



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 09:47 am BST

PDB ID : 1G50
Title : CRYSTAL STRUCTURE OF A WILD TYPE HER ALPHA LBD AT 2.9
ANGSTROM RESOLUTION
Authors : Eiler, S.; Gangloff, M.; Duclaud, S.; Moras, D.; Ruff, M.; Structural Pro-
teomics in Europe (SPINE)
Deposited on : 2000-10-30
Resolution : 2.90 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 : 2.11
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) : 2.11

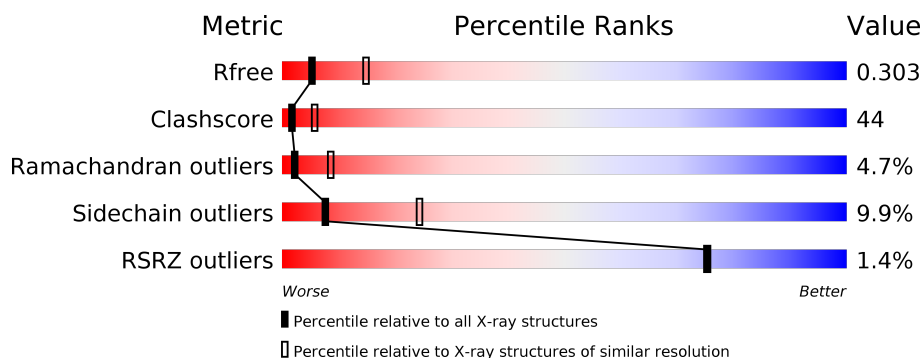
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	247	<div> <div>29%</div> <div>59%</div> <div>11%</div> <div>.</div> </div>
1	B	247	<div> <div>%</div> <div>36%</div> <div>57%</div> <div>.</div> <div>.</div> </div>
1	C	247	<div> <div>3%</div> <div>37%</div> <div>54%</div> <div>6%</div> <div>.</div> <div>.</div> </div>

2 Entry composition [i](#)

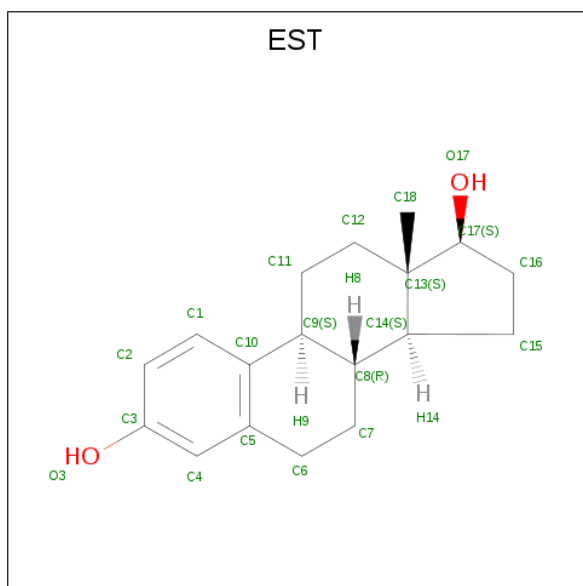
There are 3 unique types of molecules in this entry. The entry contains 6109 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	247	Total	C	N	O	S	0	0	0
			1975	1264	338	354	19			
1	B	246	Total	C	N	O	S	0	0	0
			1964	1258	335	352	19			
1	C	244	Total	C	N	O	S	0	0	0
			1945	1246	330	350	19			

- Molecule 2 is ESTRADIOL (three-letter code: EST) (formula: $C_{18}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			20	18	2		
2	C	1	Total	C	O	0	0
			20	18	2		

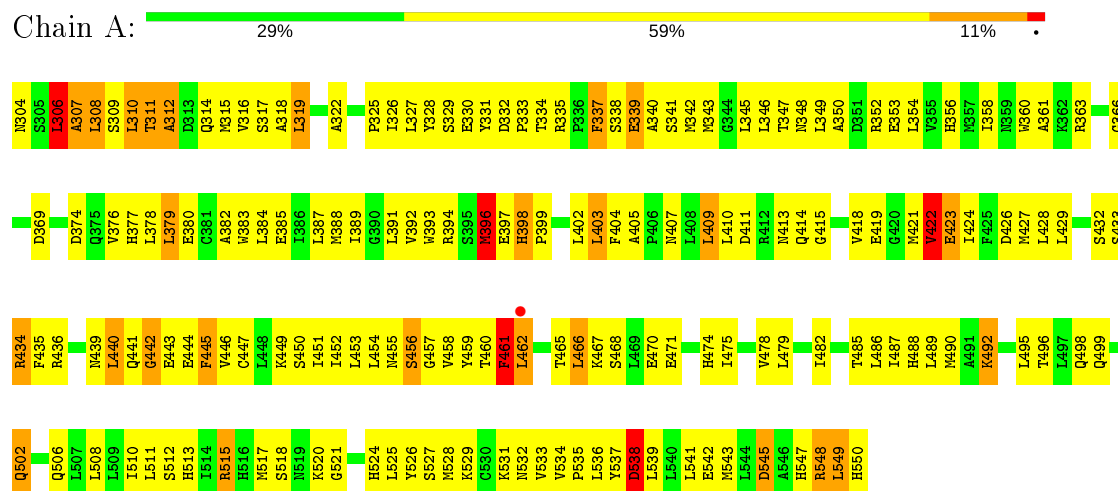
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	53	Total 53	O 53	0	0
3	C	55	Total 55	O 55	0	0

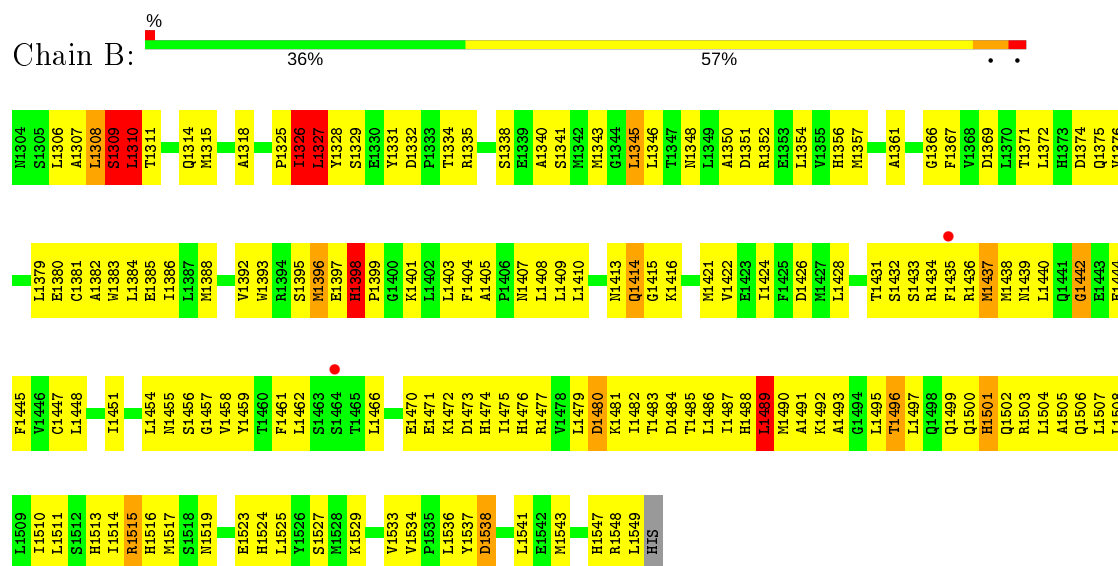
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



N2304	L2378	F2445	I2510
S2305	L2379	V2446	L2511
A2306	E2380	C2447	S2512
A2307	C2381	L2448	R2513
L2308	A2382	I2451	I2514
T2311	V2383	L2454	R2515
Q2314	L2384	I2455	R2516
M2315	E2385	S2456	M2517
M2318	I2386	G2457	S2518
A2318	M2387	V2458	N2519
L2319	M2388	Y2459	R2524
A2322	V2392	T2460	S2527
P2325	R2393	F2461	M2528
I2326	S2394	L2462	K2529
L2327	M2396	S2463	V2533
Y2328	E2397	S2464	V2534
Y2331	R2398	T2465	F2535
T2334	F2399	L2466	L2536
R2335	G2400	K2467	Y2537
P2336	K2401	S2468	D2538
F2337	L2402	E2471	L2541
S2338	L2403	K2472	E2542
E2339	F2404	D2473	M2543
A2340	A2405	R2474	R2547
S2341	P2406	I2475	ARG
M2342	M2407	R2476	LEU
M2343	L2408	L2479	HIS
G2344	L2409	D2480	
L2345	L2410	K2481	
L2346	N2413	I2482	
T2347	Q2414	T2485	
N2348	G2415	L2486	
L2349	K2416	I2487	
A2350	N2421	R2488	
D2351	V2422	I2489	
R2352	E2423	M2490	
E2353	I2424	A2491	
L2354	F2425	K2492	
V2355	D2426	A2493	
H2356	M2427	G2494	
M2357	L2428	I2495	
A2361	L2429	T2496	
G2366	A2430	L2497	
D2369	T2431	Q2498	
L2372	S2432	Q2499	
H2373	S2433	Q2500	
D2374	R2434	R2501	
Q2375	F2435	Q2502	
V2376	R2436	R2503	
H2377	M2437	L2504	
	N2438	A2505	
	N2439	Q2506	
		L2507	
		L2508	
		E2442	
		E2443	
		E2444	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.50Å 105.50Å 136.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.18 – 2.90 49.18 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.18-2.90) 91.0 (49.18-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	8.00	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.310 0.238 , 0.303	Depositor DCC
R_{free} test set	1778 reflections (9.80%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6109	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	2/2013 (0.1%)	0.74	2/2720 (0.1%)
1	B	0.76	2/2001 (0.1%)	0.72	5/2705 (0.2%)
1	C	0.68	1/1982 (0.1%)	0.69	3/2680 (0.1%)
All	All	0.66	5/5996 (0.1%)	0.72	10/8105 (0.1%)

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	B	0	2
1	C	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2495	LEU	N-CA	26.00	1.98	1.46
1	B	1310	LEU	N-CA	23.00	1.92	1.46
1	B	1327	LEU	N-CA	18.79	1.83	1.46
1	A	548	ARG	N-CA	6.64	1.59	1.46
1	A	461	PHE	N-CA	5.12	1.56	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2494	GLY	C-N-CA	-11.12	93.89	121.70
1	A	548	ARG	N-CA-CB	11.12	130.62	110.60
1	B	1309	SER	C-N-CA	-10.34	95.86	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2495	LEU	N-CA-CB	-9.75	90.90	110.40
1	B	1310	LEU	N-CA-C	-8.91	86.94	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1309	SER	Peptide
1	B	1326	ILE	Peptide
1	C	2494	GLY	Peptide

5.2 Too-close contacts

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	1975	0	2025	206	0
1	B	1964	0	2018	175	0
1	C	1945	0	1994	170	0
2	A	20	0	24	2	0
2	B	20	0	24	2	0
2	C	20	0	24	1	0
3	A	57	0	0	10	0
3	B	53	0	0	2	0
3	C	55	0	0	5	0
All	All	6109	0	6109	525	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 44.

The worst 5 of 525 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:B:1327:LEU:CA	1:B:1327:LEU:N	1.83	1.38
1:B:1310:LEU:N	1:B:1310:LEU:CA	1.92	1.32
1:B:1327:LEU:N	1:B:1327:LEU:HD23	1.46	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2495:LEU:CA	1:C:2495:LEU:N	1.98	1.27
1:B:1327:LEU:H	1:B:1327:LEU:CD2	1.62	1.12

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	245/247 (99%)	185 (76%)	43 (18%)	17 (7%)	1	3
1	B	244/247 (99%)	204 (84%)	31 (13%)	9 (4%)	3	13
1	C	242/247 (98%)	202 (84%)	32 (13%)	8 (3%)	4	15
All	All	731/741 (99%)	591 (81%)	106 (14%)	34 (5%)	2	8

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1308	LEU
1	A	306	LEU
1	A	308	LEU
1	A	339	GLU
1	A	403	LEU

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	223/223 (100%)	197 (88%)	26 (12%)	5	16
1	B	222/223 (100%)	203 (91%)	19 (9%)	10	30
1	C	220/223 (99%)	199 (90%)	21 (10%)	8	26
All	All	665/669 (99%)	599 (90%)	66 (10%)	8	24

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1345	LEU
1	B	1461	PHE
1	C	2489	LEU
1	B	1374	ASP
1	B	1414	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1439	ASN
1	B	1455	ASN
1	C	2474	HIS
1	B	1359	ASN
1	B	1375	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 carbohydrates 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
2	EST	B	1600	-	23,23,23	2.53	12 (52%)	36,36,36	1.08	2 (5%)
2	EST	A	600	-	23,23,23	2.45	10 (43%)	36,36,36	1.11	3 (8%)
2	EST	C	2600	-	23,23,23	2.61	9 (39%)	36,36,36	1.05	2 (5%)

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	EST	B	1600	-	-	-	0/4/4/4
2	EST	A	600	-	-	-	0/4/4/4
2	EST	C	2600	-	-	-	0/4/4/4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1600	EST	C5-C10	5.35	1.48	1.40
2	C	2600	EST	C1-C10	5.29	1.46	1.39
2	C	2600	EST	C5-C10	5.22	1.48	1.40
2	A	600	EST	C5-C10	5.11	1.48	1.40
2	B	1600	EST	C9-C8	4.99	1.60	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	EST	C16-C17-C13	2.67	106.66	104.53
2	B	1600	EST	C11-C9-C8	-2.60	107.89	111.39
2	C	2600	EST	C11-C9-C8	-2.57	107.92	111.39
2	A	600	EST	C11-C9-C8	-2.51	108.01	111.39
2	B	1600	EST	C16-C17-C13	2.33	106.39	104.53

There are no chirality outliers.

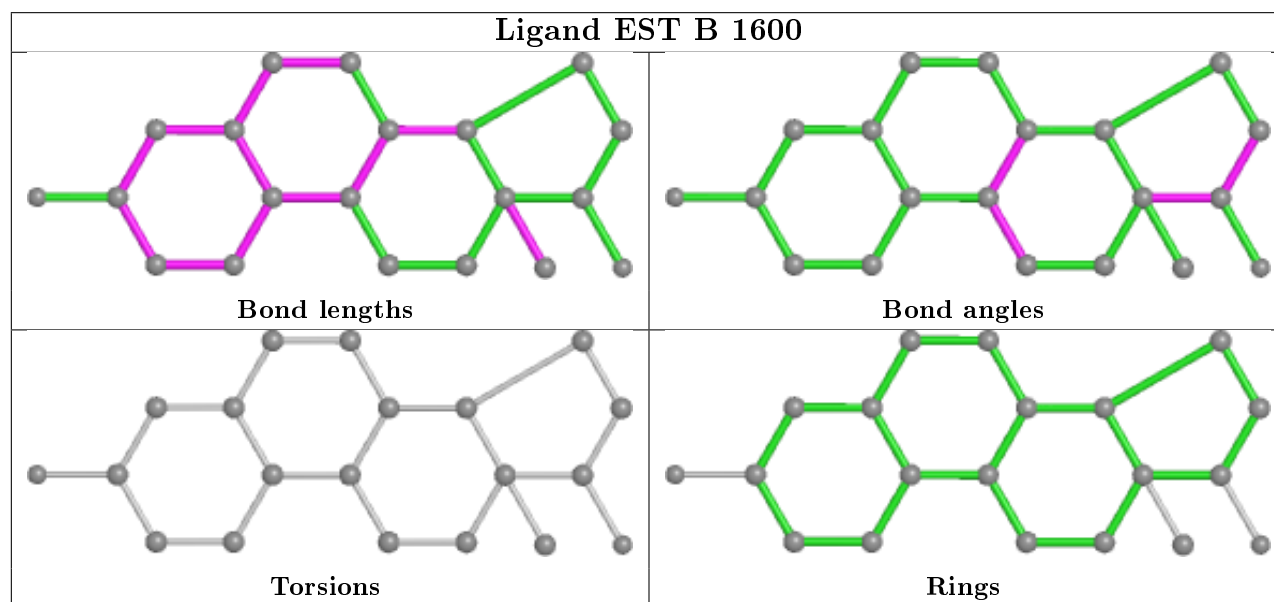
There are no torsion outliers.

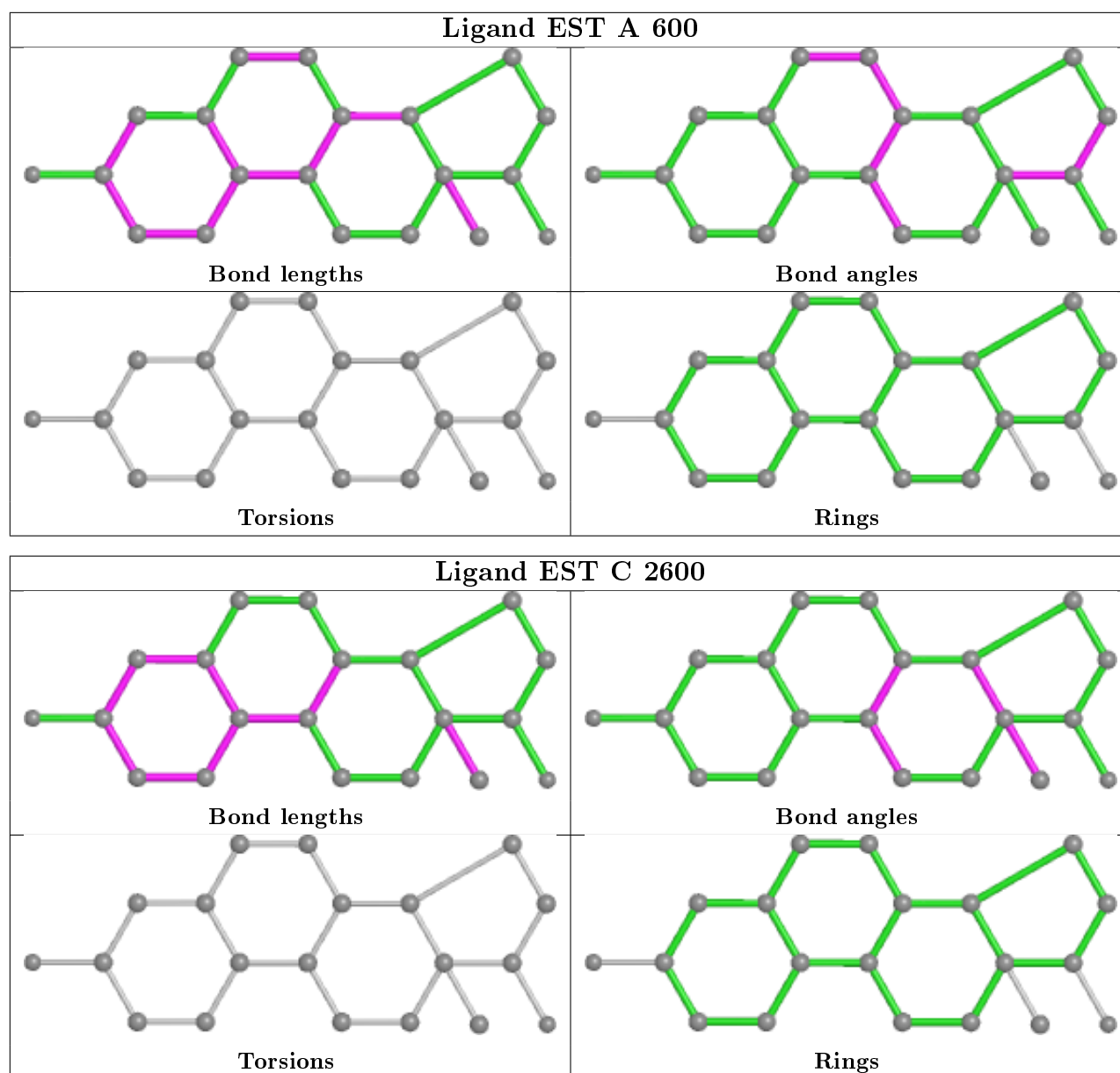
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1600	EST	2	0
2	A	600	EST	2	0
2	C	2600	EST	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	247/247 (100%)	-0.31	1 (0%) 92 93	19, 45, 78, 98	0
1	B	246/247 (99%)	-0.02	2 (0%) 86 86	46, 70, 85, 95	0
1	C	244/247 (98%)	0.12	7 (2%) 51 47	47, 70, 92, 102	0
All	All	737/741 (99%)	-0.07	10 (1%) 75 75	19, 63, 89, 102	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2334	THR	4.9
1	C	2415	GLY	2.9
1	C	2410	LEU	2.8
1	B	1464	SER	2.4
1	C	2331	TYR	2.4

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](#)

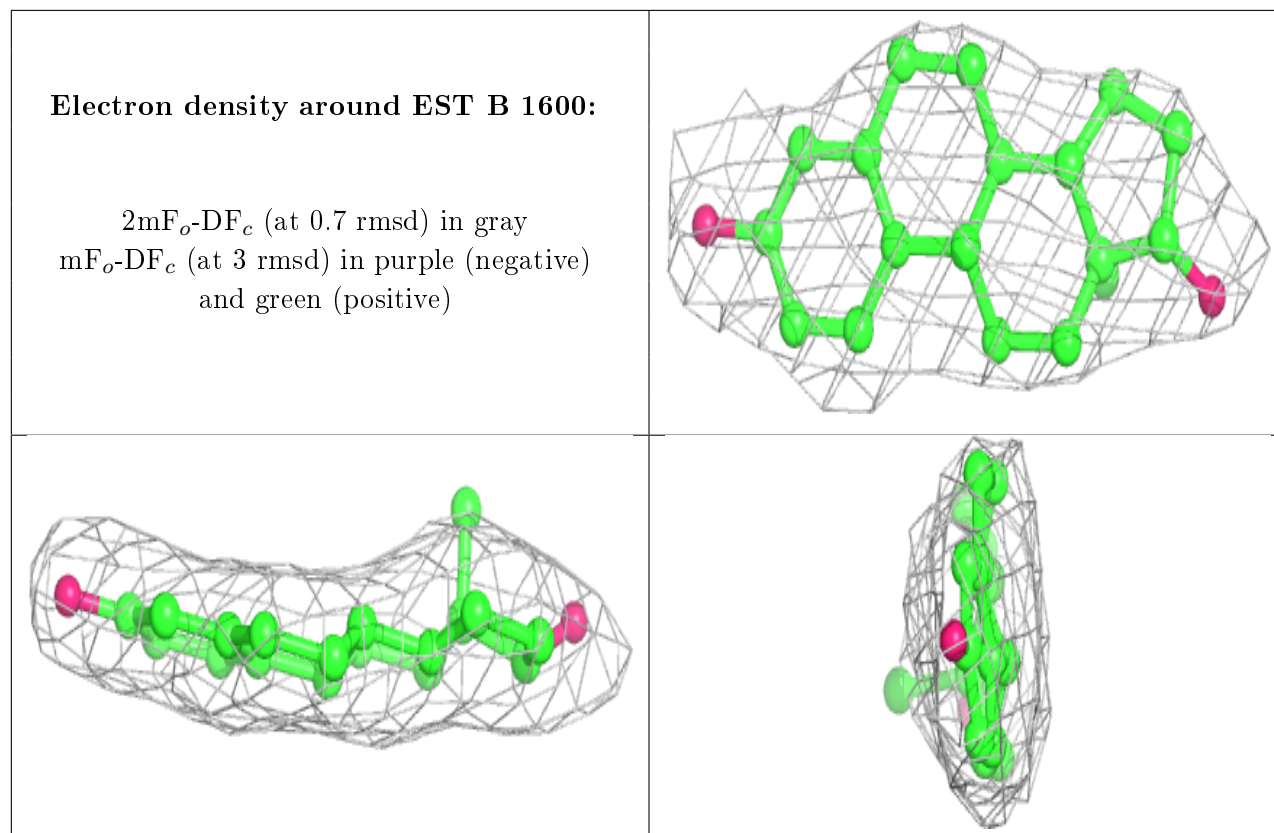
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

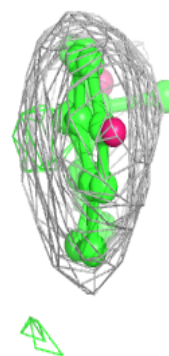
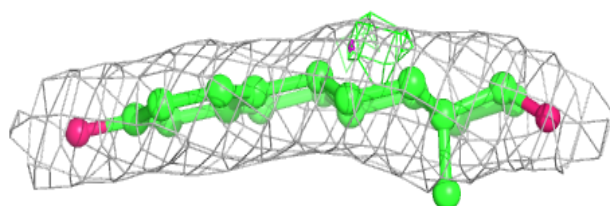
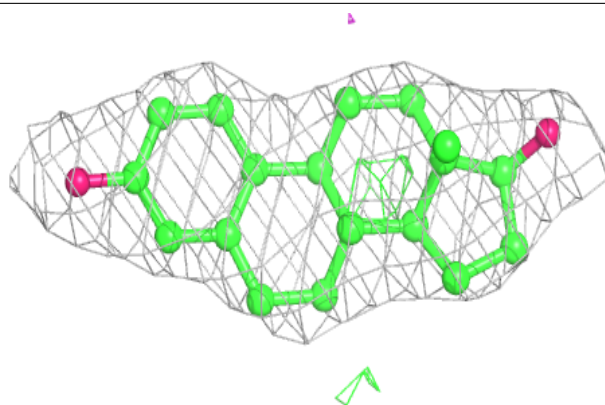
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EST	B	1600	20/20	0.96	0.21	34,36,38,39	0
2	EST	C	2600	20/20	0.96	0.19	31,36,38,38	0
2	EST	A	600	20/20	0.97	0.22	30,33,35,39	0

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.

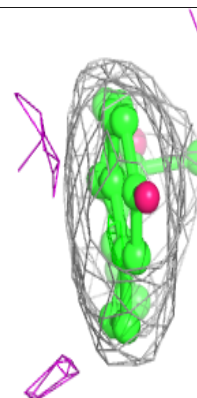
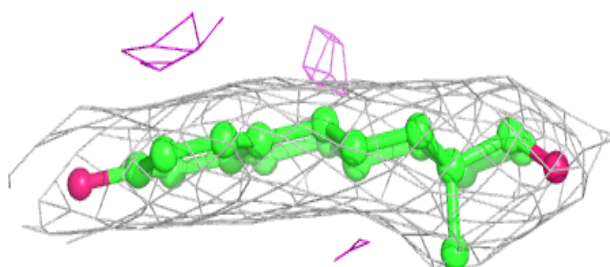
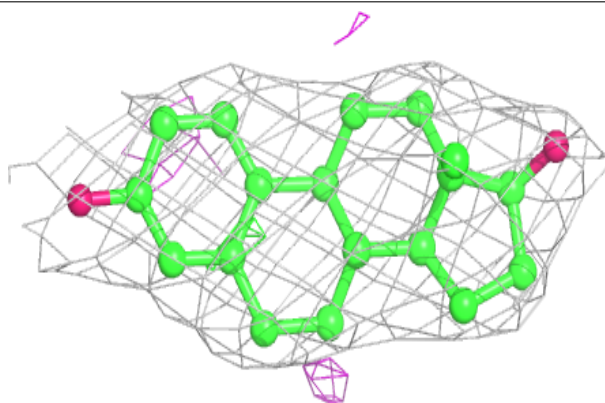


Electron density around EST C 2600:

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

**Electron density around EST 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.