



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 04:10 AM EST

PDB ID : 3FC6  
Title : hRXRalpha & mLXRalpha with an indole Pharmacophore, SB786875  
Authors : Washburn, D.G.; Hoang, T.H.; Campobasso, N.; Smallwood, A.; Parks, D.J.;  
Webb, C.L.; Frank, K.; Nord, M.; Duraiswami, C.; Evans, C.; Jaye, M.;  
Thompson, S.K.  
Deposited on : 2008-11-21  
Resolution : 2.06 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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

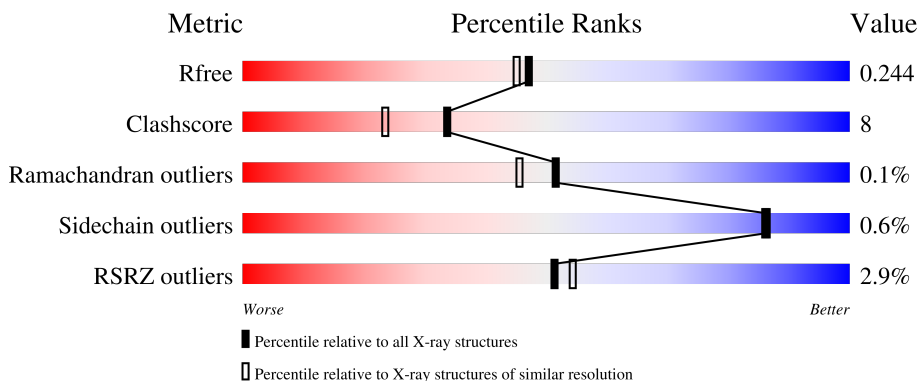
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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  $\geq 3$ , 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	242	 5% 68% 17% 14%
1	C	242	 % 75% 9% 17%
2	B	266	 3% 76% 14% 9%
2	D	266	 2% 72% 18% 9%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7497 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	Total 1635	C 1048	N 282	O 295	S 10	0	0	0
1	C	202	Total 1583	C 1007	N 274	O 292	S 10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	-	expression tag	UNP P19793
A	222	LYS	-	expression tag	UNP P19793
A	223	LYS	-	expression tag	UNP P19793
A	224	GLY	-	expression tag	UNP P19793
C	221	MET	-	expression tag	UNP P19793
C	222	LYS	-	expression tag	UNP P19793
C	223	LYS	-	expression tag	UNP P19793
C	224	GLY	-	expression tag	UNP P19793

- Molecule 2 is a protein called Nr1h3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	241	Total 1959	C 1250	N 342	O 360	S 7	0	0	0
2	D	241	Total 1959	C 1250	N 342	O 360	S 7	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

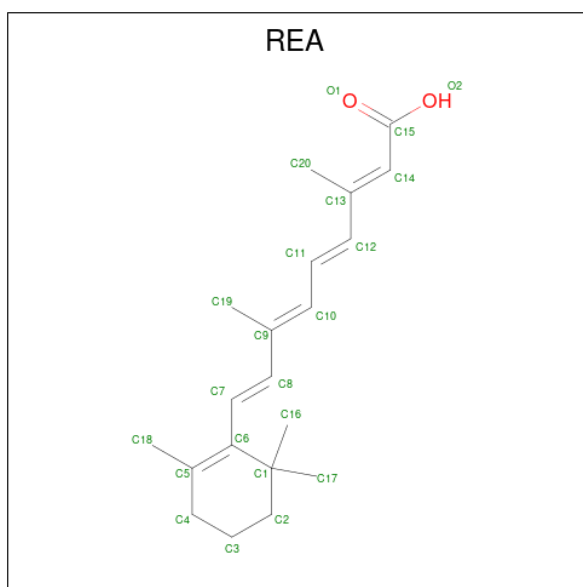
Chain	Residue	Modelled	Actual	Comment	Reference
B	180	MET	-	expression tag	UNP Q91X41
B	181	ARG	-	expression tag	UNP Q91X41
B	182	GLY	-	expression tag	UNP Q91X41
B	183	SER	-	expression tag	UNP Q91X41

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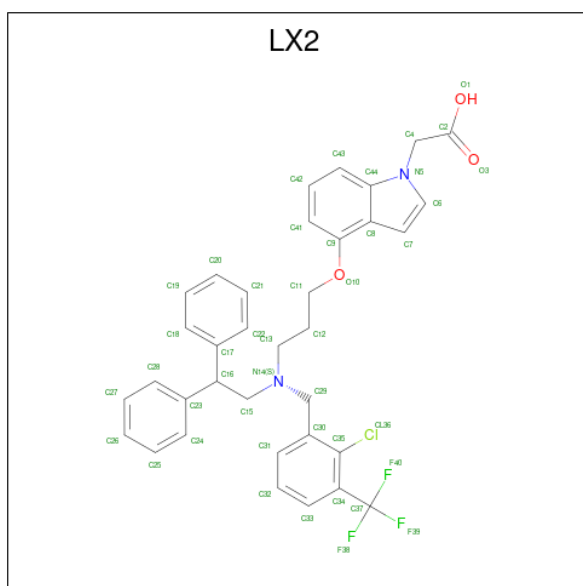
Chain	Residue	Modelled	Actual	Comment	Reference
B	184	HIS	-	expression tag	UNP Q91X41
B	185	HIS	-	expression tag	UNP Q91X41
B	186	HIS	-	expression tag	UNP Q91X41
B	187	HIS	-	expression tag	UNP Q91X41
B	188	HIS	-	expression tag	UNP Q91X41
B	189	HIS	-	expression tag	UNP Q91X41
B	190	GLY	-	expression tag	UNP Q91X41
B	191	MET	-	expression tag	UNP Q91X41
B	192	ALA	-	expression tag	UNP Q91X41
B	193	SER	-	expression tag	UNP Q91X41
B	194	LEU	-	expression tag	UNP Q91X41
B	195	VAL	-	expression tag	UNP Q91X41
B	196	PRO	-	expression tag	UNP Q91X41
B	197	ARG	-	expression tag	UNP Q91X41
B	198	GLY	-	expression tag	UNP Q91X41
B	199	SER	-	expression tag	UNP Q91X41
D	180	MET	-	expression tag	UNP Q91X41
D	181	ARG	-	expression tag	UNP Q91X41
D	182	GLY	-	expression tag	UNP Q91X41
D	183	SER	-	expression tag	UNP Q91X41
D	184	HIS	-	expression tag	UNP Q91X41
D	185	HIS	-	expression tag	UNP Q91X41
D	186	HIS	-	expression tag	UNP Q91X41
D	187	HIS	-	expression tag	UNP Q91X41
D	188	HIS	-	expression tag	UNP Q91X41
D	189	HIS	-	expression tag	UNP Q91X41
D	190	GLY	-	expression tag	UNP Q91X41
D	191	MET	-	expression tag	UNP Q91X41
D	192	ALA	-	expression tag	UNP Q91X41
D	193	SER	-	expression tag	UNP Q91X41
D	194	LEU	-	expression tag	UNP Q91X41
D	195	VAL	-	expression tag	UNP Q91X41
D	196	PRO	-	expression tag	UNP Q91X41
D	197	ARG	-	expression tag	UNP Q91X41
D	198	GLY	-	expression tag	UNP Q91X41
D	199	SER	-	expression tag	UNP Q91X41

- Molecule 3 is RETINOIC ACID (three-letter code: REA) (formula: C<sub>20</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	20	2		
3	C	1	Total	C	O	0	0
			22	20	2		

- Molecule 4 is [4-(3-{[2-chloro-3-(trifluoromethyl)benzyl](2,2-diphenylethyl)amino}propoxy)-1H-indol-1-yl]acetic acid (three-letter code: LX2) (formula: C<sub>35</sub>H<sub>32</sub>ClF<sub>3</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	B	1	Total	C	Cl	F	N	O	0	0
			44	35	1	3	2	3		

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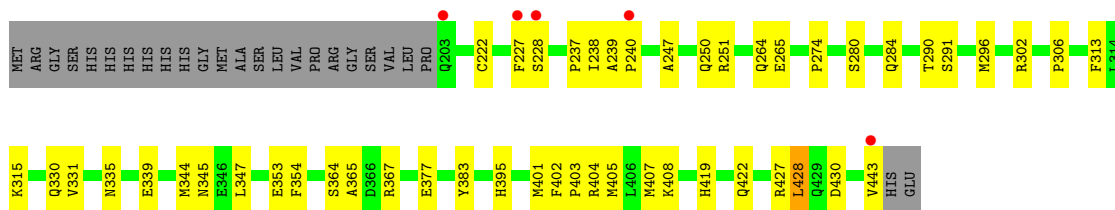
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
4	D	1	44	35	1	3	2	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	64	Total	O	0	0
			64	64		
5	C	53	Total	O	0	0
			53	53		
5	D	80	Total	O	0	0
			80	80		



Chain D:  2% 72% 18% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.16Å 90.03Å 101.64Å 90.00° 111.92° 90.00°	Depositor
Resolution (Å)	44.20 – 2.06 44.22 – 2.06	Depositor EDS
% Data completeness (in resolution range)	88.3 (44.20-2.06) 88.3 (44.22-2.06)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.06Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.199 , 0.250 0.192 , 0.244	Depositor DCC
$R_{free}$ test set	2820 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.47% 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: LX2, REA

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	0.30	0/1665	0.47	0/2247
1	C	0.36	0/1610	0.51	0/2175
2	B	0.34	0/2001	0.48	0/2711
2	D	0.37	0/2001	0.48	0/2711
All	All	0.34	0/7277	0.49	0/9844

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	1635	0	1667	29	0
1	C	1583	0	1611	18	0
2	B	1959	0	1964	36	0
2	D	1959	0	1964	45	0
3	A	22	0	27	5	0
3	C	22	0	27	3	0
4	B	44	0	31	1	0
4	D	44	0	31	5	0
5	A	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	64	0	0	4	0
5	C	53	0	0	1	0
5	D	80	0	0	3	0
All	All	7497	0	7322	124	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 (124) 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)
3:A:501:REA:H8	3:A:501:REA:H181	1.36	1.06
1:C:243:GLU:HB3	1:C:244:PRO:HD2	1.58	0.84
2:D:227:PHE:CE1	2:D:315:LYS:HD2	2.12	0.84
3:A:501:REA:H181	3:A:501:REA:C8	2.10	0.82
2:B:228:SER:HB2	5:B:150:HOH:O	1.81	0.81
2:B:207:GLU:HG3	5:B:451:HOH:O	1.81	0.79
2:B:391:VAL:HG11	2:B:405:MET:CE	2.18	0.73
2:B:429:GLN:HB2	2:B:431:LYS:HG3	1.73	0.69
2:D:227:PHE:HE1	2:D:315:LYS:HD2	1.59	0.67
2:B:402:PHE:HB3	2:B:403:PRO:HD3	1.76	0.67
3:C:501:REA:H181	3:C:501:REA:C8	2.25	0.67
1:C:449:THR:O	1:C:453:GLU:HG3	1.96	0.65
1:C:454:MET:HE1	2:D:264:GLN:HA	1.78	0.65
2:B:391:VAL:HG11	2:B:405:MET:HE2	1.78	0.64
3:C:501:REA:H181	3:C:501:REA:H8	1.80	0.64
1:A:318:ILE:HD11	1:A:357:MET:HB3	1.80	0.63
2:B:305:ASN:HB3	5:B:459:HOH:O	1.98	0.62
2:B:227:PHE:O	2:B:230:ARG:HB3	2.00	0.60
1:C:394:GLU:OE2	2:D:404:ARG:NH1	2.34	0.59
1:A:230:MET:HG3	1:A:395:LYS:HB3	1.84	0.59
2:D:353:GLU:OE2	2:D:395:HIS:NE2	2.35	0.58
2:B:222:CYS:HB3	2:B:265:GLU:HG3	1.86	0.58
2:B:391:VAL:HG11	2:B:405:MET:HE1	1.87	0.57
1:A:454:MET:HE1	2:B:264:GLN:HA	1.87	0.57
2:D:222:CYS:HB3	2:D:265:GLU:HG3	1.86	0.57
2:D:306:PRO:HG3	2:D:345:ASN:OD1	2.05	0.56
2:D:237:PRO:HG2	2:D:251:ARG:HG3	1.87	0.56
3:A:501:REA:H201	3:A:501:REA:O2	2.05	0.56
2:B:248:ARG:HD2	2:B:326:LYS:O	2.06	0.56
2:D:237:PRO:HG2	2:D:251:ARG:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:LEU:C	2:B:403:PRO:HD2	2.27	0.55
2:D:237:PRO:HG3	2:D:250:GLN:HB3	1.89	0.55
3:C:501:REA:H8	3:C:501:REA:C18	2.37	0.55
1:C:431:LYS:O	1:C:434:GLU:HG2	2.07	0.54
1:A:397:TYR:OH	2:B:407:MET:HG3	2.08	0.54
1:A:230:MET:CE	1:A:235:ILE:HD11	2.38	0.53
1:C:454:MET:CE	2:D:264:GLN:HA	2.38	0.53
2:B:400:LEU:O	2:B:403:PRO:HD2	2.09	0.53
1:A:452:MET:O	1:A:456:GLU:HG3	2.09	0.53
1:A:230:MET:CG	1:A:395:LYS:HB3	2.39	0.52
2:D:291:SER:HB3	5:D:7:HOH:O	2.07	0.52
2:B:290:THR:HG21	2:B:368:PRO:HD2	1.92	0.52
2:D:237:PRO:CD	2:D:251:ARG:HG2	2.39	0.52
1:A:422:LEU:HD12	2:B:407:MET:CE	2.40	0.52
2:B:364:SER:O	2:B:367:ARG:HG2	2.10	0.52
1:A:322:ASP:O	1:A:334:ARG:HG3	2.10	0.51
1:C:234:ARG:HD3	5:C:114:HOH:O	2.11	0.51
2:B:238:ILE:O	2:B:238:ILE:HG13	2.09	0.51
2:D:335:ASN:O	2:D:339:GLU:HG3	2.11	0.50
1:C:385:ASN:ND2	1:C:388:GLU:HB2	2.26	0.50
2:D:344:MET:SD	2:D:408:LYS:HG3	2.51	0.50
2:B:438:SER:O	2:B:442:ASP:HB2	2.12	0.49
2:D:228:SER:HB3	5:D:81:HOH:O	2.12	0.49
2:D:238:ILE:HD12	2:D:238:ILE:N	2.27	0.49
2:B:314:LEU:O	2:B:315:LYS:HB2	2.12	0.49
2:D:313:PHE:CE1	4:D:1:LX2:H11A	2.48	0.48
2:B:391:VAL:HG21	2:B:402:PHE:HB2	1.96	0.48
1:A:345:ILE:HD13	1:A:431:LYS:HD3	1.94	0.48
1:A:431:LYS:O	1:A:434:GLU:HG2	2.14	0.48
1:A:277:PHE:CE2	2:D:427:ARG:NH1	2.83	0.47
1:A:315:HIS:CB	1:A:367:LEU:HD22	2.45	0.47
2:B:317:PHE:HB3	2:B:319:TYR:CE2	2.49	0.47
1:A:273:ASP:OD2	2:D:427:ARG:NH1	2.48	0.47
2:B:335:ASN:HB2	2:B:336:PRO:HD3	1.96	0.47
2:D:402:PHE:HB3	2:D:403:PRO:CD	2.45	0.47
2:B:387:LEU:O	2:B:391:VAL:HG13	2.15	0.46
2:D:365:ALA:HB2	2:D:377:GLU:HG3	1.97	0.46
1:A:422:LEU:HD12	2:B:407:MET:HE3	1.96	0.46
1:C:448:ASP:HB3	1:C:449:THR:H	1.55	0.46
2:B:229:ASP:OD1	2:B:232:ARG:HD2	2.16	0.46
2:D:365:ALA:CB	2:D:377:GLU:HG3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:THR:CG2	2:D:367:ARG:HD2	2.45	0.45
2:D:364:SER:O	2:D:367:ARG:HG2	2.15	0.45
1:A:282:TRP:CZ3	1:A:375:LEU:HD22	2.50	0.45
1:C:277:PHE:CD1	1:C:277:PHE:C	2.89	0.45
2:D:401:MET:O	2:D:405:MET:HG3	2.17	0.45
3:A:501:REA:H161	3:A:501:REA:H7	1.69	0.45
2:D:238:ILE:HD12	2:D:238:ILE:H	1.82	0.45
2:D:443:VAL:O	2:D:443:VAL:HG23	2.17	0.45
1:A:377:ASN:HA	1:A:378:PRO:HD3	1.81	0.45
2:B:274:PRO:HD2	2:B:383:TYR:OH	2.17	0.45
1:C:338:HIS:ND1	1:C:343:GLY:HA3	2.32	0.45
1:A:302:ARG:HA	2:D:428:LEU:HD23	2.00	0.44
1:A:304:GLY:O	1:A:308:LEU:HG	2.17	0.44
1:A:349:VAL:HG13	1:A:353:LEU:HD12	1.98	0.44
1:C:243:GLU:O	1:C:244:PRO:C	2.54	0.44
2:B:327:ALA:O	2:B:431:LYS:NZ	2.43	0.44
2:D:228:SER:CB	5:D:81:HOH:O	2.64	0.44
1:A:287:PRO:O	1:A:288:HIS:HB2	2.18	0.44
2:D:274:PRO:HD2	2:D:383:TYR:OH	2.18	0.44
2:D:296:MET:HG2	4:D:1:LX2:H25	1.99	0.43
2:D:280:SER:O	2:D:284:GLN:HG3	2.19	0.43
1:A:277:PHE:HD1	2:D:430:ASP:OD1	2.01	0.43
1:C:454:MET:HE2	1:C:454:MET:HB3	1.89	0.43
2:D:237:PRO:HD2	2:D:251:ARG:HG2	1.99	0.43
1:A:454:MET:CE	2:B:264:GLN:HA	2.47	0.43
1:C:338:HIS:CE1	1:C:343:GLY:HA3	2.54	0.43
2:B:248:ARG:HD3	5:B:127:HOH:O	2.18	0.43
2:B:322:GLU:O	2:B:326:LYS:HG3	2.18	0.43
1:A:225:SER:HA	1:A:228:GLU:HG3	2.00	0.43
1:A:347:ASP:O	1:A:351:THR:HG23	2.19	0.43
1:A:392:LEU:O	1:A:396:VAL:HG23	2.19	0.43
2:B:313:PHE:CE1	4:B:1:LX2:H11A	2.53	0.43
1:C:318:ILE:HD11	1:C:357:MET:HB3	2.00	0.43
1:C:243:GLU:CB	1:C:244:PRO:HD2	2.38	0.42
2:D:302:ARG:HG2	2:D:354:PHE:CZ	2.54	0.42
2:D:419:HIS:CE1	4:D:1:LX2:H33	2.54	0.42
2:B:248:ARG:CD	2:B:326:LYS:O	2.68	0.42
2:D:330:GLN:HG2	2:D:422:GLN:OE1	2.19	0.42
2:B:368:PRO:O	2:B:369:ASN:HB2	2.20	0.42
2:D:247:ALA:O	2:D:251:ARG:HG3	2.20	0.41
1:A:448:ASP:HB3	1:A:449:THR:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:ALA:HA	2:D:240:PRO:HD3	1.71	0.41
4:D:1:LX2:H29A	4:D:1:LX2:H12A	1.66	0.41
2:D:237:PRO:HG2	2:D:251:ARG:HG2	2.02	0.41
2:B:230:ARG:HB2	2:B:314:LEU:HD13	2.02	0.41
1:C:419:LEU:HD22	2:D:407:MET:HE1	2.02	0.41
1:A:323:GLY:HA3	1:A:332:VAL:O	2.21	0.41
3:A:501:REA:H8	3:A:501:REA:C18	2.27	0.41
2:D:331:VAL:CG1	2:D:335:ASN:ND2	2.84	0.41
2:D:347:LEU:HD23	2:D:347:LEU:HA	1.78	0.41
1:A:313:PHE:CD1	1:A:313:PHE:C	2.95	0.41
1:C:289:PHE:CD1	1:C:375:LEU:HD21	2.55	0.41
2:D:313:PHE:CZ	4:D:1:LX2:H11A	2.57	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	201/242 (83%)	192 (96%)	8 (4%)	1 (0%)	29	19
1	C	196/242 (81%)	192 (98%)	4 (2%)	0	100	100
2	B	239/266 (90%)	234 (98%)	5 (2%)	0	100	100
2	D	239/266 (90%)	232 (97%)	7 (3%)	0	100	100
All	All	875/1016 (86%)	850 (97%)	24 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	LEU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/208 (85%)	177 (100%)	0	100	100
1	C	172/208 (83%)	171 (99%)	1 (1%)	86	86
2	B	218/239 (91%)	215 (99%)	3 (1%)	67	64
2	D	218/239 (91%)	217 (100%)	1 (0%)	88	89
All	All	785/894 (88%)	780 (99%)	5 (1%)	86	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	229	ASP
2	B	230	ARG
2	B	238	ILE
1	C	313	PHE
2	D	428	LEU

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

Mol	Chain	Res	Type
1	A	270	GLN
2	B	272	GLN
2	B	388	HIS
2	D	305	ASN

### 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 [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
3	REA	C	501	-	22,22,22	2.54	5 (22%)	30,30,30	1.89	6 (20%)
3	REA	A	501	-	22,22,22	2.72	5 (22%)	30,30,30	2.00	8 (26%)
4	LX2	D	1	-	44,48,48	1.01	2 (4%)	59,67,67	1.61	10 (16%)
4	LX2	B	1	-	44,48,48	1.04	2 (4%)	59,67,67	1.56	10 (16%)

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
3	REA	C	501	-	-	9/15/32/32	0/1/1/1
3	REA	A	501	-	-	9/15/32/32	0/1/1/1
4	LX2	D	1	-	-	6/33/33/33	0/5/5/5
4	LX2	B	1	-	-	3/33/33/33	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	REA	C10-C9	8.77	1.47	1.35
3	C	501	REA	C10-C9	8.06	1.46	1.35
3	A	501	REA	C11-C12	4.94	1.47	1.34
3	C	501	REA	C11-C12	4.75	1.46	1.34
3	A	501	REA	C8-C7	4.48	1.46	1.33
3	C	501	REA	C8-C7	4.44	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	REA	C14-C13	4.42	1.41	1.35
3	C	501	REA	C14-C13	3.95	1.41	1.35
4	D	1	LX2	C44-N5	-3.90	1.34	1.39
4	B	1	LX2	C44-N5	-3.89	1.34	1.39
3	A	501	REA	C5-C6	3.61	1.40	1.34
3	C	501	REA	C5-C6	3.56	1.40	1.34
4	D	1	LX2	C35-CL36	2.79	1.78	1.72
4	B	1	LX2	C35-CL36	2.73	1.78	1.72

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	LX2	C7-C8-C44	6.14	111.39	106.18
4	D	1	LX2	C7-C8-C44	6.01	111.28	106.18
4	D	1	LX2	C29-N14-C15	5.61	117.46	110.95
3	C	501	REA	C11-C10-C9	-5.24	119.83	127.31
3	C	501	REA	C7-C8-C9	-5.05	118.60	126.23
3	A	501	REA	C7-C8-C9	-4.86	118.89	126.23
3	A	501	REA	C11-C10-C9	-4.59	120.76	127.31
3	A	501	REA	C3-C4-C5	-4.55	105.96	114.08
4	B	1	LX2	C29-N14-C15	3.85	115.42	110.95
4	B	1	LX2	C2-C4-N5	-3.30	107.19	111.52
3	A	501	REA	C4-C5-C6	-3.17	118.13	122.73
3	C	501	REA	O2-C15-C14	2.91	122.53	113.50
4	B	1	LX2	C43-C44-C8	-2.89	117.02	120.94
4	B	1	LX2	C37-C34-C35	-2.81	119.87	121.78
3	A	501	REA	C15-C14-C13	-2.81	124.11	128.50
4	D	1	LX2	C12-C13-N14	-2.76	106.89	113.84
4	D	1	LX2	C37-C34-C35	-2.74	119.91	121.78
4	D	1	LX2	C43-C44-C8	-2.70	117.26	120.94
4	D	1	LX2	F40-C37-C34	-2.69	108.02	112.70
3	A	501	REA	O2-C15-C14	2.62	121.63	113.50
3	C	501	REA	C15-C14-C13	-2.57	124.48	128.50
4	B	1	LX2	C30-C35-CL36	2.53	121.83	119.18
4	B	1	LX2	F40-C37-C34	-2.42	108.49	112.70
4	D	1	LX2	O10-C9-C8	2.32	121.49	115.01
4	D	1	LX2	C31-C30-C35	2.24	119.02	117.43
3	A	501	REA	C16-C1-C6	-2.13	106.84	110.30
3	A	501	REA	C18-C5-C4	2.12	117.68	113.62
3	C	501	REA	C18-C5-C6	-2.11	122.16	124.53
4	B	1	LX2	C33-C34-C37	2.11	122.33	118.12
4	D	1	LX2	O10-C9-C41	-2.10	119.83	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	REA	C3-C4-C5	-2.09	110.34	114.08
4	D	1	LX2	C13-N14-C15	2.09	116.93	111.96
4	B	1	LX2	C31-C30-C35	2.04	118.87	117.43
4	B	1	LX2	O10-C9-C8	2.02	120.64	115.01

There are no chirality outliers.

All (27) torsion outliers are listed below:

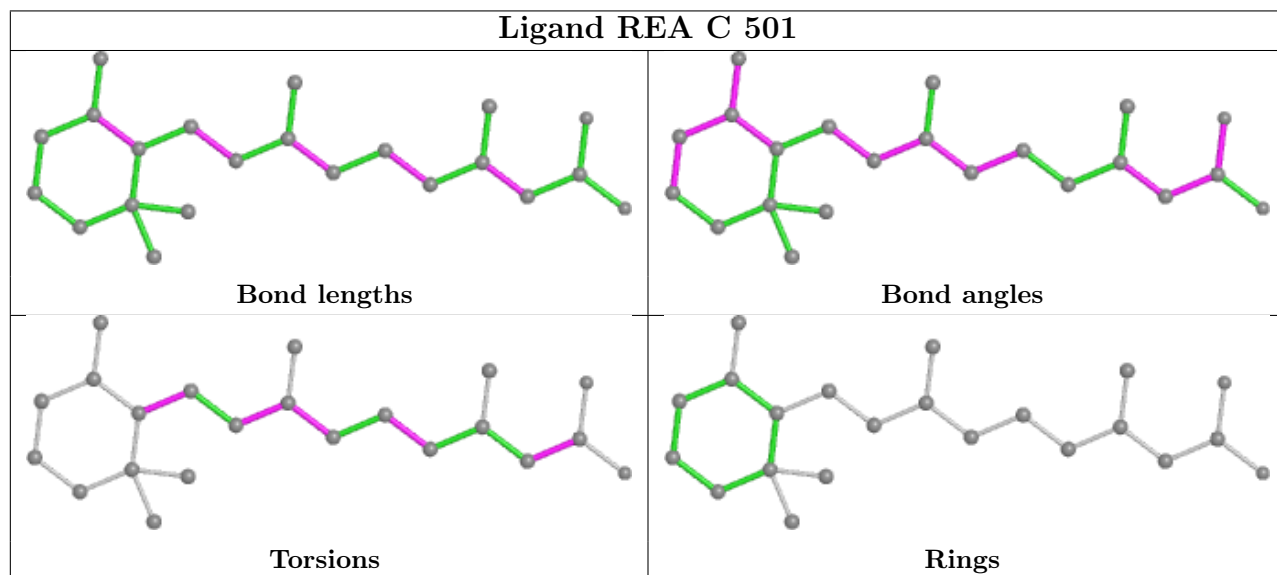
Mol	Chain	Res	Type	Atoms
3	A	501	REA	C11-C10-C9-C8
3	A	501	REA	C11-C10-C9-C19
3	A	501	REA	C10-C11-C12-C13
3	C	501	REA	C7-C8-C9-C19
3	C	501	REA	C11-C10-C9-C8
3	C	501	REA	C11-C10-C9-C19
4	B	1	LX2	C11-C12-C13-N14
4	B	1	LX2	C8-C9-O10-C11
3	A	501	REA	C7-C8-C9-C19
3	A	501	REA	C7-C8-C9-C10
3	C	501	REA	C7-C8-C9-C10
3	C	501	REA	C10-C11-C12-C13
4	B	1	LX2	C41-C9-O10-C11
3	A	501	REA	C1-C6-C7-C8
3	A	501	REA	C5-C6-C7-C8
3	C	501	REA	C1-C6-C7-C8
3	C	501	REA	C5-C6-C7-C8
4	D	1	LX2	C35-C34-C37-F40
4	D	1	LX2	C35-C34-C37-F38
4	D	1	LX2	C35-C34-C37-F39
4	D	1	LX2	C8-C9-O10-C11
4	D	1	LX2	C11-C12-C13-N14
3	C	501	REA	C13-C14-C15-O1
3	C	501	REA	C13-C14-C15-O2
4	D	1	LX2	C41-C9-O10-C11
3	A	501	REA	C13-C14-C15-O1
3	A	501	REA	C13-C14-C15-O2

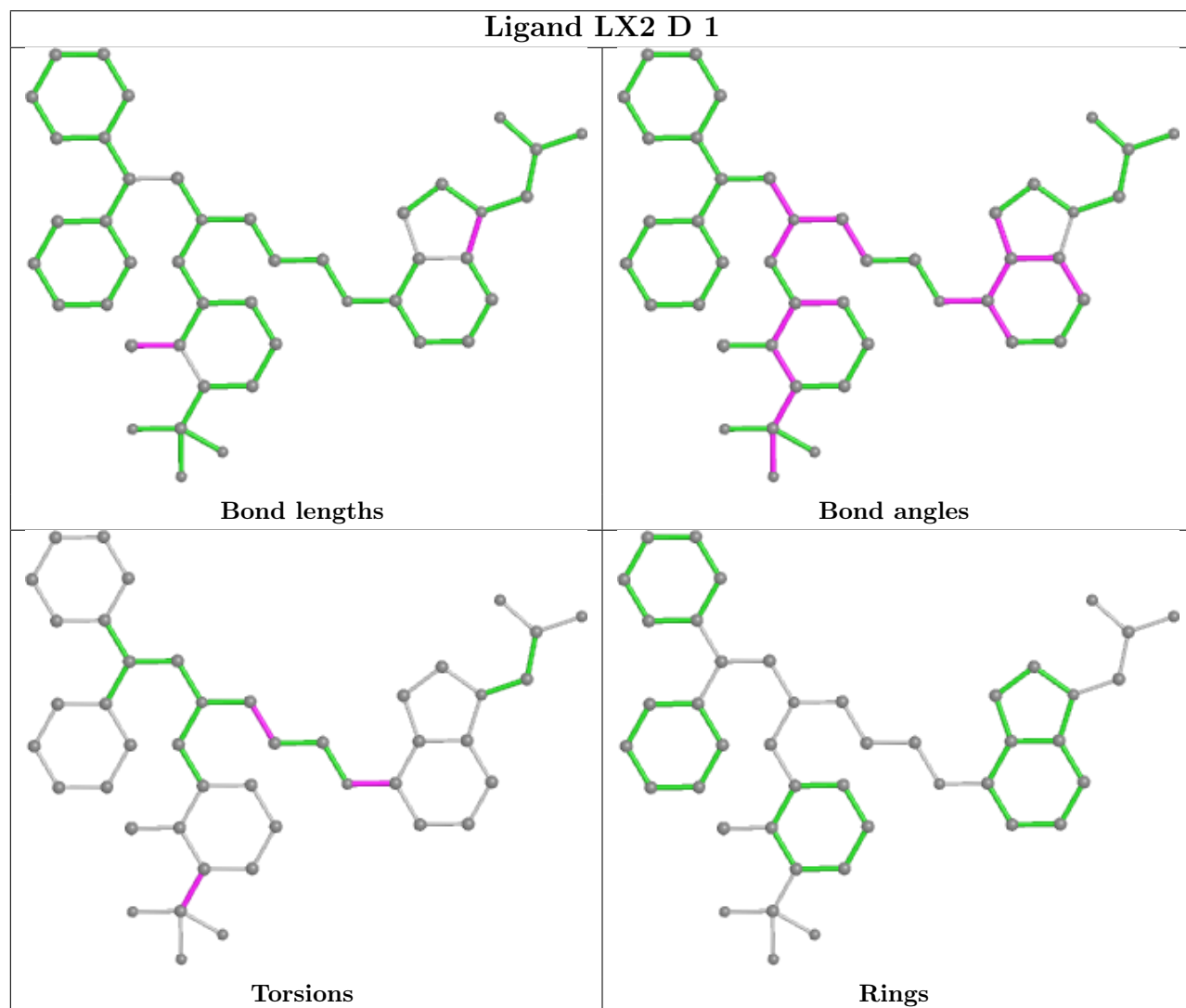
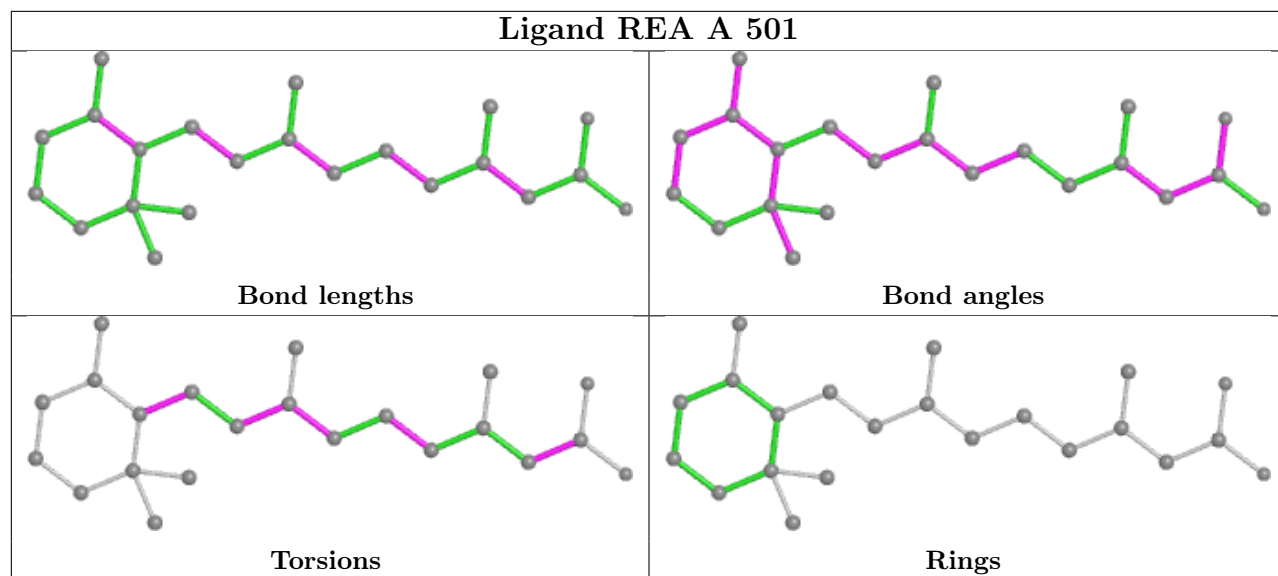
There are no ring outliers.

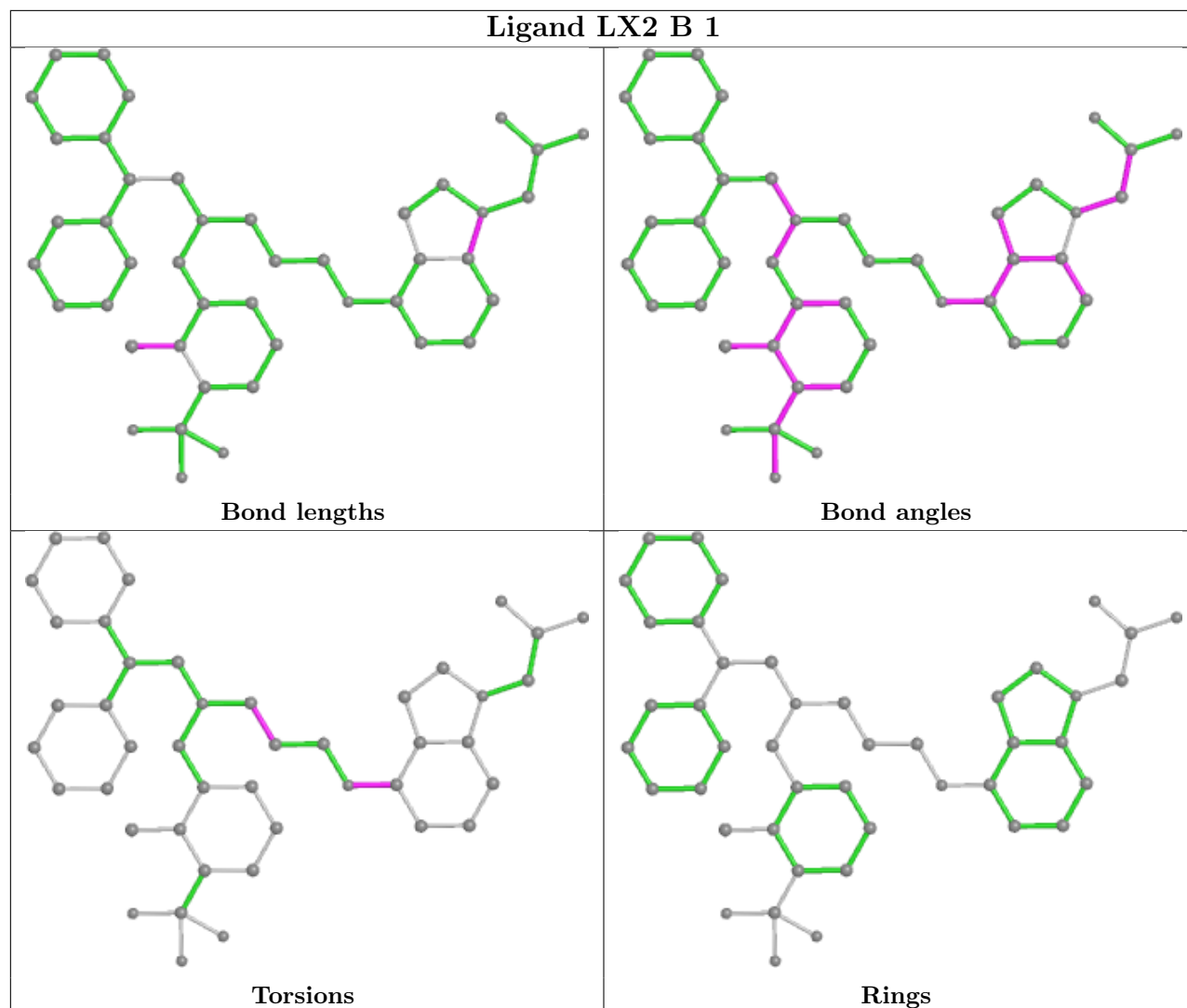
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	REA	3	0
3	A	501	REA	5	0
4	D	1	LX2	5	0
4	B	1	LX2	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	207/242 (85%)	0.22	12 (5%) 23 24	22, 38, 52, 66	0
1	C	202/242 (83%)	-0.25	2 (0%) 82 83	17, 25, 40, 57	0
2	B	241/266 (90%)	-0.12	7 (2%) 51 54	18, 28, 44, 82	0
2	D	241/266 (90%)	-0.20	5 (2%) 63 65	15, 25, 42, 55	0
All	All	891/1016 (87%)	-0.09	26 (2%) 51 54	15, 28, 48, 82	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	240	PRO	7.7
2	D	443	VAL	6.4
2	D	240	PRO	4.5
2	B	443	VAL	3.6
1	A	319	ALA	3.1
2	B	238	ILE	2.8
2	D	227	PHE	2.8
1	A	277	PHE	2.7
1	A	340	ALA	2.6
1	A	410	GLU	2.5
1	A	328	THR	2.5
1	A	267	ASN	2.3
1	A	263	ASP	2.3
2	B	242	PRO	2.3
1	A	409	PRO	2.3
1	A	331	HIS	2.2
1	A	270	GLN	2.2
2	B	203	GLN	2.2
2	B	239	ALA	2.2
1	A	327	ALA	2.1
1	A	337	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	241	ASP	2.1
2	D	203	GLN	2.1
1	C	244	PRO	2.1
2	D	228	SER	2.1
1	C	450	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](#)

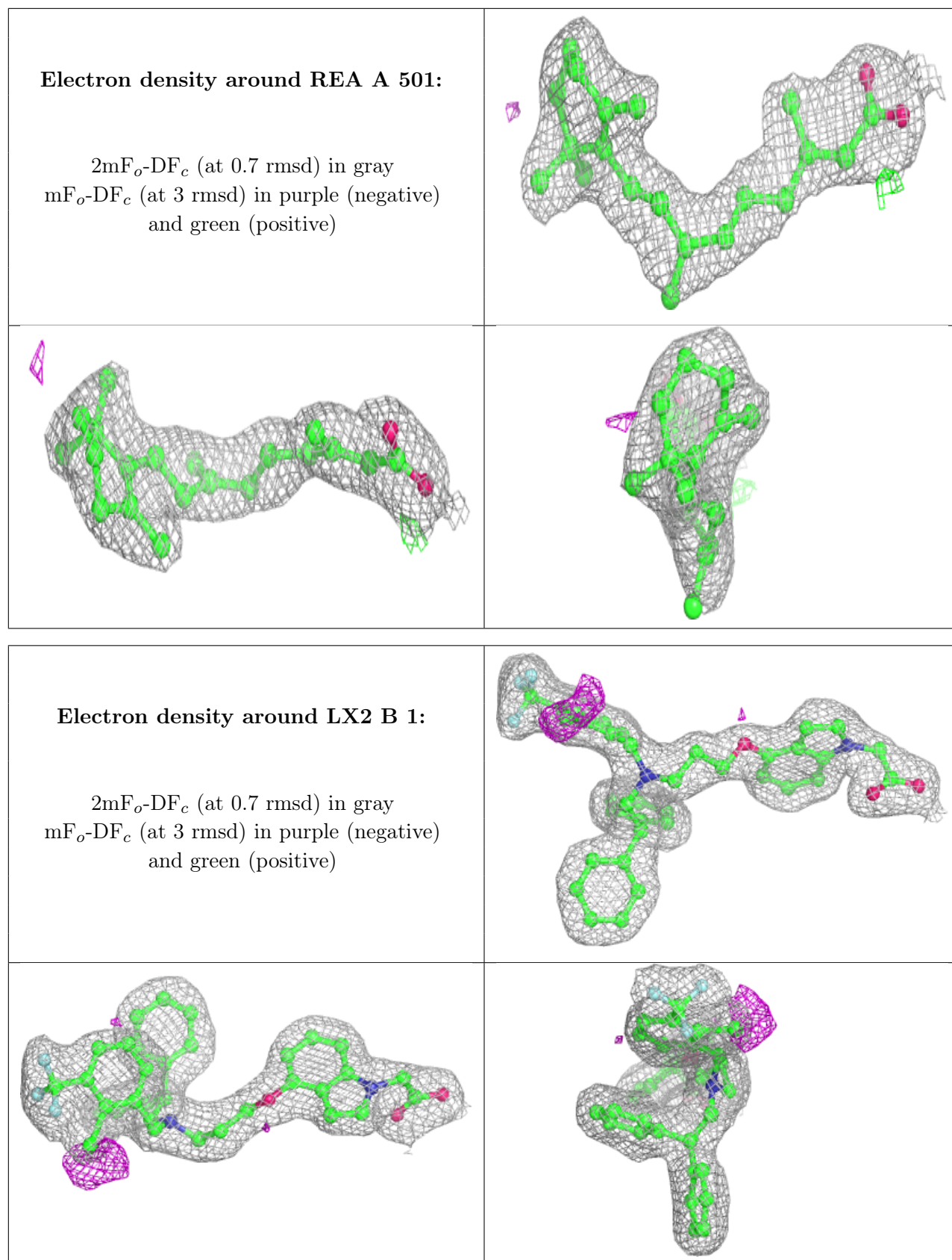
There are no monosaccharides in this entry.

## 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, 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(Å <sup>2</sup> )	Q<0.9
3	REA	A	501	22/22	0.92	0.17	31,37,41,47	0
4	LX2	B	1	44/44	0.95	0.10	16,22,33,52	0
4	LX2	D	1	44/44	0.95	0.09	16,20,31,47	0
3	REA	C	501	22/22	0.96	0.10	21,25,32,34	0

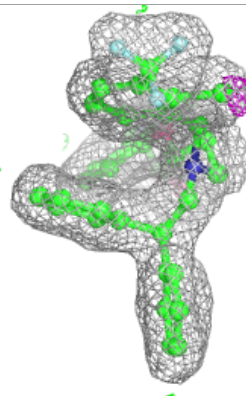
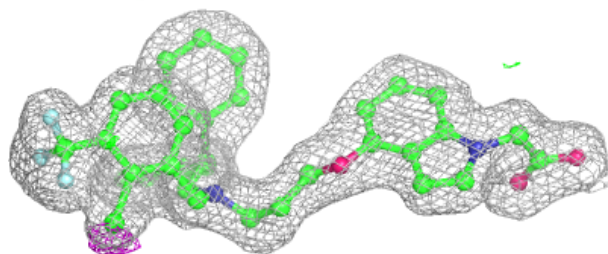
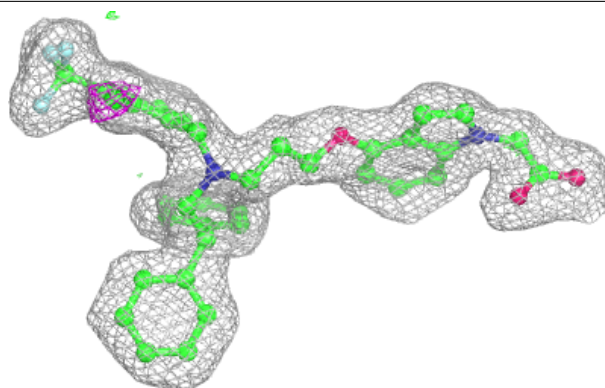
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



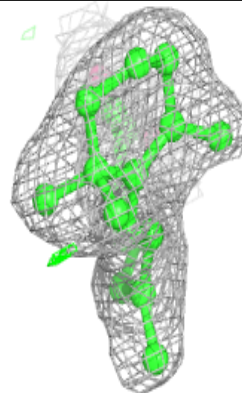
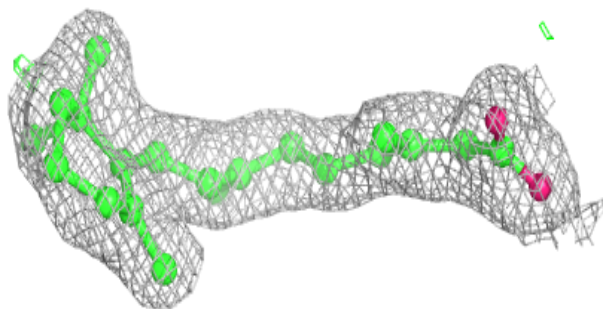
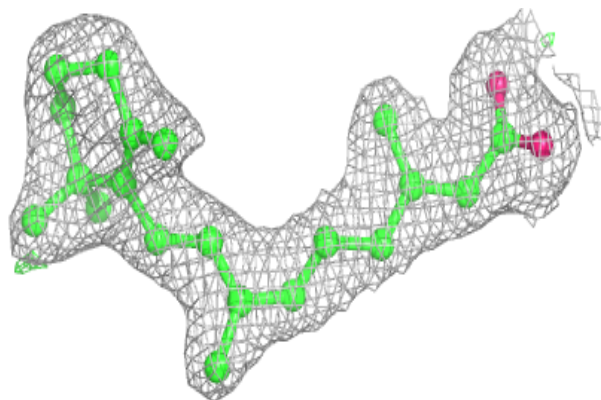


**Electron density around LX2 D 1:**

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

**Electron density around REA 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.