



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 11:30 PM JST

PDB ID : 6K9G
Title : Human LXR-beta in complex with an agonist
Authors : Zhang, Z.; Zhou, H.
Deposited on : 2019-06-15
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

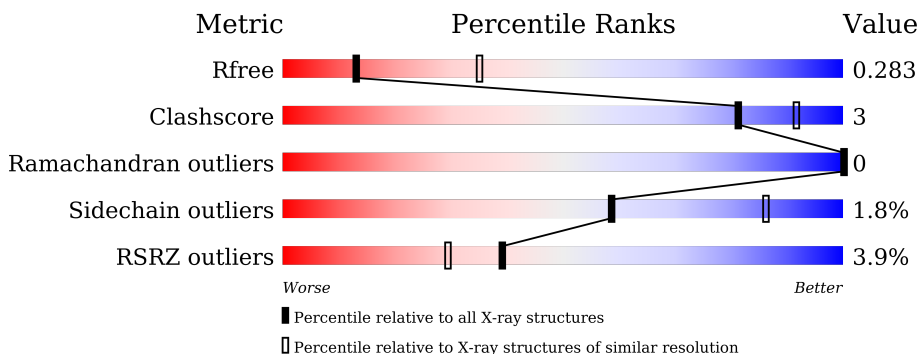
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

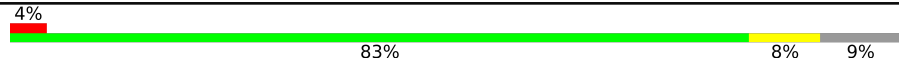

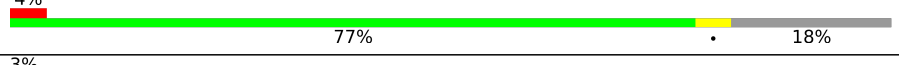

The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	274	 4% 83% 8% 9%
1	B	274	 2% 79% 17%
1	C	274	 4% 77% 18%
1	D	274	 3% 81% 16%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6943 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
			Total	C	N	O	S			
1	A	249	Total 1824	C 1182	N 319	O 316	S 7	0	0	0
1	B	228	Total 1675	C 1086	N 288	O 294	S 7	0	0	0
1	C	225	Total 1643	C 1067	N 283	O 286	S 7	0	0	0
1	D	230	Total 1640	C 1072	N 274	O 287	S 7	0	0	0

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	MET	-	initiating methionine	UNP P55055
A	208	GLY	-	expression tag	UNP P55055
A	209	HIS	-	expression tag	UNP P55055
A	210	HIS	-	expression tag	UNP P55055
A	211	HIS	-	expression tag	UNP P55055
A	212	HIS	-	expression tag	UNP P55055
A	213	HIS	-	expression tag	UNP P55055
A	214	HIS	-	expression tag	UNP P55055
A	259	ALA	GLN	engineered mutation	UNP P55055
A	261	GLY	ARG	engineered mutation	UNP P55055
A	262	SER	ASP	engineered mutation	UNP P55055
A	264	SER	ARG	engineered mutation	UNP P55055
A	462	GLY	-	expression tag	UNP P55055
A	463	SER	-	expression tag	UNP P55055
A	464	GLY	-	expression tag	UNP P55055
A	465	SER	-	expression tag	UNP P55055
A	466	GLY	-	expression tag	UNP P55055
A	467	SER	-	expression tag	UNP P55055
A	468	HIS	-	expression tag	UNP P55055
A	469	LYS	-	expression tag	UNP P55055
A	470	ILE	-	expression tag	UNP P55055

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	LEU	-	expression tag	UNP P55055
A	472	HIS	-	expression tag	UNP P55055
A	473	ARG	-	expression tag	UNP P55055
A	474	LEU	-	expression tag	UNP P55055
A	475	LEU	-	expression tag	UNP P55055
A	476	GLN	-	expression tag	UNP P55055
A	477	ASP	-	expression tag	UNP P55055
A	478	SER	-	expression tag	UNP P55055
A	479	SER	-	expression tag	UNP P55055
A	480	SER	-	expression tag	UNP P55055
B	207	MET	-	initiating methionine	UNP P55055
B	208	GLY	-	expression tag	UNP P55055
B	209	HIS	-	expression tag	UNP P55055
B	210	HIS	-	expression tag	UNP P55055
B	211	HIS	-	expression tag	UNP P55055
B	212	HIS	-	expression tag	UNP P55055
B	213	HIS	-	expression tag	UNP P55055
B	214	HIS	-	expression tag	UNP P55055
B	259	ALA	GLN	engineered mutation	UNP P55055
B	261	GLY	ARG	engineered mutation	UNP P55055
B	262	SER	ASP	engineered mutation	UNP P55055
B	264	SER	ARG	engineered mutation	UNP P55055
B	462	GLY	-	expression tag	UNP P55055
B	463	SER	-	expression tag	UNP P55055
B	464	GLY	-	expression tag	UNP P55055
B	465	SER	-	expression tag	UNP P55055
B	466	GLY	-	expression tag	UNP P55055
B	467	SER	-	expression tag	UNP P55055
B	468	HIS	-	expression tag	UNP P55055
B	469	LYS	-	expression tag	UNP P55055
B	470	ILE	-	expression tag	UNP P55055
B	471	LEU	-	expression tag	UNP P55055
B	472	HIS	-	expression tag	UNP P55055
B	473	ARG	-	expression tag	UNP P55055
B	474	LEU	-	expression tag	UNP P55055
B	475	LEU	-	expression tag	UNP P55055
B	476	GLN	-	expression tag	UNP P55055
B	477	ASP	-	expression tag	UNP P55055
B	478	SER	-	expression tag	UNP P55055
B	479	SER	-	expression tag	UNP P55055
B	480	SER	-	expression tag	UNP P55055
C	207	MET	-	initiating methionine	UNP P55055

Continued on next page...

Continued from previous page...

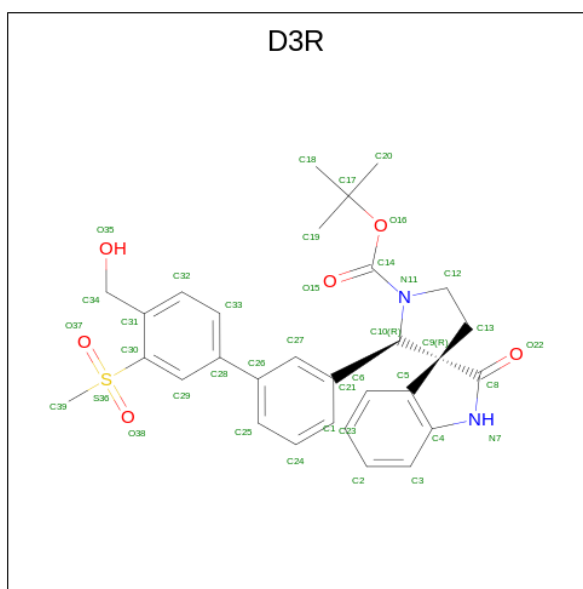
Chain	Residue	Modelled	Actual	Comment	Reference
C	208	GLY	-	expression tag	UNP P55055
C	209	HIS	-	expression tag	UNP P55055
C	210	HIS	-	expression tag	UNP P55055
C	211	HIS	-	expression tag	UNP P55055
C	212	HIS	-	expression tag	UNP P55055
C	213	HIS	-	expression tag	UNP P55055
C	214	HIS	-	expression tag	UNP P55055
C	259	ALA	GLN	engineered mutation	UNP P55055
C	261	GLY	ARG	engineered mutation	UNP P55055
C	262	SER	ASP	engineered mutation	UNP P55055
C	264	SER	ARG	engineered mutation	UNP P55055
C	462	GLY	-	expression tag	UNP P55055
C	463	SER	-	expression tag	UNP P55055
C	464	GLY	-	expression tag	UNP P55055
C	465	SER	-	expression tag	UNP P55055
C	466	GLY	-	expression tag	UNP P55055
C	467	SER	-	expression tag	UNP P55055
C	468	HIS	-	expression tag	UNP P55055
C	469	LYS	-	expression tag	UNP P55055
C	470	ILE	-	expression tag	UNP P55055
C	471	LEU	-	expression tag	UNP P55055
C	472	HIS	-	expression tag	UNP P55055
C	473	ARG	-	expression tag	UNP P55055
C	474	LEU	-	expression tag	UNP P55055
C	475	LEU	-	expression tag	UNP P55055
C	476	GLN	-	expression tag	UNP P55055
C	477	ASP	-	expression tag	UNP P55055
C	478	SER	-	expression tag	UNP P55055
C	479	SER	-	expression tag	UNP P55055
C	480	SER	-	expression tag	UNP P55055
D	207	MET	-	initiating methionine	UNP P55055
D	208	GLY	-	expression tag	UNP P55055
D	209	HIS	-	expression tag	UNP P55055
D	210	HIS	-	expression tag	UNP P55055
D	211	HIS	-	expression tag	UNP P55055
D	212	HIS	-	expression tag	UNP P55055
D	213	HIS	-	expression tag	UNP P55055
D	214	HIS	-	expression tag	UNP P55055
D	259	ALA	GLN	engineered mutation	UNP P55055
D	261	GLY	ARG	engineered mutation	UNP P55055
D	262	SER	ASP	engineered mutation	UNP P55055
D	264	SER	ARG	engineered mutation	UNP P55055

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	462	GLY	-	expression tag	UNP P55055
D	463	SER	-	expression tag	UNP P55055
D	464	GLY	-	expression tag	UNP P55055
D	465	SER	-	expression tag	UNP P55055
D	466	GLY	-	expression tag	UNP P55055
D	467	SER	-	expression tag	UNP P55055
D	468	HIS	-	expression tag	UNP P55055
D	469	LYS	-	expression tag	UNP P55055
D	470	ILE	-	expression tag	UNP P55055
D	471	LEU	-	expression tag	UNP P55055
D	472	HIS	-	expression tag	UNP P55055
D	473	ARG	-	expression tag	UNP P55055
D	474	LEU	-	expression tag	UNP P55055
D	475	LEU	-	expression tag	UNP P55055
D	476	GLN	-	expression tag	UNP P55055
D	477	ASP	-	expression tag	UNP P55055
D	478	SER	-	expression tag	UNP P55055
D	479	SER	-	expression tag	UNP P55055
D	480	SER	-	expression tag	UNP P55055

- Molecule 2 is {tert}-butyl (2' {R},3 {R})-2'-[3-[4-(hydroxymethyl)-3-methylsulfonyl-phenyl]phenyl]-2-oxidanylidene-spiro[1 {H}-indole-3,3'-pyrrolidine]-1'-carboxylate (three-letter code: D3R) (formula: C₃₀H₃₂N₂O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	39	30	2	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			39	30	2	6	1		
2	C	1	Total	C	N	O	S	0	0
			39	30	2	6	1		
2	D	1	Total	C	N	O	S	0	0
			39	30	2	6	1		

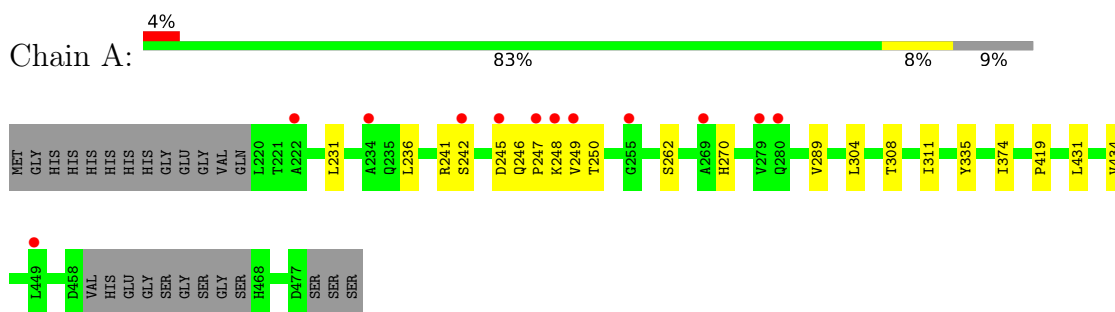
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		
3	D	1	Total	O	0	0
			1	1		

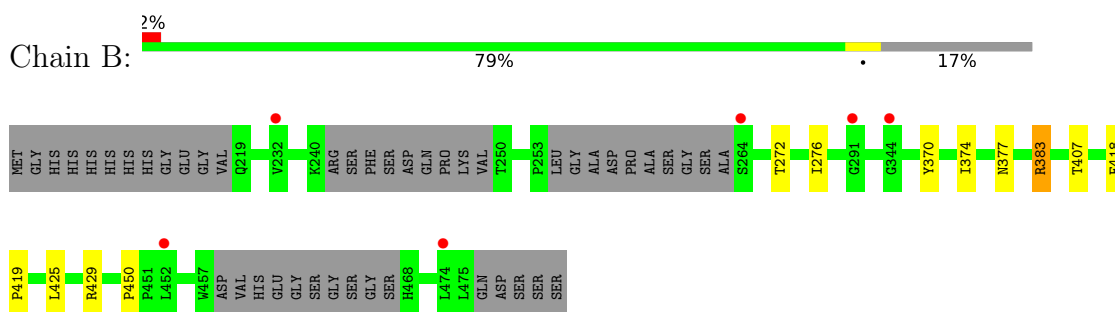
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

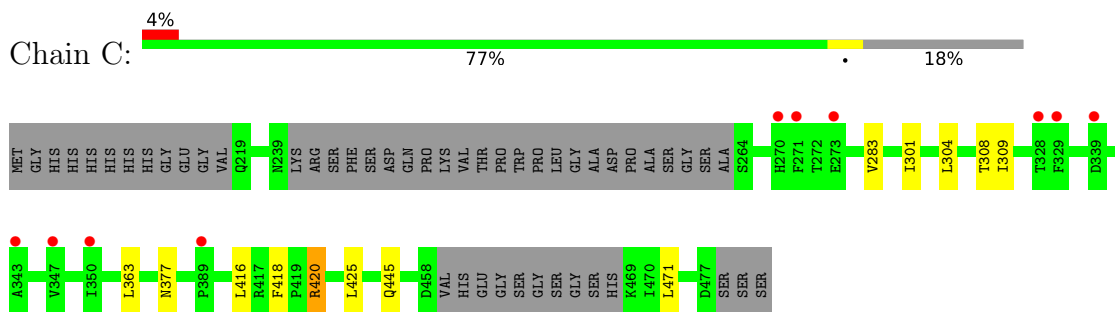
- Molecule 1: Oxysterols receptor LXR-beta



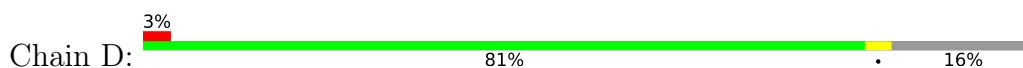
- Molecule 1: Oxysterols receptor LXR-beta

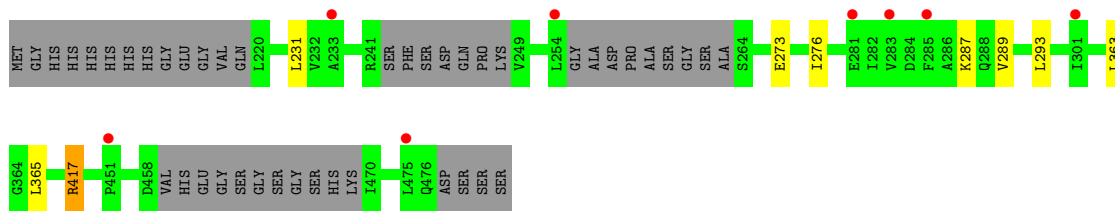


- Molecule 1: Oxysterols receptor LXR-beta



- 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, α , β , γ	67.43Å 103.74Å 152.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.80 40.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.01-2.80) 99.2 (40.55-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.39 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.261 , 0.281 0.262 , 0.283	Depositor DCC
R_{free} test set	1355 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtrriage
Anisotropy	0.472	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6943	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D3R

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	0/1861	0.59	0/2542
1	B	0.37	0/1706	0.56	0/2328
1	C	0.36	0/1673	0.58	0/2283
1	D	0.36	0/1670	0.53	0/2287
All	All	0.37	0/6910	0.56	0/9440

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1824	0	1738	14	0
1	B	1675	0	1574	10	0
1	C	1643	0	1550	8	0
1	D	1640	0	1532	4	0
2	A	39	0	0	0	0
2	B	39	0	0	0	0
2	C	39	0	0	0	0
2	D	39	0	0	0	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	D	1	0	0	0	0
All	All	6943	0	6394	35	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 3.

All (35) 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:383:ARG:HH11	1:B:383:ARG:HG3	1.00	1.09
1:B:383:ARG:HH11	1:B:383:ARG:CG	1.74	0.99
1:B:383:ARG:HG3	1:B:383:ARG:NH1	1.83	0.90
1:B:407:THR:HG21	1:B:418:PHE:HB2	1.72	0.71
1:A:242:SER:O	1:A:245:ASP:N	2.25	0.70
1:B:383:ARG:CG	1:B:383:ARG:NH1	2.44	0.66
1:A:246:GLN:N	1:A:247:PRO:HD2	2.12	0.64
1:A:249:VAL:HG12	1:A:250:THR:N	2.13	0.64
1:D:287:LYS:HA	1:D:293:LEU:HD11	1.86	0.56
1:B:370:TYR:O	1:B:374:ILE:HD12	2.05	0.55
1:C:363:LEU:HD21	1:C:420:ARG:HB3	1.89	0.53
1:A:270:HIS:NE2	1:A:335:TYR:OH	2.37	0.52
1:A:249:VAL:CG1	1:A:250:THR:N	2.73	0.52
1:A:304:LEU:O	1:A:308:THR:HG23	2.10	0.52
1:D:363:LEU:O	1:D:417:ARG:NH1	2.43	0.52
1:A:311:ILE:HG23	1:A:374:ILE:HD12	1.93	0.51
1:C:304:LEU:O	1:C:308:THR:HG23	2.13	0.49
1:A:431:LEU:HA	1:A:434:VAL:HG22	1.96	0.48
1:B:377:ASN:HD22	1:B:425:LEU:HD22	1.78	0.47
1:C:377:ASN:HD22	1:C:425:LEU:HD22	1.80	0.46
1:A:419:PRO:HG3	1:C:418:PHE:HE2	1.82	0.44
1:C:301:ILE:HG23	1:C:471:LEU:HD23	1.99	0.44
1:B:272:THR:O	1:B:276:ILE:HD12	2.18	0.43
1:C:283:VAL:HG12	1:C:304:LEU:HD13	2.00	0.43
1:C:416:LEU:O	1:C:420:ARG:NH1	2.51	0.43
1:D:231:LEU:HD21	1:D:289:VAL:HG23	2.00	0.43
1:A:246:GLN:N	1:A:247:PRO:CD	2.81	0.43
1:D:273:GLU:O	1:D:276:ILE:HG22	2.19	0.42
1:A:231:LEU:HD21	1:A:289:VAL:HG23	2.01	0.42
1:C:416:LEU:HB3	1:C:420:ARG:HH12	1.85	0.41
1:A:249:VAL:HG12	1:A:250:THR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:N	1:A:245:ASP:OD1	2.53	0.41
1:A:311:ILE:HD12	1:A:374:ILE:HG23	2.03	0.41
1:B:276:ILE:HD11	1:B:450:PRO:HG2	2.02	0.41
1:B:418:PHE:HB3	1:B:419:PRO:HD3	2.03	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	245/274 (89%)	243 (99%)	2 (1%)	0	100	100
1	B	220/274 (80%)	216 (98%)	4 (2%)	0	100	100
1	C	219/274 (80%)	214 (98%)	5 (2%)	0	100	100
1	D	222/274 (81%)	218 (98%)	4 (2%)	0	100	100
All	All	906/1096 (83%)	891 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	169/239 (71%)	165 (98%)	4 (2%)	49	81
1	B	155/239 (65%)	153 (99%)	2 (1%)	69	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	152/239 (64%)	149 (98%)	3 (2%)	55	84
1	D	148/239 (62%)	146 (99%)	2 (1%)	67	90
All	All	624/956 (65%)	613 (98%)	11 (2%)	59	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LEU
1	A	241	ARG
1	A	248	LYS
1	A	262	SER
1	B	383	ARG
1	B	429	ARG
1	C	309	ILE
1	C	420	ARG
1	C	445	GLN
1	D	365	LEU
1	D	417	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	230	GLN
1	B	266	GLN
1	B	377	ASN
1	C	270	HIS

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 monosaccharides 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	D3R	B	501	-	42,43,43	1.27	4 (9%)	60,67,67	1.63	8 (13%)
2	D3R	D	501	-	42,43,43	1.30	3 (7%)	60,67,67	1.55	9 (15%)
2	D3R	C	501	-	42,43,43	1.28	5 (11%)	60,67,67	1.91	11 (18%)
2	D3R	A	501	-	42,43,43	1.17	3 (7%)	60,67,67	1.60	11 (18%)

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	D3R	B	501	-	-	6/25/57/57	0/5/5/5
2	D3R	D	501	-	-	2/25/57/57	0/5/5/5
2	D3R	C	501	-	-	4/25/57/57	0/5/5/5
2	D3R	A	501	-	-	4/25/57/57	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	D3R	C30-S36	-5.64	1.70	1.77
2	B	501	D3R	C30-S36	-5.05	1.70	1.77
2	A	501	D3R	C30-S36	-4.89	1.71	1.77
2	C	501	D3R	C30-S36	-4.40	1.71	1.77
2	C	501	D3R	C14-N11	3.86	1.40	1.35
2	B	501	D3R	C14-N11	3.85	1.40	1.35
2	C	501	D3R	O16-C14	3.51	1.39	1.33
2	A	501	D3R	O16-C14	3.40	1.39	1.33
2	D	501	D3R	C14-N11	3.35	1.40	1.35
2	D	501	D3R	O16-C14	3.22	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	D3R	O16-C14	3.04	1.39	1.33
2	A	501	D3R	C14-N11	2.77	1.39	1.35
2	C	501	D3R	C21-C10	2.23	1.54	1.51
2	B	501	D3R	C27-C21	2.12	1.42	1.39
2	C	501	D3R	C39-S36	-2.05	1.67	1.75

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	D3R	C17-O16-C14	7.08	128.69	120.92
2	D	501	D3R	C17-O16-C14	6.95	128.56	120.92
2	C	501	D3R	O37-S36-C39	-6.49	99.16	108.49
2	B	501	D3R	O16-C14-N11	5.98	117.15	110.59
2	A	501	D3R	C17-O16-C14	5.94	127.45	120.92
2	A	501	D3R	O37-S36-C39	-5.79	100.18	108.49
2	B	501	D3R	C34-C31-C30	5.13	127.19	122.50
2	C	501	D3R	C34-C31-C30	4.99	127.06	122.50
2	B	501	D3R	O16-C14-O15	-4.40	119.18	126.40
2	C	501	D3R	C39-S36-C30	4.14	111.25	105.11
2	D	501	D3R	O37-S36-C30	4.10	113.05	108.27
2	D	501	D3R	C34-C31-C30	4.00	126.16	122.50
2	C	501	D3R	C21-C10-N11	3.88	119.15	112.35
2	C	501	D3R	O16-C14-N11	3.71	114.66	110.59
2	B	501	D3R	O37-S36-C30	3.56	112.42	108.27
2	A	501	D3R	C39-S36-C30	3.33	110.04	105.11
2	B	501	D3R	O38-S36-C30	3.31	112.12	108.27
2	D	501	D3R	O16-C14-N11	3.18	114.07	110.59
2	A	501	D3R	C34-C31-C30	3.18	125.40	122.50
2	B	501	D3R	C27-C21-C10	3.16	126.55	120.72
2	C	501	D3R	O37-S36-C30	3.14	111.93	108.27
2	D	501	D3R	O37-S36-C39	-3.13	103.99	108.49
2	B	501	D3R	C23-C21-C10	-3.02	114.34	120.70
2	C	501	D3R	O16-C14-O15	-2.90	121.64	126.40
2	A	501	D3R	O16-C14-N11	2.85	113.72	110.59
2	C	501	D3R	C27-C21-C10	2.80	125.88	120.72
2	C	501	D3R	C23-C21-C10	-2.72	114.98	120.70
2	D	501	D3R	O16-C14-O15	-2.70	121.97	126.40
2	A	501	D3R	O16-C14-O15	-2.69	121.99	126.40
2	A	501	D3R	C23-C21-C10	-2.55	115.33	120.70
2	D	501	D3R	C27-C21-C10	2.46	125.25	120.72
2	A	501	D3R	C27-C21-C10	2.41	125.16	120.72
2	D	501	D3R	C23-C21-C10	-2.37	115.72	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	D3R	C29-C30-S36	2.35	120.16	116.26
2	A	501	D3R	O37-S36-C30	2.33	110.98	108.27
2	B	501	D3R	O38-S36-O37	-2.29	113.98	117.92
2	C	501	D3R	C29-C30-S36	2.09	119.73	116.26
2	D	501	D3R	C21-C10-N11	2.06	115.96	112.35
2	A	501	D3R	C21-C10-N11	2.04	115.92	112.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

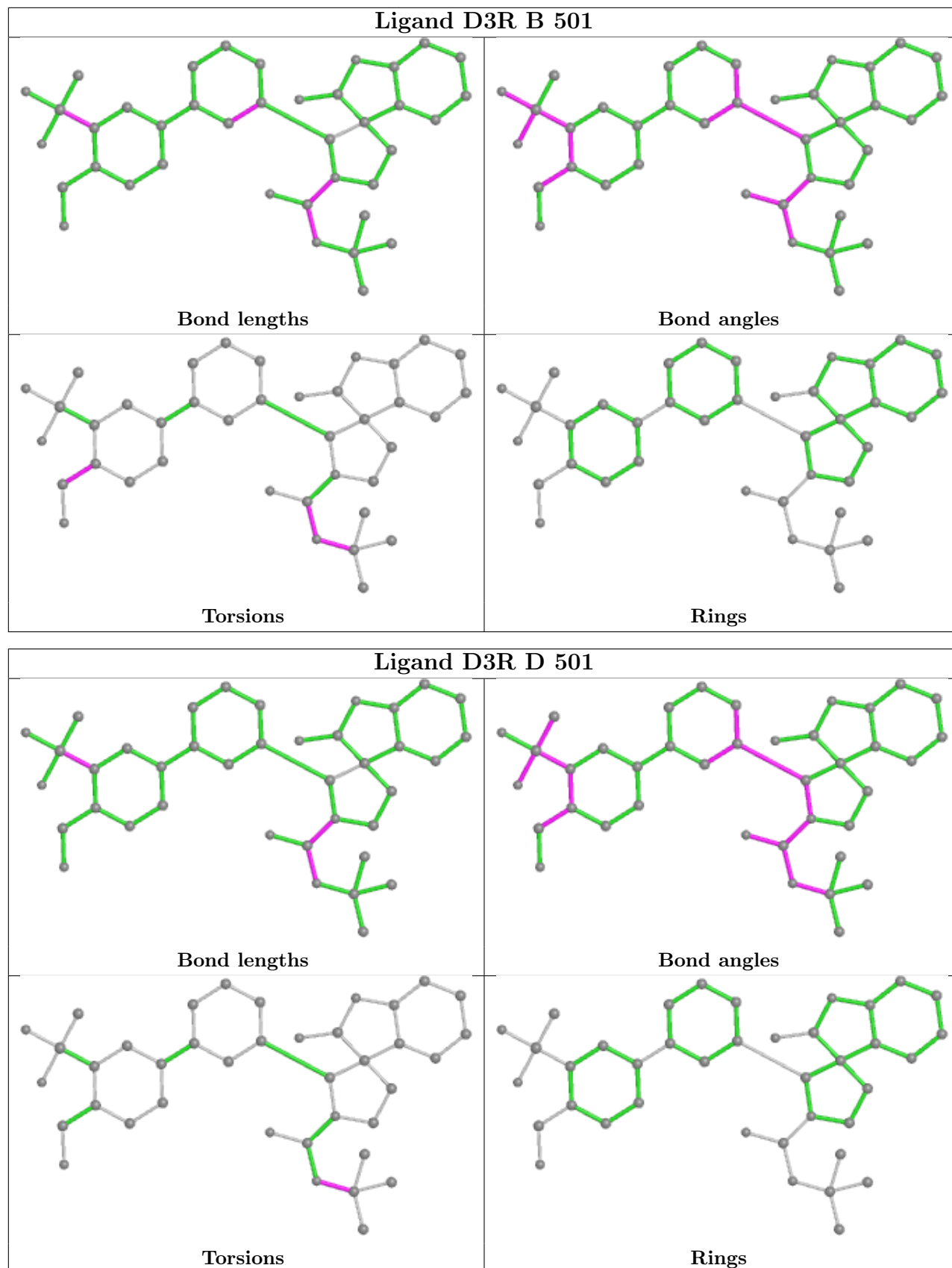
Mol	Chain	Res	Type	Atoms
2	A	501	D3R	C31-C30-S36-O38
2	A	501	D3R	C31-C30-S36-C39
2	B	501	D3R	N11-C14-O16-C17
2	C	501	D3R	C29-C30-S36-O38
2	C	501	D3R	C31-C30-S36-O38
2	C	501	D3R	C31-C30-S36-C39
2	B	501	D3R	O15-C14-O16-C17
2	B	501	D3R	C19-C17-O16-C14
2	B	501	D3R	C18-C17-O16-C14
2	B	501	D3R	C20-C17-O16-C14
2	A	501	D3R	C29-C30-S36-O38
2	D	501	D3R	C18-C17-O16-C14
2	A	501	D3R	C29-C30-S36-C39
2	C	501	D3R	C29-C30-S36-C39
2	B	501	D3R	C30-C31-C34-O35
2	D	501	D3R	C20-C17-O16-C14

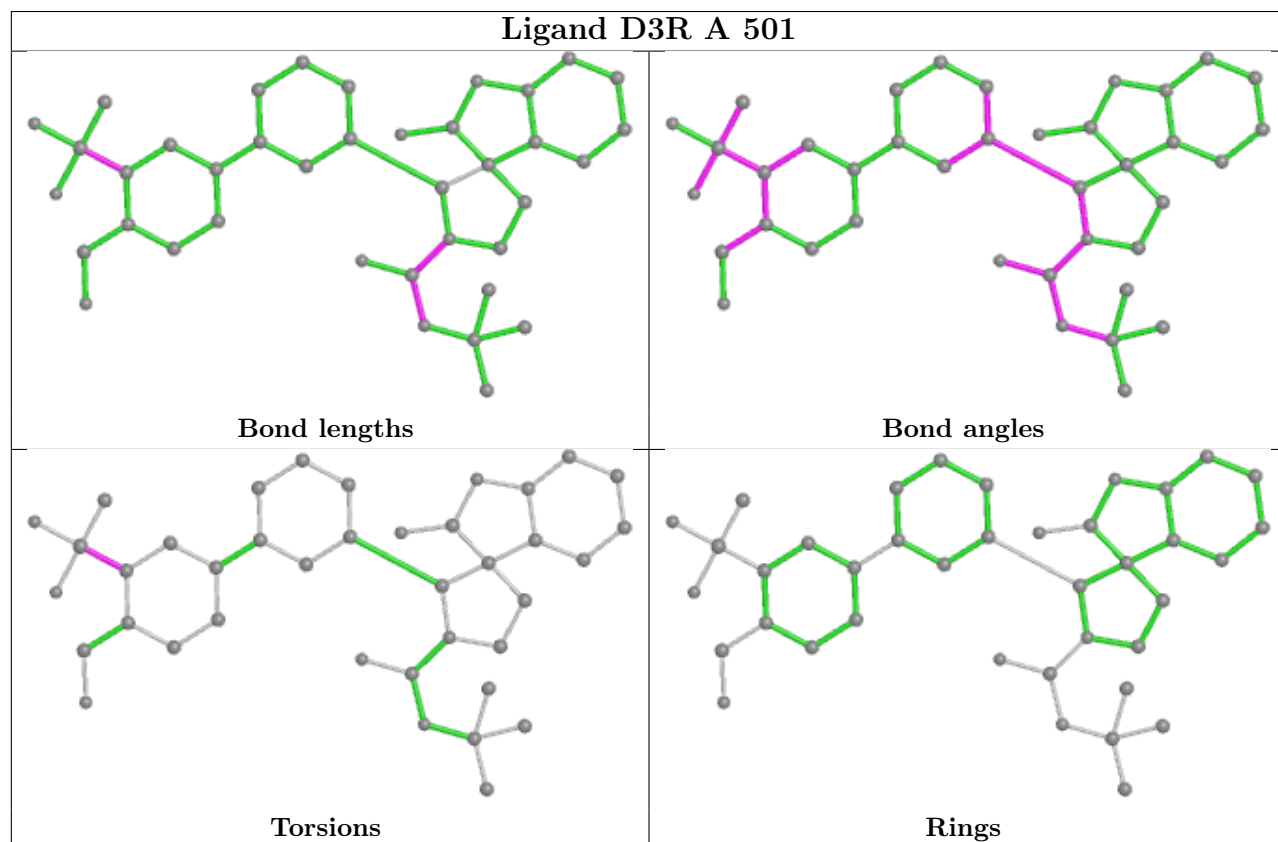
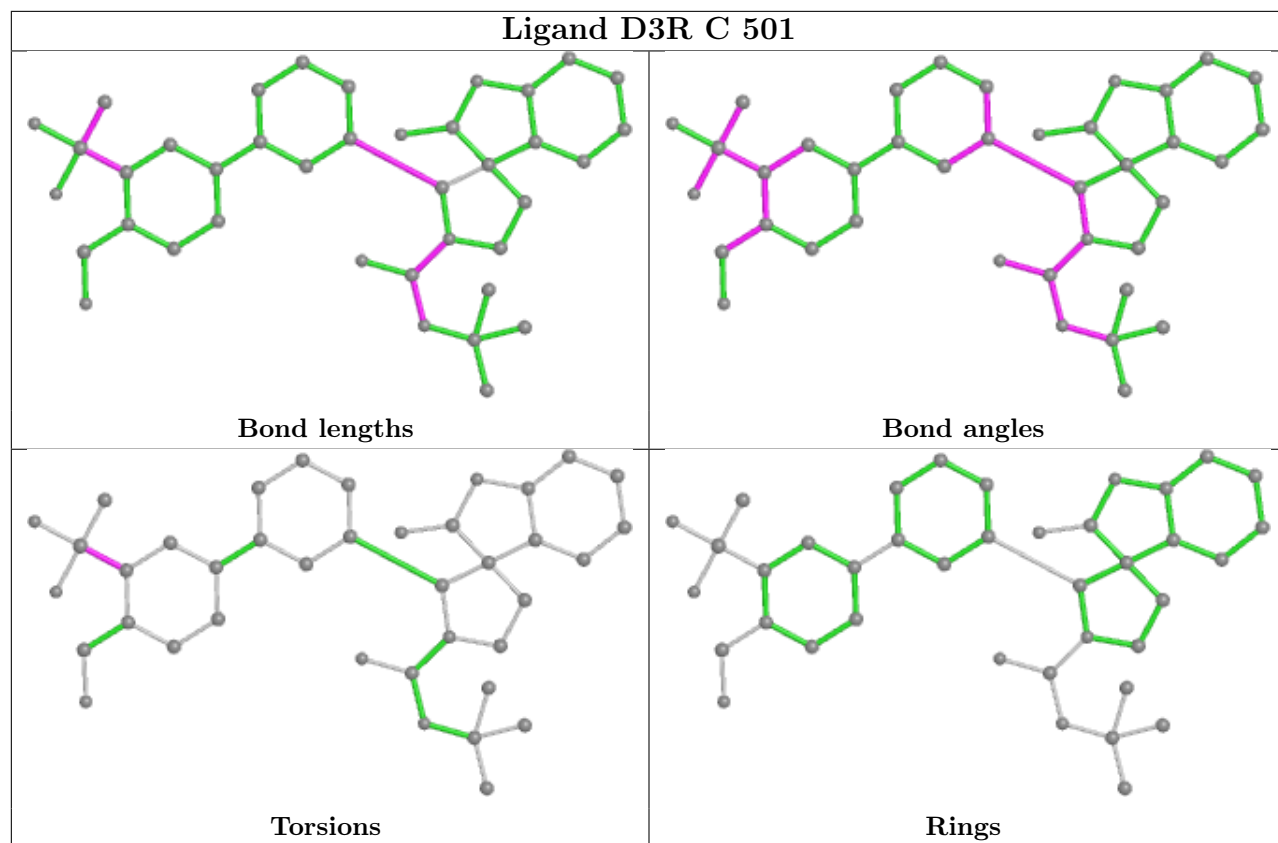
There are no ring outliers.

No monomer is involved in short contacts.

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

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	249/274 (90%)	0.14	12 (4%) 30 21	59, 81, 107, 119	0
1	B	228/274 (83%)	0.20	6 (2%) 56 46	57, 88, 125, 137	0
1	C	225/274 (82%)	0.19	10 (4%) 34 24	59, 84, 117, 136	0
1	D	230/274 (83%)	0.12	8 (3%) 44 34	61, 94, 127, 147	0
All	All	932/1096 (85%)	0.16	36 (3%) 39 29	57, 86, 123, 147	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	SER	5.4
1	C	347	VAL	4.5
1	A	245	ASP	4.3
1	B	264	SER	4.3
1	C	271	PHE	3.9
1	C	343	ALA	3.8
1	C	270	HIS	3.5
1	A	255	GLY	3.4
1	A	280	GLN	3.1
1	C	329	PHE	3.0
1	A	247	PRO	2.9
1	D	254	LEU	2.8
1	A	249	VAL	2.8
1	B	291	GLY	2.6
1	C	350	ILE	2.6
1	C	273	GLU	2.5
1	D	283	VAL	2.5
1	C	339	ASP	2.4
1	A	279	VAL	2.4
1	B	232	VAL	2.4
1	B	474	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	301	ILE	2.3
1	B	452	LEU	2.2
1	C	389	PRO	2.2
1	D	281	GLU	2.2
1	A	449	LEU	2.2
1	D	475	LEU	2.2
1	A	234	ALA	2.1
1	A	269	ALA	2.1
1	D	233	ALA	2.1
1	A	248	LYS	2.1
1	A	222	ALA	2.1
1	D	451	PRO	2.1
1	C	328	THR	2.0
1	B	344	GLY	2.0
1	D	285	PHE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

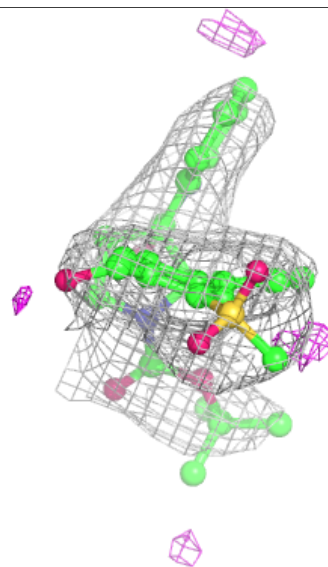
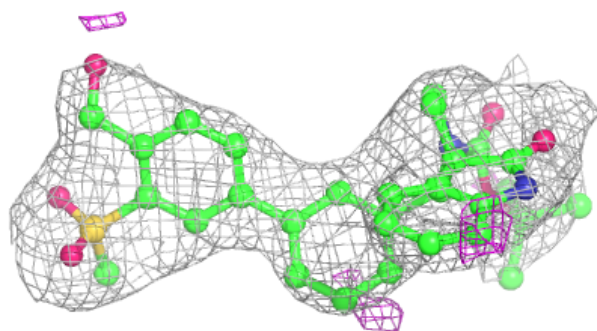
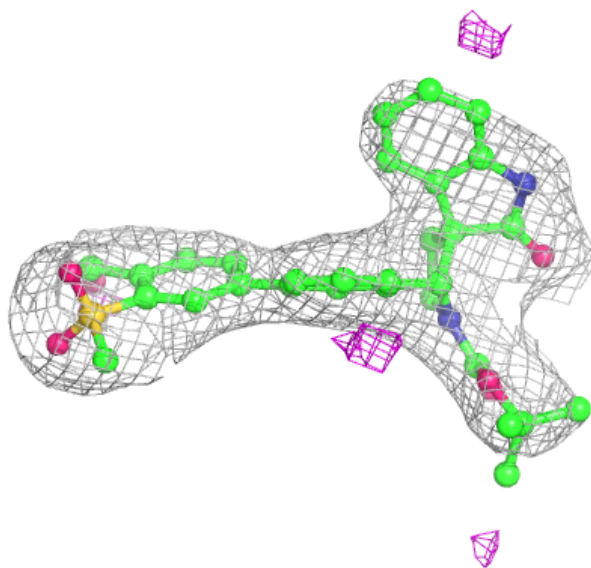
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	D3R	C	501	39/39	0.92	0.30	65,69,73,75	0
2	D3R	D	501	39/39	0.92	0.24	72,73,78,79	0
2	D3R	B	501	39/39	0.94	0.18	56,59,66,67	0
2	D3R	A	501	39/39	0.96	0.20	51,55,64,66	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.

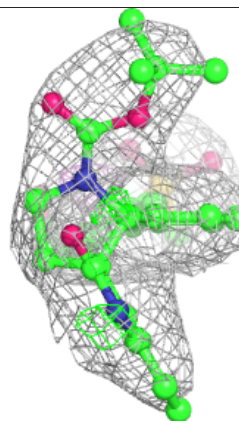
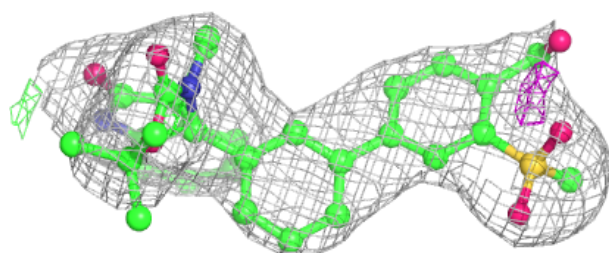
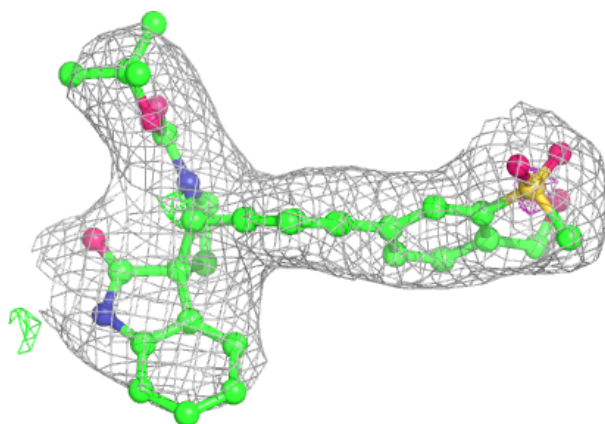
Electron density around D3R C 501:

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



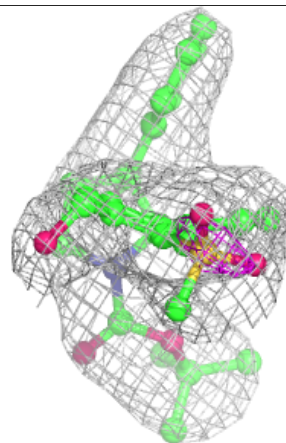
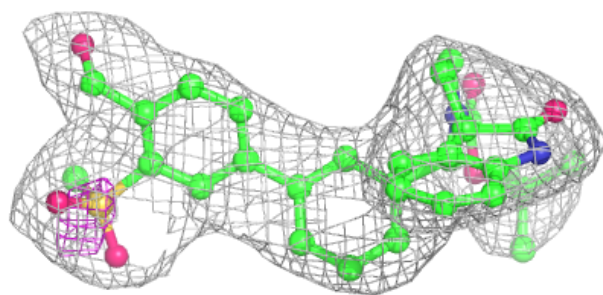
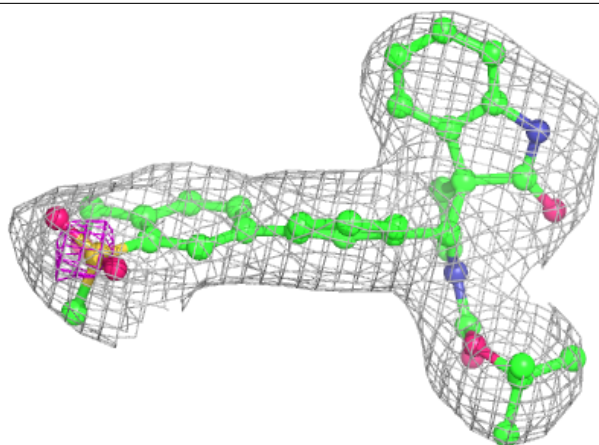
Electron density around D3R D 501:

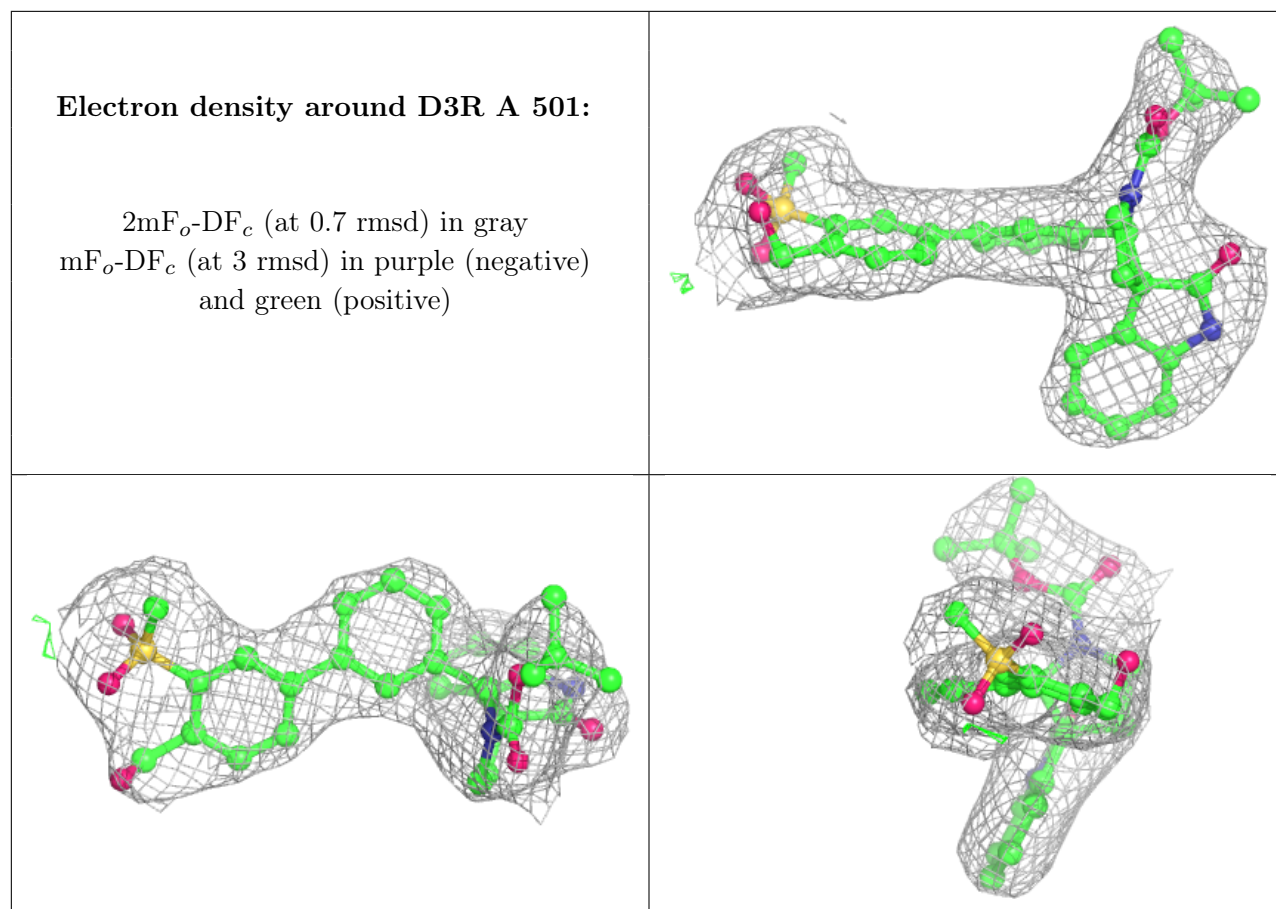
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around D3R B 501:

$2mF_o-DF_c$ (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.