



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 01:38 AM JST

PDB ID : 8GNG  
Title : Crystal structure of human adenosine A2A receptor in complex with istradefylline.  
Authors : Suzuki, M.; Saito, J.; Miyagi, H.; Yasunaga, M.  
Deposited on : 2022-08-23  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

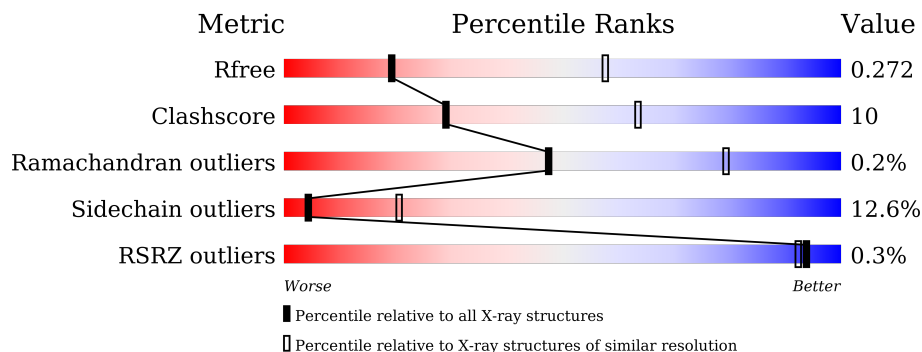
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	 58% 24% 14%
1	X	333	 57% 25% 14%
2	L	214	 77% 20%
2	Y	214	 71% 26%
3	H	226	 80% 16%
3	Z	226	 78% 17%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11322 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 Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2232	1482	368	361	21	0	0	0
1	X	285	2225	1474	370	362	19	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	expression tag	UNP P29274
A	-5	TYR	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	ASP	-	expression tag	UNP P29274
A	0	LYS	-	expression tag	UNP P29274
A	54	LEU	ALA	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	GLN	ASN	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
X	-6	ASP	-	expression tag	UNP P29274
X	-5	TYR	-	expression tag	UNP P29274
X	-4	ASP	-	expression tag	UNP P29274

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	-3	ASP	-	expression tag	UNP P29274
X	-2	ASP	-	expression tag	UNP P29274
X	-1	ASP	-	expression tag	UNP P29274
X	0	LYS	-	expression tag	UNP P29274
X	54	LEU	ALA	engineered mutation	UNP P29274
X	88	ALA	THR	engineered mutation	UNP P29274
X	122	ALA	LYS	engineered mutation	UNP P29274
X	154	GLN	ASN	engineered mutation	UNP P29274
X	239	ALA	VAL	engineered mutation	UNP P29274
X	317	HIS	-	expression tag	UNP P29274
X	318	HIS	-	expression tag	UNP P29274
X	319	HIS	-	expression tag	UNP P29274
X	320	HIS	-	expression tag	UNP P29274
X	321	HIS	-	expression tag	UNP P29274
X	322	HIS	-	expression tag	UNP P29274
X	323	HIS	-	expression tag	UNP P29274
X	324	HIS	-	expression tag	UNP P29274
X	325	HIS	-	expression tag	UNP P29274
X	326	HIS	-	expression tag	UNP P29274

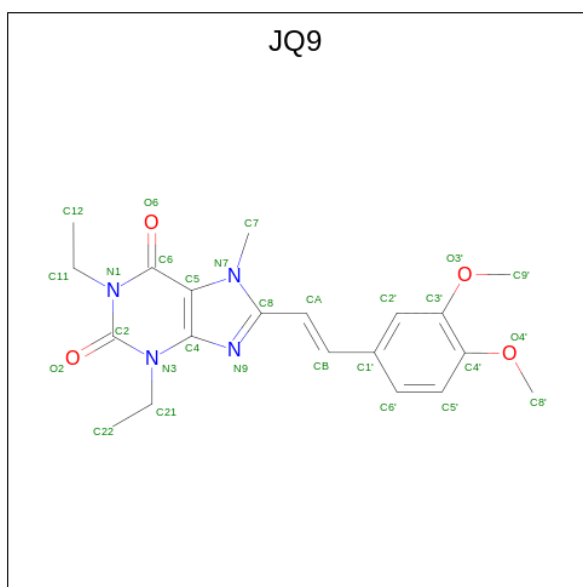
- Molecule 2 is a protein called antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1635	1023	274	332	6	0	0	0
2	Y	212	1639	1026	275	332	6	0	0	0

- Molecule 3 is a protein called antibody fab fragment heavy chain.

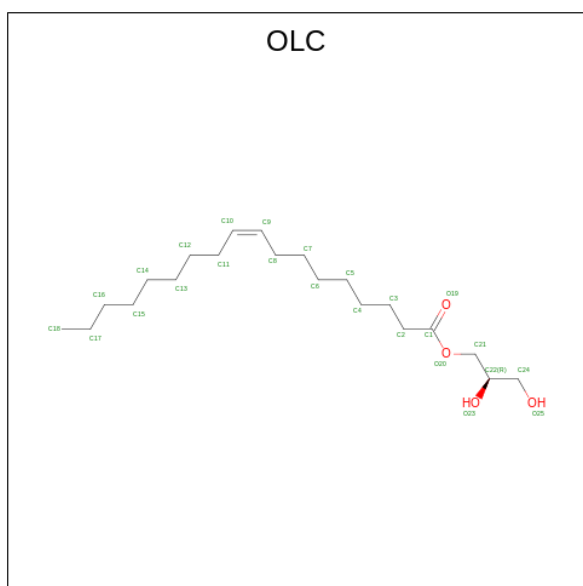
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	222	1683	1060	277	340	6	0	0	0
3	Z	222	1683	1060	277	340	6	0	0	0

- Molecule 4 is 8-[(E)-2-(3,4-dimethoxyphenyl)ethenyl]-1,3-diethyl-7-methyl-purine-2,6-dione (three-letter code: JQ9) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	28	20	4	4	0	0
4	X	1	28	20	4	4	0	0

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	15	11	4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 14 10 4	0	0
5	A	1	Total C O 21 17 4	0	0
5	A	1	Total C O 16 12 4	0	0
5	A	1	Total C O 13 9 4	0	0
5	A	1	Total C O 16 12 4	0	0
5	X	1	Total C O 16 12 4	0	0
5	X	1	Total C O 14 10 4	0	0
5	X	1	Total C O 21 17 4	0	0
5	X	1	Total C O 16 12 4	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	X	1	Total Cl 1 1	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total K 1 1	0	0
7	Y	1	Total K 1 1	0	0

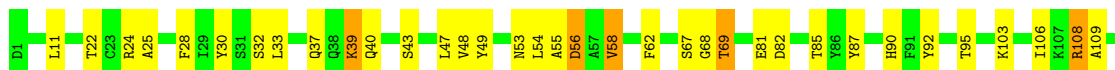
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	3	Total O 3 3	0	0

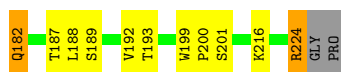
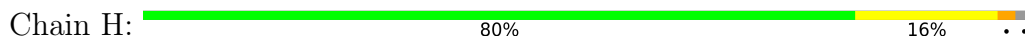




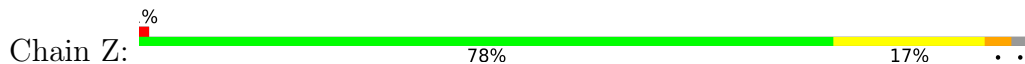
- Molecule 2: antibody fab fragment light chain



- Molecule 3: antibody fab fragment heavy chain



- Molecule 3: antibody fab fragment heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.59Å 134.84Å 42.15Å 97.72° 91.44° 89.38°	Depositor
Resolution (Å)	49.57 – 3.20 49.57 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.57-3.20) 100.0 (49.57-3.20)	Depositor EDS
$R_{merge}$	0.66	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.218 , 0.277 0.220 , 0.272	Depositor DCC
$R_{free}$ test set	1434 reflections (5.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtrriage
Anisotropy	0.670	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 31.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.054 for -h,-k-l,l 0.032 for h,-k,-l 0.014 for -h,k+l,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JQ9, OLC, CL, K

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	0.69	0/2286	0.83	0/3117
1	X	0.69	0/2278	0.86	0/3106
2	L	0.70	0/1674	0.89	0/2276
2	Y	0.72	0/1678	0.90	0/2280
3	H	0.71	0/1724	0.87	0/2349
3	Z	0.70	0/1724	0.86	0/2349
All	All	0.70	0/11364	0.87	0/15477

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2232	0	2309	57	0
1	X	2225	0	2297	62	0
2	L	1635	0	1551	20	0
2	Y	1639	0	1562	29	0
3	H	1683	0	1630	30	0
3	Z	1683	0	1630	29	0
4	A	28	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	X	28	0	0	1	0
5	A	95	0	122	2	0
5	X	67	0	88	0	0
6	A	1	0	0	0	0
6	X	1	0	0	0	0
7	L	1	0	0	0	0
7	Y	1	0	0	0	0
8	A	3	0	0	0	0
All	All	11322	0	11189	215	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 10.

All (215) 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)
2:Y:25:ALA:O	2:Y:69:THR:CG2	2.07	1.01
2:Y:39:LYS:NZ	2:Y:81:GLU:O	2.02	0.93
2:L:39:LYS:NZ	2:L:81:GLU:O	2.08	0.86
2:Y:28:PHE:CE1	2:Y:68:GLY:CA	2.60	0.84
1:A:57:VAL:HG12	1:A:58:LEU:HD13	1.59	0.84
2:Y:28:PHE:CE1	2:Y:68:GLY:HA3	2.13	0.84
2:Y:25:ALA:O	2:Y:69:THR:HG22	1.80	0.82
1:X:78:LEU:HD11	1:X:144:ASN:HB3	1.66	0.77
1:X:191:LEU:O	1:X:194:LEU:HB3	1.86	0.76
1:A:191:LEU:O	1:A:194:LEU:HB3	1.87	0.75
3:H:182:GLN:NE2	3:H:187:THR:OG1	2.21	0.74
1:A:270:MET:O	1:A:274:ILE:HG12	1.87	0.73
1:X:284:ASN:HB2	1:X:285:PRO:HD3	1.71	0.73
3:H:29:PHE:HZ	3:H:72:VAL:HG22	1.53	0.73
2:Y:28:PHE:CE1	2:Y:68:GLY:HA2	2.22	0.73
2:Y:55:ALA:O	2:Y:58:VAL:HG23	1.89	0.72
3:Z:182:GLN:NE2	3:Z:187:THR:OG1	2.23	0.71
1:A:36:ASN:ND2	2:L:32:SER:OG	2.22	0.70
2:Y:25:ALA:O	2:Y:69:THR:HG23	1.92	0.69
1:X:19:LEU:HB3	1:X:282:VAL:HG22	1.74	0.69
2:Y:87:TYR:OH	3:Z:43:LYS:HB2	1.92	0.69
1:A:144:ASN:OD1	1:A:146:CYS:SG	2.51	0.69
1:A:19:LEU:HB3	1:A:282:VAL:HG22	1.75	0.69
1:X:137:LEU:HB2	1:X:140:MET:HG3	1.75	0.69
3:H:139:CYS:SG	3:H:224:ARG:HD3	2.34	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:312:GLU:OE2	1:X:312:GLU:HA	1.93	0.67
2:Y:90:HIS:HD2	2:Y:92:TYR:H	1.42	0.67
1:X:5:GLY:O	1:X:8:VAL:HG13	1.95	0.66
3:H:2:VAL:CG2	3:H:98:ARG:NH1	2.59	0.66
2:L:90:HIS:HD2	2:L:92:TYR:H	1.43	0.64
1:X:168:PHE:CE2	1:X:172:VAL:HG11	2.32	0.64
3:H:29:PHE:CZ	3:H:72:VAL:HG22	2.34	0.63
1:A:36:ASN:HD21	2:L:32:SER:HG	1.42	0.63
1:A:168:PHE:CE2	1:A:172:VAL:HG11	2.34	0.62
1:A:276:LEU:O	1:A:279:THR:HB	2.00	0.62
3:Z:116:GLN:H	3:Z:116:GLN:NE2	1.97	0.62
3:Z:88:SER:O	3:Z:91:SER:OG	2.16	0.61
1:A:134:ALA:O	1:A:138:THR:HG22	2.01	0.60
2:L:136:LEU:HD23	2:L:144:ILE:HD11	1.83	0.60
1:X:66:ILE:HD13	1:X:166:CYS:HB3	1.83	0.60
1:X:78:LEU:HB2	1:X:140:MET:CE	2.31	0.59
1:X:78:LEU:HB2	1:X:140:MET:HE2	1.83	0.59
1:X:60:ILE:CD1	1:X:278:HIS:ND1	2.65	0.59
1:X:78:LEU:CD2	1:X:171:VAL:HB	2.32	0.58
3:H:2:VAL:HG12	3:H:24:THR:HG23	1.86	0.58
3:H:2:VAL:CG1	3:H:24:THR:HG23	2.34	0.58
3:H:12:VAL:HG11	3:H:18:VAL:CG2	2.33	0.58
1:X:221:ALA:HB3	1:X:224:THR:HB	1.86	0.58
1:A:303:ILE:HA	1:A:307:VAL:HG22	1.85	0.57
1:X:276:LEU:O	1:X:279:THR:HB	2.03	0.57
3:Z:182:GLN:HG3	3:Z:182:GLN:O	2.04	0.57
1:X:113:ASN:ND2	3:Z:30:THR:O	2.35	0.57
2:Y:28:PHE:CD1	2:Y:68:GLY:HA2	2.40	0.56
1:X:21:ILE:CD1	1:X:57:VAL:HG23	2.35	0.56
1:X:137:LEU:HB2	1:X:140:MET:CG	2.36	0.56
2:Y:37:GLN:NE2	2:Y:39:LYS:HE2	2.20	0.56
1:X:85:LEU:HD21	4:X:402:JQ9:C12	2.36	0.56
1:X:245:CYS:HA	1:X:276:LEU:HD22	1.87	0.56
3:Z:39:GLN:HE21	3:Z:45:LEU:HG	1.70	0.56
2:Y:136:LEU:HD23	2:Y:144:ILE:HD11	1.88	0.55
2:L:55:ALA:O	2:L:58:VAL:HG23	2.07	0.55
1:X:60:ILE:HD13	1:X:278:HIS:ND1	2.22	0.55
1:A:245:CYS:HA	1:A:276:LEU:HD22	1.88	0.55
1:X:134:ALA:O	1:X:138:THR:HG22	2.07	0.55
1:X:284:ASN:CB	1:X:285:PRO:HD3	2.37	0.55
3:H:148:THR:HG1	3:H:193:THR:HG1	1.55	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ILE:O	1:A:307:VAL:HG22	2.08	0.54
3:H:2:VAL:HG21	3:H:98:ARG:NH1	2.23	0.53
2:L:121:SER:OG	3:H:134:PRO:HD2	2.09	0.53
1:A:46:VAL:HG12	5:A:404:OLC:H5	1.91	0.53
1:X:176:TYR:CD1	1:X:176:TYR:C	2.82	0.53
3:Z:71:THR:OG1	3:Z:80:TYR:HB2	2.09	0.53
3:H:71:THR:OG1	3:H:80:TYR:HB2	2.09	0.52
1:X:15:ALA:O	1:X:19:LEU:HD23	2.08	0.52
3:Z:12:VAL:HG11	3:Z:18:VAL:HG23	1.91	0.52
3:Z:12:VAL:HG21	3:Z:86:LEU:HD13	1.92	0.52
1:A:168:PHE:HZ	1:A:177:MET:HE3	1.75	0.52
3:Z:154:LYS:NZ	3:Z:182:GLN:HE22	2.06	0.52
1:A:176:TYR:C	1:A:176:TYR:CD1	2.84	0.51
1:A:221:ALA:HB3	1:A:224:THR:HB	1.92	0.51
3:H:224:ARG:HD2	3:H:224:ARG:N	2.25	0.51
1:A:7:SER:O	1:A:11:THR:HG23	2.11	0.51
2:Y:183:LYS:O	2:Y:187:GLU:HG2	2.11	0.51
3:Z:103:TYR:CZ	3:Z:105:GLY:HA2	2.46	0.51
1:A:17:ALA:O	1:A:21:ILE:HG12	2.11	0.51
1:X:86:VAL:HG21	1:X:133:PHE:CD1	2.45	0.51
2:Y:28:PHE:CD1	2:Y:68:GLY:CA	2.94	0.50
1:A:237:ILE:O	1:A:241:LEU:HG	2.12	0.50
1:A:271:TYR:HA	1:A:274:ILE:HG13	1.93	0.50
3:H:12:VAL:HG11	3:H:18:VAL:HG23	1.93	0.50
1:X:15:ALA:O	1:X:18:VAL:HG12	2.12	0.50
3:H:182:GLN:O	3:H:182:GLN:HG2	2.10	0.50
1:A:21:ILE:CD1	1:A:57:VAL:HG23	2.42	0.50
3:H:103:TYR:CZ	3:H:105:GLY:HA2	2.47	0.49
1:X:233:LYS:O	1:X:237:ILE:HD12	2.12	0.49
3:H:98:ARG:NH2	3:H:112:ASP:OD2	2.45	0.49
1:A:66:ILE:HD13	1:A:166:CYS:HB3	1.95	0.49
1:A:123:GLY:O	1:A:127:ILE:HG13	2.13	0.49
1:A:138:THR:O	1:A:141:LEU:HB2	2.13	0.49
1:A:15:ALA:O	1:A:18:VAL:HG12	2.13	0.48
1:X:60:ILE:HB	1:X:61:PRO:HD3	1.95	0.48
3:Z:154:LYS:HG3	3:Z:182:GLN:HE22	1.77	0.48
1:X:36:ASN:ND2	2:Y:32:SER:OG	2.25	0.48
1:X:17:ALA:O	1:X:21:ILE:HG12	2.14	0.48
2:Y:136:LEU:HD12	2:Y:136:LEU:N	2.28	0.48
2:L:21:ILE:HD13	2:L:102:THR:HG21	1.96	0.48
1:X:312:GLU:OE2	1:X:312:GLU:CA	2.61	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:GLU:OE1	2:L:142:LYS:HE2	2.14	0.47
3:H:2:VAL:HG21	3:H:98:ARG:HD3	1.95	0.47
1:X:40:VAL:HG11	1:X:116:VAL:CG1	2.44	0.47
3:Z:148:THR:HG1	3:Z:193:THR:HG1	1.62	0.47
3:Z:199:TRP:CG	3:Z:200:PRO:HA	2.50	0.47
1:A:21:ILE:HD13	1:A:57:VAL:HG23	1.95	0.47
1:X:69:GLY:HA2	1:X:166:CYS:O	2.14	0.47
1:X:66:ILE:CD1	1:X:166:CYS:HB3	2.44	0.47
1:X:282:VAL:O	1:X:285:PRO:HD2	2.13	0.47
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.44	0.47
3:Z:18:VAL:HB	3:Z:86:LEU:HD11	1.97	0.46
2:L:29:ILE:HD11	2:L:71:PHE:CE1	2.50	0.46
3:H:29:PHE:HZ	3:H:72:VAL:CG2	2.26	0.46
1:X:33:LEU:HD22	2:Y:30:TYR:OH	2.15	0.46
3:H:154:LYS:HG3	3:H:182:GLN:HE22	1.80	0.46
1:X:243:ALA:O	1:X:247:LEU:HB2	2.16	0.46
3:Z:29:PHE:CE1	3:Z:53:PRO:HB3	2.51	0.46
1:A:138:THR:HA	1:A:141:LEU:HD12	1.98	0.45
1:X:135:ILE:HD13	1:X:185:CYS:SG	2.56	0.45
1:X:274:ILE:O	1:X:278:HIS:CD2	2.68	0.45
1:A:233:LYS:O	1:A:237:ILE:HD12	2.16	0.45
3:Z:184:ASP:OD1	3:Z:184:ASP:N	2.48	0.45
3:H:2:VAL:HG21	3:H:98:ARG:CZ	2.47	0.45
3:H:199:TRP:CG	3:H:200:PRO:HA	2.51	0.45
2:L:55:ALA:HB3	2:L:58:VAL:HG21	1.99	0.45
1:X:138:THR:N	1:X:139:PRO:CD	2.80	0.45
2:L:24:ARG:HA	2:L:69:THR:O	2.17	0.45
1:X:143:TRP:CD1	1:X:173:PRO:HG2	2.52	0.45
1:A:282:VAL:O	1:A:285:PRO:HD2	2.16	0.45
1:X:168:PHE:HZ	1:X:177:MET:HE3	1.82	0.45
3:H:29:PHE:CE2	3:H:53:PRO:HB3	2.51	0.44
1:X:61:PRO:O	1:X:65:THR:HG23	2.17	0.44
2:Y:135:PHE:HB3	2:Y:137:ASN:HD21	1.82	0.44
1:A:243:ALA:O	1:A:247:LEU:HB2	2.18	0.44
3:Z:159:GLU:HB2	3:Z:160:PRO:HA	1.98	0.44
1:X:226:GLN:HE21	1:X:226:GLN:HB3	1.55	0.44
1:A:103:TYR:HE2	1:A:199:ARG:HG2	1.82	0.44
3:Z:12:VAL:HG11	3:Z:18:VAL:CG2	2.46	0.44
1:A:62:PHE:CD2	1:A:80:ILE:HA	2.53	0.44
1:A:103:TYR:HA	1:A:200:ILE:HD11	2.00	0.44
3:H:17:SER:OG	3:H:18:VAL:N	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:47:LEU:HD21	2:Y:62:PHE:CD2	2.53	0.44
1:A:35:SER:O	1:A:37:LEU:N	2.51	0.43
2:Y:28:PHE:HE1	2:Y:68:GLY:HA3	1.75	0.43
2:Y:48:VAL:HG22	2:Y:54:LEU:HD23	1.99	0.43
2:L:110:ASP:OD2	2:L:199:LYS:NZ	2.51	0.43
1:A:138:THR:N	1:A:139:PRO:CD	2.81	0.43
1:A:186:VAL:O	1:A:190:LEU:HB2	2.18	0.43
2:L:136:LEU:HD23	2:L:144:ILE:CD1	2.47	0.43
1:X:186:VAL:O	1:X:190:LEU:HB2	2.18	0.43
1:A:174:MET:HG3	1:A:257:PHE:HB2	2.00	0.43
2:Y:56:ASP:OD1	2:Y:56:ASP:N	2.51	0.43
1:A:60:ILE:HD11	1:A:278:HIS:HB3	2.00	0.43
1:A:137:LEU:HB2	1:A:140:MET:HG3	2.01	0.43
1:A:238:ILE:CD1	1:A:287:ILE:HG21	2.49	0.43
3:Z:154:LYS:NZ	3:Z:182:GLN:NE2	2.67	0.43
1:A:61:PRO:O	1:A:65:THR:HG23	2.19	0.43
1:A:300:ARG:HD3	1:A:304:ARG:HH12	1.83	0.43
1:X:35:SER:O	1:X:37:LEU:N	2.52	0.42
1:X:103:TYR:HE2	1:X:199:ARG:HG2	1.83	0.42
1:A:247:LEU:N	1:A:248:PRO:CD	2.83	0.42
1:A:41:THR:HB	3:H:103:TYR:CE2	2.54	0.42
2:Y:49:TYR:CZ	2:Y:53:ASN:HB3	2.54	0.42
2:Y:118:PHE:HA	2:Y:119:PRO:HD3	1.93	0.42
3:Z:12:VAL:CG2	3:Z:86:LEU:HD13	2.50	0.42
2:L:55:ALA:HB3	2:L:58:VAL:CG2	2.49	0.42
1:X:123:GLY:O	1:X:127:ILE:HG13	2.18	0.42
1:X:138:THR:HA	1:X:141:LEU:CD2	2.49	0.42
1:A:116:VAL:HG13	5:A:403:OLC:H22	2.02	0.42
1:A:231:ALA:O	1:A:234:SER:HB2	2.19	0.42
2:Y:24:ARG:HA	2:Y:69:THR:O	2.19	0.42
1:A:66:ILE:CD1	1:A:166:CYS:HB3	2.49	0.42
3:Z:35:ASN:N	3:Z:35:ASN:HD22	2.18	0.42
1:A:192:LEU:HD12	1:A:192:LEU:C	2.39	0.42
1:X:78:LEU:O	1:X:82:CYS:N	2.52	0.42
3:H:154:LYS:CG	3:H:182:GLN:HE22	2.32	0.42
1:X:78:LEU:HD21	1:X:171:VAL:HB	2.01	0.42
1:X:231:ALA:HB2	3:Z:104:ASP:HA	2.01	0.42
1:A:140:MET:HE2	1:A:140:MET:HB3	1.91	0.41
3:H:119:THR:O	3:H:119:THR:HG22	2.20	0.41
1:X:192:LEU:C	1:X:192:LEU:HD12	2.40	0.41
2:L:56:ASP:OD1	2:L:56:ASP:N	2.53	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:O	1:A:82:CYS:N	2.53	0.41
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.90	0.41
1:X:304:ARG:HD2	1:X:312:GLU:HB3	2.02	0.41
3:Z:65:LYS:HE3	3:Z:65:LYS:HB2	1.65	0.41
3:Z:119:THR:O	3:Z:119:THR:HG22	2.19	0.41
3:Z:154:LYS:HZ3	3:Z:182:GLN:HE22	1.67	0.41
2:Y:119:PRO:HD2	3:Z:224:ARG:NH1	2.35	0.41
1:A:69:GLY:HA2	1:A:166:CYS:O	2.21	0.41
2:L:12:SER:HA	2:L:105:GLU:O	2.20	0.41
1:X:62:PHE:CD2	1:X:80:ILE:HA	2.56	0.41
1:X:231:ALA:O	1:X:234:SER:HB2	2.21	0.41
2:Y:108:ARG:NH2	2:Y:109:ALA:O	2.46	0.41
1:X:55:VAL:HA	1:X:59:ALA:HB3	2.03	0.41
1:X:95:LEU:HD21	1:X:238:ILE:HG22	2.02	0.41
3:H:81:ILE:HG23	3:H:81:ILE:O	2.22	0.40
1:A:183:PHE:O	1:A:188:VAL:HG23	2.21	0.40
1:A:231:ALA:HB2	3:H:104:ASP:HA	2.03	0.40
2:L:135:PHE:HB3	2:L:137:ASN:HD21	1.84	0.40
2:L:139:PHE:CZ	2:L:144:ILE:HG21	2.56	0.40
1:X:247:LEU:N	1:X:248:PRO:CD	2.85	0.40
1:X:311:GLN:O	1:X:312:GLU:HB2	2.21	0.40
1:A:103:TYR:CA	1:A:200:ILE:HD11	2.52	0.40
2:L:108:ARG:NH2	2:L:109:ALA:O	2.45	0.40
1:X:247:LEU:HD12	1:X:247:LEU:HA	1.91	0.40
3:H:174:VAL:HG22	3:H:192:VAL:HG23	2.04	0.40
2:Y:209:PHE:HB3	3:Z:138:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/333 (84%)	258 (92%)	22 (8%)	1 (0%)	34	69
1	X	279/333 (84%)	252 (90%)	25 (9%)	2 (1%)	22	61
2	L	210/214 (98%)	199 (95%)	11 (5%)	0	100	100
2	Y	210/214 (98%)	201 (96%)	9 (4%)	0	100	100
3	H	218/226 (96%)	205 (94%)	13 (6%)	0	100	100
3	Z	218/226 (96%)	209 (96%)	9 (4%)	0	100	100
All	All	1416/1546 (92%)	1324 (94%)	89 (6%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	X	36	ASN
1	X	6	SER

### 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	239/281 (85%)	208 (87%)	31 (13%)	4	19
1	X	238/281 (85%)	209 (88%)	29 (12%)	5	22
2	L	183/186 (98%)	156 (85%)	27 (15%)	3	14
2	Y	184/186 (99%)	152 (83%)	32 (17%)	2	10
3	H	192/195 (98%)	175 (91%)	17 (9%)	9	35
3	Z	192/195 (98%)	173 (90%)	19 (10%)	8	30
All	All	1228/1324 (93%)	1073 (87%)	155 (13%)	4	21

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	7	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	8	VAL
1	A	14	LEU
1	A	21	ILE
1	A	35	SER
1	A	58	LEU
1	A	86	VAL
1	A	115	LEU
1	A	120	ARG
1	A	137	LEU
1	A	138	THR
1	A	140	MET
1	A	145	ASN
1	A	163	GLN
1	A	170	ASP
1	A	172	VAL
1	A	191	LEU
1	A	193	MET
1	A	205	ARG
1	A	209	LYS
1	A	223	SER
1	A	244	LEU
1	A	249	LEU
1	A	261	ASP
1	A	267	LEU
1	A	272	LEU
1	A	274	ILE
1	A	276	LEU
1	A	282	VAL
1	A	303	ILE
2	L	22	THR
2	L	24	ARG
2	L	31	SER
2	L	33	LEU
2	L	39	LYS
2	L	40	GLN
2	L	56	ASP
2	L	69	THR
2	L	95	THR
2	L	105	GLU
2	L	108	ARG
2	L	116	SER
2	L	126	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	L	133	VAL
2	L	156	GLN
2	L	157	ASN
2	L	162	SER
2	L	168	SER
2	L	171	SER
2	L	175	MET
2	L	181	LEU
2	L	182	THR
2	L	187	GLU
2	L	190	ASN
2	L	193	THR
2	L	197	THR
2	L	210	ASN
3	H	18	VAL
3	H	35	ASN
3	H	65	LYS
3	H	67	LYS
3	H	72	VAL
3	H	75	SER
3	H	126	LYS
3	H	139	CYS
3	H	160	PRO
3	H	167	SER
3	H	172	SER
3	H	182	GLN
3	H	188	LEU
3	H	189	SER
3	H	201	SER
3	H	216	LYS
3	H	224	ARG
1	X	7	SER
1	X	14	LEU
1	X	21	ILE
1	X	35	SER
1	X	57	VAL
1	X	58	LEU
1	X	86	VAL
1	X	108	ILE
1	X	115	LEU
1	X	119	THR
1	X	137	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	X	138	THR
1	X	144	ASN
1	X	145	ASN
1	X	159	CYS
1	X	161	GLU
1	X	164	VAL
1	X	170	ASP
1	X	172	VAL
1	X	191	LEU
1	X	193	MET
1	X	226	GLN
1	X	244	LEU
1	X	249	LEU
1	X	272	LEU
1	X	276	LEU
1	X	282	VAL
1	X	291	ARG
1	X	301	LYS
2	Y	11	LEU
2	Y	22	THR
2	Y	33	LEU
2	Y	39	LYS
2	Y	40	GLN
2	Y	43	SER
2	Y	56	ASP
2	Y	58	VAL
2	Y	67	SER
2	Y	69	THR
2	Y	82	ASP
2	Y	85	THR
2	Y	95	THR
2	Y	103	LYS
2	Y	106	ILE
2	Y	108	ARG
2	Y	116	SER
2	Y	122	SER
2	Y	123	GLU
2	Y	126	THR
2	Y	133	VAL
2	Y	145	ASN
2	Y	162	SER
2	Y	168	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	Y	171	SER
2	Y	175	MET
2	Y	181	LEU
2	Y	182	THR
2	Y	190	ASN
2	Y	193	THR
2	Y	197	THR
2	Y	205	ILE
3	Z	18	VAL
3	Z	35	ASN
3	Z	41	HIS
3	Z	59	ARG
3	Z	70	LEU
3	Z	74	LYS
3	Z	75	SER
3	Z	88	SER
3	Z	89	GLU
3	Z	91	SER
3	Z	116	GLN
3	Z	126	LYS
3	Z	160	PRO
3	Z	167	SER
3	Z	189	SER
3	Z	201	SER
3	Z	205	THR
3	Z	215	THR
3	Z	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	145	ASN
1	A	264	HIS
2	L	90	HIS
2	L	210	ASN
3	H	182	GLN
1	X	226	GLN
2	Y	37	GLN
2	Y	40	GLN
2	Y	45	GLN
2	Y	90	HIS
2	Y	137	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	Y	138	ASN
2	Y	210	ASN
3	Z	116	GLN
3	Z	182	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
5	OLC	X	401	-	15,15,24	1.30	1 (6%)	16,16,25	1.34	2 (12%)
5	OLC	A	403	-	13,13,24	1.36	1 (7%)	14,14,25	1.28	2 (14%)
4	JQ9	X	402	-	27,30,30	1.63	3 (11%)	31,43,43	2.23	11 (35%)
5	OLC	A	407	-	12,12,24	1.60	1 (8%)	13,13,25	1.40	3 (23%)
5	OLC	A	408	-	15,15,24	1.37	1 (6%)	16,16,25	1.30	2 (12%)
5	OLC	X	404	-	20,20,24	1.15	1 (5%)	21,21,25	1.10	2 (9%)
5	OLC	A	402	-	14,14,24	1.33	1 (7%)	15,15,25	1.09	2 (13%)
5	OLC	X	405	-	15,15,24	1.26	1 (6%)	16,16,25	1.12	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	JQ9	A	401	-	27,30,30	1.04	1 (3%)	31,43,43	2.04	11 (35%)
5	OLC	A	405	-	15,15,24	1.26	1 (6%)	16,16,25	1.19	1 (6%)
5	OLC	X	403	-	13,13,24	1.26	1 (7%)	14,14,25	1.16	2 (14%)
5	OLC	A	404	-	20,20,24	1.15	1 (5%)	21,21,25	1.32	2 (9%)

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
5	OLC	X	401	-	-	8/15/15/24	-
5	OLC	A	403	-	-	4/13/13/24	-
4	JQ9	X	402	-	-	6/11/13/13	0/3/3/3
5	OLC	A	407	-	-	8/12/12/24	-
5	OLC	A	408	-	-	6/15/15/24	-
5	OLC	X	404	-	-	7/20/20/24	-
5	OLC	A	402	-	-	6/14/14/24	-
5	OLC	X	405	-	-	8/15/15/24	-
4	JQ9	A	401	-	-	4/11/13/13	0/3/3/3
5	OLC	A	405	-	-	5/15/15/24	-
5	OLC	X	403	-	-	5/13/13/24	-
5	OLC	A	404	-	-	6/20/20/24	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	402	JQ9	C2-N3	6.06	1.45	1.37
5	A	407	OLC	O20-C1	5.16	1.48	1.33
5	A	408	OLC	O20-C1	4.96	1.47	1.33
5	A	404	OLC	O20-C1	4.91	1.47	1.33
5	X	404	OLC	O20-C1	4.85	1.47	1.33
5	X	401	OLC	O20-C1	4.78	1.47	1.33
5	A	402	OLC	O20-C1	4.65	1.46	1.33
5	A	405	OLC	O20-C1	4.61	1.46	1.33
5	X	405	OLC	O20-C1	4.57	1.46	1.33
5	A	403	OLC	O20-C1	4.56	1.46	1.33
5	X	403	OLC	O20-C1	4.27	1.45	1.33
4	X	402	JQ9	C2-N1	2.96	1.44	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	402	JQ9	C3'-C4'	2.27	1.45	1.40
4	A	401	JQ9	O4'-C4'	2.14	1.40	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	402	JQ9	C21-N3-C2	5.06	123.97	116.75
4	X	402	JQ9	C4-N3-C2	-4.45	118.03	122.22
4	A	401	JQ9	C4-N3-C2	-4.44	118.04	122.22
5	A	404	OLC	O20-C1-C2	4.36	125.59	111.91
4	X	402	JQ9	O4'-C4'-C3'	4.13	121.16	115.41
4	X	402	JQ9	C5-N7-C8	-4.02	105.66	109.81
4	A	401	JQ9	C5-N7-C8	-4.00	105.67	109.81
4	A	401	JQ9	C8'-O4'-C4'	3.76	123.21	117.53
5	A	405	OLC	O20-C1-C2	3.69	123.48	111.91
5	X	401	OLC	O20-C1-C2	3.62	123.26	111.91
5	X	404	OLC	O20-C1-C2	3.55	123.05	111.91
5	A	408	OLC	O20-C1-C2	3.47	122.80	111.91
5	A	407	OLC	O20-C1-C2	3.38	122.50	111.91
5	A	403	OLC	O20-C1-C2	3.32	122.31	111.91
4	X	402	JQ9	O6-C6-N1	3.04	124.44	120.13
5	X	405	OLC	O20-C1-C2	3.00	121.33	111.91
5	A	403	OLC	O20-C1-O19	-2.98	116.06	123.59
4	A	401	JQ9	C7-N7-C8	2.97	130.90	124.87
4	A	401	JQ9	C2'-C3'-C4'	2.95	123.75	119.84
4	A	401	JQ9	O2-C2-N3	-2.93	118.26	122.22
4	A	401	JQ9	O3'-C3'-C2'	-2.87	119.19	124.12
5	X	403	OLC	O20-C1-C2	2.84	120.81	111.91
4	X	402	JQ9	C8'-O4'-C4'	2.81	121.78	117.53
5	A	402	OLC	O20-C1-C2	2.79	120.67	111.91
5	X	403	OLC	O20-C1-O19	-2.78	116.58	123.59
4	A	401	JQ9	C5'-C4'-C3'	-2.76	116.00	119.70
5	X	405	OLC	O20-C1-O19	-2.71	116.74	123.59
4	A	401	JQ9	CA-C8-N9	2.70	128.40	124.08
4	X	402	JQ9	C1'-CB-CA	-2.69	115.26	125.87
4	A	401	JQ9	O6-C6-N1	2.65	123.89	120.13
4	X	402	JQ9	CA-C8-N9	2.59	128.23	124.08
4	X	402	JQ9	C9'-O3'-C3'	2.56	121.40	117.53
4	X	402	JQ9	O2-C2-N1	-2.50	118.52	121.99
5	A	408	OLC	O20-C1-O19	-2.43	117.46	123.59
4	X	402	JQ9	O4'-C4'-C5'	-2.35	120.34	124.37
5	X	401	OLC	O20-C1-O19	-2.25	117.92	123.59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	407	OLC	O20-C1-O19	-2.24	117.95	123.59
5	A	404	OLC	O20-C1-O19	-2.19	118.05	123.59
4	A	401	JQ9	C5-C6-N1	-2.19	111.78	113.58
5	A	407	OLC	C21-O20-C1	2.19	125.23	117.12
5	X	404	OLC	O20-C1-O19	-2.16	118.15	123.59
5	A	402	OLC	O20-C1-O19	-2.01	118.52	123.59

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	JQ9	C22-C21-N3-C2
5	A	402	OLC	O20-C21-C22-O23
5	A	407	OLC	C21-C22-C24-O25
5	A	408	OLC	C21-C22-C24-O25
5	X	401	OLC	O20-C21-C22-O23
5	X	404	OLC	C21-C22-C24-O25
5	A	403	OLC	O19-C1-O20-C21
5	A	403	OLC	C2-C1-O20-C21
5	X	403	OLC	O19-C1-O20-C21
5	X	403	OLC	C2-C1-O20-C21
5	A	407	OLC	C2-C1-O20-C21
5	X	401	OLC	C2-C1-O20-C21
5	X	405	OLC	C2-C1-O20-C21
5	X	405	OLC	O20-C21-C22-C24
5	X	401	OLC	O19-C1-O20-C21
5	X	405	OLC	O20-C21-C22-O23
5	A	407	OLC	O19-C1-O20-C21
5	X	405	OLC	O19-C1-O20-C21
4	A	401	JQ9	C4'-C3'-O3'-C9'
5	A	404	OLC	C3-C4-C5-C6
5	A	402	OLC	C2-C1-O20-C21
5	X	401	OLC	O20-C21-C22-C24
5	A	408	OLC	C4-C5-C6-C7
5	X	405	OLC	C1-C2-C3-C4
5	A	405	OLC	C3-C4-C5-C6
5	X	405	OLC	C2-C3-C4-C5
5	A	402	OLC	O19-C1-O20-C21
5	A	408	OLC	C2-C1-O20-C21
5	A	408	OLC	O23-C22-C24-O25
4	A	401	JQ9	C2'-C3'-O3'-C9'
5	A	408	OLC	O19-C1-O20-C21

*Continued on next page...*

*Continued from previous page...*

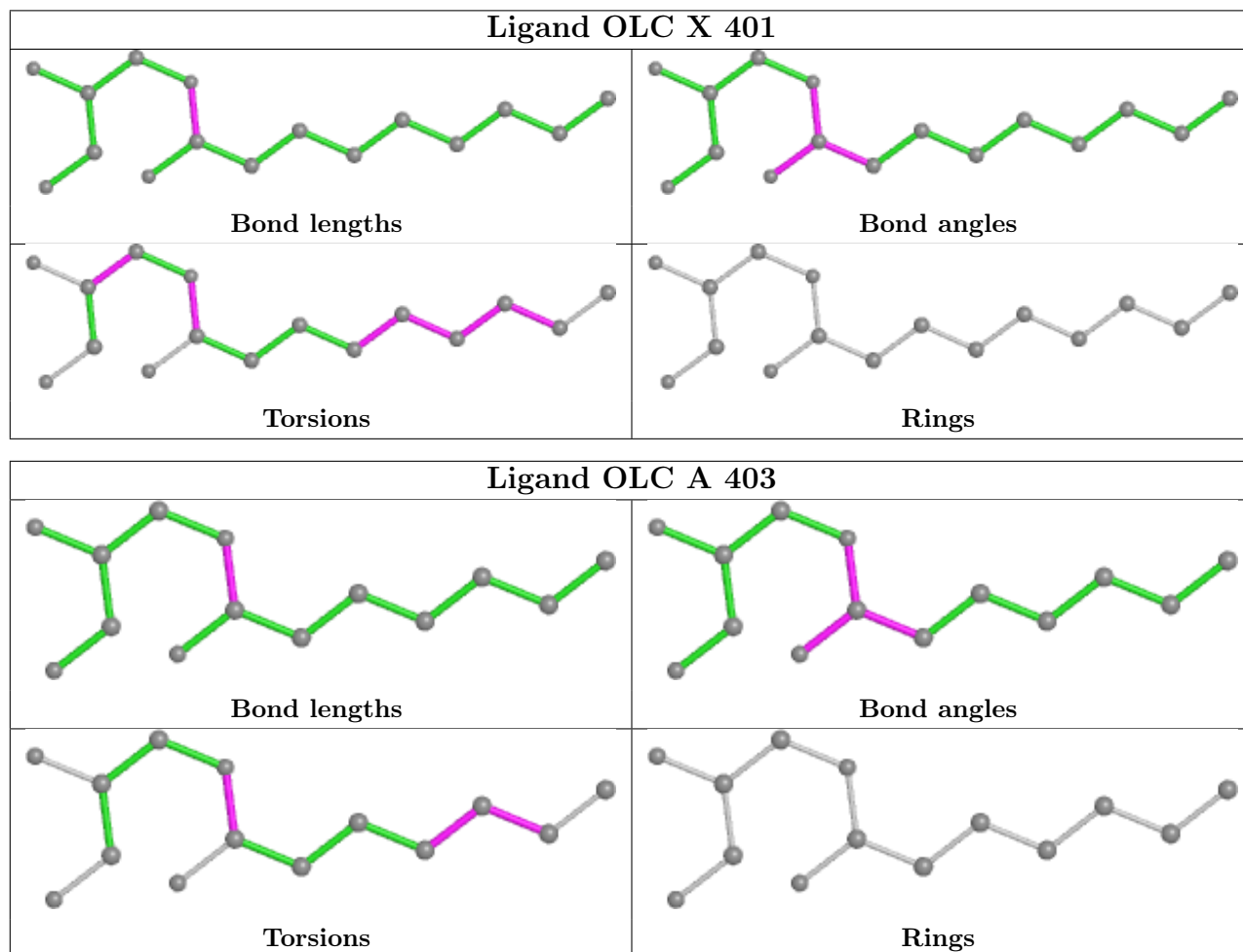
Mol	Chain	Res	Type	Atoms
5	A	402	OLC	O20-C21-C22-C24
5	X	401	OLC	C4-C5-C6-C7
5	A	404	OLC	C6-C7-C8-C9
5	X	401	OLC	C5-C6-C7-C8
5	A	404	OLC	C2-C3-C4-C5
4	X	402	JQ9	C22-C21-N3-C2
5	A	407	OLC	O23-C22-C24-O25
5	A	404	OLC	C11-C12-C13-C14
5	X	405	OLC	C4-C5-C6-C7
5	A	405	OLC	C1-C2-C3-C4
4	X	402	JQ9	C3'-C4'-O4'-C8'
5	A	408	OLC	C5-C6-C7-C8
5	A	403	OLC	C3-C4-C5-C6
5	X	401	OLC	C3-C4-C5-C6
5	X	404	OLC	O23-C22-C24-O25
5	A	407	OLC	C3-C4-C5-C6
5	A	403	OLC	C4-C5-C6-C7
4	X	402	JQ9	C12-C11-N1-C6
5	X	404	OLC	C2-C1-O20-C21
5	X	401	OLC	C6-C7-C8-C9
5	A	407	OLC	O20-C21-C22-O23
5	X	404	OLC	O19-C1-O20-C21
5	X	403	OLC	C1-C2-C3-C4
5	X	405	OLC	C3-C4-C5-C6
5	X	403	OLC	C3-C4-C5-C6
5	A	405	OLC	C5-C6-C7-C8
4	X	402	JQ9	C5'-C4'-O4'-C8'
5	X	404	OLC	C3-C4-C5-C6
5	X	404	OLC	C2-C3-C4-C5
5	A	405	OLC	C4-C5-C6-C7
5	A	404	OLC	C7-C8-C9-C10
4	X	402	JQ9	C2'-C1'-CB-CA
5	A	402	OLC	C2-C3-C4-C5
5	A	407	OLC	O20-C1-C2-C3
5	X	403	OLC	C4-C5-C6-C7
5	A	405	OLC	C2-C3-C4-C5
4	A	401	JQ9	C12-C11-N1-C6
5	A	404	OLC	C9-C10-C11-C12
5	A	402	OLC	C5-C6-C7-C8
5	A	407	OLC	O19-C1-C2-C3
5	X	404	OLC	C7-C8-C9-C10
4	X	402	JQ9	C6'-C1'-CB-CA

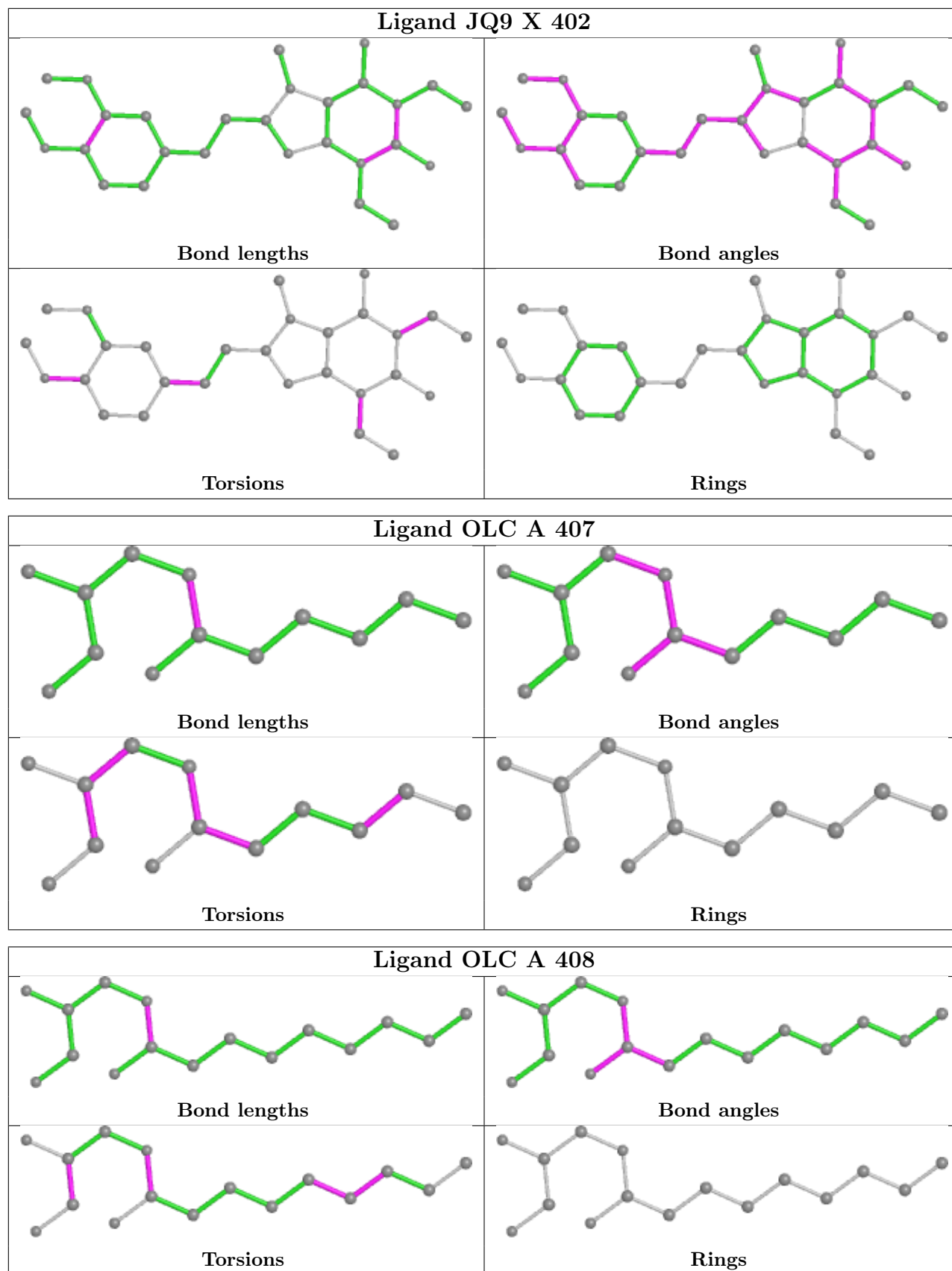
There are no ring outliers.

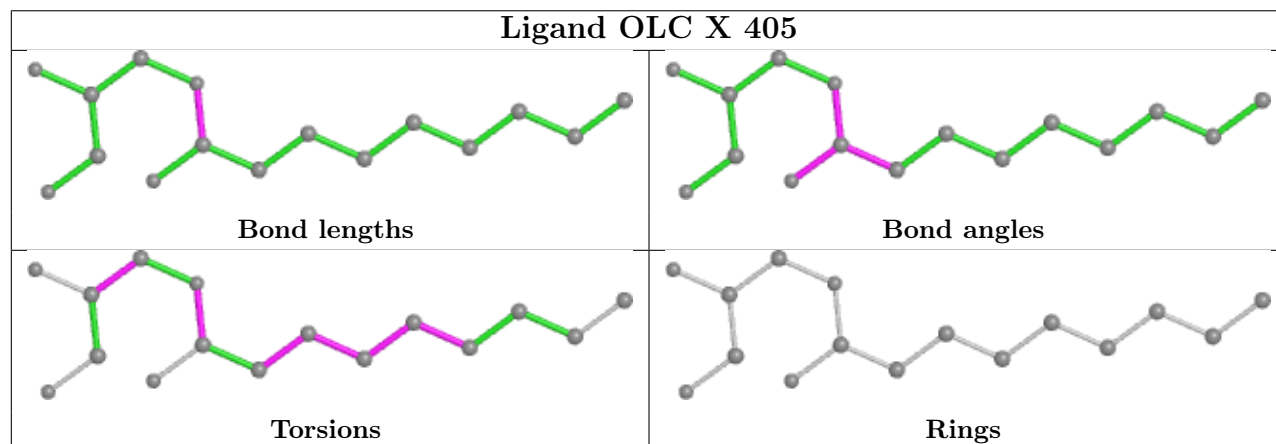
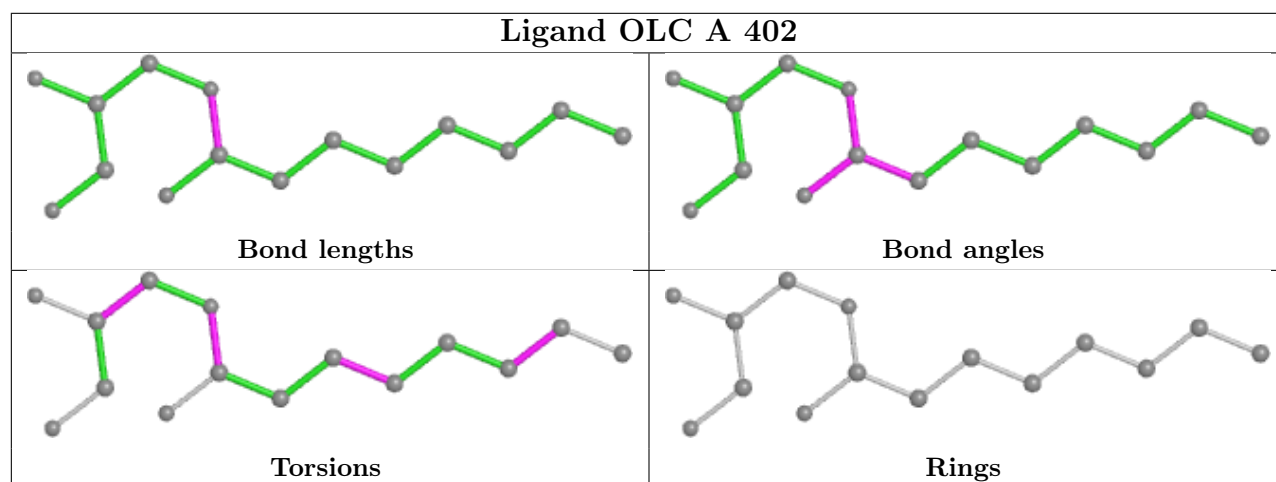
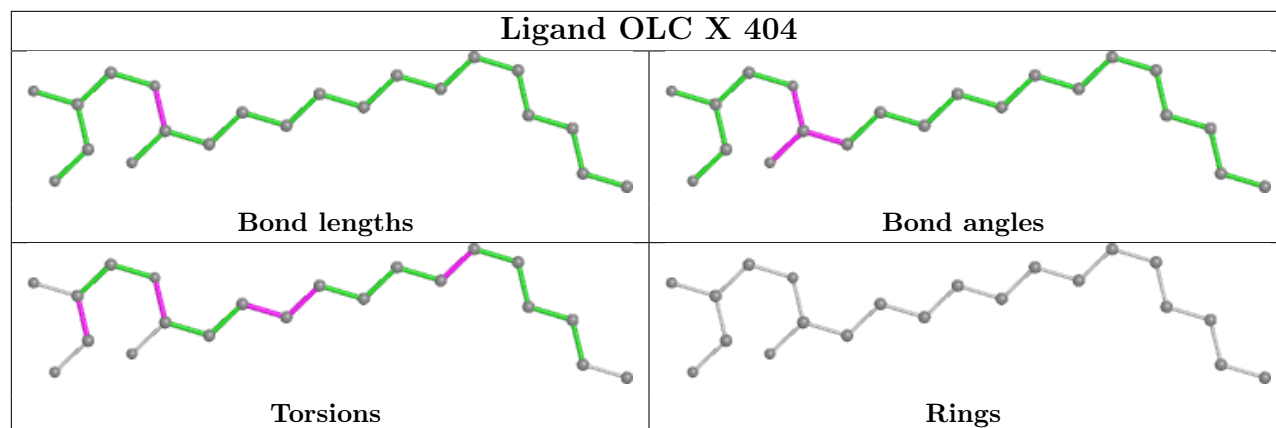
3 monomers are involved in 3 short contacts:

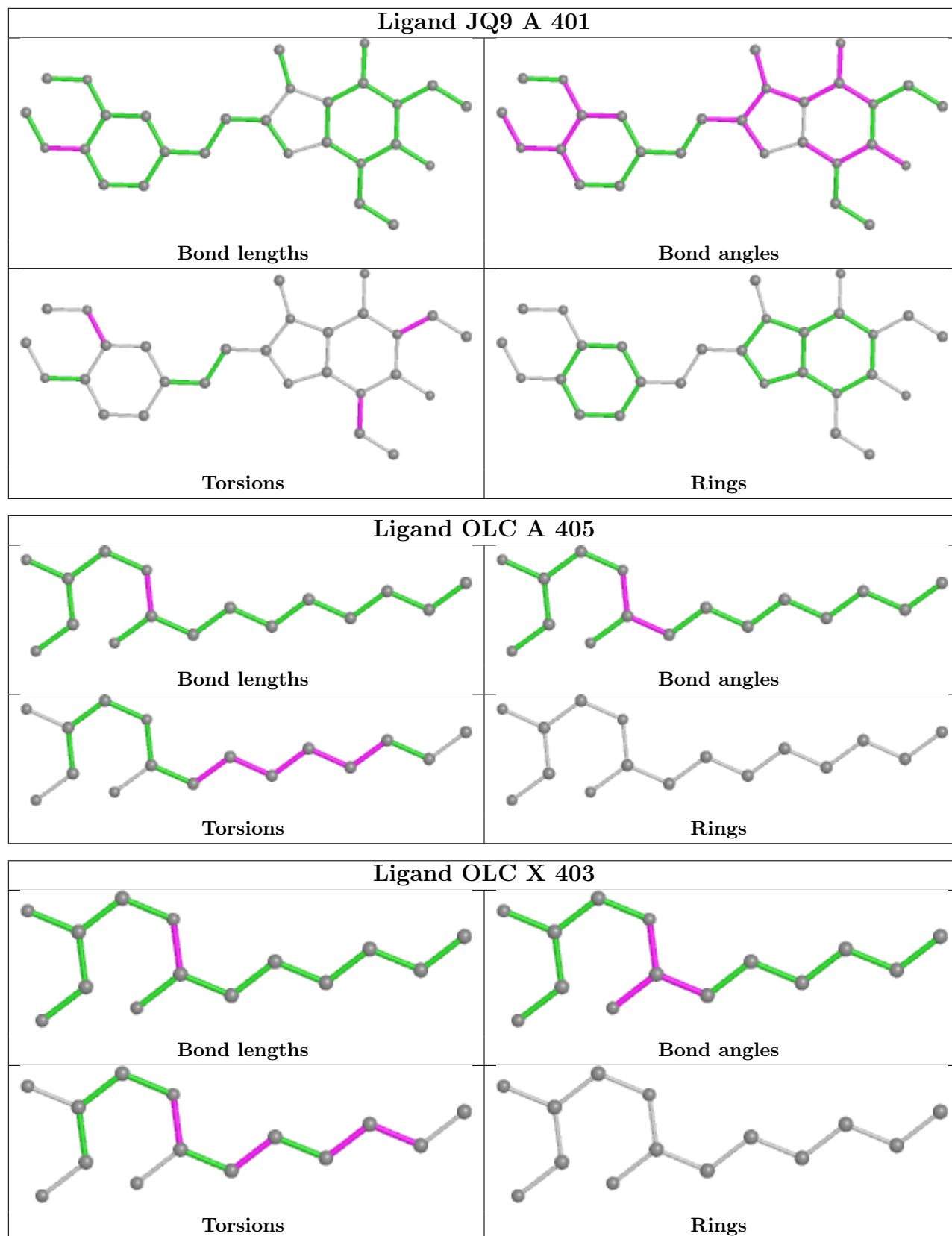
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	OLC	1	0
4	X	402	JQ9	1	0
5	A	404	OLC	1	0

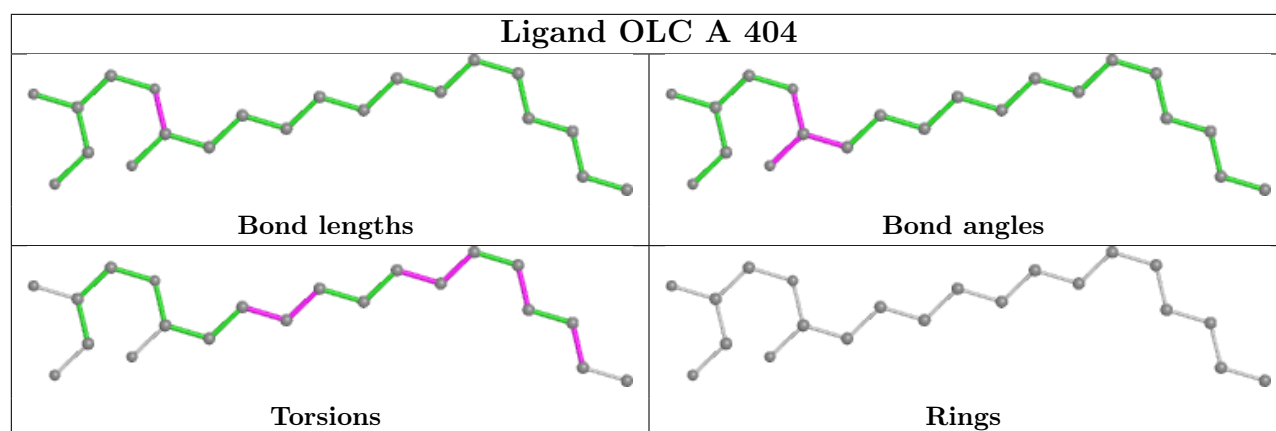
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	287/333 (86%)	-0.33	3 (1%) 82 72	36, 46, 69, 86	0
1	X	285/333 (85%)	-0.29	0 100 100	37, 47, 69, 86	0
2	L	212/214 (99%)	-0.15	0 100 100	30, 42, 59, 67	0
2	Y	212/214 (99%)	-0.12	0 100 100	34, 43, 60, 67	0
3	H	222/226 (98%)	-0.24	0 100 100	30, 42, 59, 64	0
3	Z	222/226 (98%)	-0.15	2 (0%) 84 75	33, 44, 59, 65	0
All	All	1440/1546 (93%)	-0.22	5 (0%) 94 92	30, 44, 64, 86	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	CYS	2.4
1	A	260	PRO	2.3
1	A	163	GLN	2.2
3	Z	1	GLU	2.2
3	Z	200	PRO	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands

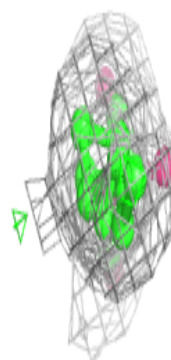
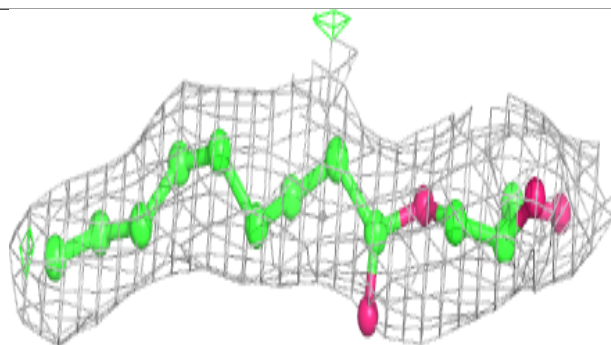
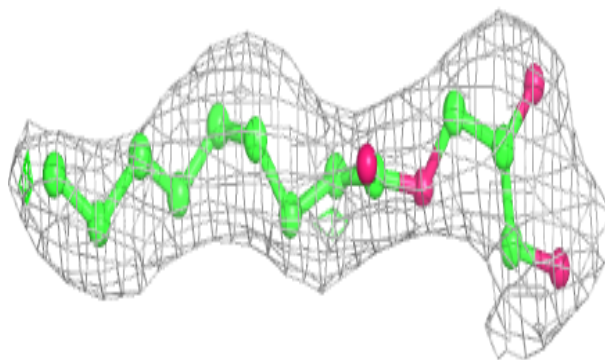
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	OLC	X	405	16/25	0.81	0.25	41,51,58,64	0
5	OLC	A	407	13/25	0.82	0.47	44,51,54,55	0
6	CL	X	406	1/1	0.84	0.15	34,34,34,34	0
5	OLC	A	405	16/25	0.85	0.20	37,41,44,48	0
5	OLC	A	402	15/25	0.85	0.39	39,42,45,46	0
6	CL	A	406	1/1	0.87	0.12	48,48,48,48	0
5	OLC	X	404	21/25	0.87	0.49	48,51,71,72	0
5	OLC	A	403	14/25	0.88	0.43	45,51,54,54	0
5	OLC	A	408	16/25	0.88	0.35	47,61,67,70	0
4	JQ9	X	402	28/28	0.88	0.30	56,63,77,78	0
5	OLC	X	403	14/25	0.89	0.36	42,51,53,54	0
5	OLC	A	404	21/25	0.90	0.36	37,41,44,45	0
5	OLC	X	401	16/25	0.91	0.28	35,44,55,56	0
4	JQ9	A	401	28/28	0.93	0.29	53,58,68,69	0
7	K	L	301	1/1	0.97	0.13	36,36,36,36	0
7	K	Y	301	1/1	0.98	0.07	34,34,34,34	0

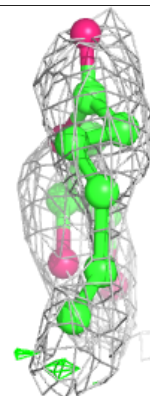
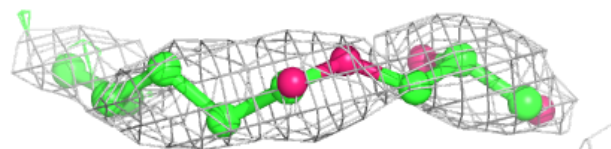
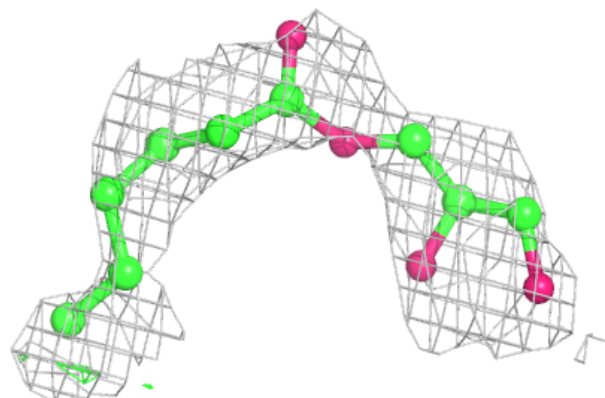
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC X 405:**

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

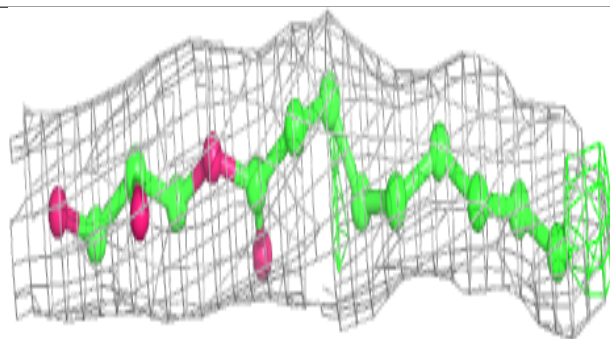
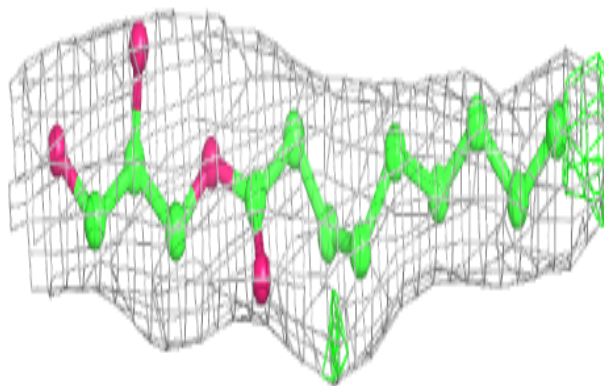
**Electron density around OLC A 407:**

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

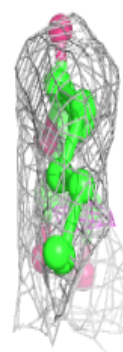
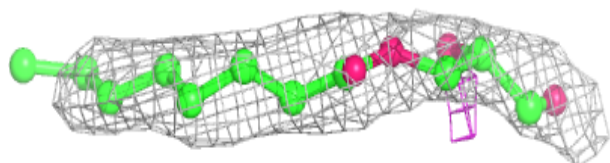
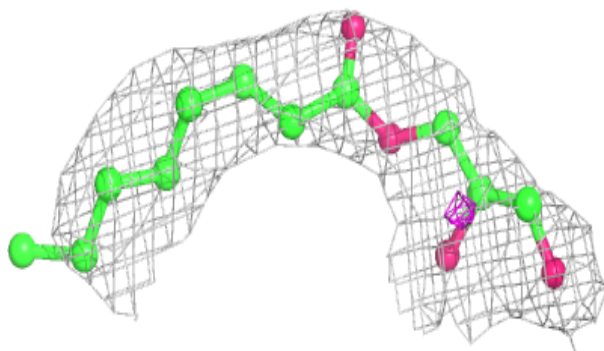


**Electron density around OLC A 405:**

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

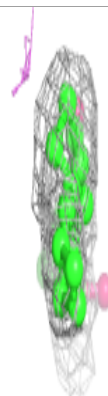
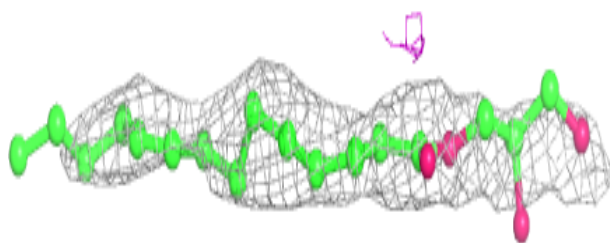
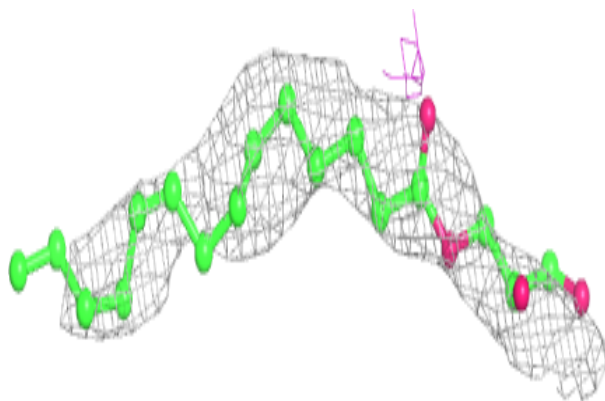
**Electron density around OLC A 402:**

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

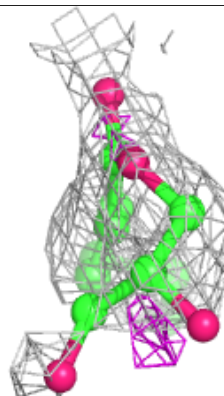
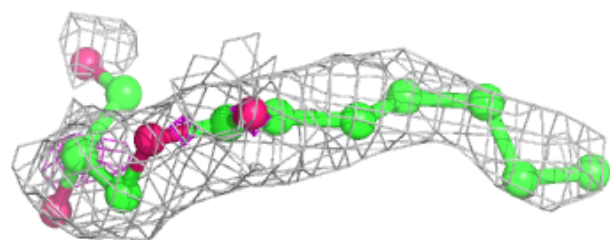
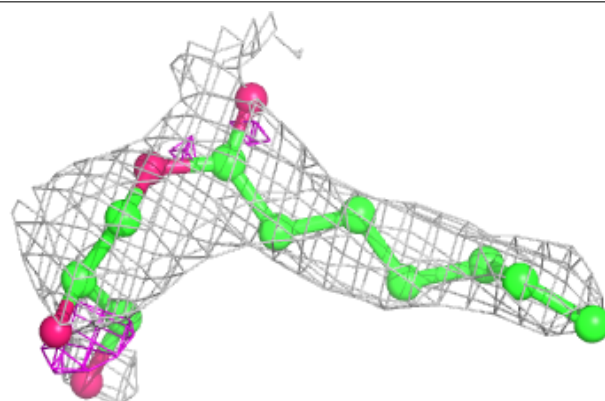


**Electron density around OLC X 404:**

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

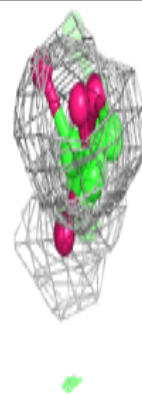
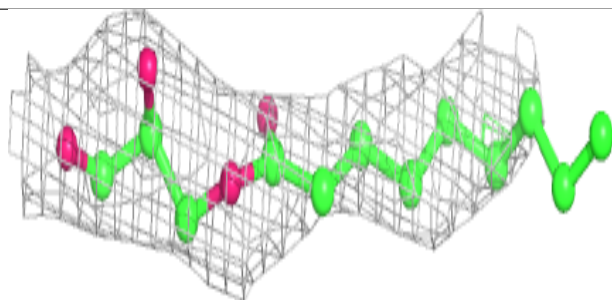
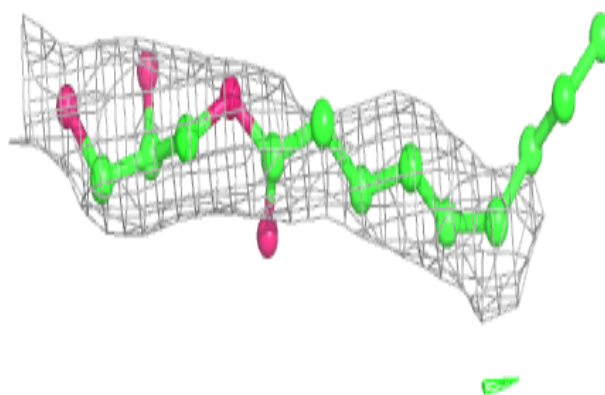
**Electron density around OLC A 403:**

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

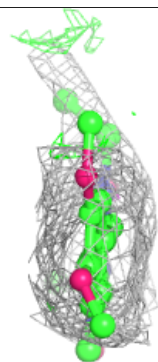
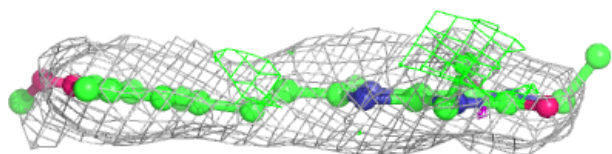
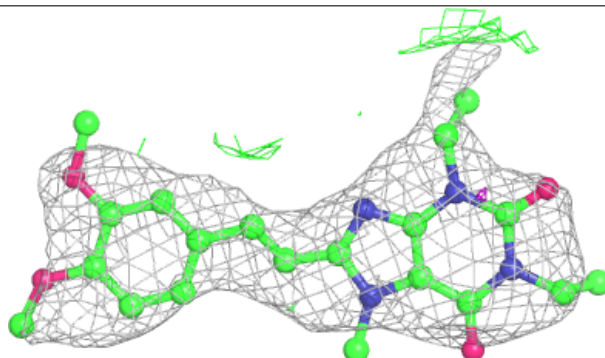


**Electron density around OLC A 408:**

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

**Electron density around JQ9 X 402:**

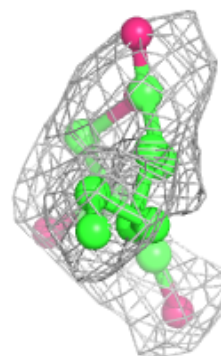
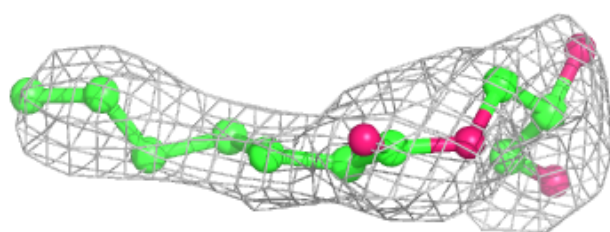
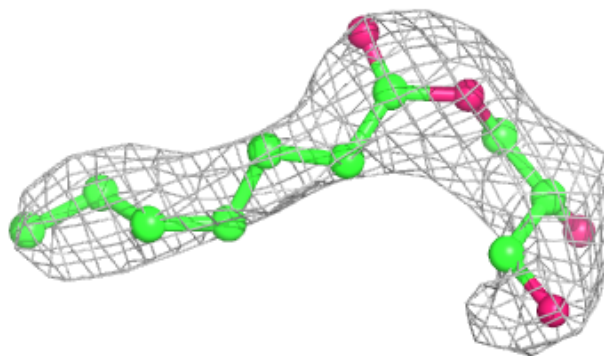
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



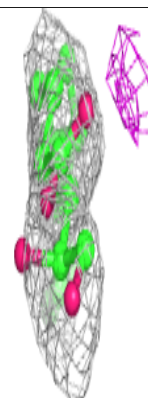
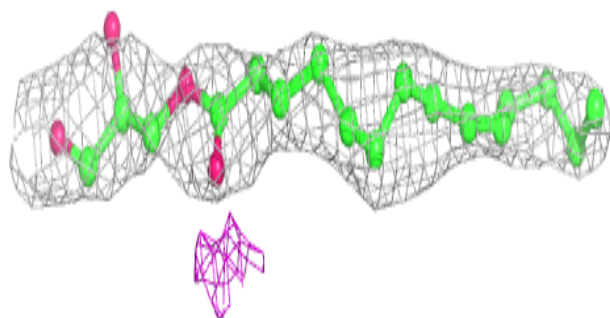
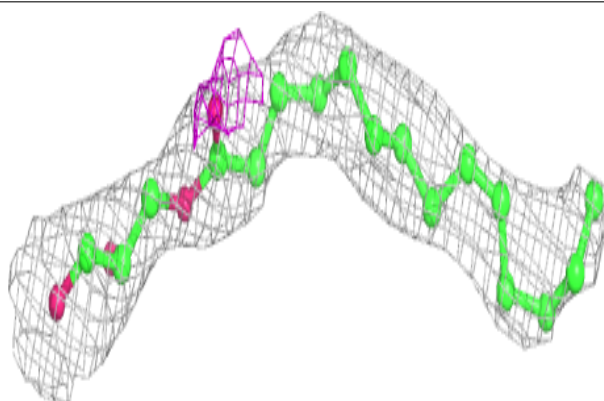


**Electron density around OLC X 403:**

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

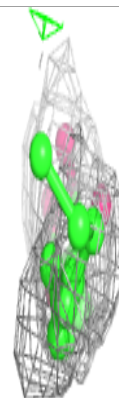
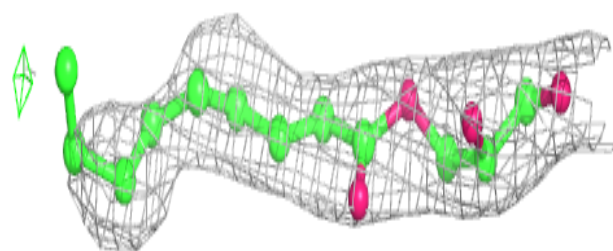
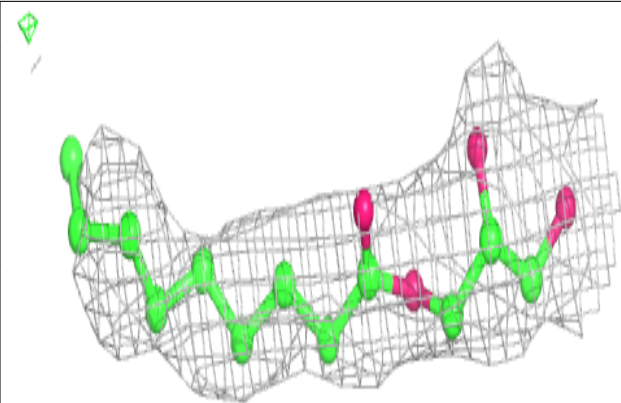
**Electron density around OLC A 404:**

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

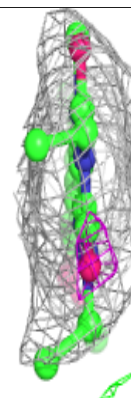
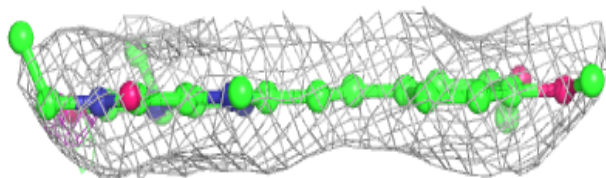
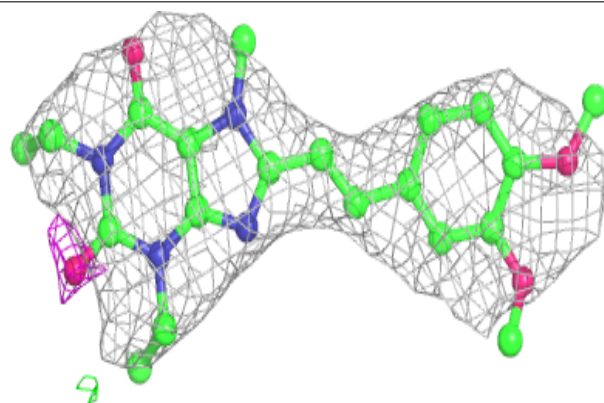


**Electron density around OLC X 401:**

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

**Electron density around JQ9 A 401:**

$2mF_o-DF_c$  (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.