wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 10:40 PM EDT

PDB ID	:	7RRY
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-20
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	:	1.87 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

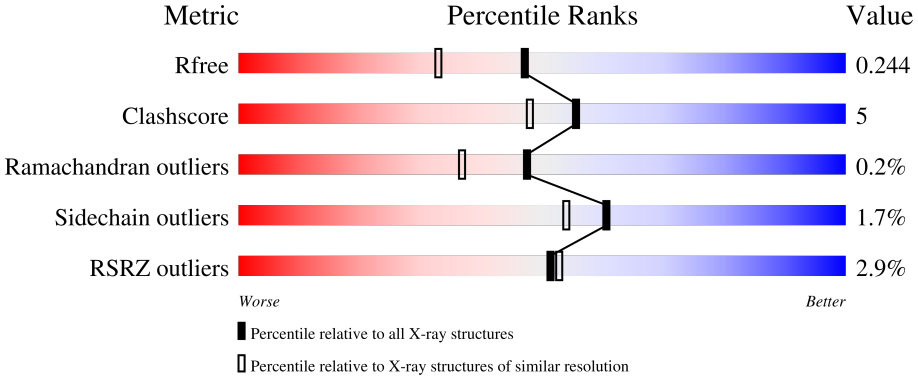
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	2%, 84%, 7%, 9%
1	B	257	3%, 79%, 5%, 14%
1	C	257	2%, 79%, 9%, 12%
1	D	257	4%, 73%, 8%, 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7470 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

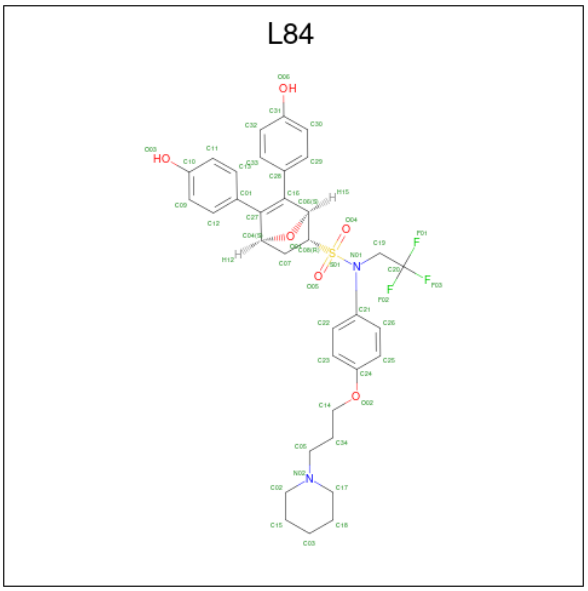
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1843	1176	321	329	17	0	2	0
1	B	221	1758	1128	304	310	16	0	2	0
1	C	227	1834	1173	321	323	17	0	4	0
1	D	209	1639	1050	280	293	16	0	0	0

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 (1S,2R,4S,5S,6S)-5,6-bis(4-hydroxyphenyl)-N-{4-[3-(piperidin-1-yl)propoxy]phenyl}-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]heptane-2-sulfonamide (three-letter code: L84) (formula: $C_{34}H_{37}F_3N_2O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	46	34	3	2	6	1	0	0
2	B	1	37	26	3	1	6	1	0	0
2	C	1	46	34	3	2	6	1	0	0
2	D	1	46	34	3	2	6	1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	B	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	54	54	54	0	0
4	B	55	55	55	0	0
4	C	65	65	65	0	0

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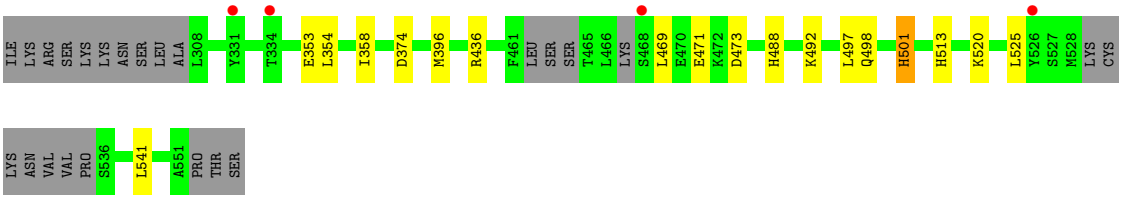
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	45	45	45	0	0

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.

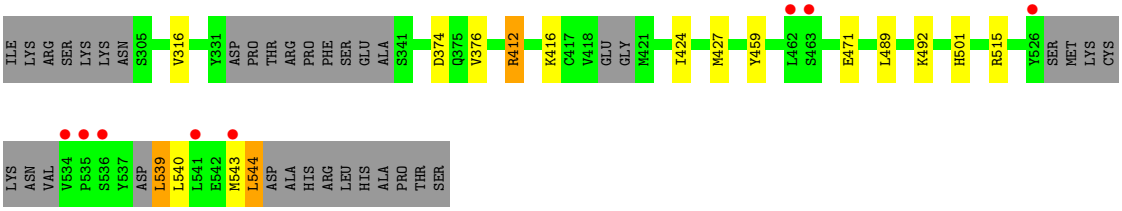
• Molecule 1: Estrogen receptor

Chain A:



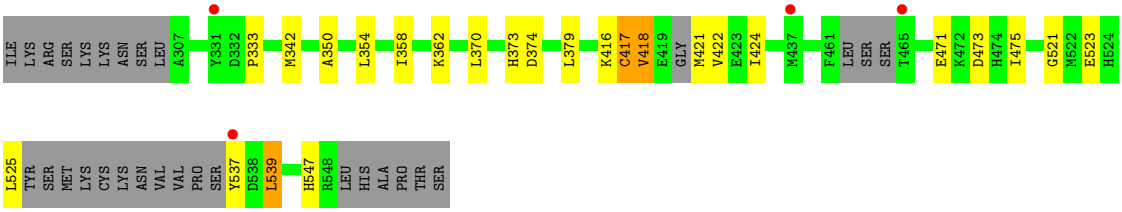
• Molecule 1: Estrogen receptor

Chain B:



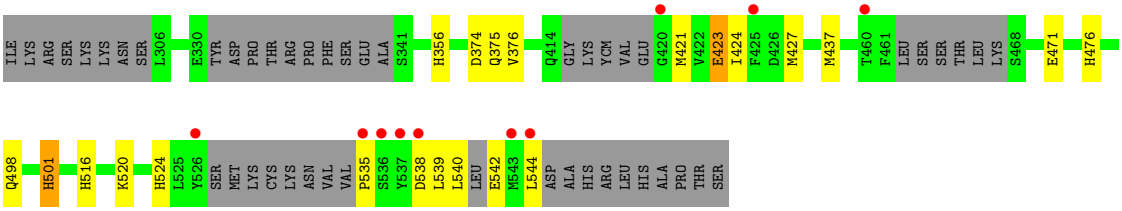
• Molecule 1: Estrogen receptor

Chain C:



• Molecule 1: Estrogen receptor

Chain D:


ILE LYS ARG SER LYS LYS ASN SER L306 E330 TYR ASP PRO THR ARG PRO PHE SER GLU ALA S341 H356 D374 Q375 V376 Q414 GLY LYS YCM VAL GLU G420 M421 V422 E423 I424 F425 D426 M427 M437 T460 F461 LEU SER SER THR LEU LYS S468 E471 H476
Q498 H501 H516 K520 H524 L525 Y526 SER MET LYS CYS LYS ASN VAL VAL P535 S536 Y537 D538 L539 L540 LEU E542 M543 L544 ASP ALA HIS ARG LEU HIS ALA PRO THR SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.42Å 59.12Å 93.52Å 86.54° 74.98° 63.19°	Depositor
Resolution (Å)	90.13 – 1.87 90.13 – 1.87	Depositor EDS
% Data completeness (in resolution range)	76.0 (90.13-1.87) 76.0 (90.13-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.207 , 0.236 0.218 , 0.244	Depositor DCC
R_{free} test set	3095 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.109 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7470	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, YCM, L84

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	0.71	0/1854	0.75	0/2502
1	B	0.72	0/1770	0.77	0/2385
1	C	0.71	0/1846	0.76	0/2490
1	D	0.75	0/1652	0.76	0/2227
All	All	0.72	0/7122	0.76	0/9604

There are no bond length outliers.

There are no bond angle outliers.

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	1843	0	1833	19	0
1	B	1758	0	1780	17	0
1	C	1834	0	1831	29	0
1	D	1639	0	1657	17	0
2	A	46	0	0	1	0
2	B	37	0	0	0	0
2	C	46	0	0	0	0
2	D	46	0	0	2	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	54	0	0	2	0
4	B	55	0	0	0	0
4	C	65	0	0	1	0
4	D	45	0	0	1	0
All	All	7470	0	7101	73	0

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.

The worst 5 of 73 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:C:539:LEU:H	1:C:539:LEU:HD12	1.23	1.04
1:D:374:ASP:OD2	1:D:471:GLU:OE1	1.78	1.01
1:A:501[A]:HIS:NE2	1:B:501:HIS:HE1	1.65	0.94
1:C:539:LEU:H	1:C:539:LEU:CD1	1.93	0.82
1:A:501[A]:HIS:CD2	1:B:501:HIS:CE1	2.69	0.80

There are no symmetry-related clashes.

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	225/257 (88%)	223 (99%)	2 (1%)	0	100	100
1	B	211/257 (82%)	209 (99%)	1 (0%)	1 (0%)	29	17
1	C	221/257 (86%)	218 (99%)	2 (1%)	1 (0%)	29	17
1	D	196/257 (76%)	195 (100%)	1 (0%)	0	100	100
All	All	853/1028 (83%)	845 (99%)	6 (1%)	2 (0%)	47	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	416	LYS
1	C	418	VAL

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	196/230 (85%)	191 (97%)	5 (3%)	46	36
1	B	191/230 (83%)	187 (98%)	4 (2%)	53	45
1	C	195/230 (85%)	193 (99%)	2 (1%)	76	73
1	D	178/230 (77%)	175 (98%)	3 (2%)	60	54
All	All	760/920 (83%)	746 (98%)	14 (2%)	60	52

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	539	LEU
1	B	544	LEU
1	D	501	HIS
1	D	423	GLU
1	D	437	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	356	HIS
1	D	398	HIS
1	D	524	HIS
1	D	516	HIS
1	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)

7 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	A	381	1	7,9,10	0.49	0	4,10,12	0.50	0
1	YCM	D	381	1	7,9,10	0.40	0	4,10,12	0.41	0
1	YCM	C	417	1	7,9,10	1.17	1 (14%)	4,10,12	1.48	1 (25%)
1	YCM	C	381	1	7,9,10	0.46	0	4,10,12	0.54	0
1	YCM	B	417	1	3,4,10	0.91	0	2,4,12	1.46	0
1	YCM	A	417	1	7,9,10	0.47	0	4,10,12	0.61	0
1	YCM	B	381	1	7,9,10	0.49	0	4,10,12	0.44	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	A	381	1	-	1/6/8/10	-
1	YCM	D	381	1	-	1/6/8/10	-
1	YCM	C	417	1	-	4/6/8/10	-
1	YCM	C	381	1	-	1/6/8/10	-
1	YCM	B	417	1	-	0/0/2/10	-
1	YCM	A	417	1	-	4/6/8/10	-
1	YCM	B	381	1	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	417	YCM	CD-SG	-2.21	1.75	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	417	YCM	CE-CD-SG	-2.39	106.56	113.59

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381	YCM	SG-CD-CE-NZ2
1	A	417	YCM	CE-CD-SG-CB
1	A	417	YCM	SG-CD-CE-OZ1
1	A	417	YCM	SG-CD-CE-NZ2
1	B	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	C	417	YCM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	L84	A	601	-	48,51,51	2.38	13 (27%)	62,75,75	2.55	18 (29%)
2	L84	B	601	-	38,41,51	2.91	17 (44%)	50,63,75	2.78	16 (32%)
2	L84	D	601	-	48,51,51	2.41	15 (31%)	62,75,75	2.30	18 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	L84	C	601	-	48,51,51	2.50	15 (31%)	62,75,75	2.91	26 (41%)

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	L84	A	601	-	-	13/34/68/68	0/7/6/6
2	L84	B	601	-	-	7/27/53/68	0/6/5/6
2	L84	D	601	-	-	9/34/68/68	0/7/6/6
2	L84	C	601	-	-	15/34/68/68	0/7/6/6

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	L84	C21-N01	-9.29	1.31	1.44
2	D	601	L84	C21-N01	-9.11	1.32	1.44
2	C	601	L84	C21-N01	-8.81	1.32	1.44
2	A	601	L84	C21-N01	-8.50	1.32	1.44
2	B	601	L84	C28-C16	-6.79	1.35	1.48

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	L84	C20-C19-N01	14.09	125.83	112.14
2	A	601	L84	C20-C19-N01	12.10	123.89	112.14
2	B	601	L84	C20-C19-N01	10.32	122.17	112.14
2	D	601	L84	C20-C19-N01	9.30	121.18	112.14
2	B	601	L84	O05-S01-N01	-7.98	97.78	107.56

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	L84	N01-C19-C20-F01
2	A	601	L84	N01-C19-C20-F02
2	A	601	L84	N01-C19-C20-F03
2	A	601	L84	C20-C19-N01-C21
2	A	601	L84	C20-C19-N01-S01

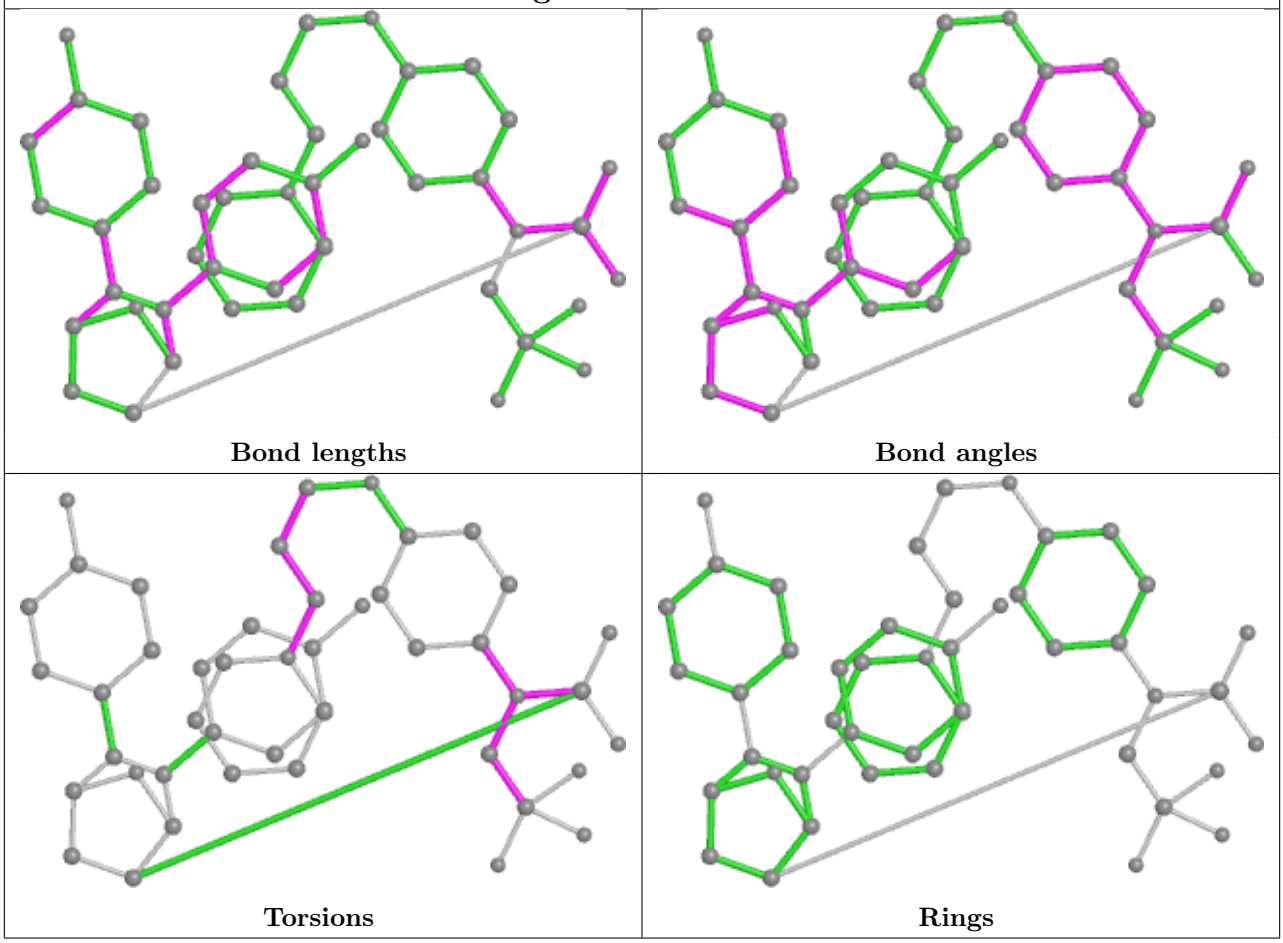
There are no ring outliers.

2 monomers are involved in 3 short contacts:

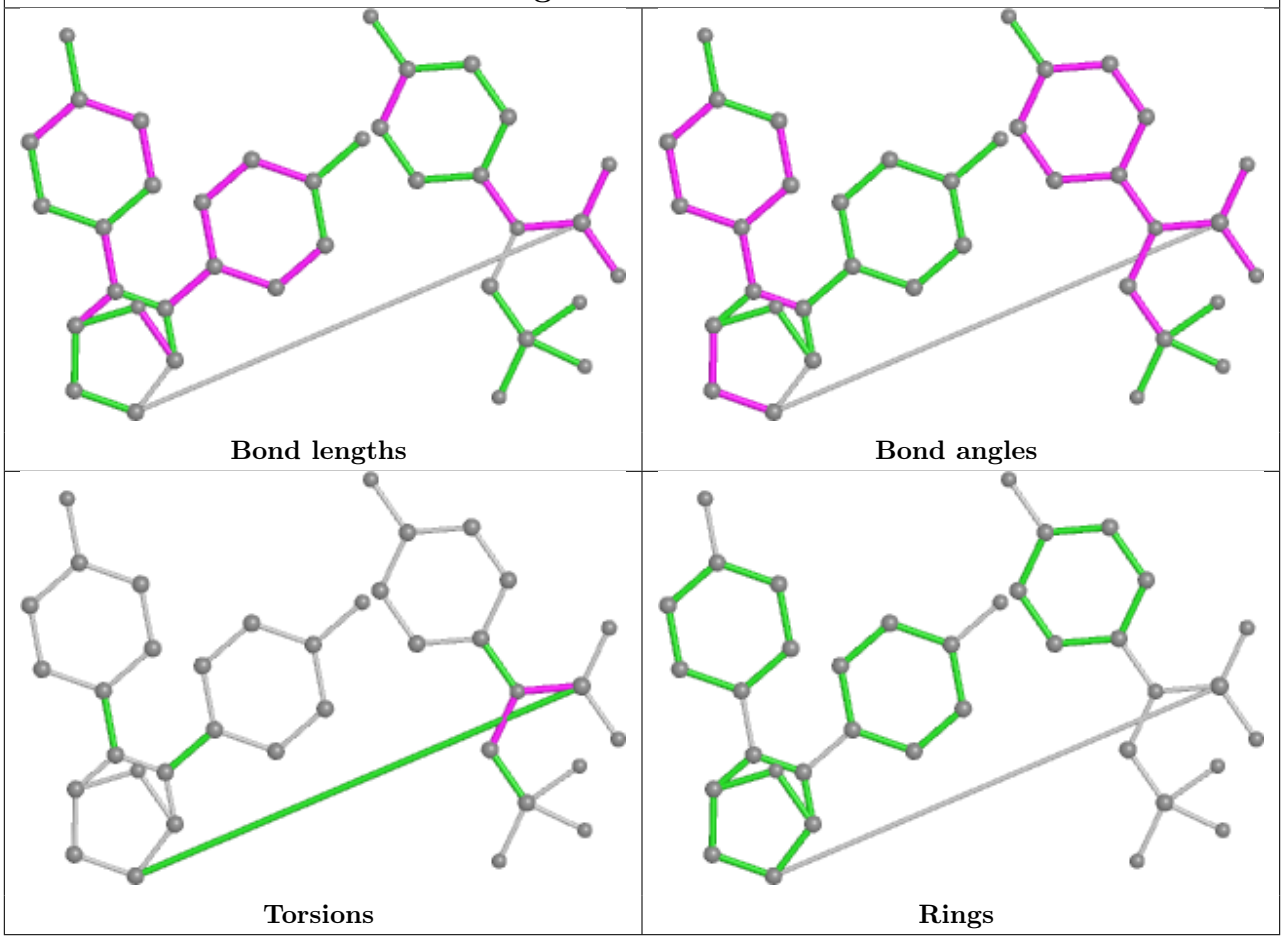
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	L84	1	0
2	D	601	L84	2	0

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 then 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.

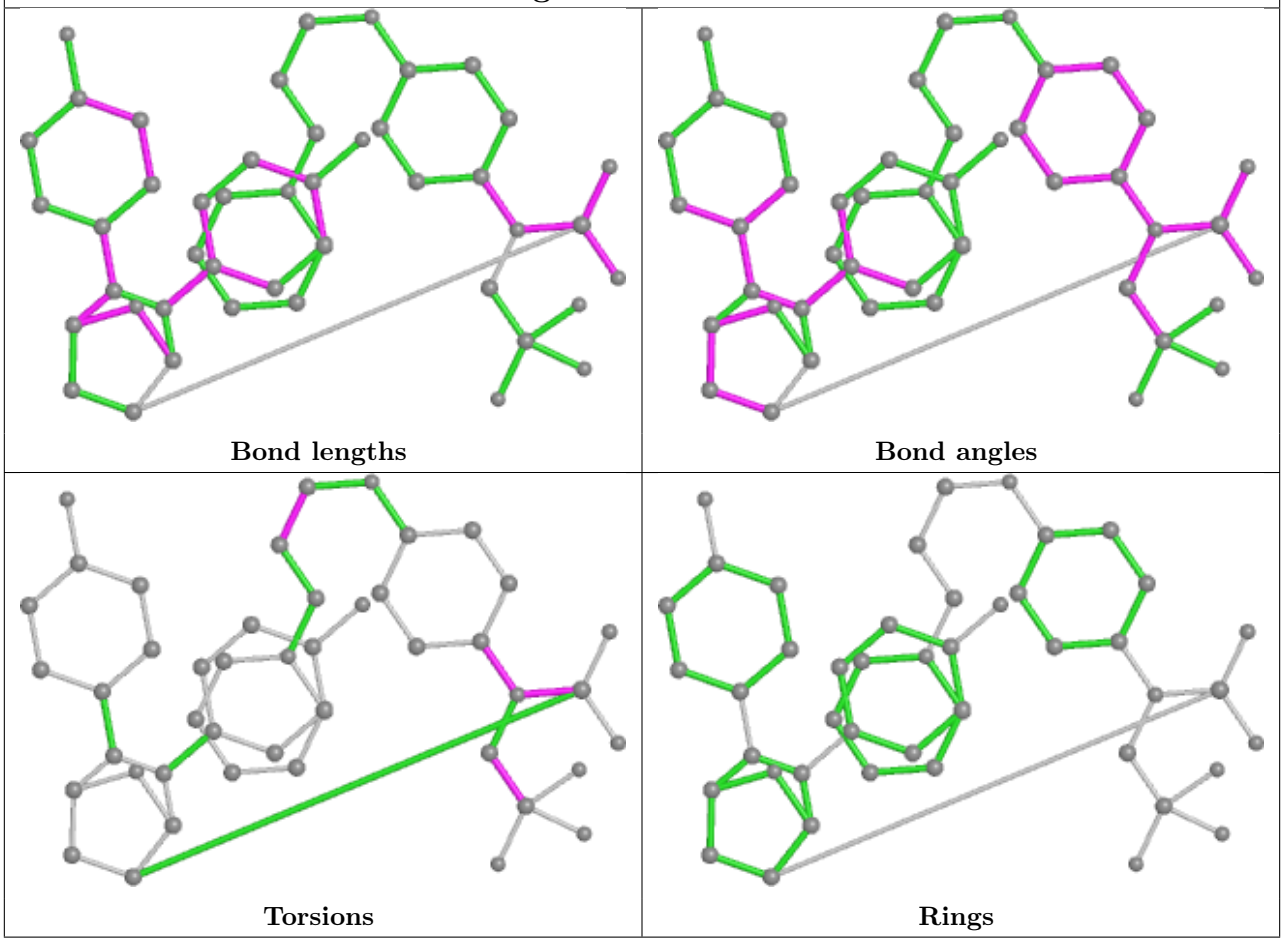
Ligand L84 A 601



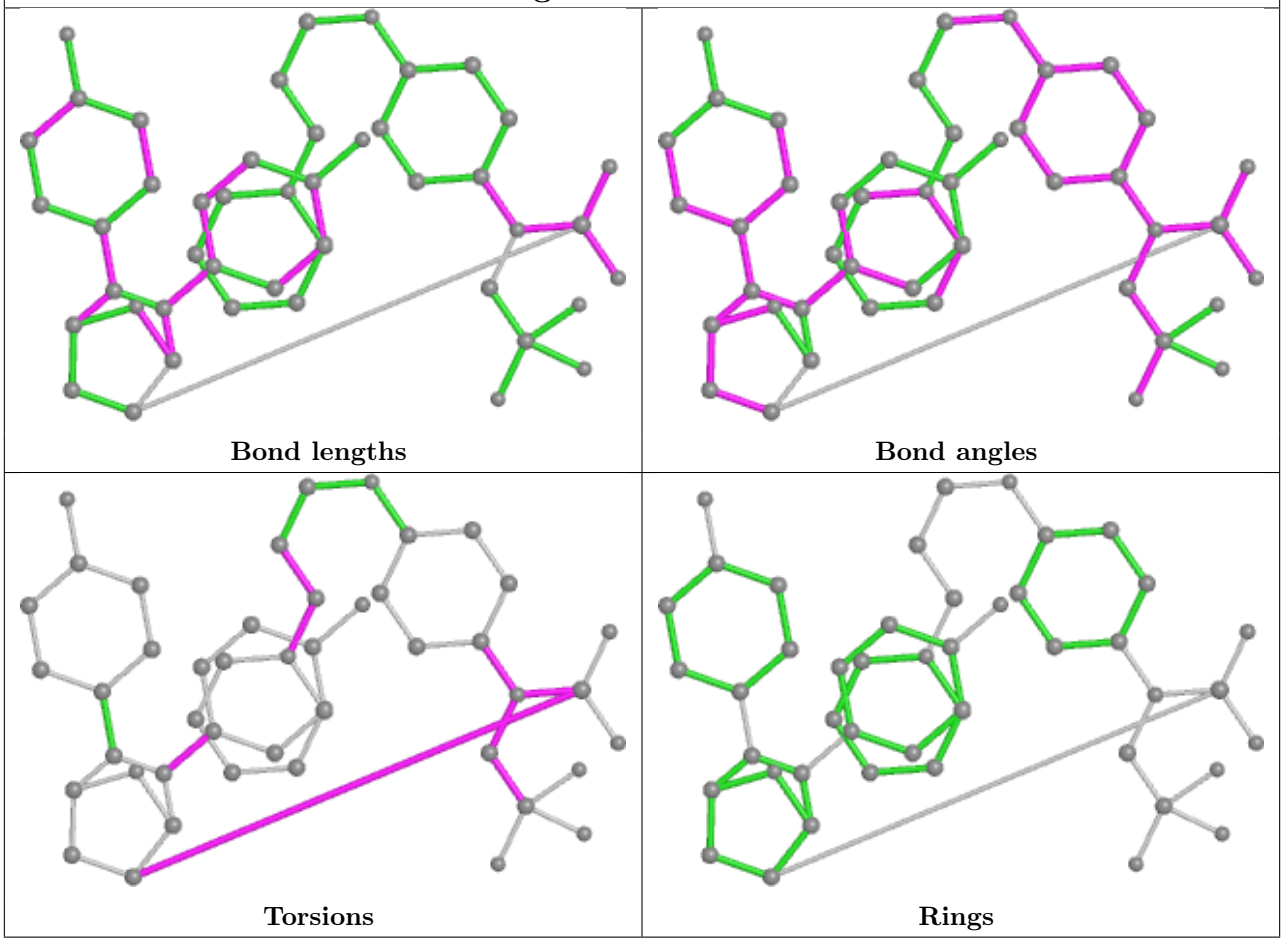
Ligand L84 B 601



Ligand L84 D 601



Ligand L84 C 601



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, 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	231/257 (89%)	0.13	4 (1%)	70	72	24, 44, 75, 110	0
1	B	219/257 (85%)	0.08	8 (3%)	41	43	23, 40, 78, 97	0
1	C	225/257 (87%)	0.04	4 (1%)	68	70	23, 39, 70, 97	0
1	D	208/257 (80%)	0.10	10 (4%)	30	32	24, 39, 75, 94	0
All	All	883/1028 (85%)	0.09	26 (2%)	51	53	23, 41, 75, 110	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	544	LEU	6.2
1	B	536	SER	3.8
1	B	535	PRO	3.4
1	D	536	SER	3.1
1	D	460	THR	3.0

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	417	10/11	0.89	0.16	77,85,91,92	0
1	YCM	C	417	10/11	0.89	0.14	70,74,82,88	0
1	YCM	B	417	5/11	0.94	0.10	97,101,102,104	0
1	YCM	D	381	10/11	0.94	0.17	34,39,68,69	0
1	YCM	A	381	10/11	0.95	0.12	27,32,64,76	0
1	YCM	B	381	10/11	0.96	0.14	27,32,64,73	0
1	YCM	C	381	10/11	0.96	0.10	25,30,51,58	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

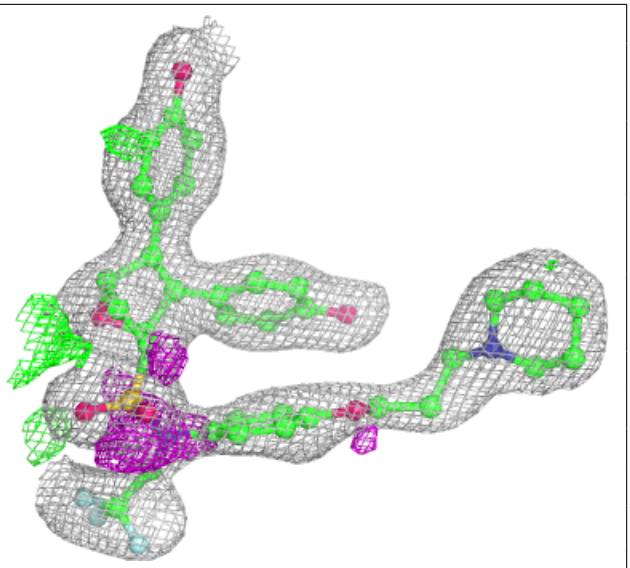
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

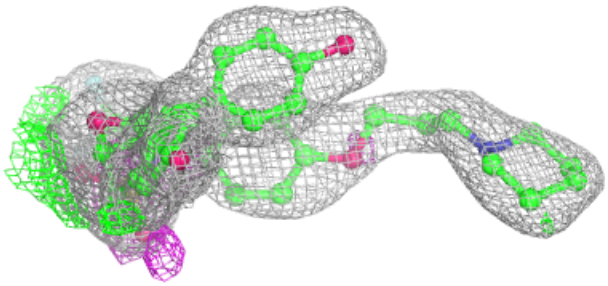
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	L84	A	601	46/46	0.91	0.13	23,46,84,92	0
2	L84	B	601	37/46	0.92	0.13	30,39,77,85	0
2	L84	C	601	46/46	0.93	0.15	24,49,81,88	0
2	L84	D	601	46/46	0.94	0.15	27,50,91,101	0
3	CL	B	602	1/1	0.98	0.09	34,34,34,34	0
3	CL	C	602	1/1	0.99	0.10	34,34,34,34	0

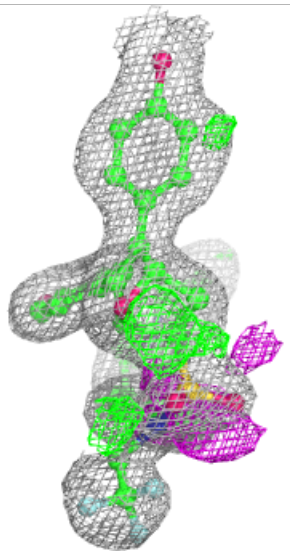
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L84 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)

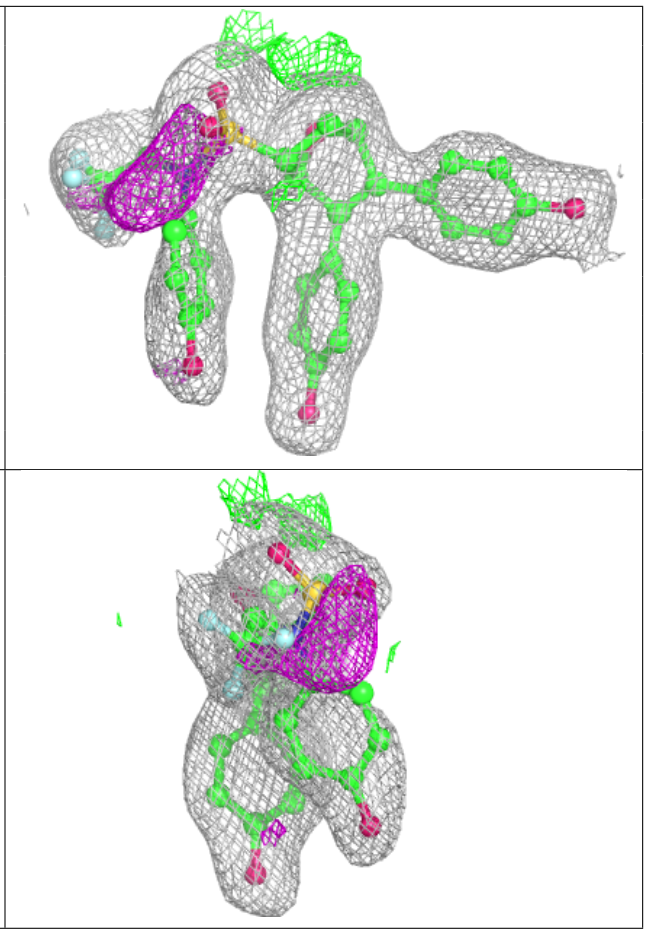


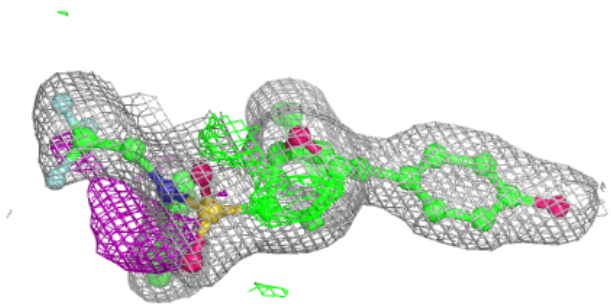




Electron density around L84 B 601:

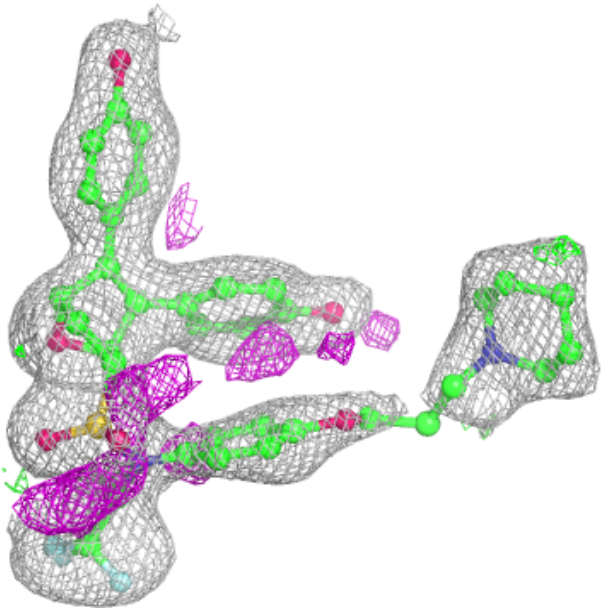
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

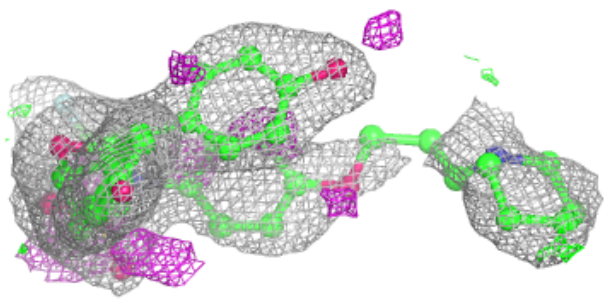


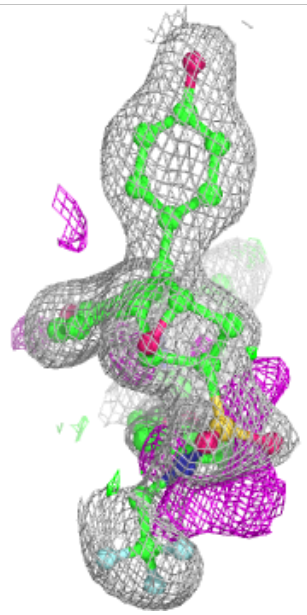


Electron density around L84 C 601:

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

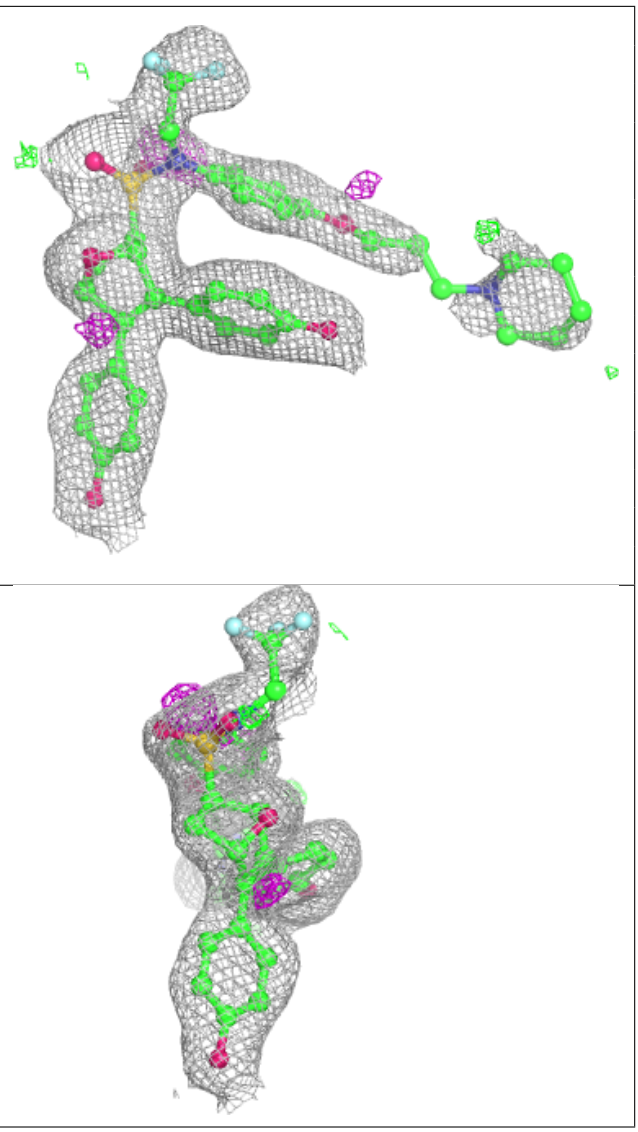






Electron density around L84 D 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.