



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:57 AM UTC

PDB ID : 1S9P / pdb_00001s9p
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

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>.

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

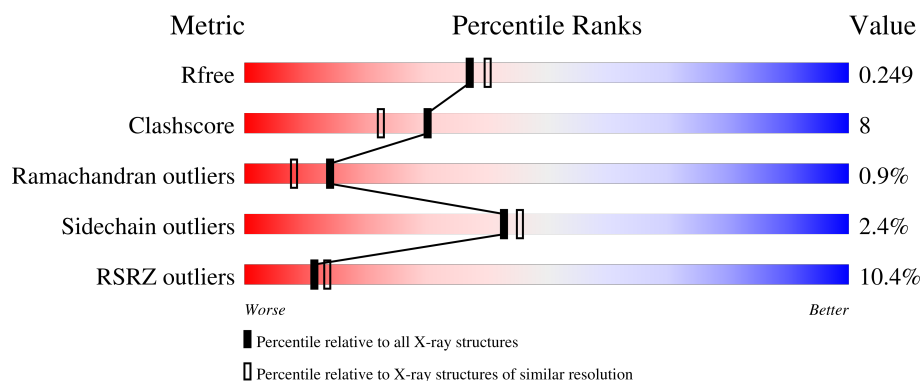
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	10% 76% 16% 5%
1	B	227	10% 79% 15% ..
1	C	227	11% 78% 19% .
1	D	227	9% 79% 19% ..

2 Entry composition [i](#)

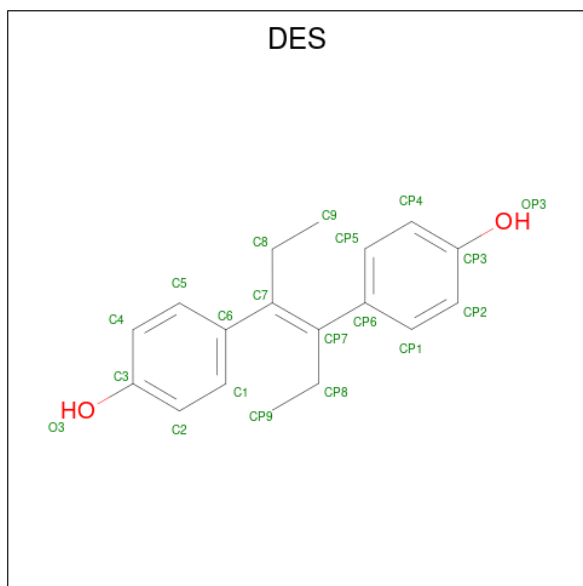
There are 3 unique types of molecules in this entry. The entry contains 7129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: DES) (formula: C₁₈H₂₀O₂).



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		

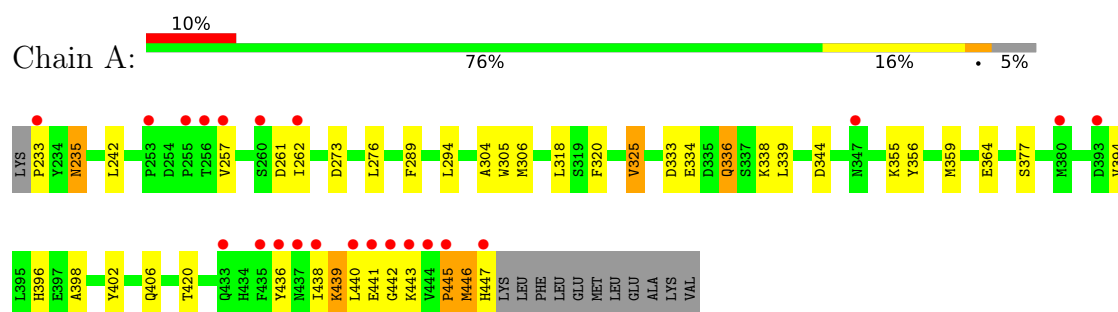
- Molecule 3 is water.

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		

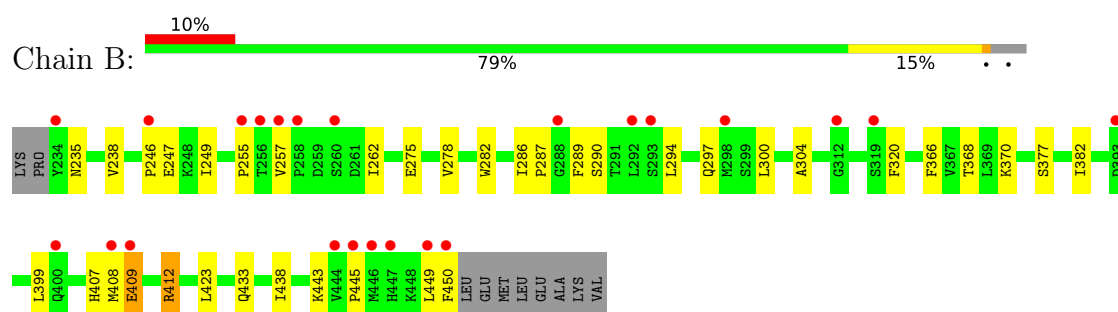
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

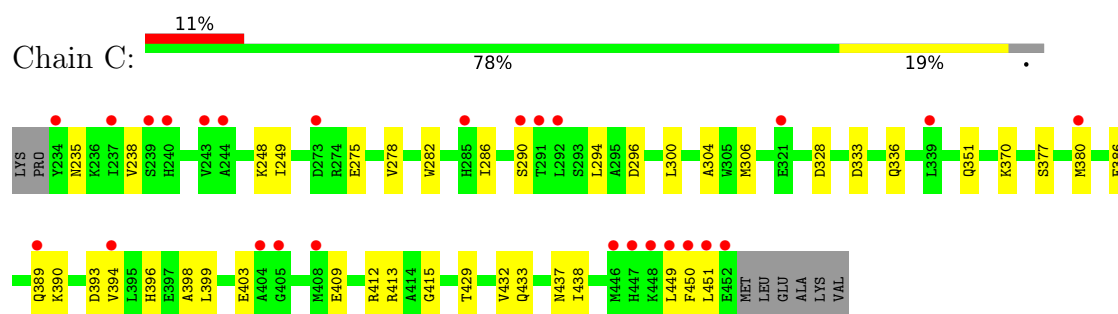
- Molecule 1: Estrogen-related receptor gamma



- Molecule 1: Estrogen-related receptor gamma

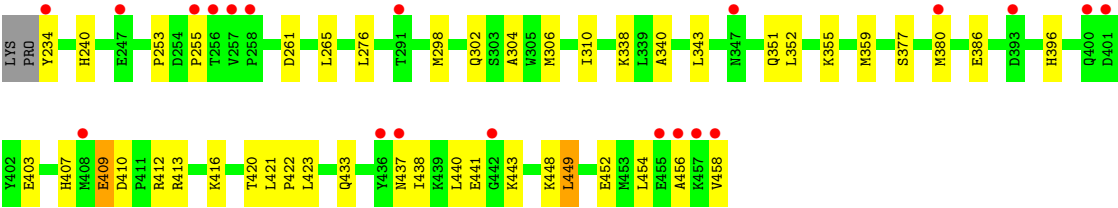


- Molecule 1: Estrogen-related receptor gamma



- 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, α , β , γ	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) 98.9 (29.30-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.51 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.251 0.226 , 0.249	Depositor DCC
R_{free} test set	2941 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: 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	0.48	0/1707	0.92	9/2312 (0.4%)
1	B	0.47	0/1725	0.87	0/2334
1	C	0.41	0/1724	0.86	0/2336
1	D	0.42	0/1803	0.88	1/2440 (0.0%)
All	All	0.44	0/6959	0.88	10/9422 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	PRO	N-CA-CB	6.46	110.03	103.25
1	A	325	VAL	N-CA-C	5.79	112.40	106.21
1	A	233	PRO	N-CA-CB	5.76	109.34	103.00
1	A	318	LEU	N-CA-C	5.72	117.52	111.28
1	D	449	LEU	N-CA-C	5.50	117.28	111.28
1	A	257	VAL	CA-C-N	5.50	125.42	119.76
1	A	257	VAL	C-N-CA	5.50	125.42	119.76
1	A	446	MET	N-CA-C	-5.20	99.72	110.80
1	A	289	PHE	N-CA-C	5.10	116.65	111.14
1	A	439	LYS	N-CA-C	-5.03	105.92	111.71

There are no chirality outliers.

There are no planarity outliers.

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	1679	0	1677	27	0
1	B	1696	0	1710	26	0
1	C	1696	0	1693	32	0
1	D	1772	0	1791	46	0
2	A	20	0	20	1	0
2	B	20	0	20	0	0
2	C	20	0	20	1	0
2	D	20	0	20	1	0
3	A	53	0	0	0	0
3	B	63	0	0	1	0
3	C	41	0	0	3	0
3	D	49	0	0	0	0
All	All	7129	0	6951	116	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 (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD11	1:D:458:VAL:O	1.51	1.11
1:C:380:MET:HG2	1:D:351:GLN:HE22	1.03	1.11
1:C:380:MET:HG2	1:D:351:GLN:NE2	1.83	0.93
1:A:355:LYS:HG3	1:A:359:MET:HE2	1.54	0.90
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:A:359:MET:HE1	1:A:420:THR:HG21	1.76	0.68
1:B:289:PHE:CE2	1:B:297:GLN:HG2	2.28	0.68
1:A:356:TYR:HA	1:A:359:MET:HE3	1.75	0.67
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:A:355:LYS:CG	1:A:359:MET:HE2	2.26	0.65
1:C:429:THR:O	1:C:433:GLN:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ASP:H	1:C:336:GLN:NE2	1.95	0.63
1:D:386:GLU:H	1:D:386:GLU:CD	2.06	0.63
1:B:438:ILE:HD12	1:B:443:LYS:HD2	1.81	0.62
1:D:355:LYS:HG3	1:D:359:MET:HE2	1.82	0.61
1:A:339:LEU:O	1:A:339:LEU:HD23	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:C:380:MET:HE3	1:D:351:GLN:NE2	2.17	0.60
1:A:294:LEU:HD11	1:D:458:VAL:C	2.25	0.60
1:C:380:MET:HE3	1:D:351:GLN:HE21	1.67	0.59
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:B:449:LEU:O	1:B:450:PHE:C	2.46	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
1:B:262:ILE:HD12	1:B:443:LYS:O	2.04	0.57
1:D:438:ILE:HG23	1:D:443:LYS:HB2	1.86	0.55
1:A:436:TYR:O	1:A:440:LEU:CB	2.56	0.54
1:C:449:LEU:C	1:C:451:LEU:H	2.15	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: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: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:359:MET:HE1	1:D:420:THR:HG21	1.92	0.52
1:D:338:LYS:HG2	1:D:343:LEU:HD22	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: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:235:ASN:HD21	1:C:398:ALA:HA	1.76	0.49
1:C:386:GLU:O	1:C:390:LYS:HG3	2.11	0.49
1:B:255:PRO:C	1:B:257:VAL:N	2.68	0.49
1:A:242:LEU:HD11	1:A:364:GLU:HG3	1.96	0.48
1:D:410:ASP:C	1:D:412:ARG:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:ARG:HB3	1:D:416:LYS:HE3	1.96	0.47
1:B:255:PRO:C	1:B:257:VAL:H	2.22	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:D:306:MET:HE1	2:D:600:DES:HP82	1.96	0.47
1:A:402:TYR:CE1	1:A:406:GLN:HG3	2.50	0.47
1:B:409:GLU:H	1:B:409:GLU:HG3	1.41	0.47
1:A:440:LEU:C	1:A:442:GLY:H	2.24	0.46
1:C:399:LEU:O	1:C:403:GLU:HG2	2.15	0.46
1:A:359:MET:HE1	1:A:420:THR:CG2	2.45	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:D:234:TYR:CD1	1:D:234:TYR:C	2.94	0.45
1:A:438:ILE:HG13	1:A:439:LYS:N	2.32	0.45
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:D:359:MET:HE1	1:D:420:THR:CG2	2.46	0.45
1:A:276:LEU:HD21	1:A:305:TRP:HB2	1.99	0.45
1:A:306:MET:HE1	2:A:459:DES:HP82	2.00	0.44
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:CD2	1:B:320:PHE:N	2.86	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:C:248:LYS:NZ	1:C:328:ASP:OD2	2.41	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: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: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:C:282:TRP:CH2	1:C:286:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:320:PHE:CE2	1:A:325:VAL:HG21	2.56	0.41
1:C:449:LEU:C	1:C:451:LEU:N	2.77	0.41
1:D:448:LYS:HD3	1:D:448:LYS:HA	1.84	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: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
1:C:296:ASP:O	1:C:300:LEU:HG	2.22	0.40
1:C:370:LYS:NZ	3:C:151:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	5	1
1	B	215/227 (95%)	204 (95%)	10 (5%)	1 (0%)	24	19
1	C	217/227 (96%)	208 (96%)	8 (4%)	1 (0%)	24	19
1	D	223/227 (98%)	219 (98%)	3 (1%)	1 (0%)	30	26
All	All	868/908 (96%)	834 (96%)	26 (3%)	8 (1%)	14	8

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 ⓘ

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%)	179 (98%)	3 (2%)	55	61
1	B	186/201 (92%)	181 (97%)	5 (3%)	39	41
1	C	183/201 (91%)	176 (96%)	7 (4%)	29	28
1	D	194/201 (96%)	191 (98%)	3 (2%)	57	63
All	All	745/804 (93%)	727 (98%)	18 (2%)	43	45

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ASP
1	A	336	GLN
1	A	344	ASP
1	B	247	GLU
1	B	408	MET
1	B	409	GLU
1	B	412	ARG
1	B	433	GLN
1	C	290	SER
1	C	294	LEU
1	C	389	GLN
1	C	393	ASP
1	C	394	VAL
1	C	409	GLU

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Mol	Chain	Res	Type
1	C	437	ASN
1	D	240	HIS
1	D	409	GLU
1	D	440	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	A	347	ASN
1	A	389	GLN
1	A	406	GLN
1	B	336	GLN
1	B	389	GLN
1	B	396	HIS
1	C	240	HIS
1	C	297	GLN
1	C	336	GLN
1	C	381	HIS
1	C	389	GLN
1	C	396	HIS
1	C	433	GLN
1	D	351	GLN
1	D	396	HIS
1	D	400	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

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	D	600	-	21,21,21	2.20	13 (61%)	28,28,28	1.17	2 (7%)
2	DES	B	459	-	21,21,21	2.21	10 (47%)	28,28,28	0.95	2 (7%)
2	DES	A	459	-	21,21,21	2.22	11 (52%)	28,28,28	0.95	2 (7%)
2	DES	C	500	-	21,21,21	2.16	10 (47%)	28,28,28	0.89	1 (3%)

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	D	600	-	-	2/16/16/16	0/2/2/2
2	DES	B	459	-	-	5/16/16/16	0/2/2/2
2	DES	A	459	-	-	3/16/16/16	0/2/2/2
2	DES	C	500	-	-	1/16/16/16	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	DES	CP2-CP1	3.51	1.44	1.38
2	A	459	DES	C6-C7	3.49	1.55	1.49
2	B	459	DES	C6-C7	3.48	1.55	1.49
2	A	459	DES	CP6-CP7	3.30	1.54	1.49
2	B	459	DES	CP6-CP7	3.30	1.54	1.49
2	C	500	DES	CP2-CP1	3.28	1.44	1.38
2	D	600	DES	CP6-CP7	3.18	1.54	1.49
2	A	459	DES	C1-C2	3.16	1.43	1.38
2	B	459	DES	C1-C2	3.14	1.43	1.38
2	D	600	DES	C6-C7	3.11	1.54	1.49
2	C	500	DES	CP6-CP7	3.10	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	DES	C6-C7	3.09	1.54	1.49
2	C	500	DES	CP1-CP6	3.05	1.44	1.39
2	A	459	DES	CP2-CP1	3.04	1.43	1.38
2	B	459	DES	CP2-CP1	3.03	1.43	1.38
2	C	500	DES	C4-C5	2.98	1.43	1.38
2	D	600	DES	C1-C2	2.98	1.43	1.38
2	D	600	DES	CP5-CP6	2.84	1.43	1.39
2	A	459	DES	C4-C5	2.82	1.43	1.38
2	C	500	DES	CP5-CP6	2.82	1.43	1.39
2	D	600	DES	CP1-CP6	2.81	1.43	1.39
2	B	459	DES	C4-C5	2.80	1.43	1.38
2	B	459	DES	CP5-CP6	2.79	1.43	1.39
2	A	459	DES	CP5-CP6	2.76	1.43	1.39
2	A	459	DES	C5-C6	2.72	1.43	1.39
2	B	459	DES	C5-C6	2.71	1.43	1.39
2	B	459	DES	CP1-CP6	2.63	1.43	1.39
2	C	500	DES	C5-C6	2.62	1.43	1.39
2	D	600	DES	C1-C6	2.61	1.43	1.39
2	A	459	DES	CP1-CP6	2.59	1.43	1.39
2	B	459	DES	C1-C6	2.53	1.43	1.39
2	A	459	DES	C1-C6	2.50	1.43	1.39
2	C	500	DES	C1-C2	2.46	1.42	1.38
2	C	500	DES	C2-C3	2.40	1.43	1.39
2	D	600	DES	CP8-CP7	2.37	1.56	1.51
2	D	600	DES	C5-C6	2.34	1.43	1.39
2	C	500	DES	C1-C6	2.26	1.42	1.39
2	D	600	DES	C4-C5	2.25	1.42	1.38
2	D	600	DES	CP2-CP3	2.20	1.43	1.39
2	D	600	DES	C2-C3	2.15	1.43	1.39
2	D	600	DES	C8-C7	2.13	1.55	1.51
2	A	459	DES	C2-C3	2.09	1.42	1.39
2	B	459	DES	C2-C3	2.06	1.42	1.39
2	A	459	DES	CP5-CP4	2.01	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	DES	CP9-CP8-CP7	3.66	118.11	112.87
2	A	459	DES	CP9-CP8-CP7	2.67	116.69	112.87
2	B	459	DES	CP9-CP8-CP7	2.66	116.68	112.87
2	C	500	DES	CP9-CP8-CP7	2.39	116.29	112.87
2	B	459	DES	C8-C7-C6	-2.35	111.10	114.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	459	DES	C8-C7-C6	-2.34	111.12	114.48
2	D	600	DES	C8-C7-C6	-2.08	111.50	114.48

There are no chirality outliers.

All (11) 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	A	459	DES	CP1-CP6-CP7-CP8
2	B	459	DES	CP1-CP6-CP7-CP8
2	D	600	DES	CP1-CP6-CP7-CP8
2	A	459	DES	CP5-CP6-CP7-CP8
2	D	600	DES	CP5-CP6-CP7-CP8
2	B	459	DES	CP5-CP6-CP7-CP8
2	A	459	DES	C1-C6-C7-C8
2	B	459	DES	C1-C6-C7-C8
2	C	500	DES	C1-C6-C7-C8

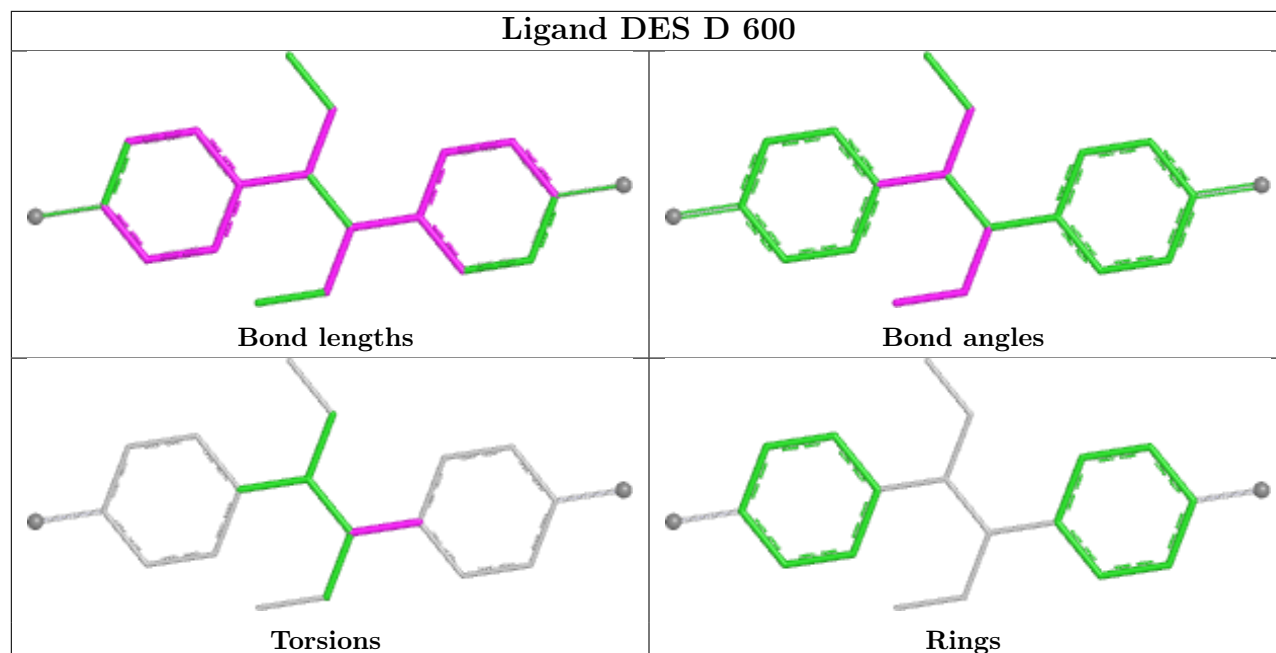
There are no ring outliers.

3 monomers are involved in 3 short contacts:

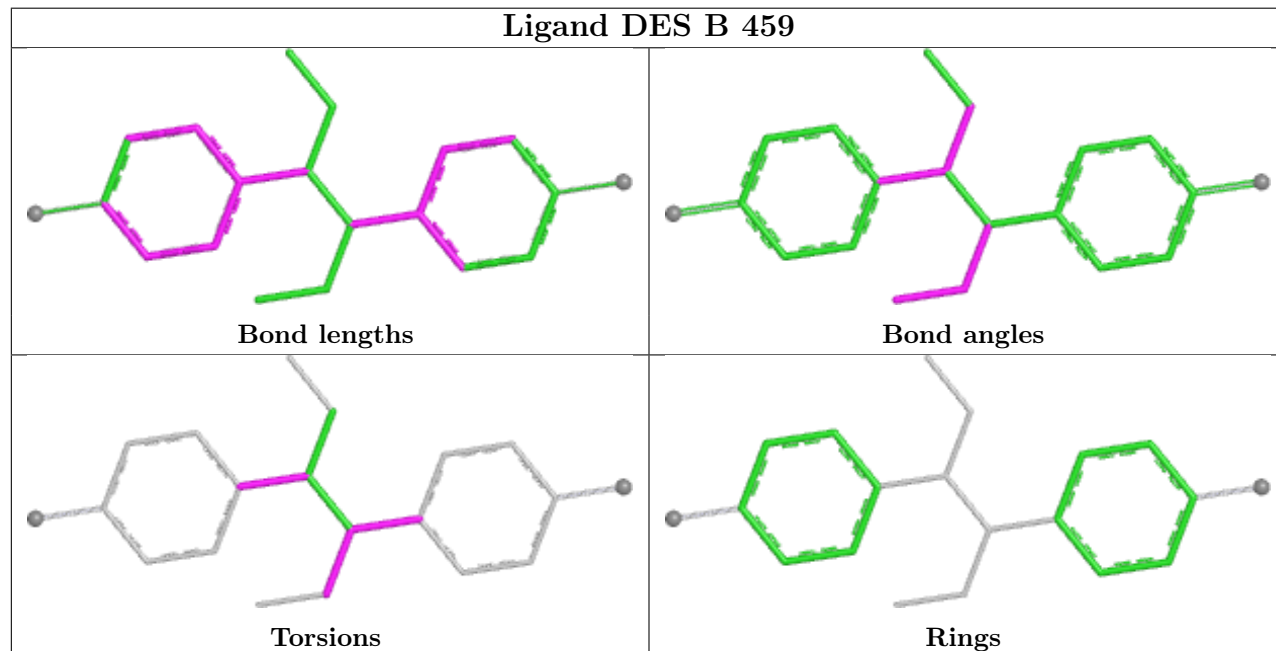
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	DES	1	0
2	A	459	DES	1	0
2	C	500	DES	1	0

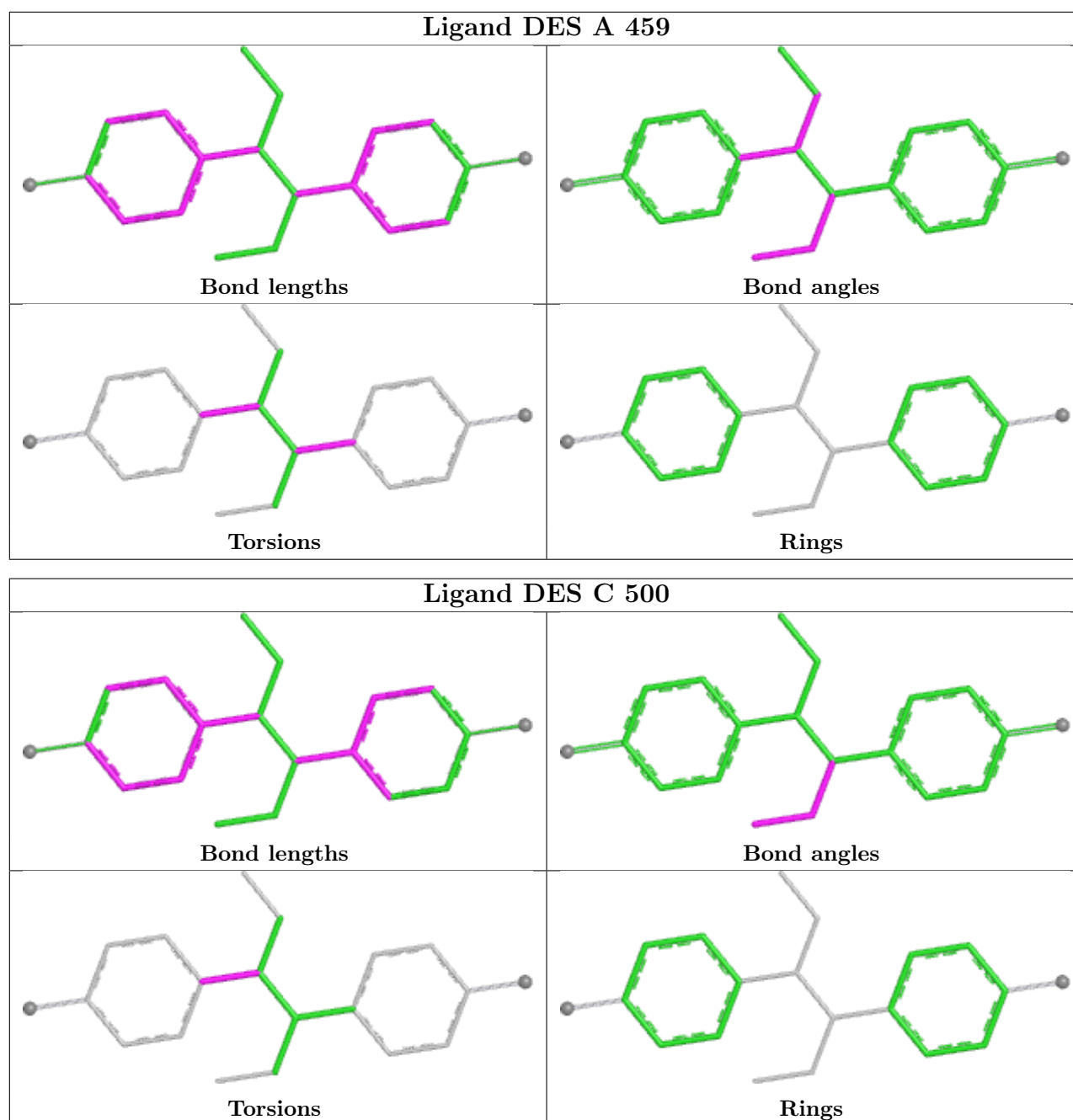
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 D 600



Ligand DES B 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, 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	215/227 (94%)	0.62	22 (10%) 12 14	25, 40, 74, 89	0
1	B	217/227 (95%)	0.66	23 (10%) 11 13	22, 41, 63, 83	0
1	C	219/227 (96%)	0.81	26 (11%) 9 10	28, 45, 64, 84	0
1	D	225/227 (99%)	0.67	20 (8%) 15 17	28, 43, 64, 85	0
All	All	876/908 (96%)	0.69	91 (10%) 11 14	22, 42, 65, 89	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	LEU	5.9
1	B	449	LEU	5.5
1	C	450	PHE	5.3
1	C	447	HIS	5.1
1	D	458	VAL	4.9
1	C	451	LEU	4.7
1	A	445	PRO	4.6
1	D	456	ALA	4.6
1	A	444	VAL	4.4
1	A	256	THR	4.2
1	B	446	MET	4.2
1	C	448	LYS	4.2
1	C	452	GLU	4.0
1	D	455	GLU	4.0
1	C	446	MET	3.9
1	D	255	PRO	3.9
1	C	449	LEU	3.8
1	B	255	PRO	3.7
1	D	234	TYR	3.7
1	A	255	PRO	3.6
1	B	256	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	401	ASP	3.5
1	D	457	LYS	3.5
1	A	441	GLU	3.4
1	C	290	SER	3.3
1	C	408	MET	3.3
1	C	234	TYR	3.3
1	D	257	VAL	3.3
1	B	293	SER	3.2
1	C	404	ALA	3.2
1	A	257	VAL	3.1
1	A	436	TYR	3.0
1	B	257	VAL	3.0
1	C	339	LEU	3.0
1	B	445	PRO	3.0
1	A	438	ILE	2.9
1	B	408	MET	2.9
1	A	260	SER	2.9
1	B	450	PHE	2.9
1	C	380	MET	2.8
1	D	380	MET	2.8
1	C	243	VAL	2.8
1	A	447	HIS	2.8
1	C	405	GLY	2.8
1	D	291	THR	2.8
1	A	253	PRO	2.7
1	D	247	GLU	2.7
1	D	437	ASN	2.7
1	C	291	THR	2.6
1	A	233	PRO	2.6
1	C	240	HIS	2.6
1	D	436	TYR	2.6
1	A	442	GLY	2.6
1	C	239	SER	2.6
1	B	234	TYR	2.6
1	B	400	GLN	2.6
1	B	288	GLY	2.6
1	A	435	PHE	2.5
1	B	260	SER	2.5
1	A	262	ILE	2.5
1	C	273	ASP	2.4
1	B	393	ASP	2.4
1	B	258	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	409	GLU	2.3
1	B	292	LEU	2.3
1	B	298	MET	2.3
1	D	258	PRO	2.3
1	D	347	ASN	2.3
1	A	443	LYS	2.3
1	D	256	THR	2.3
1	D	408	MET	2.3
1	B	319	SER	2.2
1	A	437	ASN	2.2
1	C	394	VAL	2.2
1	B	447	HIS	2.2
1	D	400	GLN	2.2
1	A	347	ASN	2.2
1	B	312	GLY	2.2
1	D	442	GLY	2.2
1	A	433	GLN	2.2
1	C	292	LEU	2.2
1	B	246	PRO	2.1
1	C	244	ALA	2.1
1	C	321	GLU	2.1
1	A	380	MET	2.1
1	A	393	ASP	2.1
1	C	389	GLN	2.1
1	C	285	HIS	2.1
1	C	237	ILE	2.1
1	B	444	VAL	2.1
1	D	393	ASP	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,

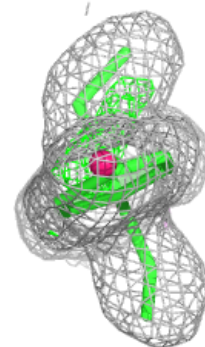
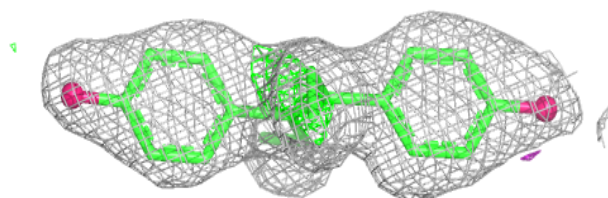
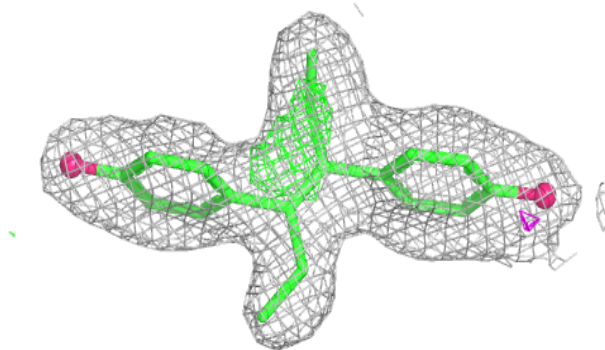
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DES	B	459	20/20	0.90	0.12	38,41,46,49	0
2	DES	C	500	20/20	0.90	0.10	31,37,41,43	0
2	DES	A	459	20/20	0.94	0.09	38,41,46,49	0
2	DES	D	600	20/20	0.94	0.08	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.

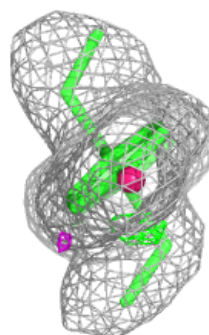
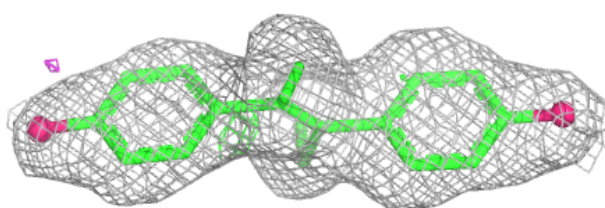
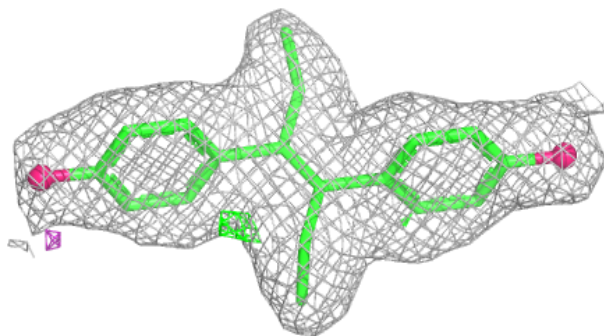
Electron density around DES B 459:

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

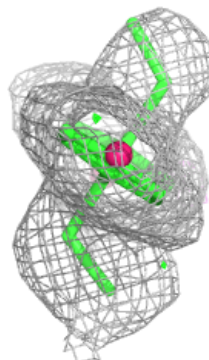
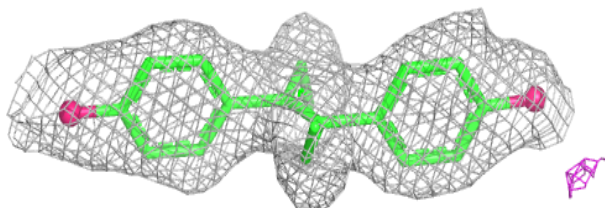
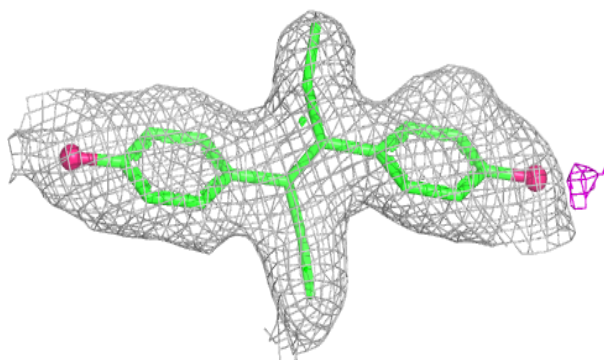


Electron density around DES C 500:

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

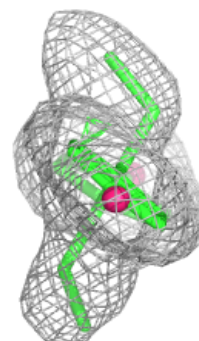
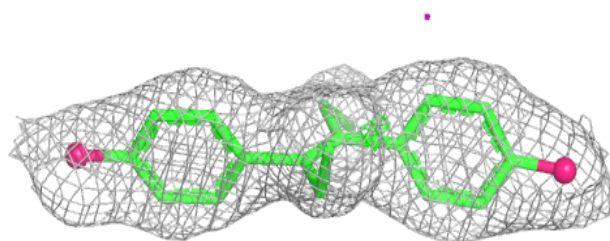
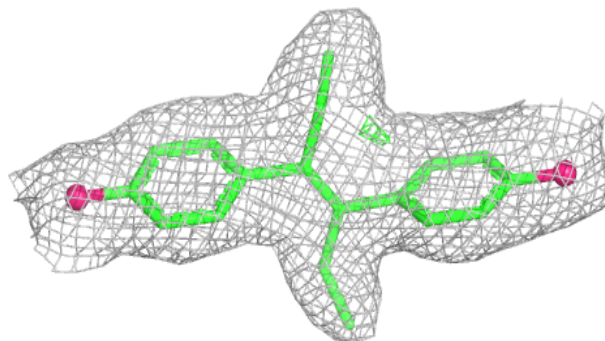
**Electron density around DES A 459:**

$2mF_o-DF_c$ (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.