wwPDB X-ray Structure Validation Summary Report (i)

Apr 26, 2026 – 03:24 AM EDT

PDB ID	:	8VZ0 / pdb_00008vz0
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with k-400
Authors	:	Min, C.K.; Nwachukwu, J.C.; Hou, Y.; Russo, R.J.; Papa, A.; Min, J.; Peng, R.; Kim, S.H.; Ziegler, Y.; Rangarajan, E.S.; Izard, T.; Katzenellenbogen, B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on	:	2024-02-09
Resolution	:	1.86 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 (1)) were used in the production of this report:

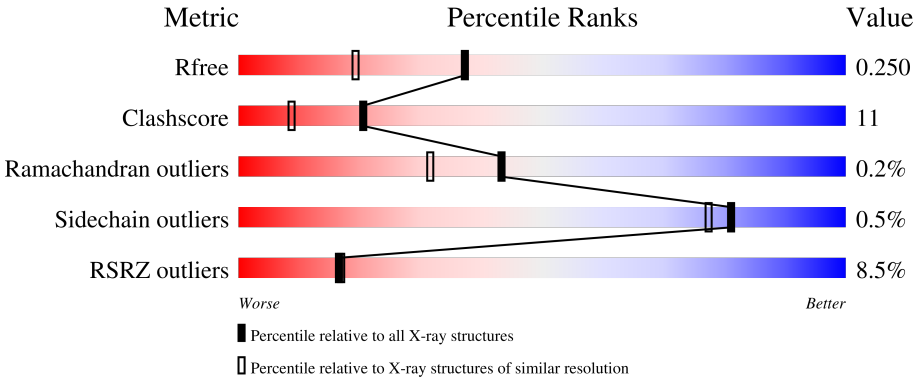
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 1.86 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	242	8% 72% 22%
1	B	242	8% 71% 19% 9%
1	C	242	10% 72% 21%
1	D	242	6% 72% 18% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14395 atoms, of which 7083 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.

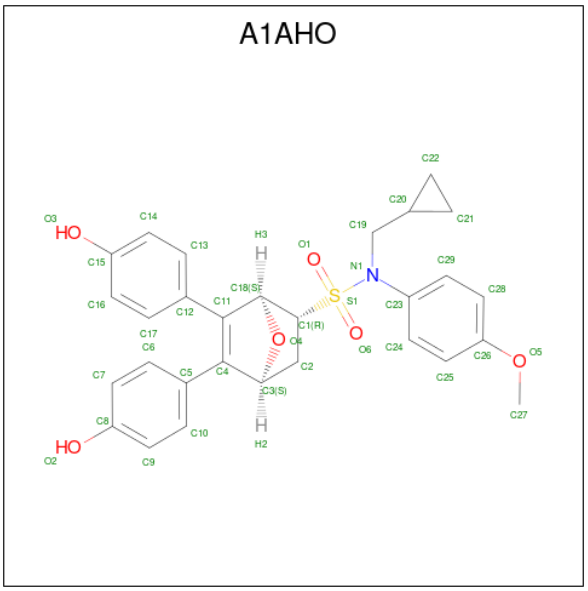
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	237	Total	C	H	N	O	S	0	1	0
			3637	1168	1818	316	318	17			
1	B	220	Total	C	H	N	O	S	0	0	0
			3320	1068	1650	289	298	15			
1	C	233	Total	C	H	N	O	S	0	3	0
			3559	1153	1768	309	313	16			
1	D	223	Total	C	H	N	O	S	0	0	0
			3481	1110	1750	298	308	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 (1S,2R,4S)-N-(cyclopropylmethyl)-5,6-bis(4-hydroxyphenyl)-N-(4-methoxyphenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (CCD ID: A1AHO) (formula: $C_{29}H_{29}NO_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			40	18	15	1	5	1		
2	B	1	Total	C	H	N	O	S	0	0
			66	29	29	1	6	1		
2	C	1	Total	C	H	N	O	S	0	0
			66	29	29	1	6	1		
2	D	1	Total	C	H	N	O	S	0	0
			58	26	24	1	6	1		

- Molecule 3 is water.

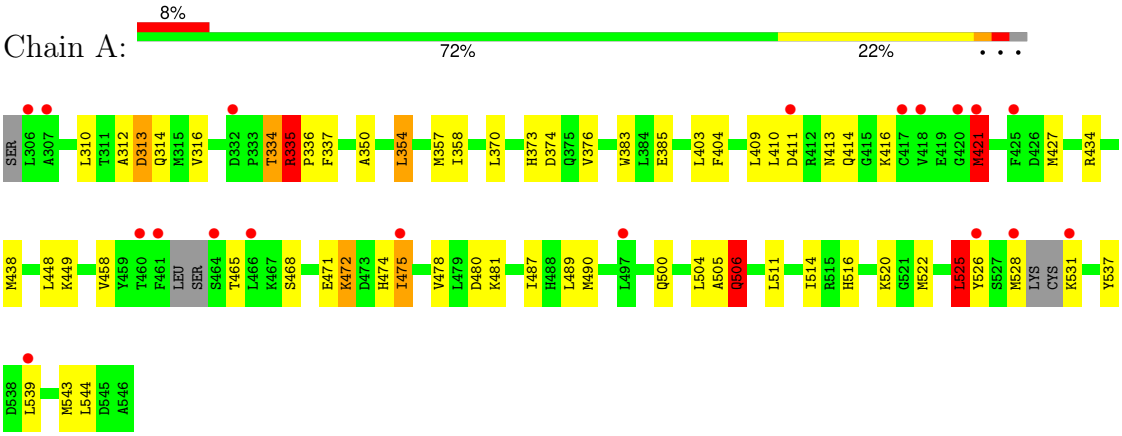
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	36	Total	O	0	0
			36	36		
3	C	47	Total	O	0	0
			47	47		
3	D	37	Total	O	0	0
			37	37		

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.

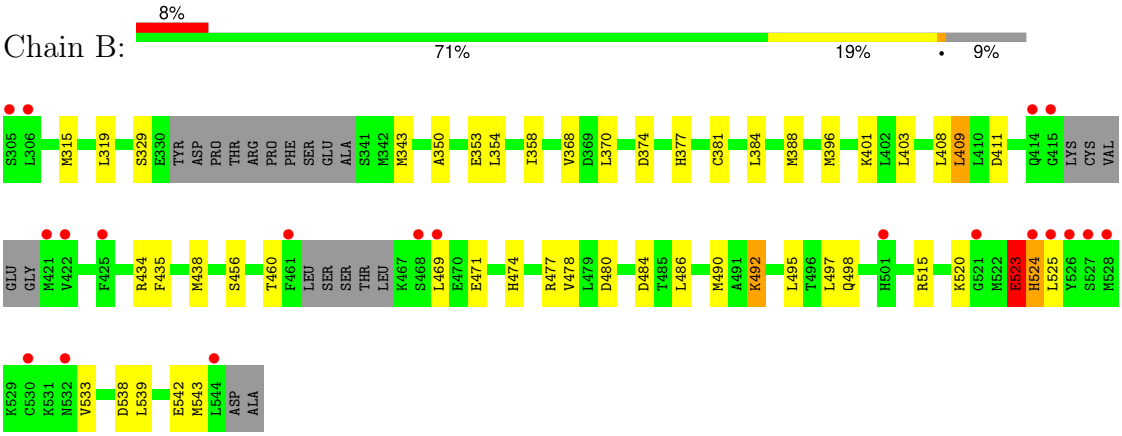
• Molecule 1: Estrogen receptor

Chain A:



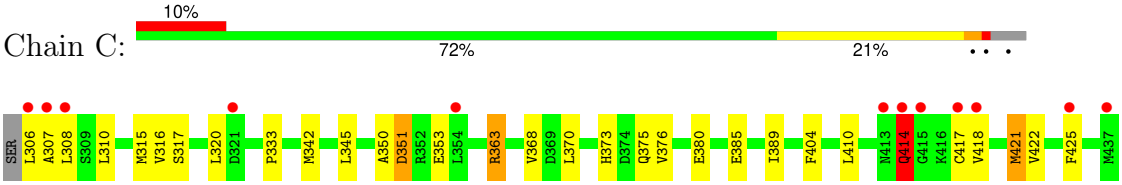
• Molecule 1: Estrogen receptor

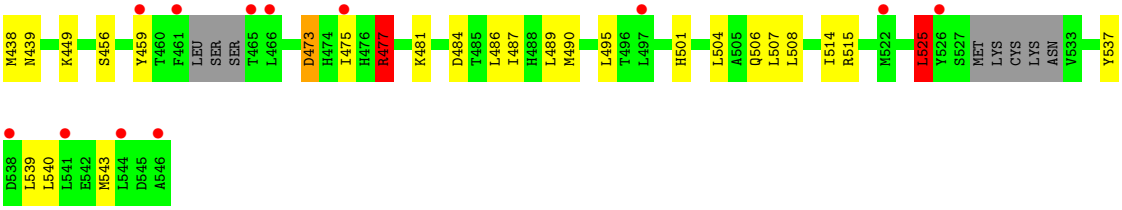
Chain B:



• Molecule 1: Estrogen receptor

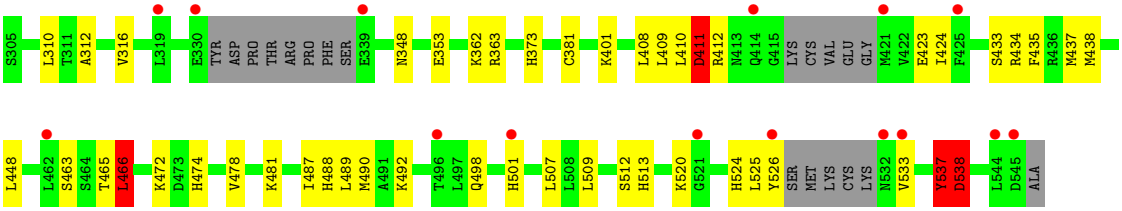
Chain C:





• Molecule 1: Estrogen receptor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.26Å 58.89Å 93.04Å 80.10° 75.02° 63.17°	Depositor
Resolution (Å)	33.05 – 1.86 33.05 – 1.86	Depositor EDS
% Data completeness (in resolution range)	59.5 (33.05-1.86) 59.6 (33.05-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.207 , 0.249 0.208 , 0.250	Depositor DCC
R_{free} test set	2400 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.124 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14395	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AHO

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	0.47	1/1864 (0.1%)	0.91	22/2527 (0.9%)
1	B	0.45	2/1696 (0.1%)	1.02	12/2297 (0.5%)
1	C	0.80	9/1839 (0.5%)	1.08	20/2495 (0.8%)
1	D	0.47	2/1759 (0.1%)	0.86	8/2378 (0.3%)
All	All	0.57	14/7158 (0.2%)	0.97	62/9697 (0.6%)

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	4
1	B	0	1
1	C	0	6
1	D	0	3
All	All	0	14

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	477	ARG	CZ-NH1	18.16	1.58	1.32
1	C	421	MET	CG-SD	-9.17	1.57	1.80
1	A	421	MET	CG-SD	-8.91	1.58	1.80
1	B	520	LYS	CD-CE	7.22	1.74	1.52
1	D	538	ASP	N-CA	6.93	1.55	1.46

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	538	ASP	OD1-CG-OD2	-20.34	74.08	122.90
1	B	523	GLU	OE1-CD-OE2	-18.01	79.67	122.90
1	B	523	GLU	CG-CD-OE1	15.89	154.94	118.40
1	C	477	ARG	NH1-CZ-NH2	-14.56	100.37	119.30
1	B	523	GLU	CG-CD-OE2	-14.33	85.44	118.40

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ASP	Sidechain
1	A	335	ARG	Sidechain
1	A	421	MET	Mainchain
1	A	506	GLN	Sidechain
1	B	523	GLU	Sidechain

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	1819	1818	1809	46	1
1	B	1670	1650	1649	33	2
1	C	1791	1768	1760	43	0
1	D	1731	1750	1749	40	0
2	A	25	15	0	4	0
2	B	37	29	0	3	0
2	C	37	29	0	2	0
2	D	34	24	0	4	0
3	A	48	0	0	7	0
3	B	36	0	0	4	0
3	C	47	0	0	7	1
3	D	37	0	0	3	1
All	All	7312	7083	6967	158	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 11.

The worst 5 of 158 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:421:MET:HE3	2:A:600:A1AHO:N1	1.73	1.04
1:D:401:LYS:NZ	1:D:411:ASP:OD2	1.94	0.98
1:C:307:ALA:N	3:C:702:HOH:O	2.06	0.87
1:D:381:CYS:SG	3:D:733:HOH:O	2.32	0.86
1:D:373:HIS:HD1	1:D:537:TYR:HH	1.19	0.86

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:B:498:GLN:NE2	1:B:542:GLU:OE1[1_455]	2.05	0.15
3:C:744:HOH:O	3:D:734:HOH:O[1_545]	2.08	0.12
1:A:481:LYS:HZ2	1:B:538:ASP:OD1[1_455]	1.57	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	232/242 (96%)	227 (98%)	4 (2%)	1 (0%)	30 17
1	B	212/242 (88%)	207 (98%)	5 (2%)	0	100 100
1	C	230/242 (95%)	226 (98%)	4 (2%)	0	100 100
1	D	215/242 (89%)	208 (97%)	6 (3%)	1 (0%)	24 13
All	All	889/968 (92%)	868 (98%)	19 (2%)	2 (0%)	43 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	538	ASP
1	A	475	ILE

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	194/218 (89%)	193 (100%)	1 (0%)	81	77
1	B	175/218 (80%)	174 (99%)	1 (1%)	78	73
1	C	187/218 (86%)	186 (100%)	1 (0%)	81	77
1	D	188/218 (86%)	187 (100%)	1 (0%)	81	77
All	All	744/872 (85%)	740 (100%)	4 (0%)	81	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	525	LEU
1	B	409	LEU
1	C	525	LEU
1	D	466	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	519	ASN
1	D	474	HIS
1	C	356	HIS
1	D	519	ASN
1	C	506	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	A1AHO	B	600	-	40,42,42	1.80	5 (12%)	52,63,63	1.26	6 (11%)
2	A1AHO	A	600	-	27,28,42	2.37	4 (14%)	33,43,63	1.91	4 (12%)
2	A1AHO	D	600	-	36,38,42	1.99	5 (13%)	47,57,63	1.25	4 (8%)
2	A1AHO	C	600	-	40,42,42	1.87	5 (12%)	52,63,63	1.03	4 (7%)

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	A1AHO	B	600	-	-	11/28/56/56	0/7/6/6
2	A1AHO	A	600	-	-	5/12/38/56	0/5/4/6
2	A1AHO	D	600	-	-	5/24/50/56	0/6/5/6
2	A1AHO	C	600	-	-	5/28/56/56	0/7/6/6

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	A1AHO	S1-N1	10.04	1.77	1.61
2	D	600	A1AHO	C19-N1	-6.97	1.34	1.47
2	C	600	A1AHO	C1-S1	5.66	1.89	1.77
2	C	600	A1AHO	S1-N1	5.60	1.79	1.67
2	B	600	A1AHO	S1-N1	5.52	1.79	1.67

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	A1AHO	O6-S1-O1	8.08	125.63	119.10
2	D	600	A1AHO	O6-S1-O1	4.18	122.32	119.17
2	A	600	A1AHO	O1-S1-C1	4.01	113.64	107.69
2	D	600	A1AHO	C24-C23-N1	-3.30	115.25	120.05
2	C	600	A1AHO	C17-C12-C11	-2.86	117.20	120.91

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	A1AHO	C18-C1-S1-O1
2	A	600	A1AHO	C2-C1-S1-O1
2	B	600	A1AHO	C20-C19-N1-C23
2	B	600	A1AHO	C20-C19-N1-S1
2	B	600	A1AHO	C18-C1-S1-O1

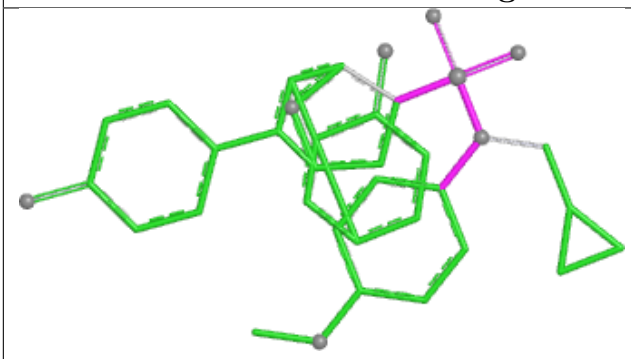
There are no ring outliers.

4 monomers are involved in 13 short contacts:

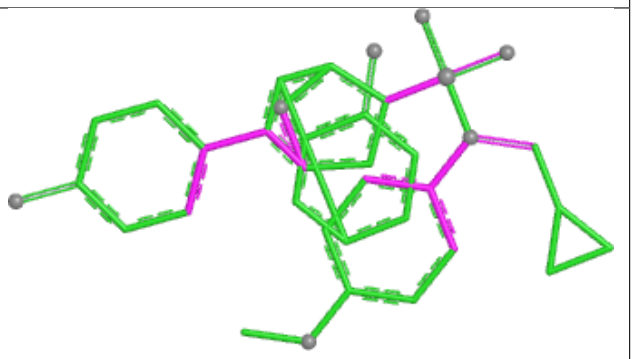
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	A1AHO	3	0
2	A	600	A1AHO	4	0
2	D	600	A1AHO	4	0
2	C	600	A1AHO	2	0

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.

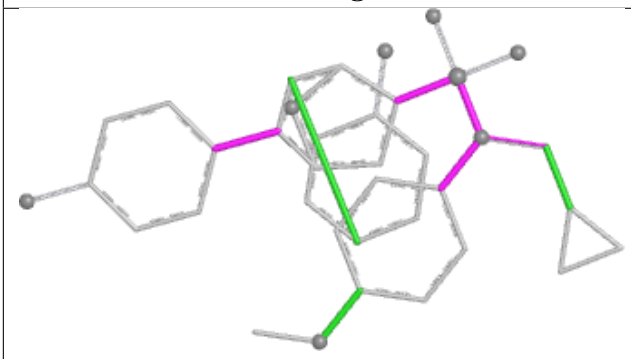
Ligand A1AHO B 600



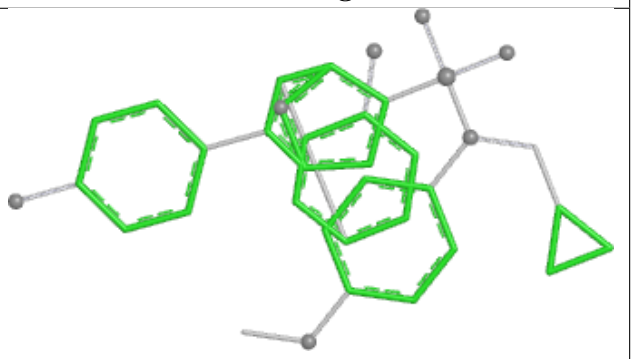
Bond lengths



Bond angles

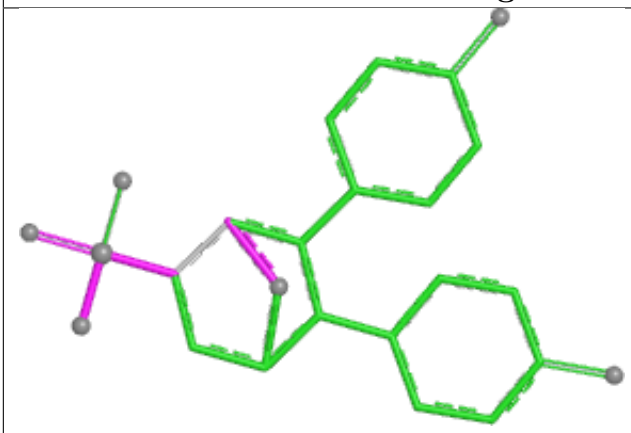


Torsions

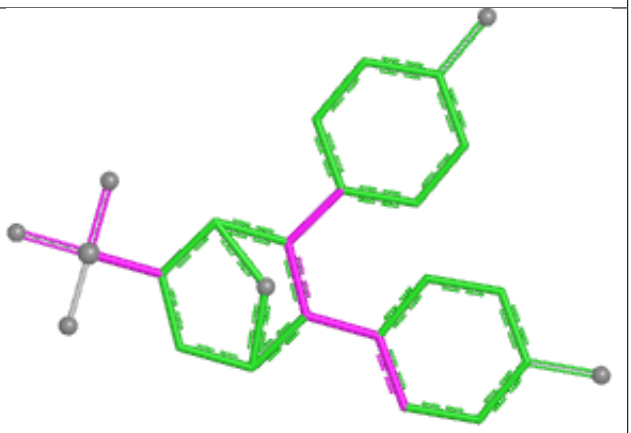


Rings

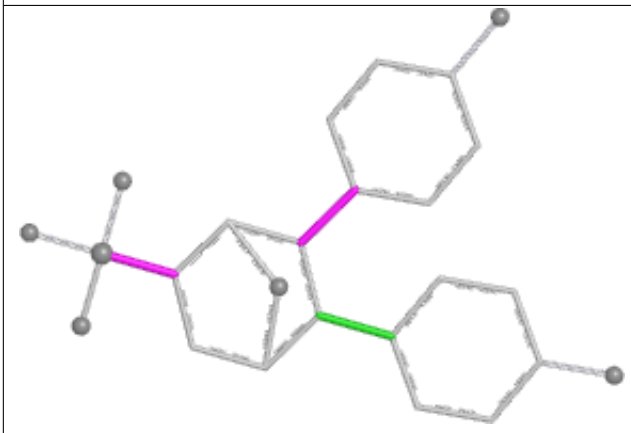
Ligand A1AHO A 600



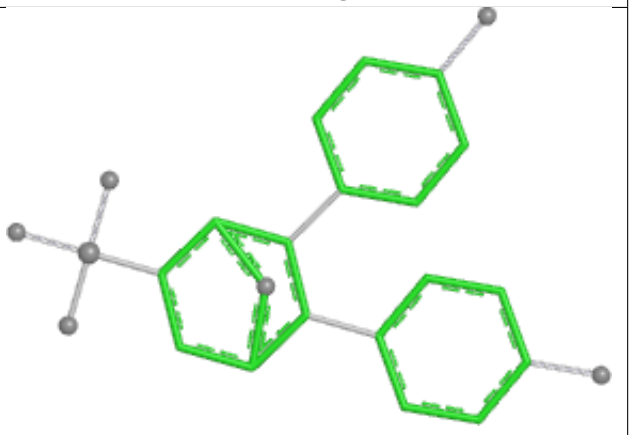
Bond lengths



Bond angles

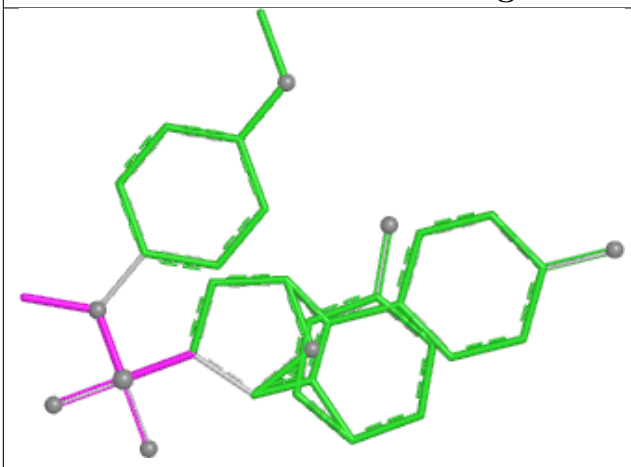


Torsions

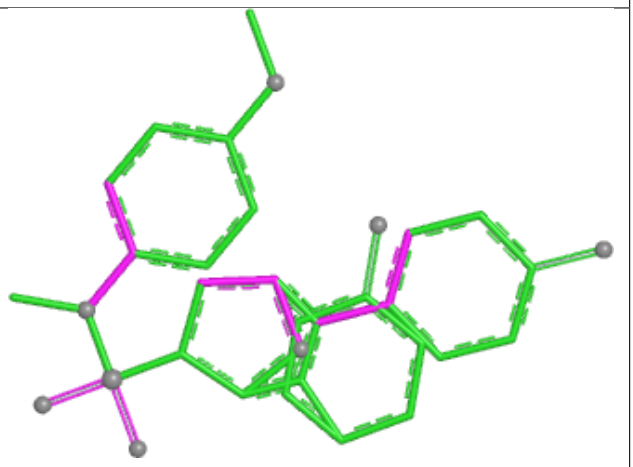


Rings

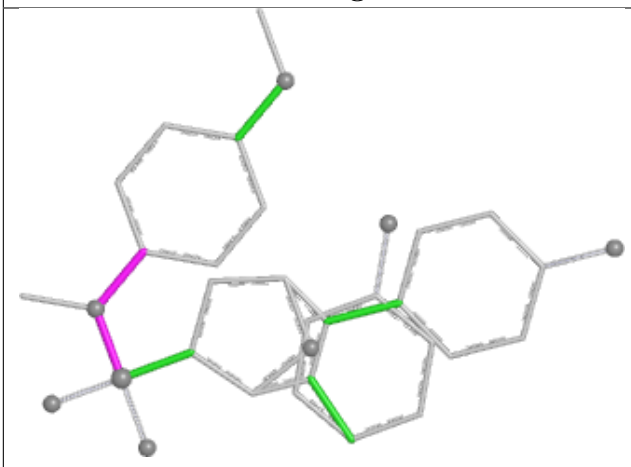
Ligand A1AHO D 600



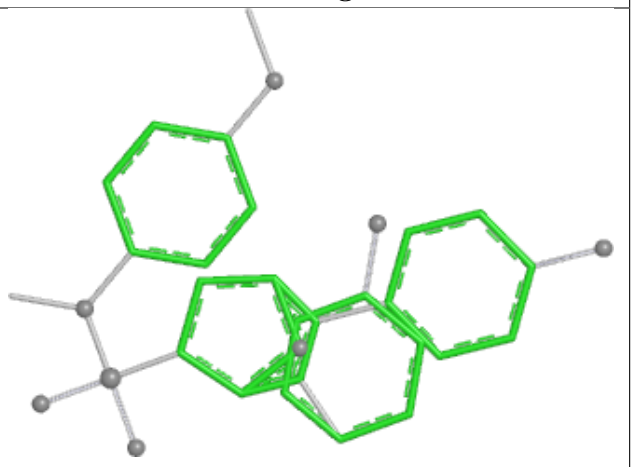
Bond lengths



Bond angles

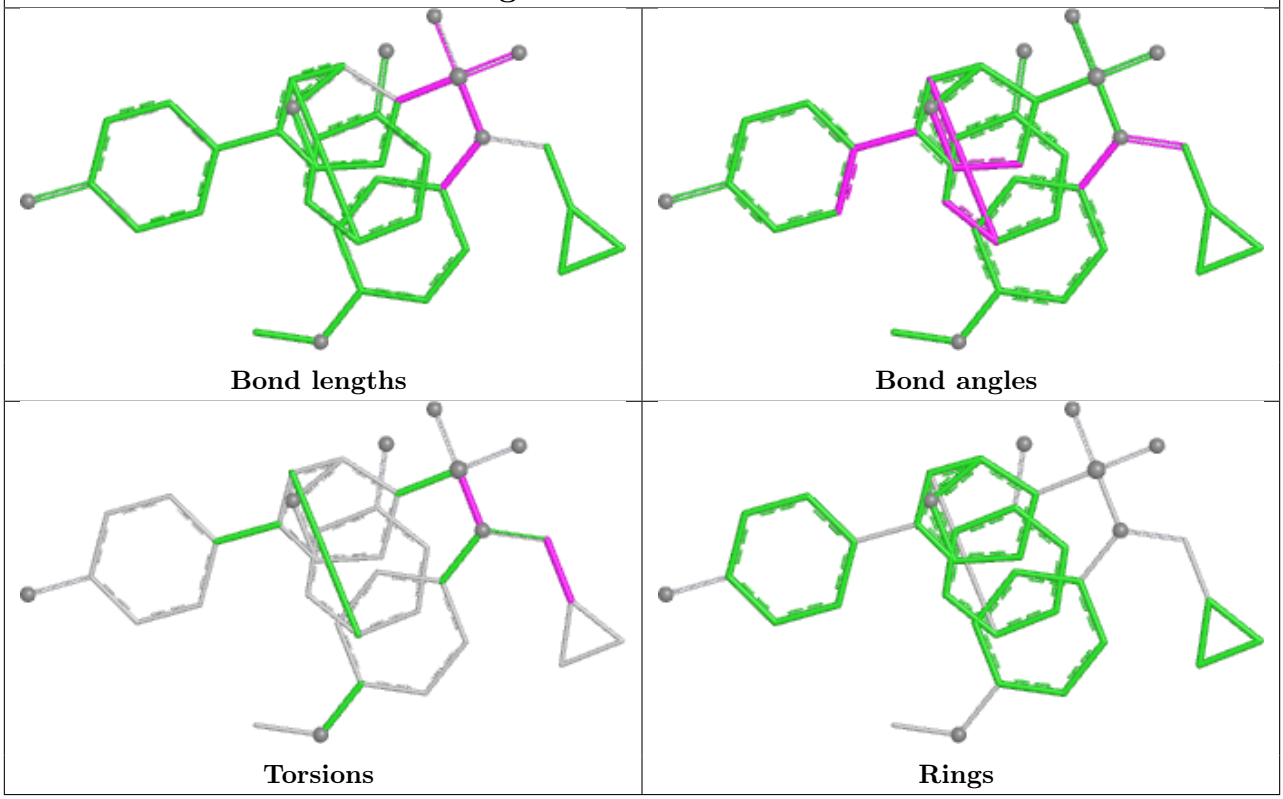


Torsions



Rings

Ligand A1AHO 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

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	237/242 (97%)	0.50	19 (8%)	18	19	27, 45, 80, 127	0
1	B	220/242 (90%)	0.56	20 (9%)	15	15	26, 45, 86, 105	0
1	C	233/242 (96%)	0.62	24 (10%)	12	12	29, 49, 80, 95	2 (0%)
1	D	223/242 (92%)	0.46	15 (6%)	24	26	28, 45, 78, 95	0
All	All	913/968 (94%)	0.53	78 (8%)	16	17	26, 46, 81, 127	2 (0%)

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	546	ALA	5.2
1	D	425	PHE	4.8
1	B	526	TYR	4.1
1	A	306	LEU	4.1
1	B	415	GLY	4.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

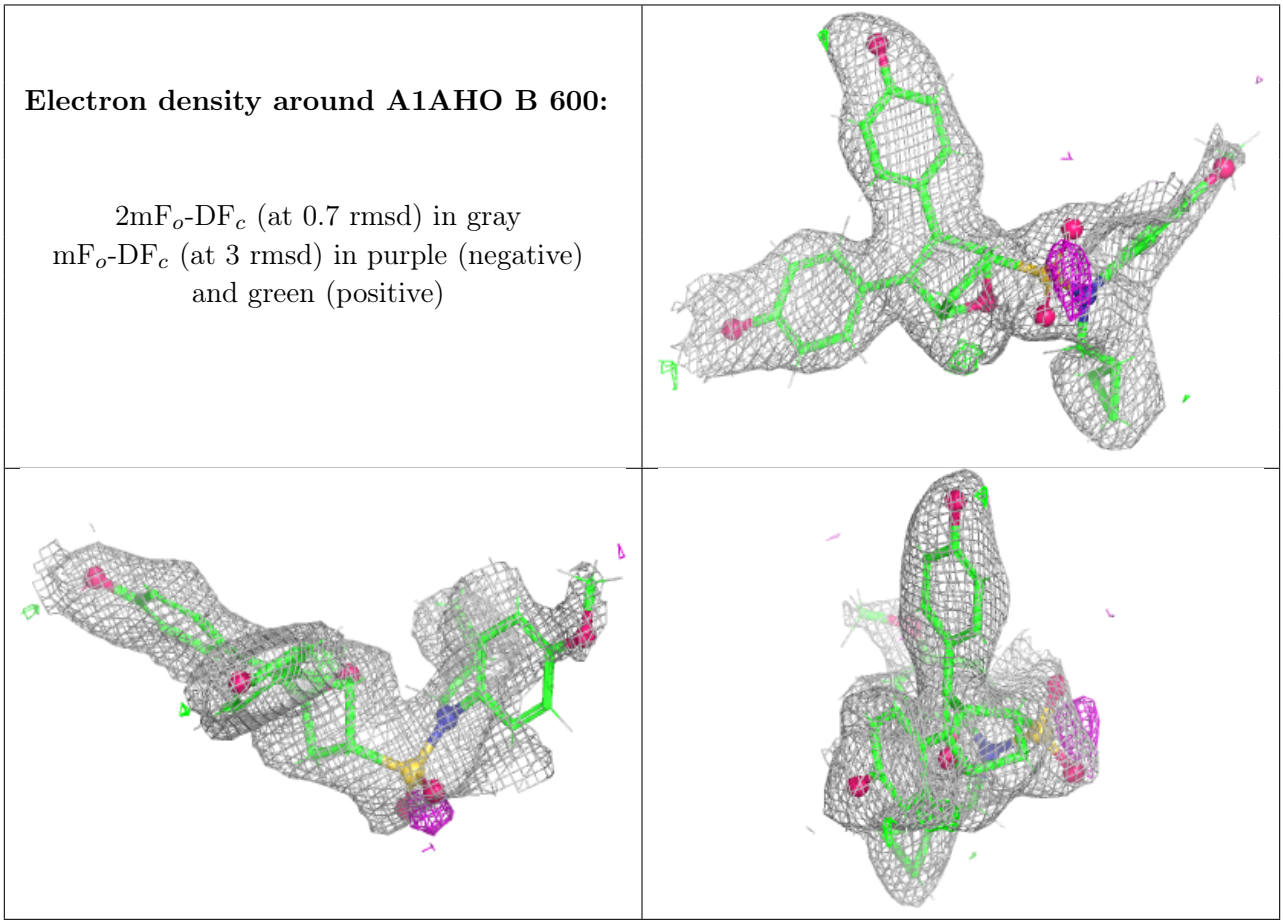
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1AHO	B	600	37/37	0.89	0.11	24,59,93,102	0
2	A1AHO	C	600	37/37	0.90	0.12	34,53,79,97	0
2	A1AHO	D	600	34/37	0.90	0.13	32,55,81,90	0
2	A1AHO	A	600	25/37	0.93	0.09	25,39,66,75	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.

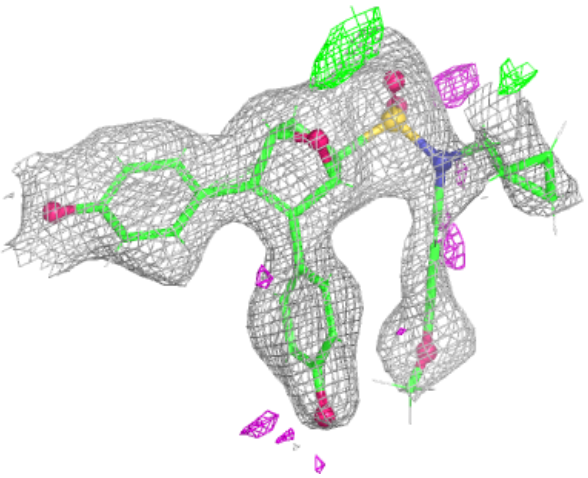
Electron density around A1AHO B 600:

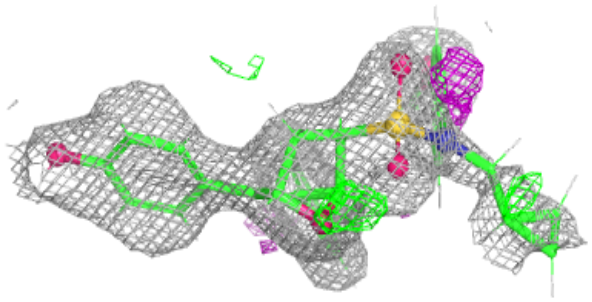
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

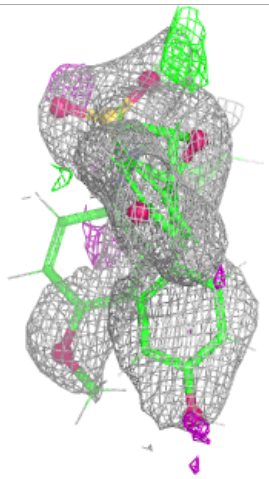


Electron density around A1AHO C 600:

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

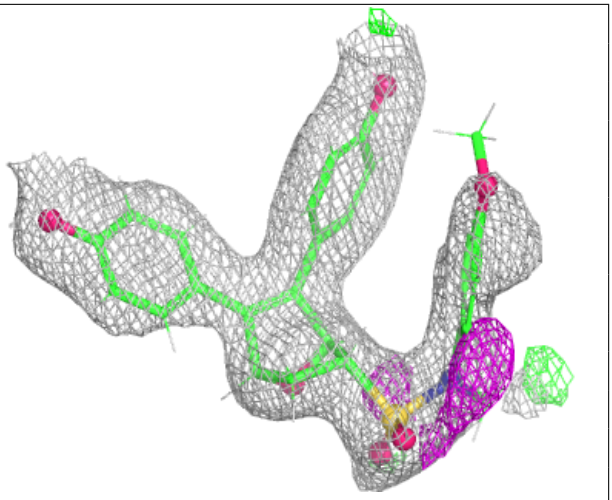


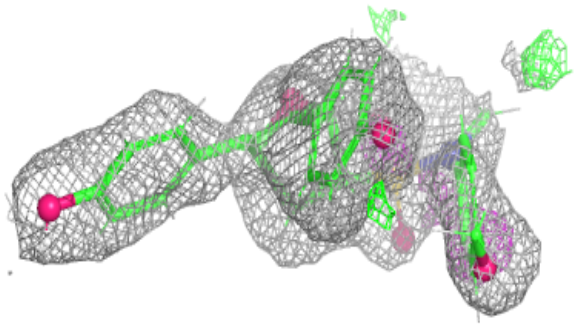


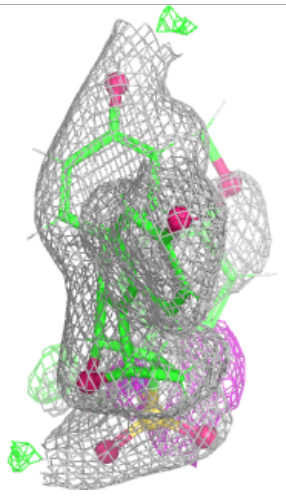


Electron density around A1AHO D 600:

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

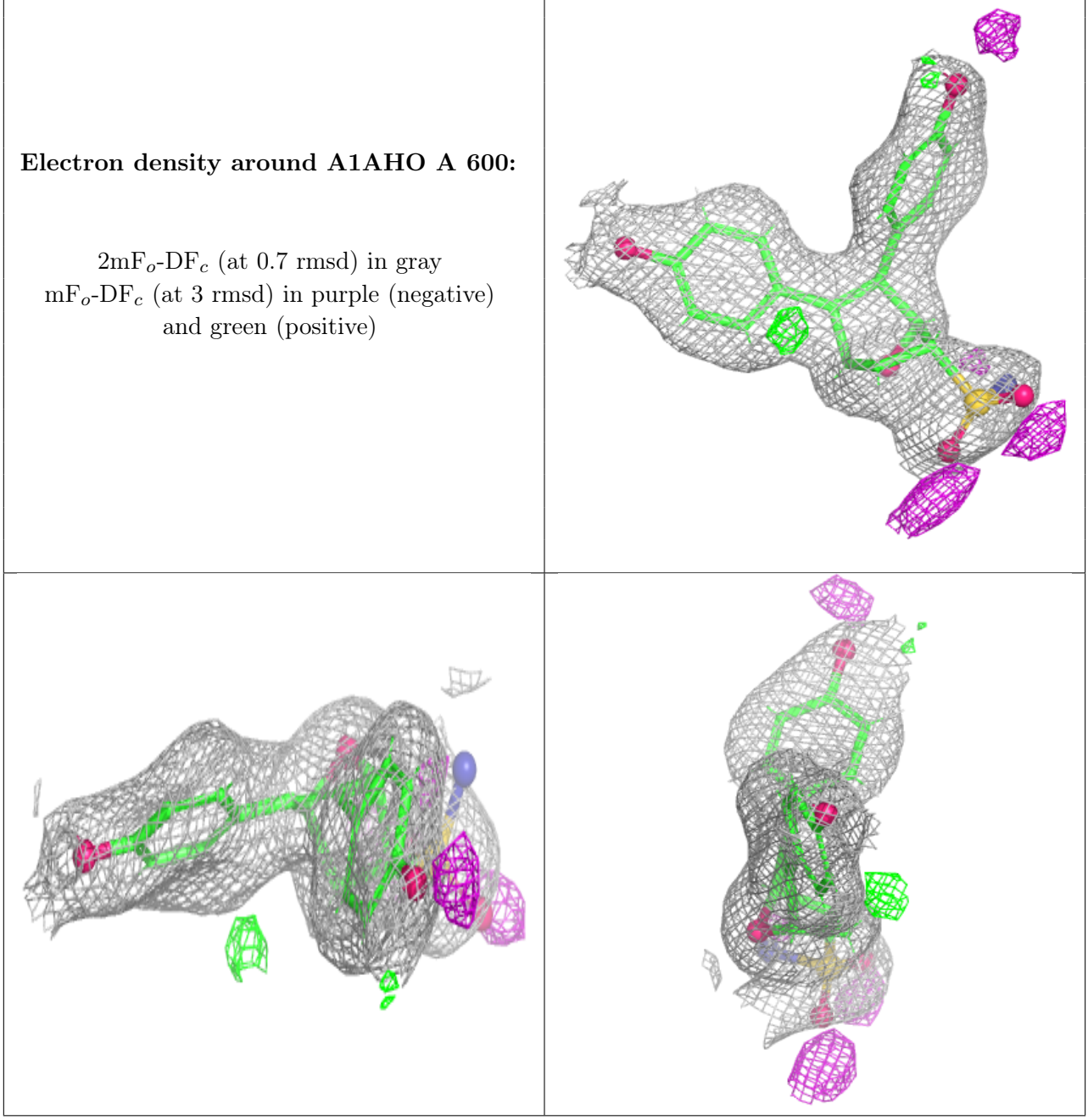






Electron density around A1AHO A 600:

$2mF_o$-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)

There are no such residues in this entry.