



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2026 – 02:14 PM EDT

PDB ID : 9OLC / pdb\_00009olc  
Title : Crystal structure of PPAR $\gamma$  ligand-binding domain in complex with NCoR1 peptide and FTX-6746  
Authors : Setser, J.W.; DeLaBarre, B.  
Deposited on : 2025-05-12  
Resolution : 2.83 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:

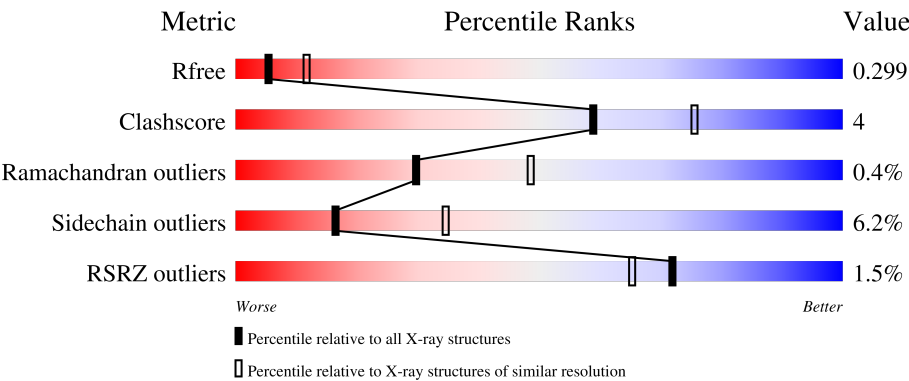
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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 <sub>free</sub>	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	278	<div><div>%</div><div><div></div><div>73%</div><div>13%</div><div>•</div><div>13%</div></div></div>
1	B	278	<div><div>%</div><div><div></div><div>75%</div><div>12%</div><div>•</div><div>12%</div></div></div>
1	C	278	<div><div>%</div><div><div></div><div>72%</div><div>14%</div><div></div><div>14%</div></div></div>
1	D	278	<div><div>2%</div><div><div></div><div>62%</div><div>9%</div><div>•</div><div>27%</div></div></div>
2	E	13	<div><div></div><div><div></div><div>85%</div><div>15%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	13	 77% 23%
2	G	13	 85% 8% 8%
2	H	13	 62% 8% 31%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7913 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 Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1951	1265	316	361	9			
1	B	245	Total	C	N	O	S	0	0	0
			1962	1270	319	364	9			
1	C	240	Total	C	N	O	S	0	0	0
			1928	1250	315	356	7			
1	D	202	Total	C	N	O	S	0	0	0
			1629	1059	263	301	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	SER	-	expression tag	UNP P37231
A	229	ASN	-	expression tag	UNP P37231
A	230	ALA	-	expression tag	UNP P37231
B	228	SER	-	expression tag	UNP P37231
B	229	ASN	-	expression tag	UNP P37231
B	230	ALA	-	expression tag	UNP P37231
C	228	SER	-	expression tag	UNP P37231
C	229	ASN	-	expression tag	UNP P37231
C	230	ALA	-	expression tag	UNP P37231
D	228	SER	-	expression tag	UNP P37231
D	229	ASN	-	expression tag	UNP P37231
D	230	ALA	-	expression tag	UNP P37231

- Molecule 2 is a protein called Nuclear receptor corepressor 1 peptide.

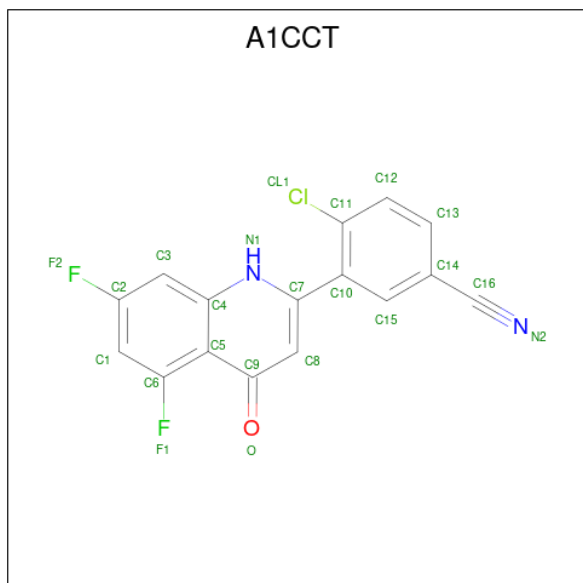
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	S	0	0	0
			102	65	18	18	1			
2	F	13	Total	C	N	O	S	0	0	0
			102	65	18	18	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	12	Total	C	N	O	S	0	0	0
			94	61	16	16	1			
2	H	9	Total	C	N	O		0	0	0
			74	48	13	13				

- Molecule 3 is (3P)-4-chloro-3-(5,7-difluoro-4-oxo-1,4-dihydroquinolin-2-yl)benzonitrile (CCD ID: A1CCT) (formula: C<sub>16</sub>H<sub>7</sub>ClF<sub>2</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			21	16	2	2	1		
3	B	1	Total	C	F	N	O	0	0
			21	16	2	2	1		
3	C	1	Total	C	F	N	O	0	0
			21	16	2	2	1		

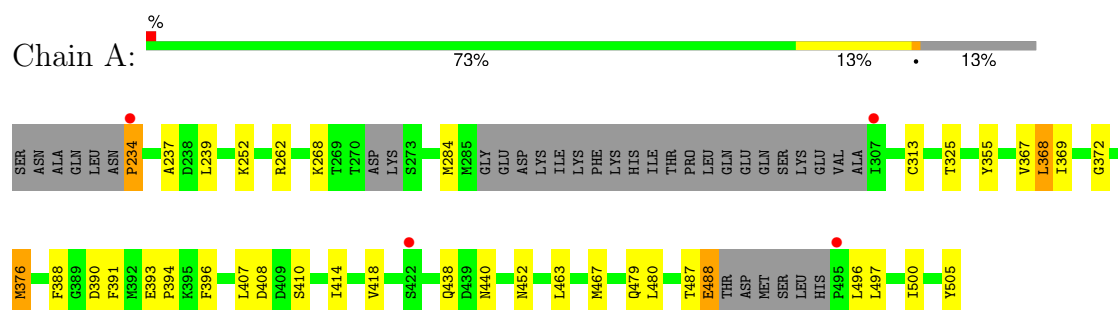
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		

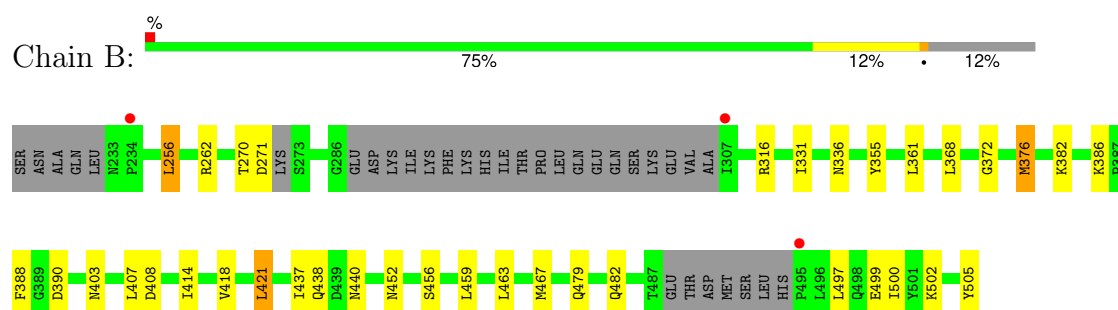
### 3 Residue-property plots [i](#)

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.

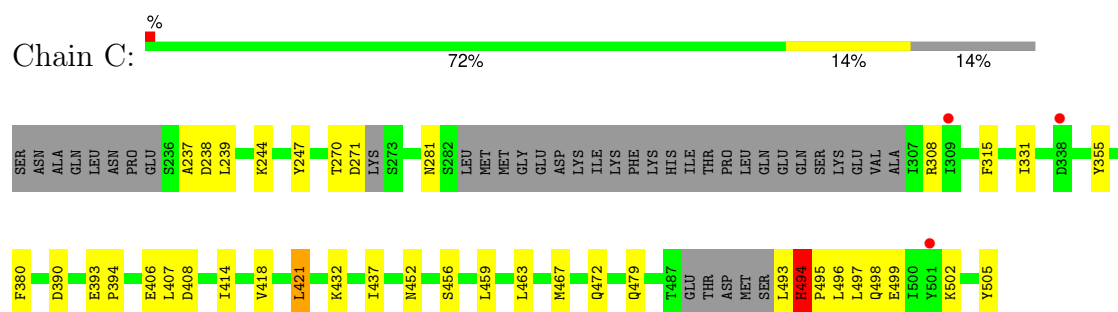
- Molecule 1: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma

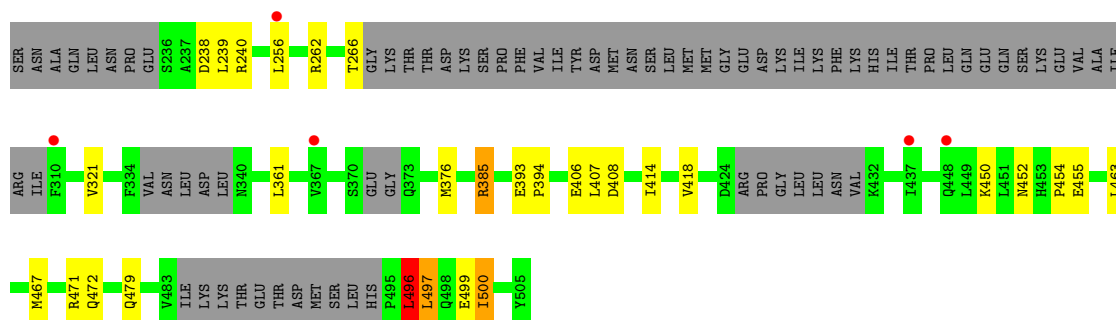


- Molecule 1: Peroxisome proliferator-activated receptor gamma



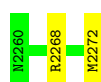
- Molecule 1: Peroxisome proliferator-activated receptor gamma





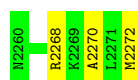
- Molecule 2: Nuclear receptor corepressor 1 peptide

Chain E: 85% 15%



- Molecule 2: Nuclear receptor corepressor 1 peptide

Chain F: 77% 23%



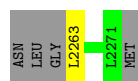
- Molecule 2: Nuclear receptor corepressor 1 peptide

Chain G: 85% 8% 8%



- Molecule 2: Nuclear receptor corepressor 1 peptide

Chain H: 62% 8% 31%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.13Å 70.33Å 92.68Å 101.19° 106.58° 104.98°	Depositor
Resolution (Å)	48.05 – 2.83 48.05 – 2.83	Depositor EDS
% Data completeness (in resolution range)	85.2 (48.05-2.83) 85.2 (48.05-2.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.231 , 0.298 0.235 , 0.299	Depositor DCC
$R_{free}$ test set	1159 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.4	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: A1CCT

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	0.52	0/1983	1.05	0/2668
1	B	0.53	0/1994	1.06	0/2684
1	C	0.50	0/1960	1.01	0/2640
1	D	0.50	0/1654	1.05	0/2221
2	E	0.51	0/101	1.07	0/133
2	F	0.53	0/101	1.07	0/133
2	G	0.48	0/93	1.06	0/122
2	H	0.47	0/73	1.03	0/96
All	All	0.51	0/7959	1.05	0/10697

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	1951	0	2011	23	0
1	B	1962	0	2017	16	0
1	C	1928	0	1983	20	0
1	D	1629	0	1668	17	0
2	E	102	0	113	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	102	0	113	1	0
2	G	94	0	107	0	0
2	H	74	0	84	1	0
3	A	21	0	0	1	0
3	B	21	0	0	0	0
3	C	21	0	0	0	0
4	A	6	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	7913	0	8096	70	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 4.

All (70) 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:244:LYS:HG3	1:D:454:PRO:HB3	1.75	0.67
1:C:237:ALA:HB1	1:D:240:ARG:HE	1.59	0.67
1:D:376:MET:SD	1:D:500:ILE:HG22	2.36	0.64
1:A:367:VAL:CG2	1:A:396:PHE:CZ	2.81	0.63
1:A:414:ILE:O	1:A:418:VAL:HG23	1.99	0.63
1:B:414:ILE:O	1:B:418:VAL:HG23	2.00	0.62
1:C:414:ILE:O	1:C:418:VAL:HG23	1.99	0.61
1:B:418:VAL:CG1	1:B:467:MET:HE1	2.30	0.61
1:D:414:ILE:O	1:D:418:VAL:HG23	2.00	0.59
1:B:331:ILE:HG21	1:B:421:LEU:CD1	2.32	0.59
1:A:418:VAL:CG1	1:A:467:MET:HE1	2.33	0.58
1:A:410:SER:OG	1:B:336:ASN:ND2	2.37	0.58
1:C:247:TYR:CE2	1:D:455:GLU:HB3	2.38	0.57
1:B:256:LEU:HD13	1:B:361:LEU:HD21	1.86	0.57
1:C:418:VAL:CG1	1:C:467:MET:HE1	2.34	0.56
1:C:331:ILE:HG21	1:C:421:LEU:CD1	2.36	0.56
1:A:418:VAL:HG12	1:A:467:MET:HE1	1.87	0.56
1:D:418:VAL:CG1	1:D:467:MET:HE1	2.35	0.56
1:B:262:ARG:NH1	1:B:403:ASN:OD1	2.39	0.55
1:B:418:VAL:HG12	1:B:467:MET:HE1	1.87	0.55
1:A:367:VAL:CG2	1:A:396:PHE:HZ	2.20	0.54
1:C:380:PHE:CZ	1:C:497:LEU:HD21	2.44	0.53
1:A:325:THR:HG21	2:F:2270:ALA:HB3	1.92	0.51
1:C:498:GLN:O	1:C:502:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:LYS:HA	1:D:454:PRO:HG3	1.93	0.51
1:C:494:HIS:O	1:C:498:GLN:HG3	2.11	0.50
1:A:376:MET:HE1	1:A:500:ILE:HG23	1.94	0.49
1:A:367:VAL:HG23	1:A:396:PHE:HZ	1.77	0.49
1:B:376:MET:HE1	1:B:500:ILE:HG23	1.95	0.49
1:C:418:VAL:HG12	1:C:467:MET:HE1	1.94	0.48
1:A:388:PHE:CE1	1:A:497:LEU:HD13	2.48	0.48
1:A:368:LEU:HG	1:A:372:GLY:HA2	1.96	0.47
1:A:393:GLU:N	1:A:394:PRO:HD2	2.29	0.47
1:A:367:VAL:HG22	1:A:396:PHE:CZ	2.49	0.47
1:D:418:VAL:HG12	1:D:467:MET:HE1	1.96	0.47
1:D:496:LEU:H	1:D:496:LEU:HD12	1.79	0.47
1:C:393:GLU:N	1:C:394:PRO:HD2	2.31	0.46
1:B:388:PHE:CE1	1:B:497:LEU:HD13	2.50	0.46
1:D:393:GLU:N	1:D:394:PRO:HD2	2.31	0.46
1:D:321:VAL:HG21	2:H:2263:LEU:HD11	1.97	0.46
1:C:244:LYS:HD2	1:D:450:LYS:O	2.16	0.45
1:A:234:PRO:HA	1:A:237:ALA:CB	2.46	0.45
1:C:408:ASP:OD1	1:C:452:ASN:ND2	2.50	0.45
1:B:355:TYR:OH	1:B:505:TYR:OXT	2.29	0.45
1:A:284:MET:HE1	1:A:496:LEU:HD21	1.98	0.45
1:A:355:TYR:OH	1:A:505:TYR:OXT	2.29	0.45
1:B:421:LEU:HD22	1:B:437:ILE:HB	1.98	0.44
1:D:497:LEU:HA	1:D:500:ILE:HG12	1.98	0.44
1:A:234:PRO:HA	1:A:237:ALA:HB3	1.98	0.44
1:C:421:LEU:HD22	1:C:437:ILE:HB	1.99	0.44
1:A:407:LEU:HD11	1:A:463:LEU:HD13	2.00	0.43
1:A:408:ASP:OD1	1:A:452:ASN:ND2	2.51	0.43
1:D:408:ASP:OD1	1:D:452:ASN:ND2	2.51	0.43
1:C:432:LYS:HD2	1:C:432:LYS:HA	1.92	0.43
1:C:407:LEU:HD11	1:C:463:LEU:HD13	2.01	0.43
1:D:262:ARG:O	1:D:266:THR:N	2.49	0.43
1:C:355:TYR:OH	1:C:505:TYR:OXT	2.30	0.42
1:A:313:CYS:SG	3:A:601:A1CCT:C8	3.07	0.42
1:D:238:ASP:OD1	1:D:239:LEU:N	2.51	0.42
1:B:408:ASP:OD1	1:B:452:ASN:ND2	2.53	0.42
1:C:238:ASP:OD1	1:C:239:LEU:N	2.53	0.42
1:B:407:LEU:HD11	1:B:463:LEU:HD13	2.02	0.41
1:D:407:LEU:HD11	1:D:463:LEU:HD13	2.01	0.41
1:A:487:THR:O	1:A:488:GLU:C	2.63	0.41
1:C:456:SER:HB3	1:C:459:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:PHE:CE1	1:A:480:LEU:HD11	2.56	0.41
1:A:438:GLN:C	1:A:440:ASN:N	2.79	0.40
1:B:456:SER:HB3	1:B:459:LEU:HB2	2.04	0.40
1:B:368:LEU:HD13	1:B:372:GLY:HA2	2.03	0.40
1:B:438:GLN:C	1:B:440:ASN:N	2.80	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	235/278 (84%)	230 (98%)	5 (2%)	0	100	100
1	B	237/278 (85%)	234 (99%)	3 (1%)	0	100	100
1	C	232/278 (84%)	225 (97%)	5 (2%)	2 (1%)	14	27
1	D	190/278 (68%)	185 (97%)	3 (2%)	2 (1%)	11	23
2	E	11/13 (85%)	11 (100%)	0	0	100	100
2	F	11/13 (85%)	11 (100%)	0	0	100	100
2	G	10/13 (77%)	10 (100%)	0	0	100	100
2	H	7/13 (54%)	7 (100%)	0	0	100	100
All	All	933/1164 (80%)	913 (98%)	16 (2%)	4 (0%)	30	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	495	PRO
1	D	496	LEU
1	C	494	HIS
1	D	385	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/250 (87%)	207 (95%)	11 (5%)	22	44
1	B	219/250 (88%)	206 (94%)	13 (6%)	18	37
1	C	215/250 (86%)	201 (94%)	14 (6%)	15	32
1	D	180/250 (72%)	169 (94%)	11 (6%)	17	35
2	E	11/11 (100%)	9 (82%)	2 (18%)	2	2
2	F	11/11 (100%)	9 (82%)	2 (18%)	2	2
2	G	10/11 (91%)	9 (90%)	1 (10%)	7	16
2	H	8/11 (73%)	8 (100%)	0	100	100
All	All	872/1044 (84%)	818 (94%)	54 (6%)	16	34

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	PRO
1	A	239	LEU
1	A	252	LYS
1	A	262	ARG
1	A	268	LYS
1	A	368	LEU
1	A	369	ILE
1	A	376	MET
1	A	390	ASP
1	A	479	GLN
1	A	488	GLU
1	B	256	LEU
1	B	270	THR
1	B	271	ASP
1	B	316	ARG
1	B	376	MET
1	B	382	LYS
1	B	386	LYS
1	B	390	ASP

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Mol	Chain	Res	Type
1	B	421	LEU
1	B	479	GLN
1	B	482	GLN
1	B	499	GLU
1	B	502	LYS
1	C	270	THR
1	C	271	ASP
1	C	281	ASN
1	C	308	ARG
1	C	315	PHE
1	C	390	ASP
1	C	406	GLU
1	C	421	LEU
1	C	472	GLN
1	C	479	GLN
1	C	493	LEU
1	C	494	HIS
1	C	496	LEU
1	C	499	GLU
1	D	256	LEU
1	D	361	LEU
1	D	385	ARG
1	D	406	GLU
1	D	471	ARG
1	D	472	GLN
1	D	479	GLN
1	D	496	LEU
1	D	497	LEU
1	D	499	GLU
1	D	500	ILE
2	E	2268	ARG
2	E	2272	MET
2	F	2268	ARG
2	F	2272	MET
2	G	2272	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	340	ASN
1	B	245	HIS

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Mol	Chain	Res	Type
1	D	245	HIS
1	D	311	GLN
1	D	373	GLN

### 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 ⓘ

3 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	$\# Z  > 2$
3	A1CCT	C	601	1	22,23,24	0.72	0	30,33,35	1.58	4 (13%)
3	A1CCT	A	601	1	22,23,24	0.95	0	30,33,35	2.10	9 (30%)
3	A1CCT	B	601	1	22,23,24	0.83	1 (4%)	30,33,35	2.06	9 (30%)

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
3	A1CCT	C	601	1	-	0/6/6/6	0/3/3/3
3	A1CCT	A	601	1	-	0/6/6/6	0/3/3/3
3	A1CCT	B	601	1	-	1/6/6/6	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	A1CCT	C4-N1	-2.04	1.36	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	A1CCT	C1-C6-C5	-6.85	117.41	123.96
3	B	601	A1CCT	C1-C6-C5	-5.62	118.58	123.96
3	C	601	A1CCT	C1-C6-C5	-5.28	118.91	123.96
3	A	601	A1CCT	C12-C11-C10	-4.38	116.06	120.36
3	A	601	A1CCT	C6-C1-C2	3.73	120.64	116.67
3	B	601	A1CCT	C15-C10-C7	-3.56	114.93	120.43
3	B	601	A1CCT	C6-C1-C2	3.51	120.41	116.67
3	B	601	A1CCT	C11-C10-C7	3.42	126.00	120.81
3	C	601	A1CCT	O-C9-C5	-3.16	116.94	122.10
3	B	601	A1CCT	F2-C2-C1	2.95	122.47	118.28
3	B	601	A1CCT	F1-C6-C1	2.94	124.52	118.64
3	B	601	A1CCT	C3-C2-C1	-2.91	119.97	123.50
3	A	601	A1CCT	C8-C7-N1	2.79	122.61	118.98
3	C	601	A1CCT	C6-C1-C2	2.71	119.56	116.67
3	A	601	A1CCT	C11-C10-C15	2.70	122.37	119.25
3	A	601	A1CCT	C15-C10-C7	-2.62	116.39	120.43
3	A	601	A1CCT	C10-C7-C8	-2.45	120.33	123.59
3	C	601	A1CCT	C11-C10-C7	2.34	124.35	120.81
3	B	601	A1CCT	O-C9-C5	-2.30	118.34	122.10
3	A	601	A1CCT	F1-C6-C1	2.09	122.81	118.64
3	A	601	A1CCT	F2-C2-C1	2.07	121.22	118.28
3	B	601	A1CCT	C12-C11-C10	-2.02	118.38	120.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	A1CCT	C11-C10-C7-C8

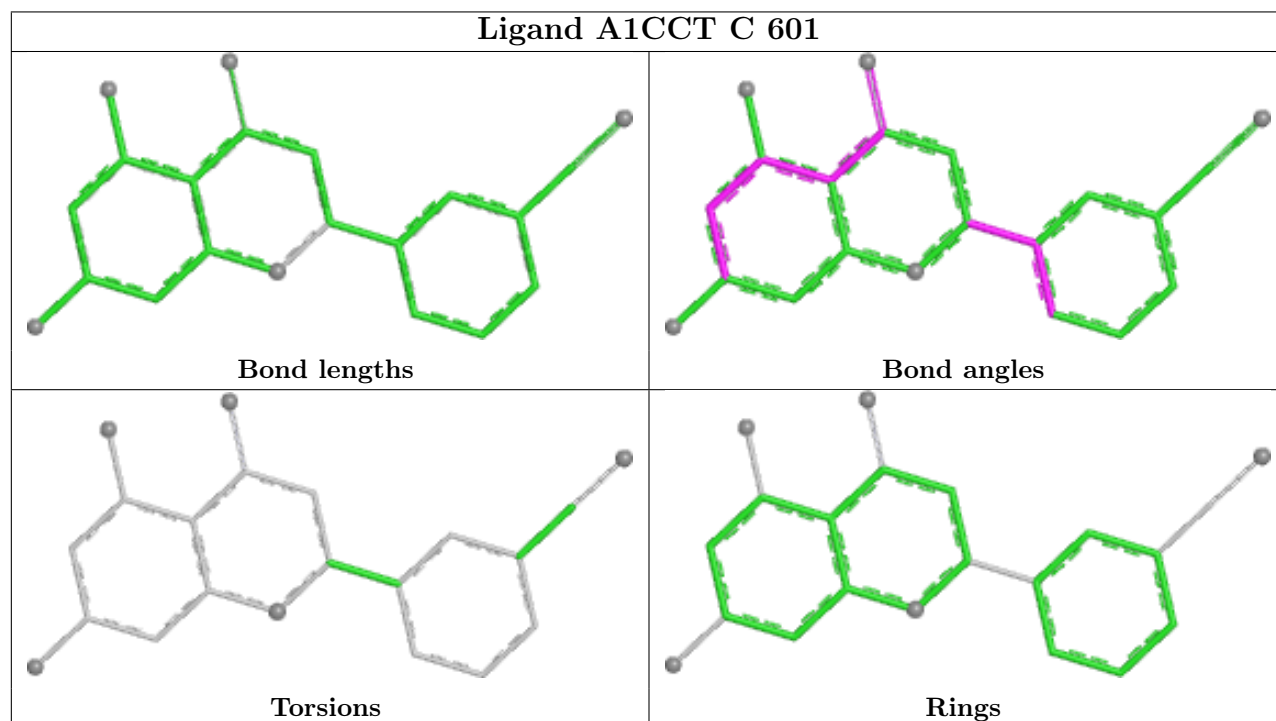
There are no ring outliers.

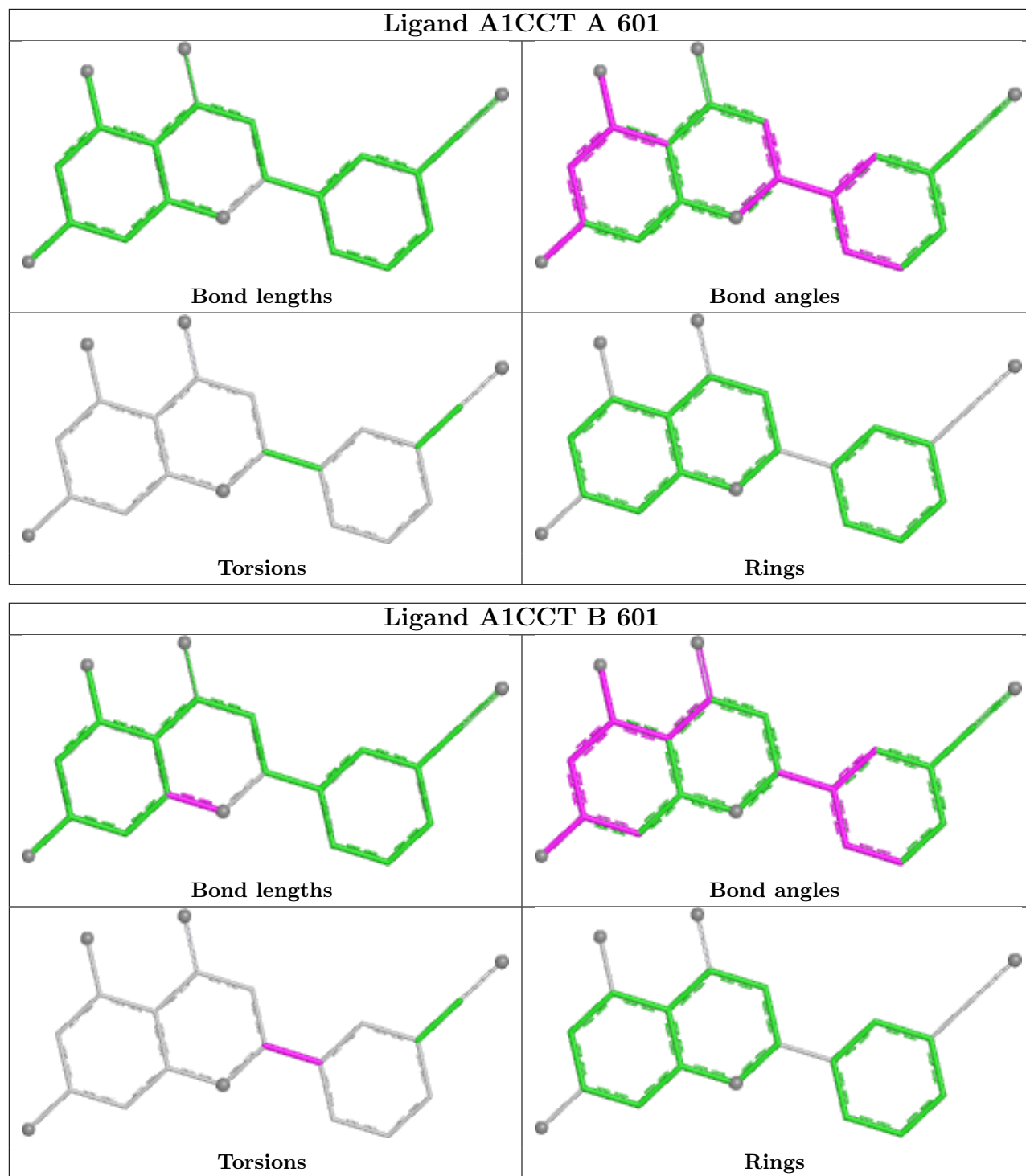


1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	A1CCT	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	243/278 (87%)	0.12	4 (1%) 70 64	45, 69, 106, 138	0
1	B	245/278 (88%)	-0.05	3 (1%) 76 71	43, 64, 106, 144	0
1	C	240/278 (86%)	0.20	3 (1%) 75 69	55, 82, 119, 158	0
1	D	202/278 (72%)	0.62	5 (2%) 58 49	78, 123, 160, 219	0
2	E	13/13 (100%)	0.22	0 100 100	58, 68, 119, 119	0
2	F	13/13 (100%)	0.43	0 100 100	63, 75, 104, 139	0
2	G	12/13 (92%)	0.12	0 100 100	67, 98, 111, 123	0
2	H	9/13 (69%)	0.60	0 100 100	116, 150, 165, 182	0
All	All	977/1164 (83%)	0.21	15 (1%) 72 65	43, 79, 143, 219	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	PRO	3.6
1	A	307	ILE	3.5
1	B	307	ILE	3.0
1	B	234	PRO	2.7
1	A	422	SER	2.7
1	D	448	GLN	2.6
1	A	495	PRO	2.6
1	C	338	ASP	2.6
1	C	501	TYR	2.4
1	B	495	PRO	2.3
1	C	309	ILE	2.3
1	D	256	LEU	2.2
1	D	310	PHE	2.2
1	D	367	VAL	2.1
1	D	437	ILE	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](#)

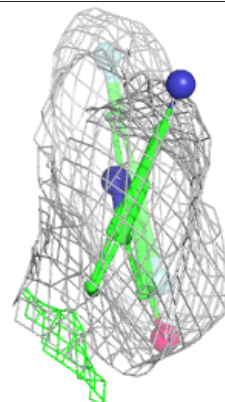
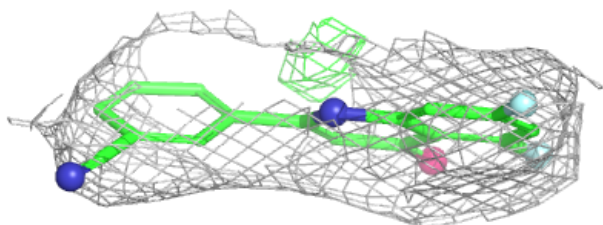
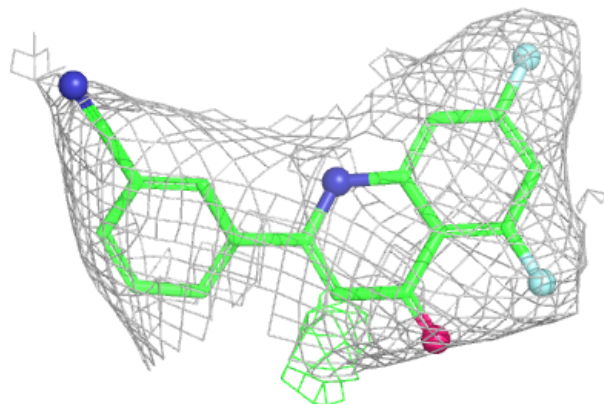
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1CCT	A	601	21/22	0.92	0.08	53,59,72,87	0
3	A1CCT	C	601	21/22	0.93	0.07	62,67,75,82	0
3	A1CCT	B	601	21/22	0.96	0.06	47,53,61,62	0

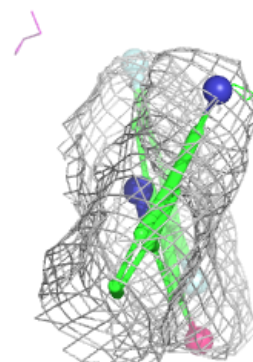
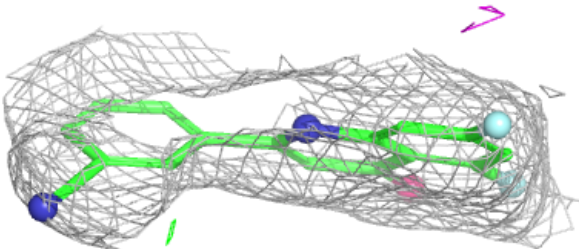
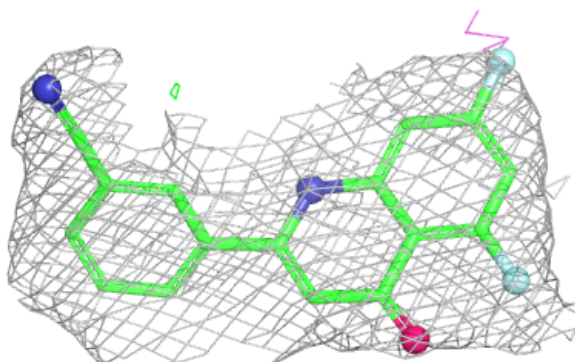
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1CCT 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)

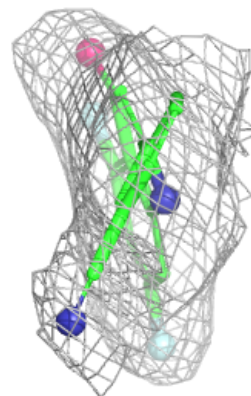
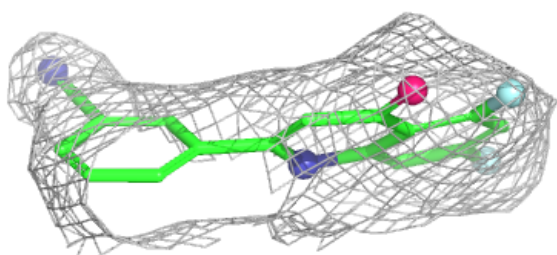
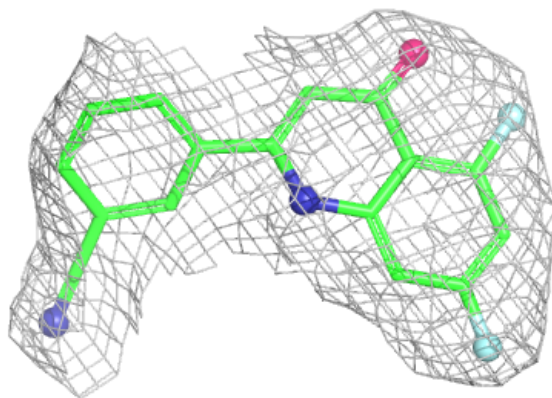
**Electron density around A1CCT C 601:**

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



**Electron density around A1CCT 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.