



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:54 PM UTC

PDB ID : 4DQM / pdb_00004dqm
Title : Revealing a marine natural product as a novel agonist for retinoic acid receptors with a unique binding mode and antitumor activity
Authors : Wang, S.; Wang, Z.; Lin, S.; Zheng, W.; Wang, R.; Jin, S.; Chen, J.; Jin, L.; Li, Y.
Deposited on : 2012-02-16
Resolution : 2.75 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

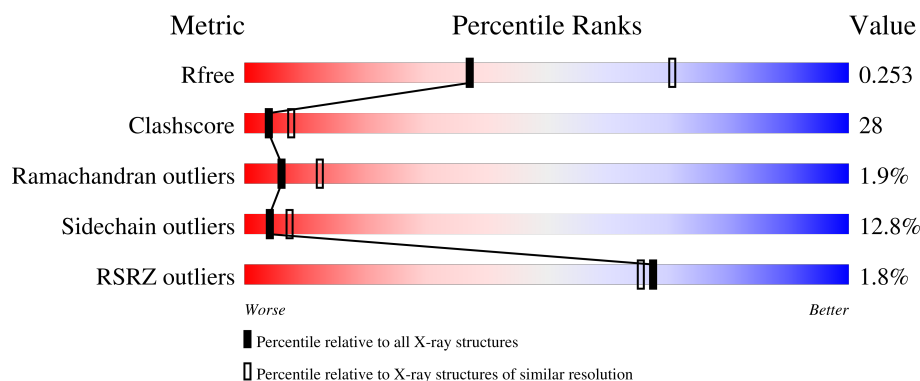
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	234	2% 58% 36% 6%
1	C	234	2% 65% 26% 8%
2	B	10	40% 40% 20%
2	D	10	10% 40% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LUF	A	501	-	-	X	-
3	LUF	C	501	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3940 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.

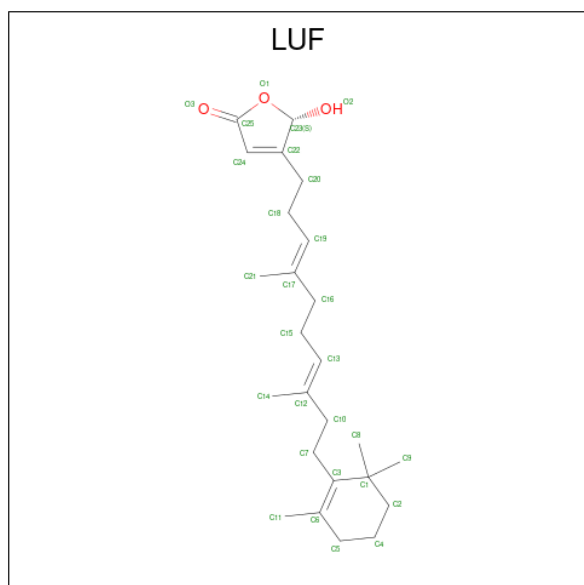
- Molecule 1 is a protein called Retinoic acid receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	1	0	0
			1847	1172	311	348	16			
1	C	234	Total	C	N	O	S	0	0	0
			1846	1172	310	348	16			

- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			81	52	13	16			
2	D	10	Total	C	N	O	0	0	0
			81	52	13	16			

- Molecule 3 is (5S)-4-[(3E,7E)-4,8-dimethyl-10-(2,6,6-trimethylcyclohex-1-en-1-yl)deca-3,7-dien-1-yl]-5-hydroxyfuran-2(5H)-one (CCD ID: LUF) (formula: C₂₅H₃₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	25	3		
3	C	1	Total	C	O	0	0
			26	23	3		

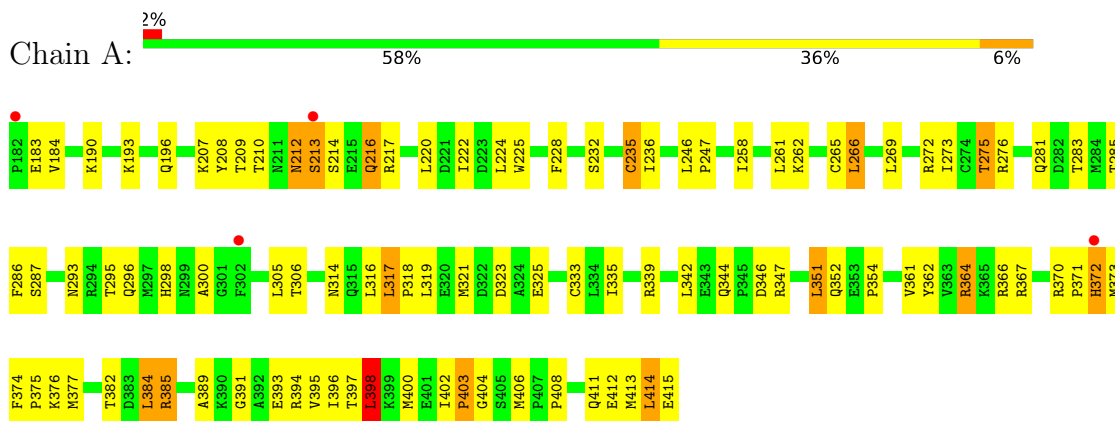
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	C	19	Total	O	0	0
			19	19		

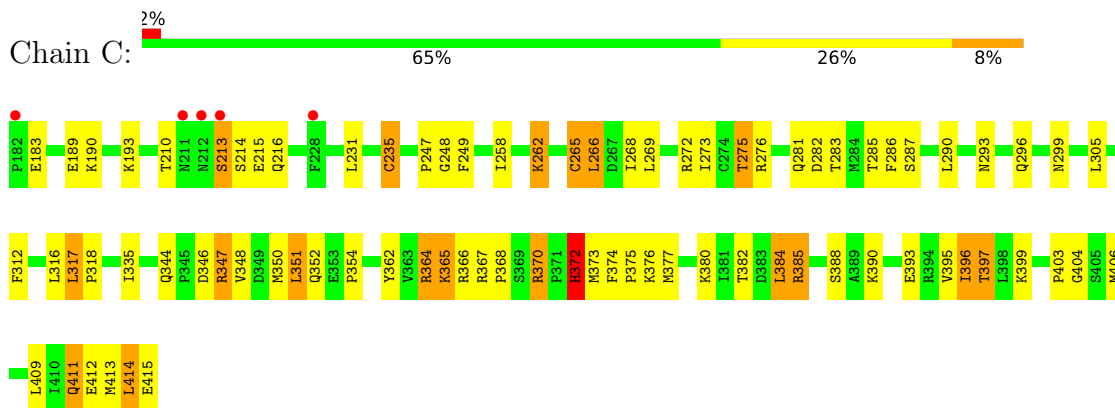
3 Residue-property plots

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: Retinoic acid receptor alpha



- Molecule 1: Retinoic acid receptor alpha



- Molecule 2: Nuclear receptor coactivator 1



- Molecule 2: Nuclear receptor coactivator 1



K1432
S1433
L1434
L1435
Q1436
Q1437
L1438
L1439
T1440
E1441

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	54.12Å 104.46Å 113.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 2.75 47.46 – 2.75	Depositor EDS
% Data completeness (in resolution range)	84.9 (47.46-2.75) 90.1 (47.46-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.259 0.210 , 0.253	Depositor DCC
R_{free} test set	922 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.0	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	3940	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: LUF

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	0.99	2/1877 (0.1%)	1.15	4/2537 (0.2%)
1	C	0.96	1/1875 (0.1%)	1.12	1/2532 (0.0%)
2	B	1.07	0/80	1.18	0/106
2	D	1.26	0/80	0.96	0/106
All	All	0.98	3/3912 (0.1%)	1.14	5/5281 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	CYS	CB-SG	-10.31	1.47	1.81
1	A	235	CYS	CA-C	-5.74	1.45	1.52
1	C	372	HIS	CG-CD2	5.12	1.41	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	CYS	N-CA-C	-7.62	102.91	111.07
1	A	235	CYS	CB-CA-C	-7.47	99.15	110.88
1	A	333	CYS	CA-CB-SG	7.43	131.49	114.40
1	A	398	LEU	N-CA-C	-5.55	105.30	112.68
1	C	265	CYS	N-CA-C	5.25	117.00	111.28

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	1847	0	1903	88	0
1	C	1846	0	1901	87	0
2	B	81	0	90	7	0
2	D	81	0	90	25	0
3	A	28	0	38	33	0
3	C	26	0	31	32	0
4	A	12	0	0	1	0
4	C	19	0	0	3	0
All	All	3940	0	4053	221	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 28.

All (221) 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:235:CYS:SG	3:A:501:LUF:H19	1.46	1.54
1:C:235:CYS:SG	3:C:501:LUF:H19	1.73	1.29
1:A:235:CYS:SG	3:A:501:LUF:C21	2.22	1.27
1:A:287:SER:N	3:A:501:LUF:O3	1.68	1.25
1:C:281:GLN:C	1:C:282:ASP:CA	2.18	1.17
3:A:501:LUF:H19	3:A:501:LUF:H17	1.18	1.16
3:A:501:LUF:C22	3:A:501:LUF:H20	1.76	1.16
3:A:501:LUF:C21	3:A:501:LUF:C22	2.29	1.09
3:A:501:LUF:C21	3:A:501:LUF:C20	2.32	1.07
3:A:501:LUF:H19	3:A:501:LUF:C20	1.84	1.06
1:C:287:SER:N	3:C:501:LUF:O3	1.87	1.05
1:C:286:PHE:CA	3:C:501:LUF:O3	2.14	0.95
1:A:286:PHE:CA	3:A:501:LUF:O3	2.16	0.94
1:A:273:ILE:HB	3:A:501:LUF:H28	1.48	0.94
3:A:501:LUF:H10	3:A:501:LUF:H12	1.48	0.93
1:C:262:LYS:HZ2	1:C:413:MET:C	1.77	0.92
2:D:1437:GLN:O	2:D:1441:GLU:HG3	1.71	0.89
3:C:501:LUF:C21	3:C:501:LUF:C22	2.51	0.89
1:A:273:ILE:HB	3:A:501:LUF:C19	2.03	0.88
1:C:286:PHE:HB3	3:C:501:LUF:O3	1.75	0.86
1:C:286:PHE:CB	3:C:501:LUF:O3	2.24	0.86
1:A:287:SER:H	3:A:501:LUF:C25	1.88	0.85
1:A:286:PHE:C	3:A:501:LUF:O3	2.19	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1435:LEU:HA	2:D:1438:LEU:HD12	1.58	0.84
1:C:412:GLU:OE2	2:D:1433:SER:O	1.96	0.84
1:C:262:LYS:NZ	1:C:413:MET:C	2.37	0.82
1:C:409:LEU:HD13	2:D:1434:LEU:CD2	2.10	0.82
1:C:395:VAL:HG23	3:C:501:LUF:H4	1.60	0.81
1:A:286:PHE:HA	3:A:501:LUF:O3	1.80	0.81
1:C:293:ASN:H	1:C:296:GLN:HE21	1.27	0.81
1:A:222:ILE:HD11	1:A:403:PRO:HD3	1.63	0.80
1:C:266:LEU:HD11	3:C:501:LUF:C11	2.11	0.80
3:C:501:LUF:C22	3:C:501:LUF:H20	2.11	0.80
1:C:364:ARG:NH2	4:C:610:HOH:O	2.12	0.79
1:C:286:PHE:HA	3:C:501:LUF:O3	1.82	0.79
1:C:266:LEU:HD11	3:C:501:LUF:H39	1.66	0.78
1:C:235:CYS:SG	3:C:501:LUF:C21	2.67	0.78
2:D:1434:LEU:C	2:D:1434:LEU:HD23	2.10	0.77
2:D:1433:SER:O	2:D:1434:LEU:HB3	1.85	0.76
1:C:409:LEU:HD13	2:D:1434:LEU:HD21	1.66	0.76
1:C:273:ILE:HB	3:C:501:LUF:C19	2.17	0.75
1:C:412:GLU:CD	2:D:1433:SER:O	2.31	0.74
3:A:501:LUF:H19	3:A:501:LUF:C22	2.08	0.73
3:A:501:LUF:C21	3:A:501:LUF:H17	1.88	0.73
1:C:190:LYS:HD2	1:C:247:PRO:HG3	1.70	0.73
3:A:501:LUF:H20	3:A:501:LUF:C24	2.18	0.72
2:D:1440:THR:C	2:D:1441:GLU:HG2	2.16	0.71
1:C:286:PHE:C	3:C:501:LUF:O3	2.33	0.71
3:A:501:LUF:C21	3:A:501:LUF:C23	2.68	0.70
2:D:1437:GLN:NE2	2:D:1441:GLU:OE2	2.24	0.70
2:B:1433:SER:OG	2:B:1436:GLN:HB2	1.92	0.70
2:D:1440:THR:O	2:D:1441:GLU:HG2	1.92	0.70
1:A:262:LYS:NZ	1:A:412:GLU:O	2.25	0.69
3:C:501:LUF:H19	3:C:501:LUF:O2	1.93	0.69
1:C:262:LYS:NZ	1:C:412:GLU:O	2.25	0.69
1:C:281:GLN:HB3	1:C:283:THR:HG23	1.72	0.69
1:C:412:GLU:OE2	2:D:1434:LEU:HB3	1.93	0.68
1:A:293:ASN:OD1	1:A:296:GLN:HG3	1.94	0.68
1:A:196:GLN:HG3	1:A:323:ASP:OD2	1.95	0.67
1:A:339:ARG:HH12	1:A:385:ARG:HH22	1.43	0.66
1:C:293:ASN:H	1:C:296:GLN:NE2	1.94	0.66
1:C:395:VAL:CG2	3:C:501:LUF:H4	2.26	0.66
1:A:415:GLU:HA	4:A:607:HOH:O	1.97	0.65
1:C:344:GLN:OE1	1:C:347:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ARG:HD2	1:C:373:MET:HG2	1.77	0.65
1:C:395:VAL:CG2	3:C:501:LUF:C5	2.74	0.65
3:C:501:LUF:H19	3:C:501:LUF:C22	2.23	0.65
1:C:287:SER:H	3:C:501:LUF:C25	2.08	0.65
1:C:269:LEU:HB3	3:C:501:LUF:H14	1.78	0.65
1:C:362:TYR:CZ	1:C:366:ARG:HD2	2.31	0.65
3:C:501:LUF:C22	3:C:501:LUF:C19	2.76	0.64
2:D:1433:SER:O	2:D:1434:LEU:CB	2.46	0.64
3:C:501:LUF:C21	3:C:501:LUF:O2	2.46	0.63
1:A:374:PHE:HB3	1:A:375:PRO:HD3	1.80	0.63
1:C:395:VAL:HG22	3:C:501:LUF:H1	1.81	0.62
1:A:286:PHE:CB	3:A:501:LUF:O3	2.48	0.62
2:D:1437:GLN:NE2	2:D:1441:GLU:CD	2.58	0.61
1:A:266:LEU:HD11	3:A:501:LUF:H39	1.82	0.61
1:C:189:GLU:HB2	4:C:607:HOH:O	2.00	0.61
1:A:367:ARG:HD2	1:A:373:MET:HG2	1.81	0.61
1:A:208:TYR:O	1:A:208:TYR:CD1	2.54	0.60
1:A:351:LEU:O	1:A:354:PRO:HD2	2.02	0.60
1:A:293:ASN:H	1:A:296:GLN:HE21	1.49	0.60
3:A:501:LUF:H19	3:A:501:LUF:C23	2.31	0.60
1:A:220:LEU:HD11	1:A:225:TRP:HB2	1.83	0.60
1:C:372:HIS:C	1:C:375:PRO:HD2	2.27	0.60
1:C:281:GLN:C	1:C:282:ASP:CB	2.74	0.60
1:C:365:LYS:HB2	1:C:365:LYS:NZ	2.17	0.59
1:A:362:TYR:CZ	1:A:366:ARG:HD2	2.37	0.59
2:D:1437:GLN:OE1	2:D:1441:GLU:OE2	2.21	0.59
1:A:370:ARG:HE	1:A:373:MET:HE3	1.67	0.58
1:C:273:ILE:HD13	3:C:501:LUF:H22	1.85	0.58
1:A:286:PHE:HB3	3:A:501:LUF:O3	2.04	0.58
3:A:501:LUF:H10	3:A:501:LUF:C10	2.23	0.58
1:A:314:ASN:HA	1:A:317:LEU:HD22	1.87	0.57
3:A:501:LUF:H20	3:A:501:LUF:C23	2.31	0.57
1:A:235:CYS:SG	3:A:501:LUF:H18	2.38	0.56
1:A:395:VAL:HG22	3:A:501:LUF:H4	1.88	0.56
1:A:339:ARG:HB2	1:A:342:LEU:HG	1.88	0.56
1:A:364:ARG:NH2	1:A:371:PRO:HB3	2.21	0.56
3:A:501:LUF:C21	3:A:501:LUF:O2	2.30	0.56
1:C:335:ILE:O	1:C:352:GLN:HG3	2.06	0.56
2:D:1437:GLN:CD	2:D:1441:GLU:OE2	2.49	0.55
1:C:412:GLU:OE1	2:D:1433:SER:O	2.24	0.55
1:C:262:LYS:NZ	1:C:414:LEU:N	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HB2	1:A:318:PRO:HD3	1.89	0.54
1:C:265:CYS:O	1:C:269:LEU:HG	2.07	0.54
1:A:272:ARG:O	1:A:275:THR:HB	2.08	0.54
1:A:228:PHE:HE2	3:A:501:LUF:H8	1.72	0.53
1:C:262:LYS:HZ2	1:C:414:LEU:N	2.06	0.53
1:A:339:ARG:NH1	1:A:385:ARG:HH22	2.07	0.52
1:A:370:ARG:HE	1:A:373:MET:CE	2.23	0.52
1:C:365:LYS:HB2	1:C:365:LYS:HZ3	1.73	0.52
1:A:398:LEU:HD12	1:A:406:MET:HE1	1.91	0.52
1:A:235:CYS:HB3	1:A:269:LEU:HD22	1.93	0.51
1:A:413:MET:C	1:A:414:LEU:HD23	2.36	0.51
1:C:362:TYR:CE1	1:C:366:ARG:HD2	2.45	0.51
1:C:351:LEU:O	1:C:354:PRO:HD2	2.10	0.51
1:A:269:LEU:HB3	3:A:501:LUF:H14	1.92	0.51
1:C:293:ASN:N	1:C:296:GLN:HE21	2.02	0.51
1:A:408:PRO:HA	1:A:411:GLN:HE21	1.76	0.51
1:A:389:ALA:C	1:A:391:GLY:H	2.18	0.51
1:C:399:LYS:HE3	1:C:406:MET:HG2	1.91	0.51
3:C:501:LUF:H10	3:C:501:LUF:H12	1.93	0.51
1:A:217:ARG:HG2	1:A:295:THR:HG23	1.93	0.50
2:B:1433:SER:C	2:B:1437:GLN:OE1	2.54	0.50
1:A:372:HIS:CD2	1:A:372:HIS:H	2.30	0.50
2:D:1437:GLN:HE22	2:D:1441:GLU:CD	2.18	0.50
1:C:258:ILE:HG23	2:D:1435:LEU:HD21	1.93	0.50
1:C:266:LEU:HD13	1:C:388:SER:HB2	1.93	0.50
1:A:408:PRO:HB2	2:B:1434:LEU:HD11	1.93	0.49
2:B:1433:SER:O	2:B:1434:LEU:C	2.55	0.49
2:D:1434:LEU:HD23	2:D:1435:LEU:N	2.27	0.49
1:A:414:LEU:HD23	1:A:414:LEU:N	2.28	0.49
1:C:374:PHE:HB3	1:C:375:PRO:HD3	1.95	0.49
2:D:1434:LEU:CD2	2:D:1434:LEU:C	2.85	0.49
1:C:317:LEU:HB2	1:C:318:PRO:HD3	1.93	0.49
1:C:268:ILE:HG22	1:C:272:ARG:HD2	1.93	0.49
1:A:184:VAL:HG11	1:A:361:VAL:HG21	1.95	0.48
1:A:319:LEU:N	1:A:319:LEU:HD12	2.27	0.48
1:C:365:LYS:O	1:C:368:PRO:HD3	2.13	0.48
1:C:312:PHE:CZ	1:C:384:LEU:HD13	2.48	0.48
1:C:406:MET:HB2	1:C:411:GLN:HG2	1.95	0.48
1:A:408:PRO:O	1:A:411:GLN:HB2	2.13	0.48
1:A:212:ASN:O	1:A:214:SER:N	2.46	0.48
1:A:406:MET:HB2	1:A:411:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:HA	1:A:385:ARG:HD3	1.61	0.48
1:C:335:ILE:HG23	1:C:348:VAL:HG13	1.96	0.48
1:A:276:ARG:HD2	1:A:285:THR:O	2.14	0.47
1:C:231:LEU:HD11	1:C:290:LEU:HD23	1.95	0.47
1:C:367:ARG:CD	1:C:373:MET:HG2	2.43	0.47
1:A:265:CYS:O	1:A:269:LEU:HG	2.15	0.47
1:A:281:GLN:HB3	1:A:283:THR:HG23	1.96	0.47
1:C:305:LEU:HD21	1:C:390:LYS:HB3	1.95	0.47
1:C:266:LEU:CD1	3:C:501:LUF:H39	2.42	0.47
3:C:501:LUF:H12	3:C:501:LUF:H37	1.96	0.47
1:A:398:LEU:C	1:A:400:MET:N	2.71	0.47
1:C:281:GLN:O	1:C:282:ASP:HB3	2.14	0.47
2:D:1432:LYS:O	2:D:1434:LEU:N	2.48	0.47
1:A:224:LEU:HB3	1:A:300:ALA:HB2	1.95	0.46
1:A:321:MET:HA	1:A:325:GLU:OE2	2.14	0.46
1:C:272:ARG:O	1:C:275:THR:HB	2.15	0.46
2:B:1433:SER:N	2:B:1437:GLN:OE1	2.49	0.46
3:C:501:LUF:H20	3:C:501:LUF:C24	2.45	0.46
1:A:402:ILE:HB	1:A:403:PRO:CD	2.46	0.46
1:A:258:ILE:HG23	2:B:1435:LEU:HD23	1.97	0.46
1:A:339:ARG:HH12	1:A:385:ARG:NH2	2.11	0.46
1:A:362:TYR:CE1	1:A:366:ARG:HD2	2.51	0.46
3:C:501:LUF:C21	3:C:501:LUF:C23	2.94	0.46
1:C:396:ILE:CG2	1:C:397:THR:N	2.79	0.45
1:C:365:LYS:NZ	1:C:365:LYS:CB	2.78	0.45
1:A:305:LEU:O	1:A:306:THR:C	2.58	0.45
1:A:364:ARG:HD2	1:A:364:ARG:HA	1.41	0.45
2:B:1433:SER:O	2:B:1436:GLN:N	2.50	0.45
1:A:232:SER:O	1:A:236:ILE:HG13	2.17	0.44
1:A:212:ASN:O	1:A:213:SER:C	2.60	0.44
1:A:212:ASN:HD22	1:A:212:ASN:HA	1.63	0.44
1:C:231:LEU:CD1	1:C:290:LEU:HD23	2.47	0.44
2:D:1435:LEU:C	2:D:1435:LEU:HD13	2.43	0.44
1:A:391:GLY:O	1:A:395:VAL:HG23	2.17	0.43
1:C:273:ILE:CD1	3:C:501:LUF:H22	2.48	0.43
3:C:501:LUF:H19	3:C:501:LUF:C23	2.45	0.43
1:C:335:ILE:HG22	1:C:352:GLN:HB2	2.00	0.43
1:C:281:GLN:O	1:C:282:ASP:CA	2.63	0.43
1:A:298:HIS:HA	1:A:306:THR:OG1	2.19	0.43
1:A:382:THR:HG23	1:C:382:THR:HA	2.01	0.43
1:A:216:GLN:H	1:A:216:GLN:HG3	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ARG:HD2	1:C:364:ARG:HA	1.53	0.43
1:A:335:ILE:HG22	1:A:352:GLN:HB2	2.00	0.43
1:C:248:GLY:O	1:C:249:PHE:C	2.58	0.43
1:A:319:LEU:HD23	1:A:377:MET:HG2	2.01	0.42
1:C:372:HIS:CD2	1:C:372:HIS:H	2.36	0.42
1:C:380:LYS:HA	1:C:380:LYS:HD3	1.75	0.42
1:A:269:LEU:HB3	3:A:501:LUF:C15	2.49	0.42
1:A:402:ILE:HB	1:A:403:PRO:HD2	2.00	0.42
1:C:395:VAL:HG22	3:C:501:LUF:C4	2.49	0.42
1:A:398:LEU:C	1:A:400:MET:H	2.28	0.42
1:A:246:LEU:O	1:A:247:PRO:C	2.62	0.42
1:C:385:ARG:HA	1:C:385:ARG:HD3	1.47	0.42
1:A:370:ARG:HA	1:A:371:PRO:HD3	1.85	0.42
1:A:411:GLN:HA	1:A:415:GLU:OE1	2.19	0.42
1:A:376:LYS:HD3	1:A:376:LYS:HA	1.99	0.41
1:A:382:THR:HA	1:C:382:THR:HG23	2.01	0.41
3:A:501:LUF:H22	3:A:501:LUF:H26	1.83	0.41
1:C:372:HIS:HB3	4:C:612:HOH:O	2.21	0.41
1:C:372:HIS:O	1:C:375:PRO:HD2	2.19	0.41
1:A:209:THR:HB	1:A:210:THR:H	1.70	0.41
1:C:213:SER:C	1:C:215:GLU:H	2.28	0.41
1:A:261:LEU:O	1:A:262:LYS:C	2.64	0.41
1:A:384:LEU:HD12	1:A:384:LEU:HA	1.91	0.41
1:C:377:MET:O	1:C:380:LYS:HB2	2.21	0.41
1:A:394:ARG:O	1:A:398:LEU:HB2	2.21	0.41
1:C:299:ASN:N	1:C:299:ASN:HD22	2.19	0.40
1:A:235:CYS:HB3	1:A:269:LEU:CD2	2.50	0.40
1:C:370:ARG:HG2	1:C:370:ARG:HH11	1.87	0.40
1:A:207:LYS:O	1:A:208:TYR:HB3	2.21	0.40
1:C:276:ARG:HD2	1:C:285:THR:O	2.22	0.40
1:C:406:MET:CB	1:C:411:GLN:HG2	2.51	0.40
1:C:409:LEU:HD13	2:D:1434:LEU:HD22	2.01	0.40
2:D:1440:THR:C	2:D:1441:GLU:CG	2.92	0.40
1:A:228:PHE:CE2	3:A:501:LUF:H8	2.54	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	232/234 (99%)	214 (92%)	15 (6%)	3 (1%)	9	18
1	C	230/234 (98%)	216 (94%)	11 (5%)	3 (1%)	9	18
2	B	8/10 (80%)	7 (88%)	0	1 (12%)	0	0
2	D	8/10 (80%)	5 (62%)	1 (12%)	2 (25%)	0	0
All	All	478/488 (98%)	442 (92%)	27 (6%)	9 (2%)	6	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	SER
2	D	1434	LEU
1	A	403	PRO
1	C	403	PRO
1	C	404	GLY
2	D	1433	SER
2	B	1434	LEU
1	C	213	SER
1	A	404	GLY

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	210/210 (100%)	188 (90%)	22 (10%)	6	13
1	C	209/210 (100%)	181 (87%)	28 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	10/10 (100%)	8 (80%)	2 (20%)	1	2
2	D	10/10 (100%)	6 (60%)	4 (40%)	0	0
All	All	439/440 (100%)	383 (87%)	56 (13%)	4	7

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	GLU
1	A	190	LYS
1	A	193	LYS
1	A	212	ASN
1	A	216	GLN
1	A	266	LEU
1	A	275	THR
1	A	316	LEU
1	A	317	LEU
1	A	344	GLN
1	A	346	ASP
1	A	347	ARG
1	A	351	LEU
1	A	364	ARG
1	A	372	HIS
1	A	384	LEU
1	A	385	ARG
1	A	393	GLU
1	A	396	ILE
1	A	397	THR
1	A	398	LEU
1	A	414	LEU
2	B	1432	LYS
2	B	1437	GLN
1	C	183	GLU
1	C	193	LYS
1	C	210	THR
1	C	214	SER
1	C	216	GLN
1	C	235	CYS
1	C	262	LYS
1	C	266	LEU
1	C	275	THR
1	C	316	LEU

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Mol	Chain	Res	Type
1	C	317	LEU
1	C	346	ASP
1	C	347	ARG
1	C	350	MET
1	C	351	LEU
1	C	364	ARG
1	C	365	LYS
1	C	370	ARG
1	C	372	HIS
1	C	376	LYS
1	C	384	LEU
1	C	385	ARG
1	C	393	GLU
1	C	396	ILE
1	C	397	THR
1	C	411	GLN
1	C	414	LEU
1	C	415	GLU
2	D	1432	LYS
2	D	1435	LEU
2	D	1436	GLN
2	D	1441	GLU

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

Mol	Chain	Res	Type
1	A	212	ASN
1	A	245	GLN
1	A	296	GLN
1	A	299	ASN
1	A	411	GLN
2	B	1436	GLN
1	C	195	HIS
1	C	204	GLN
1	C	281	GLN
1	C	296	GLN
1	C	299	ASN
1	C	411	GLN
2	D	1436	GLN
2	D	1437	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 ⓘ

2 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	LUF	C	501	-	24,26,29	1.59	3 (12%)	32,35,40	3.47	16 (50%)
3	LUF	A	501	-	29,29,29	1.69	4 (13%)	38,40,40	3.29	16 (42%)

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	LUF	C	501	-	-	5/11/37/46	0/2/2/2
3	LUF	A	501	-	-	8/17/46/46	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	LUF	O1-C25	5.71	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	LUF	O1-C25	5.33	1.45	1.36
3	A	501	LUF	C1-C3	-4.10	1.48	1.53
3	C	501	LUF	C7-C3	3.27	1.56	1.51
3	A	501	LUF	O1-C23	-2.85	1.42	1.46
3	C	501	LUF	C16-C17	2.13	1.54	1.51
3	A	501	LUF	C23-C22	-2.13	1.49	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	LUF	O1-C25-C24	10.05	114.88	108.17
3	A	501	LUF	C23-C22-C24	9.35	115.44	109.13
3	C	501	LUF	C23-O1-C25	-9.25	102.12	109.31
3	C	501	LUF	C22-C24-C25	-7.65	104.39	108.62
3	A	501	LUF	C7-C3-C1	7.64	121.29	116.81
3	A	501	LUF	C4-C5-C6	-7.05	101.48	114.06
3	A	501	LUF	C5-C6-C3	-6.87	114.09	122.36
3	A	501	LUF	C2-C1-C3	-6.63	101.83	110.61
3	C	501	LUF	C4-C5-C6	-4.73	105.62	114.06
3	C	501	LUF	C5-C6-C3	-4.32	117.16	122.36
3	A	501	LUF	C11-C6-C5	3.92	121.95	113.60
3	A	501	LUF	O1-C25-O3	3.88	125.62	120.93
3	A	501	LUF	C23-O1-C25	-3.46	106.62	109.31
3	A	501	LUF	C21-C17-C16	3.42	121.16	115.23
3	C	501	LUF	C15-C13-C12	-3.32	120.03	127.62
3	C	501	LUF	C7-C3-C1	3.25	118.72	116.81
3	A	501	LUF	O3-C25-C24	-3.23	124.46	130.80
3	C	501	LUF	O3-C25-C24	-3.20	125.54	130.85
3	C	501	LUF	C21-C17-C19	-3.19	114.21	122.23
3	C	501	LUF	C16-C17-C19	3.14	131.50	123.13
3	C	501	LUF	C11-C6-C5	2.88	119.74	113.60
3	A	501	LUF	C22-C24-C25	-2.67	103.71	108.89
3	C	501	LUF	O2-C23-O1	-2.66	103.77	109.80
3	A	501	LUF	C15-C13-C12	-2.65	121.56	127.62
3	A	501	LUF	C14-C12-C10	2.53	119.62	115.23
3	C	501	LUF	C10-C7-C3	-2.51	108.63	113.64
3	C	501	LUF	C4-C2-C1	-2.48	105.64	114.43
3	A	501	LUF	C18-C19-C17	-2.47	121.98	127.62
3	A	501	LUF	O1-C23-C22	-2.35	101.98	103.57
3	C	501	LUF	O1-C23-C22	2.32	107.64	104.39
3	A	501	LUF	O2-C23-O1	2.21	113.78	110.65
3	C	501	LUF	C9-C1-C8	2.02	114.41	108.63

There are no chirality outliers.

All (13) torsion outliers are listed below:

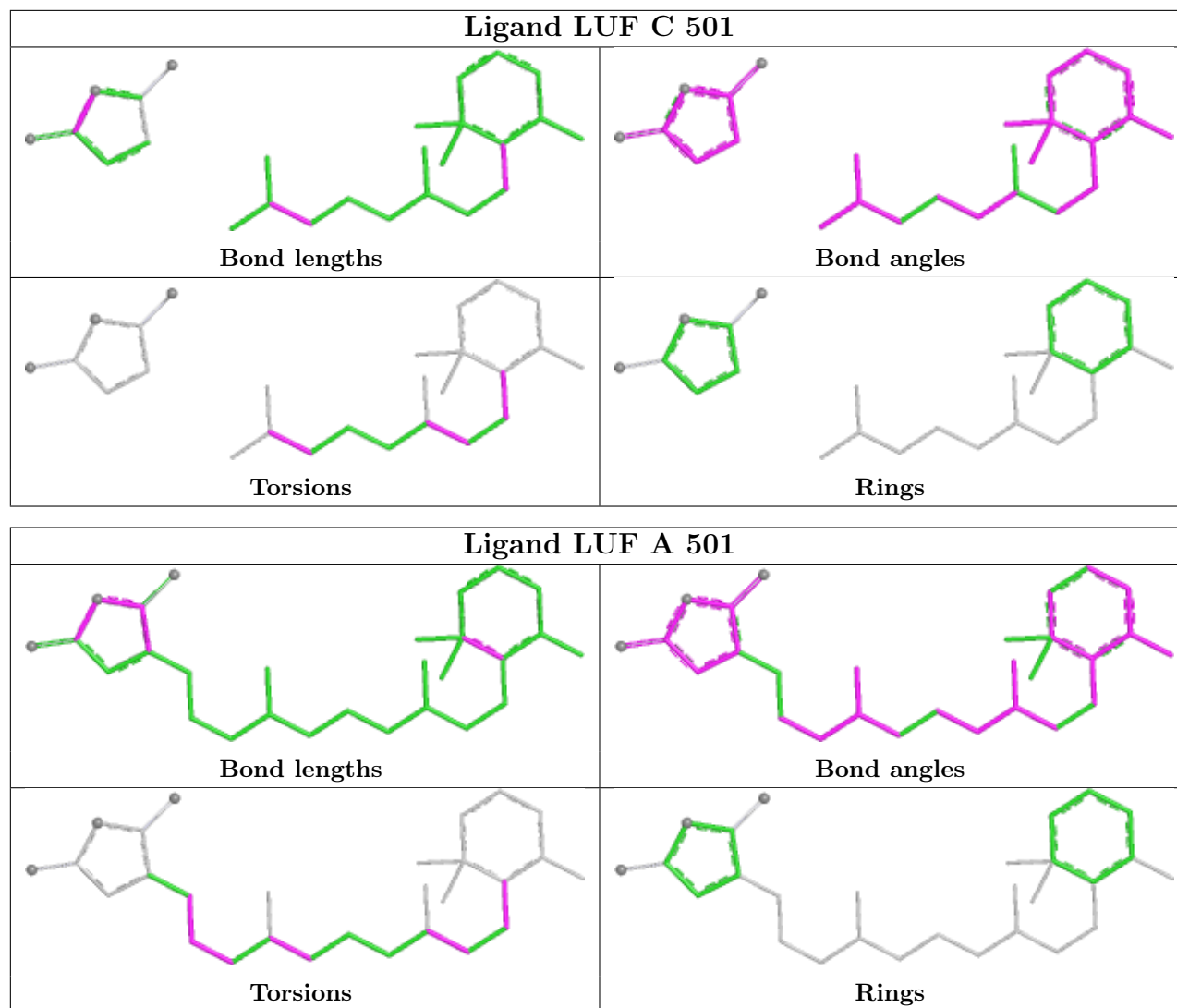
Mol	Chain	Res	Type	Atoms
3	A	501	LUF	C6-C3-C7-C10
3	A	501	LUF	C7-C10-C12-C13
3	A	501	LUF	C7-C10-C12-C14
3	A	501	LUF	C20-C18-C19-C17
3	C	501	LUF	C7-C10-C12-C14
3	C	501	LUF	C7-C10-C12-C13
3	A	501	LUF	C19-C18-C20-C22
3	C	501	LUF	C6-C3-C7-C10
3	A	501	LUF	C15-C16-C17-C21
3	A	501	LUF	C1-C3-C7-C10
3	C	501	LUF	C1-C3-C7-C10
3	C	501	LUF	C15-C16-C17-C21
3	A	501	LUF	C15-C16-C17-C19

There are no ring outliers.

2 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	LUF	32	0
3	A	501	LUF	33	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, 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	234/234 (100%)	0.02	4 (1%) 69 67	34, 58, 95, 114	1 (0%)
1	C	234/234 (100%)	-0.01	5 (2%) 63 61	34, 57, 96, 116	0
2	B	10/10 (100%)	0.14	0 100 100	54, 63, 71, 97	0
2	D	10/10 (100%)	0.41	0 100 100	55, 60, 76, 83	0
All	All	488/488 (100%)	0.02	9 (1%) 67 65	34, 58, 95, 116	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	PRO	4.3
1	A	182	PRO	3.8
1	C	213	SER	3.0
1	A	372	HIS	2.9
1	C	212	ASN	2.7
1	C	211	ASN	2.4
1	A	302	PHE	2.1
1	A	213	SER	2.1
1	C	228	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

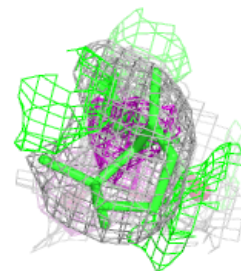
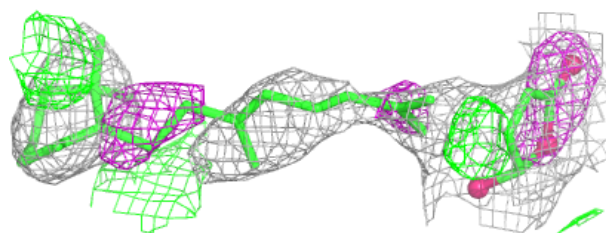
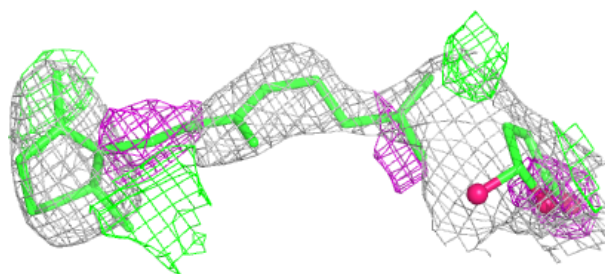
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

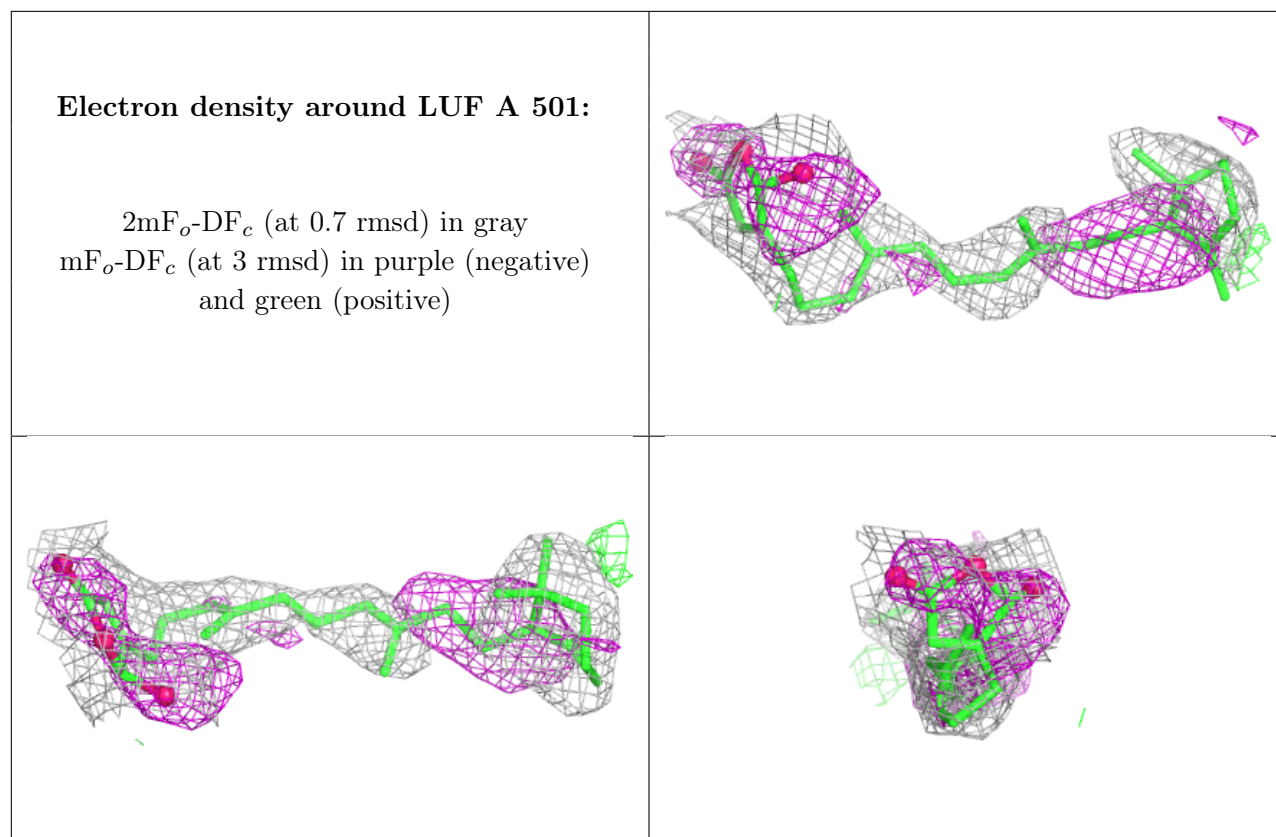
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LUF	C	501	26/28	0.80	0.16	38,49,60,60	0
3	LUF	A	501	28/28	0.84	0.14	36,49,58,59	0

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 LUF 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.