



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:16 PM UTC

PDB ID : 9B2B / pdb\_00009b2b  
Title : Estrogen Receptor Alpha Ligand Binding Domain in Complex with a Complete Estrogen Receptor Antagonists that Favors Tetramer Formation  
Authors : Fink, E.C.; Chawla, R.; Wells, K.S.; Barratt, S.; Myles, D.C.; Pena, G.; Robello, B.W.; Ng, R.; Fanning, S.W.  
Deposited on : 2024-03-14  
Resolution : 2.08 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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

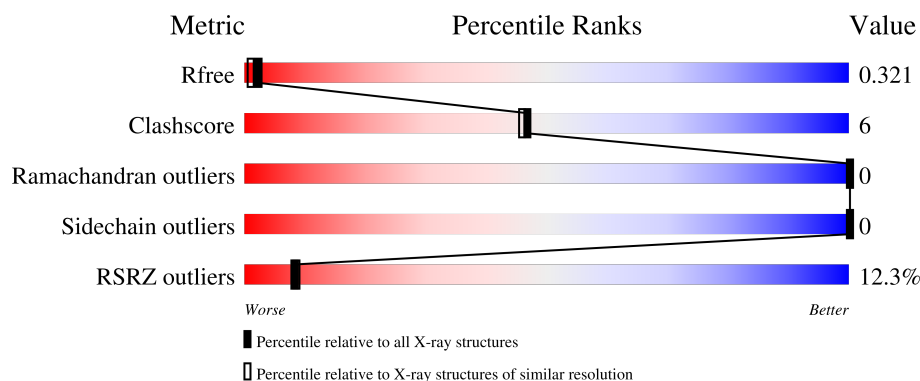
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	255	<div> <div>12%</div> <div>77%</div> <div>13%</div> <div>10%</div> </div>
1	B	255	<div> <div>11%</div> <div>77%</div> <div>13%</div> <div>10%</div> </div>
1	C	255	<div> <div>9%</div> <div>73%</div> <div>12%</div> <div>15%</div> </div>
1	D	255	<div> <div>12%</div> <div>76%</div> <div>10%</div> <div>14%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7588 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.

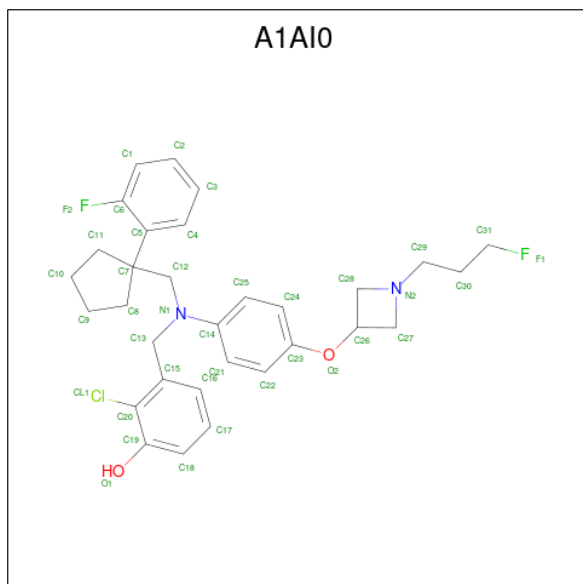
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1804	1155	306	328	15			
1	B	230	Total	C	N	O	S	0	2	0
			1804	1156	305	327	16			
1	C	216	Total	C	N	O	S	0	2	0
			1701	1091	294	301	15			
1	D	219	Total	C	N	O	S	0	2	0
			1728	1107	299	307	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	-	initiating methionine	UNP P03372
A	381	SER	CYS	engineered mutation	UNP P03372
A	417	SER	CYS	engineered mutation	UNP P03372
A	530	SER	CYS	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	300	MET	-	initiating methionine	UNP P03372
B	381	SER	CYS	engineered mutation	UNP P03372
B	417	SER	CYS	engineered mutation	UNP P03372
B	530	SER	CYS	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	300	MET	-	initiating methionine	UNP P03372
C	381	SER	CYS	engineered mutation	UNP P03372
C	417	SER	CYS	engineered mutation	UNP P03372
C	530	SER	CYS	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	300	MET	-	initiating methionine	UNP P03372
D	381	SER	CYS	engineered mutation	UNP P03372
D	417	SER	CYS	engineered mutation	UNP P03372
D	530	SER	CYS	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is 2-chloro-3-{{[1-(2-fluorophenyl)cyclopentyl]methyl}(4-{[1-(3-fluoropropyl)azetidin-3-yl]oxy}phenyl)amino]methyl}phenol (CCD ID: A1AI0) (formula: C<sub>31</sub>H<sub>35</sub>ClF<sub>2</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 38	C 31	Cl 1	F 2	N 2	O 2	0	0
2	B	1	Total 38	C 31	Cl 1	F 2	N 2	O 2	0	0
2	C	1	Total 38	C 31	Cl 1	F 2	N 2	O 2	0	0
2	D	1	Total 38	C 31	Cl 1	F 2	N 2	O 2	0	0

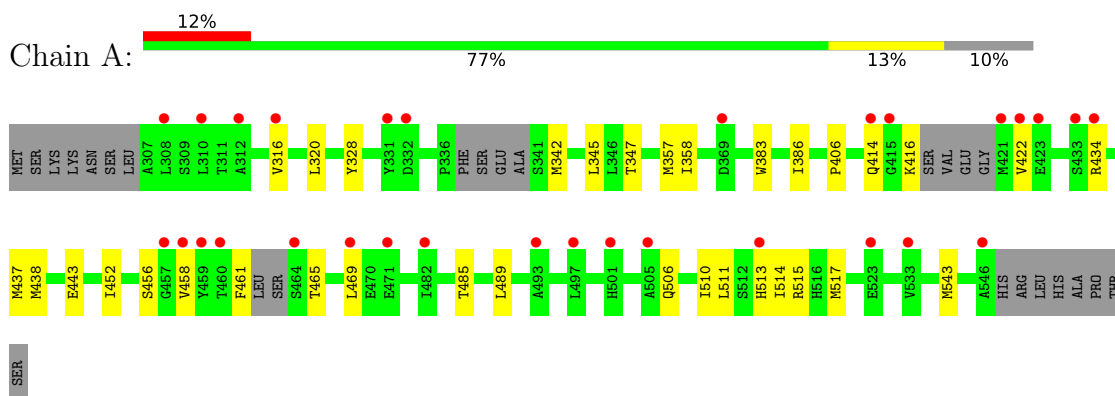
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	98	Total	O	0	0
			98	98		
3	C	104	Total	O	0	0
			104	104		
3	D	105	Total	O	0	0
			105	105		

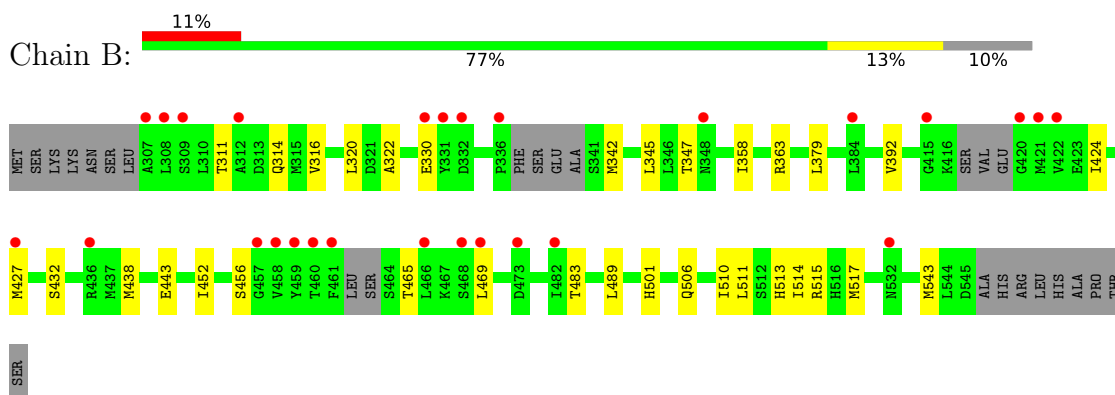
### 3 Residue-property plots [i](#)

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.

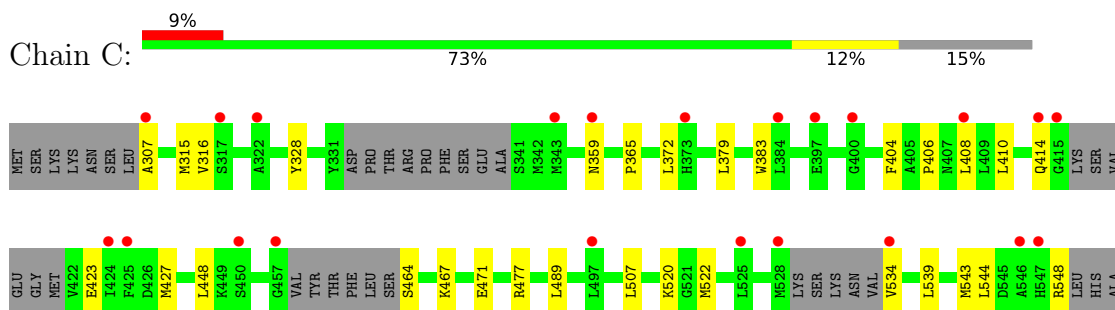
- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.10Å 57.42Å 174.80Å 90.00° 102.16° 90.00°	Depositor
Resolution (Å)	49.19 – 2.08 49.19 – 2.08	Depositor EDS
% Data completeness (in resolution range)	88.8 (49.19-2.08) 89.4 (49.19-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.259 , 0.318 0.264 , 0.321	Depositor DCC
$R_{free}$ test set	2613 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.000 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 93.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5311e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1AI0

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	0.33	0/1835	0.51	0/2481
1	B	0.34	0/1835	0.53	0/2480
1	C	0.42	0/1729	0.57	0/2335
1	D	0.39	0/1757	0.55	0/2373
All	All	0.37	0/7156	0.54	0/9669

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	1804	0	1820	24	0
1	B	1804	0	1819	23	0
1	C	1701	0	1719	21	0
1	D	1728	0	1744	20	0
2	A	38	0	0	1	0
2	B	38	0	0	1	0
2	C	38	0	0	0	0
2	D	38	0	0	1	0
3	A	92	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	98	0	0	1	0
3	C	104	0	0	5	0
3	D	105	0	0	1	0
All	All	7588	0	7102	82	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 6.

All (82) 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:D:488:HIS:ND1	3:D:701:HOH:O	2.20	0.75
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.67	0.74
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.70	0.74
1:B:358:ILE:HD12	1:B:543:MET:HE3	1.70	0.73
1:D:379:LEU:HD12	1:D:544:LEU:HD11	1.72	0.72
1:C:372:LEU:HD23	1:D:372:LEU:HD23	1.73	0.70
1:C:404:PHE:HB2	1:C:408:LEU:HD22	1.78	0.66
1:D:383:TRP:CZ2	1:D:522:MET:HE1	2.31	0.66
1:B:358:ILE:CD1	1:B:543:MET:HE3	2.26	0.66
1:C:383:TRP:CZ2	1:C:522:MET:HE1	2.31	0.66
1:C:379:LEU:HD12	1:C:544:LEU:HD11	1.79	0.65
1:B:342:MET:HA	1:B:345:LEU:HD12	1.78	0.64
1:D:404:PHE:HB2	1:D:408:LEU:HD22	1.78	0.64
1:A:438:MET:HE1	1:A:506:GLN:HB3	1.78	0.64
1:C:427:MET:HE1	1:C:520:LYS:HD3	1.81	0.63
1:B:438:MET:HE1	1:B:506:GLN:HB3	1.81	0.62
1:A:342:MET:HE1	1:A:414:GLN:HB3	1.82	0.60
1:C:548:ARG:HB2	1:D:369:ASP:HA	1.83	0.60
1:A:434:ARG:HH12	1:A:513:HIS:CE1	2.20	0.59
1:C:534:VAL:N	3:C:701:HOH:O	2.36	0.57
1:D:539:LEU:HG	1:D:543:MET:HE2	1.86	0.57
1:C:427:MET:CE	1:C:520:LYS:HD3	2.36	0.56
1:A:416:LYS:HG2	1:A:422:VAL:HG11	1.89	0.55
1:C:448:LEU:HD11	1:C:507:LEU:HD22	1.89	0.54
1:C:464:SER:N	3:C:702:HOH:O	2.41	0.53
1:D:467:LYS:O	1:D:471:GLU:HG2	2.09	0.53
1:C:539:LEU:HG	1:C:543:MET:HE2	1.89	0.52
1:B:392:VAL:HG13	1:B:432:SER:HA	1.92	0.52
1:A:434:ARG:NH1	1:A:513:HIS:CE1	2.78	0.52
1:B:320:LEU:HD11	1:B:443:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:MET:HA	1:A:345:LEU:HD12	1.91	0.51
1:A:358:ILE:CD1	1:A:543:MET:HE3	2.41	0.50
1:A:514:ILE:HA	1:A:517:MET:HE2	1.94	0.49
1:C:467:LYS:O	1:C:471:GLU:HG2	2.13	0.49
1:A:358:ILE:HD12	1:A:543:MET:HE3	1.94	0.49
1:D:525:LEU:HG	2:D:601:A1AI0:C2	2.44	0.48
1:C:307:ALA:N	3:C:708:HOH:O	2.47	0.47
1:B:465:THR:O	1:B:469:LEU:HD13	2.14	0.47
1:A:437:MET:HE3	1:A:437:MET:HB2	1.82	0.47
1:D:487:ILE:HA	1:D:490:MET:CE	2.45	0.47
1:A:320:LEU:HD11	1:A:443:GLU:OE1	2.15	0.47
1:A:456:SER:HA	1:A:515:ARG:NH2	2.30	0.47
1:B:330:GLU:O	3:B:701:HOH:O	2.21	0.47
1:B:483:THR:HG22	1:D:501:HIS:HD2	1.79	0.47
1:A:434:ARG:HD3	1:A:510:ILE:HG12	1.98	0.46
1:D:328:TYR:CE2	1:D:406:PRO:HB2	2.50	0.46
1:C:410:LEU:HD22	1:C:414:GLN:OE1	2.16	0.45
1:D:448:LEU:HD11	1:D:507:LEU:HD22	1.99	0.45
1:A:465:THR:O	1:A:469:LEU:HD13	2.16	0.45
1:B:347:THR:HG23	2:B:601:A1AI0:C28	2.47	0.45
1:B:424:ILE:HD13	1:B:427[A]:MET:HE3	1.98	0.45
1:A:485:THR:O	1:A:489:LEU:HD23	2.16	0.45
1:B:501:HIS:CD2	1:D:483:THR:HG22	2.51	0.45
1:B:452:ILE:HD11	1:B:511:LEU:HD22	1.99	0.44
1:D:358:ILE:CD1	1:D:379:LEU:HD13	2.48	0.44
1:A:452:ILE:HD11	1:A:511:LEU:HD22	1.98	0.44
1:B:514:ILE:HA	1:B:517:MET:CE	2.48	0.44
1:A:458:VAL:HA	1:A:461:PHE:HE1	1.83	0.44
1:C:307:ALA:N	3:C:711:HOH:O	2.51	0.43
1:C:477:ARG:NE	3:C:713:HOH:O	2.51	0.43
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.53	0.43
1:A:514:ILE:HA	1:A:517:MET:CE	2.47	0.43
1:B:427[B]:MET:HE2	1:B:427[B]:MET:HB3	1.92	0.43
1:A:357:MET:HE1	1:A:383:TRP:O	2.18	0.43
1:B:510:ILE:HA	1:B:513:HIS:CD2	2.54	0.43
1:A:357:MET:HE2	1:A:386:ILE:HB	2.01	0.43
1:B:456:SER:HA	1:B:515:ARG:NH2	2.33	0.43
1:D:379:LEU:HD23	1:D:379:LEU:HA	1.85	0.43
1:D:383:TRP:HZ2	1:D:522:MET:HE1	1.82	0.42
1:C:328:TYR:CE2	1:C:406:PRO:HB2	2.55	0.42
1:A:328:TYR:OH	1:C:359:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HG12	1:B:379:LEU:HD13	2.02	0.41
1:B:483:THR:HG22	1:D:501:HIS:CD2	2.55	0.41
1:C:423:GLU:CB	1:C:520:LYS:HE2	2.50	0.41
1:C:316:VAL:HG21	1:C:489:LEU:HD21	2.02	0.41
1:C:315:MET:HE1	1:C:365:PRO:HD2	2.02	0.41
1:D:315:MET:HE3	1:D:319:LEU:HG	2.02	0.41
1:B:514:ILE:HA	1:B:517:MET:HE2	2.03	0.41
1:B:311:THR:OG1	1:B:314:GLN:HG3	2.21	0.40
1:B:322:ALA:HA	1:B:363:ARG:HE	1.87	0.40
1:A:347:THR:HG23	2:A:601:A1AI0:C27	2.52	0.40
1:A:328:TYR:CE2	1:A:406:PRO:HB2	2.56	0.40

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	222/255 (87%)	220 (99%)	2 (1%)	0	100	100
1	B	223/255 (88%)	220 (99%)	3 (1%)	0	100	100
1	C	207/255 (81%)	206 (100%)	1 (0%)	0	100	100
1	D	210/255 (82%)	207 (99%)	3 (1%)	0	100	100
All	All	862/1020 (84%)	853 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	199/230 (86%)	199 (100%)	0	100	100
1	B	199/230 (86%)	199 (100%)	0	100	100
1	C	185/230 (80%)	185 (100%)	0	100	100
1	D	189/230 (82%)	189 (100%)	0	100	100
All	All	772/920 (84%)	772 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	356	HIS
1	A	455	ASN
1	A	500	GLN
1	A	501	HIS
1	A	513	HIS
1	A	516	HIS
1	B	348	ASN
1	B	513	HIS
1	C	359	ASN
1	C	375	GLN
1	D	476	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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	A1AI0	D	601	-	41,42,42	5.91	32 (78%)	45,59,59	2.04	13 (28%)
2	A1AI0	A	601	-	41,42,42	6.28	29 (70%)	45,59,59	1.57	5 (11%)
2	A1AI0	B	601	-	41,42,42	5.87	31 (75%)	45,59,59	1.60	13 (28%)
2	A1AI0	C	601	-	41,42,42	5.87	31 (75%)	45,59,59	1.73	10 (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	A1AI0	D	601	-	-	8/25/44/44	0/5/5/5
2	A1AI0	A	601	-	-	5/25/44/44	0/5/5/5
2	A1AI0	B	601	-	-	6/25/44/44	0/5/5/5
2	A1AI0	C	601	-	-	5/25/44/44	0/5/5/5

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1AI0	C29-N2	-16.44	1.10	1.47
2	B	601	A1AI0	C29-N2	-14.84	1.13	1.47
2	D	601	A1AI0	C29-N2	-14.53	1.14	1.47
2	C	601	A1AI0	C29-N2	-14.34	1.14	1.47
2	C	601	A1AI0	C20-C15	13.73	1.53	1.39
2	D	601	A1AI0	C20-C15	13.30	1.52	1.39
2	A	601	A1AI0	C27-N2	-13.12	1.35	1.49
2	A	601	A1AI0	C28-N2	-12.24	1.36	1.49
2	B	601	A1AI0	C20-C15	11.88	1.51	1.39
2	D	601	A1AI0	C5-C6	11.87	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	A1AI0	C5-C6	11.66	1.55	1.39
2	C	601	A1AI0	C5-C6	11.34	1.54	1.39
2	A	601	A1AI0	C20-C15	11.03	1.50	1.39
2	A	601	A1AI0	C5-C6	10.25	1.53	1.39
2	D	601	A1AI0	C22-C21	10.08	1.55	1.38
2	C	601	A1AI0	C22-C21	9.69	1.54	1.38
2	B	601	A1AI0	C22-C21	9.31	1.53	1.38
2	A	601	A1AI0	C27-C26	-9.05	1.37	1.53
2	D	601	A1AI0	C2-C1	8.87	1.54	1.38
2	B	601	A1AI0	C17-C16	8.81	1.54	1.38
2	C	601	A1AI0	C24-C23	8.78	1.55	1.38
2	D	601	A1AI0	C3-C4	8.77	1.53	1.38
2	C	601	A1AI0	C2-C1	8.77	1.53	1.38
2	B	601	A1AI0	C2-C1	8.66	1.53	1.38
2	A	601	A1AI0	C22-C21	8.64	1.52	1.38
2	D	601	A1AI0	C24-C23	8.60	1.54	1.38
2	C	601	A1AI0	C3-C4	8.48	1.53	1.38
2	B	601	A1AI0	C3-C4	8.46	1.53	1.38
2	A	601	A1AI0	C17-C16	8.34	1.53	1.38
2	D	601	A1AI0	C17-C16	8.32	1.53	1.38
2	C	601	A1AI0	C17-C16	8.31	1.53	1.38
2	C	601	A1AI0	C25-C14	8.28	1.55	1.39
2	B	601	A1AI0	C24-C23	8.14	1.54	1.38
2	B	601	A1AI0	C18-C19	8.08	1.53	1.39
2	B	601	A1AI0	C28-N2	-8.01	1.40	1.49
2	A	601	A1AI0	C3-C4	7.86	1.52	1.38
2	D	601	A1AI0	C18-C19	7.83	1.53	1.39
2	B	601	A1AI0	C27-N2	-7.82	1.41	1.49
2	D	601	A1AI0	C25-C14	7.81	1.54	1.39
2	C	601	A1AI0	C18-C19	7.64	1.52	1.39
2	A	601	A1AI0	C25-C14	7.58	1.53	1.39
2	B	601	A1AI0	C25-C14	7.45	1.53	1.39
2	A	601	A1AI0	C28-C26	-7.38	1.40	1.53
2	C	601	A1AI0	C27-N2	-7.37	1.41	1.49
2	D	601	A1AI0	C27-C26	-7.19	1.40	1.53
2	D	601	A1AI0	C27-N2	-7.19	1.41	1.49
2	B	601	A1AI0	C28-C26	-7.07	1.40	1.53
2	D	601	A1AI0	C28-N2	-7.03	1.41	1.49
2	C	601	A1AI0	C27-C26	-6.87	1.41	1.53
2	B	601	A1AI0	C27-C26	-6.73	1.41	1.53
2	C	601	A1AI0	C28-N2	-6.66	1.42	1.49
2	A	601	A1AI0	C24-C23	6.53	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1AI0	C18-C19	6.51	1.50	1.39
2	C	601	A1AI0	C28-C26	-6.44	1.41	1.53
2	A	601	A1AI0	C2-C1	6.33	1.49	1.38
2	D	601	A1AI0	C28-C26	-6.32	1.42	1.53
2	A	601	A1AI0	C19-C20	-6.26	1.32	1.40
2	A	601	A1AI0	C4-C5	-5.95	1.31	1.39
2	A	601	A1AI0	C17-C18	-5.92	1.28	1.38
2	A	601	A1AI0	C16-C15	-5.74	1.30	1.39
2	D	601	A1AI0	C19-C20	-5.48	1.33	1.40
2	C	601	A1AI0	C19-C20	-5.48	1.33	1.40
2	B	601	A1AI0	C19-C20	-5.35	1.33	1.40
2	A	601	A1AI0	C25-C24	-4.98	1.30	1.38
2	A	601	A1AI0	C21-C14	-4.83	1.30	1.39
2	B	601	A1AI0	C4-C5	-4.66	1.33	1.39
2	C	601	A1AI0	C16-C15	-4.20	1.32	1.39
2	C	601	A1AI0	C4-C5	-4.20	1.33	1.39
2	D	601	A1AI0	C16-C15	-4.15	1.32	1.39
2	D	601	A1AI0	C4-C5	-4.09	1.33	1.39
2	C	601	A1AI0	C14-N1	4.04	1.50	1.38
2	B	601	A1AI0	C16-C15	-4.02	1.33	1.39
2	B	601	A1AI0	C25-C24	-3.89	1.32	1.38
2	B	601	A1AI0	C17-C18	-3.78	1.32	1.38
2	D	601	A1AI0	C17-C18	-3.77	1.32	1.38
2	C	601	A1AI0	C17-C18	-3.75	1.32	1.38
2	D	601	A1AI0	C14-N1	3.71	1.49	1.38
2	B	601	A1AI0	C12-N1	3.63	1.51	1.46
2	A	601	A1AI0	C7-C5	3.36	1.58	1.54
2	A	601	A1AI0	C3-C2	-3.35	1.30	1.38
2	C	601	A1AI0	C12-N1	3.34	1.50	1.46
2	B	601	A1AI0	C21-C14	-3.34	1.33	1.39
2	D	601	A1AI0	C25-C24	-3.26	1.33	1.38
2	A	601	A1AI0	C1-C6	-3.22	1.31	1.37
2	D	601	A1AI0	C12-N1	3.19	1.50	1.46
2	B	601	A1AI0	C14-N1	3.06	1.47	1.38
2	A	601	A1AI0	C8-C7	-3.03	1.51	1.55
2	C	601	A1AI0	C21-C14	-2.97	1.33	1.39
2	B	601	A1AI0	C8-C7	-2.94	1.51	1.55
2	A	601	A1AI0	C14-N1	2.84	1.46	1.38
2	D	601	A1AI0	C20-CL1	2.83	1.78	1.72
2	B	601	A1AI0	C22-C23	-2.83	1.33	1.38
2	C	601	A1AI0	O2-C23	2.78	1.43	1.38
2	C	601	A1AI0	C13-C15	2.76	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	A1AI0	C21-C14	-2.75	1.34	1.39
2	C	601	A1AI0	C25-C24	-2.72	1.34	1.38
2	D	601	A1AI0	O2-C23	2.71	1.43	1.38
2	B	601	A1AI0	C7-C5	2.67	1.57	1.54
2	A	601	A1AI0	C11-C7	-2.60	1.52	1.55
2	B	601	A1AI0	C20-CL1	2.58	1.78	1.72
2	D	601	A1AI0	C13-C15	2.51	1.55	1.51
2	C	601	A1AI0	C20-CL1	2.49	1.78	1.72
2	A	601	A1AI0	C22-C23	-2.49	1.34	1.38
2	C	601	A1AI0	O1-C19	2.48	1.41	1.36
2	A	601	A1AI0	C13-C15	2.47	1.55	1.51
2	B	601	A1AI0	C13-C15	2.46	1.55	1.51
2	C	601	A1AI0	C1-C6	-2.43	1.33	1.37
2	D	601	A1AI0	O1-C19	2.41	1.41	1.36
2	C	601	A1AI0	C22-C23	-2.38	1.34	1.38
2	D	601	A1AI0	C11-C7	-2.38	1.52	1.55
2	C	601	A1AI0	C8-C7	-2.35	1.52	1.55
2	D	601	A1AI0	C1-C6	-2.34	1.33	1.37
2	B	601	A1AI0	C3-C2	-2.33	1.33	1.38
2	B	601	A1AI0	O2-C23	2.31	1.42	1.38
2	D	601	A1AI0	C22-C23	-2.28	1.34	1.38
2	D	601	A1AI0	C3-C2	-2.27	1.33	1.38
2	D	601	A1AI0	C8-C7	-2.22	1.52	1.55
2	B	601	A1AI0	C1-C6	-2.21	1.33	1.37
2	C	601	A1AI0	C3-C2	-2.19	1.33	1.38
2	B	601	A1AI0	C11-C7	-2.14	1.52	1.55
2	C	601	A1AI0	C11-C7	-2.10	1.52	1.55
2	A	601	A1AI0	C20-CL1	2.09	1.77	1.72
2	D	601	A1AI0	C13-N1	2.02	1.49	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	A1AI0	C23-O2-C26	-6.22	107.92	119.18
2	A	601	A1AI0	C19-C20-C15	-5.65	117.31	121.97
2	D	601	A1AI0	C4-C5-C7	-5.39	116.41	121.92
2	C	601	A1AI0	C11-C7-C8	5.00	108.68	102.40
2	D	601	A1AI0	C11-C7-C8	4.99	108.67	102.40
2	B	601	A1AI0	C4-C5-C7	-4.21	117.62	121.92
2	C	601	A1AI0	C23-O2-C26	-4.07	111.82	119.18
2	B	601	A1AI0	C16-C15-C20	3.68	120.22	117.33
2	C	601	A1AI0	C4-C5-C6	3.51	121.22	116.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	A1AI0	C16-C15-C20	3.31	119.93	117.33
2	D	601	A1AI0	C11-C7-C5	-3.30	106.55	113.15
2	D	601	A1AI0	F2-C6-C5	3.24	122.58	119.01
2	A	601	A1AI0	C18-C19-C20	3.18	123.55	119.56
2	C	601	A1AI0	C16-C15-C20	3.08	119.75	117.33
2	A	601	A1AI0	C11-C7-C8	3.07	106.25	102.40
2	C	601	A1AI0	C4-C5-C7	-3.04	118.82	121.92
2	C	601	A1AI0	C1-C6-C5	-3.03	119.46	123.46
2	C	601	A1AI0	C15-C13-N1	-2.97	108.27	113.79
2	D	601	A1AI0	C1-C6-C5	-2.94	119.57	123.46
2	B	601	A1AI0	C13-C15-C20	-2.84	117.04	121.67
2	D	601	A1AI0	C15-C13-N1	-2.75	108.68	113.79
2	B	601	A1AI0	F2-C6-C5	2.72	122.01	119.01
2	B	601	A1AI0	C13-N1-C14	-2.67	116.10	120.72
2	D	601	A1AI0	C4-C5-C6	2.54	119.85	116.28
2	B	601	A1AI0	C15-C20-CL1	-2.53	116.56	119.16
2	B	601	A1AI0	C1-C6-C5	-2.53	120.12	123.46
2	D	601	A1AI0	C25-C14-N1	-2.47	117.96	121.39
2	B	601	A1AI0	C11-C7-C8	2.47	105.50	102.40
2	C	601	A1AI0	F2-C6-C5	2.41	121.67	119.01
2	A	601	A1AI0	C11-C7-C5	-2.37	108.41	113.15
2	C	601	A1AI0	C15-C20-CL1	-2.34	116.76	119.16
2	B	601	A1AI0	C19-C20-C15	-2.27	120.10	121.97
2	D	601	A1AI0	C9-C8-C7	2.18	107.67	105.00
2	B	601	A1AI0	C21-C14-N1	-2.15	118.40	121.39
2	C	601	A1AI0	C8-C7-C5	-2.12	108.91	113.15
2	B	601	A1AI0	C19-C20-CL1	2.09	123.33	118.60
2	A	601	A1AI0	C16-C15-C20	2.07	118.95	117.33
2	B	601	A1AI0	C11-C7-C5	-2.04	109.07	113.15
2	D	601	A1AI0	C15-C20-CL1	-2.02	117.09	119.16
2	B	601	A1AI0	C15-C13-N1	-2.01	110.06	113.79
2	D	601	A1AI0	C10-C11-C7	2.00	107.45	105.00

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	A1AI0	C27-C26-O2-C23
2	A	601	A1AI0	N2-C29-C30-C31
2	A	601	A1AI0	C29-C30-C31-F1
2	B	601	A1AI0	C28-C26-O2-C23
2	B	601	A1AI0	C29-C30-C31-F1

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Mol	Chain	Res	Type	Atoms
2	C	601	A1AI0	N2-C29-C30-C31
2	D	601	A1AI0	C6-C5-C7-C12
2	D	601	A1AI0	N2-C29-C30-C31
2	D	601	A1AI0	C29-C30-C31-F1
2	B	601	A1AI0	N2-C29-C30-C31
2	B	601	A1AI0	C22-C23-O2-C26
2	B	601	A1AI0	C24-C23-O2-C26
2	A	601	A1AI0	C22-C23-O2-C26
2	A	601	A1AI0	C24-C23-O2-C26
2	D	601	A1AI0	C22-C23-O2-C26
2	B	601	A1AI0	C27-C26-O2-C23
2	D	601	A1AI0	C6-C5-C7-C11
2	D	601	A1AI0	C24-C23-O2-C26
2	C	601	A1AI0	C29-C30-C31-F1
2	C	601	A1AI0	N1-C12-C7-C5
2	C	601	A1AI0	C28-C26-O2-C23
2	D	601	A1AI0	C28-C26-O2-C23
2	D	601	A1AI0	C27-C26-O2-C23
2	C	601	A1AI0	N1-C12-C7-C11

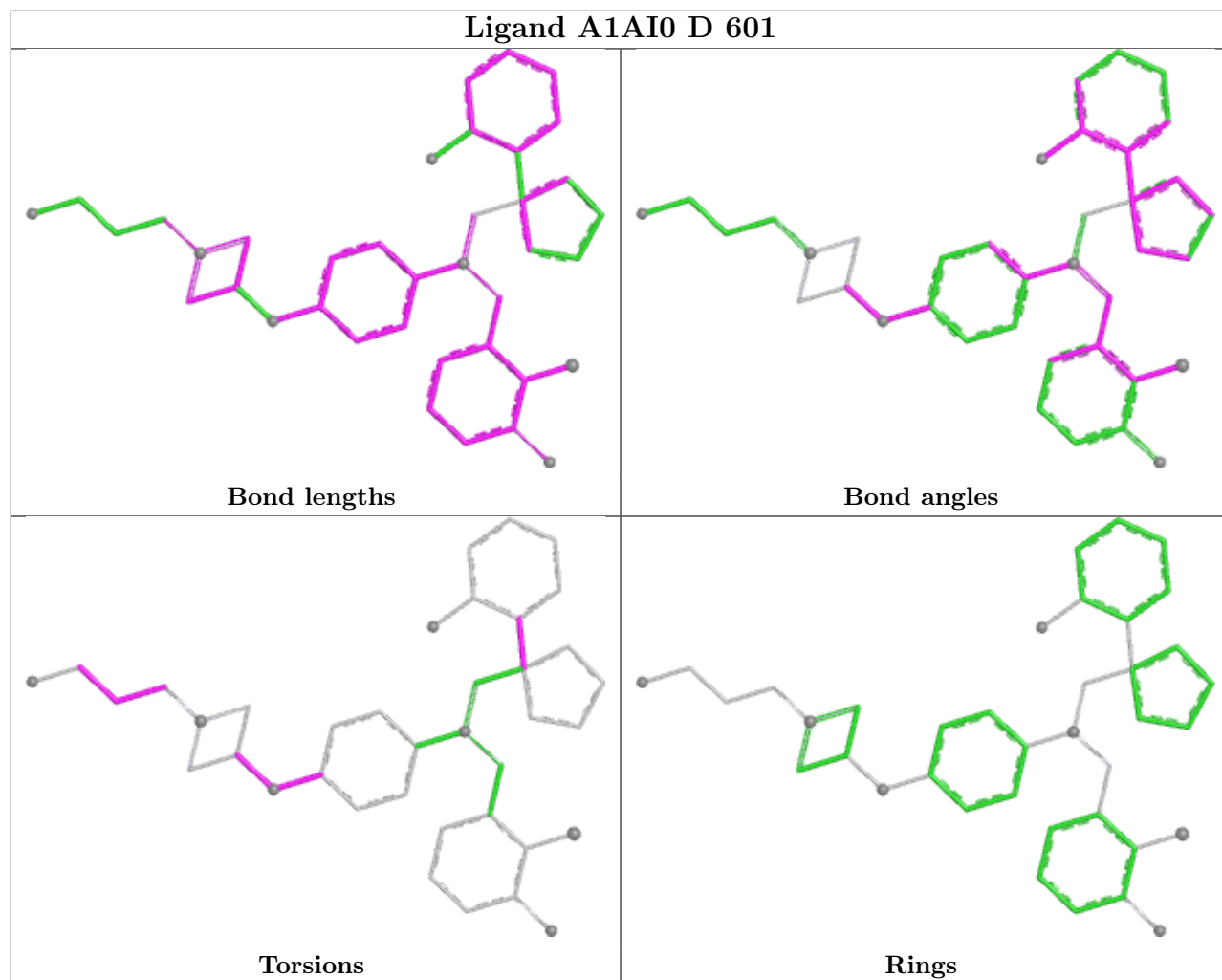
There are no ring outliers.

3 monomers are involved in 3 short contacts:

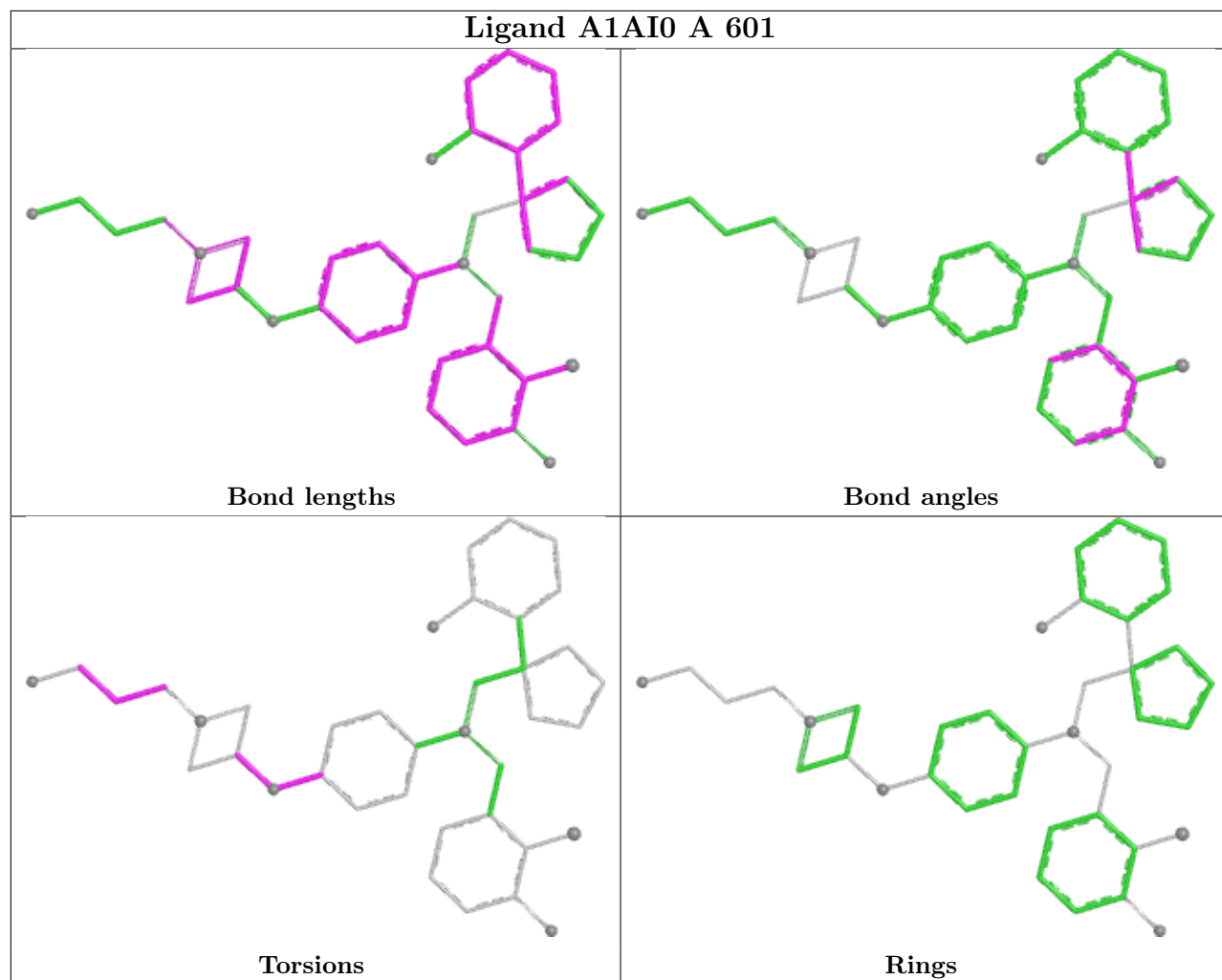
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	A1AI0	1	0
2	A	601	A1AI0	1	0
2	B	601	A1AI0	1	0

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.

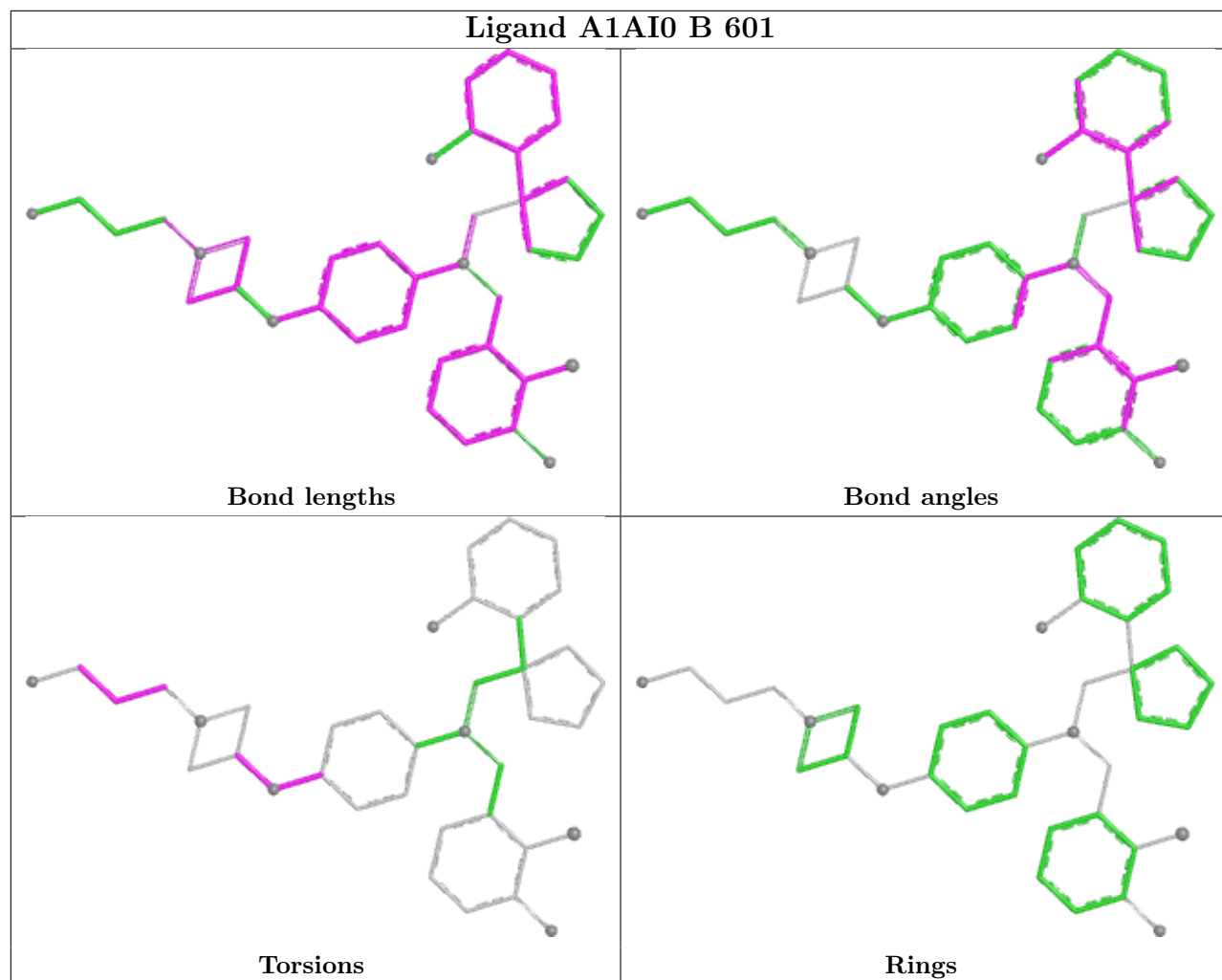
## Ligand A1AI0 D 601

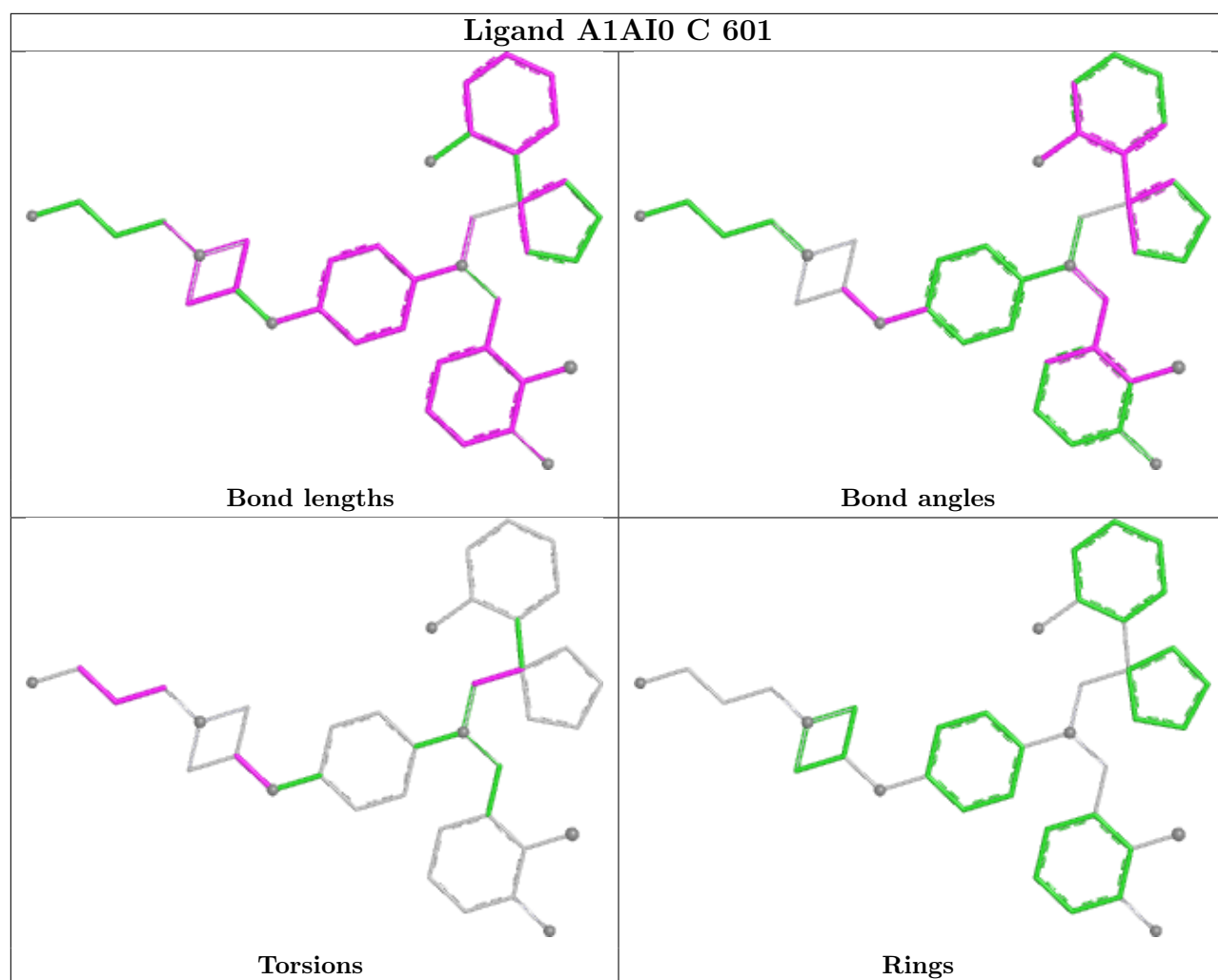


## Ligand A1AI0 A 601



## Ligand A1AI0 B 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	230/255 (90%)	1.07	30 (13%)	7 8	15, 28, 47, 57	1 (0%)
1	B	230/255 (90%)	0.83	27 (11%)	9 9	14, 26, 48, 62	3 (1%)
1	C	216/255 (84%)	0.87	22 (10%)	12 13	7, 25, 43, 67	1 (0%)
1	D	219/255 (85%)	1.11	31 (14%)	6 6	12, 28, 50, 78	2 (0%)
All	All	895/1020 (87%)	0.97	110 (12%)	8 8	7, 27, 48, 78	7 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	550	HIS	6.1
1	C	373	HIS	5.2
1	B	422	VAL	4.8
1	B	473[A]	ASP	4.8
1	C	528	MET	4.7
1	D	533	VAL	4.5
1	C	414	GLN	4.4
1	D	497	LEU	4.3
1	C	415	GLY	4.0
1	A	423	GLU	3.9
1	B	460	THR	3.8
1	B	421	MET	3.6
1	A	458	VAL	3.5
1	D	528	MET	3.5
1	C	359	ASN	3.5
1	C	322	ALA	3.5
1	B	457	GLY	3.4
1	A	497	LEU	3.4
1	A	482	ILE	3.4
1	A	331	TYR	3.4
1	A	415	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	523	GLU	3.3
1	D	450[A]	SER	3.3
1	A	493	ALA	3.3
1	A	312	ALA	3.3
1	B	312	ALA	3.2
1	D	414	GLN	3.2
1	D	343	MET	3.2
1	B	307	ALA	3.2
1	A	464	SER	3.2
1	A	421	MET	3.1
1	C	457	GLY	3.1
1	D	425	PHE	3.1
1	D	534	VAL	3.1
1	A	460	THR	3.0
1	A	471	GLU	3.0
1	A	457	GLY	3.0
1	D	468	SER	3.0
1	A	422	VAL	3.0
1	A	533	VAL	3.0
1	D	342	MET	3.0
1	A	414	GLN	2.9
1	B	348	ASN	2.9
1	A	332	ASP	2.9
1	D	549	LEU	2.8
1	B	420	GLY	2.8
1	C	307	ALA	2.8
1	A	316	VAL	2.8
1	B	332	ASP	2.8
1	B	331	TYR	2.8
1	B	466	LEU	2.8
1	B	436	ARG	2.7
1	C	400	GLY	2.7
1	A	546	ALA	2.7
1	A	310	LEU	2.7
1	C	317	SER	2.7
1	C	534	VAL	2.6
1	A	434	ARG	2.6
1	A	505	ALA	2.6
1	D	351	ASP	2.6
1	B	482	ILE	2.6
1	D	328	TYR	2.6
1	C	497	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	397	GLU	2.5
1	B	458	VAL	2.5
1	C	424	ILE	2.5
1	D	514	ILE	2.5
1	B	336	PRO	2.5
1	A	459	TYR	2.5
1	C	450[A]	SER	2.5
1	C	408	LEU	2.4
1	D	380	GLU	2.4
1	A	433	SER	2.4
1	D	491	ALA	2.4
1	D	415	GLY	2.4
1	A	308	LEU	2.3
1	B	330	GLU	2.3
1	D	397	GLU	2.3
1	D	500	GLN	2.3
1	D	541	LEU	2.3
1	C	343	MET	2.3
1	B	308	LEU	2.3
1	B	427[A]	MET	2.3
1	B	469	LEU	2.3
1	B	459	TYR	2.3
1	A	501	HIS	2.2
1	C	547	HIS	2.2
1	C	525	LEU	2.2
1	A	369	ASP	2.2
1	B	532	ASN	2.2
1	D	535	PRO	2.2
1	D	493	ALA	2.2
1	B	461	PHE	2.1
1	A	469	LEU	2.1
1	B	384	LEU	2.1
1	D	486	LEU	2.1
1	B	468	SER	2.1
1	C	425	PHE	2.1
1	D	311	THR	2.1
1	B	415	GLY	2.1
1	C	546	ALA	2.1
1	D	309	SER	2.1
1	D	519	ASN	2.1
1	D	522	MET	2.0
1	C	384	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	525	LEU	2.0
1	A	513	HIS	2.0
1	D	521	GLY	2.0
1	B	309	SER	2.0
1	D	457	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

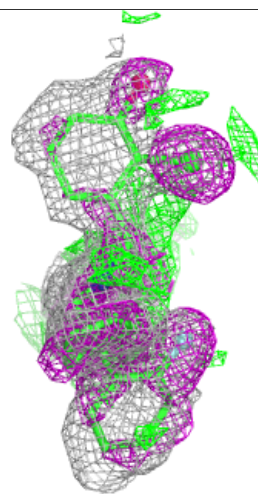
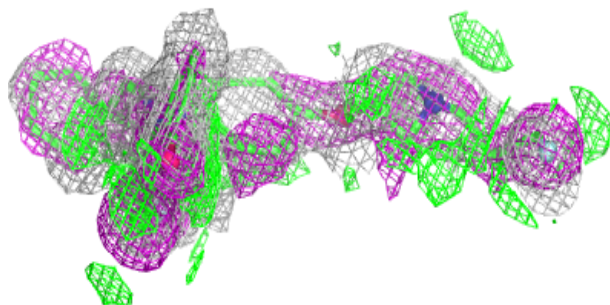
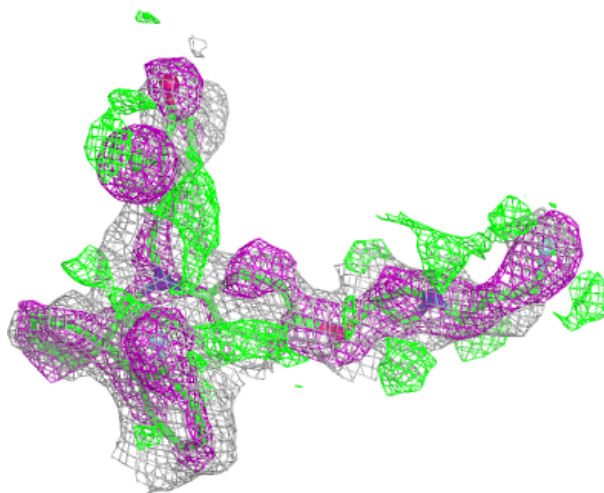
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	A1AI0	A	601	38/38	0.77	0.14	0,0,0,0	0
2	A1AI0	C	601	38/38	0.84	0.14	26,45,51,55	0
2	A1AI0	D	601	38/38	0.85	0.14	24,43,53,55	0
2	A1AI0	B	601	38/38	0.91	0.13	16,22,39,43	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.

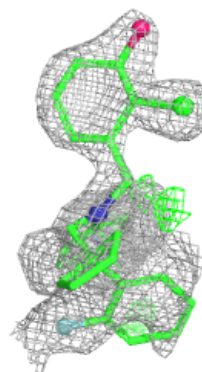
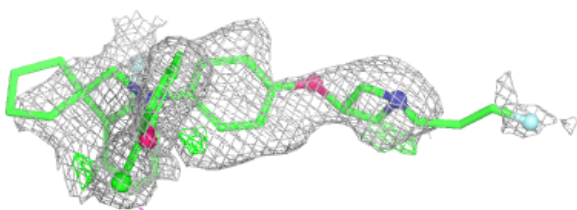
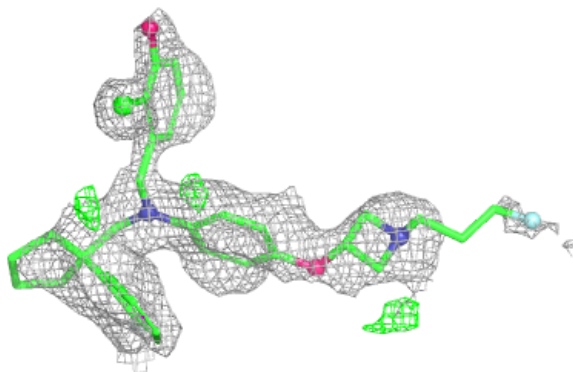
**Electron density around A1AI0 A 601:**

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

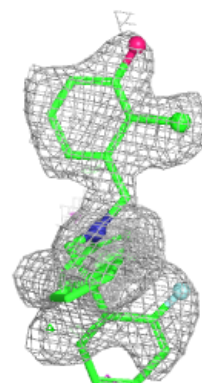
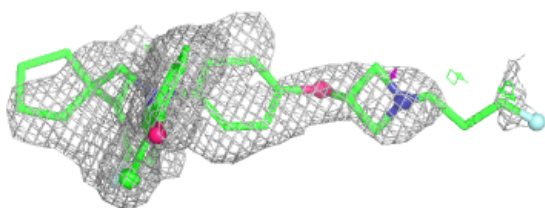
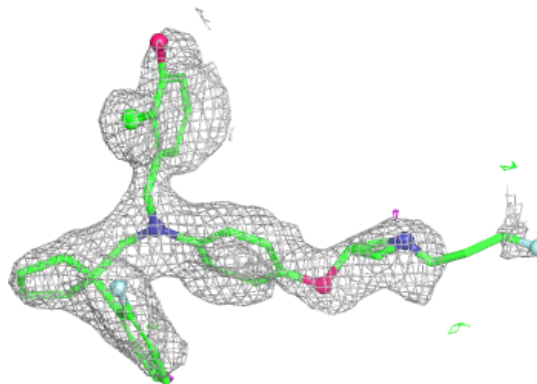


**Electron density around A1AI0 C 601:**

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

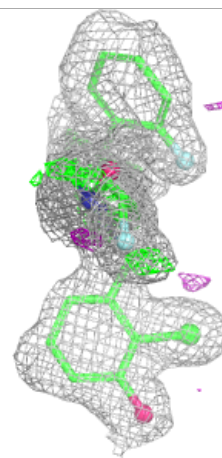
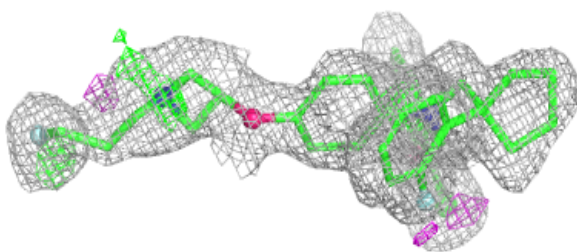
**Electron density around A1AI0 D 601:**

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



**Electron density around A1AI0 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.