



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:29 am BST

PDB ID : 1DMH  
Title : STRUCTURE OF CATECHOL 1,2-DIOXYGENASE FROM ACINETO-  
BACTER SP. ADP1 WITH BOUND 4-METHYLCATECHOL  
Authors : Vetting, M.W.; Ohlendorf, D.H.  
Deposited on : 1999-12-14  
Resolution : 1.70 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 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

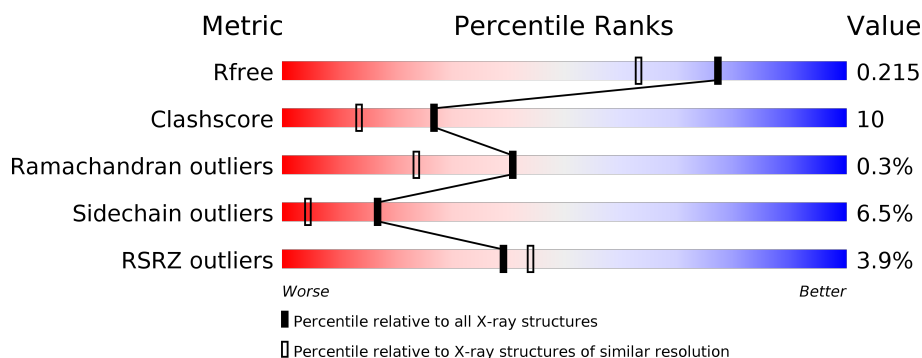
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	311	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>...</div> </div> </div>
1	B	311	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>16%</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
3	MCT	A	401	-	-	X	-
3	MCT	B	401	-	-	X	-
4	LIO	A	1999	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5190 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.

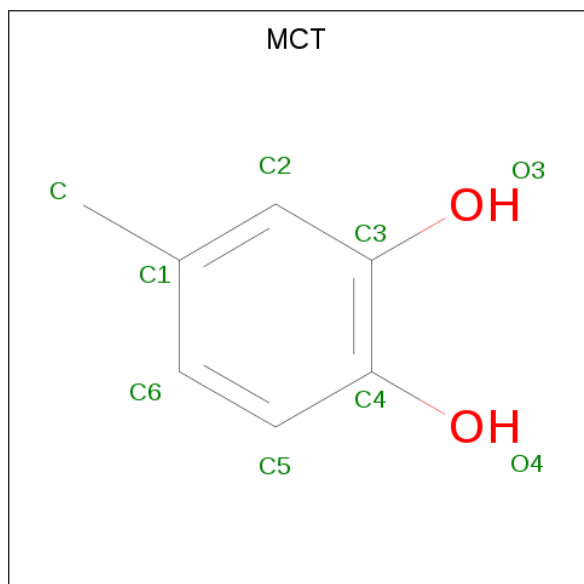
- Molecule 1 is a protein called CATECHOL 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2407	1509	423	469	6			
1	B	309	Total	C	N	O	S	0	0	0
			2407	1509	423	469	6			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

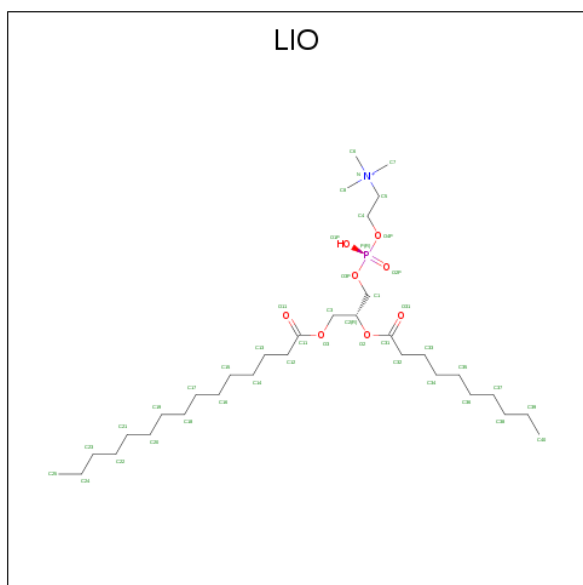
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 4-METHYLCATECHOL (three-letter code: MCT) (formula: C<sub>7</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0

- Molecule 4 is [1-PENTADECANOYL-2-DECANOYL-GLYCEROL-3-YL]PHOSPHONYL CHOLINE (three-letter code: LIO) (formula:  $C_{33}H_{67}NO_8P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 43 33 1 8 1	0	0
4	B	1	Total C N O P 43 33 1 8 1	0	0

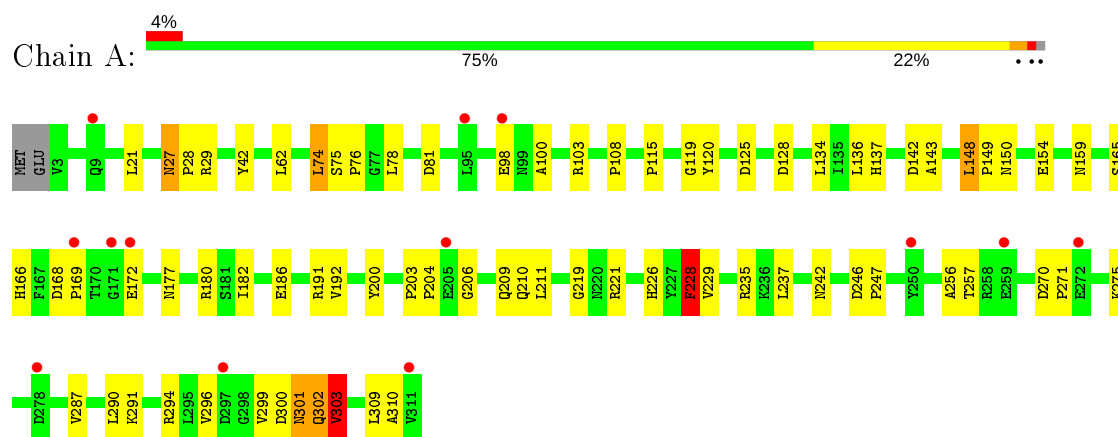
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	126	Total O 126 126	0	0
5	B	144	Total O 144 144	0	0

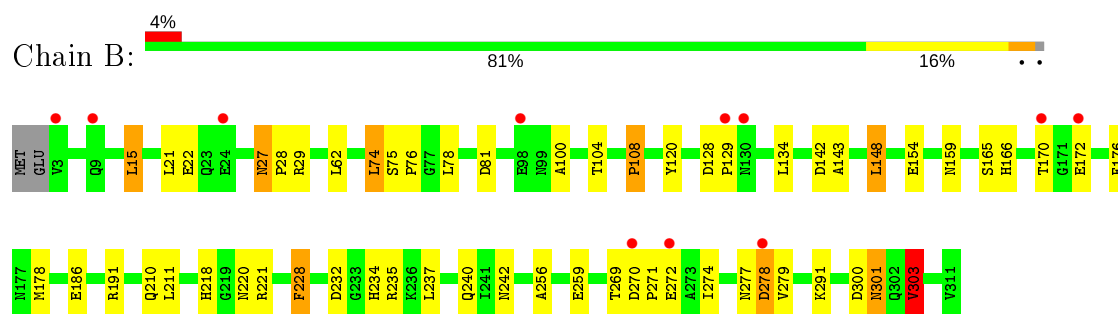
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: CATECHOL 1,2-DIOXYGENASE



#### • Molecule 1: CATECHOL 1,2-DIOXYGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.80Å 88.00Å 84.40Å 90.00° 96.30° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.91 – 1.69	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-1.70) 85.8 (19.91-1.69)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.185 , 0.218 0.184 , 0.215	Depositor DCC
$R_{free}$ test set	7315 reflections (9.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5190	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LIO, FE, MCT

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	0.54	0/2463	0.81	3/3351 (0.1%)
1	B	0.53	0/2463	0.77	2/3351 (0.1%)
All	All	0.53	0/4926	0.79	5/6702 (0.1%)

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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	172	GLU	CA-C-O	5.78	132.24	120.10
1	A	303	VAL	CB-CA-C	-5.29	101.35	111.40
1	B	303	VAL	CB-CA-C	-5.08	101.75	111.40
1	A	228	PHE	N-CA-C	-5.07	97.31	111.00
1	B	15	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	TYR	Sidechain



## 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	2407	0	2300	50	0
1	B	2407	0	2300	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	9	0	6	4	0
3	B	9	0	6	6	0
4	A	43	0	66	0	0
4	B	43	0	66	0	0
5	A	126	0	0	1	0
5	B	144	0	0	5	0
All	All	5190	0	4744	99	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 (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:401:MCT:C3	5:B:503:HOH:O	1.76	1.24
1:B:170:THR:OG1	1:B:172:GLU:HG3	1.67	0.93
1:B:218:HIS:HD2	1:B:220:ASN:H	1.03	0.92
1:B:166:HIS:CE1	1:B:176:PHE:H	1.91	0.88
1:B:166:HIS:HE1	1:B:176:PHE:H	1.22	0.86
1:B:218:HIS:CD2	1:B:220:ASN:H	1.94	0.84
1:A:235:ARG:HH11	1:A:301:ASN:HD21	1.24	0.84
1:B:235:ARG:HH11	1:B:301:ASN:HD21	1.31	0.79
1:B:301:ASN:HD22	1:B:301:ASN:H	1.32	0.78
3:B:401:MCT:C4	5:B:503:HOH:O	2.13	0.74
1:A:103:ARG:HH21	1:A:302:GLN:HE21	1.35	0.73
3:B:401:MCT:O3	5:B:503:HOH:O	1.92	0.72
1:B:27:ASN:HD22	1:B:27:ASN:C	1.92	0.72
1:A:115:PRO:HG2	1:A:180:ARG:HD3	1.71	0.72
1:B:143:ALA:H	1:B:234:HIS:HE1	1.37	0.70
1:A:301:ASN:HD22	1:A:301:ASN:H	1.38	0.70
1:A:182:ILE:HD11	1:A:192:VAL:HG12	1.75	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:HB2	1:A:228:PHE:HB2	1.73	0.69
1:A:186:GLU:CD	1:A:186:GLU:H	1.96	0.69
1:B:240:GLN:NE2	5:B:752:HOH:O	2.26	0.68
1:B:74:LEU:HD22	1:B:78:LEU:HG	1.74	0.68
1:B:170:THR:OG1	1:B:172:GLU:CG	2.41	0.67
1:A:301:ASN:HD22	1:A:301:ASN:N	1.92	0.67
1:B:142:ASP:HB3	1:B:148:LEU:HG	1.76	0.66
1:B:242:ASN:HB3	5:B:613:HOH:O	1.97	0.63
1:B:218:HIS:HD2	1:B:220:ASN:N	1.87	0.62
1:B:186:GLU:H	1:B:186:GLU:CD	2.02	0.62
1:A:242:ASN:HB3	5:A:662:HOH:O	1.98	0.62
1:A:74:LEU:HD22	1:A:78:LEU:HG	1.83	0.61
1:A:27:ASN:HD22	1:A:27:ASN:C	2.02	0.60
1:B:274:ILE:HG23	1:B:279:VAL:HG23	1.83	0.60
1:A:206:GLY:O	1:A:210:GLN:HG2	2.03	0.58
1:B:100:ALA:CB	1:B:291:LYS:HD3	2.34	0.58
1:A:242:ASN:ND2	1:A:257:THR:HG22	2.17	0.58
1:B:300:ASP:CG	1:B:303:VAL:HG22	2.24	0.58
1:B:143:ALA:H	1:B:234:HIS:CE1	2.21	0.57
1:A:142:ASP:HB3	1:A:148:LEU:HG	1.86	0.57
1:A:182:ILE:CD1	1:A:192:VAL:CG1	2.83	0.56
1:B:159:ASN:HB3	1:B:178:MET:HE1	1.86	0.56
1:B:166:HIS:HE1	1:B:176:PHE:N	1.99	0.55
1:A:226:HIS:CE1	3:A:401:MCT:O3	2.58	0.55
1:A:125:ASP:H	1:A:177:ASN:HD21	1.53	0.55
1:A:182:ILE:HD11	1:A:192:VAL:CG1	2.36	0.55
1:B:76:PRO:HG3	3:B:401:MCT:C	2.36	0.55
1:B:154:GLU:HB2	1:B:228:PHE:HB2	1.88	0.55
1:A:209:GLN:HE22	1:A:219:GLY:HA3	1.73	0.54
1:A:100:ALA:CB	1:A:291:LYS:HD3	2.38	0.53
1:A:115:PRO:HG2	1:A:180:ARG:CD	2.39	0.52
1:B:221:ARG:HH11	3:B:401:MCT:C3	2.23	0.52
1:A:242:ASN:HD21	1:A:257:THR:HG22	1.75	0.51
1:A:300:ASP:CG	1:A:303:VAL:HG22	2.31	0.51
1:A:182:ILE:CD1	1:A:192:VAL:HG12	2.40	0.51
1:B:27:ASN:C	1:B:27:ASN:ND2	2.62	0.51
1:B:104:THR:HG21	1:B:240:GLN:HG2	1.93	0.50
1:A:301:ASN:ND2	1:A:301:ASN:H	2.07	0.49
1:A:309:LEU:HD23	1:A:310:ALA:N	2.28	0.49
1:B:301:ASN:HD22	1:B:301:ASN:N	2.05	0.49
1:A:229:VAL:HG21	1:A:290:LEU:HD22	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HH11	3:A:401:MCT:C3	2.25	0.48
1:B:27:ASN:ND2	1:B:29:ARG:H	2.11	0.48
1:B:235:ARG:HH11	1:B:301:ASN:ND2	2.06	0.47
1:A:137:HIS:CE1	1:A:287:VAL:HG22	2.50	0.47
1:B:108:PRO:HD3	3:B:401:MCT:H3	1.96	0.47
1:A:128:ASP:OD2	1:A:159:ASN:HB2	2.15	0.47
1:A:76:PRO:HG3	3:A:401:MCT:H3	1.97	0.46
1:B:259:GLU:HA	1:B:259:GLU:OE1	2.16	0.46
1:A:221:ARG:NH2	1:A:256:ALA:HB3	2.30	0.45
1:A:143:ALA:CB	1:A:294:ARG:HG3	2.46	0.45
1:A:149:PRO:O	1:A:150:ASN:HB2	2.15	0.45
1:A:301:ASN:N	1:A:301:ASN:ND2	2.63	0.45
1:B:142:ASP:O	1:B:291:LYS:NZ	2.49	0.45
1:B:232:ASP:O	1:B:234:HIS:HD2	2.00	0.45
1:B:277:ASN:O	1:B:279:VAL:HG13	2.18	0.43
1:B:120:TYR:HA	1:B:191:ARG:O	2.18	0.43
1:B:27:ASN:HD22	1:B:28:PRO:N	2.16	0.43
1:A:275:LYS:HE3	1:A:275:LYS:HB2	1.69	0.43
1:A:200:TYR:CG	3:A:401:MCT:H5	2.53	0.43
1:B:221:ARG:NH2	1:B:256:ALA:HB3	2.33	0.43
1:B:301:ASN:ND2	1:B:301:ASN:H	2.08	0.43
1:A:246:ASP:HA	1:A:247:PRO:HD3	1.89	0.43
1:A:75:SER:HB3	1:A:76:PRO:CD	2.49	0.43
1:A:242:ASN:CG	1:A:257:THR:HG22	2.39	0.43
1:B:165:SER:O	1:B:166:HIS:HB2	2.19	0.43
1:A:27:ASN:HA	1:A:28:PRO:HD2	1.80	0.42
1:A:290:LEU:HD12	1:A:290:LEU:N	2.34	0.42
1:B:270:ASP:OD1	1:B:272:GLU:HB2	2.19	0.42
1:A:270:ASP:HA	1:A:271:PRO:HD3	1.86	0.42
1:A:296:VAL:O	1:A:299:VAL:HG22	2.19	0.42
1:B:270:ASP:HA	1:B:271:PRO:HD3	1.82	0.42
1:A:165:SER:O	1:A:166:HIS:HB2	2.20	0.42
1:A:27:ASN:ND2	1:A:29:ARG:H	2.18	0.42
1:B:75:SER:HB3	1:B:76:PRO:CD	2.50	0.42
1:A:120:TYR:HA	1:A:191:ARG:O	2.20	0.42
1:B:277:ASN:O	1:B:278:ASP:C	2.58	0.41
1:B:128:ASP:HA	1:B:129:PRO:HD3	1.84	0.41
1:A:168:ASP:HA	1:A:169:PRO:HD2	1.91	0.41
1:A:203:PRO:HA	1:A:204:PRO:HD2	1.92	0.41
1:A:27:ASN:ND2	1:A:27:ASN:C	2.72	0.40
1:B:170:THR:CB	1:B:172:GLU:HG3	2.48	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	307/311 (99%)	300 (98%)	6 (2%)	1 (0%)	41	24
1	B	307/311 (99%)	298 (97%)	8 (3%)	1 (0%)	41	24
All	All	614/622 (99%)	598 (97%)	14 (2%)	2 (0%)	41	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	278	ASP
1	A	119	GLY

### 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	252/254 (99%)	236 (94%)	16 (6%)	18	5
1	B	252/254 (99%)	235 (93%)	17 (7%)	16	4
All	All	504/508 (99%)	471 (94%)	33 (6%)	17	4

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	27	ASN
1	A	62	LEU
1	A	74	LEU
1	A	81	ASP
1	A	98	GLU
1	A	108	PRO
1	A	134	LEU
1	A	136	LEU
1	A	148	LEU
1	A	211	LEU
1	A	228	PHE
1	A	237	LEU
1	A	301	ASN
1	A	302	GLN
1	A	303	VAL
1	B	15	LEU
1	B	21	LEU
1	B	22	GLU
1	B	27	ASN
1	B	62	LEU
1	B	74	LEU
1	B	81	ASP
1	B	108	PRO
1	B	134	LEU
1	B	148	LEU
1	B	210	GLN
1	B	211	LEU
1	B	228	PHE
1	B	237	LEU
1	B	269	THR
1	B	301	ASN
1	B	303	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	49	ASN
1	A	150	ASN
1	A	177	ASN
1	A	209	GLN
1	A	210	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	301	ASN
1	A	302	GLN
1	B	27	ASN
1	B	35	HIS
1	B	49	ASN
1	B	64	GLN
1	B	68	ASN
1	B	150	ASN
1	B	166	HIS
1	B	174	GLN
1	B	177	ASN
1	B	209	GLN
1	B	210	GLN
1	B	218	HIS
1	B	234	HIS
1	B	240	GLN
1	B	301	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	MCT	B	401	2	9,9,9	2.38	1 (11%)	12,12,12	1.59	4 (33%)
4	LIO	A	1999	-	42,42,42	1.56	4 (9%)	48,50,50	1.64	6 (12%)
3	MCT	A	401	2	9,9,9	2.12	1 (11%)	12,12,12	1.61	4 (33%)
4	LIO	B	999	-	42,42,42	1.52	4 (9%)	48,50,50	1.68	6 (12%)

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	MCT	B	401	2	-	-	0/1/1/1
4	LIO	A	1999	-	-	19/46/46/46	-
3	MCT	A	401	2	-	-	0/1/1/1
4	LIO	B	999	-	-	25/46/46/46	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	MCT	C6-C5	6.58	1.50	1.38
3	A	401	MCT	C6-C5	5.65	1.49	1.38
4	A	1999	LIO	O2-C31	5.28	1.49	1.34
4	A	1999	LIO	O3-C11	5.14	1.48	1.33
4	B	999	LIO	O2-C31	5.13	1.48	1.34
4	B	999	LIO	O3-C11	4.96	1.47	1.33
4	A	1999	LIO	C1-C2	-3.86	1.38	1.50
4	A	1999	LIO	C3-C2	-3.86	1.38	1.50
4	B	999	LIO	C1-C2	-3.84	1.38	1.50
4	B	999	LIO	C3-C2	-3.81	1.39	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	LIO	O2-C31-C32	6.24	124.96	111.50
4	A	1999	LIO	O2-C31-C32	5.85	124.12	111.50
4	A	1999	LIO	O3-C3-C2	5.51	124.47	108.43
4	B	999	LIO	O3-C3-C2	5.22	123.62	108.43
4	B	999	LIO	C2-O2-C31	3.86	127.30	117.79
4	A	1999	LIO	C2-O2-C31	3.60	126.66	117.79
3	A	401	MCT	C3-C2-C1	-3.27	118.26	121.01
3	B	401	MCT	C3-C2-C1	-2.80	118.66	121.01

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	LIO	O2-C31-O31	-2.54	117.56	123.70
4	A	1999	LIO	O2-C31-O31	-2.52	117.62	123.70
4	B	999	LIO	O4P-C4-C5	2.44	121.97	109.16
3	B	401	MCT	C2-C3-C4	2.37	121.96	119.86
4	A	1999	LIO	O4P-C4-C5	2.31	121.32	109.16
3	B	401	MCT	C6-C5-C4	-2.29	118.15	120.50
3	A	401	MCT	C2-C3-C4	2.27	121.88	119.86
3	B	401	MCT	C6-C1-C2	2.27	121.36	117.95
3	A	401	MCT	C6-C1-C2	2.24	121.31	117.95
4	B	999	LIO	O2-C2-C3	2.20	116.38	108.40
4	A	1999	LIO	O2-C2-C3	2.20	116.38	108.40
3	A	401	MCT	C6-C5-C4	-2.17	118.27	120.50

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	999	LIO	C12-C11-O3-C3
4	B	999	LIO	O11-C11-O3-C3
4	B	999	LIO	C32-C31-O2-C2
4	B	999	LIO	O31-C31-O2-C2
4	A	1999	LIO	C12-C11-O3-C3
4	A	1999	LIO	O11-C11-O3-C3
4	A	1999	LIO	C32-C31-O2-C2
4	A	1999	LIO	O31-C31-O2-C2
4	B	999	LIO	C31-C32-C33-C34
4	A	1999	LIO	C33-C34-C35-C36
4	B	999	LIO	C16-C17-C18-C19
4	A	1999	LIO	C17-C18-C19-C20
4	A	1999	LIO	C36-C37-C38-C39
4	B	999	LIO	C17-C18-C19-C20
4	B	999	LIO	C1-C2-C3-O3
4	B	999	LIO	O3P-C1-C2-C3
4	B	999	LIO	C32-C33-C34-C35
4	B	999	LIO	C36-C37-C38-C39
4	A	1999	LIO	C1-C2-C3-O3
4	B	999	LIO	C12-C13-C14-C15
4	A	1999	LIO	O3P-C1-C2-C3
4	B	999	LIO	C13-C14-C15-C16
4	A	1999	LIO	C22-C23-C24-C25
4	B	999	LIO	C33-C34-C35-C36
4	B	999	LIO	O3P-C1-C2-O2

*Continued on next page...*



*Continued from previous page...*

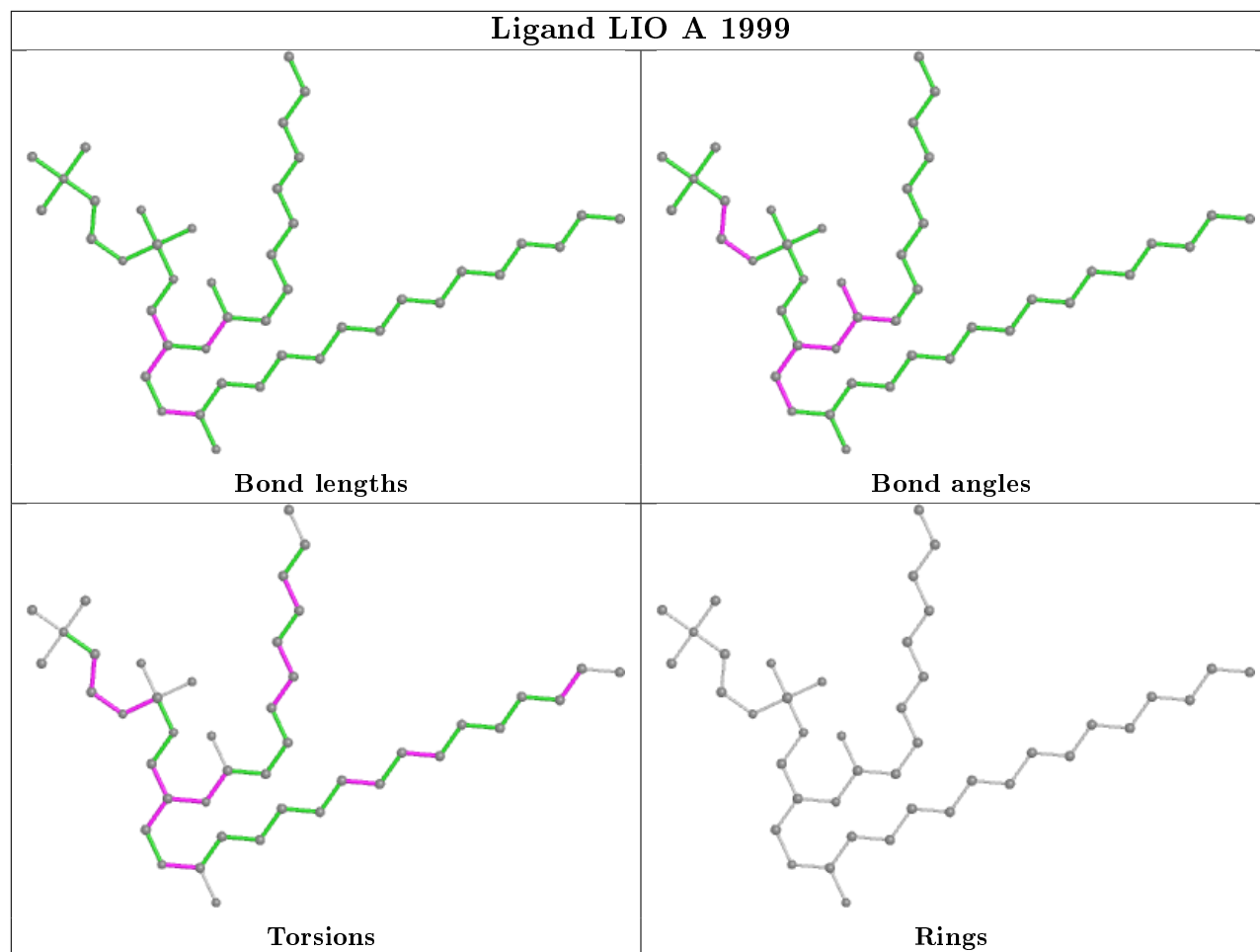
Mol	Chain	Res	Type	Atoms
4	A	1999	LIO	C34-C35-C36-C37
4	B	999	LIO	C5-C4-O4P-P
4	A	1999	LIO	C5-C4-O4P-P
4	B	999	LIO	C34-C35-C36-C37
4	A	1999	LIO	O3P-C1-C2-O2
4	B	999	LIO	O4P-C4-C5-N
4	A	1999	LIO	O4P-C4-C5-N
4	B	999	LIO	O2-C2-C3-O3
4	A	1999	LIO	C15-C16-C17-C18
4	B	999	LIO	C3-C2-O2-C31
4	A	1999	LIO	C1-C2-O2-C31
4	A	1999	LIO	C3-C2-O2-C31
4	B	999	LIO	C37-C38-C39-C40
4	A	1999	LIO	O2-C2-C3-O3
4	B	999	LIO	C4-O4P-P-O3P
4	A	1999	LIO	C4-O4P-P-O3P
4	B	999	LIO	C1-C2-O2-C31
4	B	999	LIO	O2-C31-C32-C33
4	B	999	LIO	O31-C31-C32-C33

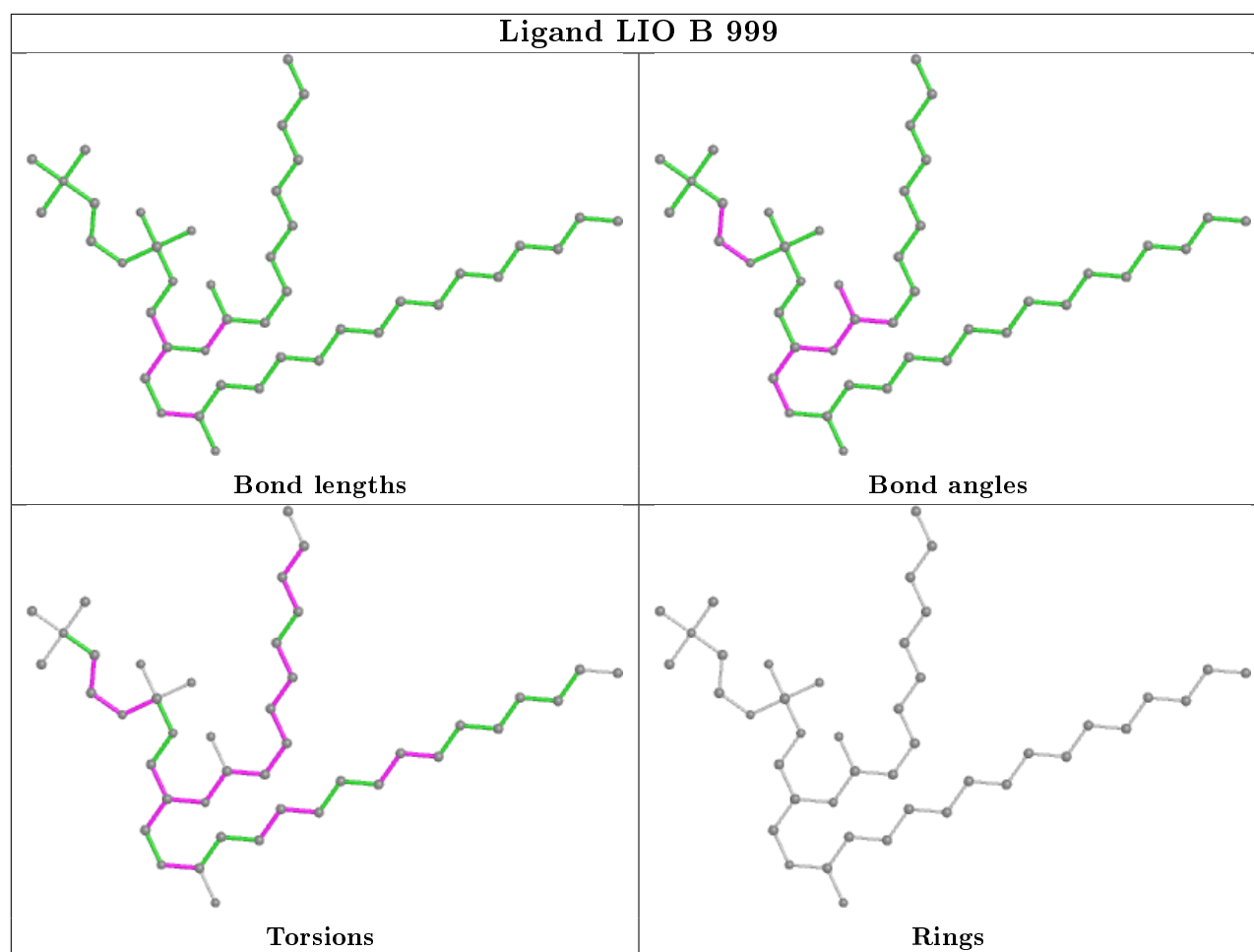
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	MCT	6	0
3	A	401	MCT	4	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, 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	309/311 (99%)	0.09	13 (4%) 36 40	9, 19, 39, 52	0
1	B	309/311 (99%)	-0.07	11 (3%) 42 47	9, 18, 40, 57	0
All	All	618/622 (99%)	0.01	24 (3%) 39 44	9, 19, 40, 57	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	GLU	5.4
1	B	129	PRO	3.5
1	B	270	ASP	3.4
1	A	272	GLU	3.4
1	A	171	GLY	3.3
1	A	297	ASP	3.1
1	A	169	PRO	2.9
1	B	172	GLU	2.8
1	A	311	VAL	2.8
1	B	272	GLU	2.7
1	A	250	TYR	2.7
1	A	278	ASP	2.6
1	A	98	GLU	2.6
1	B	130	ASN	2.6
1	B	170	THR	2.5
1	B	278	ASP	2.5
1	B	98	GLU	2.5
1	A	259	GLU	2.4
1	A	205	GLU	2.3
1	A	9	GLN	2.2
1	B	24	GLU	2.1
1	B	3	VAL	2.1
1	B	9	GLN	2.0
1	A	95	LEU	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](#)

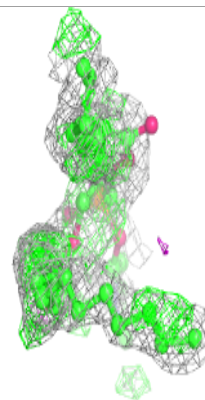
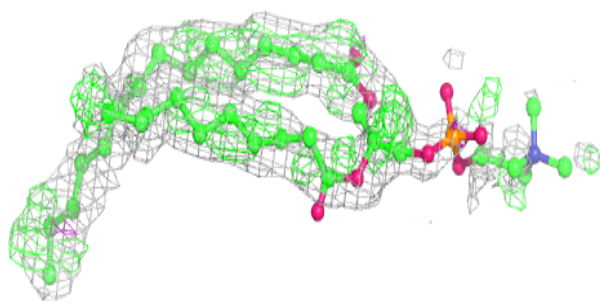
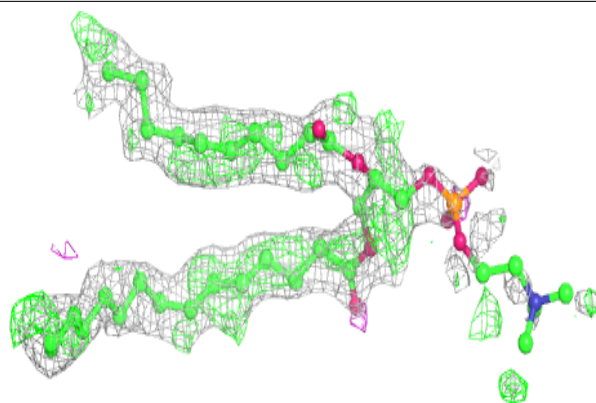
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	LIO	B	999	43/43	0.38	0.40	14,25,46,46	43
4	LIO	A	1999	43/43	0.39	0.42	12,25,45,45	43
3	MCT	B	401	9/9	0.90	0.23	19,19,20,21	9
3	MCT	A	401	9/9	0.92	0.24	21,22,22,22	9
2	FE	A	400	1/1	0.99	0.04	15,15,15,15	0
2	FE	B	400	1/1	1.00	0.04	14,14,14,14	0

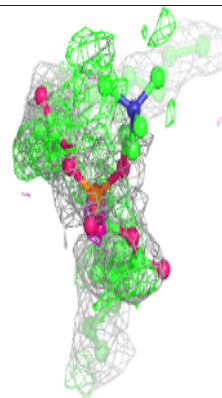
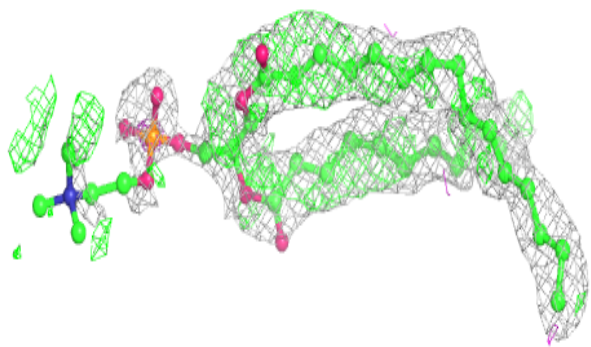
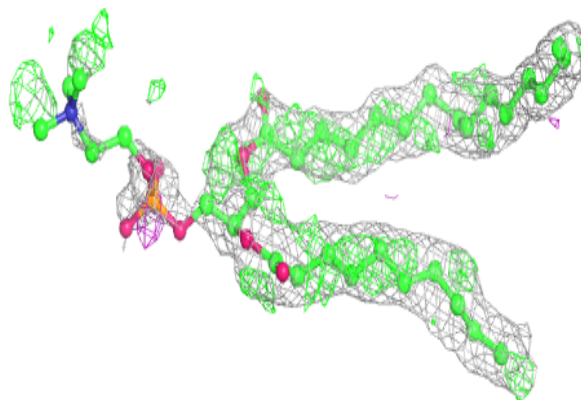
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LIO B 999:**

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

**Electron density around LIO A 1999:**

$2mF_o-DF_c$  (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.