



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:12 am BST

PDB ID : 1J7E
Title : A Structural Basis for the Unique Binding Features of the Human Vitamin D-binding Protein
Authors : Verboven, C.; Rabijns, A.; De Maeyer, M.; Van Baelen, H.; Bouillon, R.; De Ranter, C.
Deposited on : 2001-05-16
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

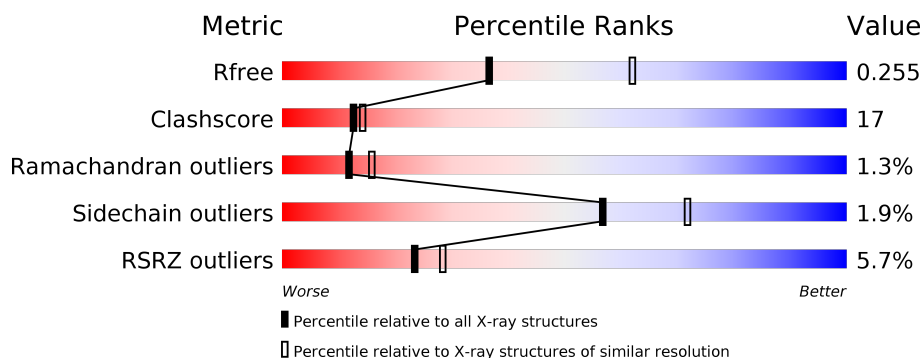
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	458	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>• 5%</div> </div> </div>
1	B	458	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>• •</div> </div> </div>

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
2	JY	A	501	-	-	-	X
2	JY	B	502	-	-	-	X
3	OLA	B	503	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7170 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.

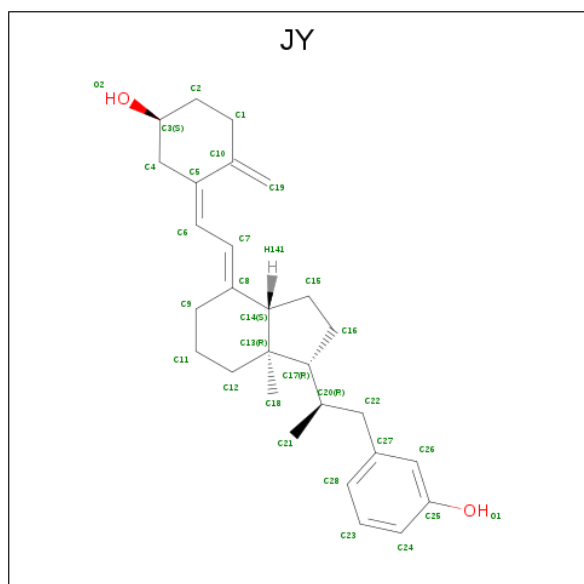
- Molecule 1 is a protein called vitamin D binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3385	2129	549	673	34			
1	B	447	Total	C	N	O	S	0	0	0
			3419	2143	553	688	35			

There are 2 discrepancies between the modelled and reference sequences:

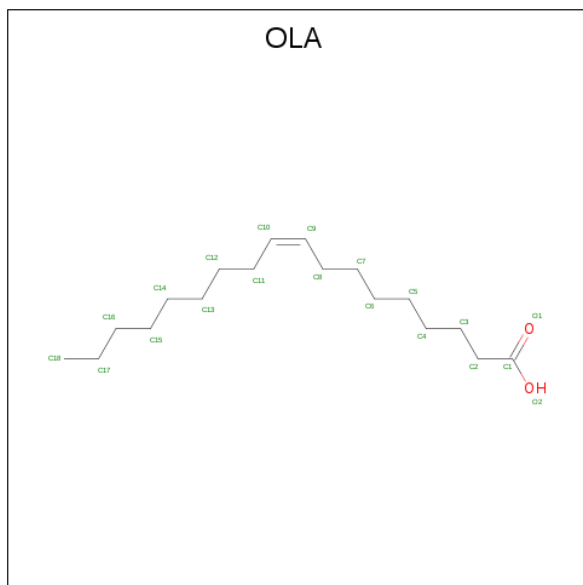
Chain	Residue	Modelled	Actual	Comment	Reference
A	420	THR	LYS	VARIANT	UNP P02774
B	420	THR	LYS	VARIANT	UNP P02774

- Molecule 2 is 3-(2-{4-[2-(5-HYDROXY-2-METHYLENE-CYCLOHEXYLIDENE)-ETHYLIDENE]-7A-METHYL-OCTAHYDRO-INDEN-1-YL}-PROPYL)-PHENOL (three-letter code: JY) (formula: C₂₈H₃₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			30	28	2		
2	B	1	Total	C	O	0	0
			30	28	2		

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).

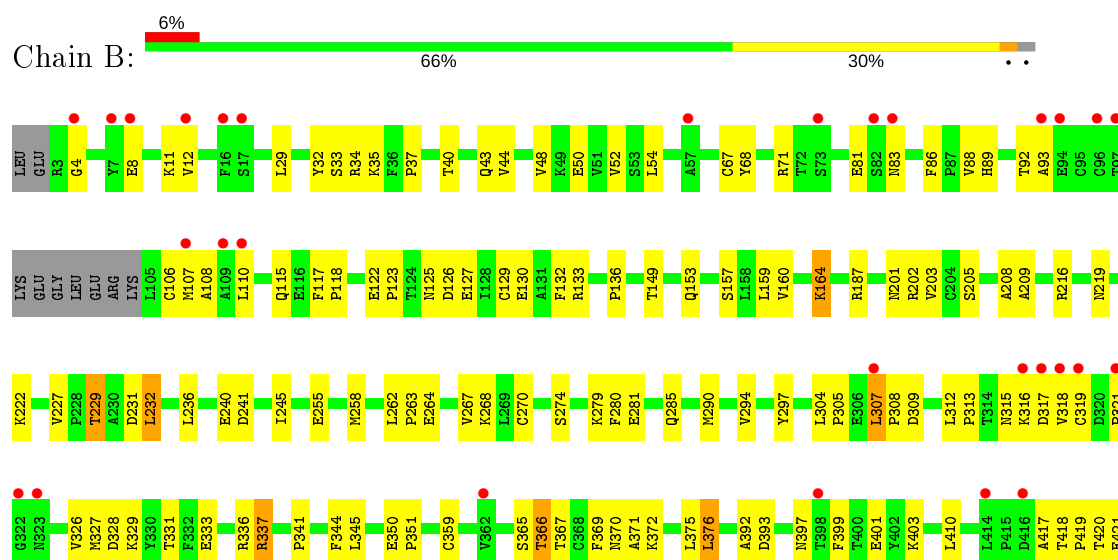


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		
4	B	97	Total	O	0	0
			97	97		

- Molecule 1: vitamin D binding protein



L422	A423	K424	I425	V426	S430	D431	F432	C437	S448	E449	I450	E453	L454	K455	M456	I457	I458
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	131.98Å 131.98Å 73.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 2.55 29.51 – 2.37	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.51-2.55) 93.9 (29.51-2.37)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.263 0.206 , 0.255	Depositor DCC
R_{free} test set	1925 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: OLA, JY

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	0.36	0/3447	0.58	0/4661
1	B	0.36	0/3485	0.57	0/4727
All	All	0.36	0/6932	0.58	0/9388

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	TYR	Sidechain

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	3385	0	3326	119	0
1	B	3419	0	3282	113	0
2	A	30	0	37	2	0
2	B	30	0	37	1	0
3	A	20	0	34	0	0
3	B	40	0	68	3	0
4	A	149	0	0	13	1
4	B	97	0	0	6	0
All	All	7170	0	6784	229	1

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 17.

All (229) 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:286:GLU:HG2	1:A:291:ASP:HB3	1.41	1.01
1:B:316:LYS:HE3	1:B:365:SER:HB2	1.40	1.00
1:B:115:GLN:HE21	1:B:117:PHE:H	1.00	0.93
1:A:315:ASN:ND2	1:A:317:ASP:HB2	1.88	0.89
1:A:374:PRO:O	1:A:378:LYS:HD3	1.81	0.81
1:A:118:PRO:HG3	4:A:506:HOH:O	1.80	0.81
1:B:115:GLN:HE21	1:B:117:PHE:N	1.77	0.80
1:A:238:LEU:HD13	1:A:269:LEU:HD23	1.64	0.78
1:B:222:LYS:HE3	4:B:579:HOH:O	1.83	0.78
1:A:98:LYS:NZ	1:A:104:LYS:HB2	1.99	0.78
1:A:204:CYS:HB3	4:A:611:HOH:O	1.83	0.77
1:B:115:GLN:NE2	1:B:117:PHE:H	1.80	0.76
1:A:315:ASN:HD21	1:A:317:ASP:HB2	1.50	0.75
1:A:286:GLU:CG	1:A:291:ASP:HB3	2.17	0.75
1:B:316:LYS:NZ	1:B:366:THR:HB	2.02	0.74
1:A:317:ASP:HB3	1:A:326:VAL:HG21	1.70	0.73
1:A:135:ASP:CG	1:A:138:GLU:HB3	2.09	0.72
1:A:98:LYS:HG3	1:A:103:ARG:HB3	1.70	0.72
1:B:153:GLN:H	1:B:201:ASN:HD22	1.38	0.71
1:A:350:GLU:HB3	1:A:351:PRO:HD3	1.73	0.71
1:A:210:TYR:HB3	1:A:214:LYS:HB2	1.73	0.70
1:B:118:PRO:HG2	1:B:202:ARG:NH2	2.06	0.69
1:A:307:LEU:HD12	1:A:307:LEU:N	2.09	0.67
1:B:317:ASP:HB3	1:B:326:VAL:HG21	1.77	0.67
1:A:21:LYS:HD2	1:A:22:GLU:N	2.10	0.66
1:B:126:ASP:O	1:B:130:GLU:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:PRO:HB2	1:B:318:VAL:HG11	1.77	0.66
1:A:98:LYS:HZ1	1:A:104:LYS:HB2	1.59	0.65
1:B:118:PRO:HG3	4:B:507:HOH:O	1.97	0.65
1:A:210:TYR:CD1	1:A:214:LYS:HE3	2.32	0.65
1:B:399:PHE:CE2	1:B:403:LYS:HE3	2.32	0.65
1:A:181:VAL:HG23	4:A:598:HOH:O	1.97	0.64
1:A:32:TYR:OH	2:A:501:JY:H141	1.98	0.64
1:B:88:VAL:HG13	1:B:92:THR:OG1	1.99	0.62
1:B:327:MET:O	1:B:331:THR:HG23	1.98	0.62
1:B:270:CYS:O	1:B:274:SER:HB2	1.99	0.62
1:B:316:LYS:HZ1	1:B:366:THR:HB	1.65	0.61
1:A:90:PRO:HG2	1:B:418:THR:HG22	1.82	0.61
1:B:89:HIS:O	1:B:92:THR:HG23	2.01	0.61
1:A:114:PRO:HD2	1:A:444:LEU:CD1	2.31	0.60
1:B:307:LEU:HB3	1:B:308:PRO:CD	2.31	0.60
1:B:118:PRO:CG	1:B:202:ARG:HH22	2.14	0.60
1:B:208:ALA:HA	3:B:504:OLA:H32	1.82	0.60
1:B:341:PRO:HG2	1:B:344:PHE:HD1	1.67	0.59
1:A:40:THR:OG1	1:A:43:GLN:HG3	2.02	0.59
1:A:180:THR:HB	4:A:598:HOH:O	2.02	0.58
1:B:279:LYS:NZ	4:B:587:HOH:O	2.36	0.58
1:A:195:LEU:HD11	1:A:294:VAL:HG21	1.85	0.58
1:A:8:GLU:HA	1:A:11:LYS:HB3	1.86	0.58
1:A:89:HIS:CE1	1:A:112:HIS:HB3	2.39	0.58
1:A:153:GLN:H	1:A:201:ASN:HD22	1.50	0.57
1:B:125:ASN:ND2	1:B:187:ARG:HH21	2.01	0.57
1:A:47:LEU:O	1:A:51:VAL:HG23	2.05	0.57
1:B:359:CYS:HB3	1:B:369:PHE:CE1	2.39	0.57
1:A:8:GLU:HA	1:A:11:LYS:CB	2.36	0.56
1:B:371:ALA:O	1:B:375:LEU:HD23	2.06	0.56
1:A:199:LEU:HD21	1:A:293:PHE:CD1	2.41	0.56
1:B:123:PRO:HB3	1:B:127:GLU:OE2	2.05	0.56
1:A:416:ASP:HB2	4:A:550:HOH:O	2.06	0.55
1:A:286:GLU:HG2	1:A:291:ASP:CB	2.25	0.55
1:A:409:ARG:HD2	4:A:596:HOH:O	2.06	0.55
1:A:153:GLN:H	1:A:201:ASN:ND2	2.05	0.55
1:A:219:ASN:ND2	4:A:540:HOH:O	2.35	0.55
1:A:428:LYS:NZ	1:A:428:LYS:HB3	2.22	0.54
1:B:33:SER:O	1:B:149:THR:HG22	2.07	0.54
1:A:263:PRO:HG2	4:A:518:HOH:O	2.07	0.53
1:B:227:VAL:C	1:B:229:THR:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:NE	1:A:202:ARG:HA	2.22	0.53
1:A:50:GLU:O	1:A:53:SER:HB3	2.08	0.53
1:B:81:GLU:HG2	1:B:83:ASN:H	1.72	0.53
1:A:113:GLN:HB2	1:B:419:PRO:HD2	1.90	0.53
1:A:69:ASP:N	1:A:72:THR:HG1	2.06	0.53
1:A:315:ASN:O	1:A:318:VAL:HG22	2.08	0.53
1:B:319:CYS:O	1:B:321:PRO:HD3	2.08	0.53
1:A:120:TYR:HD1	1:A:146:GLU:HG2	1.74	0.53
1:A:33:SER:HB3	1:A:149:THR:HG23	1.91	0.52
1:A:413:LYS:O	1:A:414:LEU:HD23	2.09	0.52
1:B:341:PRO:HG2	1:B:344:PHE:CD1	2.44	0.52
1:A:35:LYS:O	1:A:89:HIS:HE1	1.93	0.52
1:A:440:ASN:HB2	4:A:582:HOH:O	2.09	0.52
1:B:307:LEU:HB3	1:B:308:PRO:HD2	1.91	0.52
1:A:124:THR:OG1	1:A:127:GLU:HG3	2.10	0.52
1:B:329:LYS:O	1:B:333:GLU:HG2	2.10	0.52
1:B:34:ARG:HD2	1:B:159:LEU:HD12	1.92	0.52
1:B:187:ARG:HH11	1:B:187:ARG:HG2	1.75	0.52
1:B:32:TYR:OH	2:B:502:JY:H141	2.09	0.52
1:A:98:LYS:HG3	1:A:103:ARG:NE	2.25	0.51
1:B:216:ARG:NH1	1:B:240:GLU:HG2	2.26	0.51
1:B:350:GLU:HB3	1:B:351:PRO:HD3	1.92	0.51
1:A:98:LYS:HZ2	1:A:104:LYS:HB2	1.73	0.51
1:A:375:LEU:O	1:A:379:GLU:HG3	2.11	0.50
1:A:54:LEU:HD12	1:A:54:LEU:C	2.31	0.50
1:B:132:PHE:O	1:B:136:PRO:HG3	2.11	0.50
1:A:8:GLU:C	1:A:10:ASN:H	2.15	0.50
1:B:122:GLU:CD	1:B:187:ARG:HH12	2.14	0.50
1:A:130:GLU:O	1:A:133:ARG:HG2	2.12	0.50
1:A:214:LYS:HD3	1:A:350:GLU:CD	2.32	0.50
1:B:153:GLN:H	1:B:201:ASN:ND2	2.05	0.50
1:A:341:PRO:HG2	1:A:437:CYS:HA	1.94	0.50
1:B:118:PRO:HG2	1:B:202:ARG:HH22	1.69	0.50
1:B:50:GLU:HG3	1:B:86:PHE:CZ	2.46	0.50
1:B:92:THR:HG22	1:B:110:LEU:HD12	1.94	0.50
1:B:203:VAL:HG12	1:B:297:TYR:CE2	2.47	0.50
1:A:114:PRO:HD2	1:A:444:LEU:HD11	1.94	0.49
1:A:439:ILE:HA	4:A:523:HOH:O	2.11	0.49
1:B:312:LEU:HD13	1:B:376:LEU:HG	1.93	0.49
1:B:35:LYS:O	1:B:37:PRO:HD3	2.12	0.49
1:B:264:GLU:HG2	1:B:268:LYS:NZ	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:SER:HB3	1:B:149:THR:HG23	1.94	0.49
1:B:281:GLU:O	1:B:285:GLN:HG3	2.13	0.49
1:A:456:ASN:ND2	1:A:457:ILE:H	2.11	0.49
1:B:365:SER:HB3	1:B:369:PHE:HE1	1.78	0.49
1:B:8:GLU:O	1:B:12:VAL:HG22	2.12	0.48
1:A:307:LEU:CD1	1:A:307:LEU:N	2.76	0.48
1:A:95:CYS:SG	1:A:106:CYS:C	2.92	0.48
1:A:103:ARG:C	1:A:105:LEU:H	2.16	0.48
1:B:129:CYS:O	1:B:133:ARG:HG3	2.13	0.48
1:A:15:GLU:O	1:A:19:LEU:HD13	2.14	0.48
1:B:232:LEU:HD22	1:B:329:LYS:HA	1.96	0.48
1:B:258:MET:HE3	1:B:262:LEU:HD11	1.94	0.48
1:B:315:ASN:OD1	1:B:317:ASP:HB2	2.14	0.48
1:B:350:GLU:HB3	1:B:351:PRO:CD	2.44	0.47
1:A:399:PHE:O	1:A:402:TYR:HB3	2.14	0.47
1:A:155:PRO:HG2	1:A:158:LEU:HB2	1.95	0.47
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.80	0.47
1:A:270:CYS:O	1:A:274:SER:HB2	2.13	0.47
1:A:158:LEU:HD21	1:A:196:LEU:HG	1.95	0.47
1:B:341:PRO:HG3	1:B:437:CYS:HA	1.96	0.47
1:A:44:VAL:O	1:A:48:VAL:HG23	2.15	0.47
1:B:290:MET:O	1:B:294:VAL:HG23	2.15	0.47
1:B:48:VAL:O	1:B:52:VAL:HG23	2.15	0.47
1:A:98:LYS:HG3	1:A:103:ARG:HE	1.79	0.47
1:B:153:GLN:HG3	1:B:205:SER:OG	2.15	0.47
1:B:372:LYS:HG2	1:B:376:LEU:HD22	1.96	0.46
1:A:24:PHE:CZ	1:A:55:THR:HG21	2.51	0.46
1:A:392:ALA:O	1:A:393:ASP:HB2	2.15	0.46
1:B:106:CYS:C	1:B:108:ALA:H	2.19	0.46
1:B:365:SER:C	1:B:367:THR:H	2.19	0.46
1:A:199:LEU:HD11	1:A:293:PHE:HE1	1.80	0.46
1:B:227:VAL:CG2	1:B:280:PHE:CE1	2.99	0.46
1:B:258:MET:O	1:B:262:LEU:HG	2.16	0.46
1:A:222:LYS:HE2	1:A:439:ILE:O	2.16	0.46
1:A:435:ASN:O	1:A:441:SER:HB3	2.15	0.46
1:B:29:LEU:HA	1:B:48:VAL:HG21	1.97	0.46
1:A:8:GLU:C	1:A:10:ASN:N	2.69	0.46
1:B:71:ARG:HH11	1:B:71:ARG:HG2	1.81	0.46
1:B:157:SER:OG	1:B:255:GLU:HB3	2.16	0.46
1:A:195:LEU:O	1:A:195:LEU:HD13	2.16	0.46
1:A:450:ILE:O	1:A:454:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PRO:HD2	1:A:444:LEU:HD12	1.98	0.45
1:A:18:HIS:ND1	1:A:19:LEU:HD12	2.32	0.45
1:A:12:VAL:HG12	1:A:55:THR:HG23	1.97	0.45
1:B:241:ASP:O	1:B:245:ILE:HG13	2.17	0.45
1:A:366:THR:HG22	1:A:370:ASN:HD21	1.82	0.45
1:A:427:ASN:ND2	4:A:581:HOH:O	2.49	0.45
1:B:263:PRO:O	1:B:267:VAL:HG23	2.17	0.44
1:A:21:LYS:C	1:A:21:LYS:HD2	2.38	0.44
1:B:258:MET:HB2	4:B:544:HOH:O	2.18	0.44
1:B:450:ILE:O	1:B:454:LEU:HG	2.17	0.44
1:B:236:LEU:O	1:B:240:GLU:HG3	2.17	0.44
1:B:54:LEU:HD23	1:B:54:LEU:C	2.36	0.44
1:B:304:LEU:HD22	1:B:336:ARG:O	2.17	0.44
1:B:316:LYS:O	1:B:319:CYS:HB2	2.17	0.44
1:B:312:LEU:CD1	1:B:376:LEU:HG	2.47	0.44
1:B:309:ASP:HA	1:B:337:ARG:CZ	2.48	0.44
1:B:399:PHE:CZ	1:B:403:LYS:HE3	2.53	0.44
1:A:386:LYS:NZ	1:A:457:ILE:HB	2.33	0.44
1:A:424:LYS:HZ1	1:B:448:SER:CB	2.30	0.44
1:A:199:LEU:HD11	1:A:293:PHE:CE1	2.52	0.43
1:B:40:THR:O	1:B:44:VAL:HG23	2.18	0.43
1:A:98:LYS:HB2	1:A:103:ARG:HH21	1.82	0.43
1:A:76:SER:HA	2:A:501:JY:O2	2.18	0.43
1:B:304:LEU:HA	1:B:305:PRO:HD3	1.79	0.43
1:A:30:VAL:O	1:A:34:ARG:HG3	2.18	0.43
1:A:116:GLU:OE1	1:A:444:LEU:HB2	2.19	0.43
1:A:122:GLU:HA	1:A:123:PRO:HD3	1.90	0.43
1:A:236:LEU:HB3	1:A:237:PRO:HD3	2.01	0.43
1:A:203:VAL:CG2	1:A:246:LEU:HD21	2.49	0.43
1:B:367:THR:HA	1:B:370:ASN:HD22	1.83	0.43
1:A:307:LEU:HB3	1:A:308:PRO:CD	2.49	0.43
1:A:263:PRO:HA	1:A:289:ALA:HB1	2.01	0.42
1:A:359:CYS:SG	1:A:368:CYS:O	2.77	0.42
1:A:46:GLN:O	1:A:49:LYS:HB3	2.18	0.42
1:B:392:ALA:O	1:B:393:ASP:HB2	2.19	0.42
1:B:315:ASN:O	1:B:318:VAL:HG22	2.19	0.42
1:B:420:THR:CG2	1:B:424:LYS:HE3	2.49	0.42
1:B:92:THR:HG22	1:B:110:LEU:CD1	2.48	0.42
1:A:272:ASN:N	1:A:272:ASN:HD22	2.16	0.42
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.91	0.42
1:B:403:LYS:HE2	1:B:430:SER:OG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:N	1:A:237:PRO:CD	2.82	0.42
1:A:55:THR:O	1:A:59:CYS:SG	2.78	0.42
1:A:98:LYS:CG	1:A:103:ARG:NE	2.82	0.42
1:A:98:LYS:HE3	1:A:103:ARG:HB3	2.02	0.42
1:B:219:ASN:ND2	4:B:543:HOH:O	2.51	0.42
1:B:262:LEU:N	1:B:263:PRO:CD	2.81	0.42
1:B:365:SER:HB3	1:B:369:PHE:CE1	2.55	0.42
1:B:92:THR:OG1	1:B:93:ALA:N	2.53	0.41
1:B:209:ALA:O	3:B:504:OLA:H132	2.20	0.41
1:B:432:PHE:CD1	1:B:453:GLU:HG3	2.55	0.41
1:A:195:LEU:HD11	1:A:294:VAL:CG2	2.50	0.41
1:B:397:ASN:HB3	1:B:401:GLU:HB3	2.03	0.41
1:A:216:ARG:NH2	1:A:240:GLU:OE2	2.37	0.41
1:A:428:LYS:HB3	1:A:428:LYS:HZ3	1.82	0.41
1:B:216:ARG:NH2	1:B:328:ASP:OD2	2.53	0.41
1:A:378:LYS:N	1:A:378:LYS:HD2	2.35	0.41
1:A:384:ILE:O	1:A:388:GLN:HG3	2.20	0.41
1:B:122:GLU:HA	1:B:123:PRO:HD3	1.91	0.41
1:B:40:THR:OG1	1:B:43:GLN:HG3	2.19	0.41
1:B:410:LEU:HD12	1:B:426:VAL:HG22	2.02	0.41
1:A:449:GLU:OE2	1:B:424:LYS:HE2	2.21	0.41
1:B:71:ARG:HG2	1:B:71:ARG:NH1	2.35	0.41
1:A:251:GLU:HA	4:A:622:HOH:O	2.21	0.41
1:A:103:ARG:HG2	1:A:104:LYS:H	1.85	0.41
1:A:107:MET:C	1:A:109:ALA:H	2.25	0.41
3:B:504:OLA:H141	4:B:597:HOH:O	2.20	0.41
1:A:348:VAL:C	1:A:351:PRO:HD2	2.41	0.41
1:A:396:GLU:OE1	1:A:396:GLU:N	2.41	0.41
1:B:160:VAL:O	1:B:164:LYS:HB2	2.20	0.41
1:B:312:LEU:HA	1:B:313:PRO:HD3	1.93	0.41
1:A:133:ARG:HG3	1:A:134:LYS:N	2.35	0.41
1:A:342:GLU:HG3	4:A:503:HOH:O	2.21	0.41
1:B:92:THR:HA	1:B:110:LEU:HD11	2.01	0.41
1:B:270:CYS:O	1:B:274:SER:CB	2.67	0.41
1:B:417:ALA:HA	1:B:421:GLU:OE2	2.20	0.41
1:B:365:SER:O	1:B:369:PHE:HD1	2.05	0.40
1:A:336:ARG:HH21	1:A:337:ARG:HH21	1.70	0.40
1:A:456:ASN:HD22	1:A:456:ASN:HA	1.69	0.40
1:B:366:THR:O	1:B:370:ASN:ND2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:574:HOH:O	4:A:606:HOH:O[3_654]	2.03	0.17

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	427/458 (93%)	404 (95%)	21 (5%)	2 (0%)	29	40
1	B	443/458 (97%)	412 (93%)	22 (5%)	9 (2%)	7	8
All	All	870/916 (95%)	816 (94%)	43 (5%)	11 (1%)	12	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	CYS
1	B	4	GLY
1	B	366	THR
1	B	11	LYS
1	B	68	TYR
1	A	306	GLU
1	A	316	LYS
1	B	107	MET
1	B	455	LYS
1	B	232	LEU
1	B	307	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	394/415 (95%)	385 (98%)	9 (2%)	50	65
1	B	390/415 (94%)	384 (98%)	6 (2%)	65	77
All	All	784/830 (94%)	769 (98%)	15 (2%)	57	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	49	LYS
1	A	54	LEU
1	A	98	LYS
1	A	106	CYS
1	A	195	LEU
1	A	202	ARG
1	A	286	GLU
1	A	456	ASN
1	B	164	LYS
1	B	229	THR
1	B	231	ASP
1	B	337	ARG
1	B	376	LEU
1	B	422	LEU

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

Mol	Chain	Res	Type
1	A	89	HIS
1	A	153	GLN
1	A	201	ASN
1	A	244	ASN
1	A	272	ASN
1	A	285	GLN
1	A	315	ASN
1	A	370	ASN
1	A	456	ASN
1	B	115	GLN
1	B	125	ASN
1	B	201	ASN
1	B	370	ASN
1	B	388	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	OLA	B	504	-	16,19,19	0.56	0	15,19,19	0.26	0
3	OLA	A	502	-	16,19,19	0.48	0	15,19,19	0.27	0
2	JY	B	502	-	33,33,33	2.06	13 (39%)	48,48,48	1.49	10 (20%)
3	OLA	B	503	-	16,19,19	0.51	0	15,19,19	0.26	0
2	JY	A	501	-	33,33,33	2.03	13 (39%)	48,48,48	1.46	9 (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
3	OLA	B	504	-	-	11/15/17/17	-
3	OLA	A	502	-	-	8/15/17/17	-
2	JY	B	502	-	-	5/13/54/54	0/4/4/4
3	OLA	B	503	-	-	11/15/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JY	A	501	-	-	6/13/54/54	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	JY	C20-C17	4.14	1.61	1.54
2	A	501	JY	C20-C17	4.05	1.61	1.54
2	A	501	JY	C10-C5	3.32	1.53	1.47
2	B	502	JY	C18-C13	3.13	1.59	1.54
2	B	502	JY	C10-C5	3.05	1.53	1.47
2	B	502	JY	C22-C20	2.96	1.57	1.54
2	A	501	JY	C6-C5	2.95	1.45	1.36
2	A	501	JY	C18-C13	2.95	1.59	1.54
2	B	502	JY	C2-C3	2.90	1.58	1.51
2	A	501	JY	C2-C3	2.89	1.58	1.51
2	B	502	JY	C6-C5	2.89	1.44	1.36
2	B	502	JY	C24-C25	2.67	1.44	1.38
2	A	501	JY	C24-C25	2.61	1.43	1.38
2	B	502	JY	C12-C13	2.60	1.58	1.54
2	A	501	JY	C13-C17	2.59	1.59	1.55
2	A	501	JY	C12-C13	2.58	1.58	1.54
2	B	502	JY	C7-C6	2.51	1.51	1.42
2	A	501	JY	C22-C20	2.48	1.56	1.54
2	B	502	JY	C4-C3	2.46	1.56	1.52
2	A	501	JY	C4-C3	2.41	1.56	1.52
2	B	502	JY	C13-C17	2.36	1.59	1.55
2	A	501	JY	C7-C6	2.36	1.50	1.42
2	B	502	JY	C26-C25	2.26	1.42	1.39
2	A	501	JY	C26-C25	2.26	1.42	1.39
2	A	501	JY	C26-C27	2.05	1.42	1.39
2	B	502	JY	C28-C27	2.01	1.43	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	JY	C14-C13-C17	-4.33	95.11	99.72
2	A	501	JY	C14-C13-C17	-3.88	95.59	99.72
2	A	501	JY	C22-C20-C17	3.29	114.62	109.86
2	B	502	JY	C22-C20-C17	3.16	114.44	109.86
2	B	502	JY	C21-C20-C22	-2.84	107.85	110.91
2	A	501	JY	C21-C20-C22	-2.83	107.86	110.91
2	A	501	JY	C18-C13-C12	-2.78	106.19	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	JY	C18-C13-C12	-2.70	106.33	110.59
2	A	501	JY	C7-C6-C5	-2.68	122.19	126.54
2	B	502	JY	C15-C14-C13	-2.67	101.83	104.21
2	A	501	JY	C2-C3-C4	2.64	113.92	110.31
2	A	501	JY	C13-C17-C20	2.60	123.56	119.49
2	A	501	JY	C18-C13-C17	2.55	116.47	111.71
2	B	502	JY	C13-C17-C20	2.51	123.42	119.49
2	B	502	JY	C18-C13-C17	2.46	116.31	111.71
2	B	502	JY	C7-C6-C5	-2.32	122.76	126.54
2	B	502	JY	C16-C17-C13	-2.15	101.25	103.84
2	B	502	JY	C2-C3-C4	2.11	113.20	110.31
2	A	501	JY	C15-C14-C13	-2.06	102.38	104.21

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	504	OLA	C1-C2-C3-C4
3	A	502	OLA	C1-C2-C3-C4
3	B	503	OLA	C1-C2-C3-C4
2	B	502	JY	C16-C17-C20-C22
2	A	501	JY	C16-C17-C20-C22
2	B	502	JY	C16-C17-C20-C21
2	B	502	JY	C13-C17-C20-C22
2	A	501	JY	C16-C17-C20-C21
2	A	501	JY	C13-C17-C20-C22
3	B	504	OLA	C11-C12-C13-C14
3	B	504	OLA	C12-C13-C14-C15
3	B	503	OLA	C13-C14-C15-C16
3	B	503	OLA	C12-C13-C14-C15
3	B	503	OLA	C14-C15-C16-C17
3	A	502	OLA	C5-C6-C7-C8
3	B	503	OLA	C5-C6-C7-C8
3	B	503	OLA	C6-C7-C8-C9
3	A	502	OLA	C11-C12-C13-C14
3	B	504	OLA	C13-C14-C15-C16
3	B	504	OLA	C5-C6-C7-C8
3	B	503	OLA	C2-C3-C4-C5
3	B	504	OLA	C6-C7-C8-C9
3	B	504	OLA	C10-C11-C12-C13
3	A	502	OLA	C3-C4-C5-C6
3	B	504	OLA	C14-C15-C16-C17

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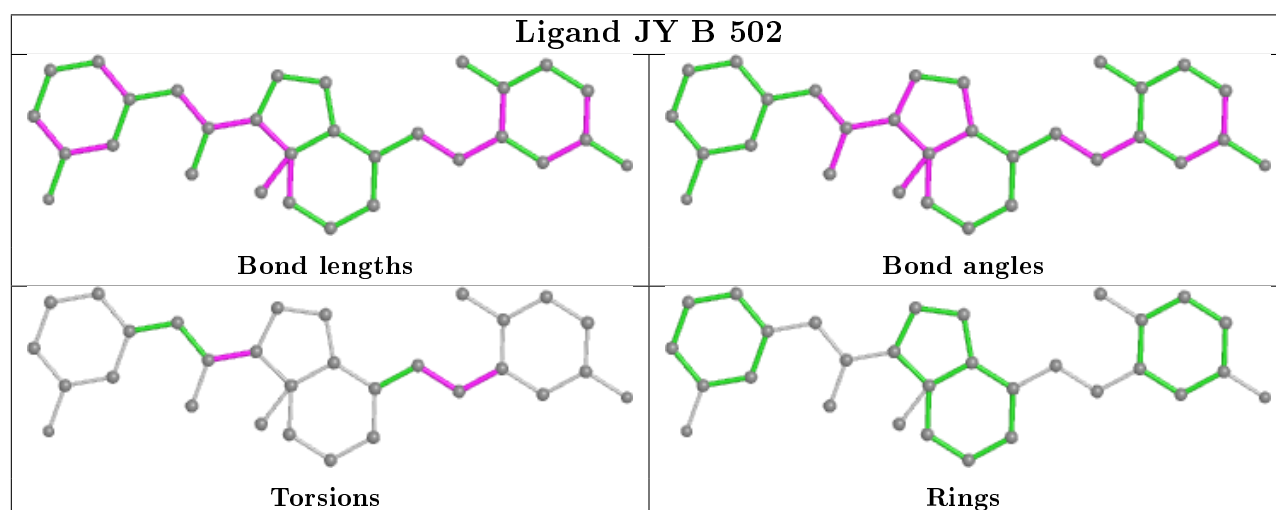
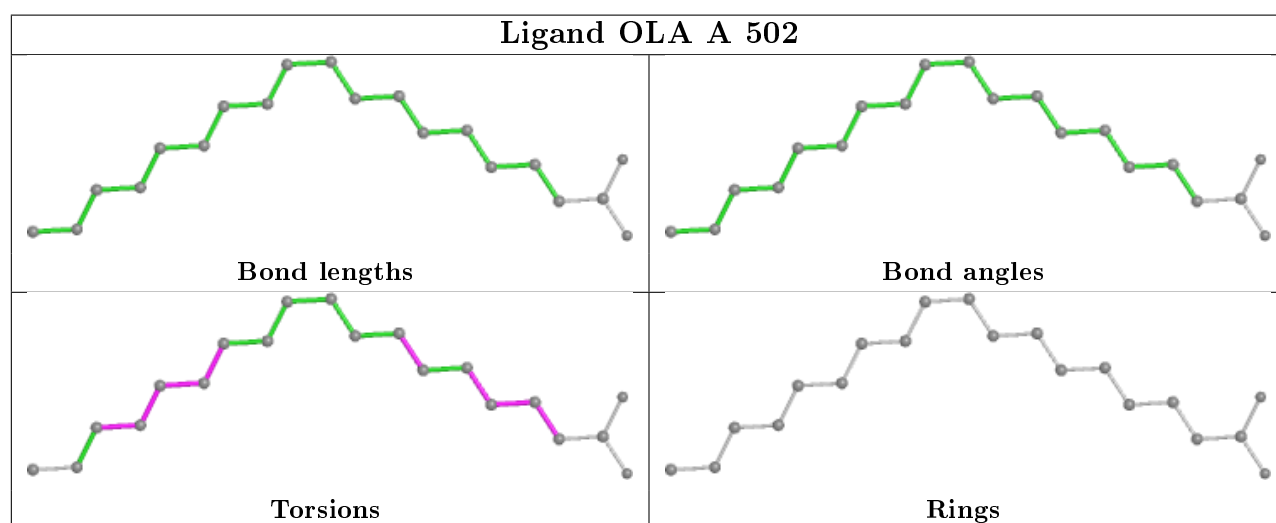
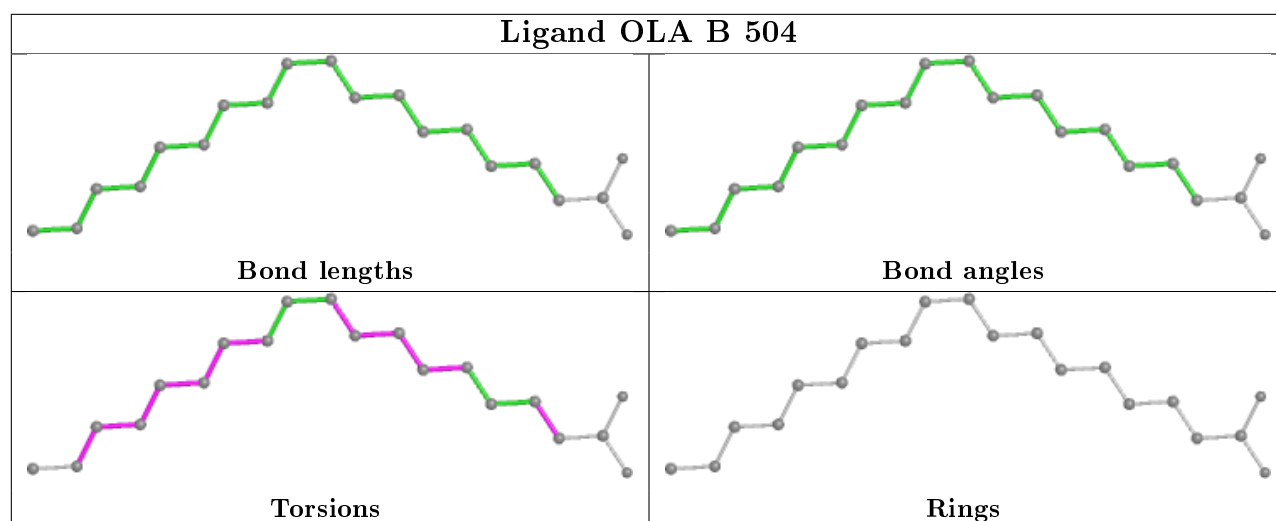
Mol	Chain	Res	Type	Atoms
3	A	502	OLA	C2-C3-C4-C5
3	B	504	OLA	C15-C16-C17-C18
3	B	503	OLA	C15-C16-C17-C18
3	A	502	OLA	C13-C14-C15-C16
2	B	502	JY	C5-C6-C7-C8
2	A	501	JY	C5-C6-C7-C8
2	B	502	JY	C4-C5-C6-C7
3	B	503	OLA	C4-C5-C6-C7
3	B	503	OLA	C3-C4-C5-C6
3	B	503	OLA	C11-C12-C13-C14
3	B	504	OLA	C7-C8-C9-C10
2	A	501	JY	C4-C5-C6-C7
2	A	501	JY	C17-C20-C22-C27
3	A	502	OLA	C12-C13-C14-C15
3	A	502	OLA	C14-C15-C16-C17
3	B	504	OLA	C4-C5-C6-C7

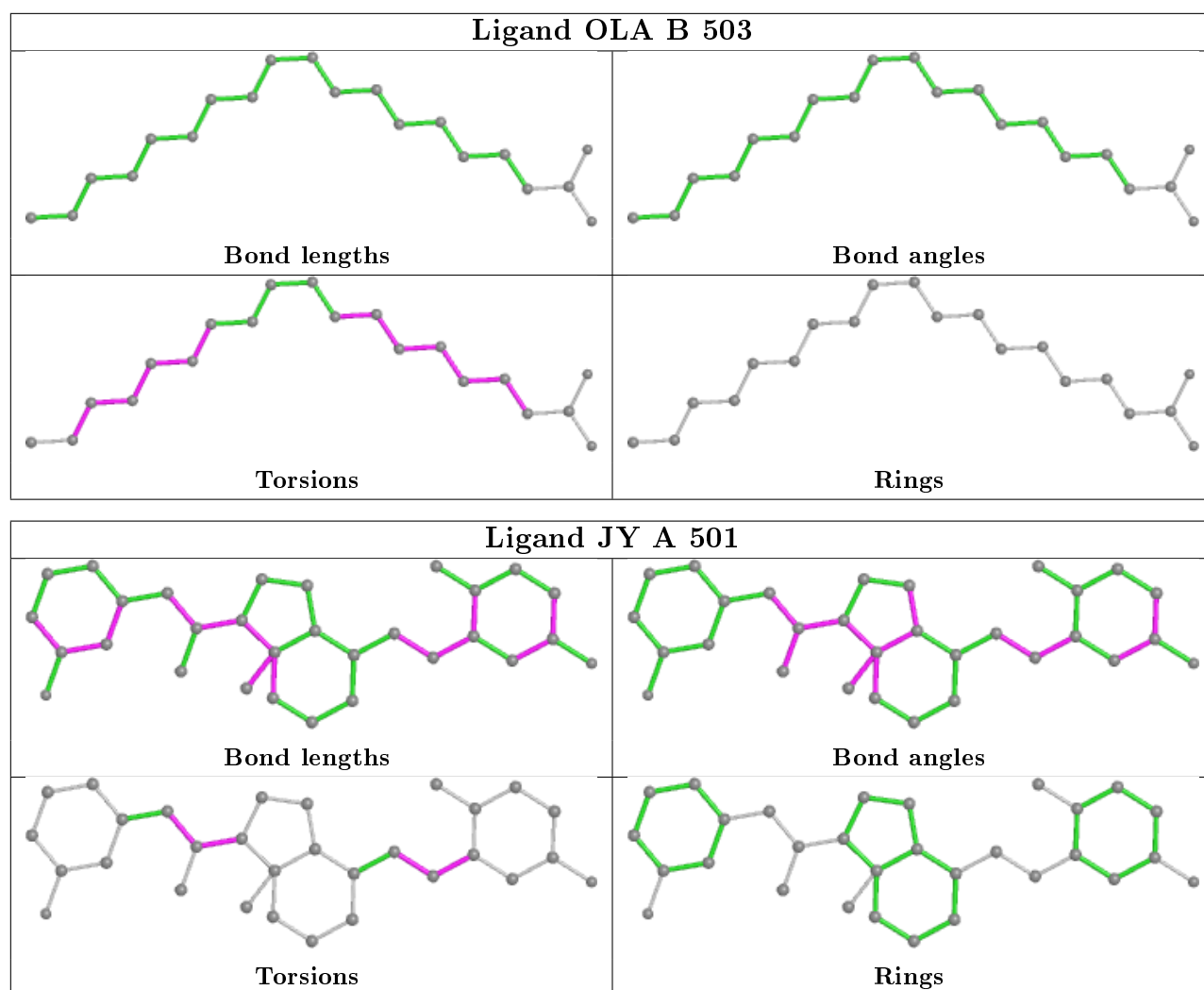
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	OLA	3	0
2	B	502	JY	1	0
2	A	501	JY	2	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 ⓘ

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	435/458 (94%)	0.01	21 (4%)	30 37	29, 53, 107, 166	0
1	B	447/458 (97%)	0.09	29 (6%)	18 22	33, 57, 124, 147	0
All	All	882/916 (96%)	0.05	50 (5%)	23 28	29, 55, 114, 166	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	MET	5.9
1	B	321	PRO	5.7
1	A	7	TYR	5.0
1	B	7	TYR	4.9
1	B	82	SER	4.7
1	B	83	ASN	4.6
1	B	110	LEU	4.2
1	B	4	GLY	4.0
1	A	97	THR	3.9
1	B	97	THR	3.9
1	A	322	GLY	3.9
1	B	8	GLU	3.8
1	B	109	ALA	3.8
1	B	96	CYS	3.8
1	A	321	PRO	3.5
1	B	94	GLU	3.4
1	A	223	LEU	3.2
1	A	21	LYS	3.1
1	B	318	VAL	2.9
1	A	221	ILE	2.9
1	A	375	LEU	2.8
1	B	362	VAL	2.8
1	B	322	GLY	2.7
1	B	398	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	19	LEU	2.7
1	B	12	VAL	2.7
1	A	306	GLU	2.7
1	A	457	ILE	2.6
1	A	58	CYS	2.6
1	A	70	THR	2.6
1	A	54	LEU	2.6
1	B	17	SER	2.5
1	B	73	SER	2.5
1	A	78	LYS	2.5
1	B	416	ASP	2.5
1	B	323	ASN	2.4
1	B	316	LYS	2.3
1	B	414	LEU	2.3
1	A	55	THR	2.3
1	B	16	PHE	2.3
1	B	307	LEU	2.3
1	B	317	ASP	2.2
1	A	335	SER	2.1
1	A	77	ALA	2.1
1	B	57	ALA	2.1
1	A	96	CYS	2.1
1	A	298	PHE	2.1
1	B	93	ALA	2.1
1	A	52	VAL	2.0
1	B	319	CYS	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](#)

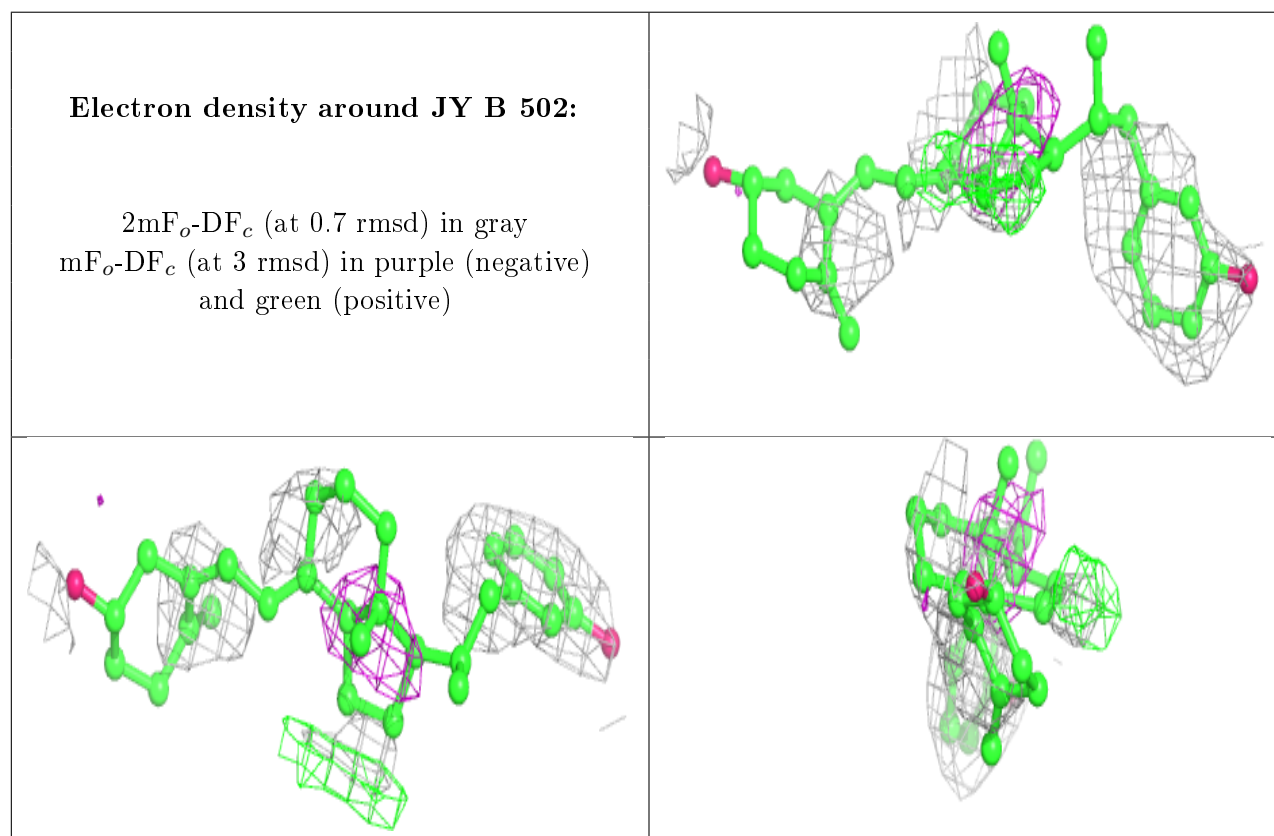
There are no carbohydrates in this entry.

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.

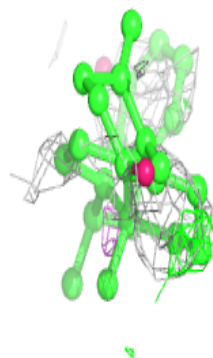
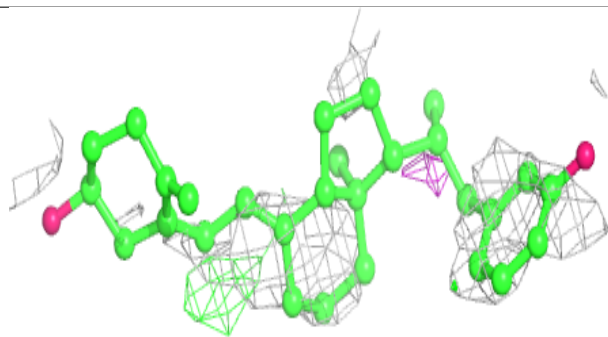
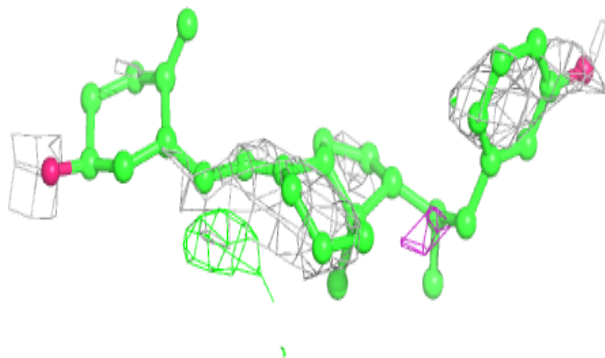
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	JY	B	502	30/30	0.44	0.53	110,141,145,148	0
2	JY	A	501	30/30	0.47	0.62	145,153,156,157	0
3	OLA	B	503	20/20	0.58	0.42	81,90,121,121	0
3	OLA	B	504	20/20	0.63	0.34	79,88,94,97	0
3	OLA	A	502	20/20	0.70	0.37	58,79,109,110	0

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.



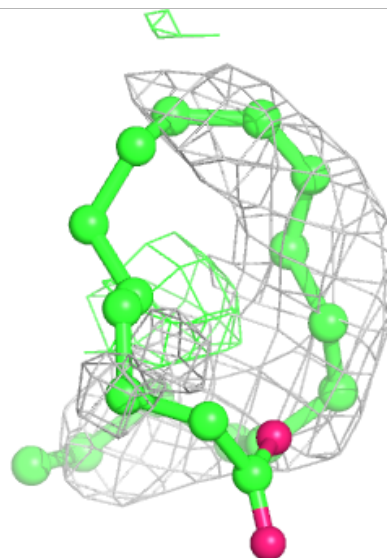
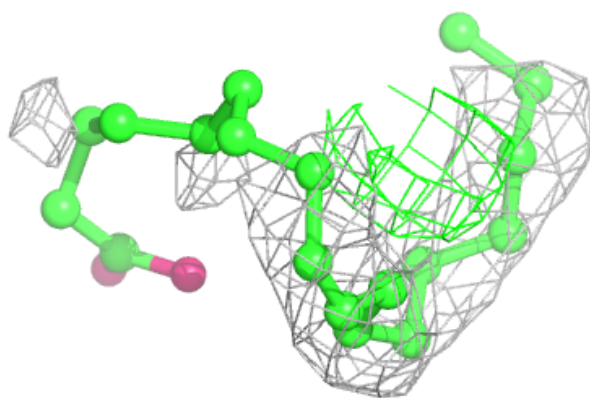
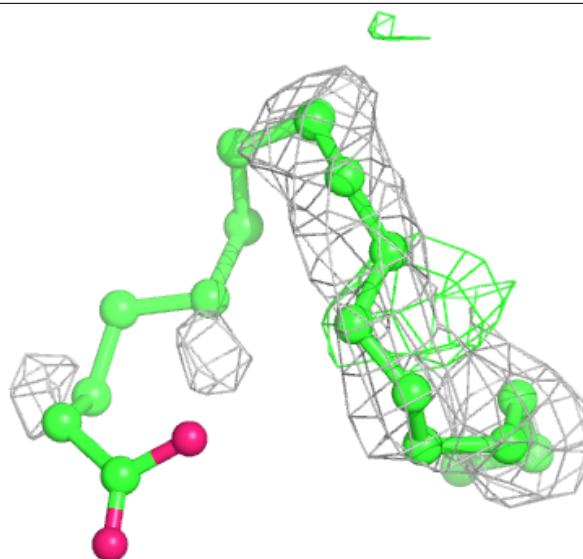
Electron density around JY A 501:

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



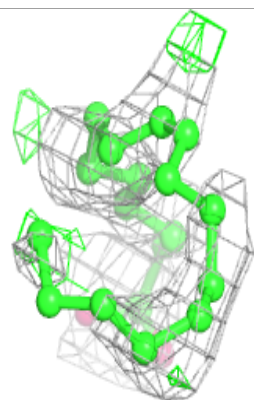
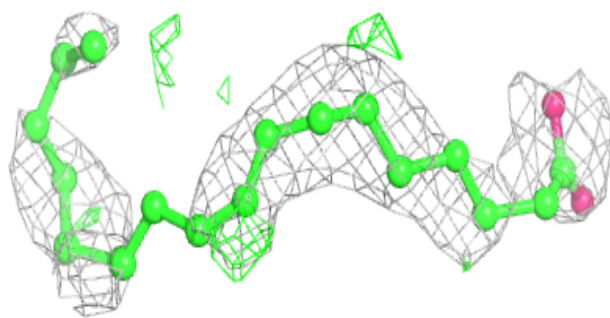
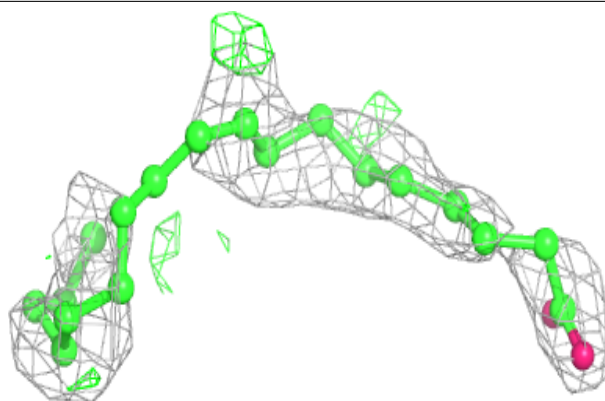
Electron density around OLA B 503:

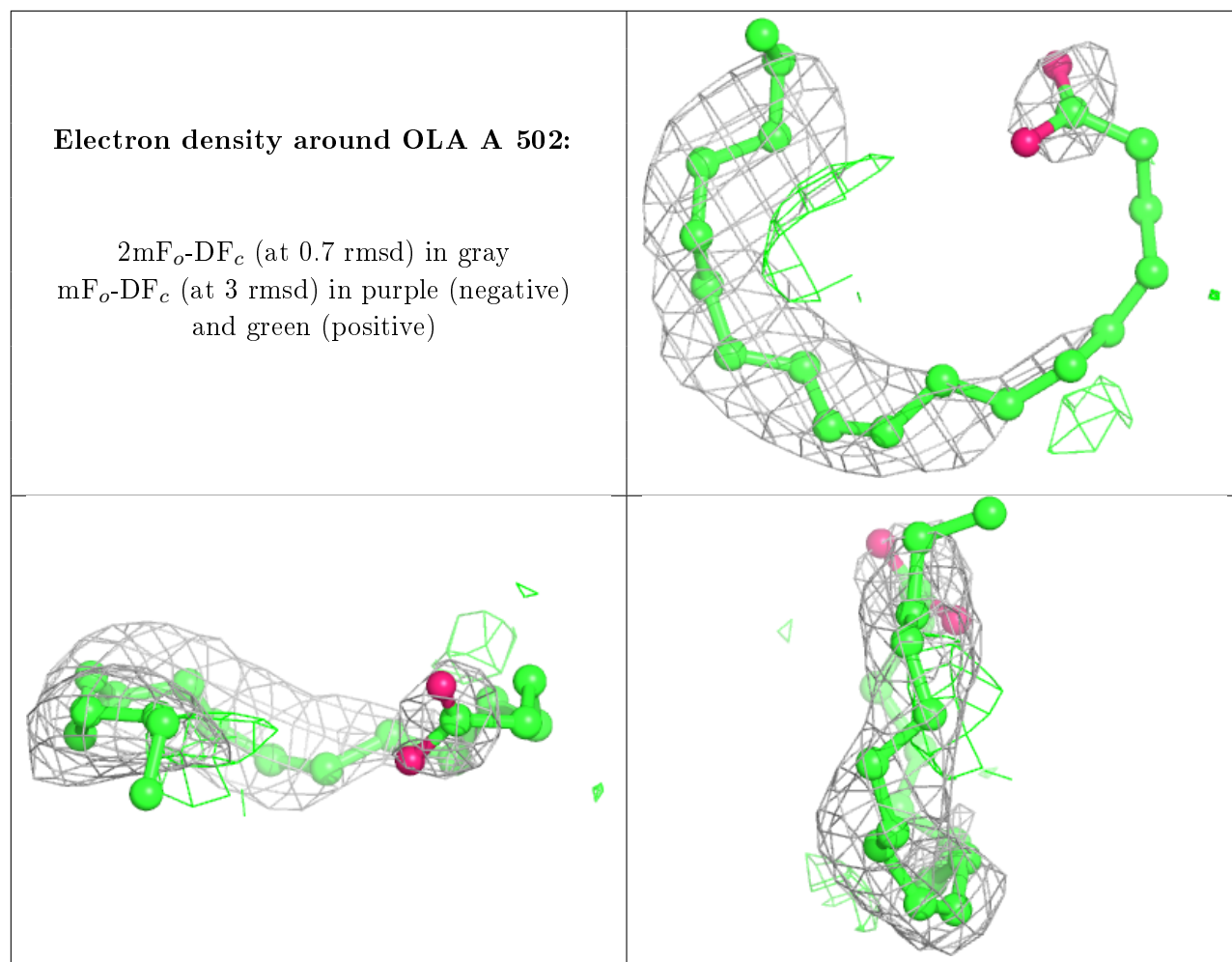
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLA B 504:

$2mF_o-DF_c$ (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.