



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2020 – 02:08 PM JST

PDB ID : 6L8L
Title : C-Src in complex with ibrutinib
Authors : Guo, M.; Dai, S.; Chen, L.; Chen, Y.
Deposited on : 2019-11-06
Resolution : 2.89 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 ⓘ 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 : 2.14.6
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) : 2.14.6

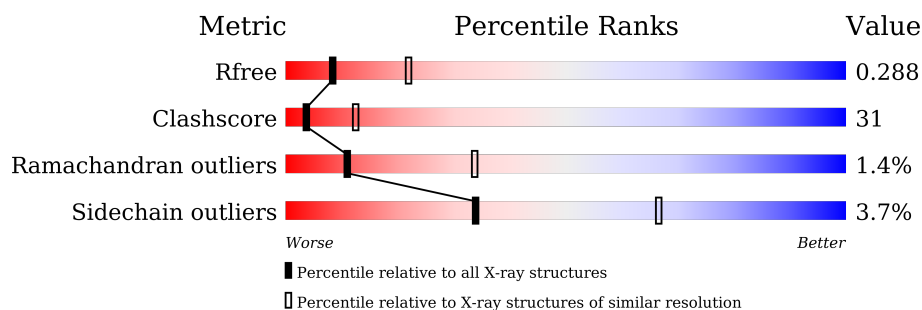
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	286	<div> <div>59%</div> <div>29%</div> <div>• 10%</div> </div>
1	B	286	<div> <div>60%</div> <div>27%</div> <div>•• 10%</div> </div>
1	C	286	<div> <div>65%</div> <div>22%</div> <div>• 10%</div> </div>
1	D	286	<div> <div>57%</div> <div>29%</div> <div>• 10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	1E8	A	600	-	-	X	-
2	1E8	B	600	-	-	X	-
2	1E8	C	600	-	-	X	-
2	1E8	D	600	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8393 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.

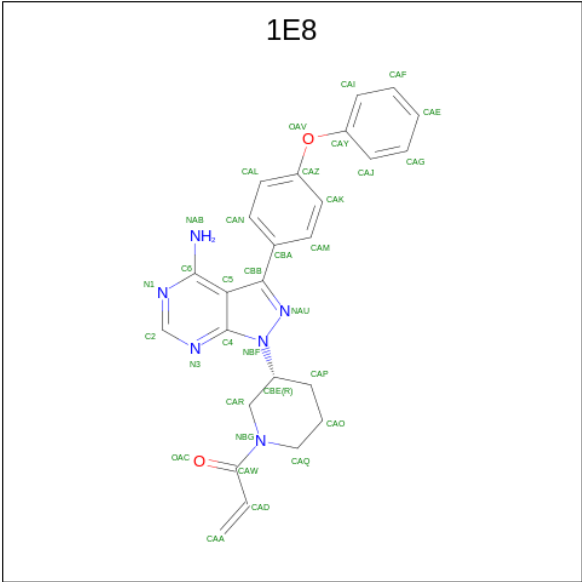
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2074	1331	348	378	17			
1	B	256	Total	C	N	O	S	0	0	0
			2055	1319	343	376	17			
1	C	258	Total	C	N	O	S	0	0	0
			2072	1330	345	380	17			
1	D	256	Total	C	N	O	S	0	0	0
			2050	1318	343	372	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523
C	248	GLY	-	expression tag	UNP P00523
C	249	HIS	-	expression tag	UNP P00523
C	250	MET	-	expression tag	UNP P00523
D	248	GLY	-	expression tag	UNP P00523
D	249	HIS	-	expression tag	UNP P00523
D	250	MET	-	expression tag	UNP P00523

- Molecule 2 is 1-((3R)-3-[4-amino-3-(4-phenoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]piperidin-1-yl)prop-2-en-1-one (three-letter code: 1E8) (formula: C₂₅H₂₄N₆O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	25	6	2		
2	B	1	Total	C	N	O	0	0
			33	25	6	2		
2	C	1	Total	C	N	O	0	0
			33	25	6	2		
2	D	1	Total	C	N	O	0	0
			33	25	6	2		

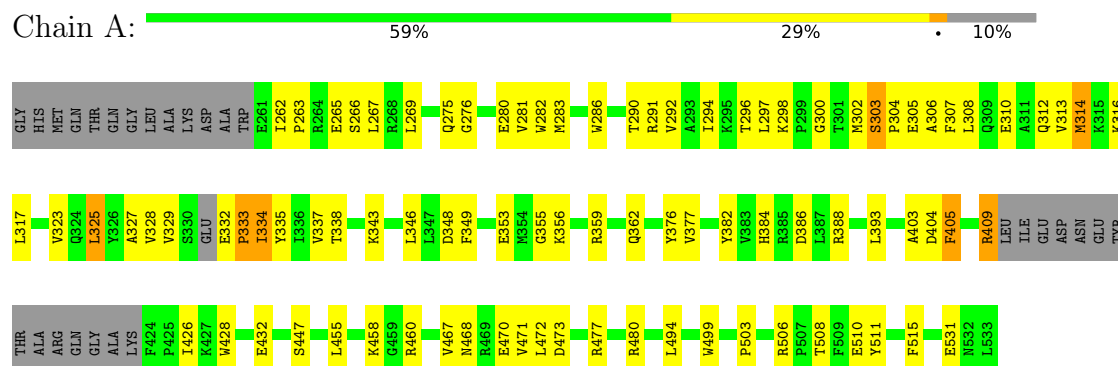
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	C	3	Total	O	0	0
			3	3		
3	D	5	Total	O	0	0
			5	5		

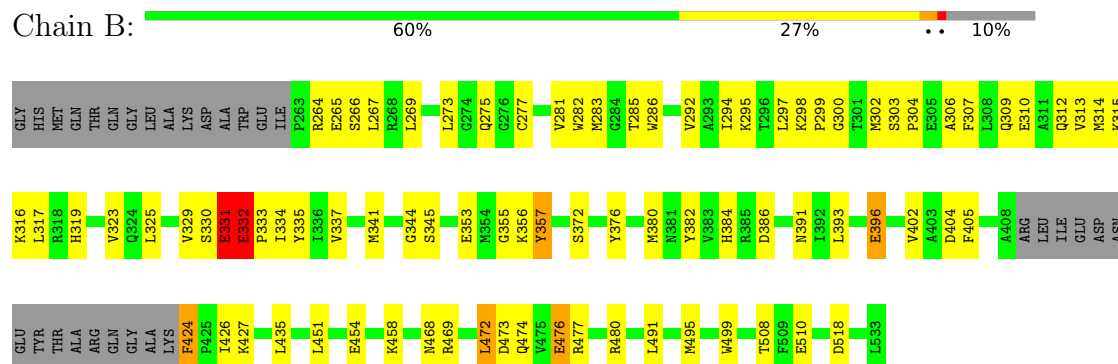
3 Residue-property plots

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. 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. 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.

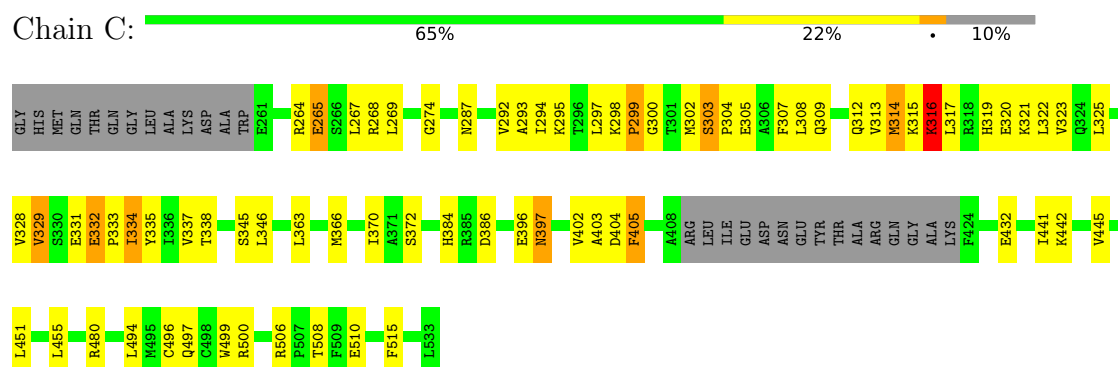
- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



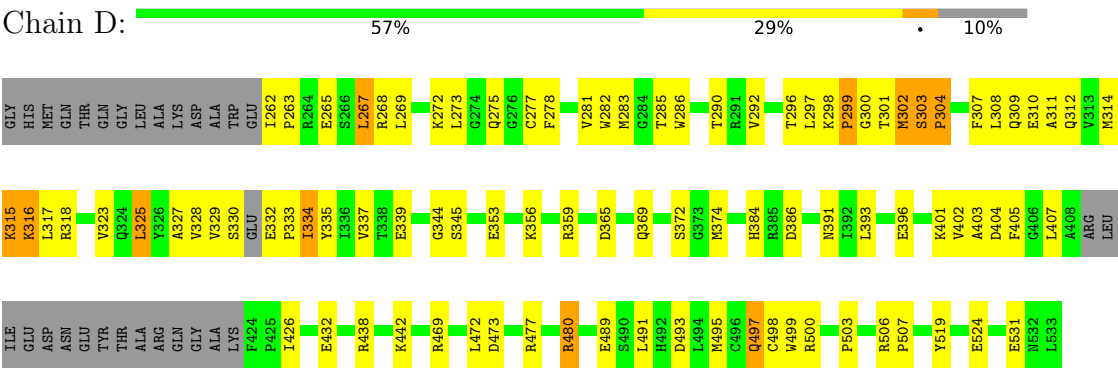
- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



● Molecule 1: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.60Å 63.41Å 113.92Å 89.97° 89.94° 90.03°	Depositor
Resolution (Å)	42.38 – 2.89 42.38 – 2.89	Depositor EDS
% Data completeness (in resolution range)	95.0 (42.38-2.89) 94.7 (42.38-2.89)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.77 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.238 , 0.286 0.246 , 0.288	Depositor DCC
R_{free} test set	1390 reflections (5.47%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.409 for h,-k,-l 0.408 for -h,k,-l 0.460 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8393	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1E8

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	0.51	1/2123 (0.0%)	0.71	0/2871
1	B	0.54	0/2105	0.71	0/2848
1	C	0.55	1/2122 (0.0%)	0.66	0/2872
1	D	0.52	0/2099	0.70	0/2840
All	All	0.53	2/8449 (0.0%)	0.70	0/11431

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	PRO	C-N	-5.60	1.21	1.34
1	C	329	VAL	C-N	5.20	1.46	1.34

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	2074	0	2067	139	0
1	B	2055	0	2046	156	0
1	C	2072	0	2062	98	0
1	D	2050	0	2045	123	0
2	A	33	0	24	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	33	0	24	28	0
2	C	33	0	24	26	0
2	D	33	0	24	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	2	0
All	All	8393	0	8316	522	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 31.

The worst 5 of 522 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:332:GLU:HB3	1:A:333:PRO:CD	1.35	1.45
1:C:274:GLY:HA3	2:C:600:1E8:CAD	1.51	1.36
1:C:298:LYS:CG	1:C:299:PRO:HD2	1.58	1.34
1:C:302:MET:CE	1:C:334:ILE:HG21	1.64	1.28
1:B:304:PRO:CB	1:B:331:GLU:HB2	1.67	1.24

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	252/286 (88%)	237 (94%)	14 (6%)	1 (0%)	34	64
1	B	252/286 (88%)	232 (92%)	18 (7%)	2 (1%)	19	48
1	C	254/286 (89%)	232 (91%)	16 (6%)	6 (2%)	6	20
1	D	250/286 (87%)	229 (92%)	16 (6%)	5 (2%)	7	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1008/1144 (88%)	930 (92%)	64 (6%)	14 (1%)	11	34

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	304	PRO
1	B	331	GLU
1	C	265	GLU
1	C	316	LYS
1	C	334	ILE

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	224/245 (91%)	218 (97%)	6 (3%)	44	75
1	B	222/245 (91%)	209 (94%)	13 (6%)	19	47
1	C	224/245 (91%)	219 (98%)	5 (2%)	52	80
1	D	221/245 (90%)	212 (96%)	9 (4%)	30	62
All	All	891/980 (91%)	858 (96%)	33 (4%)	34	66

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	424	PHE
1	B	476	GLU
1	D	438	ARG
1	B	435	LEU
1	B	472	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	275	GLN
1	B	312	GLN
1	B	324	GLN
1	C	526	GLN
1	D	497	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1E8	A	600	-	35,37,37	1.99	9 (25%)	41,52,52	3.41	7 (17%)
2	1E8	B	600	-	35,37,37	1.99	9 (25%)	41,52,52	3.41	7 (17%)
2	1E8	C	600	-	35,37,37	1.99	9 (25%)	41,52,52	3.40	7 (17%)
2	1E8	D	600	-	35,37,37	1.99	9 (25%)	41,52,52	3.41	7 (17%)

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	1E8	A	600	-	-	3/14/28/28	0/5/5/5
2	1E8	B	600	-	-	2/14/28/28	0/5/5/5
2	1E8	C	600	-	-	4/14/28/28	0/5/5/5
2	1E8	D	600	-	-	4/14/28/28	0/5/5/5

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	1E8	CBE-NBF	-5.33	1.41	1.49
2	D	600	1E8	CBE-NBF	-5.29	1.41	1.49
2	C	600	1E8	CBE-NBF	-5.27	1.41	1.49
2	B	600	1E8	CBE-NBF	-5.24	1.41	1.49
2	A	600	1E8	CAA-CAD	4.74	1.53	1.30

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	1E8	C5-C6-NAB	14.05	148.04	122.67
2	B	600	1E8	C5-C6-NAB	14.04	148.03	122.67
2	A	600	1E8	C5-C6-NAB	14.04	148.03	122.67
2	D	600	1E8	C5-C6-NAB	14.04	148.03	122.67
2	B	600	1E8	NAB-C6-N1	-12.84	91.92	118.57

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

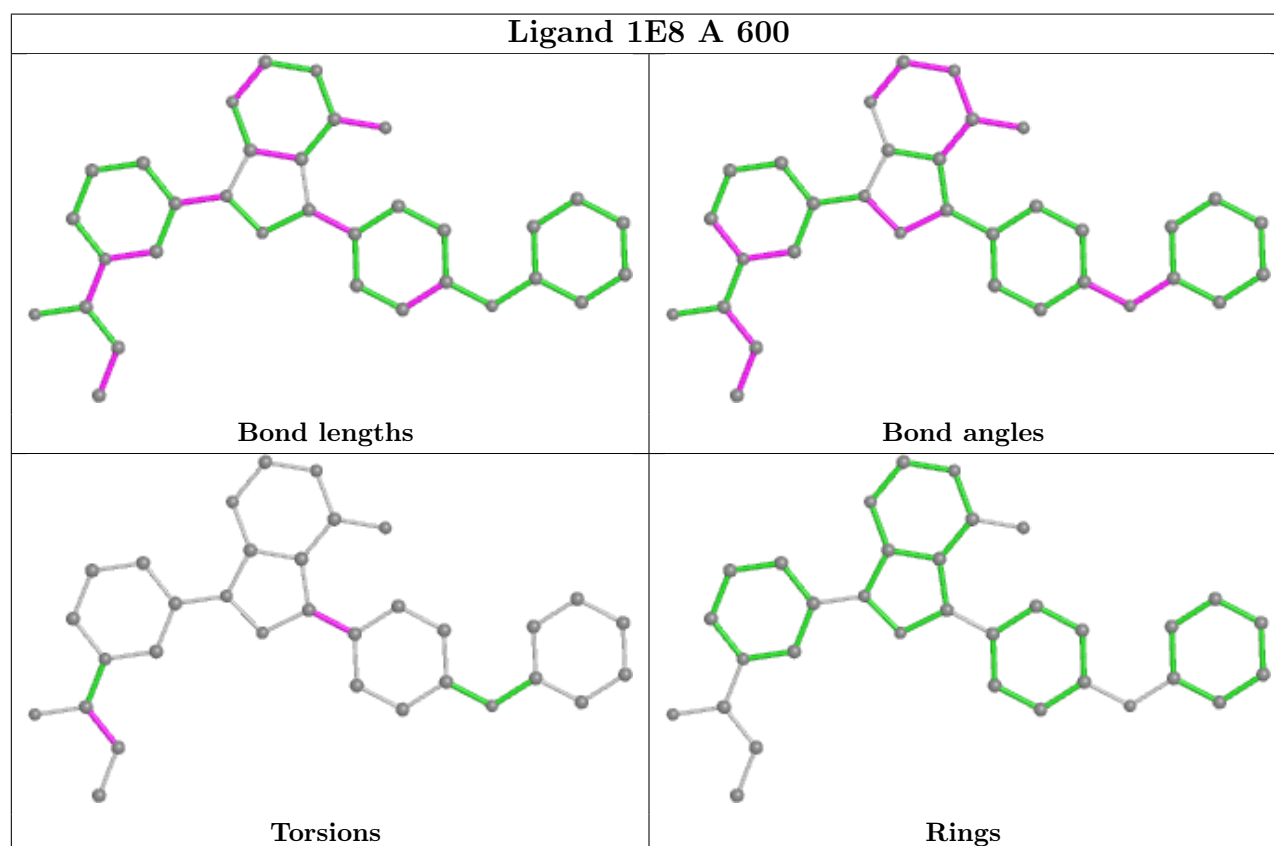
Mol	Chain	Res	Type	Atoms
2	B	600	1E8	CAM-CBA-CBB-NAU
2	B	600	1E8	CAN-CBA-CBB-NAU
2	C	600	1E8	CAA-CAD-CAW-NBG
2	D	600	1E8	CAN-CBA-CBB-NAU
2	D	600	1E8	CAM-CBA-CBB-NAU

There are no ring outliers.

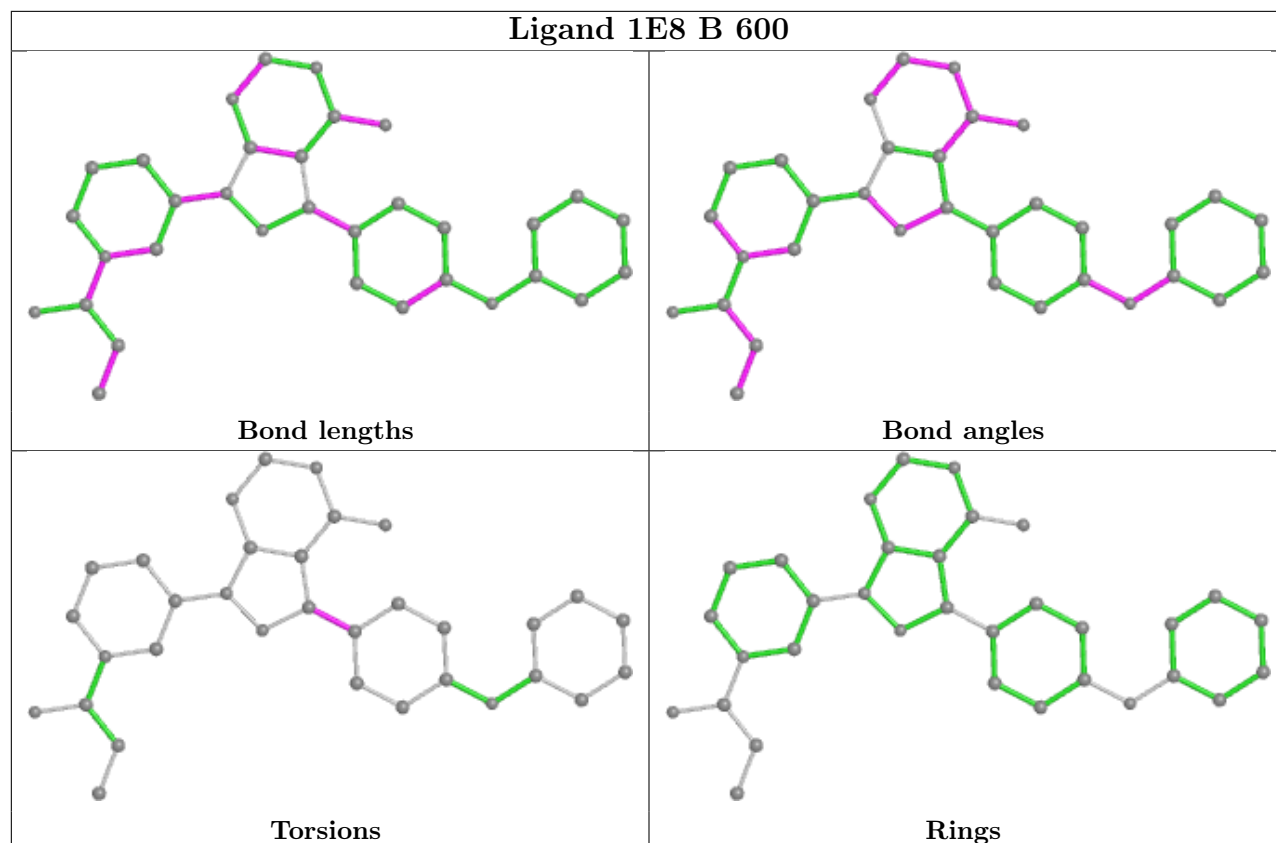
4 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	1E8	20	0
2	B	600	1E8	28	0
2	C	600	1E8	26	0
2	D	600	1E8	16	0

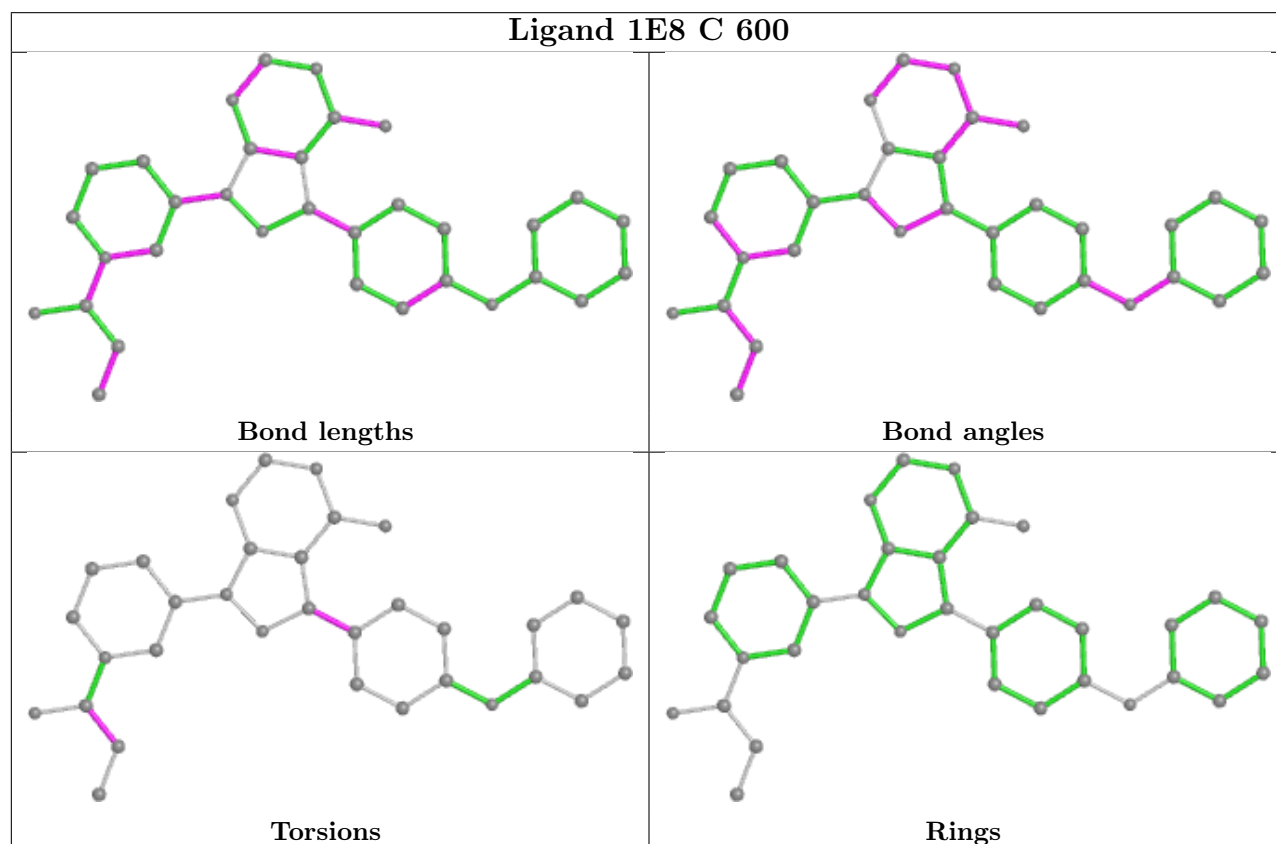
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

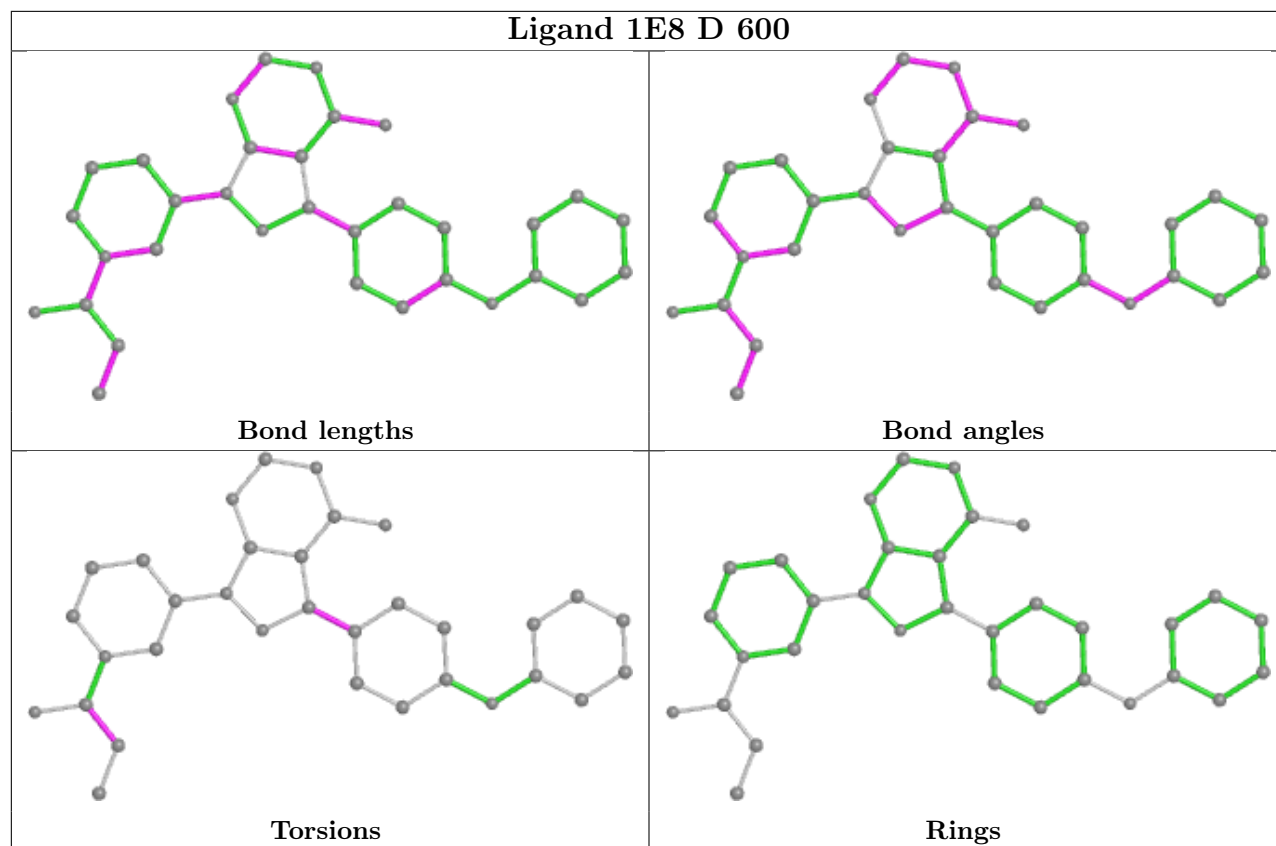


Ligand 1E8 B 600



Ligand 1E8 C 600





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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

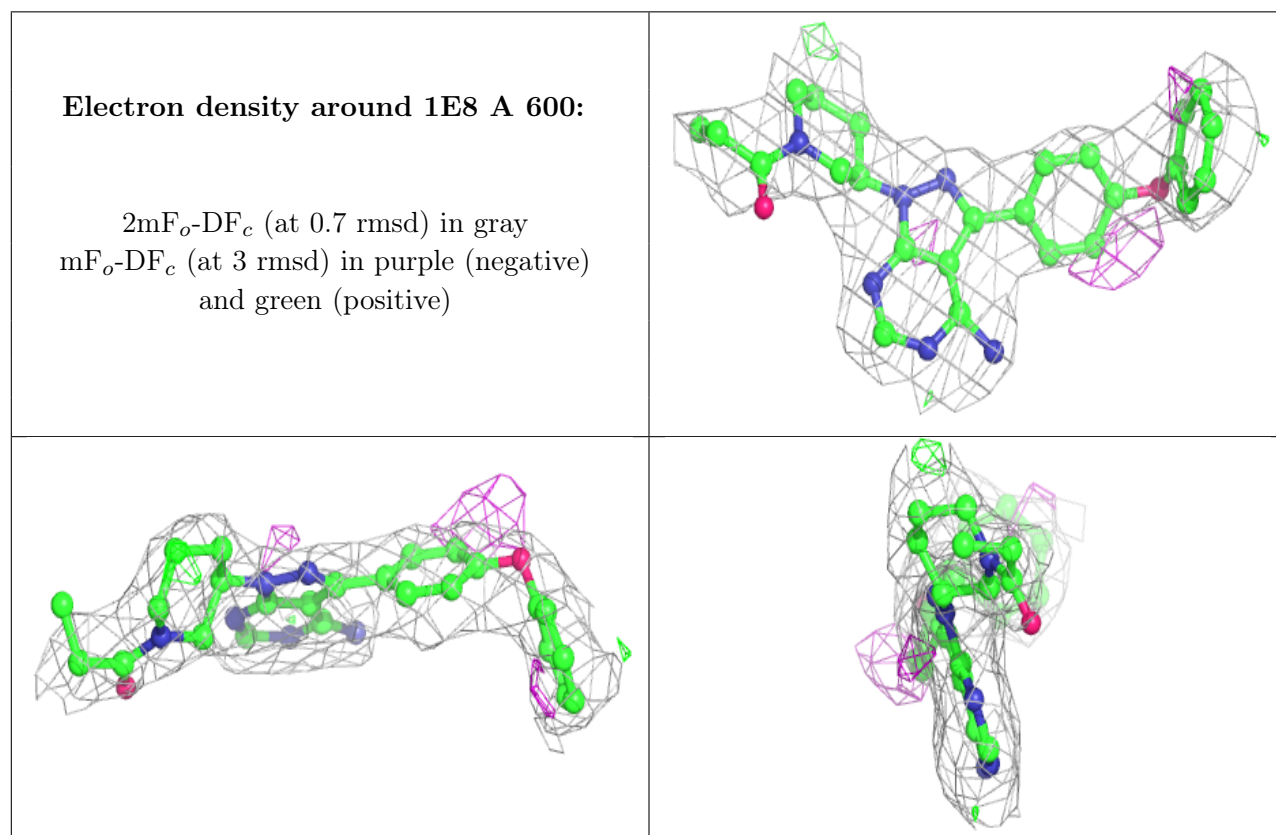
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

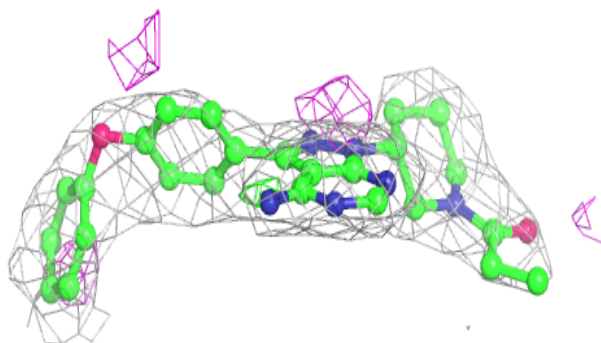
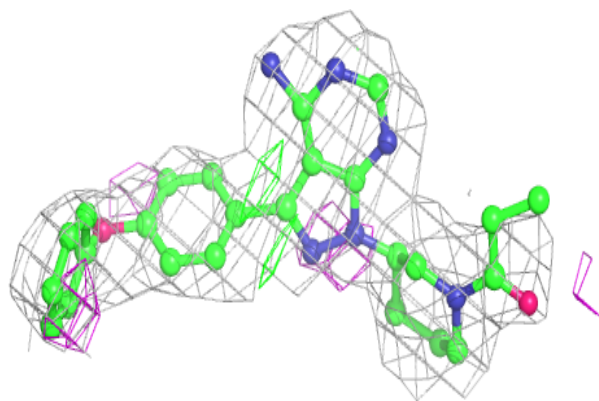
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

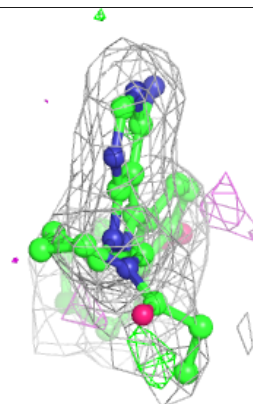
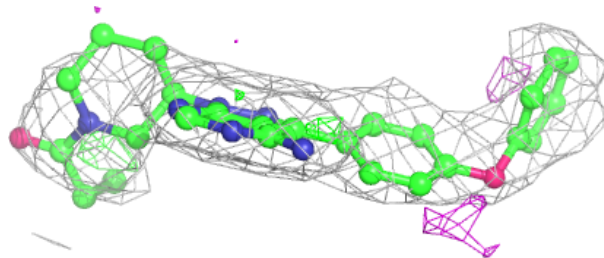
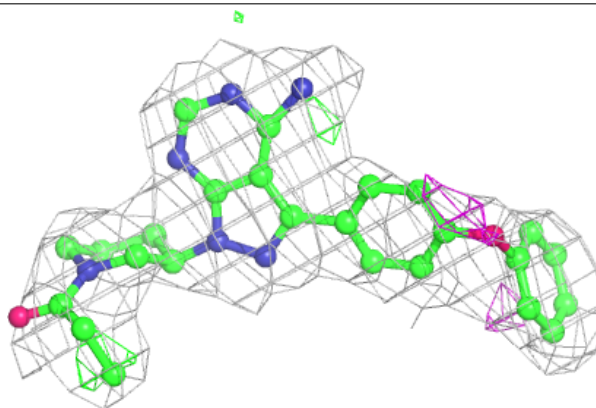


Electron density around 1E8 B 600:

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

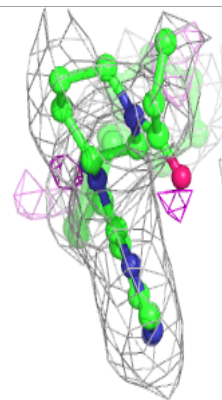
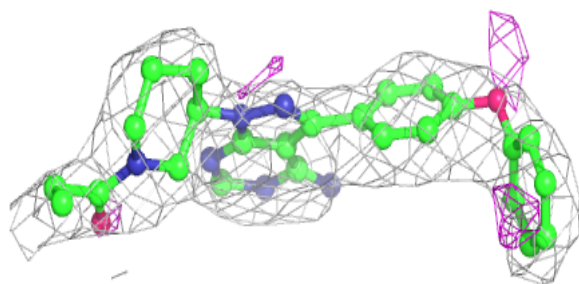
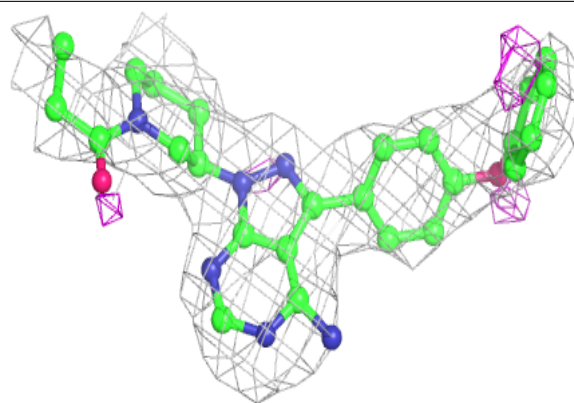
**Electron density around 1E8 C 600:**

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



Electron density around 1E8 D 600:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.