



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:57 AM UTC

PDB ID : 6YXF / pdb_00006yxf
Title : Cryogenic human adiponectin receptor 2 (ADIPOR2) with Gd-DO3 ligand determined by Serial Crystallography (SSX) using CrystalDirect
Authors : Healey, R.D.; Basu, S.; Humm, A.S.; Leyrat, C.; Dupeux, F.; Pica, A.; Granier, S.; Marquez, J.A.
Deposited on : 2020-05-01
Resolution : 3.02 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

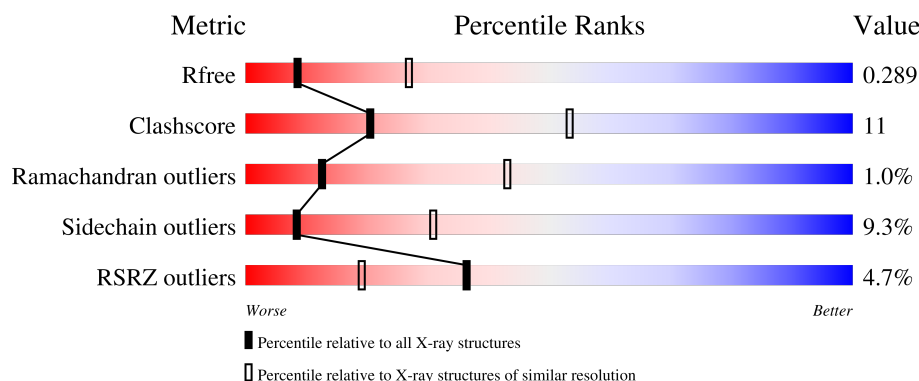
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	292	4% 63% 31% • •
2	H	228	5% 72% 25% •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4426 atoms, of which 87 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 Adiponectin receptor protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	2282	1533	371	361	17	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q86V24
A	-3	GLY	-	expression tag	UNP Q86V24
A	-2	SER	-	expression tag	UNP Q86V24
A	-1	GLU	-	expression tag	UNP Q86V24
A	0	PHE	-	expression tag	UNP Q86V24

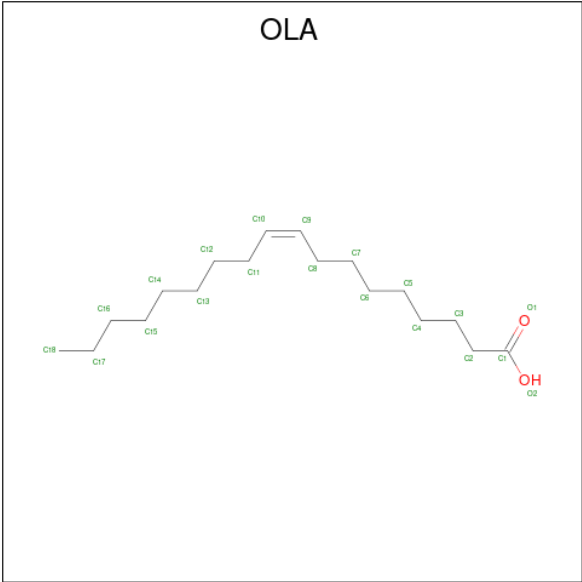
- Molecule 2 is a protein called V REGION HEAVY and LIGHT CHAINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	228	1755	1113	288	347	7	0	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

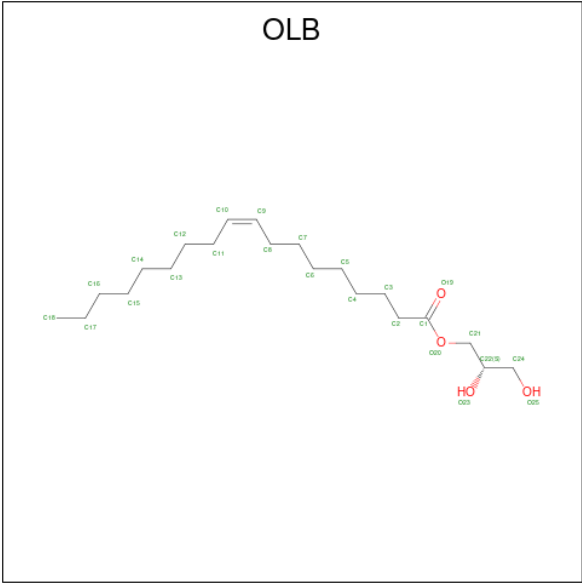
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLB) (formula: C₂₁H₄₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	11	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		

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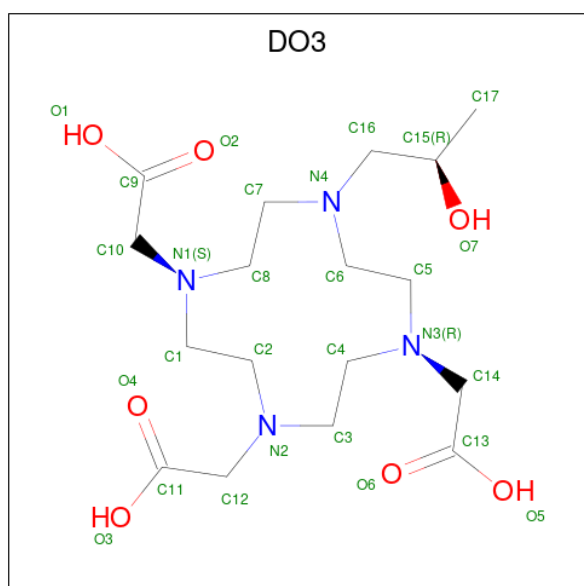
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 25	C 21	O 4	0	0
5	A	1	Total 25	C 21	O 4	0	0
5	A	1	Total 25	C 21	O 4	0	0
5	H	1	Total 25	C 21	O 4	0	0

- Molecule 6 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Gd 2 2	0	0
6	H	1	Total Gd 1 1	0	0

- Molecule 7 is 10-((2R)-2-HYDROXYPROPYL)-1,4,7,10-TETRAAZACYCLODODECAN E 1,4,7-TRIACETIC ACID (CCD ID: DO3) (formula: C₁₇H₃₂N₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	A	1	Total 57	C 17	H 29	N 4	O 7	0	0
7	A	1	Total 57	C 17	H 29	N 4	O 7	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	H	1	Total	C	H	N	O	0	0
			57	17	29	4	7		

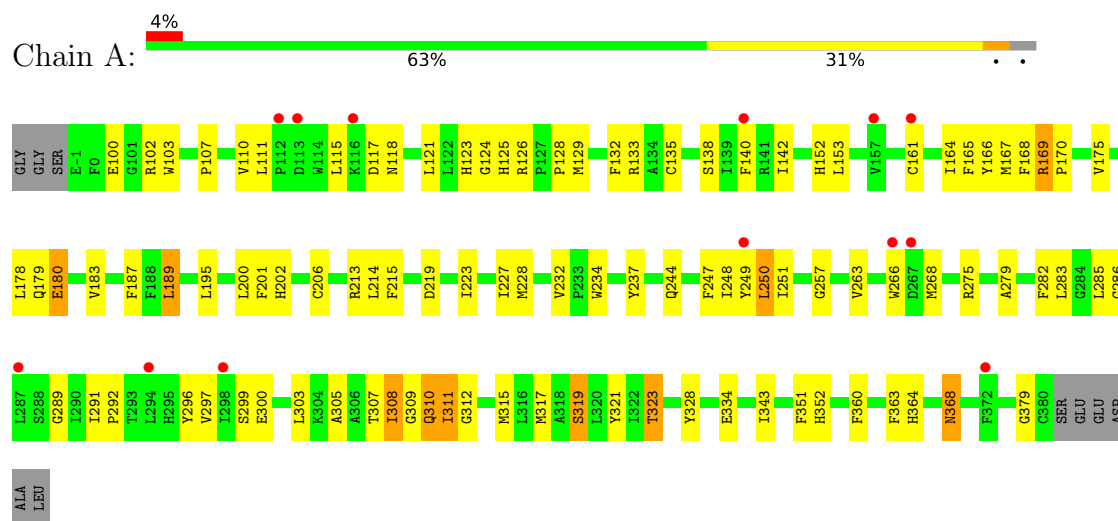
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	14	Total	O	0	0
			14	14		
8	H	30	Total	O	0	0
			30	30		

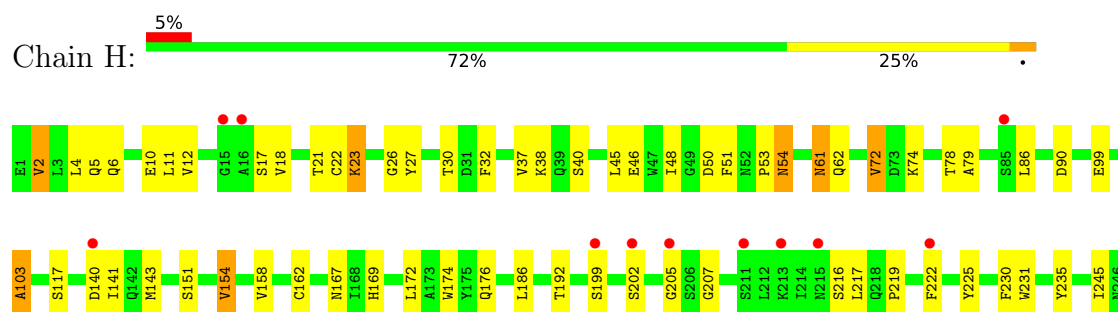
3 Residue-property plots [i](#)

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

• Molecule 1: Adiponectin receptor protein 2



• Molecule 2: V REGION HEAVY and LIGHT CHAINS



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	74.64Å 100.65Å 111.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 3.02 48.67 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.67-3.02) 98.7 (48.67-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3 (29-NOV-2019)	Depositor
R, R_{free}	0.214 , 0.259 0.229 , 0.289	Depositor DCC
R_{free} test set	956 reflections (5.59%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4426	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DO3, OLA, OLB, GD, ZN

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	0.94	0/2366	1.30	13/3216 (0.4%)
2	H	0.90	1/1799 (0.1%)	1.16	9/2441 (0.4%)
All	All	0.92	1/4165 (0.0%)	1.24	22/5657 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	46	GLU	CA-C	-5.46	1.45	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	PHE	CA-CB-CG	-8.34	105.46	113.80
2	H	50	ASP	CA-CB-CG	7.74	120.33	112.60
2	H	230	PHE	CA-CB-CG	6.68	120.48	113.80
1	A	164	ILE	N-CA-C	-6.57	104.45	110.82
1	A	179	GLN	CA-C-N	6.24	128.93	120.38
1	A	179	GLN	C-N-CA	6.24	128.93	120.38
2	H	205	GLY	N-CA-C	6.12	118.26	112.08
2	H	90	ASP	CA-CB-CG	-6.10	106.50	112.60
2	H	74	LYS	CA-C-N	5.82	129.15	120.31
2	H	74	LYS	C-N-CA	5.82	129.15	120.31
2	H	2	VAL	N-CA-CB	5.81	117.17	110.49
1	A	140	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	379	GLY	N-CA-C	5.62	119.39	112.14
2	H	192	THR	N-CA-C	5.52	117.10	109.15
2	H	61	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	307	THR	N-CA-C	-5.50	104.97	110.97
1	A	153	LEU	N-CA-C	-5.40	104.81	111.40
1	A	178	LEU	CA-C-N	5.36	128.24	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	LEU	C-N-CA	5.36	128.24	120.79
1	A	175	VAL	N-CA-C	-5.26	105.58	110.53
1	A	219	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	368	ASN	N-CA-C	-5.09	106.75	113.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2282	0	2260	62	0
2	H	1755	0	1673	27	0
3	A	1	0	0	0	0
4	A	20	0	33	5	0
5	A	125	0	200	12	0
5	H	25	0	40	2	0
6	A	2	0	0	0	0
6	H	1	0	0	0	0
7	A	56	58	55	5	0
7	H	28	29	28	6	0
8	A	14	0	0	2	0
8	H	30	0	0	0	0
All	All	4339	87	4289	96	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 11.

All (96) 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:170:PRO:HA	5:A:404:OLB:H24	1.52	0.91
7:H:303:DO3:HC31	7:H:303:DO3:O3	1.76	0.83
1:A:118:ASN:HD22	1:A:121:LEU:HG	1.48	0.78
1:A:223:ILE:HD11	4:A:402:OLA:H21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:GLN:HB2	2:H:186:LEU:HD11	1.68	0.75
7:A:410:DO3:O3	7:A:410:DO3:H101	1.87	0.74
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.71	0.71
5:A:404:OLB:H31	5:A:407:OLB:H36	1.72	0.70
1:A:126:ARG:NH1	1:A:138:SER:OG	2.26	0.69
7:H:303:DO3:HC61	7:H:303:DO3:O2	1.96	0.66
1:A:227:ILE:HD12	1:A:285:LEU:HD23	1.77	0.66
1:A:102:ARG:NH1	2:H:235:TYR:OH	2.28	0.65
2:H:30:THR:HA	2:H:53:PRO:HB2	1.79	0.65
7:A:410:DO3:HC51	8:A:504:HOH:O	1.96	0.64
1:A:202:HIS:CD2	1:A:352:HIS:HE1	2.16	0.64
1:A:319:SER:O	1:A:323:THR:HG23	2.00	0.62
5:A:404:OLB:H3A	5:A:407:OLB:C9	2.32	0.60
1:A:282:PHE:HB2	4:A:402:OLA:H9	1.84	0.59
1:A:142:ILE:HG23	1:A:343:ILE:HG21	1.86	0.58
2:H:154:VAL:HG13	2:H:245:ILE:HG21	1.86	0.58
1:A:202:HIS:CD2	1:A:352:HIS:CE1	2.91	0.58
1:A:132:PHE:HB2	5:H:301:OLB:H2A	1.86	0.57
1:A:289:GLY:HA3	5:A:403:OLB:H241	1.85	0.57
2:H:143:MET:HE3	2:H:162:CYS:SG	2.45	0.57
1:A:124:GLY:HA2	8:A:504:HOH:O	2.06	0.56
7:H:303:DO3:HC72	7:H:303:DO3:C9	2.35	0.56
1:A:232:VAL:HG22	1:A:250:LEU:HD21	1.86	0.56
2:H:23:LYS:HA	2:H:78:THR:HG22	1.88	0.56
1:A:118:ASN:HD21	1:A:334:GLU:HG3	1.70	0.55
1:A:247:PHE:CZ	1:A:251:ILE:HD11	2.42	0.55
7:H:303:DO3:HC42	7:H:303:DO3:N4	2.22	0.55
2:H:18:VAL:HG22	2:H:86:LEU:HD11	1.89	0.55
1:A:165:PHE:HB3	5:A:405:OLB:H20	1.90	0.54
1:A:223:ILE:CD1	4:A:402:OLA:H21	2.38	0.53
1:A:234:TRP:NE1	1:A:310:GLN:OE1	2.36	0.53
1:A:315:MET:HG2	5:A:403:OLB:H5	1.91	0.53
1:A:161:CYS:HB3	5:A:405:OLB:O19	2.10	0.52
1:A:296:TYR:CE1	1:A:300:GLU:HG3	2.45	0.52
1:A:291:ILE:HB	1:A:292:PRO:CD	2.39	0.52
1:A:132:PHE:HA	1:A:135:CYS:HB2	1.91	0.51
1:A:291:ILE:HB	1:A:292:PRO:HD3	1.92	0.51
2:H:99:GLU:HG2	2:H:103:ALA:HA	1.92	0.51
1:A:166:TYR:CE2	1:A:169:ARG:NH1	2.78	0.51
2:H:51:PHE:CE2	2:H:72:VAL:HB	2.45	0.51
1:A:170:PRO:HA	5:A:404:OLB:C24	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PHE:CB	4:A:402:OLA:H9	2.41	0.50
2:H:154:VAL:HG11	2:H:219:PRO:HG3	1.94	0.49
1:A:152:HIS:CD2	1:A:195:LEU:HD22	2.47	0.49
2:H:54:ASN:ND2	7:H:303:DO3:HC61	2.28	0.49
1:A:180:GLU:HG2	1:A:237:TYR:OH	2.13	0.48
1:A:166:TYR:CZ	1:A:169:ARG:NH1	2.82	0.48
1:A:286:GLY:HA3	1:A:321:TYR:CE1	2.49	0.48
2:H:6:GLN:HA	2:H:21:THR:O	2.13	0.48
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.95	0.48
1:A:312:GLY:HA2	1:A:315:MET:HE2	1.96	0.48
1:A:103:TRP:CD1	1:A:129:MET:SD	3.06	0.47
2:H:2:VAL:HG22	2:H:27:TYR:HB3	1.96	0.47
1:A:249:TYR:CD2	1:A:292:PRO:HB3	2.48	0.47
1:A:107:PRO:HA	1:A:123:HIS:HA	1.97	0.47
7:A:410:DO3:C13	7:A:410:DO3:H171	2.44	0.47
2:H:32:PHE:HB3	2:H:99:GLU:O	2.15	0.47
1:A:202:HIS:HD2	1:A:352:HIS:HE1	1.61	0.47
2:H:176:GLN:HG3	2:H:225:TYR:CZ	2.50	0.46
1:A:351:PHE:CE1	4:A:402:OLA:H72	2.49	0.46
2:H:37:VAL:HG11	2:H:45:LEU:HD23	1.96	0.46
1:A:201:PHE:HB2	1:A:215:PHE:HB3	1.98	0.46
1:A:100:GLU:CD	2:H:231:TRP:HE1	2.23	0.46
2:H:222:PHE:HB3	2:H:245:ILE:HG12	1.98	0.46
1:A:115:LEU:HD21	1:A:206:CYS:HA	1.99	0.45
1:A:286:GLY:HA3	1:A:321:TYR:CZ	2.51	0.45
1:A:311:ILE:O	1:A:315:MET:HG3	2.17	0.45
2:H:172:LEU:HD21	2:H:174:TRP:NE1	2.32	0.45
1:A:213:ARG:HH12	7:A:411:DO3:HC12	1.82	0.45
1:A:247:PHE:CE2	1:A:251:ILE:HD11	2.53	0.44
1:A:266:TRP:CE2	1:A:268:MET:HB2	2.53	0.44
1:A:364:HIS:CE1	1:A:368:ASN:HD21	2.36	0.44
1:A:128:PRO:HA	1:A:206:CYS:O	2.18	0.44
2:H:172:LEU:CD2	2:H:174:TRP:NE1	2.81	0.43
1:A:308:ILE:HG13	1:A:308:ILE:O	2.17	0.43
1:A:213:ARG:HH22	7:A:411:DO3:HC81	1.85	0.42
2:H:176:GLN:HG3	2:H:225:TYR:CE2	2.54	0.42
1:A:183:VAL:HG12	5:A:406:OLB:H19	2.01	0.42
1:A:279:ALA:O	1:A:283:LEU:HB2	2.20	0.42
2:H:158:VAL:HG13	2:H:217:LEU:HD11	2.01	0.42
1:A:189:LEU:HD23	5:A:406:OLB:H38	2.02	0.41
2:H:54:ASN:OD1	7:H:303:DO3:O7	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:MET:SD	1:A:257:GLY:HA3	2.60	0.41
2:H:22:CYS:HB3	2:H:79:ALA:HB3	2.02	0.41
1:A:275:ARG:HG3	1:A:328:TYR:CE1	2.55	0.41
1:A:248:ILE:HA	1:A:251:ILE:HD12	2.02	0.41
1:A:187:PHE:CE2	1:A:363:PHE:HB2	2.56	0.41
1:A:111:LEU:HD11	1:A:125:HIS:CG	2.56	0.41
1:A:165:PHE:HD2	5:A:405:OLB:H23	1.86	0.41
1:A:305:ALA:O	1:A:308:ILE:O	2.39	0.40
2:H:167:ASN:HD21	5:H:301:OLB:H22	1.84	0.40
1:A:168:PHE:HB2	5:A:405:OLB:H32	2.04	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	281/292 (96%)	260 (92%)	20 (7%)	1 (0%)	30	63
2	H	224/228 (98%)	207 (92%)	13 (6%)	4 (2%)	6	29
All	All	505/520 (97%)	467 (92%)	33 (6%)	5 (1%)	12	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
2	H	207	GLY
2	H	54	ASN
2	H	103	ALA
2	H	216	SER

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	240/246 (98%)	219 (91%)	21 (9%)	9	33
2	H	189/189 (100%)	170 (90%)	19 (10%)	7	27
All	All	429/435 (99%)	389 (91%)	40 (9%)	8	31

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	VAL
1	A	117	ASP
1	A	133	ARG
1	A	167	MET
1	A	169	ARG
1	A	180	GLU
1	A	189	LEU
1	A	200	LEU
1	A	214	LEU
1	A	244	GLN
1	A	250	LEU
1	A	263	VAL
1	A	297	VAL
1	A	299	SER
1	A	303	LEU
1	A	308	ILE
1	A	310	GLN
1	A	311	ILE
1	A	317	MET
1	A	319	SER
1	A	323	THR
2	H	4	LEU
2	H	5	GLN
2	H	10	GLU
2	H	11	LEU
2	H	12	VAL
2	H	17	SER

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Mol	Chain	Res	Type
2	H	23	LYS
2	H	40	SER
2	H	61	ASN
2	H	62	GLN
2	H	72	VAL
2	H	117	SER
2	H	140	ASP
2	H	141	ILE
2	H	151	SER
2	H	154	VAL
2	H	169	HIS
2	H	199	SER
2	H	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	364	HIS
2	H	246	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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
7	DO3	H	303	6	28,28,28	0.48	0	36,36,36	1.29	5 (13%)
5	OLB	A	404	-	24,24,24	0.26	0	25,25,25	0.47	0
5	OLB	A	406	-	24,24,24	0.30	0	25,25,25	0.21	0
4	OLA	A	402	-	19,19,19	0.37	0	19,19,19	0.39	0
7	DO3	A	410	6	28,28,28	0.44	0	36,36,36	1.15	4 (11%)
5	OLB	A	403	-	24,24,24	0.22	0	25,25,25	0.25	0
5	OLB	A	405	-	24,24,24	0.33	0	25,25,25	0.31	0
7	DO3	A	411	6	28,28,28	0.38	0	36,36,36	1.22	5 (13%)
5	OLB	A	407	-	24,24,24	0.27	0	25,25,25	0.31	0
5	OLB	H	301	-	24,24,24	0.26	0	25,25,25	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DO3	H	303	6	-	18/36/36/36	1/1/1/1
5	OLB	A	404	-	-	11/24/24/24	-
5	OLB	A	406	-	-	3/24/24/24	-
4	OLA	A	402	-	-	4/17/17/17	-
7	DO3	A	410	6	-	13/36/36/36	1/1/1/1
5	OLB	A	403	-	-	5/24/24/24	-
5	OLB	A	405	-	-	8/24/24/24	-
7	DO3	A	411	6	-	19/36/36/36	1/1/1/1
5	OLB	A	407	-	-	4/24/24/24	-
5	OLB	H	301	-	-	6/24/24/24	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	303	DO3	C11-C12-N2	3.35	124.37	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	411	DO3	C12-N2-C3	3.19	119.61	111.91
7	A	410	DO3	C7-N4-C16	2.77	118.36	111.89
7	H	303	DO3	C3-N2-C2	2.76	118.00	111.44
7	H	303	DO3	C1-C2-N2	2.37	118.59	112.98
7	A	410	DO3	C13-C14-N3	2.36	121.24	113.77
7	A	411	DO3	C4-C3-N2	2.35	118.55	112.98
7	A	410	DO3	C6-N4-C16	2.26	117.18	111.89
7	A	410	DO3	C7-C8-N1	2.26	118.35	112.98
7	H	303	DO3	C2-C1-N1	2.25	118.32	112.98
7	A	411	DO3	C8-C7-N4	2.21	118.22	112.98
7	A	411	DO3	C11-C12-N2	2.18	120.68	113.77
7	H	303	DO3	C13-C14-N3	2.09	120.40	113.77
7	A	411	DO3	C7-C8-N1	2.01	117.75	112.98

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	OLB	O20-C21-C22-C24
5	A	404	OLB	C21-C22-C24-O25
5	A	406	OLB	O20-C21-C22-C24
5	H	301	OLB	O20-C21-C22-O23
7	A	410	DO3	C9-C10-N1-C1
7	A	410	DO3	N1-C10-C9-O1
7	A	411	DO3	N1-C10-C9-O1
7	A	411	DO3	N1-C10-C9-O2
7	H	303	DO3	C11-C12-N2-C3
7	H	303	DO3	C13-C14-N3-C5
7	H	303	DO3	N1-C10-C9-O1
7	H	303	DO3	O5-C13-C14-N3
7	H	303	DO3	C17-C15-C16-N4
7	A	411	DO3	C1-C2-N2-C12
7	A	411	DO3	C4-C3-N2-C12
7	A	410	DO3	C5-C6-N4-C16
5	A	404	OLB	O20-C21-C22-O23
5	A	406	OLB	O20-C21-C22-O23
7	A	410	DO3	N1-C10-C9-O2
7	A	410	DO3	O3-C11-C12-N2
7	A	410	DO3	O4-C11-C12-N2
7	A	411	DO3	O3-C11-C12-N2
7	A	411	DO3	O4-C11-C12-N2
7	A	411	DO3	O5-C13-C14-N3

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Mol	Chain	Res	Type	Atoms
7	A	411	DO3	O6-C13-C14-N3
7	H	303	DO3	N1-C10-C9-O2
7	H	303	DO3	O6-C13-C14-N3
5	H	301	OLB	O20-C21-C22-C24
5	A	403	OLB	C12-C13-C14-C15
4	A	402	OLA	C1-C2-C3-C4
7	A	411	DO3	N2-C3-C4-N3
5	A	405	OLB	C21-C22-C24-O25
5	A	405	OLB	C1-C2-C3-C4
7	A	411	DO3	N4-C7-C8-N1
7	H	303	DO3	N2-C3-C4-N3
5	A	403	OLB	C14-C15-C16-C17
5	A	405	OLB	C4-C5-C6-C7
5	H	301	OLB	C2-C3-C4-C5
5	A	404	OLB	C11-C12-C13-C14
5	A	405	OLB	O23-C22-C24-O25
7	A	410	DO3	N1-C1-C2-N2
7	A	411	DO3	C15-C16-N4-C6
7	H	303	DO3	C15-C16-N4-C6
7	A	410	DO3	C8-C7-N4-C16
5	A	403	OLB	C1-C2-C3-C4
5	A	404	OLB	C15-C16-C17-C18
5	A	404	OLB	C2-C3-C4-C5
5	A	403	OLB	C11-C12-C13-C14
5	H	301	OLB	C5-C6-C7-C8
5	A	404	OLB	C13-C14-C15-C16
7	A	410	DO3	C13-C14-N3-C5
7	A	410	DO3	C1-C2-N2-C12
7	A	411	DO3	C4-C3-N2-C2
7	A	411	DO3	C6-C5-N3-C4
7	A	410	DO3	C1-C2-N2-C3
7	H	303	DO3	C2-C1-N1-C8
7	H	303	DO3	O7-C15-C16-N4
5	A	407	OLB	C1-C2-C3-C4
5	A	404	OLB	O23-C22-C24-O25
7	H	303	DO3	C4-C3-N2-C12
7	A	411	DO3	C6-C5-N3-C14
5	A	403	OLB	C2-C3-C4-C5
7	H	303	DO3	C11-C12-N2-C2
7	A	411	DO3	C1-C2-N2-C3
7	A	411	DO3	C3-C4-N3-C5
7	A	410	DO3	C9-C10-N1-C8

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Mol	Chain	Res	Type	Atoms
7	H	303	DO3	C1-C2-N2-C3
5	A	405	OLB	C7-C8-C9-C10
4	A	402	OLA	C11-C12-C13-C14
7	A	410	DO3	C13-C14-N3-C4
5	A	405	OLB	C11-C12-C13-C14
7	H	303	DO3	C4-C3-N2-C2
5	A	404	OLB	C9-C10-C11-C12
7	A	411	DO3	C2-C1-N1-C8
5	A	407	OLB	C10-C11-C12-C13
5	A	404	OLB	C14-C15-C16-C17
4	A	402	OLA	O1-C1-C2-C3
7	H	303	DO3	C5-C6-N4-C7
4	A	402	OLA	O2-C1-C2-C3
5	A	406	OLB	C7-C8-C9-C10
5	A	405	OLB	C2-C3-C4-C5
5	H	301	OLB	C7-C8-C9-C10
5	A	407	OLB	C4-C5-C6-C7
7	A	411	DO3	N3-C5-C6-N4
7	A	411	DO3	C3-C4-N3-C14
5	A	407	OLB	C7-C8-C9-C10
5	H	301	OLB	C14-C15-C16-C17
7	H	303	DO3	C2-C1-N1-C10
5	A	404	OLB	C7-C8-C9-C10
5	A	405	OLB	C10-C11-C12-C13
7	H	303	DO3	C3-C4-N3-C14

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	411	DO3	C1-C2-C3-C4-C5-C6-C7-C8-N1-N2-N3-N4
7	H	303	DO3	C1-C2-C3-C4-C5-C6-C7-C8-N1-N2-N3-N4
7	A	410	DO3	C1-C2-C3-C4-C5-C6-C7-C8-N1-N2-N3-N4

10 monomers are involved in 30 short contacts:

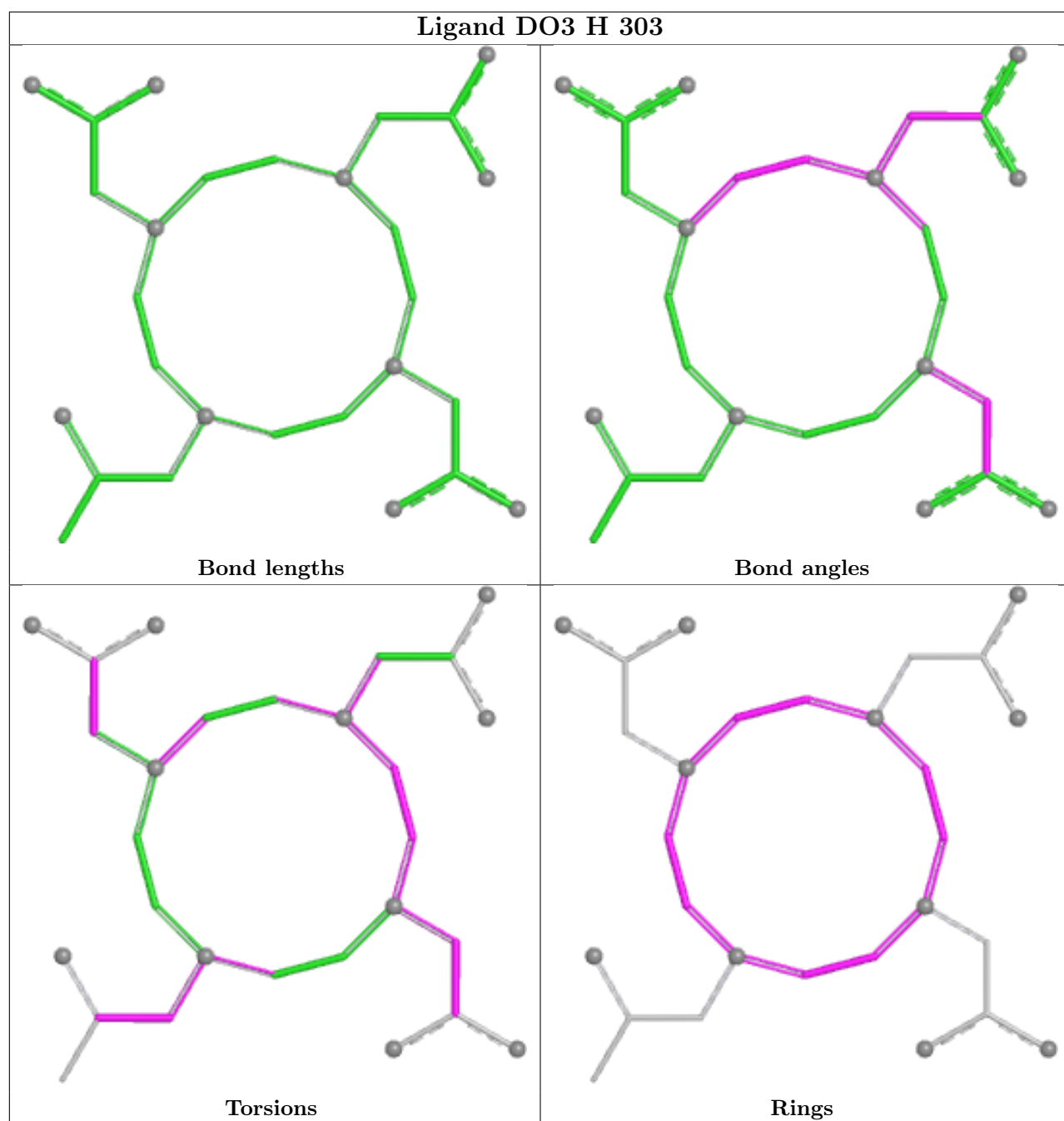
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	303	DO3	6	0
5	A	404	OLB	4	0
5	A	406	OLB	2	0
4	A	402	OLA	5	0
7	A	410	DO3	3	0
5	A	403	OLB	2	0

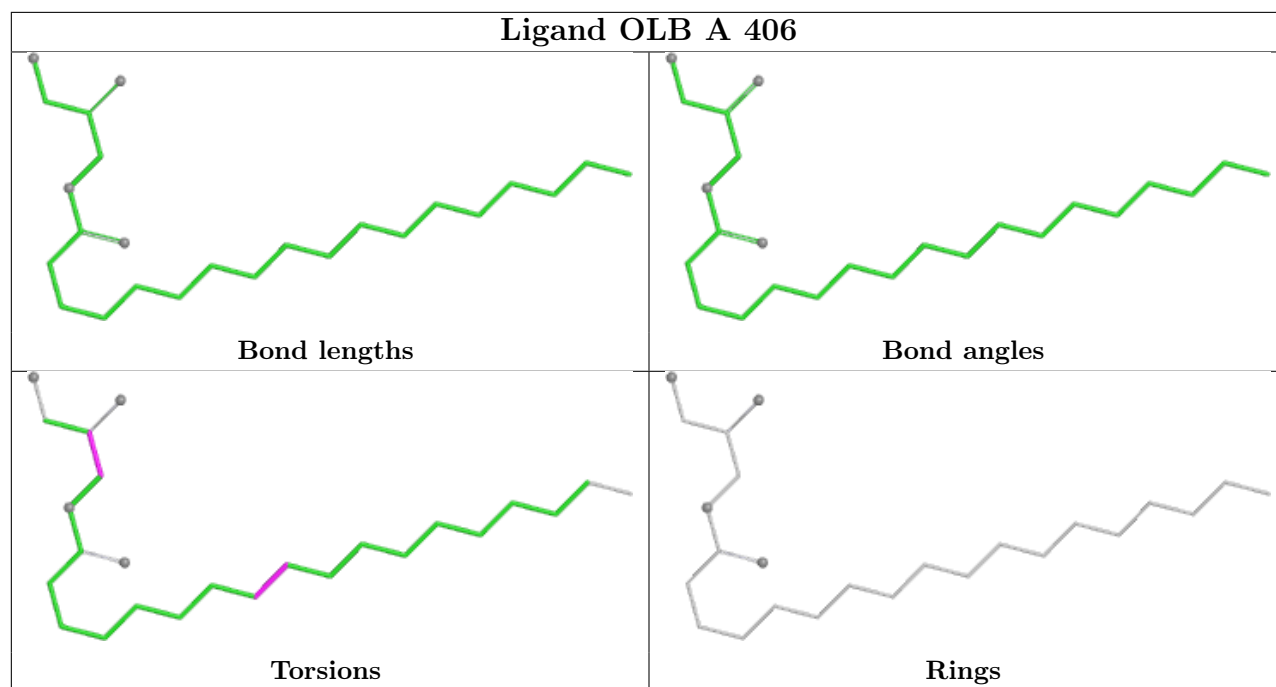
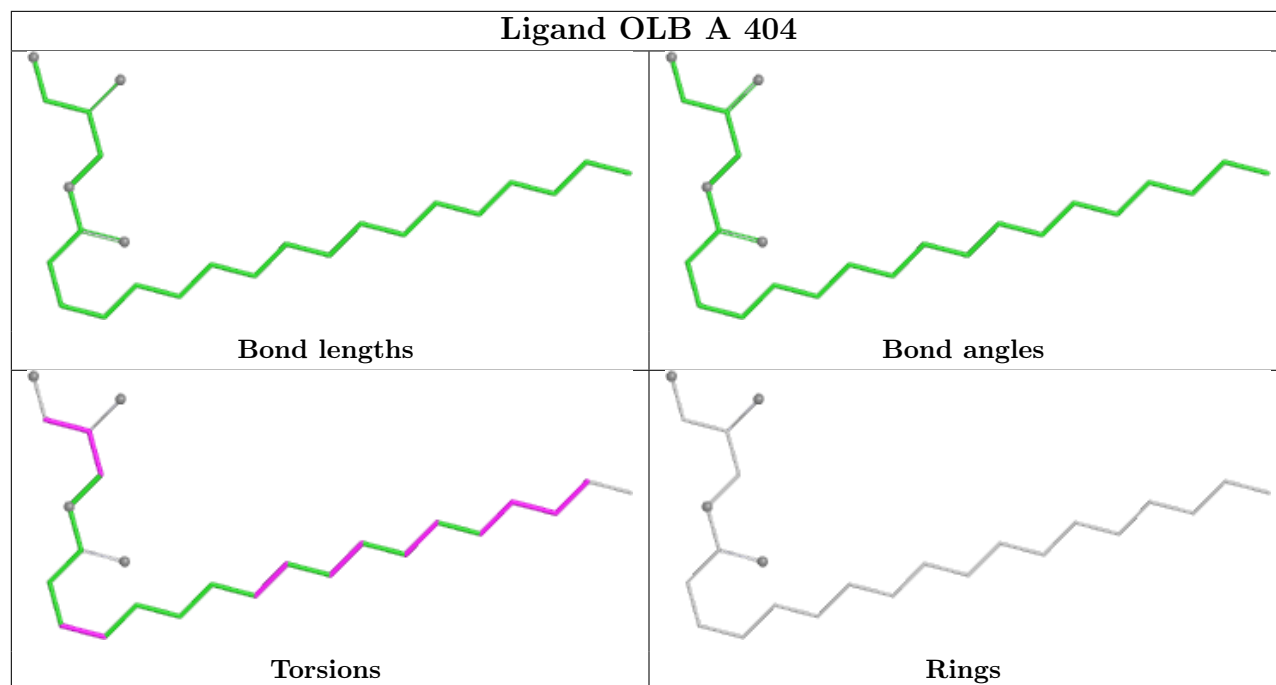
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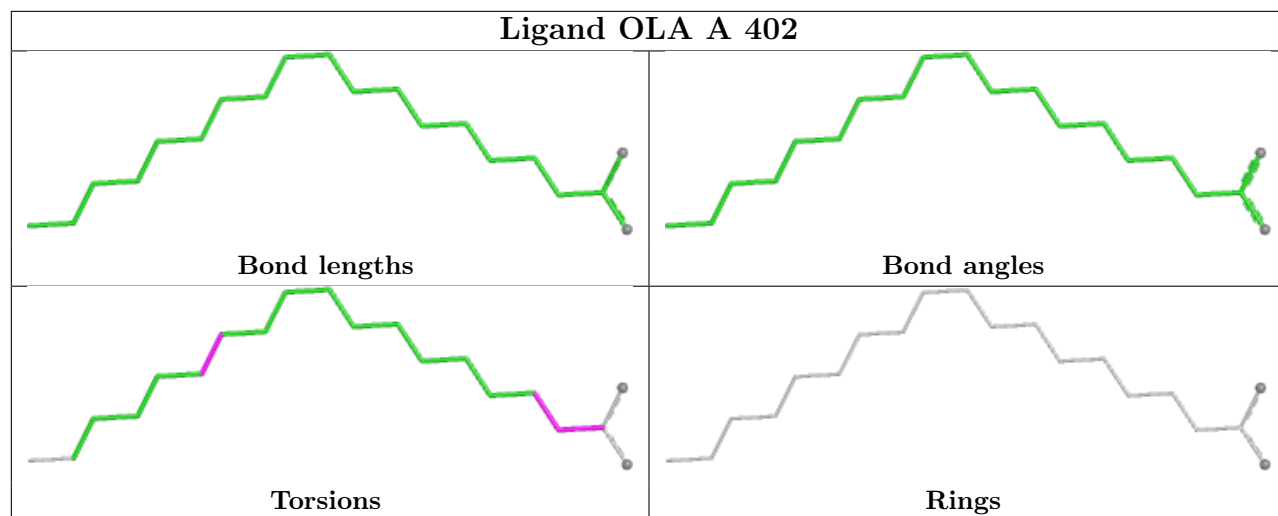
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	OLB	4	0
7	A	411	DO3	2	0
5	A	407	OLB	2	0
5	H	301	OLB	2	0

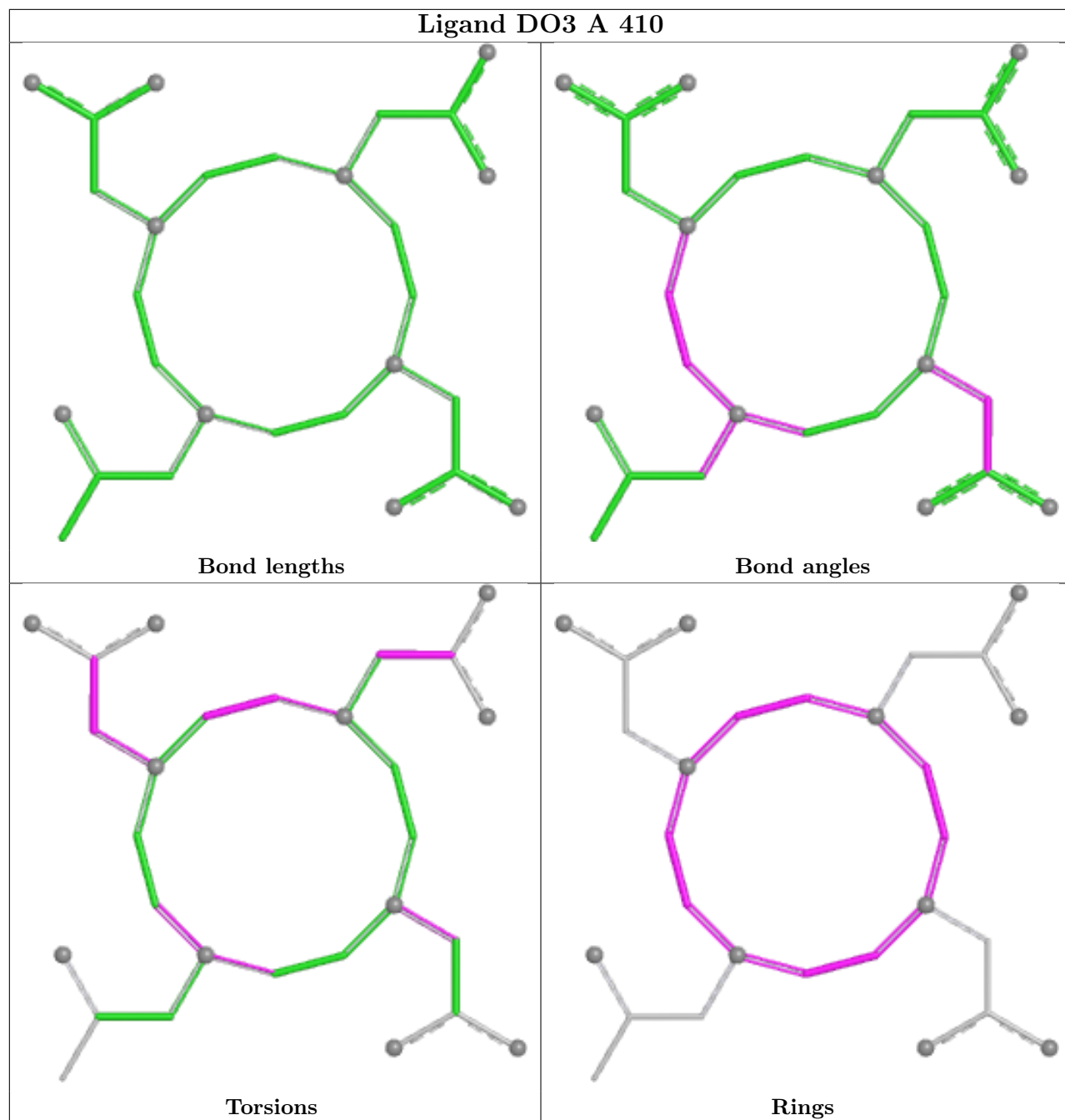
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

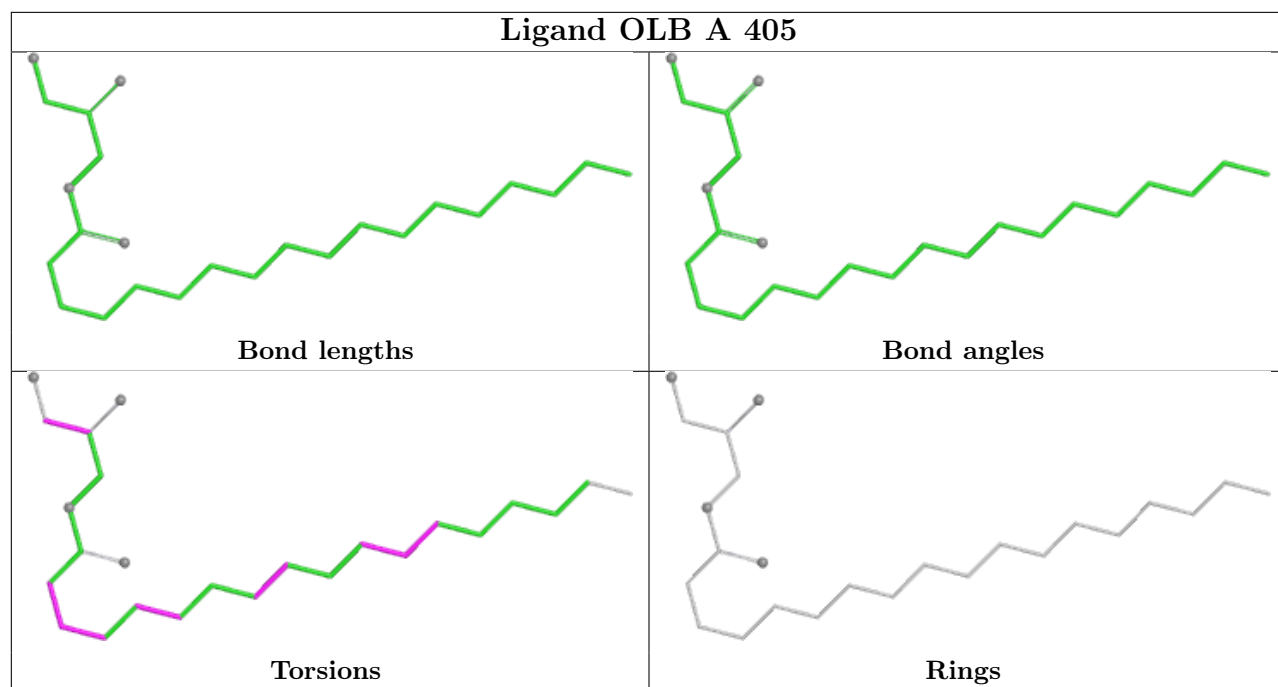
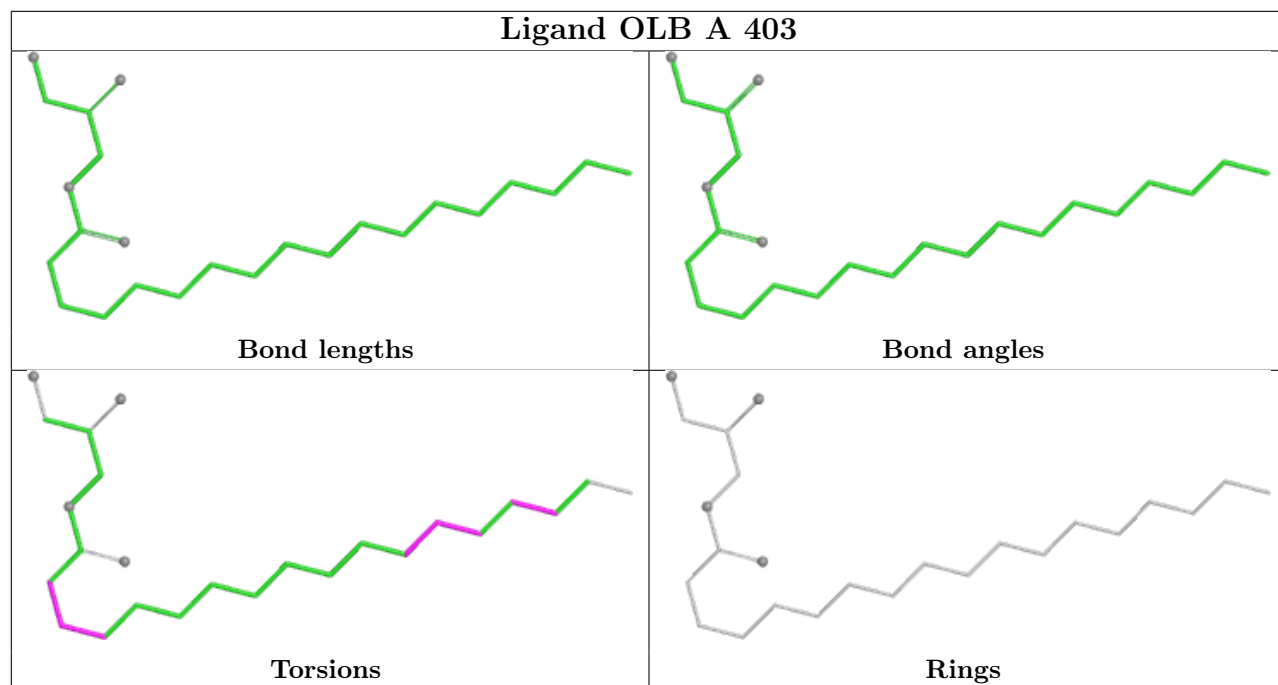




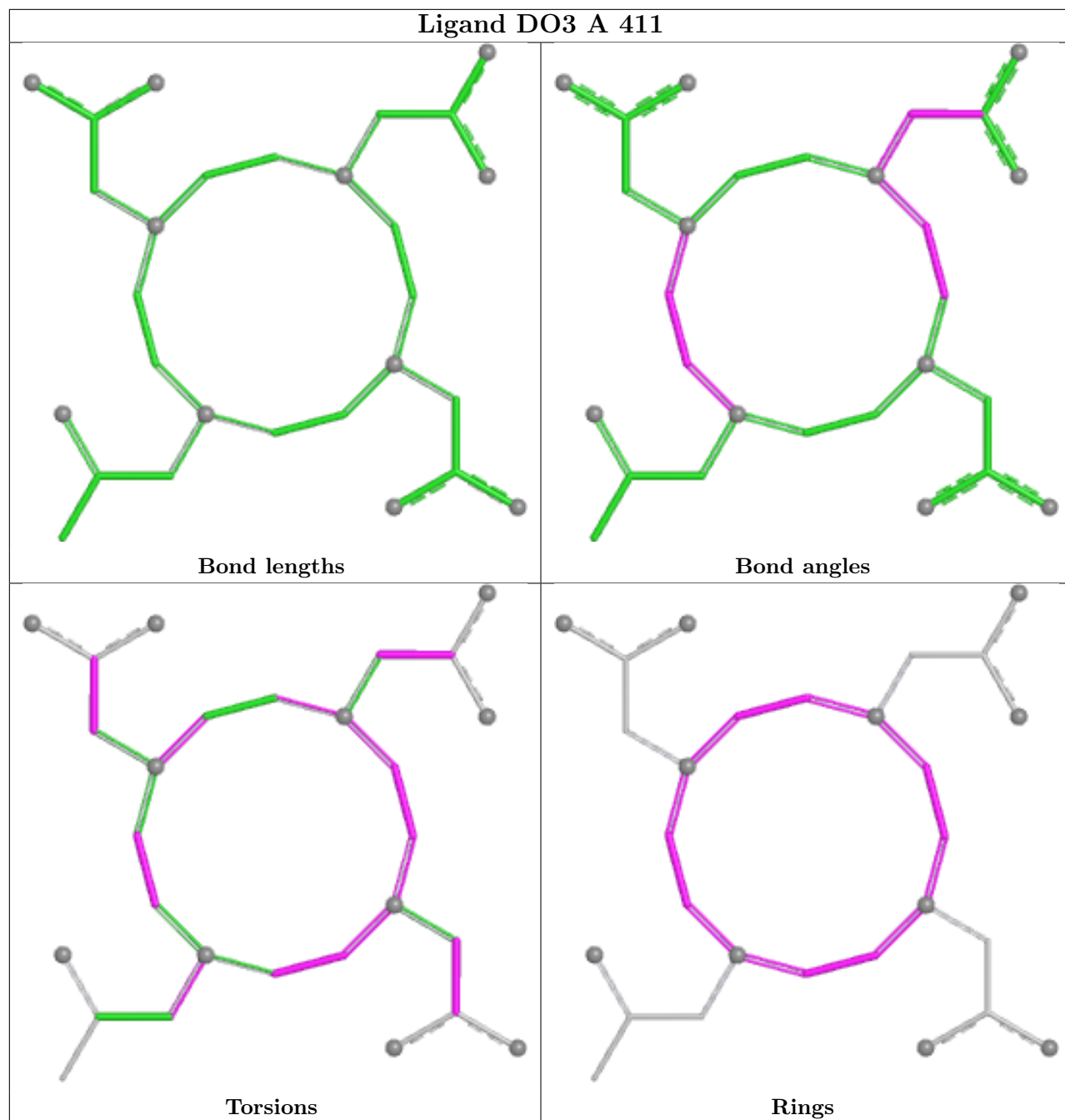


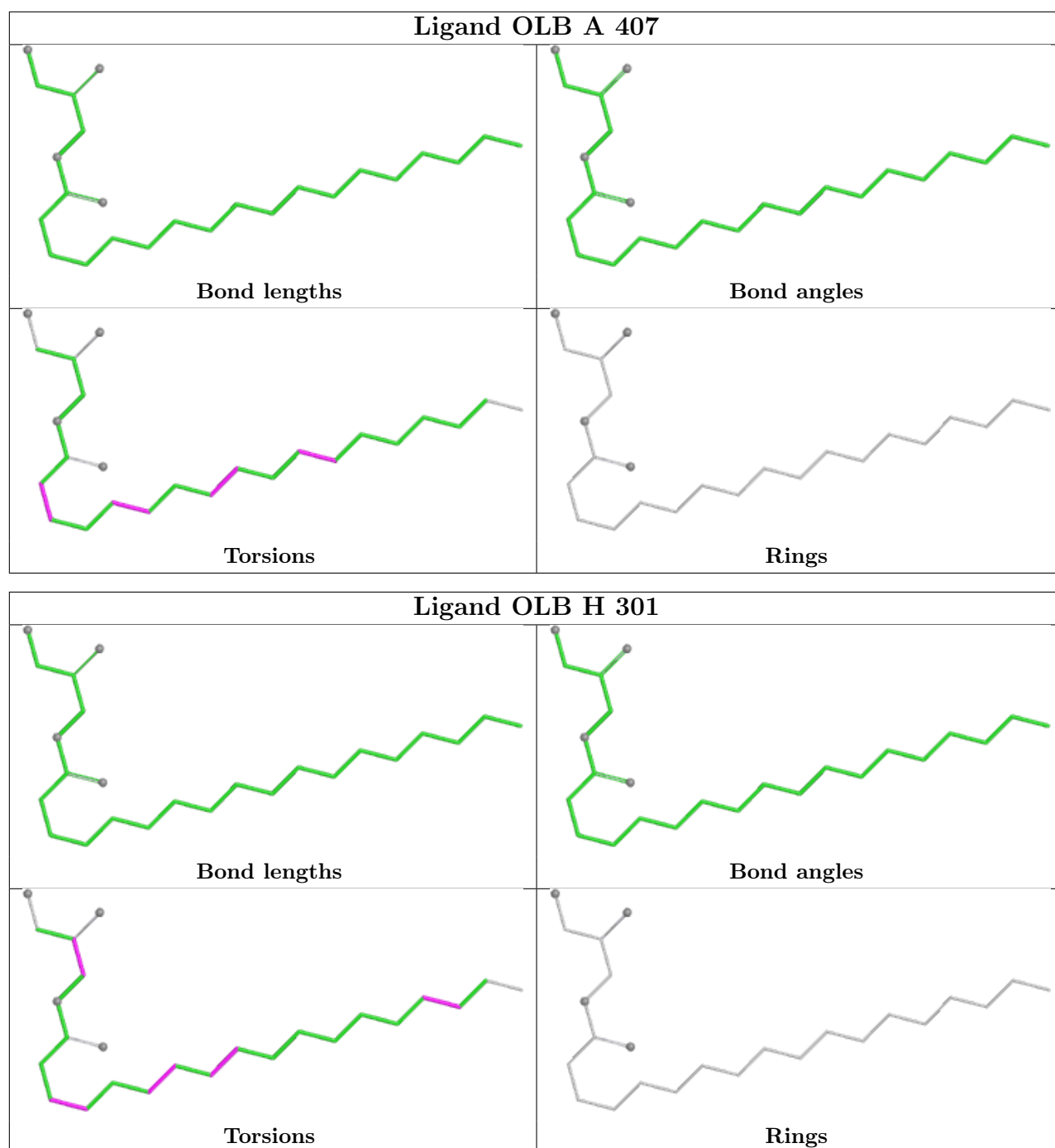
Ligand DO3 A 410





Ligand DO3 A 411





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	121:GLY	C	140:ASP	N	39.03

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	283/292 (96%)	0.38	13 (4%)	37	20	58, 77, 104, 119	1 (0%)
2	H	228/228 (100%)	0.25	11 (4%)	35	18	59, 78, 92, 99	0
All	All	511/520 (98%)	0.32	24 (4%)	36	19	58, 77, 99, 119	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	PRO	7.3
2	H	15	GLY	5.3
1	A	294	LEU	5.3
2	H	199	SER	5.1
1	A	113	ASP	4.9
1	A	140	PHE	4.2
2	H	202	SER	4.2
2	H	222	PHE	4.0
1	A	298	ILE	3.5
2	H	211	SER	3.1
2	H	205	GLY	3.0
1	A	116	LYS	2.9
2	H	85	SER	2.7
1	A	267	ASP	2.6
1	A	372	PHE	2.5
2	H	215	ASN	2.5
1	A	287	LEU	2.2
2	H	140	ASP	2.2
1	A	249	TYR	2.1
1	A	266	TRP	2.1
2	H	16	ALA	2.1
2	H	213	LYS	2.1
1	A	157	VAL	2.0
1	A	161	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

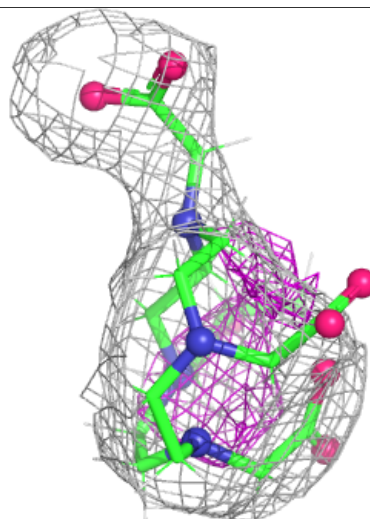
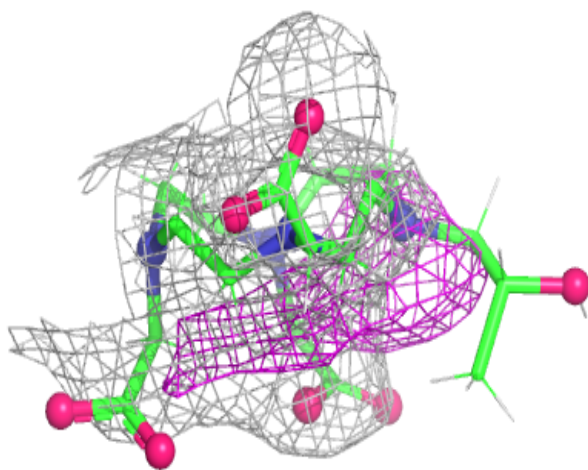
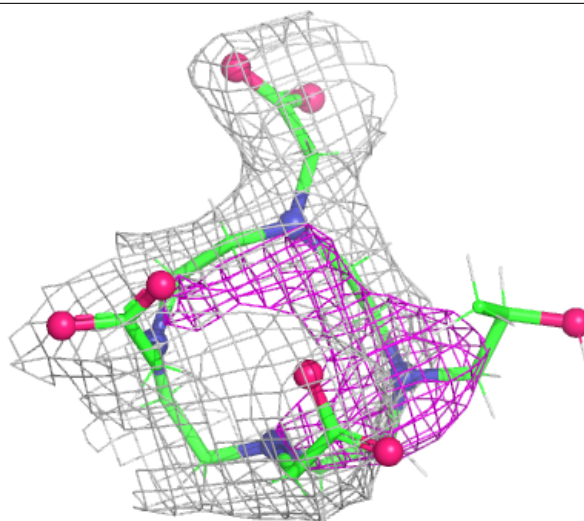
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	DO3	A	411	28/28	0.24	0.15	106,111,133,134	0
7	DO3	H	303	28/28	0.24	0.18	110,120,144,144	0
7	DO3	A	410	28/28	0.47	0.15	109,124,149,149	0
5	OLB	A	405	25/25	0.56	0.34	88,99,105,105	0
5	OLB	A	406	25/25	0.84	0.22	100,106,113,113	0
5	OLB	A	404	25/25	0.85	0.21	82,90,96,96	0
5	OLB	A	403	25/25	0.85	0.33	83,90,93,96	11
5	OLB	H	301	25/25	0.86	0.23	79,84,91,91	0
6	GD	H	302	1/1	0.89	0.17	190,190,190,190	0
5	OLB	A	407	25/25	0.90	0.19	92,99,104,104	0
6	GD	A	409	1/1	0.90	0.21	300,300,300,300	0
4	OLA	A	402	20/20	0.91	0.14	64,66,70,70	0
6	GD	A	408	1/1	0.95	0.07	278,278,278,278	0
3	ZN	A	401	1/1	0.98	0.10	62,62,62,62	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.

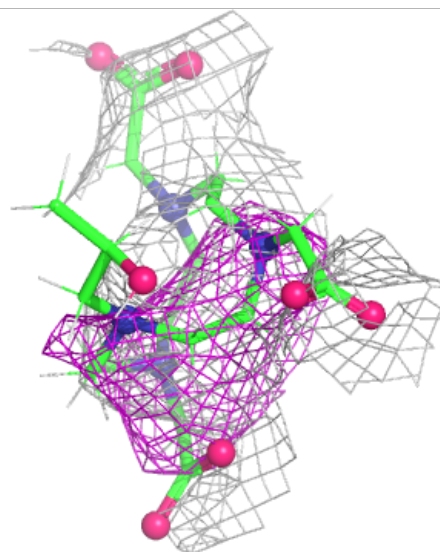
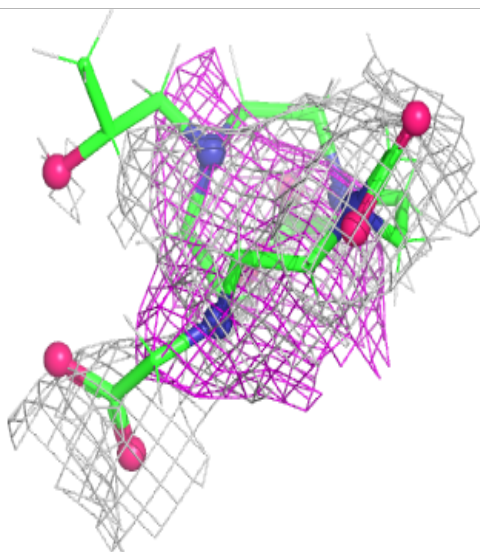
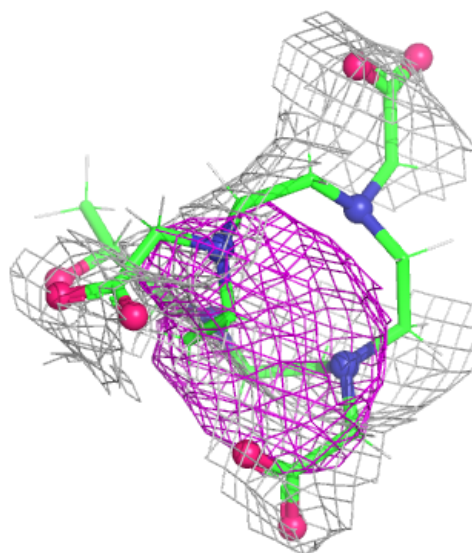
Electron density around DO3 A 411:

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



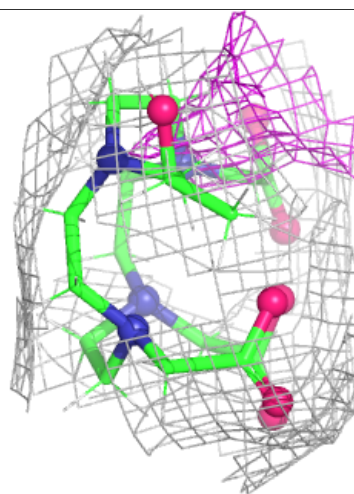
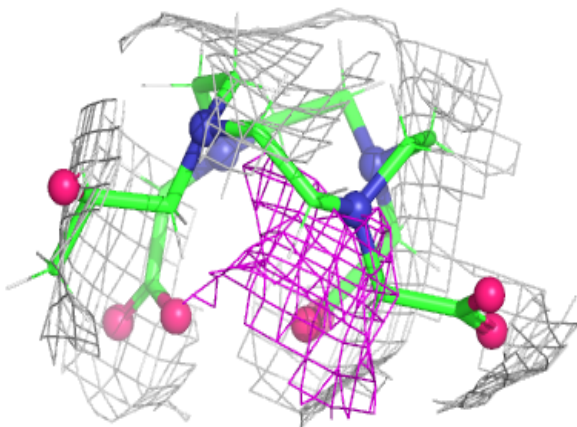
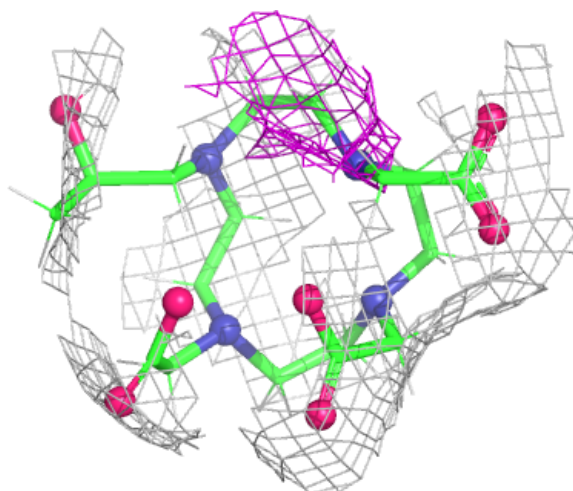
Electron density around DO3 H 303:

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



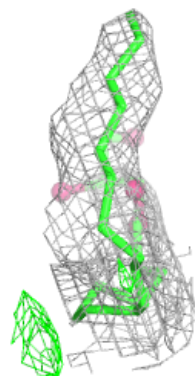
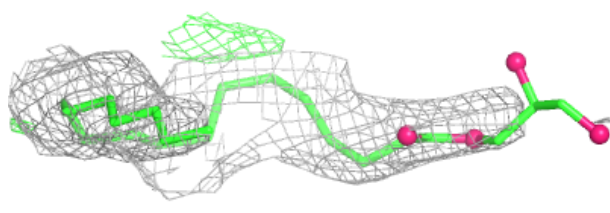
Electron density around DO3 A 410:

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

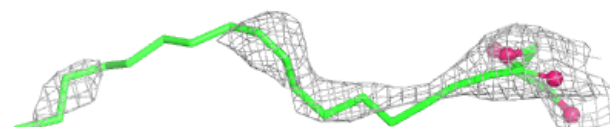
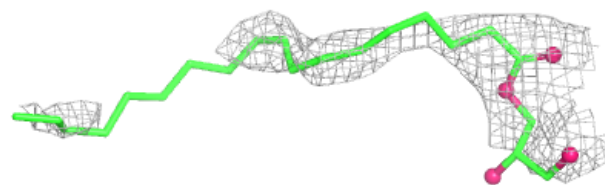


Electron density around OLB A 405:

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

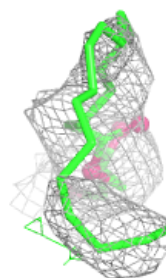
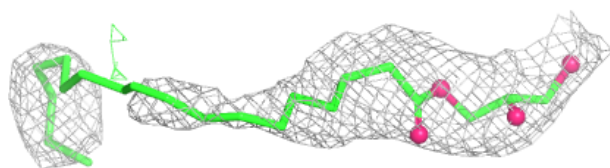
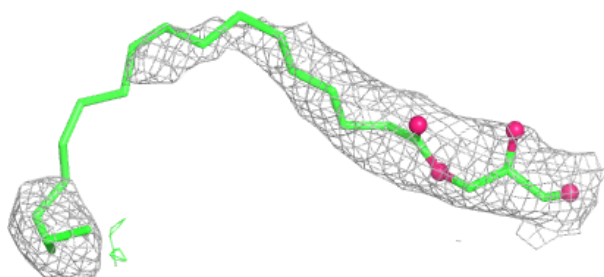
**Electron density around OLB A 406:**

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

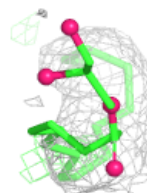
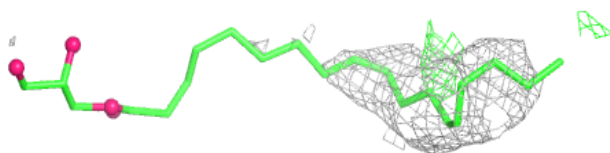
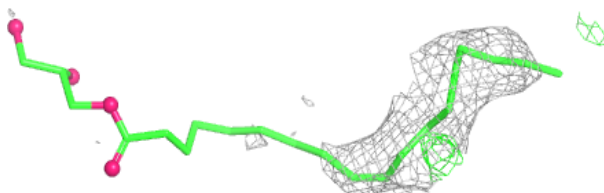


Electron density around OLB A 404:

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

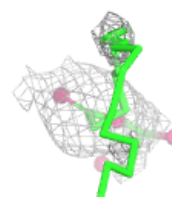
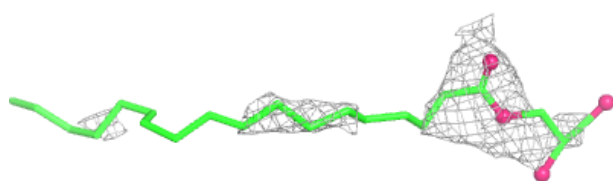
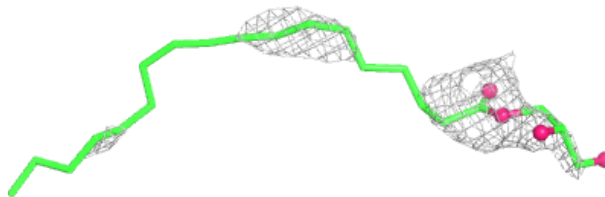
**Electron density around OLB A 403:**

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



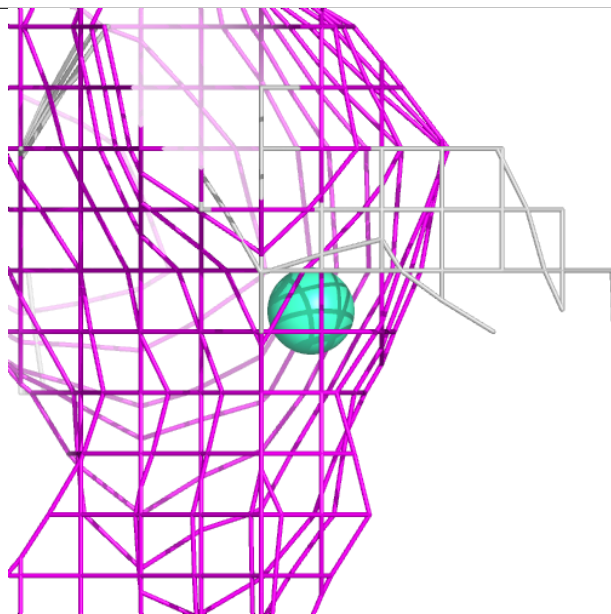
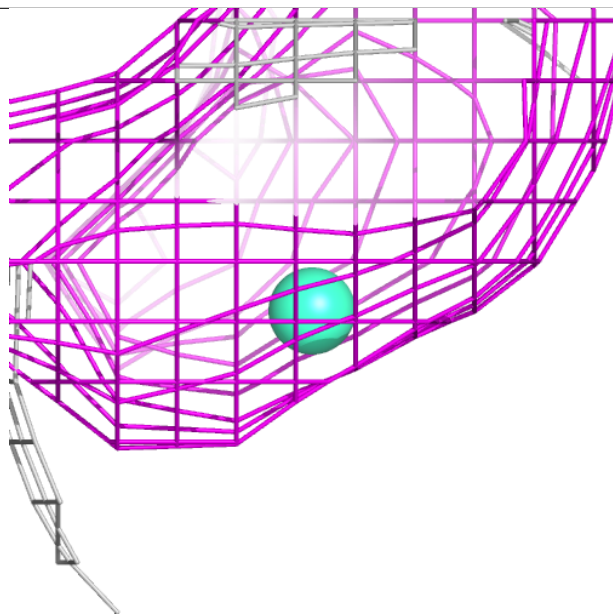
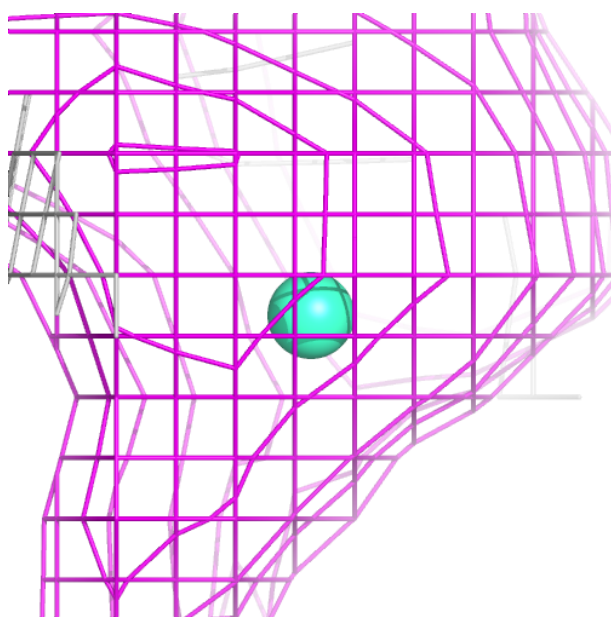
Electron density around OLB H 301:

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



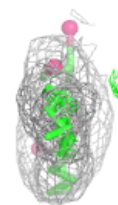
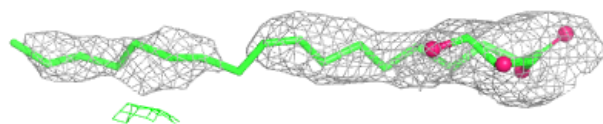
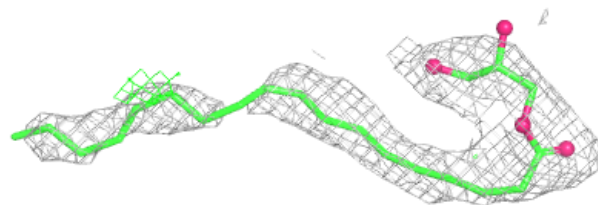
Electron density around GD H 302:

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



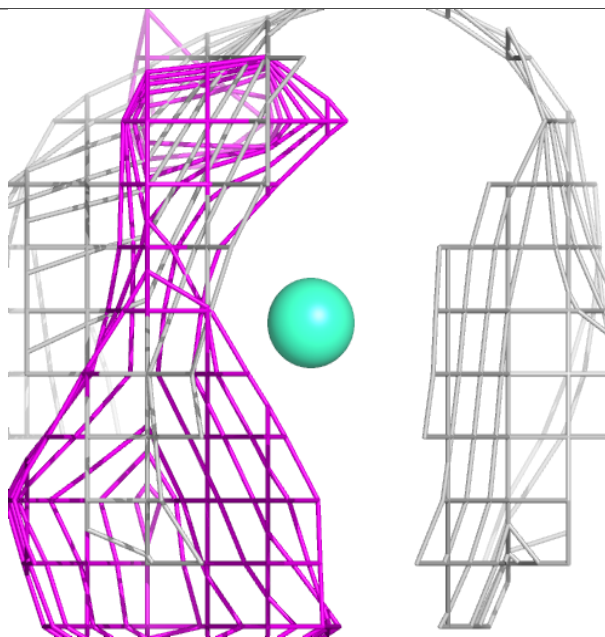
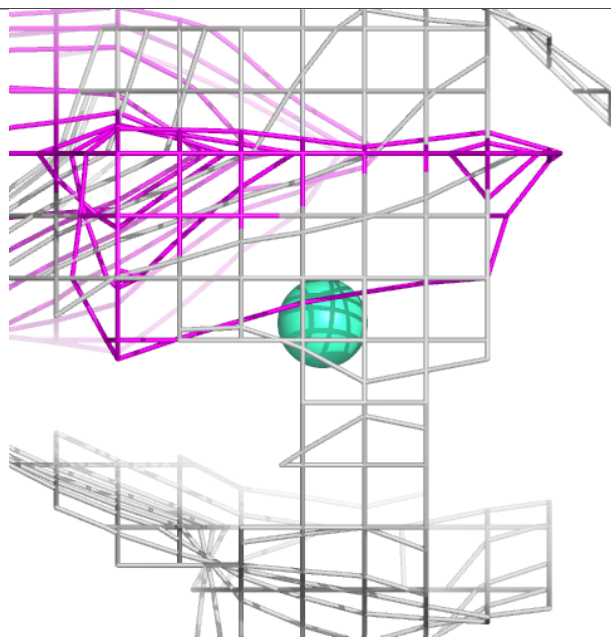
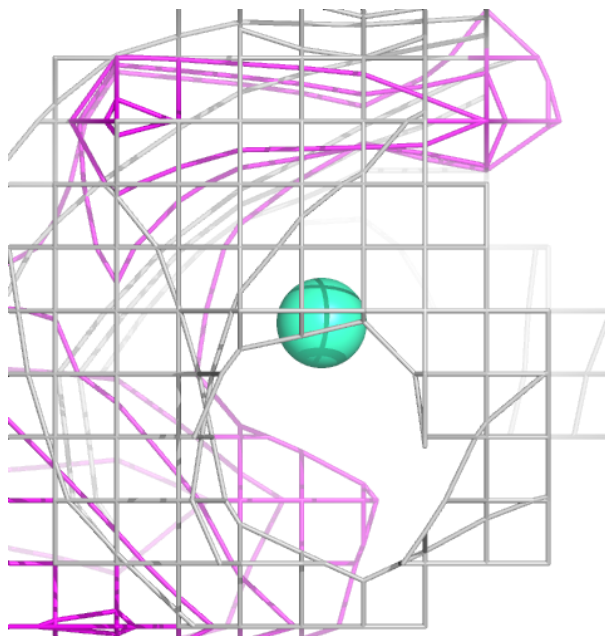
Electron density around OLB A 407:

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



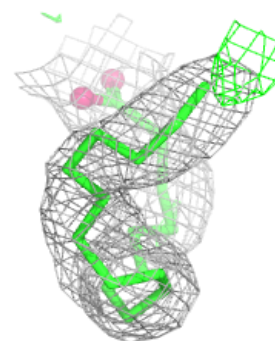
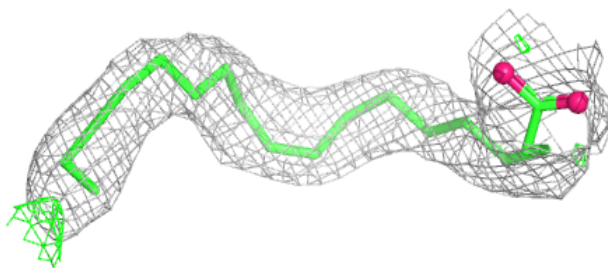
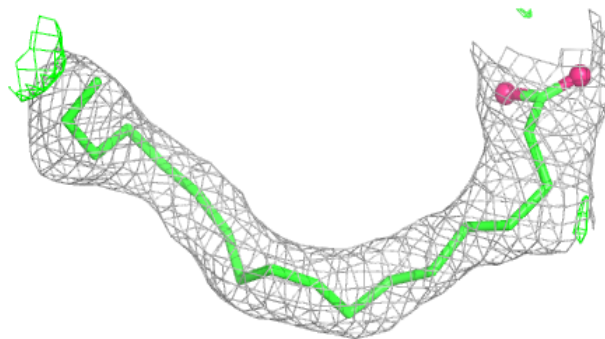
Electron density around GD A 409:

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



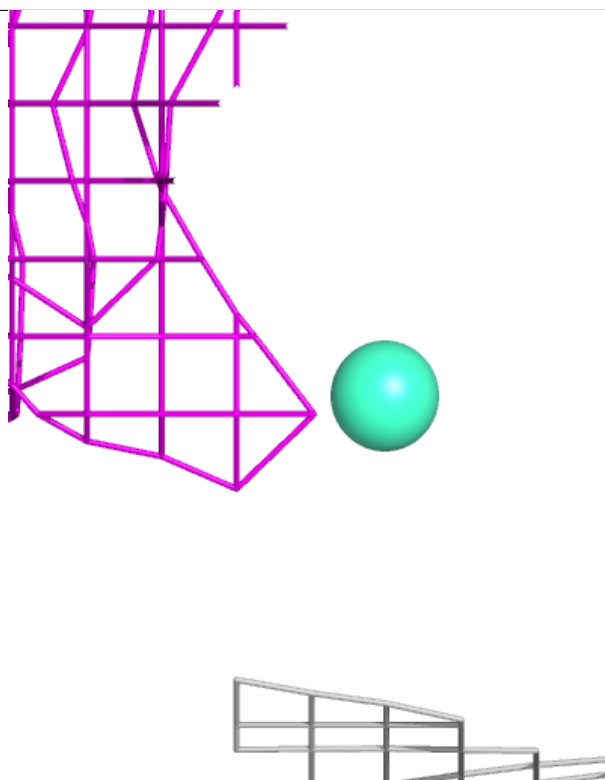
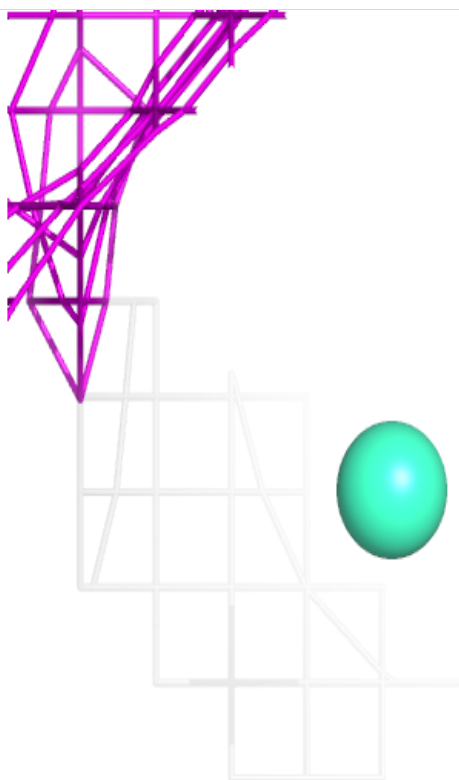
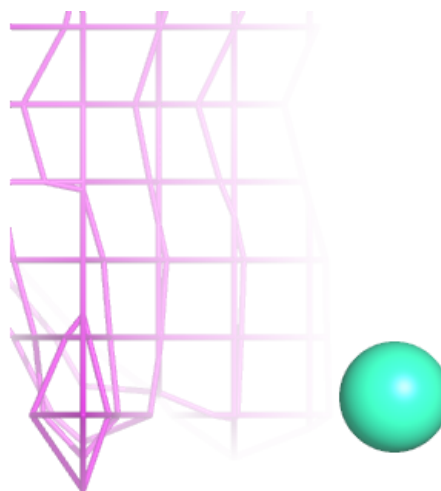
Electron density around OLA A 402:

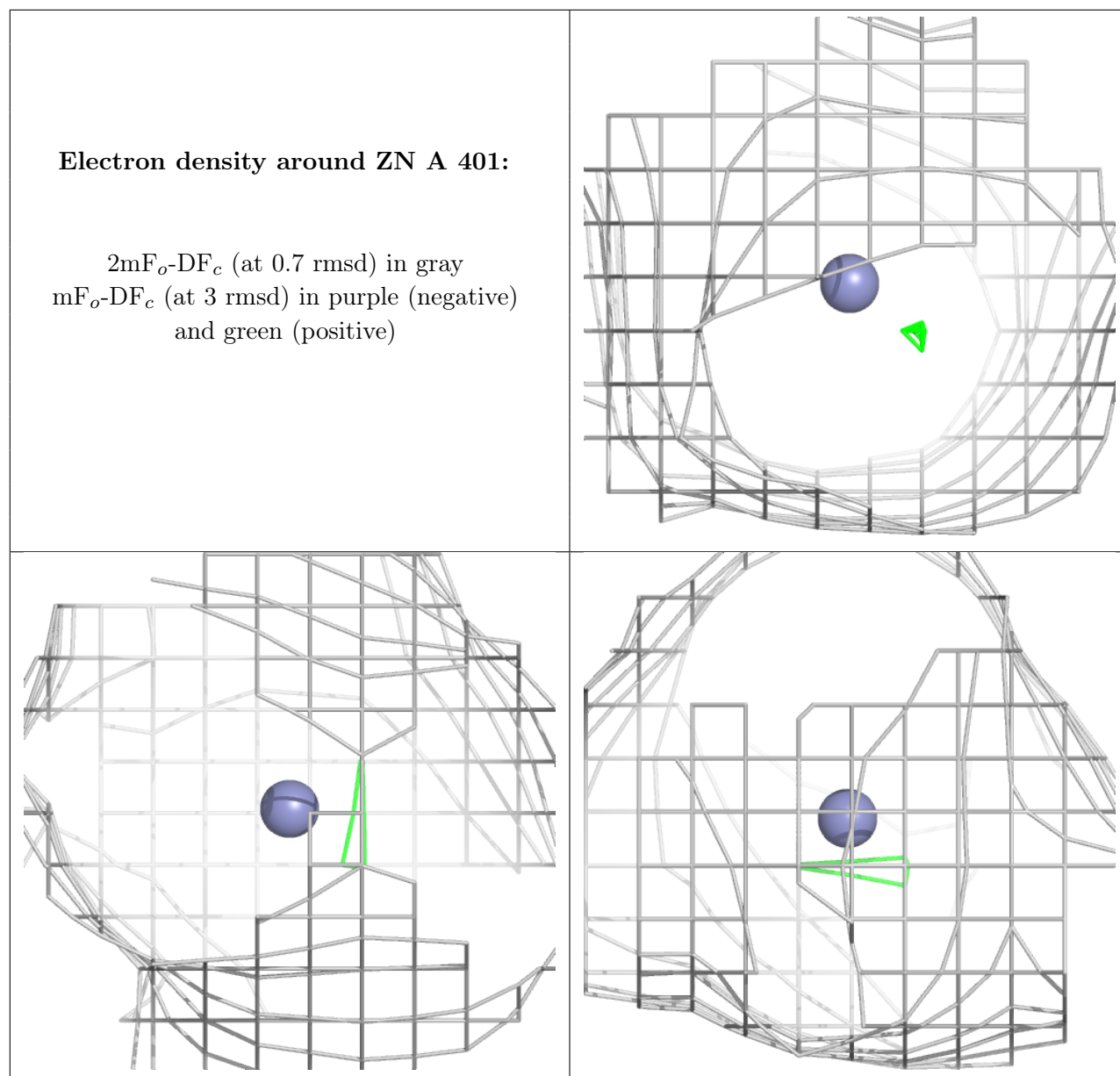
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GD A 408:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.