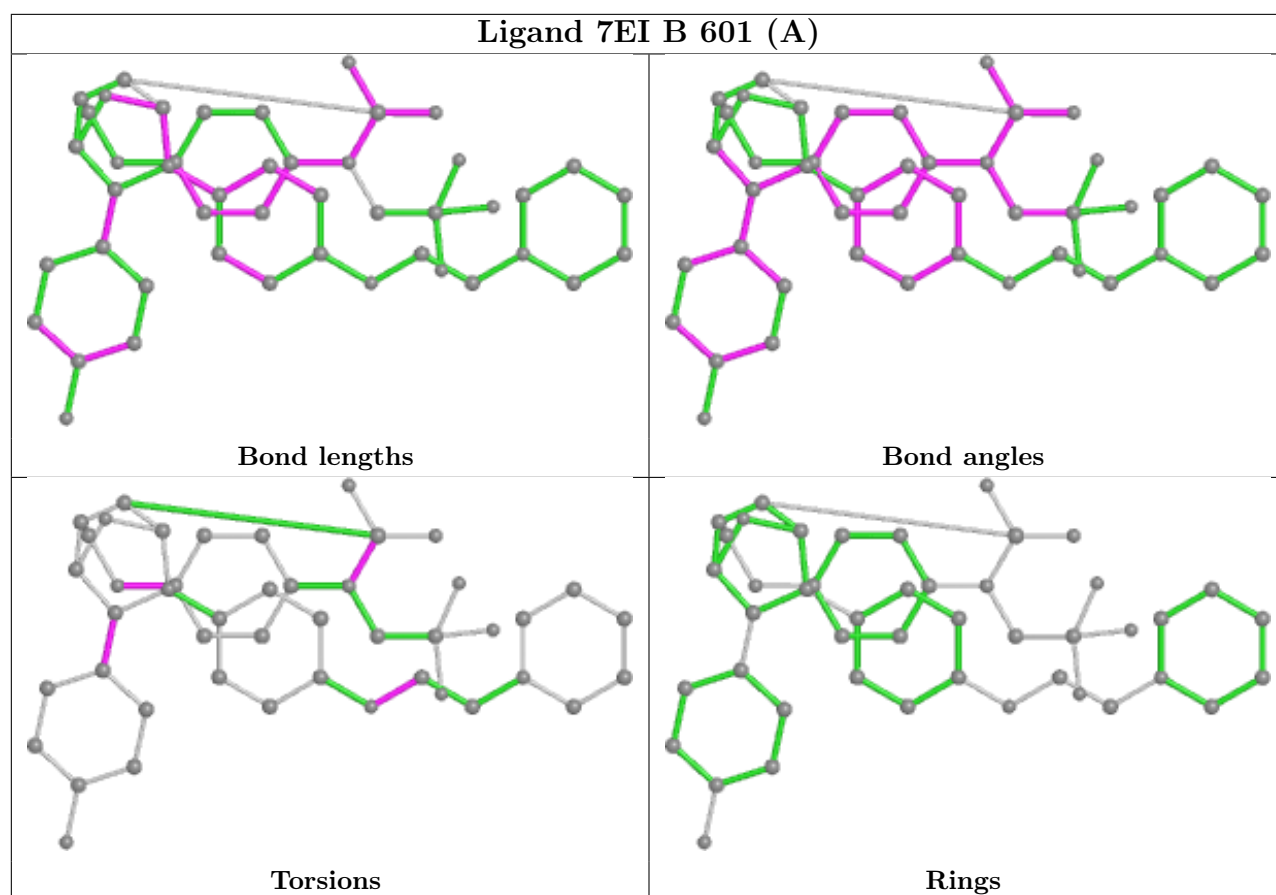
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601[B]	7EI	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	227/257 (88%)	0.25	14 (6%) 20 17	14, 26, 50, 76	0
1	B	226/257 (87%)	0.27	17 (7%) 14 12	12, 24, 61, 74	0
1	C	228/257 (88%)	0.14	9 (3%) 39 37	12, 24, 48, 66	0
2	D	217/257 (84%)	0.25	15 (6%) 16 14	13, 24, 57, 85	0
All	All	898/1028 (87%)	0.23	55 (6%) 21 18	12, 25, 55, 85	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	VAL	7.2
1	B	546	ALA	5.7
1	B	306	LEU	5.5
1	A	546	ALA	5.3
2	D	533	VAL	5.3
1	B	532	ASN	5.3
1	C	533	VAL	5.1
2	D	421	MET	4.6
1	B	337	PHE	4.4
1	B	462	LEU	4.2
1	C	306	LEU	4.2
1	A	415	GLY	4.1
2	D	527	SER	3.9
1	B	413	ASN	3.8
1	B	533	VAL	3.8
1	A	413	ASN	3.7
1	B	525	LEU	3.6
2	D	468	SER	3.6
2	D	526	TYR	3.6
1	C	461	PHE	3.4
1	A	421	MET	3.4

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
2	D	524	HIS	3.4
2	D	525	LEU	3.3
1	C	413	ASN	3.3
1	B	524	HIS	3.2
2	D	459	TYR	3.1
2	D	306	LEU	3.1
1	B	331	TYR	3.1
2	D	469	LEU	3.0
1	A	464	SER	2.9
2	D	528	MET	2.9
2	D	467	LYS	2.9
1	A	492	LYS	2.8
1	B	421	MET	2.7
1	C	463	SER	2.7
2	D	331	TYR	2.7
1	C	464	SER	2.5
1	B	335	ARG	2.5
1	A	459	TYR	2.5
1	C	525	LEU	2.5
1	A	525	LEU	2.4
1	B	397	GLU	2.4
1	B	338	SER	2.3
1	A	334	THR	2.3
1	A	416	LYS	2.3
1	C	546	ALA	2.3
2	D	461	PHE	2.1
1	B	545	ASP	2.1
1	A	437	MET	2.1
1	B	437	MET	2.1
1	A	425	PHE	2.0
1	A	461	PHE	2.0
1	B	334	THR	2.0
1	C	437	MET	2.0
2	D	534	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
1	YCM	A	381	10/11	0.90	0.14	18,21,32,36	0
1	YCM	C	381	10/11	0.91	0.11	19,22,33,35	0
1	YCM	B	381	10/11	0.94	0.12	18,20,31,33	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

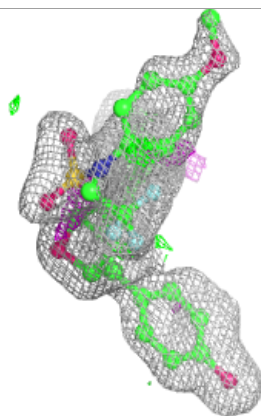
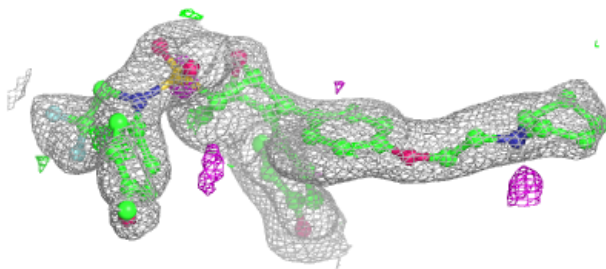
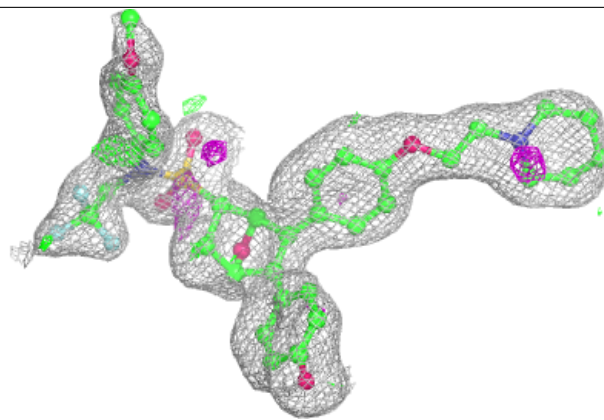
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	7EI	B	601[A]	46/46	0.88	0.16	18,25,30,30	46
3	7EI	B	601[B]	42/46	0.88	0.16	24,32,36,37	42
3	7EI	D	601	46/46	0.88	0.13	23,33,45,47	0
3	7EI	C	601	46/46	0.90	0.12	19,31,42,45	0
3	7EI	A	601	46/46	0.90	0.12	21,31,39,41	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.

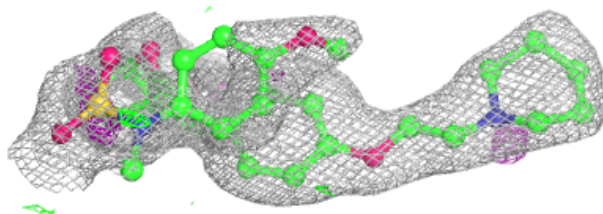
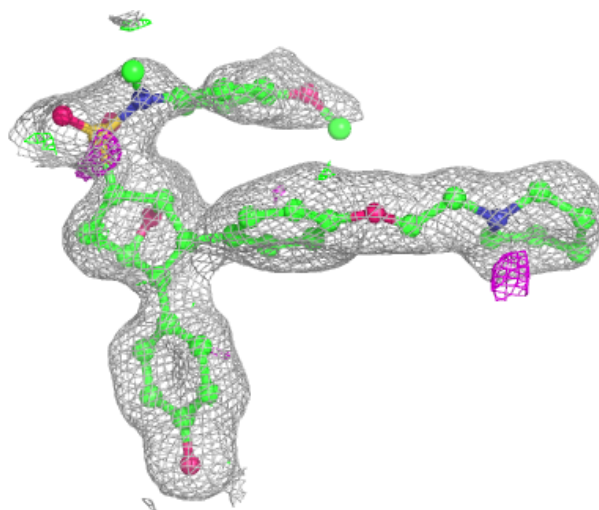
**Electron density around 7EI B 601 (A):**

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



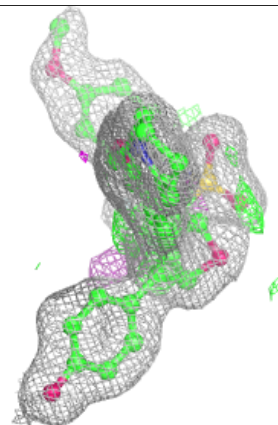
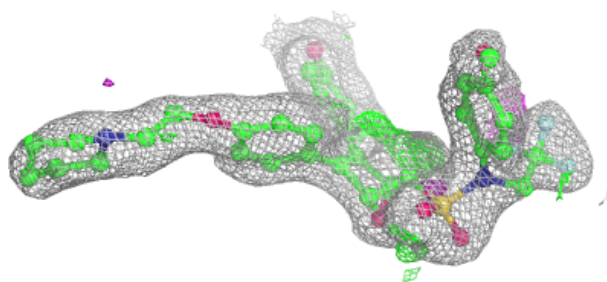
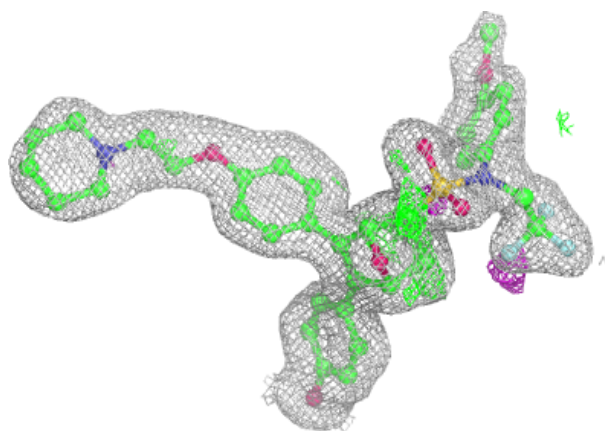
**Electron density around 7EI B 601 (B):**

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

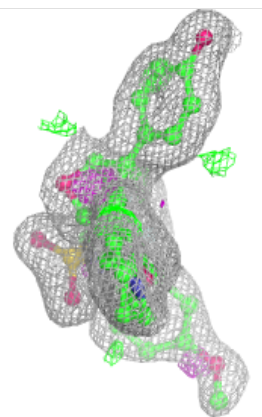
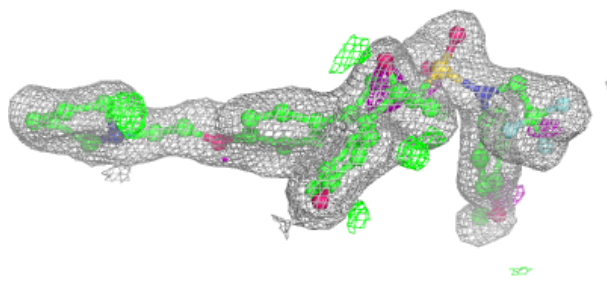
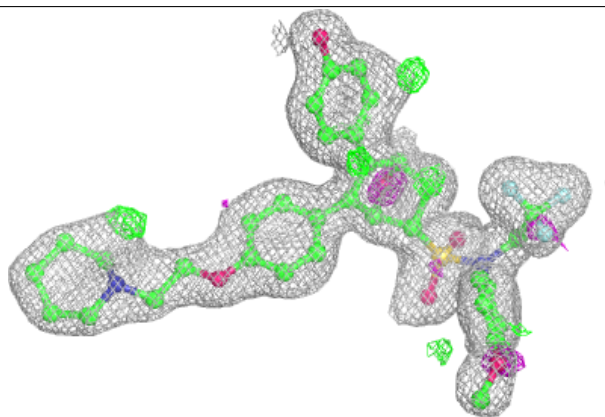


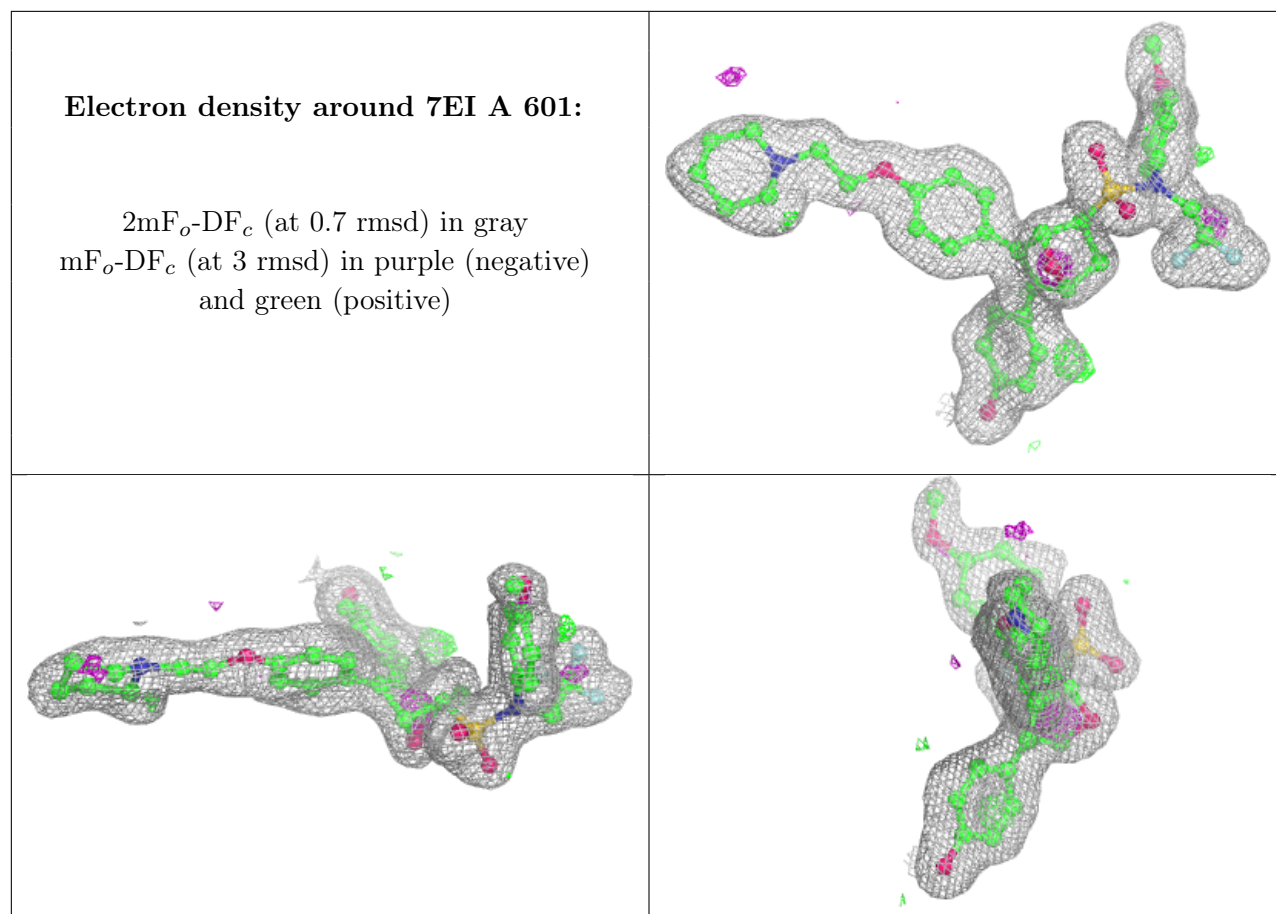
**Electron density around 7EI D 601:**

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

**Electron density around 7EI 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.