



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 12:30 PM EDT

PDB ID : 7RS0
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-18
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 : 2021-08-10
Resolution : 1.67 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
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)	:	2.23.1

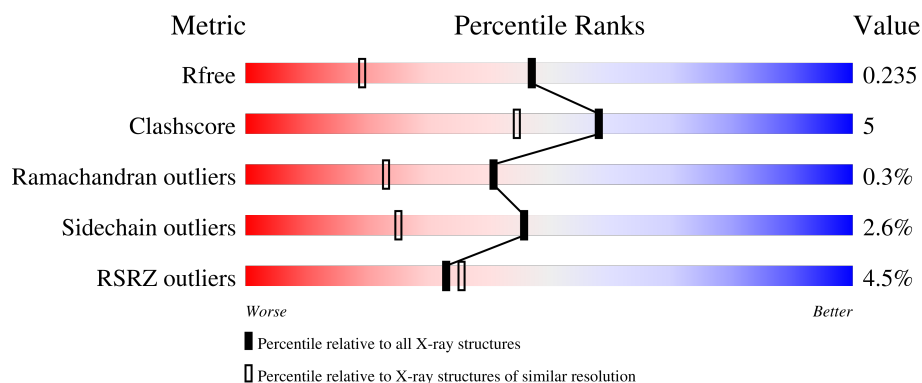
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	 7% 81% 11% • 6%
1	B	257	 2% 77% 9% 14%
1	C	257	 5% 84% 7% • 8%
1	D	257	 2% 77% 5% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7685 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
1	A	242	Total	C	N	O	S	0	1	0
			1936	1237	327	353	19			
1	B	221	Total	C	N	O	S	0	0	0
			1754	1123	299	315	17			
1	C	236	Total	C	N	O	S	0	1	0
			1889	1208	318	346	17			
1	D	210	Total	C	N	O	S	0	0	0
			1677	1076	286	300	15			

There are 8 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
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is (1R,2S,4R,5R,6R)-5-(4-hydroxyphenyl)-N-(4-methoxyphenyl)-6-(4-propoxyp henyl)-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]heptane-2-sulfonamide (three-letter code: 7I9) (formula: C₃₆H₄₁F₃N₂O₆S) (labeled as "Ligand of Interest" by depositor).



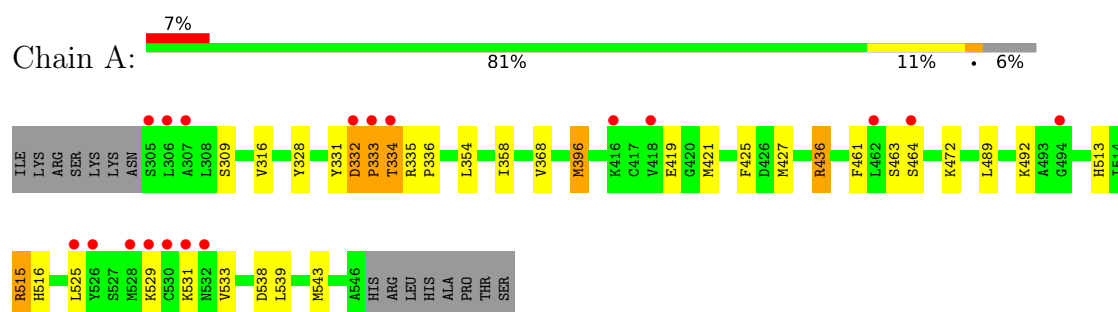
- Molecule 3 is water.



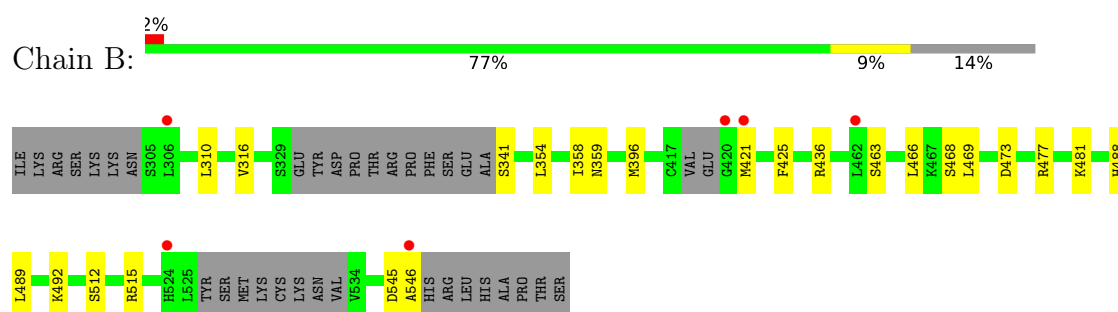
3 Residue-property plots [i](#)

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.

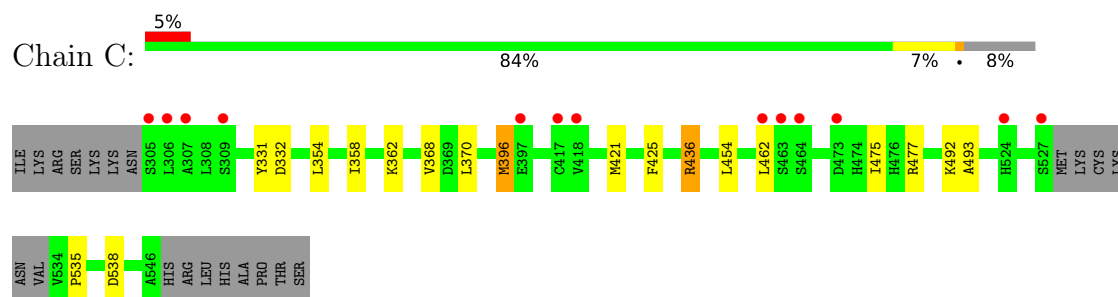
• Molecule 1: Estrogen receptor



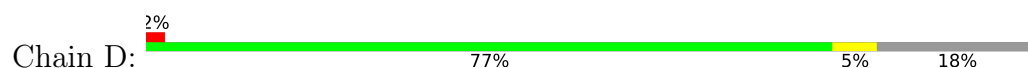
• Molecule 1: Estrogen receptor

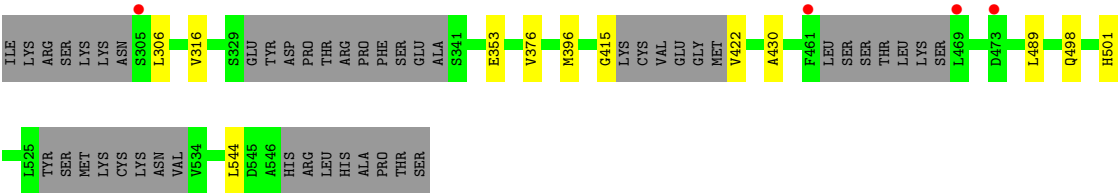


• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.27Å 58.80Å 92.67Å 79.95° 75.46° 63.10°	Depositor
Resolution (Å)	89.48 – 1.67 89.48 – 1.67	Depositor EDS
% Data completeness (in resolution range)	57.1 (89.48-1.67) 57.1 (89.48-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.227 0.202 , 0.235	Depositor DCC
R_{free} test set	3158 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.084 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7685	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7I9, 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	0.44	0/1961	0.64	1/2649 (0.0%)
1	B	0.44	0/1771	0.66	1/2387 (0.0%)
1	C	0.47	0/1913	0.66	1/2585 (0.0%)
1	D	0.48	0/1693	0.65	0/2283
All	All	0.46	0/7338	0.65	3/9904 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	436	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	436	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	TYR	Peptide
1	A	333	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1936	0	1977	22	1
1	B	1754	0	1807	14	1
1	C	1889	0	1921	13	0
1	D	1677	0	1719	8	0
2	A	26	0	0	6	0
2	B	34	0	0	7	0
2	C	28	0	0	6	0
2	D	33	0	0	5	0
3	A	70	0	0	4	0
3	B	78	0	0	3	0
3	C	85	0	0	0	0
3	D	75	0	0	0	0
All	All	7685	0	7424	71	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 5.

All (71) 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)
2:C:601:7I9:C01	2:C:601:7I9:C05	1.75	1.42
2:B:601:7I9:C01	2:B:601:7I9:C05	1.75	1.41
2:A:601:7I9:C01	2:A:601:7I9:C05	1.75	1.38
2:C:601:7I9:S42	2:C:601:7I9:C03	2.11	1.38
2:D:601:7I9:C01	2:D:601:7I9:C05	1.75	1.37
2:D:601:7I9:C03	2:D:601:7I9:S42	2.12	1.36
2:B:601:7I9:S42	2:B:601:7I9:C03	2.12	1.36
2:A:601:7I9:S42	2:A:601:7I9:C03	2.12	1.35
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.57	0.84
1:A:515:ARG:NH1	1:B:512:SER:OG	2.15	0.80
1:B:473:ASP:OD2	1:B:477:ARG:NH1	2.17	0.78
2:A:601:7I9:S42	2:A:601:7I9:C02	2.75	0.74
2:D:601:7I9:S42	2:D:601:7I9:C04	2.75	0.74
1:B:546:ALA:O	3:B:701:HOH:O	2.08	0.71
2:B:601:7I9:S42	2:B:601:7I9:C04	2.77	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:7I9:S42	2:C:601:7I9:C02	2.80	0.68
1:A:533:VAL:HG12	2:A:601:7I9:O21	1.93	0.68
2:C:601:7I9:S42	2:C:601:7I9:C04	2.79	0.66
1:A:333:PRO:O	1:A:335:ARG:HG3	1.96	0.64
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.81	0.62
1:B:488:HIS:NE2	1:B:492:LYS:HD2	2.16	0.61
2:A:601:7I9:S42	2:A:601:7I9:C04	2.84	0.60
1:A:332:ASP:O	3:A:701:HOH:O	2.17	0.60
1:A:515:ARG:NE	3:A:702:HOH:O	2.33	0.59
2:B:601:7I9:S42	2:B:601:7I9:C02	2.88	0.58
1:D:415:GLY:C	1:D:422:VAL:HG22	2.24	0.58
1:B:310:LEU:O	1:B:481:LYS:CE	2.54	0.56
1:B:477:ARG:NH2	3:B:702:HOH:O	2.28	0.55
1:A:461:PHE:HB2	1:A:472:LYS:HE3	1.90	0.53
2:C:601:7I9:C01	2:C:601:7I9:C08	2.76	0.53
1:C:462:LEU:CD2	1:D:430:ALA:HB2	2.39	0.53
2:D:601:7I9:S42	2:D:601:7I9:C02	2.90	0.53
1:A:427:MET:CE	1:A:516:HIS:HD2	2.22	0.53
1:C:462:LEU:HD21	1:D:430:ALA:HB2	1.91	0.53
1:B:463:SER:HB3	1:B:468:SER:OG	2.10	0.51
1:A:539:LEU:HG	1:A:543:MET:CE	2.41	0.50
1:A:427:MET:HE1	1:A:516:HIS:CD2	2.48	0.49
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.95	0.48
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.94	0.48
1:C:396:MET:O	1:C:436:ARG:HD3	2.13	0.48
1:C:454:LEU:HD22	1:C:475:ILE:HD12	1.96	0.47
1:A:396:MET:O	1:A:436:ARG:HD3	2.15	0.47
1:B:354:LEU:O	1:B:358:ILE:HD13	2.16	0.46
1:D:376:VAL:CG2	1:D:544:LEU:HD12	2.45	0.46
1:A:515:ARG:NH2	3:A:702:HOH:O	2.49	0.45
1:C:421:MET:SD	2:C:601:7I9:N22	2.89	0.45
1:B:469:LEU:HD13	1:C:493:ALA:O	2.16	0.45
1:B:310:LEU:O	1:B:481:LYS:HE3	2.17	0.45
1:A:525:LEU:HD23	1:A:525:LEU:C	2.37	0.44
1:C:362:LYS:HD2	1:C:368:VAL:HG12	1.99	0.44
1:A:427:MET:HE2	1:A:513:HIS:CE1	2.52	0.44
1:A:354:LEU:O	1:A:358:ILE:HD13	2.17	0.44
1:C:331:TYR:CE2	1:C:332:ASP:HB2	2.53	0.43
1:D:353:GLU:OE1	2:D:601:7I9:O20	2.37	0.43
1:A:539:LEU:HG	1:A:543:MET:HE1	1.99	0.43
1:C:492:LYS:HB3	1:C:492:LYS:HE2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MET:CE	1:A:516:HIS:CD2	3.01	0.43
1:A:427:MET:HE1	1:A:516:HIS:HD2	1.83	0.43
1:A:334:THR:HG23	1:A:334:THR:O	2.19	0.42
1:B:421:MET:HG3	2:B:601:7I9:C24	2.50	0.42
1:C:354:LEU:O	1:C:358:ILE:HD13	2.19	0.42
1:A:421:MET:SD	2:A:601:7I9:N22	2.93	0.42
1:A:368:VAL:HG22	3:A:706:HOH:O	2.20	0.41
2:B:601:7I9:C01	2:B:601:7I9:C08	2.81	0.41
1:B:421:MET:HG3	2:B:601:7I9:F47	2.11	0.41
1:C:370:LEU:CD1	1:C:475:ILE:HD11	2.40	0.41
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.56	0.40
1:B:341:SER:N	3:B:710:HOH:O	2.54	0.40
1:C:354:LEU:HD21	1:C:535:PRO:HB3	2.04	0.40
1:A:316:VAL:HG21	1:A:489:LEU:HD21	2.03	0.40
1:A:335:ARG:HA	1:A:336:PRO:C	2.42	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:328:TYR:OH	1:B:359:ASN:ND2[1_545]	1.84	0.36

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	240/257 (93%)	233 (97%)	4 (2%)	3 (1%)	12	2
1	B	212/257 (82%)	210 (99%)	2 (1%)	0	100	100
1	C	232/257 (90%)	230 (99%)	2 (1%)	0	100	100
1	D	199/257 (77%)	198 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	883/1028 (86%)	871 (99%)	9 (1%)	3 (0%)	41	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	SER
1	A	529	LYS
1	A	332	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/231 (94%)	208 (95%)	10 (5%)	27	9
1	B	197/231 (85%)	192 (98%)	5 (2%)	47	26
1	C	212/231 (92%)	208 (98%)	4 (2%)	57	38
1	D	187/231 (81%)	185 (99%)	2 (1%)	73	61
All	All	814/924 (88%)	793 (97%)	21 (3%)	46	25

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	SER
1	A	334	THR
1	A	396	MET
1	A	419	GLU
1	A	425	PHE
1	A	464	SER
1	A	492	LYS
1	A	515	ARG
1	A	531	LYS
1	A	538	ASP
1	B	396	MET
1	B	425	PHE

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Mol	Chain	Res	Type
1	B	466	LEU
1	B	515	ARG
1	B	545	ASP
1	C	396	MET
1	C	425	PHE
1	C	477	ARG
1	C	538	ASP
1	D	306	LEU
1	D	396	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	502	GLN
1	A	513	HIS
1	A	516	HIS
1	B	413	ASN
1	B	513	HIS
1	B	524	HIS
1	C	413	ASN
1	C	513	HIS
1	C	519	ASN
1	D	513	HIS
1	D	519	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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	D	381	1	7,9,10	0.46	0	4,10,12	0.45	0
1	YCM	B	381	1	7,9,10	0.44	0	4,10,12	0.48	0
1	YCM	A	381	1	7,9,10	0.54	0	4,10,12	0.53	0
1	YCM	C	381	1	7,9,10	0.58	0	4,10,12	0.53	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	D	381	1	-	1/6/8/10	-
1	YCM	B	381	1	-	1/6/8/10	-
1	YCM	A	381	1	-	1/6/8/10	-
1	YCM	C	381	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	7I9	B	601	-	34,37,53	7.53	24 (70%)	43,56,77	4.92	9 (20%)
2	7I9	A	601	-	27,29,53	8.38	24 (88%)	33,44,77	5.88	11 (33%)
2	7I9	D	601	-	33,36,53	7.64	24 (72%)	42,55,77	5.02	13 (30%)
2	7I9	C	601	-	29,31,53	8.10	22 (75%)	35,46,77	5.21	8 (22%)

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	7I9	B	601	-	-	15/25/53/71	0/5/4/6
2	7I9	A	601	-	-	9/14/40/71	0/5/4/6
2	7I9	D	601	-	-	14/24/52/71	0/5/4/6
2	7I9	C	601	-	-	9/16/42/71	0/5/4/6

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	7I9	C04-C03	-24.76	1.23	1.54
2	B	601	7I9	C04-C03	-24.63	1.23	1.54
2	D	601	7I9	C04-C03	-24.57	1.23	1.54
2	A	601	7I9	C04-C03	-24.31	1.24	1.54
2	C	601	7I9	C05-C01	20.84	1.75	1.34
2	A	601	7I9	C05-C01	20.71	1.75	1.34
2	B	601	7I9	C05-C01	20.70	1.75	1.34
2	D	601	7I9	C05-C01	20.56	1.75	1.34
2	B	601	7I9	C04-C06	-9.45	1.32	1.53
2	D	601	7I9	C04-C06	-9.23	1.33	1.53
2	C	601	7I9	C04-C06	-8.73	1.34	1.53
2	D	601	7I9	C14-C13	8.45	1.54	1.38
2	B	601	7I9	C14-C13	8.41	1.54	1.38
2	A	601	7I9	C15-C08	8.32	1.53	1.39
2	A	601	7I9	C11-C10	8.23	1.53	1.38
2	B	601	7I9	C14-C09	8.17	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	7I9	C11-C10	8.07	1.53	1.38
2	A	601	7I9	C14-C13	8.07	1.53	1.38
2	D	601	7I9	C11-C10	8.06	1.53	1.38
2	C	601	7I9	C14-C13	8.06	1.53	1.38
2	D	601	7I9	C14-C09	8.06	1.53	1.39
2	A	601	7I9	C14-C09	8.02	1.53	1.39
2	A	601	7I9	C04-C06	-8.02	1.35	1.53
2	D	601	7I9	C10-C09	7.97	1.52	1.39
2	A	601	7I9	C16-C15	7.96	1.53	1.38
2	D	601	7I9	C15-C08	7.89	1.52	1.39
2	B	601	7I9	C15-C08	7.84	1.52	1.39
2	C	601	7I9	C14-C09	7.79	1.52	1.39
2	D	601	7I9	C13-C12	7.78	1.54	1.38
2	A	601	7I9	C10-C09	7.73	1.52	1.39
2	C	601	7I9	C10-C09	7.71	1.52	1.39
2	C	601	7I9	C15-C08	7.68	1.52	1.39
2	B	601	7I9	C13-C12	7.65	1.54	1.38
2	B	601	7I9	C10-C09	7.63	1.52	1.39
2	B	601	7I9	C19-C08	7.63	1.52	1.39
2	C	601	7I9	C16-C15	7.63	1.52	1.38
2	A	601	7I9	C19-C08	7.60	1.52	1.39
2	D	601	7I9	C19-C08	7.60	1.52	1.39
2	C	601	7I9	C11-C10	7.60	1.52	1.38
2	C	601	7I9	C19-C08	7.57	1.52	1.39
2	B	601	7I9	C16-C15	7.48	1.52	1.38
2	C	601	7I9	C13-C12	7.40	1.53	1.38
2	D	601	7I9	C11-C12	7.36	1.53	1.38
2	A	601	7I9	C18-C17	7.36	1.53	1.38
2	D	601	7I9	C16-C15	7.36	1.52	1.38
2	A	601	7I9	C16-C17	7.36	1.53	1.38
2	C	601	7I9	C18-C17	7.35	1.52	1.38
2	B	601	7I9	C16-C17	7.34	1.52	1.38
2	D	601	7I9	C16-C17	7.25	1.52	1.38
2	A	601	7I9	C19-C18	7.19	1.51	1.38
2	C	601	7I9	C16-C17	7.18	1.52	1.38
2	B	601	7I9	C11-C12	7.17	1.53	1.38
2	C	601	7I9	C19-C18	7.16	1.51	1.38
2	C	601	7I9	C11-C12	7.15	1.53	1.38
2	D	601	7I9	C18-C17	7.10	1.52	1.38
2	A	601	7I9	C11-C12	7.07	1.52	1.38
2	D	601	7I9	C19-C18	7.03	1.51	1.38
2	A	601	7I9	C13-C12	6.97	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	7I9	C18-C17	6.88	1.52	1.38
2	B	601	7I9	C19-C18	6.71	1.51	1.38
2	A	601	7I9	O07-C02	5.05	1.50	1.43
2	A	601	7I9	S42-N22	4.66	1.70	1.59
2	D	601	7I9	O07-C06	4.61	1.55	1.44
2	C	601	7I9	S42-N22	4.55	1.70	1.59
2	B	601	7I9	O07-C06	4.53	1.54	1.44
2	B	601	7I9	O07-C02	4.44	1.49	1.43
2	C	601	7I9	O07-C06	4.43	1.54	1.44
2	C	601	7I9	O07-C02	4.41	1.49	1.43
2	D	601	7I9	O07-C02	4.28	1.49	1.43
2	A	601	7I9	O07-C06	4.27	1.54	1.44
2	B	601	7I9	O43-S42	4.06	1.47	1.43
2	D	601	7I9	O43-S42	4.03	1.47	1.43
2	D	601	7I9	O44-S42	3.82	1.46	1.43
2	C	601	7I9	C02-C01	-3.55	1.46	1.50
2	B	601	7I9	O44-S42	3.50	1.46	1.43
2	B	601	7I9	C24-C45	3.25	1.54	1.50
2	A	601	7I9	C02-C01	-3.00	1.47	1.50
2	B	601	7I9	C02-C01	-2.95	1.47	1.50
2	D	601	7I9	C24-C45	2.93	1.54	1.50
2	D	601	7I9	C09-C01	2.70	1.53	1.48
2	C	601	7I9	C09-C01	2.66	1.53	1.48
2	D	601	7I9	C06-C05	-2.58	1.47	1.51
2	B	601	7I9	C09-C01	2.56	1.53	1.48
2	A	601	7I9	C09-C01	2.53	1.53	1.48
2	D	601	7I9	C02-C01	-2.35	1.48	1.50
2	A	601	7I9	O21-C12	2.35	1.42	1.37
2	A	601	7I9	O43-S42	2.32	1.47	1.43
2	A	601	7I9	O44-S42	2.31	1.47	1.43
2	A	601	7I9	C06-C05	-2.31	1.48	1.51
2	B	601	7I9	C06-C05	-2.29	1.48	1.51
2	C	601	7I9	O43-S42	2.11	1.46	1.43
2	C	601	7I9	O44-S42	2.08	1.46	1.43
2	D	601	7I9	O21-C12	2.07	1.42	1.37
2	B	601	7I9	O21-C12	2.05	1.42	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	7I9	O44-S42-O43	-29.45	101.19	119.23
2	D	601	7I9	O44-S42-O43	-28.21	101.09	119.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	7I9	O44-S42-O43	-27.44	101.58	119.22
2	C	601	7I9	O44-S42-O43	-27.08	102.64	119.23
2	B	601	7I9	C06-C04-C03	11.70	110.95	100.61
2	A	601	7I9	C06-C04-C03	11.70	110.95	100.61
2	D	601	7I9	C06-C04-C03	10.51	109.90	100.61
2	C	601	7I9	C06-C04-C03	8.99	108.55	100.61
2	A	601	7I9	O07-C06-C05	-5.90	93.79	101.99
2	B	601	7I9	O07-C06-C04	-5.51	93.81	104.64
2	C	601	7I9	O07-C06-C04	-5.16	94.50	104.64
2	C	601	7I9	C08-C05-C01	-5.06	115.70	128.81
2	B	601	7I9	O44-S42-N22	4.78	112.36	107.49
2	A	601	7I9	O44-S42-N22	4.74	112.64	107.72
2	C	601	7I9	O43-S42-N22	4.61	112.51	107.72
2	D	601	7I9	O07-C06-C04	-4.38	96.03	104.64
2	D	601	7I9	O44-S42-N22	4.34	111.91	107.49
2	A	601	7I9	C08-C05-C06	4.31	128.47	121.44
2	B	601	7I9	C06-C05-C01	-4.31	97.92	106.97
2	C	601	7I9	O44-S42-N22	4.21	112.08	107.72
2	D	601	7I9	C06-C05-C01	-4.17	98.22	106.97
2	D	601	7I9	O43-S42-N22	4.04	111.61	107.49
2	C	601	7I9	C06-C05-C01	-3.98	98.61	106.97
2	D	601	7I9	C09-C01-C02	3.72	127.39	121.27
2	A	601	7I9	O07-C06-C04	-3.71	97.34	104.64
2	B	601	7I9	C08-C05-C01	-3.59	119.50	128.81
2	B	601	7I9	O43-S42-N22	3.58	111.14	107.49
2	D	601	7I9	C24-N22-S42	3.26	123.88	118.44
2	B	601	7I9	C10-C09-C01	-3.17	116.81	120.91
2	D	601	7I9	C08-C05-C01	-3.15	120.66	128.81
2	D	601	7I9	C09-C01-C05	-3.13	120.70	128.81
2	B	601	7I9	C09-C01-C02	3.01	126.22	121.27
2	A	601	7I9	C09-C01-C02	-2.85	116.59	121.27
2	A	601	7I9	C06-C05-C01	-2.77	101.15	106.97
2	A	601	7I9	O43-S42-N22	2.35	110.15	107.72
2	D	601	7I9	C10-C09-C01	-2.33	117.90	120.91
2	A	601	7I9	C09-C01-C05	-2.30	122.85	128.81
2	C	601	7I9	C09-C01-C02	2.24	124.95	121.27
2	D	601	7I9	C19-C08-C15	2.20	121.71	118.59
2	A	601	7I9	C19-C08-C05	-2.09	118.20	120.91
2	D	601	7I9	F47-C45-C24	-2.05	108.77	112.13

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	7I9	C02-C03-S42-O43
2	B	601	7I9	N22-C24-C45-F46
2	B	601	7I9	N22-C24-C45-F47
2	B	601	7I9	N22-C24-C45-F48
2	B	601	7I9	C24-N22-S42-C03
2	B	601	7I9	C24-N22-S42-O44
2	B	601	7I9	C1-N22-S42-O44
2	D	601	7I9	N22-C24-C45-F46
2	D	601	7I9	N22-C24-C45-F47
2	D	601	7I9	N22-C24-C45-F48
2	D	601	7I9	C24-N22-S42-C03
2	D	601	7I9	C24-N22-S42-O44
2	D	601	7I9	C1-N22-S42-O44
2	A	601	7I9	C13-C12-O21-C32
2	A	601	7I9	C11-C12-O21-C32
2	B	601	7I9	C13-C12-O21-C32
2	B	601	7I9	C11-C12-O21-C32
2	C	601	7I9	C13-C12-O21-C32
2	A	601	7I9	C01-C05-C08-C15
2	C	601	7I9	C11-C12-O21-C32
2	A	601	7I9	C02-C01-C09-C14
2	B	601	7I9	C1-N22-S42-C03
2	D	601	7I9	C1-N22-S42-C03
2	A	601	7I9	C01-C05-C08-C19
2	C	601	7I9	C01-C05-C08-C15
2	C	601	7I9	C33-C32-O21-C12
2	B	601	7I9	O21-C32-C33-C34
2	C	601	7I9	C01-C05-C08-C19
2	D	601	7I9	C33-C32-O21-C12
2	D	601	7I9	C01-C05-C08-C19
2	B	601	7I9	C05-C01-C09-C10
2	B	601	7I9	C01-C05-C08-C19
2	D	601	7I9	C01-C05-C08-C15
2	A	601	7I9	C02-C01-C09-C10
2	D	601	7I9	C13-C12-O21-C32
2	D	601	7I9	C11-C12-O21-C32
2	C	601	7I9	C04-C03-S42-O44
2	B	601	7I9	C01-C05-C08-C15
2	B	601	7I9	C05-C01-C09-C14
2	B	601	7I9	C33-C32-O21-C12
2	D	601	7I9	C05-C01-C09-C10
2	C	601	7I9	C05-C01-C09-C10
2	C	601	7I9	C05-C01-C09-C14

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Mol	Chain	Res	Type	Atoms
2	D	601	7I9	C05-C01-C09-C14
2	C	601	7I9	C02-C01-C09-C14
2	A	601	7I9	C02-C03-S42-O44
2	A	601	7I9	C04-C03-S42-O44

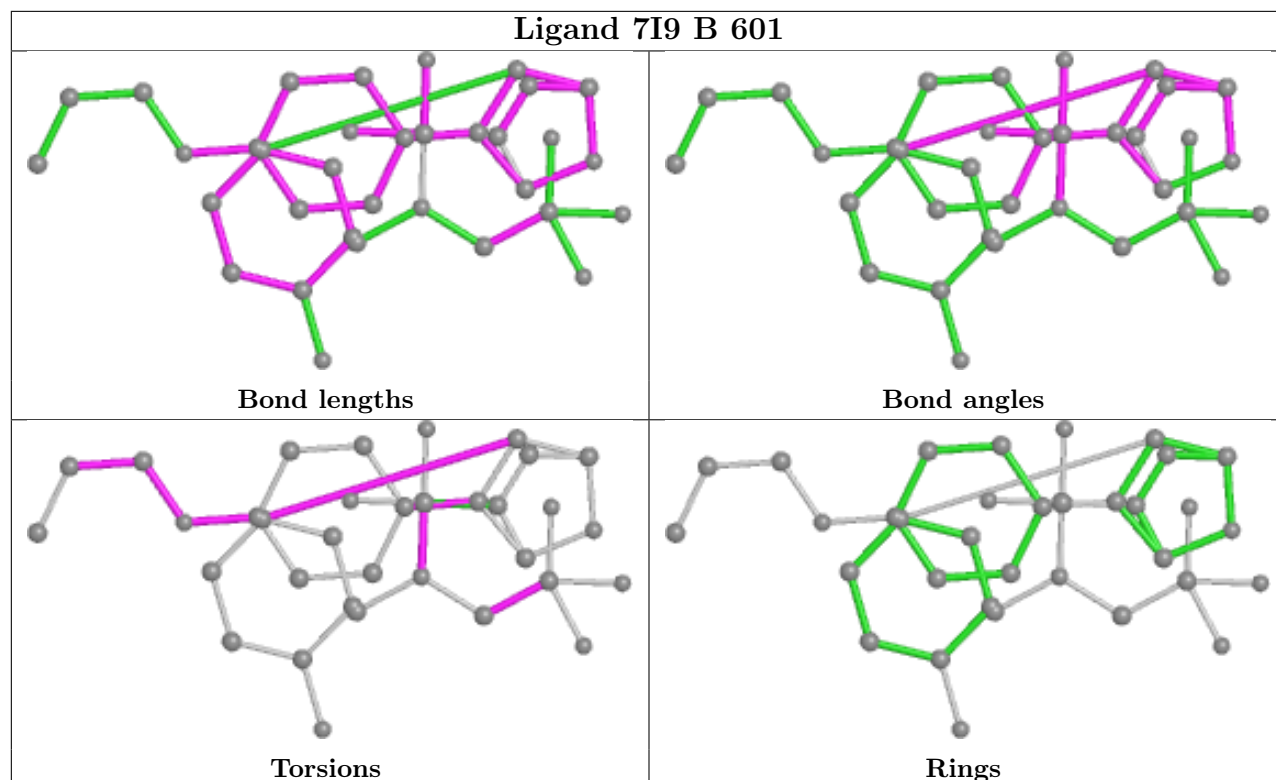
There are no ring outliers.

4 monomers are involved in 24 short contacts:

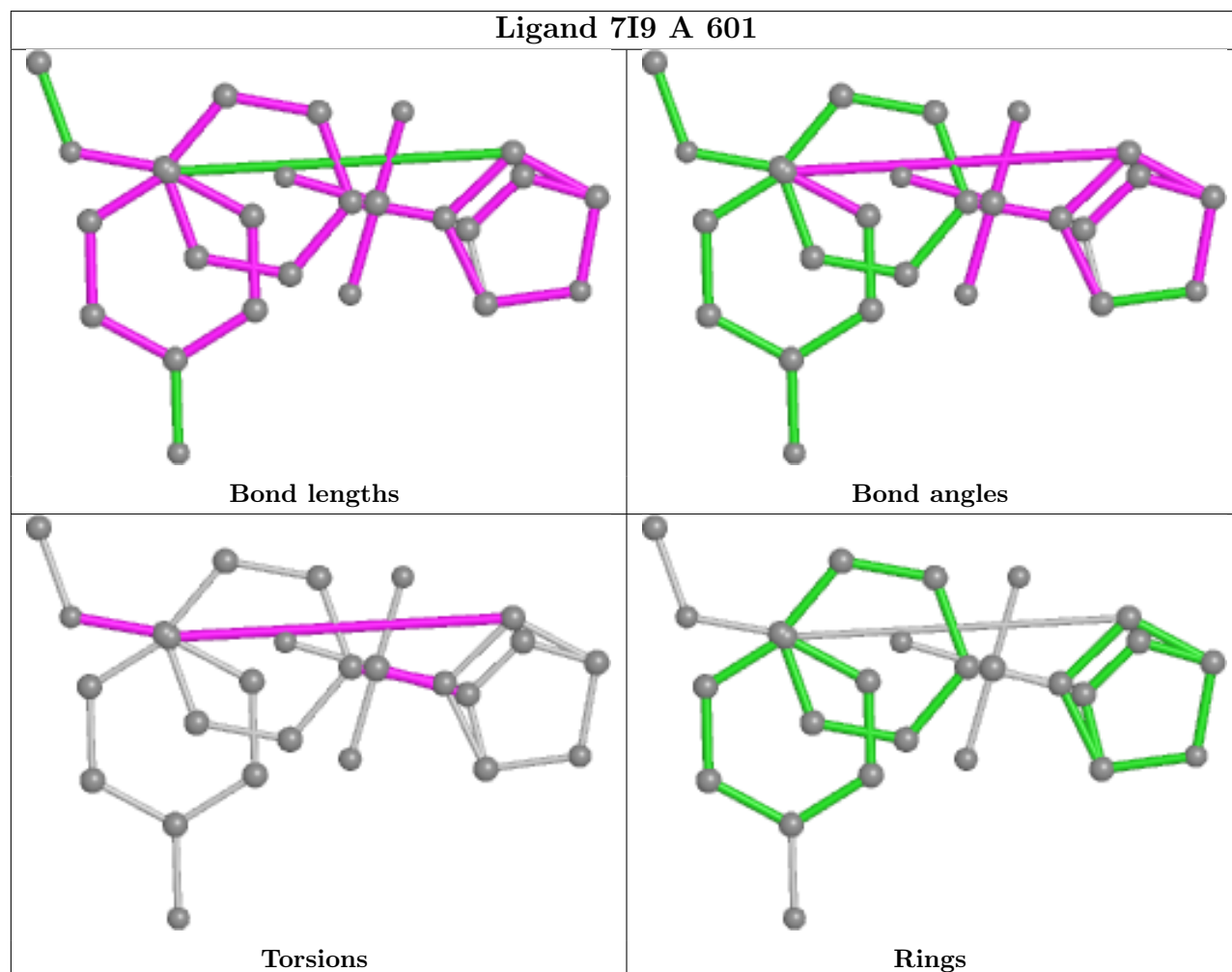
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	7I9	7	0
2	A	601	7I9	6	0
2	D	601	7I9	5	0
2	C	601	7I9	6	0

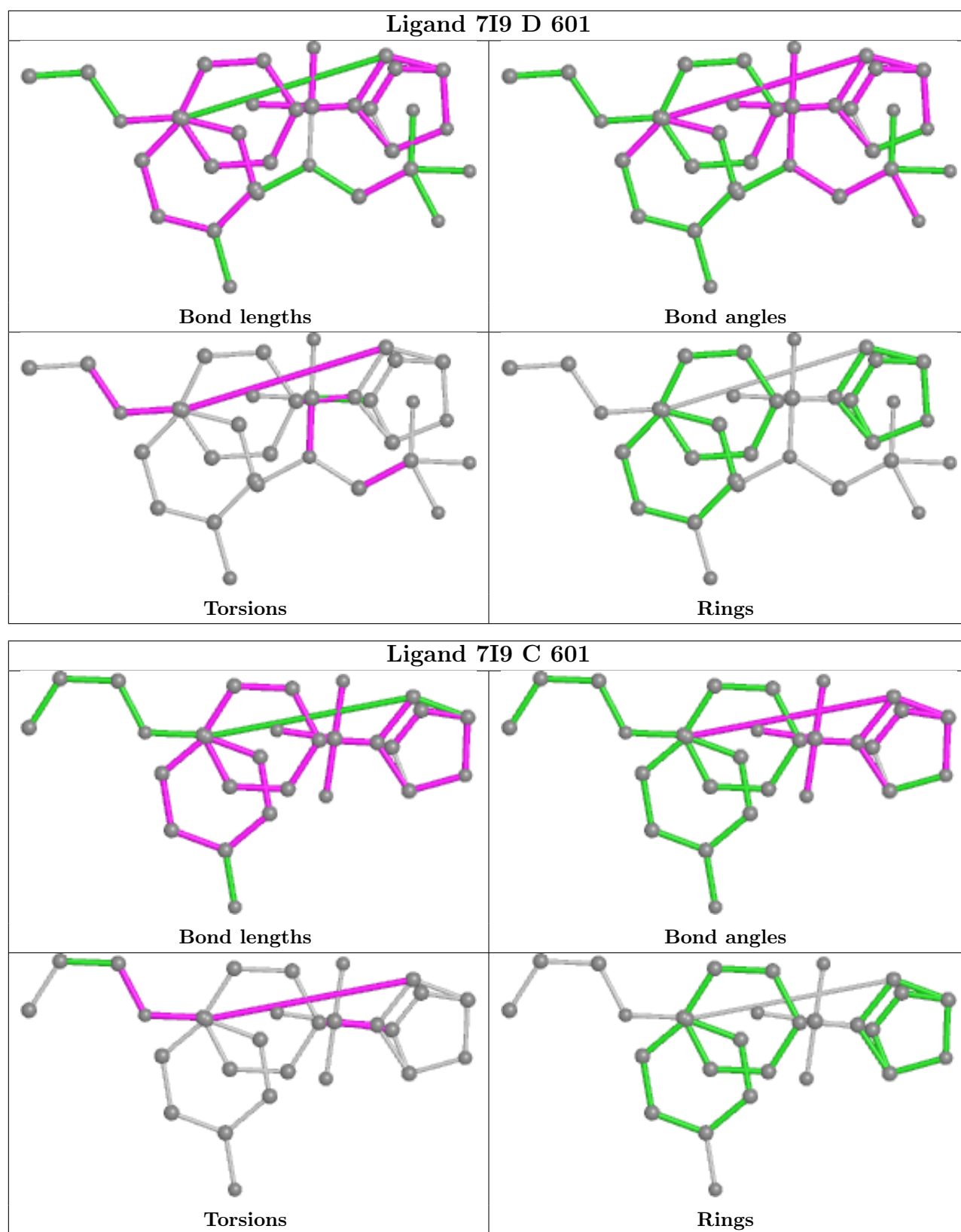
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 7I9 B 601



Ligand 7I9 A 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	241/257 (93%)	0.53	18 (7%) 14 15	18, 42, 85, 131	0
1	B	220/257 (85%)	0.13	6 (2%) 54 57	18, 36, 78, 104	0
1	C	235/257 (91%)	0.37	13 (5%) 25 26	18, 36, 69, 106	0
1	D	209/257 (81%)	0.16	4 (1%) 66 70	19, 36, 75, 91	0
All	All	905/1028 (88%)	0.30	41 (4%) 33 35	18, 38, 78, 131	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	SER	8.8
1	C	305	SER	8.5
1	A	530	CYS	8.2
1	A	462	LEU	6.4
1	A	333	PRO	5.9
1	B	306	LEU	5.5
1	A	531	LYS	5.3
1	D	461	PHE	4.8
1	C	462	LEU	4.7
1	C	464	SER	4.7
1	C	527	SER	4.6
1	A	306	LEU	4.5
1	B	421	MET	4.2
1	D	469	LEU	4.2
1	A	334	THR	4.1
1	A	307	ALA	4.0
1	C	306	LEU	3.8
1	A	525	LEU	3.7
1	A	529	LYS	3.7
1	D	305	SER	3.4
1	A	332	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	309	SER	3.3
1	B	462	LEU	3.2
1	A	416	LYS	3.1
1	A	494	GLY	3.0
1	C	524	HIS	3.0
1	A	528	MET	2.9
1	A	464	SER	2.7
1	C	417	CYS	2.7
1	A	532	ASN	2.7
1	B	420	GLY	2.5
1	C	463	SER	2.4
1	A	418	VAL	2.4
1	C	307	ALA	2.3
1	D	473	ASP	2.3
1	B	546	ALA	2.2
1	C	418	VAL	2.1
1	B	524	HIS	2.1
1	C	397[A]	GLU	2.1
1	A	526	TYR	2.0
1	C	473	ASP	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, 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
1	YCM	A	381	10/11	0.96	0.12	20,26,49,70	0
1	YCM	C	381	10/11	0.97	0.10	21,26,55,72	0
1	YCM	D	381	10/11	0.97	0.11	28,31,70,75	0
1	YCM	B	381	10/11	0.98	0.09	23,27,55,74	0

6.3 Carbohydrates [i](#)

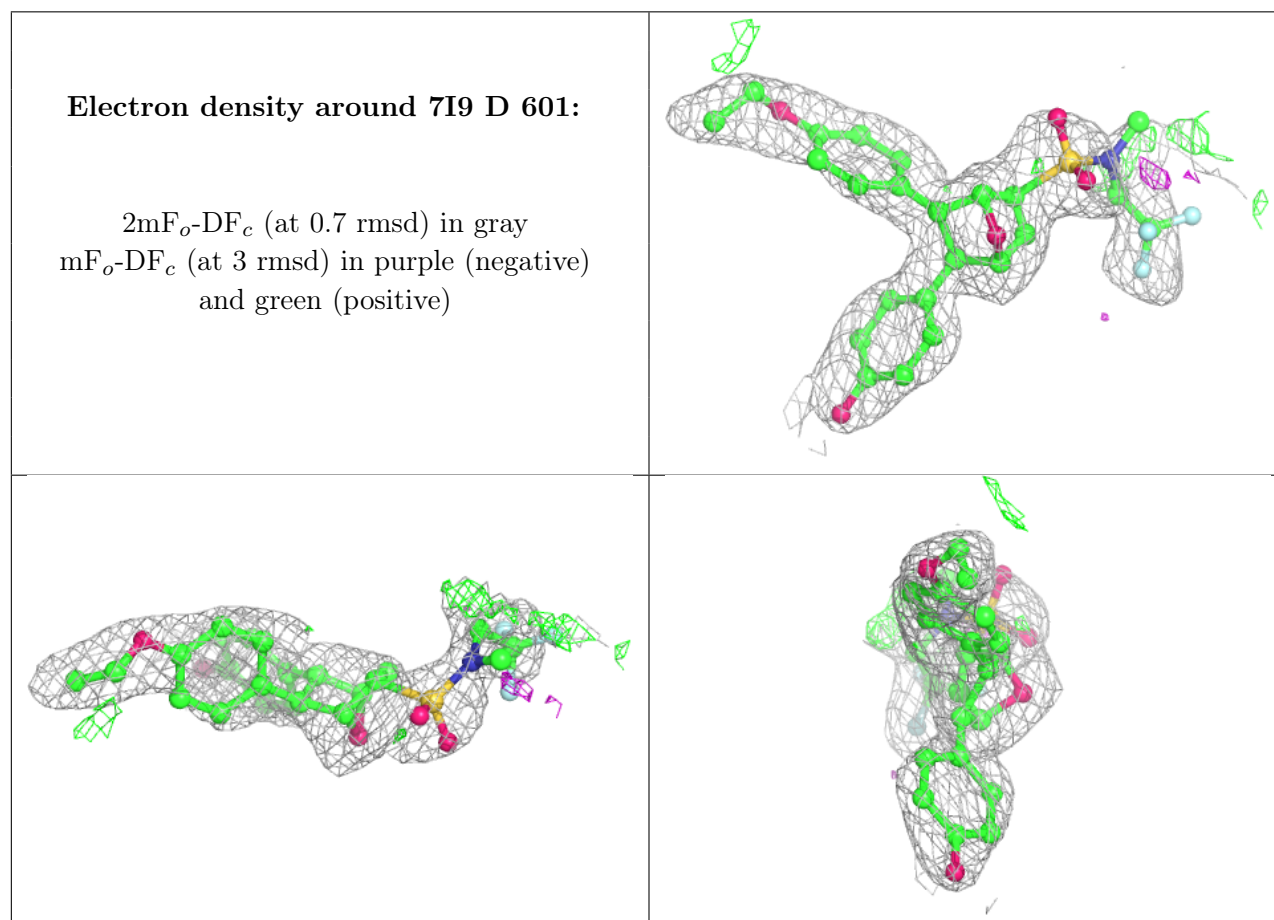
There are no monosaccharides in this entry.

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, 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.

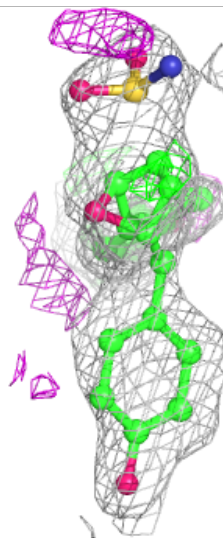
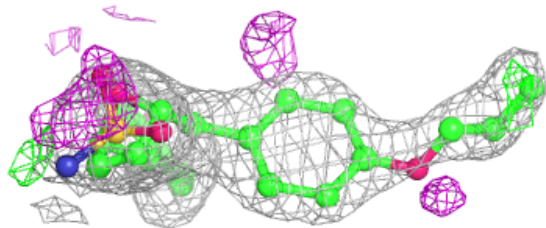
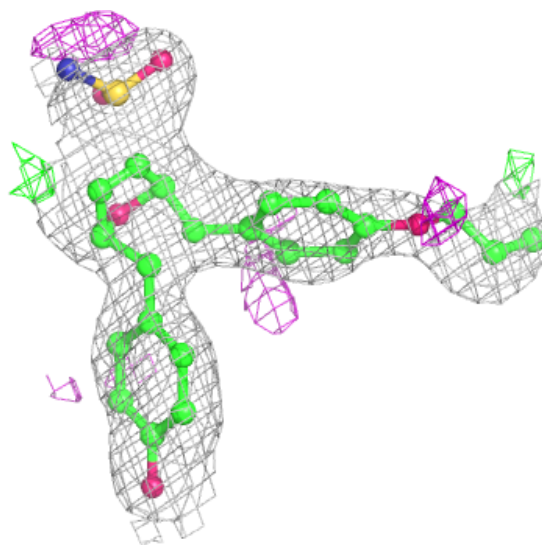
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	7I9	D	601	33/48	0.84	0.18	38,68,108,119	0
2	7I9	C	601	28/48	0.86	0.15	34,59,83,90	0
2	7I9	A	601	26/48	0.87	0.14	31,52,77,94	0
2	7I9	B	601	34/48	0.88	0.16	38,68,131,181	0

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.



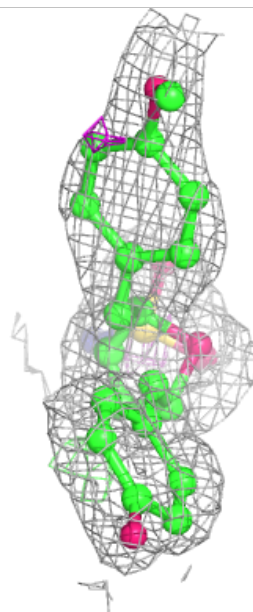
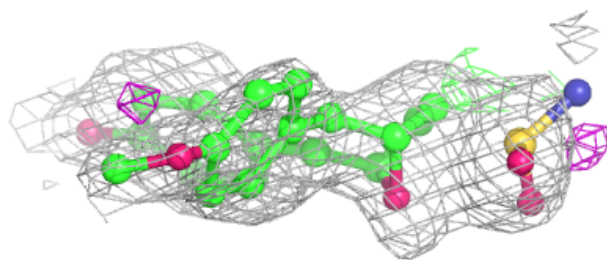
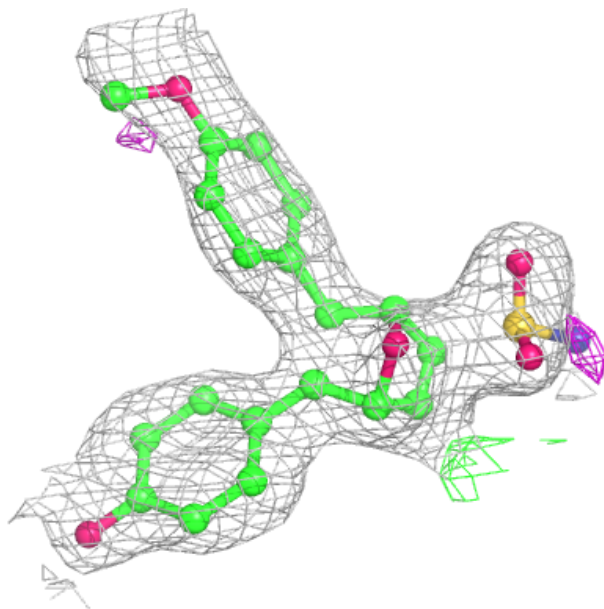
Electron density around 7I9 C 601:

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



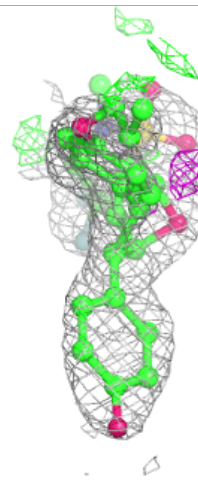
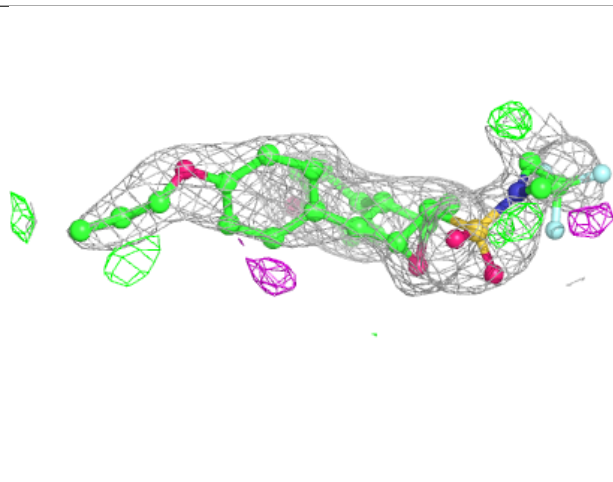
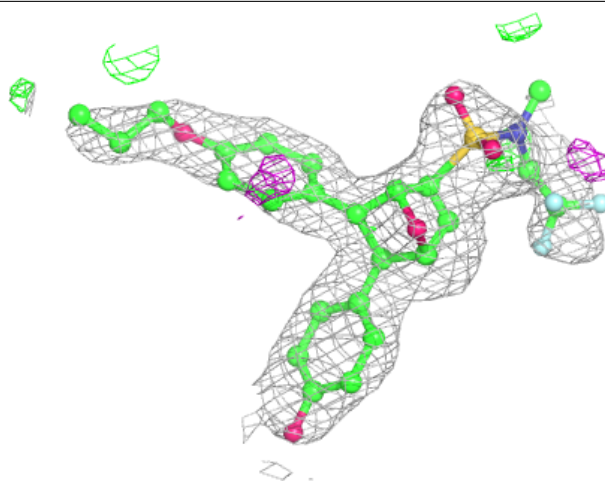
Electron density around 7I9 A 601:

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



Electron density around 7I9 B 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.