



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:35 am BST

PDB ID : 1PQ9  
Title : HUMAN LXR BETA HORMONE RECEPTOR COMPLEXED WITH  
T0901317 COMPLEX  
Authors : Farnegardh, M.; Bonn, T.; Sun, S.; Ljunggren, J.; Ahola, H.; Wilhelmsson, A.;  
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Deposited on : 2003-06-18  
Resolution : 2.10 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

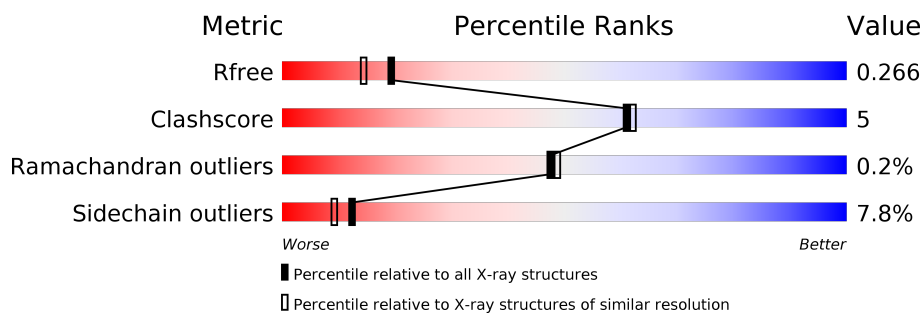
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	253	
1	B	253	
1	C	253	
1	D	253	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7779 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.

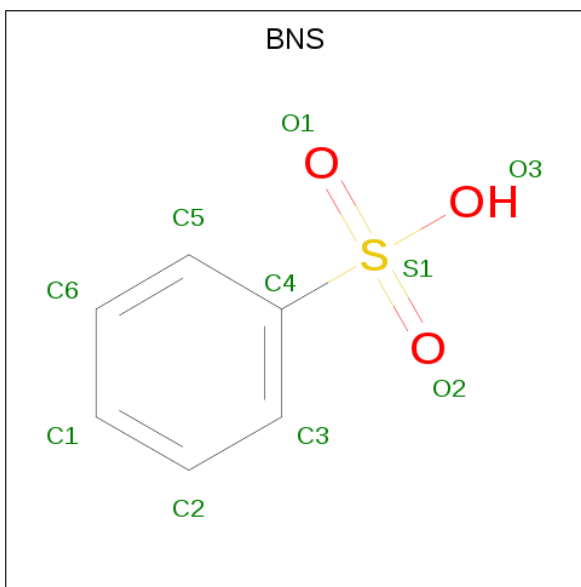
- Molecule 1 is a protein called Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1891	1210	331	343	7			
1	B	238	Total	C	N	O	S	0	0	0
			1925	1230	337	351	7			
1	C	231	Total	C	N	O	S	0	0	0
			1884	1204	333	340	7			
1	D	219	Total	C	N	O	S	0	0	0
			1774	1133	313	321	7			

There are 16 discrepancies between the modelled and reference sequences:

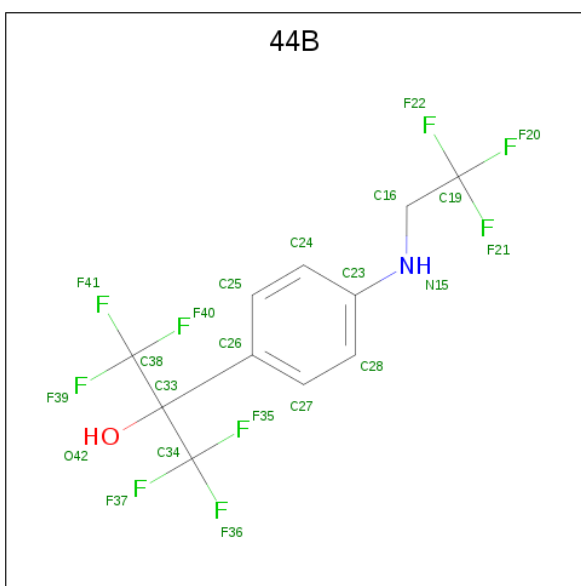
Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	CLONING ARTIFACT	UNP P55055
A	210	SER	-	CLONING ARTIFACT	UNP P55055
A	211	HIS	-	CLONING ARTIFACT	UNP P55055
A	212	MET	-	CLONING ARTIFACT	UNP P55055
B	209	GLY	-	CLONING ARTIFACT	UNP P55055
B	210	SER	-	CLONING ARTIFACT	UNP P55055
B	211	HIS	-	CLONING ARTIFACT	UNP P55055
B	212	MET	-	CLONING ARTIFACT	UNP P55055
C	209	GLY	-	CLONING ARTIFACT	UNP P55055
C	210	SER	-	CLONING ARTIFACT	UNP P55055
C	211	HIS	-	CLONING ARTIFACT	UNP P55055
C	212	MET	-	CLONING ARTIFACT	UNP P55055
D	209	GLY	-	CLONING ARTIFACT	UNP P55055
D	210	SER	-	CLONING ARTIFACT	UNP P55055
D	211	HIS	-	CLONING ARTIFACT	UNP P55055
D	212	MET	-	CLONING ARTIFACT	UNP P55055

- Molecule 2 is benzenesulfonic acid (three-letter code: BNS) (formula: C<sub>6</sub>H<sub>6</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			9	6	2	1		
2	B	1	Total	C	O	S	0	0
			9	6	2	1		
2	C	1	Total	C	O	S	0	0
			9	6	2	1		
2	D	1	Total	C	O	S	0	0
			9	6	2	1		

- Molecule 3 is 1,1,1,3,3,3-HEXAFLUORO-2-{4-[(2,2,2-TRIFLUOROETHYL)AMINO]PHE  
NYL}PROPAN-2-OL (three-letter code: 44B) (formula: C<sub>11</sub>H<sub>8</sub>F<sub>9</sub>NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	B	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	C	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	D	1	Total	C	F	N	O	0	0
			22	11	9	1	1		

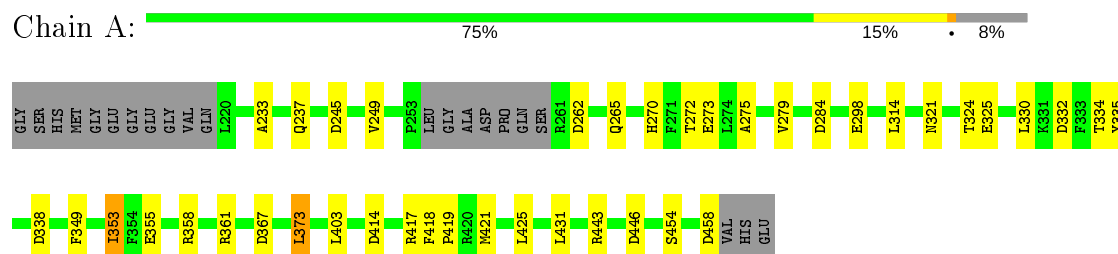
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	73	Total	O	0	0
			73	73		
4	C	52	Total	O	0	0
			52	52		
4	D	21	Total	O	0	0
			21	21		

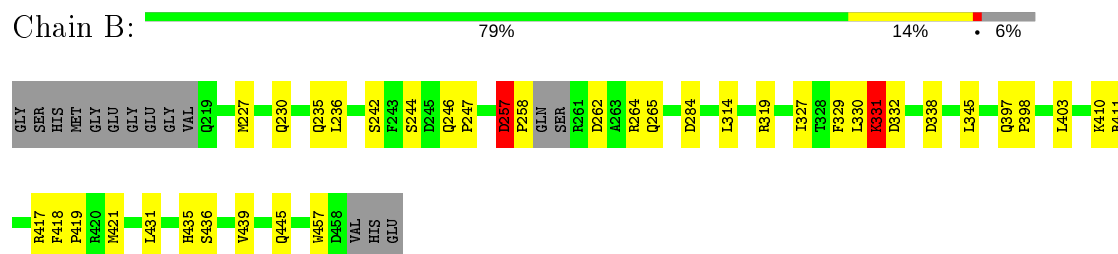
### 3 Residue-property plots

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. 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. 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.

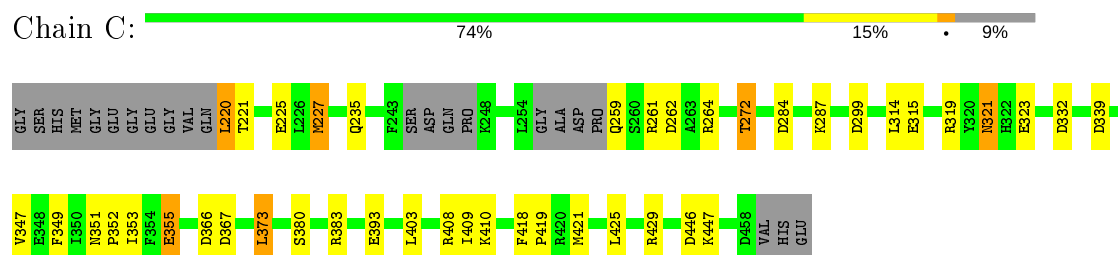
#### • Molecule 1: Oxysterols receptor LXR-beta



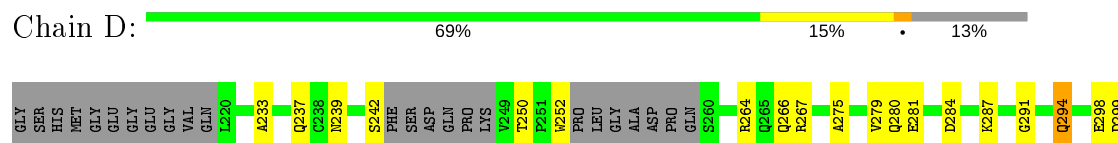
#### • Molecule 1: Oxysterols receptor LXR-beta



#### • Molecule 1: Oxysterols receptor LXR-beta



#### • Molecule 1: Oxysterols receptor LXR-beta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.87Å 103.61Å 176.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.84 – 2.10 55.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (55.84-2.10) 99.7 (55.84-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.28	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.214 , 0.254 0.269 , 0.266	Depositor DCC
$R_{free}$ test set	3227 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.9	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	0.92	EDS
Total number of atoms	7779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BNS, 44B

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	0.62	0/1928	0.80	8/2607 (0.3%)
1	B	0.66	0/1963	0.82	4/2656 (0.2%)
1	C	0.68	1/1919 (0.1%)	0.84	10/2591 (0.4%)
1	D	0.59	0/1804	0.75	4/2436 (0.2%)
All	All	0.64	1/7614 (0.0%)	0.80	26/10290 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	THR	CB-CG2	-5.35	1.34	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	MET	CG-SD-CE	-8.11	87.23	100.20
1	B	284	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	338	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	332	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	446	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	446	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	339	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	366	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	262	ASP	CB-CG-OD2	5.56	123.31	118.30
1	D	458	ASP	CB-CG-OD2	5.53	123.27	118.30
1	D	299	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	332	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	284	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	338	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	257	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	332	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	429	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	299	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	245	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	284	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	458	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	338	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	367	ASP	CB-CG-OD2	5.05	122.84	118.30
1	C	284	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	367	ASP	CB-CG-OD2	5.00	122.80	118.30

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	1891	0	1913	12	0
1	B	1925	0	1936	16	0
1	C	1884	0	1905	18	0
1	D	1774	0	1788	19	0
2	A	9	0	5	1	0
2	B	9	0	5	1	0
2	C	9	0	5	2	0
2	D	9	0	5	1	0
3	A	22	0	8	1	0
3	B	22	0	8	0	0
3	C	22	0	8	2	0
3	D	22	0	8	1	0
4	A	35	0	0	0	0
4	B	73	0	0	0	0
4	C	52	0	0	0	0
4	D	21	0	0	0	0
All	All	7779	0	7594	69	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 5.

All (69) 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:352:PRO:HA	1:C:355:GLU:HG3	1.49	0.94
1:D:233:ALA:O	1:D:237:GLN:HG3	1.87	0.74
1:D:360:MET:HE1	1:D:424:LYS:HD2	1.72	0.72
2:C:3500:BNS:O1	3:C:3501:44B:N15	2.25	0.70
1:C:351:ASN:O	1:C:355:GLU:HG2	1.93	0.69
1:C:315:GLU:OE1	1:C:319:ARG:NH1	2.27	0.68
1:C:352:PRO:HA	1:C:355:GLU:CG	2.23	0.67
1:D:242:SER:OG	1:D:281:GLU:OE2	2.10	0.66
1:A:403:LEU:HD21	1:A:421:MET:HE2	1.81	0.63
1:A:349:PHE:CE1	1:A:353:ILE:HD11	2.36	0.60
1:A:373:LEU:HD22	1:A:425:LEU:HD21	1.85	0.59
1:B:246:GLN:NE2	1:B:330:LEU:O	2.35	0.59
1:B:257:ASP:CB	1:B:258:PRO:CD	2.82	0.57
1:C:321:ASN:HD21	1:C:323:GLU:HB3	1.70	0.56
1:D:250:THR:CG2	1:D:266:GLN:HE21	2.19	0.56
1:D:321:ASN:C	1:D:321:ASN:HD22	2.10	0.55
1:D:252:TRP:CZ2	1:D:267:ARG:HD3	2.42	0.54
1:A:321:ASN:ND2	1:A:324:THR:OG1	2.34	0.54
1:C:403:LEU:HD21	1:C:421:MET:HE2	1.89	0.54
1:B:257:ASP:CB	1:B:258:PRO:HD2	2.38	0.53
1:C:221:THR:O	1:C:225:GLU:HG3	2.09	0.53
1:C:409:ILE:O	1:C:410:LYS:C	2.48	0.51
1:C:373:LEU:HD22	1:C:425:LEU:HD21	1.92	0.51
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.93	0.50
1:B:257:ASP:HB3	1:B:258:PRO:CD	2.42	0.50
1:D:410:LYS:HD3	1:D:411:ARG:HG3	1.93	0.50
1:D:410:LYS:HZ1	1:D:411:ARG:HE	1.58	0.50
1:A:355:GLU:HG3	1:A:358:ARG:NH1	2.26	0.49
1:A:349:PHE:O	1:A:353:ILE:HD13	2.12	0.49
1:A:249:VAL:HG13	1:A:273:GLU:HB2	1.96	0.48
1:D:291:GLY:O	1:D:294:GLN:HG2	2.13	0.48
1:D:373:LEU:HD22	1:D:425:LEU:HD21	1.95	0.48
1:B:329:PHE:CZ	2:B:2500:BNS:O1	2.67	0.47
1:D:360:MET:CE	1:D:424:LYS:HD2	2.43	0.47
1:A:270:HIS:NE2	1:A:335:TYR:OH	2.38	0.47
1:B:246:GLN:HB3	1:B:247:PRO:HD3	1.96	0.47
1:B:410:LYS:HG2	1:B:411:ARG:HG2	1.95	0.47
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:ASN:O	1:C:355:GLU:CG	2.62	0.46
1:D:410:LYS:NZ	1:D:411:ARG:HE	2.13	0.45
1:C:349:PHE:CZ	1:C:353:ILE:HD11	2.52	0.45
1:C:352:PRO:CA	1:C:355:GLU:HG3	2.35	0.45
1:B:257:ASP:HB3	1:B:258:PRO:HD2	1.99	0.45
2:C:3500:BNS:O1	3:C:3501:44B:C23	2.64	0.45
1:A:414:ASP:OD2	1:A:417:ARG:HB2	2.17	0.44
1:B:330:LEU:O	1:B:331:LYS:HB2	2.17	0.44
1:D:403:LEU:O	1:D:407:THR:HG23	2.18	0.44
1:B:403:LEU:HD21	1:B:421:MET:HE2	2.00	0.43
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.99	0.43
1:D:388:GLU:CD	1:D:391:ARG:HD3	2.39	0.43
1:B:435:HIS:HE1	1:B:457:TRP:CD2	2.38	0.42
1:C:220:LEU:HD13	1:C:225:GLU:HG2	2.00	0.42
2:D:4500:BNS:O2	3:D:4501:44B:N15	2.47	0.42
1:B:330:LEU:O	1:B:331:LYS:CB	2.67	0.42
2:A:1500:BNS:S1	3:A:1501:44B:N15	2.92	0.42
1:D:321:ASN:HD21	1:D:323:GLU:HB2	1.85	0.42
1:A:275:ALA:O	1:A:279:VAL:HG23	2.19	0.41
1:B:397:GLN:HB3	1:B:398:PRO:HD3	2.02	0.41
1:B:436:SER:HA	1:B:439:VAL:HG22	2.01	0.41
1:C:353:ILE:HD13	1:C:353:ILE:HG21	1.83	0.41
1:C:380:SER:O	1:C:383:ARG:HG2	2.19	0.41
1:C:349:PHE:CE2	1:C:353:ILE:HD11	2.56	0.41
1:B:417:ARG:O	1:B:421:MET:HG3	2.21	0.41
1:D:417:ARG:HH11	1:D:417:ARG:HG2	1.86	0.41
1:D:304:LEU:HD23	1:D:304:LEU:HA	1.86	0.40
1:D:313:LEU:CD2	1:D:353:ILE:HD12	2.51	0.40
1:A:233:ALA:O	1:A:237:GLN:HG3	2.21	0.40
1:C:418:PHE:HB3	1:C:419:PRO:CD	2.52	0.40
1:D:275:ALA:O	1:D:279:VAL:HG23	2.22	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	228/253 (90%)	224 (98%)	4 (2%)	0	100	100
1	B	234/253 (92%)	229 (98%)	3 (1%)	2 (1%)	17	12
1	C	225/253 (89%)	221 (98%)	4 (2%)	0	100	100
1	D	209/253 (83%)	202 (97%)	7 (3%)	0	100	100
All	All	896/1012 (88%)	876 (98%)	18 (2%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	ASP
1	B	331	LYS

### 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	206/222 (93%)	193 (94%)	13 (6%)	18	15
1	B	208/222 (94%)	191 (92%)	17 (8%)	11	8
1	C	204/222 (92%)	188 (92%)	16 (8%)	12	9
1	D	191/222 (86%)	174 (91%)	17 (9%)	9	6
All	All	809/888 (91%)	746 (92%)	63 (8%)	12	9

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	A	272	THR
1	A	298	GLU
1	A	314	LEU
1	A	325	GLU
1	A	330	LEU

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Mol	Chain	Res	Type
1	A	334	THR
1	A	353	ILE
1	A	361	ARG
1	A	373	LEU
1	A	431	LEU
1	A	443	ARG
1	A	454	SER
1	B	227	MET
1	B	230	GLN
1	B	235	GLN
1	B	236	LEU
1	B	242	SER
1	B	244	SER
1	B	257	ASP
1	B	262	ASP
1	B	264	ARG
1	B	265	GLN
1	B	314	LEU
1	B	319	ARG
1	B	327	ILE
1	B	331	LYS
1	B	345	LEU
1	B	431	LEU
1	B	445	GLN
1	C	220	LEU
1	C	227	MET
1	C	235	GLN
1	C	259	GLN
1	C	261	ARG
1	C	264	ARG
1	C	272	THR
1	C	287	LYS
1	C	314	LEU
1	C	321	ASN
1	C	347	VAL
1	C	355	GLU
1	C	373	LEU
1	C	393	GLU
1	C	408	ARG
1	C	447	LYS
1	D	239	ASN
1	D	264	ARG

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Mol	Chain	Res	Type
1	D	280	GLN
1	D	287	LYS
1	D	294	GLN
1	D	298	GLU
1	D	305	LYS
1	D	314	LEU
1	D	321	ASN
1	D	342	ARG
1	D	360	MET
1	D	373	LEU
1	D	417	ARG
1	D	423	MET
1	D	439	VAL
1	D	442	LEU
1	D	443	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	A	300	GLN
1	A	321	ASN
1	A	396	GLN
1	B	239	ASN
1	B	246	GLN
1	B	288	GLN
1	C	230	GLN
1	C	259	GLN
1	C	321	ASN
1	C	346	GLN
1	D	239	ASN
1	D	266	GLN
1	D	280	GLN
1	D	294	GLN
1	D	321	ASN

### 5.3.3 RNA ⓘ

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](#)

8 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	BNS	C	3500	-	6,9,10	2.26	2 (33%)	10,11,14	0.54	0
3	44B	D	4501	-	22,22,22	1.85	8 (36%)	36,36,36	1.43	4 (11%)
3	44B	A	1501	-	22,22,22	1.53	3 (13%)	36,36,36	1.43	6 (16%)
3	44B	B	2501	-	22,22,22	1.69	5 (22%)	36,36,36	1.13	2 (5%)
2	BNS	D	4500	-	6,9,10	2.24	2 (33%)	10,11,14	0.99	1 (10%)
3	44B	C	3501	-	22,22,22	1.71	5 (22%)	36,36,36	1.32	3 (8%)
2	BNS	A	1500	-	6,9,10	2.05	2 (33%)	10,11,14	1.10	1 (10%)
2	BNS	B	2500	-	6,9,10	2.08	2 (33%)	10,11,14	0.77	0

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	BNS	C	3500	-	-	4/4/4/6	0/1/1/1
3	44B	D	4501	-	-	0/30/30/30	0/1/1/1
3	44B	A	1501	-	-	4/30/30/30	0/1/1/1
3	44B	B	2501	-	-	2/30/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BNS	D	4500	-	-	4/4/4/6	0/1/1/1
3	44B	C	3501	-	-	2/30/30/30	0/1/1/1
2	BNS	A	1500	-	-	3/4/4/6	0/1/1/1
2	BNS	B	2500	-	-	4/4/4/6	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3501	44B	C23-N15	4.19	1.51	1.38
3	D	4501	44B	C27-C26	4.06	1.45	1.39
3	B	2501	44B	C23-N15	3.68	1.49	1.38
3	A	1501	44B	C23-N15	3.57	1.49	1.38
3	B	2501	44B	C27-C26	3.54	1.44	1.39
3	D	4501	44B	C23-N15	3.50	1.48	1.38
3	C	3501	44B	C27-C26	3.44	1.44	1.39
2	C	3500	BNS	C5-C4	3.39	1.43	1.38
3	B	2501	44B	C25-C26	3.36	1.44	1.39
3	A	1501	44B	C27-C26	3.27	1.44	1.39
3	C	3501	44B	C25-C26	3.23	1.44	1.39
3	D	4501	44B	C25-C26	3.23	1.44	1.39
2	D	4500	BNS	C5-C4	3.21	1.43	1.38
2	B	2500	BNS	C5-C4	3.10	1.43	1.38
2	D	4500	BNS	C3-C4	2.95	1.42	1.38
2	C	3500	BNS	C3-C4	2.79	1.42	1.38
2	A	1500	BNS	C5-C4	2.76	1.42	1.38
2	B	2500	BNS	C3-C4	2.65	1.42	1.38
2	A	1500	BNS	C3-C4	2.58	1.42	1.38
3	D	4501	44B	C28-C23	2.54	1.43	1.39
3	B	2501	44B	C24-C23	2.40	1.43	1.39
3	D	4501	44B	C33-C26	2.38	1.57	1.53
3	C	3501	44B	C24-C23	2.35	1.43	1.39
3	D	4501	44B	C38-C33	2.27	1.59	1.54
3	A	1501	44B	C38-C33	2.25	1.59	1.54
3	C	3501	44B	C28-C27	2.21	1.42	1.38
3	B	2501	44B	C28-C23	2.17	1.42	1.39
3	D	4501	44B	C28-C27	2.15	1.42	1.38
3	D	4501	44B	O42-C33	2.14	1.46	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1501	44B	C19-C16-N15	-4.81	105.45	111.95
3	D	4501	44B	C19-C16-N15	-4.77	105.51	111.95
3	C	3501	44B	C19-C16-N15	-4.11	106.40	111.95
3	B	2501	44B	C19-C16-N15	-3.27	107.54	111.95
3	C	3501	44B	F22-C19-C16	-2.95	103.75	111.85
3	D	4501	44B	C27-C26-C33	2.90	126.78	120.30
3	B	2501	44B	C16-N15-C23	-2.73	114.86	122.52
3	C	3501	44B	C16-N15-C23	-2.60	115.22	122.52
2	A	1500	BNS	O2-S1-C4	2.56	110.41	104.58
3	A	1501	44B	C16-N15-C23	-2.36	115.91	122.52
3	D	4501	44B	C24-C23-N15	-2.27	116.26	120.97
3	A	1501	44B	F41-C38-C33	2.25	116.15	111.85
2	D	4500	BNS	O1-S1-C4	-2.24	99.48	104.58
3	A	1501	44B	C38-C33-C26	-2.21	106.58	110.34
3	D	4501	44B	C25-C26-C33	-2.15	115.49	120.30
3	A	1501	44B	F20-C19-F22	2.13	114.25	106.43
3	A	1501	44B	C27-C26-C33	2.02	124.80	120.30

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2501	44B	C28-C23-N15-C16
3	B	2501	44B	C24-C23-N15-C16
3	A	1501	44B	N15-C16-C19-F22
3	C	3501	44B	C28-C23-N15-C16
2	C	3500	BNS	C3-C4-S1-O2
2	C	3500	BNS	C5-C4-S1-O2
2	D	4500	BNS	C3-C4-S1-O1
2	D	4500	BNS	C5-C4-S1-O1
2	A	1500	BNS	C3-C4-S1-O1
2	A	1500	BNS	C3-C4-S1-O2
2	A	1500	BNS	C5-C4-S1-O1
2	B	2500	BNS	C3-C4-S1-O1
2	B	2500	BNS	C5-C4-S1-O1
3	C	3501	44B	C24-C23-N15-C16
3	A	1501	44B	C28-C23-N15-C16
3	A	1501	44B	C24-C23-N15-C16
3	A	1501	44B	N15-C16-C19-F21
2	C	3500	BNS	C3-C4-S1-O1
2	C	3500	BNS	C5-C4-S1-O1
2	D	4500	BNS	C3-C4-S1-O2
2	D	4500	BNS	C5-C4-S1-O2

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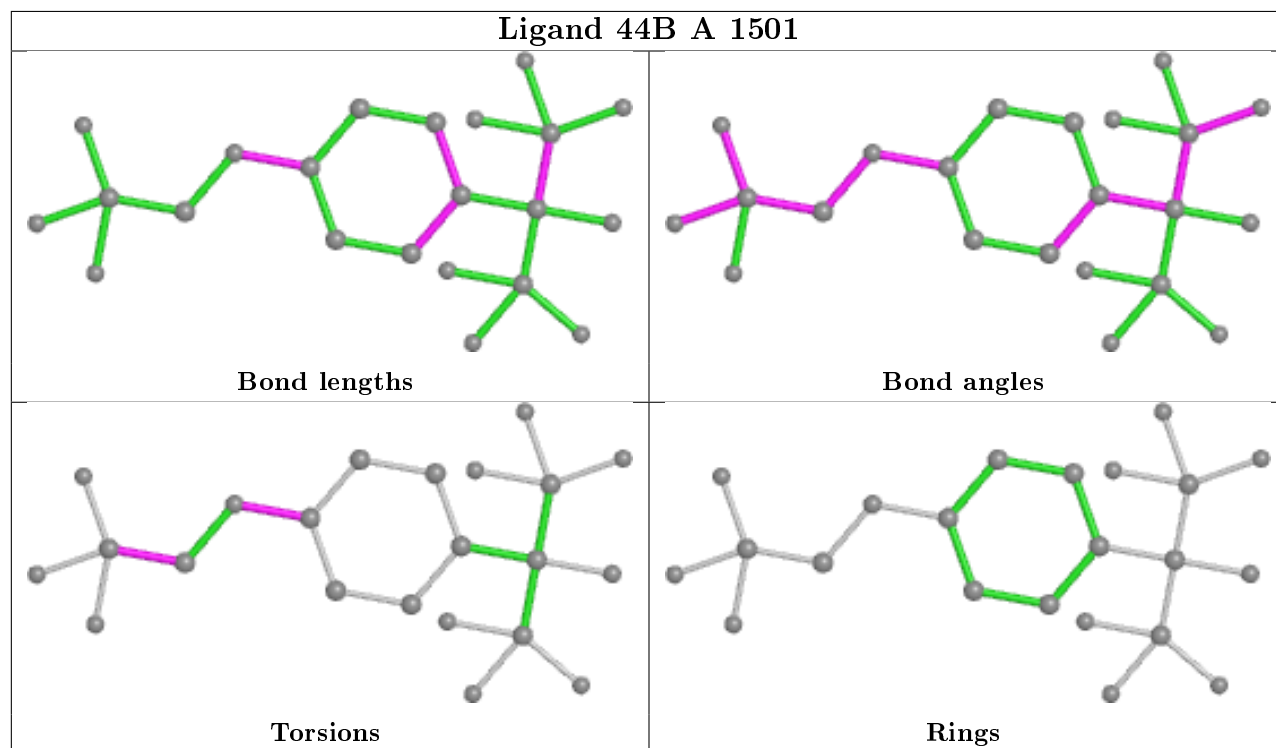
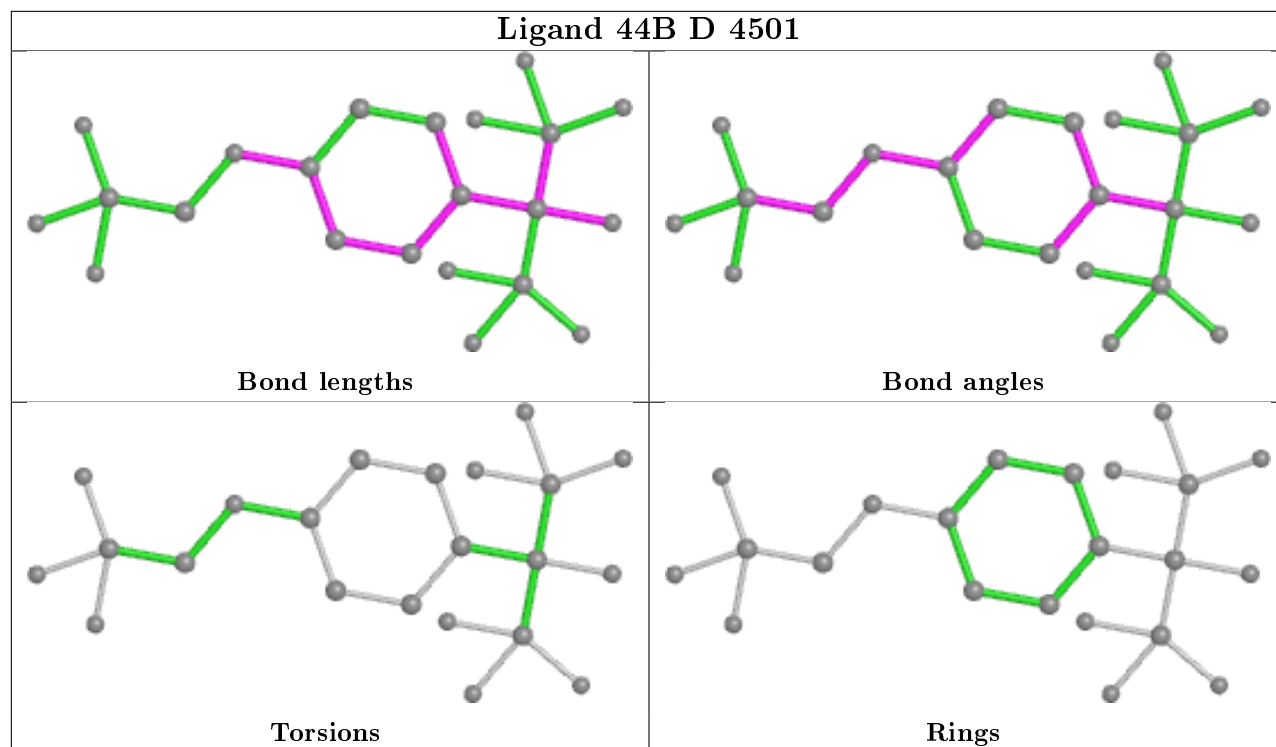
Mol	Chain	Res	Type	Atoms
2	B	2500	BNS	C3-C4-S1-O2
2	B	2500	BNS	C5-C4-S1-O2

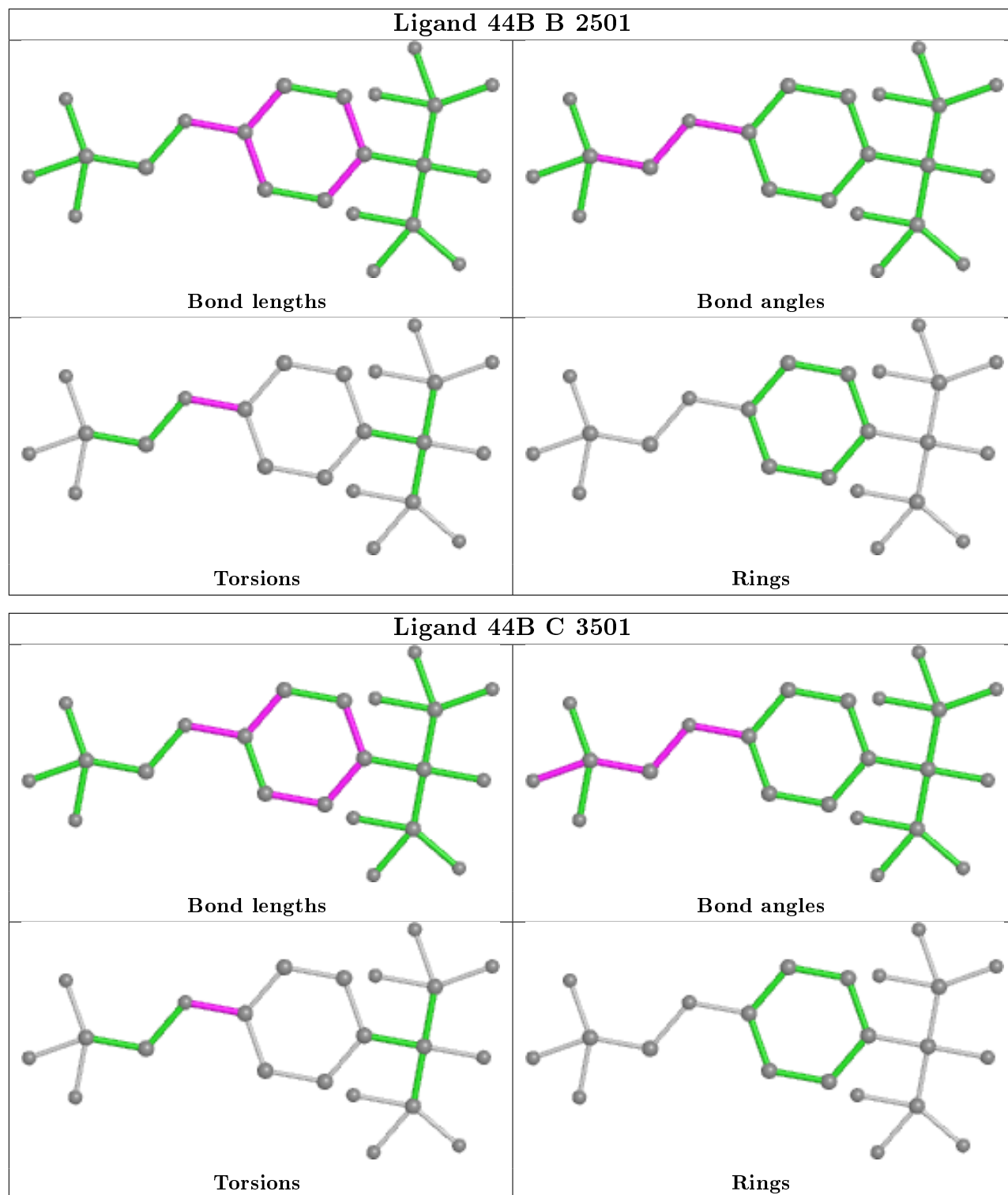
There are no ring outliers.

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3500	BNS	2	0
3	D	4501	44B	1	0
3	A	1501	44B	1	0
2	D	4500	BNS	1	0
3	C	3501	44B	2	0
2	A	1500	BNS	1	0
2	B	2500	BNS	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 ⓘ

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

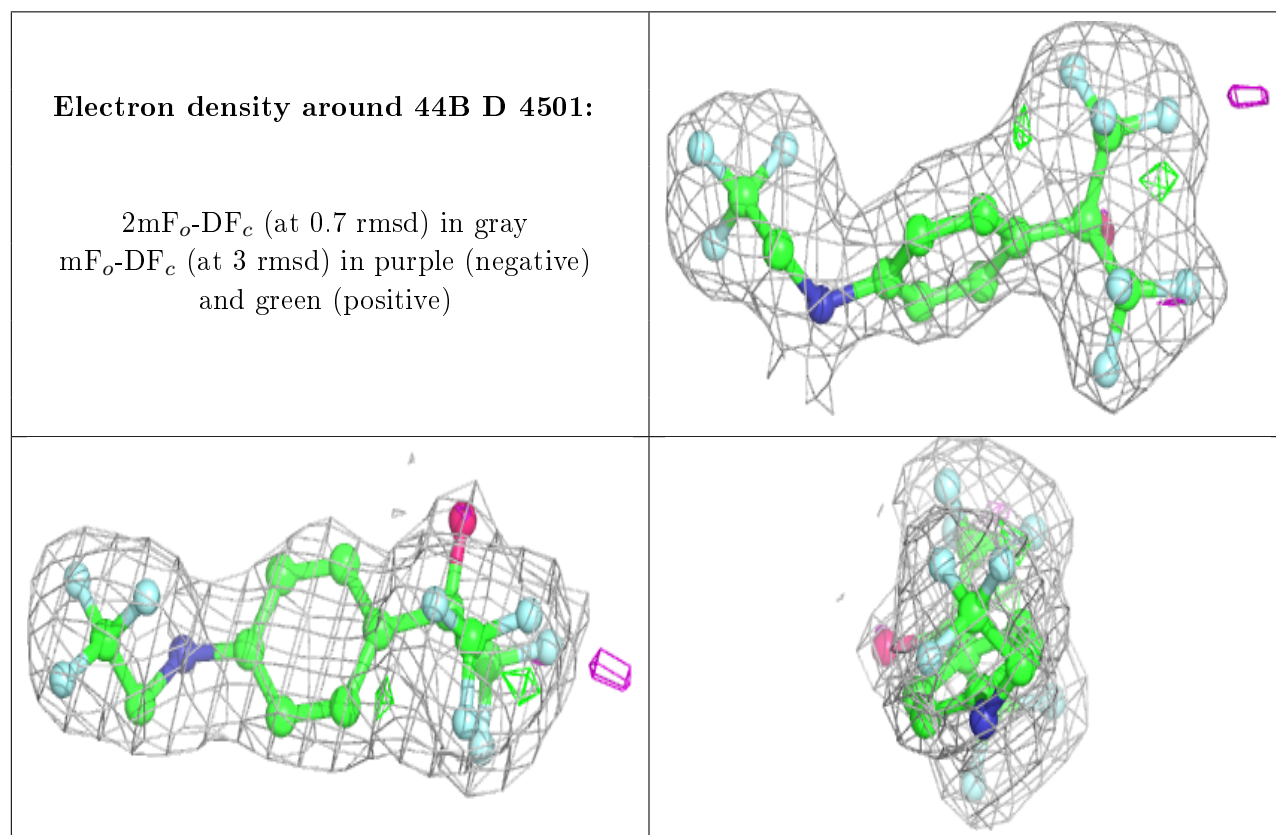
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

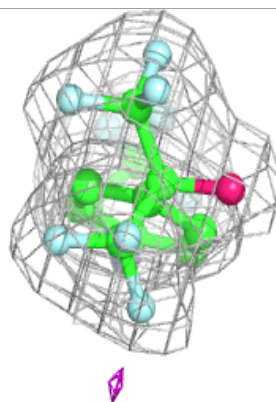
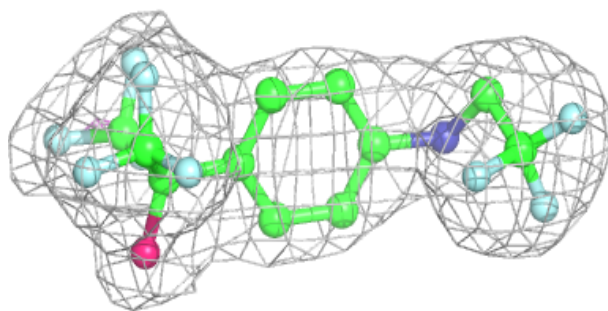
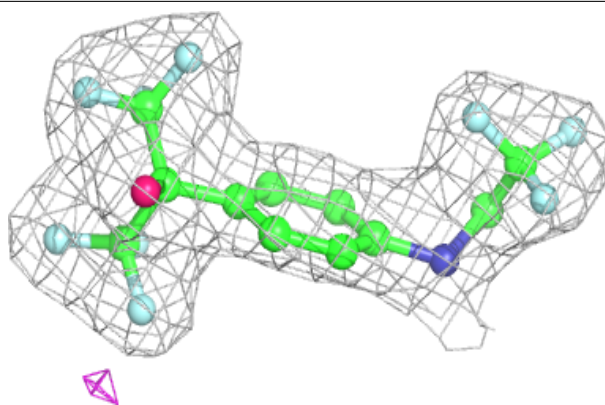
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

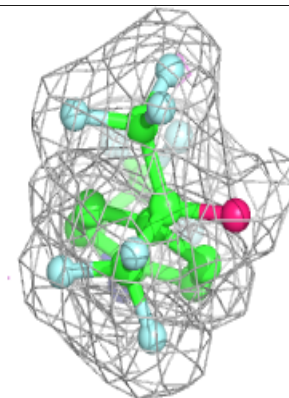
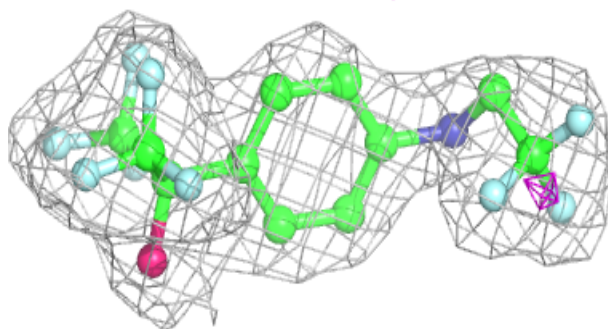
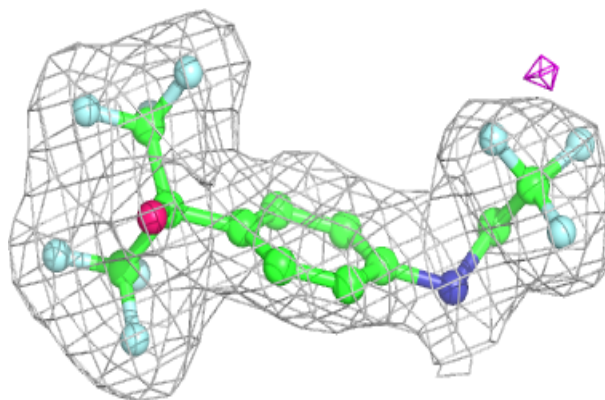


**Electron density around 44B A 1501:**

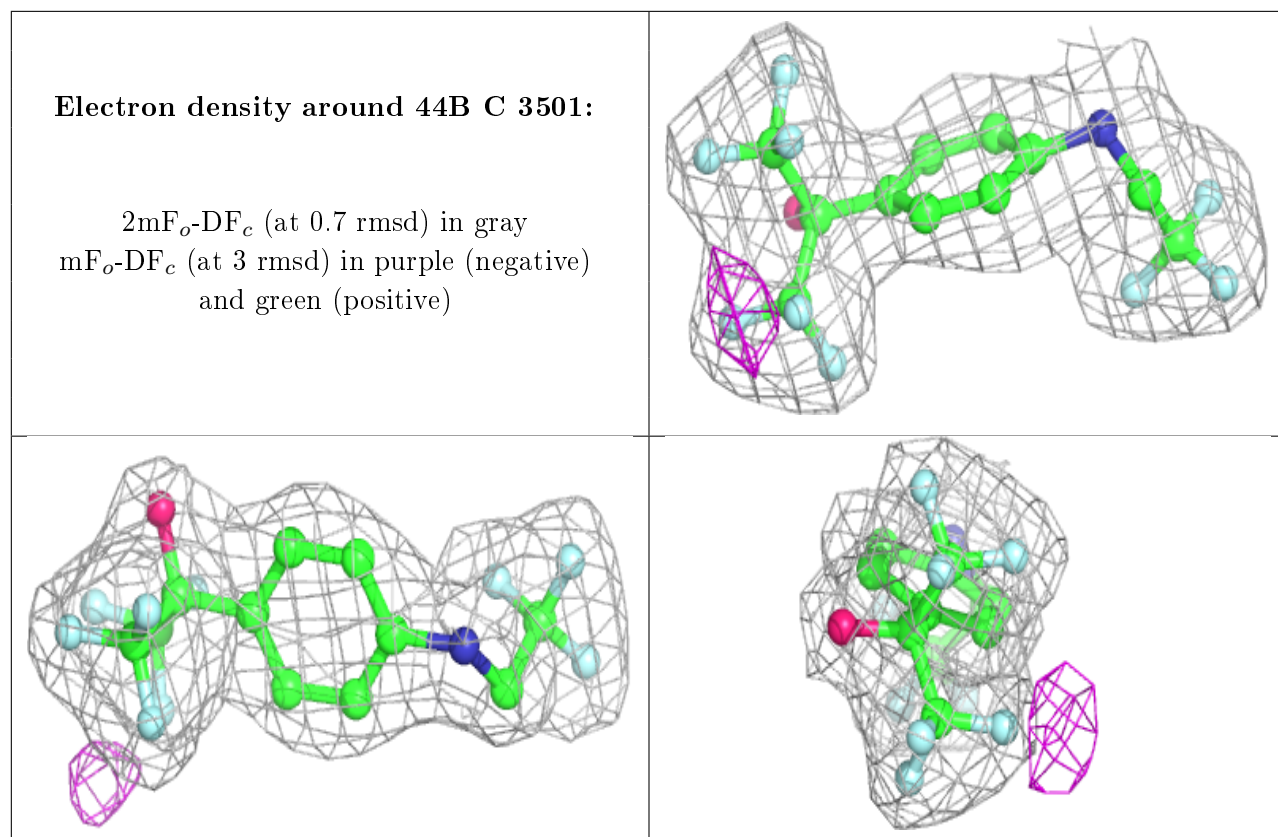
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 44B B 2501:**

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







## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.