



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:33 am BST

PDB ID : 1S9P  
Title : crystal structure of the ligand-binding domain of the estrogen-related receptor gamma in complex with diethylstilbestrol  
Authors : Greschik, H.; Flaig, R.; Renaud, J.P.; Moras, D.  
Deposited on : 2004-02-05  
Resolution : 2.13 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.

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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

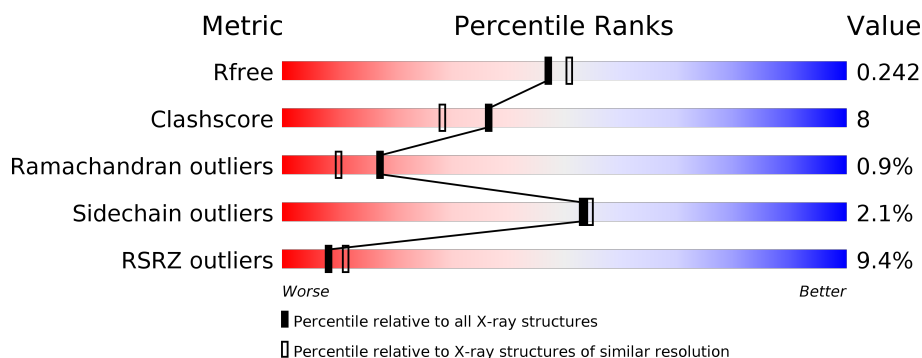
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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  $\geq 3$ , 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	227	<div> <div>11%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	B	227	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>•</div> </div> </div>
1	C	227	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>•</div> </div> </div>
1	D	227	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

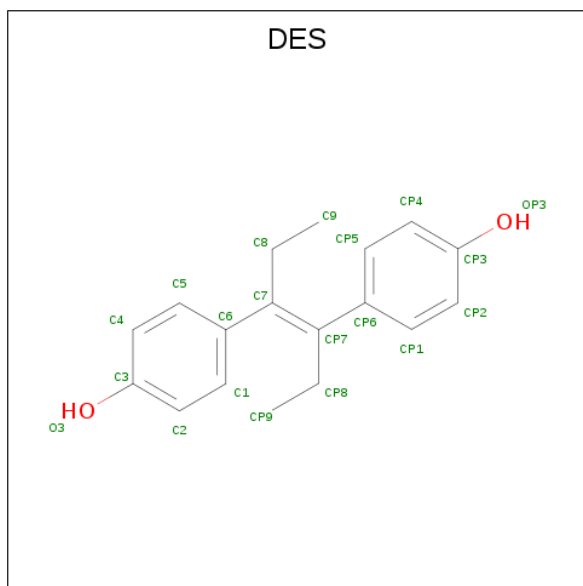
There are 3 unique types of molecules in this entry. The entry contains 7129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-related receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1679	1072	274	323	10			
1	B	217	Total	C	N	O	S	0	0	0
			1696	1084	277	325	10			
1	C	219	Total	C	N	O	S	0	0	0
			1696	1083	277	326	10			
1	D	225	Total	C	N	O	S	0	0	0
			1772	1137	287	336	12			

- Molecule 2 is DIETHYLSTILBESTROL (three-letter code: DES) (formula: C<sub>18</sub>H<sub>20</sub>O<sub>2</sub>).



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		

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

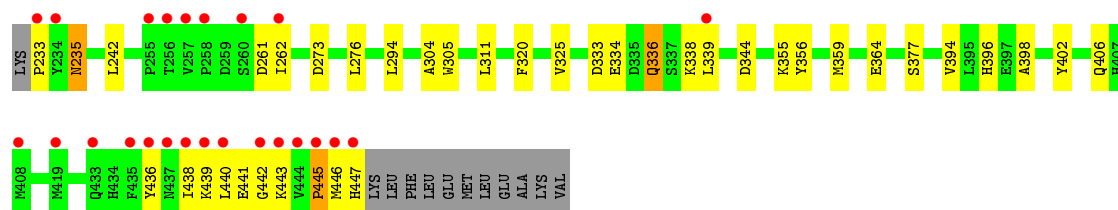
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	63	Total	O	0	0
			63	63		
3	C	41	Total	O	0	0
			41	41		
3	D	49	Total	O	0	0
			49	49		

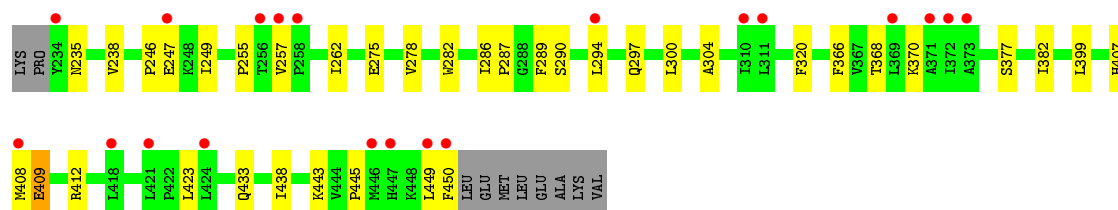
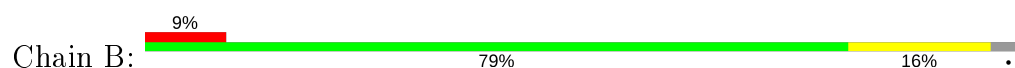
### 3 Residue-property plots [i](#)

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.

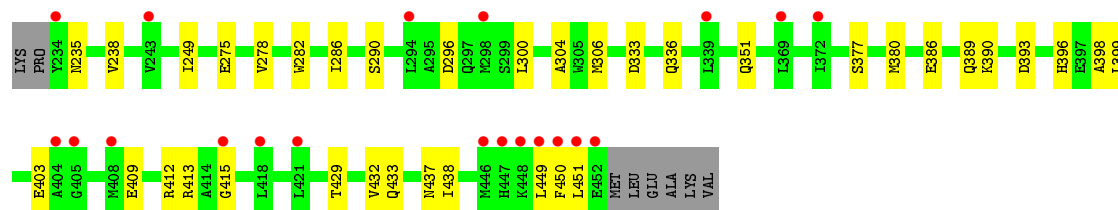
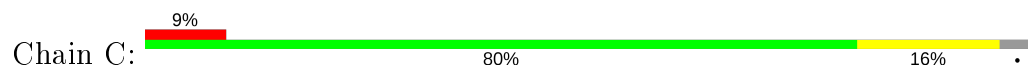
#### • Molecule 1: Estrogen-related receptor gamma



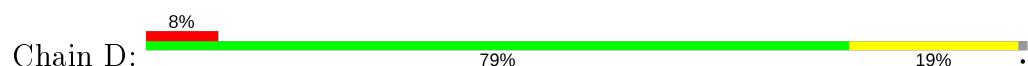
#### • Molecule 1: Estrogen-related receptor gamma

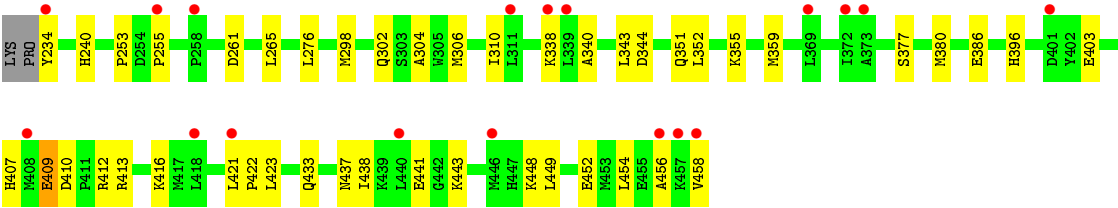


#### • Molecule 1: Estrogen-related receptor gamma



#### • Molecule 1: Estrogen-related receptor gamma





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.00Å 77.46Å 95.77Å 90.00° 97.55° 90.00°	Depositor
Resolution (Å)	29.30 – 2.13 29.30 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.30-2.13) 99.0 (29.30-2.13)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.51 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.251 0.218 , 0.242	Depositor DCC
$R_{free}$ test set	2941 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: DES

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	0.37	0/1707	0.61	2/2312 (0.1%)
1	B	0.35	0/1725	0.56	0/2334
1	C	0.31	0/1724	0.54	0/2336
1	D	0.34	0/1803	0.55	0/2440
All	All	0.34	0/6959	0.57	2/9422 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	PRO	N-CA-CB	5.61	110.03	103.30
1	A	233	PRO	N-CA-CB	5.03	109.34	103.30

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	1679	0	1677	27	0
1	B	1696	0	1710	26	0
1	C	1696	0	1693	27	0
1	D	1772	0	1791	42	0
2	A	20	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	20	0	0
2	C	20	0	20	1	0
2	D	20	0	20	0	0
3	A	53	0	0	0	0
3	B	63	0	0	1	0
3	C	41	0	0	2	0
3	D	49	0	0	0	0
All	All	7129	0	6951	109	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 8.

All (109) 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:380:MET:HG2	1:D:351:GLN:HE22	1.03	1.11
1:A:294:LEU:HD11	1:D:458:VAL:O	1.51	1.11
1:C:380:MET:HG2	1:D:351:GLN:NE2	1.83	0.93
1:A:304:ALA:HB2	1:A:377:SER:HB3	1.57	0.85
1:A:294:LEU:CD1	1:D:458:VAL:O	2.29	0.81
1:C:304:ALA:HB2	1:C:377:SER:HB3	1.65	0.76
1:D:355:LYS:HG3	1:D:359:MET:CE	2.18	0.73
1:C:333:ASP:H	1:C:336:GLN:HE21	1.35	0.73
1:C:433:GLN:HE22	1:D:433:GLN:HE22	1.37	0.73
1:D:304:ALA:HB2	1:D:377:SER:HB3	1.76	0.68
1:B:289:PHE:CE2	1:B:297:GLN:HG2	2.28	0.68
1:C:380:MET:CG	1:D:351:GLN:HE22	1.95	0.66
1:D:407:HIS:HA	1:D:409:GLU:OE2	1.95	0.66
1:B:304:ALA:HB2	1:B:377:SER:HB3	1.79	0.65
1:C:429:THR:O	1:C:433:GLN:HG3	1.97	0.65
1:C:333:ASP:H	1:C:336:GLN:NE2	1.95	0.63
1:B:438:ILE:HD12	1:B:443:LYS:HD2	1.81	0.62
1:A:339:LEU:HD23	1:A:339:LEU:O	2.00	0.61
1:C:396:HIS:CE1	1:D:412:ARG:HG2	2.36	0.61
1:C:249:ILE:HD11	1:C:278:VAL:HG21	1.81	0.60
1:D:261:ASP:O	1:D:265:LEU:HG	2.00	0.60
1:A:396:HIS:CE1	1:B:412:ARG:HG2	2.38	0.59
3:C:73:HOH:O	1:D:355:LYS:HE2	2.01	0.59
1:B:290:SER:HA	1:B:297:GLN:NE2	2.18	0.58
1:A:439:LYS:HE2	1:A:447:HIS:CB	2.33	0.58
1:B:246:PRO:HB3	1:B:278:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:GLU:CD	1:D:386:GLU:H	2.06	0.58
1:B:262:ILE:HD12	1:B:443:LYS:O	2.04	0.57
1:A:355:LYS:O	1:A:359:MET:HE2	2.04	0.57
1:D:438:ILE:HG23	1:D:443:LYS:HB2	1.86	0.55
1:A:294:LEU:HD11	1:D:458:VAL:C	2.25	0.55
1:A:436:TYR:O	1:A:440:LEU:CB	2.56	0.54
1:D:352:LEU:HD13	1:D:423:LEU:HG	1.89	0.54
1:D:448:LYS:O	1:D:452:GLU:HG3	2.07	0.54
1:B:262:ILE:CD1	1:B:443:LYS:HG2	2.38	0.54
1:B:249:ILE:HD13	1:B:275:GLU:HA	1.89	0.54
1:B:449:LEU:O	1:B:450:PHE:C	2.46	0.53
1:C:403:GLU:OE1	1:C:413:ARG:HD3	2.09	0.53
1:B:423:LEU:HD11	3:B:117:HOH:O	2.08	0.53
1:A:356:TYR:CD1	1:A:359:MET:HE3	2.44	0.53
1:D:276:LEU:HD22	1:D:454:LEU:HD12	1.89	0.53
1:D:338:LYS:CG	1:D:343:LEU:HD22	2.38	0.53
1:D:338:LYS:HG2	1:D:343:LEU:HD22	1.92	0.51
1:D:355:LYS:HG3	1:D:359:MET:HE1	1.92	0.51
1:B:366:PHE:CZ	1:B:370:LYS:HE2	2.46	0.51
1:C:449:LEU:O	1:C:451:LEU:N	2.44	0.50
1:A:333:ASP:OD1	1:A:336:GLN:HB2	2.11	0.50
1:A:355:LYS:CG	1:A:359:MET:HE1	2.42	0.50
1:B:282:TRP:CH2	1:B:286:ILE:HD11	2.47	0.50
1:D:437:ASN:O	1:D:441:GLU:HG3	2.12	0.50
1:C:449:LEU:C	1:C:451:LEU:H	2.15	0.50
1:C:386:GLU:O	1:C:390:LYS:HG3	2.11	0.49
1:C:235:ASN:HD21	1:C:398:ALA:HA	1.76	0.49
1:A:242:LEU:HD11	1:A:364:GLU:HG3	1.96	0.48
1:D:412:ARG:HB3	1:D:416:LYS:HE3	1.96	0.47
1:B:300:LEU:HD23	1:B:382:ILE:HD11	1.96	0.47
1:C:433:GLN:HE22	1:D:433:GLN:NE2	2.10	0.47
1:A:402:TYR:CE1	1:A:406:GLN:HG3	2.50	0.47
1:B:409:GLU:HG3	1:B:409:GLU:H	1.41	0.47
1:C:399:LEU:O	1:C:403:GLU:HG2	2.15	0.46
1:C:412:ARG:HA	3:C:179:HOH:O	2.15	0.46
1:C:304:ALA:HB2	1:C:377:SER:CB	2.41	0.46
1:C:438:ILE:HG13	2:C:500:DES:OP3	2.16	0.46
1:D:304:ALA:HB2	1:D:377:SER:CB	2.44	0.46
1:C:351:GLN:NE2	1:D:380:MET:HG2	2.31	0.46
1:B:255:PRO:C	1:B:257:VAL:N	2.68	0.45
1:A:438:ILE:HG13	1:A:439:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:HIS:ND1	1:B:409:GLU:OE2	2.48	0.45
1:D:298:MET:O	1:D:302:GLN:HG3	2.17	0.45
1:A:276:LEU:HD21	1:A:305:TRP:HB2	1.99	0.45
1:B:235:ASN:OD1	1:B:238:VAL:HG23	2.18	0.44
1:D:338:LYS:CE	1:D:343:LEU:HD22	2.48	0.44
1:A:261:ASP:OD1	1:A:262:ILE:N	2.50	0.44
1:D:276:LEU:HD22	1:D:454:LEU:CD1	2.48	0.43
1:C:415:GLY:HA3	1:D:396:HIS:CE1	2.53	0.43
1:D:253:PRO:O	1:D:255:PRO:HD3	2.17	0.43
1:B:320:PHE:N	1:B:320:PHE:CD2	2.86	0.43
1:A:355:LYS:HG3	1:A:359:MET:HE1	2.00	0.43
1:D:410:ASP:C	1:D:412:ARG:H	2.22	0.43
1:A:355:LYS:HG3	1:A:359:MET:CE	2.49	0.43
1:B:294:LEU:HD12	1:B:297:GLN:OE1	2.18	0.43
1:B:246:PRO:CB	1:B:278:VAL:CG1	2.96	0.43
1:B:368:THR:HG21	1:B:399:LEU:HB2	2.00	0.43
1:D:403:GLU:OE1	1:D:413:ARG:HD3	2.19	0.42
1:D:351:GLN:HE21	1:D:351:GLN:HB2	1.66	0.42
1:A:355:LYS:HG2	1:A:359:MET:HE1	2.01	0.42
1:A:334:GLU:O	1:A:338:LYS:HG3	2.19	0.42
1:A:438:ILE:HG13	1:A:439:LYS:H	1.84	0.42
1:D:355:LYS:HG3	1:D:359:MET:HE2	1.98	0.42
1:B:255:PRO:C	1:B:257:VAL:H	2.22	0.42
1:A:394:VAL:HG11	1:D:449:LEU:CD1	2.50	0.42
1:D:261:ASP:HA	1:D:340:ALA:HA	2.00	0.42
1:D:421:LEU:N	1:D:422:PRO:CD	2.83	0.42
1:A:440:LEU:C	1:A:442:GLY:H	2.24	0.42
1:C:282:TRP:CH2	1:C:286:ILE:HD11	2.55	0.41
1:B:249:ILE:HD11	1:B:278:VAL:HG21	2.01	0.41
1:B:294:LEU:HD12	1:B:294:LEU:HA	1.93	0.41
1:D:306:MET:O	1:D:310:ILE:HG12	2.21	0.41
1:C:235:ASN:OD1	1:C:238:VAL:HG23	2.20	0.41
1:C:249:ILE:HD13	1:C:275:GLU:HA	2.03	0.41
1:D:448:LYS:HD3	1:D:448:LYS:HA	1.84	0.41
1:A:320:PHE:CE2	1:A:325:VAL:HG21	2.56	0.41
1:C:306:MET:HG2	1:C:432:VAL:HG23	2.03	0.40
1:D:265:LEU:HD13	1:D:438:ILE:HG21	2.03	0.40
1:A:304:ALA:HB2	1:A:377:SER:CB	2.40	0.40
1:D:234:TYR:C	1:D:234:TYR:CD1	2.94	0.40
1:A:235:ASN:ND2	1:A:398:ALA:HA	2.36	0.40
1:B:286:ILE:HA	1:B:287:PRO:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ASP:O	1:C:300:LEU:HG	2.22	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	213/227 (94%)	203 (95%)	5 (2%)	5 (2%)	6	1
1	B	215/227 (95%)	204 (95%)	10 (5%)	1 (0%)	29	22
1	C	217/227 (96%)	208 (96%)	8 (4%)	1 (0%)	29	22
1	D	223/227 (98%)	219 (98%)	3 (1%)	1 (0%)	34	29
All	All	868/908 (96%)	834 (96%)	26 (3%)	8 (1%)	17	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	MET
1	A	443	LYS
1	C	450	PHE
1	A	445	PRO
1	D	456	ALA
1	A	235	ASN
1	A	441	GLU
1	B	445	PRO

### 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	182/201 (90%)	178 (98%)	4 (2%)	52	53
1	B	186/201 (92%)	182 (98%)	4 (2%)	52	53
1	C	183/201 (91%)	178 (97%)	5 (3%)	44	43
1	D	194/201 (96%)	191 (98%)	3 (2%)	65	68
All	All	745/804 (93%)	729 (98%)	16 (2%)	53	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ASP
1	A	311	LEU
1	A	336	GLN
1	A	344	ASP
1	B	247	GLU
1	B	408	MET
1	B	409	GLU
1	B	433	GLN
1	C	290	SER
1	C	389	GLN
1	C	393	ASP
1	C	409	GLU
1	C	437	ASN
1	D	240	HIS
1	D	344	ASP
1	D	409	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	A	347	ASN
1	A	389	GLN
1	B	389	GLN
1	B	396	HIS
1	C	302	GLN
1	C	336	GLN
1	C	351	GLN
1	C	389	GLN

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Mol	Chain	Res	Type
1	C	396	HIS
1	C	433	GLN
1	D	351	GLN
1	D	396	HIS
1	D	400	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 carbohydrates 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	DES	B	459	-	21,21,21	2.06	10 (47%)	28,28,28	0.93	2 (7%)
2	DES	C	500	-	21,21,21	2.00	10 (47%)	28,28,28	0.87	1 (3%)
2	DES	A	459	-	21,21,21	2.06	10 (47%)	28,28,28	0.93	2 (7%)
2	DES	D	600	-	21,21,21	2.05	13 (61%)	28,28,28	1.15	2 (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	DES	B	459	-	-	4/16/16/16	0/2/2/2
2	DES	C	500	-	-	1/16/16/16	0/2/2/2
2	DES	A	459	-	-	3/16/16/16	0/2/2/2
2	DES	D	600	-	-	2/16/16/16	0/2/2/2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	459	DES	C6-C7	3.29	1.55	1.49
2	B	459	DES	C6-C7	3.29	1.55	1.49
2	D	600	DES	CP2-CP1	3.15	1.44	1.38
2	A	459	DES	CP6-CP7	3.11	1.54	1.49
2	B	459	DES	CP6-CP7	3.11	1.54	1.49
2	D	600	DES	CP6-CP7	3.00	1.54	1.49
2	C	500	DES	CP2-CP1	2.94	1.44	1.38
2	D	600	DES	C6-C7	2.93	1.54	1.49
2	C	500	DES	CP6-CP7	2.92	1.54	1.49
2	C	500	DES	C6-C7	2.91	1.54	1.49
2	A	459	DES	C1-C2	2.84	1.43	1.38
2	B	459	DES	C1-C2	2.82	1.43	1.38
2	C	500	DES	CP1-CP6	2.77	1.44	1.39
2	A	459	DES	CP2-CP1	2.73	1.43	1.38
2	B	459	DES	CP2-CP1	2.72	1.43	1.38
2	C	500	DES	C4-C5	2.68	1.43	1.38
2	D	600	DES	C1-C2	2.67	1.43	1.38
2	D	600	DES	CP5-CP6	2.58	1.43	1.39
2	C	500	DES	CP5-CP6	2.56	1.43	1.39
2	D	600	DES	CP1-CP6	2.55	1.43	1.39
2	B	459	DES	CP5-CP6	2.54	1.43	1.39
2	A	459	DES	C4-C5	2.54	1.43	1.38
2	B	459	DES	C4-C5	2.52	1.43	1.38
2	A	459	DES	CP5-CP6	2.51	1.43	1.39
2	A	459	DES	C5-C6	2.47	1.43	1.39
2	B	459	DES	C5-C6	2.47	1.43	1.39
2	B	459	DES	CP1-CP6	2.40	1.43	1.39
2	C	500	DES	C2-C3	2.39	1.43	1.38
2	C	500	DES	C5-C6	2.39	1.43	1.39
2	D	600	DES	C1-C6	2.38	1.43	1.39
2	A	459	DES	CP1-CP6	2.36	1.43	1.39
2	B	459	DES	C1-C6	2.31	1.43	1.39
2	A	459	DES	C1-C6	2.28	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	DES	CP8-CP7	2.23	1.56	1.51
2	C	500	DES	C1-C2	2.22	1.42	1.38
2	D	600	DES	CP2-CP3	2.19	1.43	1.38
2	D	600	DES	C2-C3	2.14	1.43	1.38
2	D	600	DES	C5-C6	2.14	1.43	1.39
2	A	459	DES	C2-C3	2.08	1.42	1.38
2	C	500	DES	C1-C6	2.07	1.42	1.39
2	B	459	DES	C2-C3	2.06	1.42	1.38
2	D	600	DES	C4-C5	2.03	1.42	1.38
2	D	600	DES	C8-C7	2.00	1.55	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	DES	CP9-CP8-CP7	3.57	118.11	112.88
2	A	459	DES	CP9-CP8-CP7	2.60	116.69	112.88
2	B	459	DES	CP9-CP8-CP7	2.60	116.68	112.88
2	B	459	DES	C8-C7-C6	-2.33	111.10	114.45
2	C	500	DES	CP9-CP8-CP7	2.33	116.29	112.88
2	A	459	DES	C8-C7-C6	-2.32	111.12	114.45
2	D	600	DES	C8-C7-C6	-2.06	111.50	114.45

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	459	DES	CP6-CP7-CP8-CP9
2	B	459	DES	C7-CP7-CP8-CP9
2	B	459	DES	CP1-CP6-CP7-CP8
2	A	459	DES	CP1-CP6-CP7-CP8
2	D	600	DES	CP1-CP6-CP7-CP8
2	B	459	DES	C1-C6-C7-C8
2	C	500	DES	C1-C6-C7-C8
2	A	459	DES	CP5-CP6-CP7-CP8
2	A	459	DES	C1-C6-C7-C8
2	D	600	DES	CP5-CP6-CP7-CP8

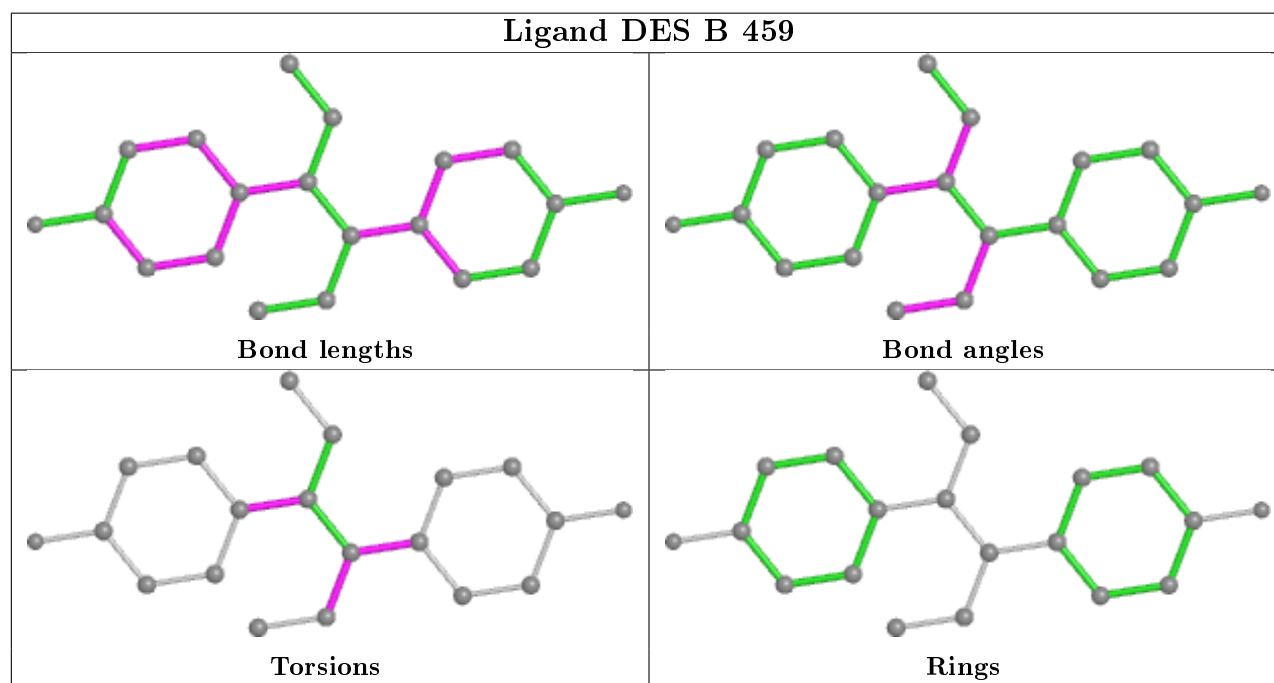
There are no ring outliers.

1 monomer is involved in 1 short contact:

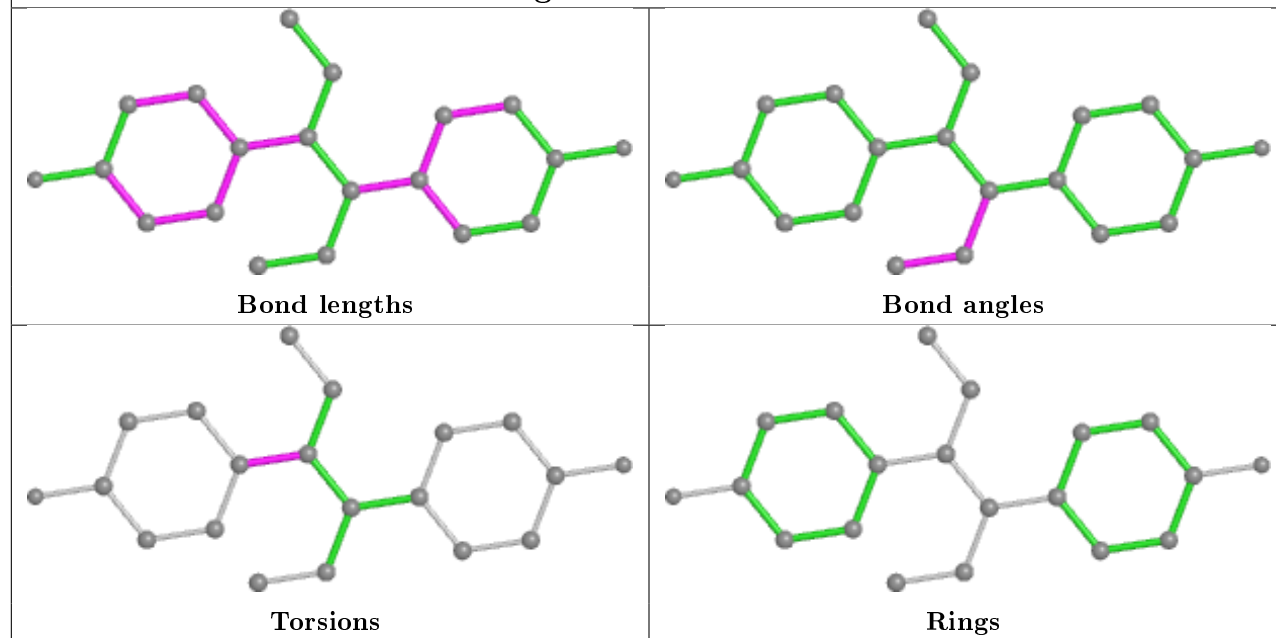


Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	DES	1	0

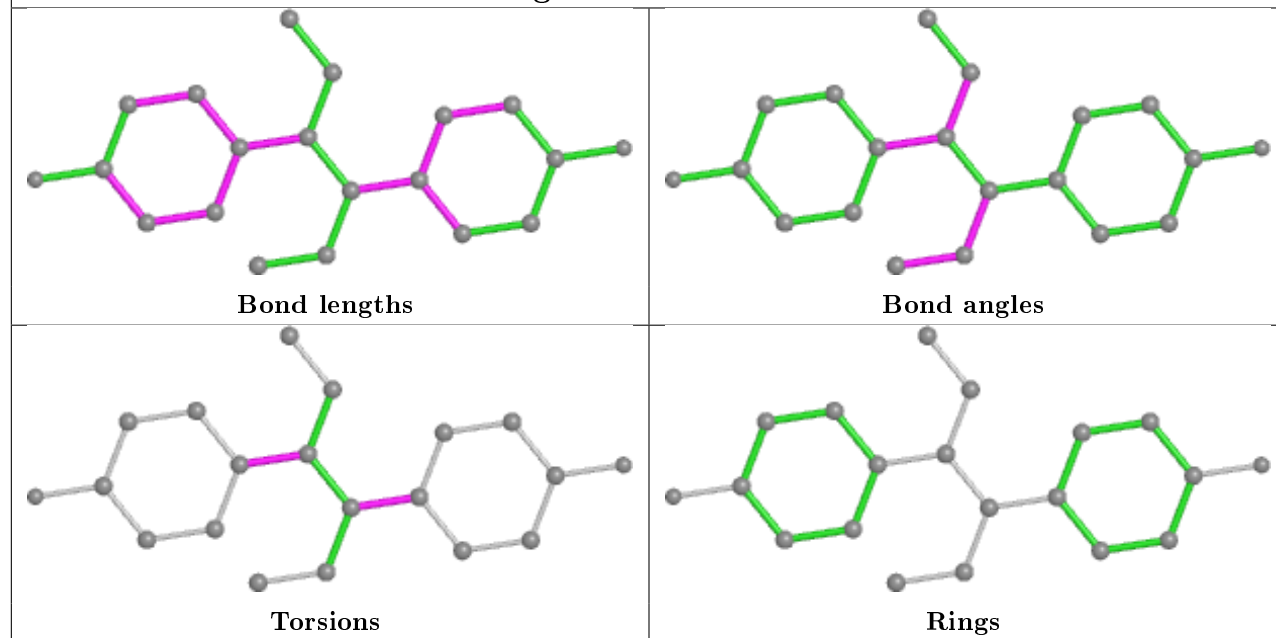
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

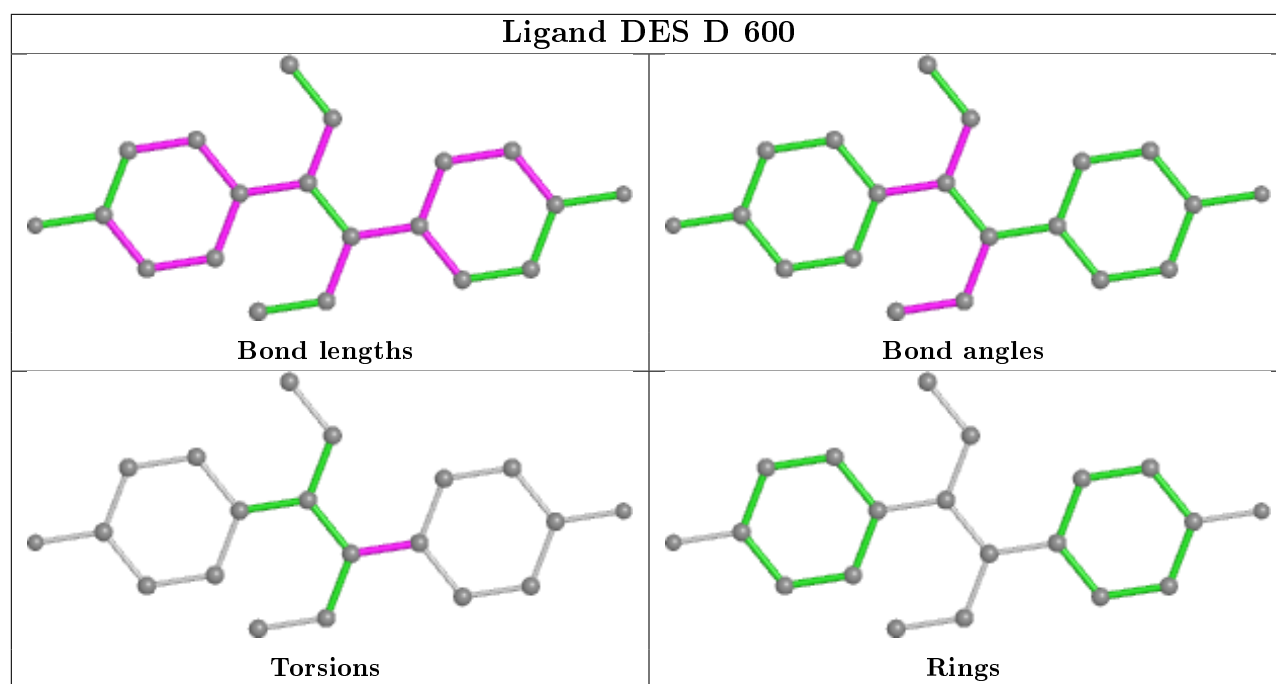


## Ligand DES C 500



## Ligand DES A 459





## 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	215/227 (94%)	0.57	24 (11%) 5 6	25, 40, 74, 89	0
1	B	217/227 (95%)	0.48	20 (9%) 9 12	22, 41, 63, 83	0
1	C	219/227 (96%)	0.52	20 (9%) 9 12	28, 45, 64, 84	0
1	D	225/227 (99%)	0.47	18 (8%) 12 15	28, 43, 64, 85	0
All	All	876/908 (96%)	0.51	82 (9%) 8 11	22, 42, 65, 89	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	VAL	10.6
1	C	452	GLU	8.3
1	A	256	THR	7.6
1	C	450	PHE	7.0
1	C	451	LEU	6.8
1	A	446	MET	6.3
1	B	449	LEU	6.0
1	A	257	VAL	5.7
1	A	233	PRO	5.7
1	C	294	LEU	5.6
1	C	234	TYR	5.2
1	A	444	VAL	4.9
1	A	442	GLY	4.6
1	C	449	LEU	4.5
1	C	446	MET	4.5
1	D	234	TYR	4.4
1	A	258	PRO	4.4
1	D	408	MET	4.3
1	B	447	HIS	4.1
1	B	294	LEU	4.1
1	C	448	LYS	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	436	TYR	3.9
1	D	418	LEU	3.9
1	B	446	MET	3.9
1	A	440	LEU	3.9
1	D	255	PRO	3.8
1	A	447	HIS	3.8
1	B	450	PHE	3.7
1	D	456	ALA	3.6
1	A	443	LYS	3.6
1	C	447	HIS	3.6
1	A	408	MET	3.4
1	A	255	PRO	3.4
1	B	234	TYR	3.4
1	B	256	THR	3.3
1	D	369	LEU	3.2
1	D	421	LEU	3.2
1	D	258	PRO	3.2
1	B	372	ILE	3.2
1	B	421	LEU	2.9
1	C	404	ALA	2.9
1	D	440	LEU	2.9
1	A	234	TYR	2.8
1	D	339	LEU	2.8
1	C	408	MET	2.8
1	A	437	ASN	2.8
1	C	421	LEU	2.8
1	A	262	ILE	2.8
1	D	457	LYS	2.8
1	C	418	LEU	2.7
1	A	445	PRO	2.7
1	B	408	MET	2.7
1	B	258	PRO	2.6
1	D	446	MET	2.6
1	C	405	GLY	2.6
1	A	439	LYS	2.6
1	C	339	LEU	2.6
1	B	373	ALA	2.6
1	D	311	LEU	2.6
1	C	243	VAL	2.5
1	A	260	SER	2.5
1	A	435	PHE	2.5
1	A	438	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	310	ILE	2.4
1	B	311	LEU	2.4
1	C	372	ILE	2.4
1	D	372	ILE	2.4
1	B	369	LEU	2.4
1	C	415	GLY	2.4
1	D	338	LYS	2.4
1	C	369	LEU	2.3
1	B	257	VAL	2.3
1	B	371	ALA	2.2
1	C	298	MET	2.2
1	A	339	LEU	2.1
1	B	247	GLU	2.1
1	B	424	LEU	2.1
1	D	401	ASP	2.1
1	B	418	LEU	2.1
1	A	419	MET	2.1
1	A	433	GLN	2.0
1	D	373	ALA	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](#)

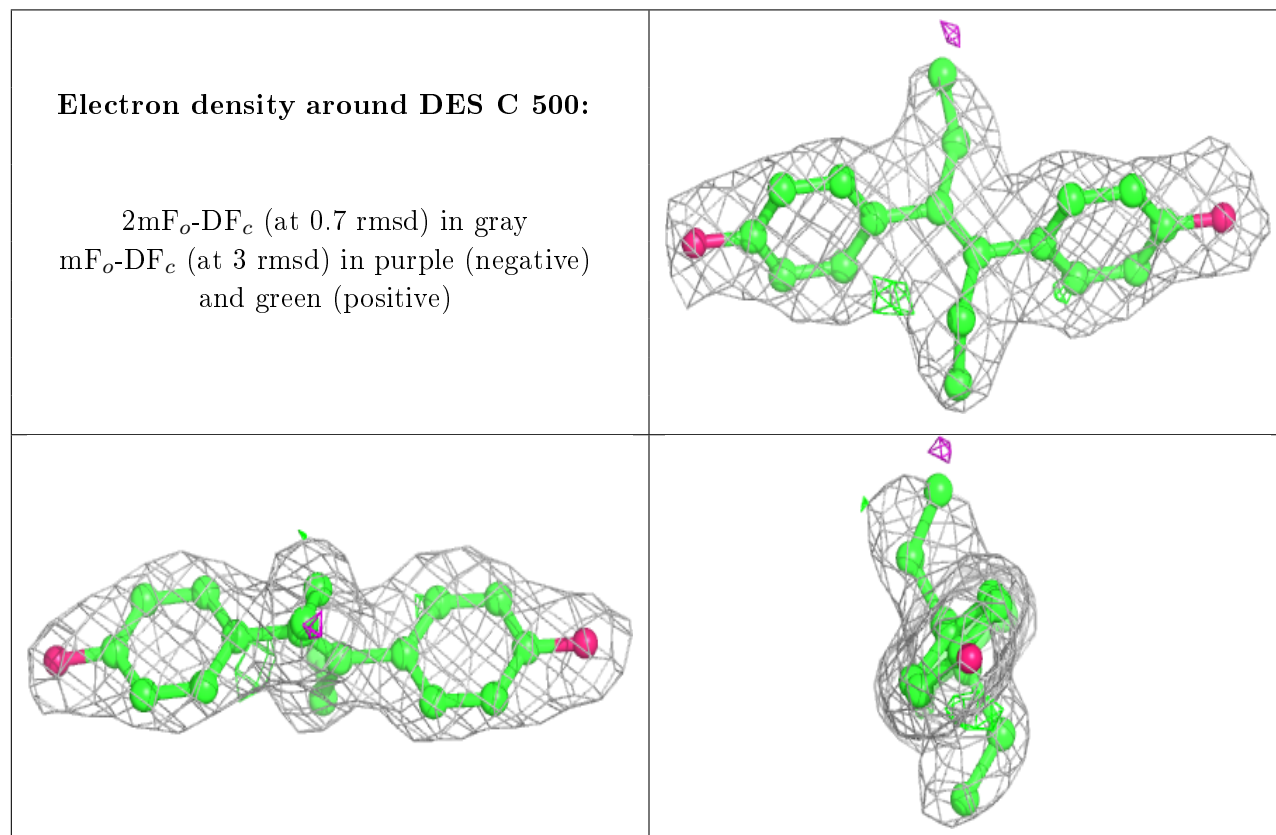
There are no carbohydrates in this entry.

## 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, 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.

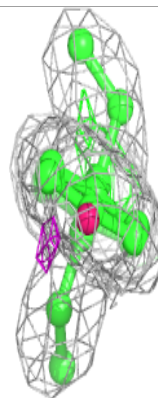
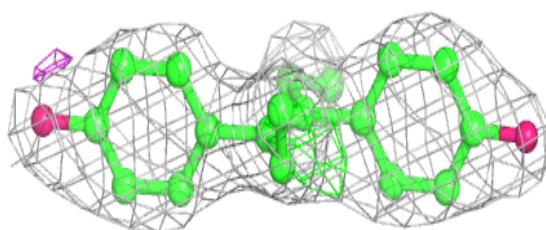
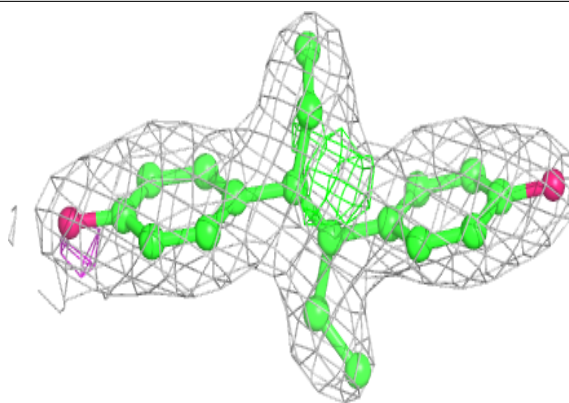
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DES	C	500	20/20	0.90	0.16	31,37,41,43	0
2	DES	B	459	20/20	0.92	0.21	38,41,46,49	0
2	DES	A	459	20/20	0.92	0.16	38,41,46,49	0
2	DES	D	600	20/20	0.95	0.15	29,37,42,43	0

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.

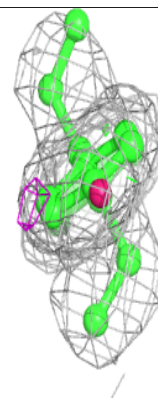
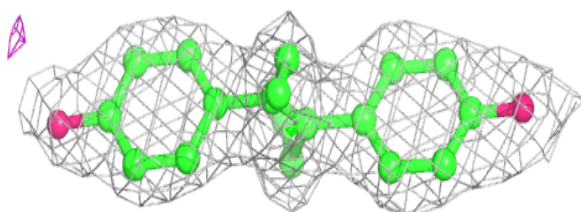
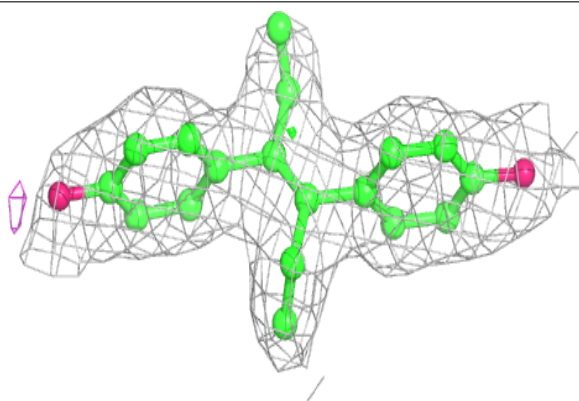


**Electron density around DES B 459:**

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

**Electron density around DES A 459:**

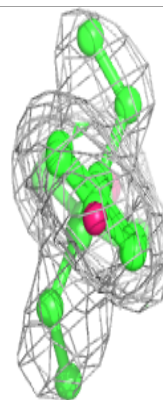
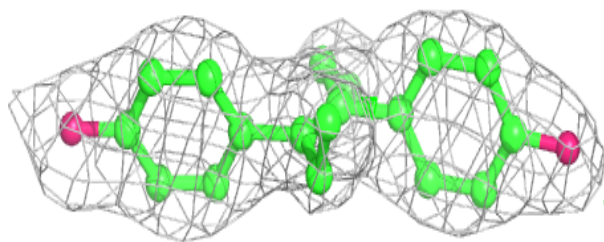
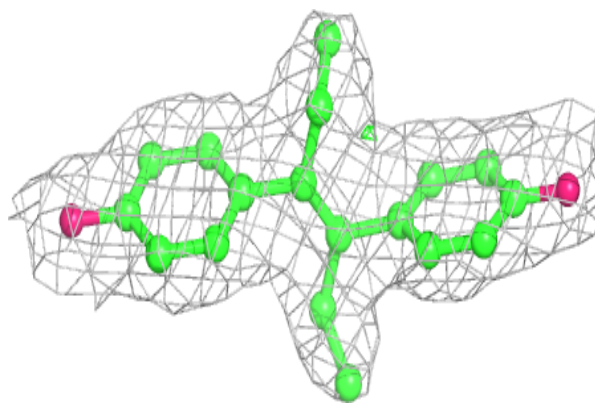
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around DES D 600:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.