



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:32 AM UTC

PDB ID : 1DLM / pdb_00001dlm
Title : STRUCTURE OF CATECHOL 1,2-DIOXYGENASE FROM ACINETO-
BACTER CALCOACETICUS NATIVE DATA
Authors : Vetting, M.W.; Ohlendorf, D.H.
Deposited on : 1999-12-11
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

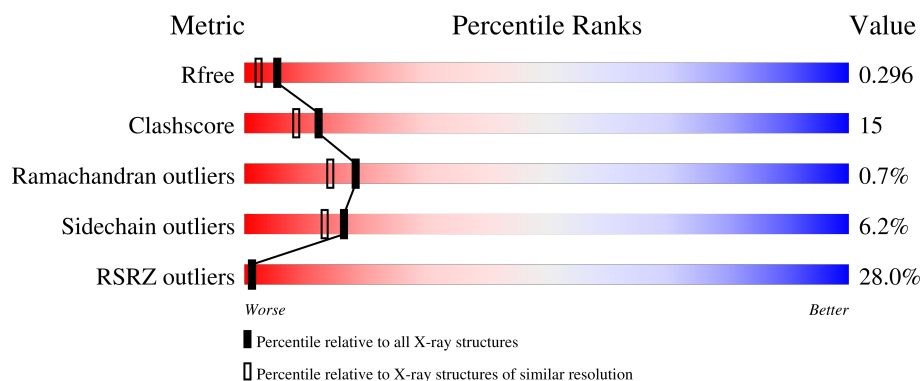
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	311	14% 66% 29% ...
1	B	311	42% 71% 25% ...

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5085 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.

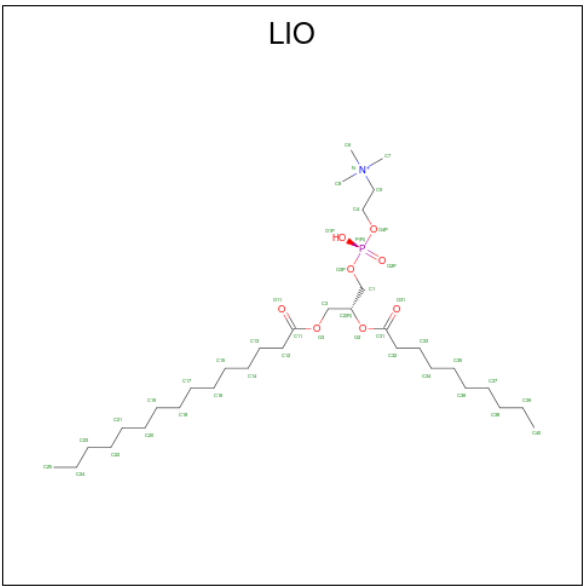
- Molecule 1 is a protein called CATECHOL 1,2-DIOXYGENASE.

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 (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is [1-PENTADECANOYL-2-DECANOYL-GLYCEROL-3-YL]PHOSPHONYL CHOLINE (CCD ID: LIO) (formula: C₃₃H₆₇NO₈P).



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

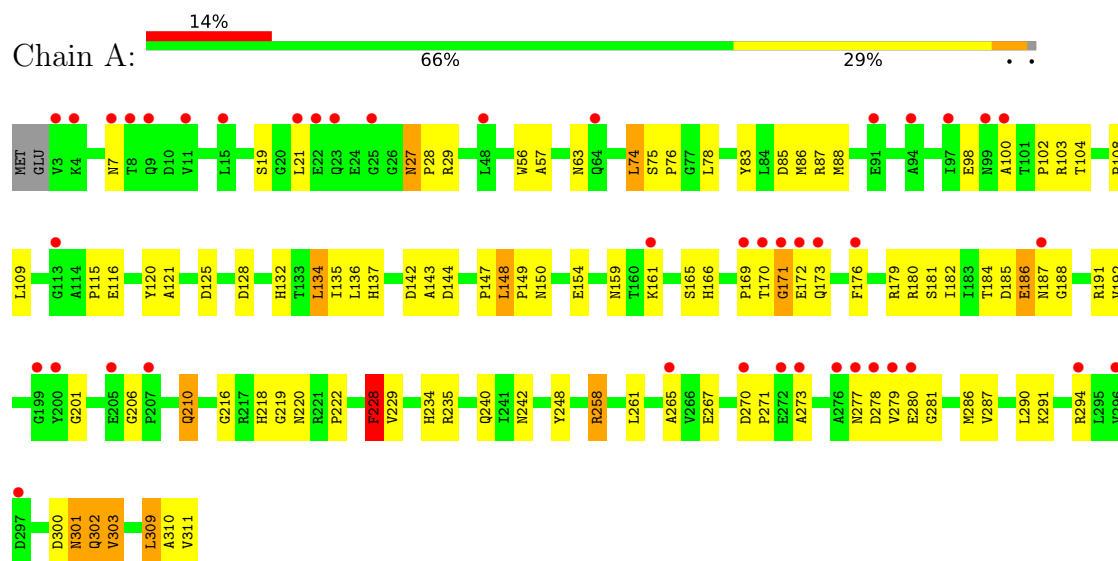
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total 88	O 88	0	0
4	B	95	Total 95	O 95	0	0

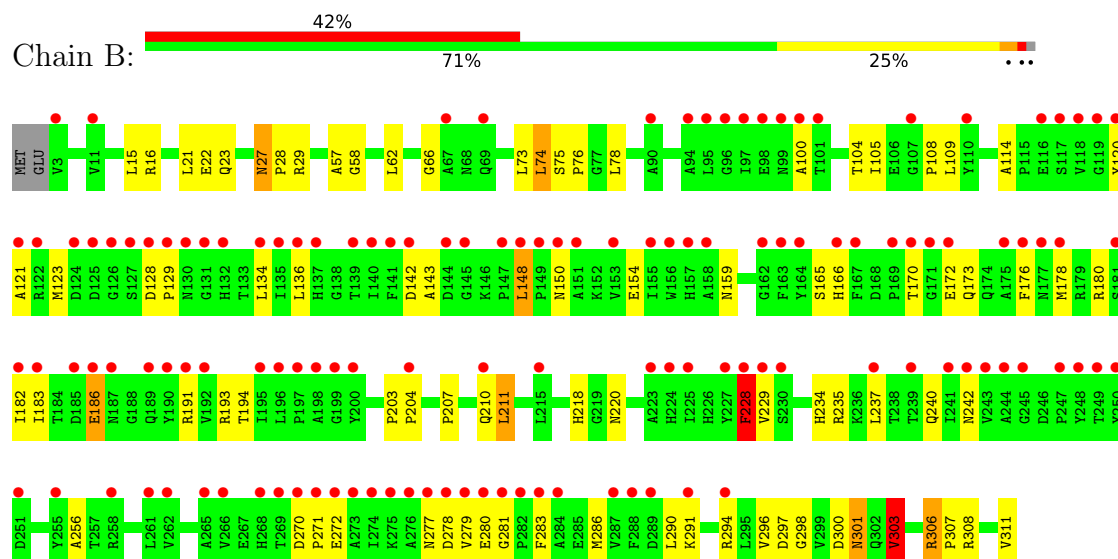
3 Residue-property plots [i](#)

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: 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, α , β , γ	52.60Å 87.60Å 84.20Å 90.00° 96.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 83.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 1.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.243 0.268 , 0.296	Depositor DCC
R_{free} test set	4718 reflections (9.21%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5085	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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: FE, LIO

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	0.44	0/2463	0.96	5/3351 (0.1%)
1	B	0.44	0/2463	0.96	6/3351 (0.2%)
All	All	0.44	0/4926	0.96	11/6702 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLN	N-CA-C	6.68	120.42	109.06
1	B	211	LEU	N-CA-C	-6.67	103.94	111.14
1	B	57	ALA	N-CA-C	-6.50	104.28	111.36
1	A	109	LEU	N-CA-C	6.14	120.09	112.59
1	B	228	PHE	N-CA-C	-6.08	98.48	108.76
1	A	228	PHE	N-CA-C	-5.83	98.59	108.26
1	A	57	ALA	N-CA-C	-5.52	105.35	111.36
1	B	109	LEU	N-CA-C	5.47	119.26	112.59
1	A	273	ALA	N-CA-C	-5.38	105.50	111.36
1	B	303	VAL	CB-CA-C	-5.28	103.24	111.26
1	B	173	GLN	N-CA-C	5.18	118.67	109.96

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	2407	0	2299	77	1
1	B	2407	0	2299	75	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	66	0	0
3	B	43	0	66	0	0
4	A	88	0	0	2	0
4	B	95	0	0	4	0
All	All	5085	0	4730	149	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (149) 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:B:170:THR:OG1	1:B:172:GLU:HG3	1.57	1.05
1:A:170:THR:O	1:A:172:GLU:HG3	1.60	0.99
1:A:235:ARG:HH11	1:A:301:ASN:HD21	1.22	0.88
1:B:301:ASN:HD22	1:B:301:ASN:H	1.25	0.85
1:B:235:ARG:HH11	1:B:301:ASN:HD21	1.25	0.84
1:B:170:THR:OG1	1:B:172:GLU:CG	2.26	0.83
1:B:306:ARG:HD3	4:B:552:HOH:O	1.82	0.80
1:B:170:THR:CB	1:B:172:GLU:HG3	2.14	0.77
1:A:218:HIS:HD2	1:A:220:ASN:H	1.30	0.77
1:B:218:HIS:HD2	1:B:220:ASN:H	1.34	0.76
1:A:229:VAL:HG21	1:A:290:LEU:HD22	1.67	0.74
1:A:103:ARG:HH21	1:A:302:GLN:HE21	1.34	0.73
1:A:206:GLY:O	1:A:210:GLN:HG2	1.89	0.73
1:A:300:ASP:CG	1:A:303:VAL:HG22	2.14	0.72
1:B:301:ASN:HD22	1:B:301:ASN:N	1.86	0.72
1:B:74:LEU:HD22	1:B:78:LEU:HG	1.73	0.71
1:A:19:SER:HB2	1:A:21:LEU:HD13	1.74	0.70
1:A:218:HIS:CD2	1:A:220:ASN:H	2.10	0.70
1:B:27:ASN:HD22	1:B:27:ASN:C	1.98	0.69
1:A:154:GLU:HB2	1:A:228:PHE:HB2	1.73	0.69
1:B:277:ASN:O	1:B:279:VAL:N	2.27	0.67
1:B:300:ASP:CG	1:B:303:VAL:HG22	2.19	0.67
1:B:218:HIS:CD2	1:B:220:ASN:H	2.12	0.67
1:A:143:ALA:H	1:A:234:HIS:HE1	1.41	0.66
1:A:277:ASN:O	1:A:279:VAL:N	2.28	0.66
1:A:279:VAL:HG12	1:A:281:GLY:H	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD22	1:A:78:LEU:HG	1.78	0.65
1:A:301:ASN:HD22	1:A:301:ASN:N	1.93	0.64
1:B:123:MET:HB3	1:B:180:ARG:HG3	1.80	0.63
1:A:128:ASP:OD2	1:A:159:ASN:HB2	1.99	0.63
1:B:154:GLU:HB2	1:B:228:PHE:HB2	1.80	0.62
1:A:27:ASN:C	1:A:27:ASN:HD22	2.05	0.62
1:B:16:ARG:HD2	4:B:664:HOH:O	1.99	0.62
1:B:58:GLY:O	1:B:62:LEU:HD22	1.99	0.62
1:A:182:ILE:HD11	1:A:192:VAL:HG12	1.81	0.62
1:B:294:ARG:HG3	1:B:294:ARG:HH11	1.65	0.61
1:A:137:HIS:CE1	1:A:287:VAL:HG22	2.36	0.60
1:B:142:ASP:HB3	1:B:148:LEU:HG	1.84	0.60
1:A:115:PRO:HG2	1:A:180:ARG:HD3	1.83	0.59
1:A:104:THR:HG21	1:A:240:GLN:HG2	1.83	0.59
1:A:301:ASN:HD22	1:A:301:ASN:H	1.51	0.59
1:B:165:SER:O	1:B:166:HIS:HB2	2.03	0.59
1:A:279:VAL:HG12	1:A:280:GLU:N	2.18	0.58
1:A:19:SER:CB	1:A:21:LEU:HD13	2.34	0.58
1:A:116:GLU:HB3	1:A:181:SER:HB2	1.87	0.57
1:B:159:ASN:HB3	1:B:178:MET:HE1	1.85	0.57
1:B:270:ASP:OD2	1:B:272:GLU:HB2	2.03	0.57
1:B:186:GLU:H	1:B:186:GLU:CD	2.13	0.55
1:A:102:PRO:HG2	1:A:261:LEU:HD21	1.89	0.55
1:B:27:ASN:C	1:B:27:ASN:ND2	2.65	0.55
1:B:306:ARG:HG2	1:B:307:PRO:CD	2.37	0.55
1:A:143:ALA:H	1:A:234:HIS:CE1	2.22	0.54
1:A:265:ALA:HA	1:A:286:MET:HG2	1.89	0.54
1:A:83:TYR:HA	1:A:86:MET:HE2	1.89	0.54
1:A:240:GLN:NE2	4:A:572:HOH:O	2.41	0.54
1:A:143:ALA:CB	1:A:294:ARG:HG3	2.38	0.54
1:A:185:ASP:C	1:A:187:ASN:H	2.15	0.54
1:B:104:THR:HG21	1:B:240:GLN:HG2	1.89	0.54
1:B:143:ALA:H	1:B:234:HIS:HE1	1.56	0.53
1:B:306:ARG:HG2	1:B:307:PRO:HD2	1.90	0.53
1:B:58:GLY:O	1:B:62:LEU:CD2	2.57	0.53
1:A:170:THR:O	1:A:171:GLY:C	2.52	0.53
1:A:184:THR:HB	1:A:188:GLY:HA2	1.90	0.53
1:A:186:GLU:H	1:A:186:GLU:CD	2.16	0.52
1:A:134:LEU:HD23	1:A:135:ILE:N	2.25	0.52
1:B:279:VAL:HG12	1:B:281:GLY:H	1.75	0.52
1:B:207:PRO:HA	1:B:210:GLN:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:TYR:HA	1:B:191:ARG:O	2.10	0.51
1:A:115:PRO:HG2	1:A:180:ARG:CD	2.42	0.50
1:B:279:VAL:HG12	1:B:280:GLU:N	2.25	0.50
1:A:27:ASN:C	1:A:27:ASN:ND2	2.69	0.50
1:A:56:TRP:CG	1:B:306:ARG:HG3	2.47	0.49
1:A:27:ASN:HD22	1:A:28:PRO:N	2.10	0.49
1:A:120:TYR:CG	1:A:121:ALA:N	2.80	0.49
1:B:143:ALA:H	1:B:234:HIS:CE1	2.30	0.49
1:A:182:ILE:HD11	1:A:192:VAL:CG1	2.43	0.49
1:A:301:ASN:H	1:A:301:ASN:ND2	2.12	0.48
1:B:123:MET:HB3	1:B:180:ARG:CG	2.43	0.48
1:B:301:ASN:H	1:B:301:ASN:ND2	2.00	0.48
1:B:280:GLU:N	1:B:280:GLU:CD	2.73	0.47
1:A:216:GLY:O	1:B:23:GLN:HG2	2.14	0.47
1:B:128:ASP:OD2	1:B:159:ASN:HB2	2.14	0.47
1:A:309:LEU:HD23	1:A:310:ALA:N	2.30	0.47
1:B:100:ALA:CB	1:B:291:LYS:HB3	2.45	0.47
1:B:193:ARG:NH2	1:B:280:GLU:OE1	2.38	0.46
1:A:182:ILE:CD1	1:A:192:VAL:CG1	2.94	0.46
1:A:222:PRO:HB3	1:A:248:TYR:C	2.40	0.46
1:A:169:PRO:C	1:A:171:GLY:H	2.22	0.46
1:A:311:VAL:HG12	1:A:311:VAL:OXT	2.14	0.46
1:B:134:LEU:HD12	1:B:194:THR:CG2	2.45	0.46
1:B:290:LEU:HD12	1:B:290:LEU:N	2.30	0.46
1:A:85:ASP:HA	1:A:88:MET:HE3	1.96	0.46
1:B:211:LEU:O	1:B:211:LEU:HD23	2.15	0.46
1:A:27:ASN:ND2	1:A:29:ARG:H	2.14	0.45
1:B:240:GLN:NE2	4:B:542:HOH:O	2.49	0.45
1:A:185:ASP:C	1:A:187:ASN:N	2.73	0.45
1:B:182:ILE:N	1:B:182:ILE:HD12	2.32	0.45
1:A:170:THR:O	1:A:172:GLU:CG	2.47	0.45
1:A:165:SER:O	1:A:166:HIS:HB2	2.17	0.45
1:B:100:ALA:HB3	1:B:291:LYS:HB3	1.98	0.45
1:A:185:ASP:O	1:A:187:ASN:N	2.50	0.44
1:B:120:TYR:CG	1:B:121:ALA:N	2.85	0.44
1:A:279:VAL:CG1	1:A:280:GLU:N	2.80	0.43
1:B:73:LEU:O	1:B:76:PRO:HG2	2.18	0.43
1:B:150:ASN:HA	1:B:183:ILE:CG2	2.48	0.43
1:B:270:ASP:HA	1:B:271:PRO:HD3	1.87	0.43
1:A:120:TYR:HA	1:A:191:ARG:O	2.19	0.43
1:B:27:ASN:ND2	1:B:29:ARG:H	2.16	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:THR:HB	1:B:172:GLU:HG3	1.97	0.43
1:A:149:PRO:O	1:A:150:ASN:HB2	2.17	0.43
1:A:270:ASP:HA	1:A:271:PRO:HD3	1.86	0.43
1:B:75:SER:HB3	1:B:76:PRO:CD	2.48	0.43
1:B:235:ARG:HH11	1:B:301:ASN:ND2	2.05	0.43
1:B:311:VAL:OXT	1:B:311:VAL:HG12	2.17	0.43
1:A:27:ASN:HA	1:A:28:PRO:HD2	1.86	0.43
1:A:100:ALA:HB3	1:A:291:LYS:HB3	1.99	0.43
1:B:128:ASP:HA	1:B:129:PRO:HD3	1.89	0.43
1:A:176:PHE:HA	1:A:179:ARG:HD2	2.01	0.42
1:B:134:LEU:HD21	1:B:286:MET:HG3	2.00	0.42
1:B:296:VAL:O	1:B:297:ASP:HB2	2.19	0.42
1:B:306:ARG:O	1:B:308:ARG:HG3	2.19	0.42
1:A:144:ASP:CG	1:A:294:ARG:HH22	2.27	0.42
1:A:228:PHE:HD1	1:A:228:PHE:HA	1.72	0.42
1:B:203:PRO:HA	1:B:204:PRO:HD2	1.89	0.42
1:B:229:VAL:HG21	1:B:290:LEU:HD22	2.02	0.42
1:A:132:HIS:NE2	1:A:267:GLU:OE2	2.52	0.42
1:B:211:LEU:HD23	1:B:211:LEU:C	2.45	0.42
1:B:100:ALA:CB	1:B:291:LYS:HD3	2.50	0.42
1:B:105:ILE:HG12	1:B:256:ALA:HB2	2.01	0.42
1:B:123:MET:CG	1:B:194:THR:HB	2.50	0.42
1:A:137:HIS:O	1:A:287:VAL:HA	2.19	0.42
1:A:290:LEU:HD12	1:A:290:LEU:N	2.35	0.42
1:B:294:ARG:HG3	1:B:294:ARG:NH1	2.30	0.41
1:A:100:ALA:CB	1:A:291:LYS:HD3	2.49	0.41
1:B:280:GLU:CD	1:B:280:GLU:H	2.28	0.41
1:A:142:ASP:HB3	1:A:148:LEU:HG	2.03	0.41
1:A:201:GLY:HA2	1:A:219:GLY:O	2.20	0.41
1:A:258:ARG:HB2	1:A:261:LEU:HD12	2.03	0.41
1:B:242:ASN:HB3	4:B:632:HOH:O	2.20	0.41
1:A:83:TYR:O	1:A:87:ARG:HG3	2.21	0.41
1:A:75:SER:HB3	1:A:76:PRO:CD	2.51	0.41
1:B:277:ASN:ND2	1:B:283:PHE:CZ	2.88	0.41
1:B:27:ASN:HD22	1:B:28:PRO:N	2.18	0.41
1:B:114:ALA:HA	1:B:176:PHE:CD1	2.56	0.41
1:A:63:ASN:HA	1:B:66:GLY:HA2	2.03	0.40
1:A:218:HIS:CD2	1:A:220:ASN:HB2	2.56	0.40
1:A:125:ASP:OD1	1:A:125:ASP:C	2.65	0.40
1:A:242:ASN:HB3	4:A:624:HOH:O	2.21	0.40
1:B:228:PHE:HD1	1:B:228:PHE:HA	1.80	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:OH	1:B:298:GLY:O[2_547]	2.18	0.02

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%)	291 (95%)	13 (4%)	3 (1%)	12	8
1	B	307/311 (99%)	295 (96%)	11 (4%)	1 (0%)	36	35
All	All	614/622 (99%)	586 (95%)	24 (4%)	4 (1%)	18	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ASP
1	B	278	ASP
1	A	171	GLY
1	A	186	GLU

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%)	235 (93%)	17 (7%)	15	11
1	B	252/254 (99%)	238 (94%)	14 (6%)	19	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	504/508 (99%)	473 (94%)	31 (6%)	16	13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	27	ASN
1	A	74	LEU
1	A	98	GLU
1	A	108	PRO
1	A	134	LEU
1	A	136	LEU
1	A	147	PRO
1	A	148	LEU
1	A	161	LYS
1	A	210	GLN
1	A	228	PHE
1	A	258	ARG
1	A	301	ASN
1	A	302	GLN
1	A	303	VAL
1	A	309	LEU
1	B	15	LEU
1	B	21	LEU
1	B	22	GLU
1	B	27	ASN
1	B	74	LEU
1	B	108	PRO
1	B	136	LEU
1	B	148	LEU
1	B	186	GLU
1	B	228	PHE
1	B	237	LEU
1	B	301	ASN
1	B	303	VAL
1	B	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	23	GLN
1	A	27	ASN
1	A	35	HIS
1	A	49	ASN
1	A	69	GLN
1	A	150	ASN
1	A	174	GLN
1	A	218	HIS
1	A	220	ASN
1	A	234	HIS
1	A	240	GLN
1	A	301	ASN
1	A	302	GLN
1	B	23	GLN
1	B	27	ASN
1	B	35	HIS
1	B	49	ASN
1	B	64	GLN
1	B	68	ASN
1	B	69	GLN
1	B	150	ASN
1	B	177	ASN
1	B	209	GLN
1	B	213	ASN
1	B	214	GLN
1	B	218	HIS
1	B	234	HIS
1	B	240	GLN
1	B	301	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	LIO	A	1999	-	42,42,42	1.34	2 (4%)	48,50,50	1.56	6 (12%)
3	LIO	B	999	-	42,42,42	1.32	2 (4%)	48,50,50	1.57	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	LIO	A	1999	-	-	22/46/46/46	-
3	LIO	B	999	-	-	23/46/46/46	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1999	LIO	O3-C11	5.26	1.48	1.33
3	B	999	LIO	O3-C11	5.07	1.48	1.33
3	A	1999	LIO	O2-C31	5.04	1.48	1.34
3	B	999	LIO	O2-C31	5.02	1.48	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	LIO	O2-C31-C32	5.44	123.26	111.48
3	A	1999	LIO	O2-C31-C32	5.44	123.25	111.48
3	A	1999	LIO	O3-C3-C2	5.10	123.09	108.40
3	B	999	LIO	O3-C3-C2	5.07	123.01	108.40
3	B	999	LIO	C2-O2-C31	3.33	125.76	117.80
3	A	1999	LIO	C2-O2-C31	3.19	125.42	117.80
3	A	1999	LIO	O2-C31-O31	-2.35	118.21	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	LIO	O2-C31-O31	-2.34	118.24	123.70
3	B	999	LIO	O4P-C4-C5	2.29	120.69	109.65
3	B	999	LIO	C3-C2-C1	-2.27	106.48	111.78
3	A	1999	LIO	C3-C2-C1	-2.26	106.52	111.78
3	A	1999	LIO	O4P-C4-C5	2.14	119.96	109.65

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1999	LIO	C12-C11-O3-C3
3	A	1999	LIO	O11-C11-O3-C3
3	A	1999	LIO	C32-C31-O2-C2
3	A	1999	LIO	O31-C31-O2-C2
3	B	999	LIO	C12-C11-O3-C3
3	B	999	LIO	O11-C11-O3-C3
3	B	999	LIO	C32-C31-O2-C2
3	B	999	LIO	O31-C31-O2-C2
3	B	999	LIO	C11-C12-C13-C14
3	A	1999	LIO	C11-C12-C13-C14
3	B	999	LIO	C31-C32-C33-C34
3	A	1999	LIO	C1-C2-C3-O3
3	A	1999	LIO	C33-C34-C35-C36
3	A	1999	LIO	C36-C37-C38-C39
3	B	999	LIO	C13-C14-C15-C16
3	B	999	LIO	C20-C21-C22-C23
3	B	999	LIO	C36-C37-C38-C39
3	A	1999	LIO	C18-C19-C20-C21
3	B	999	LIO	C12-C13-C14-C15
3	A	1999	LIO	C34-C35-C36-C37
3	A	1999	LIO	O3P-C1-C2-C3
3	B	999	LIO	C1-C2-C3-O3
3	A	1999	LIO	C15-C16-C17-C18
3	B	999	LIO	C32-C33-C34-C35
3	A	1999	LIO	O3P-C1-C2-O2
3	B	999	LIO	O3P-C1-C2-O2
3	A	1999	LIO	C37-C38-C39-C40
3	A	1999	LIO	C5-C4-O4P-P
3	A	1999	LIO	O4P-C4-C5-N
3	B	999	LIO	O4P-C4-C5-N
3	B	999	LIO	O3P-C1-C2-C3
3	B	999	LIO	C16-C17-C18-C19

Continued on next page...

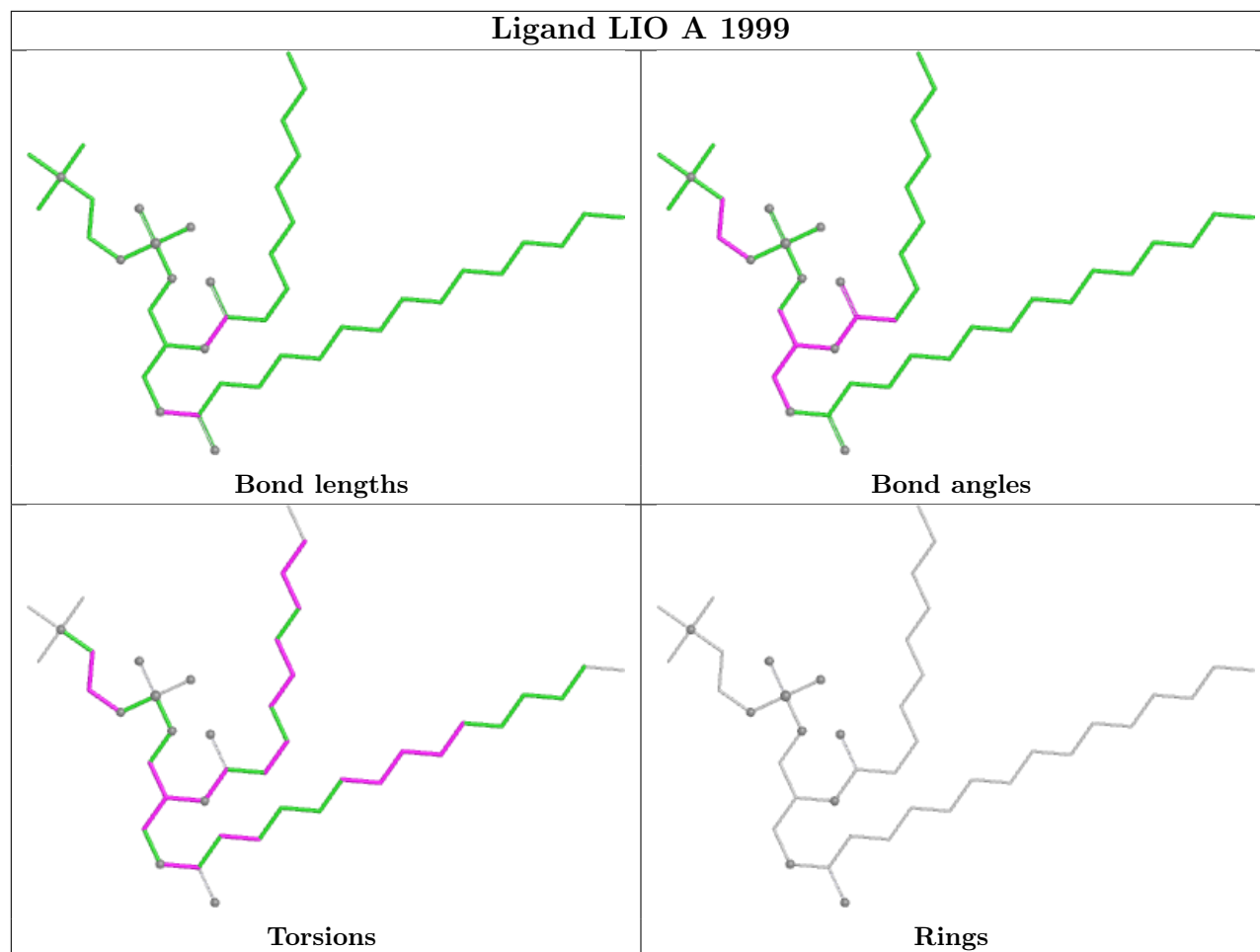
Continued from previous page...

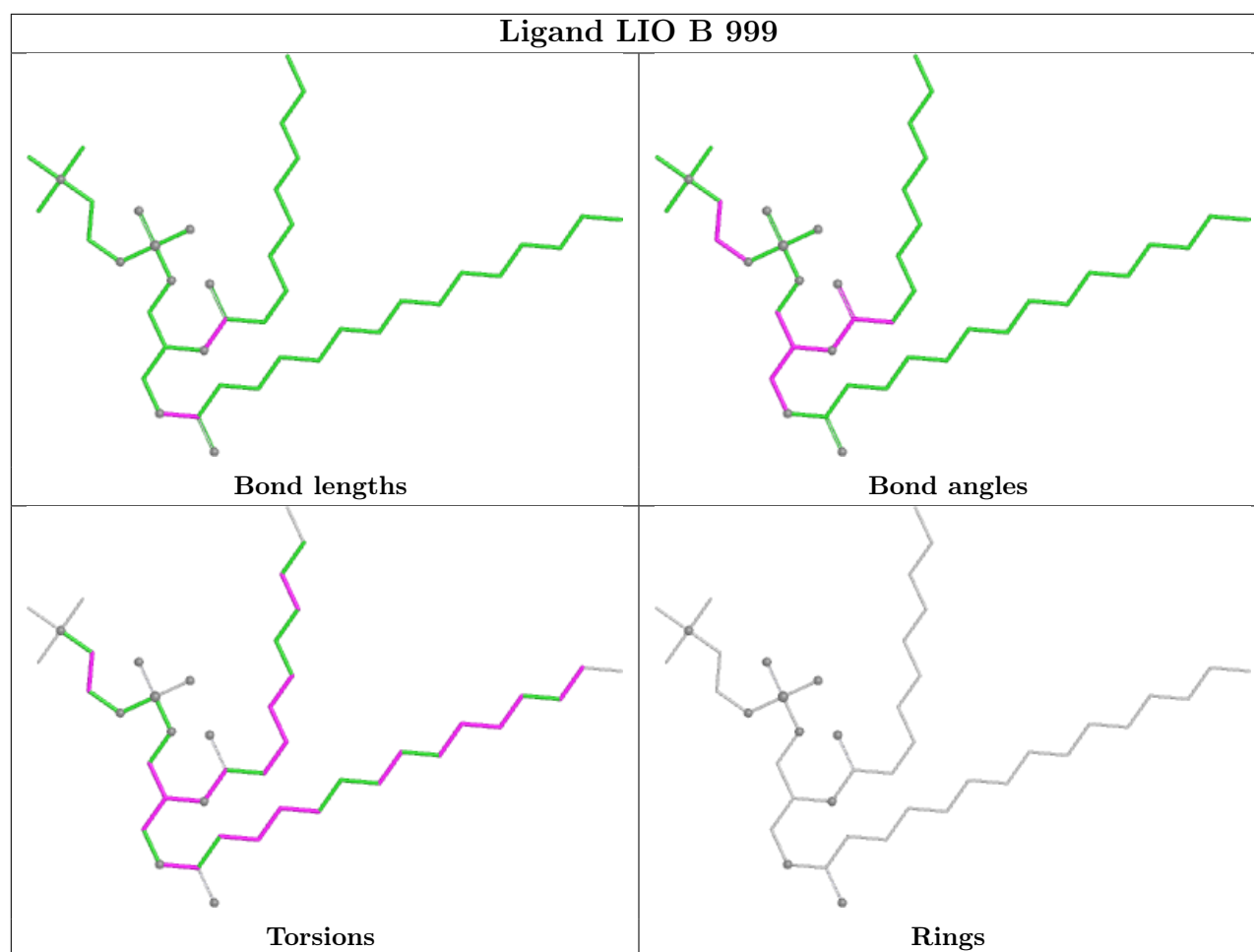
Mol	Chain	Res	Type	Atoms
3	B	999	LIO	C18-C19-C20-C21
3	B	999	LIO	O2-C2-C3-O3
3	B	999	LIO	C19-C20-C21-C22
3	A	1999	LIO	O2-C2-C3-O3
3	A	1999	LIO	C31-C32-C33-C34
3	A	1999	LIO	C1-C2-O2-C31
3	A	1999	LIO	C3-C2-O2-C31
3	B	999	LIO	C1-C2-O2-C31
3	B	999	LIO	C3-C2-O2-C31
3	A	1999	LIO	C17-C18-C19-C20
3	B	999	LIO	C33-C34-C35-C36
3	A	1999	LIO	C16-C17-C18-C19
3	B	999	LIO	C22-C23-C24-C25

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/311 (99%)	1.02	43 (13%) 6 5	12, 23, 46, 65	0
1	B	309/311 (99%)	1.83	130 (42%) 0 1	12, 22, 47, 66	0
All	All	618/622 (99%)	1.43	173 (27%) 1 1	12, 23, 47, 66	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	5.8
1	B	273	ALA	5.4
1	A	172	GLU	5.3
1	B	274	ILE	5.1
1	B	276	ALA	4.8
1	B	272	GLU	4.4
1	B	175	ALA	4.4
1	A	171	GLY	4.4
1	B	100	ALA	4.3
1	B	266	VAL	4.2
1	B	134	LEU	4.2
1	B	269	THR	4.0
1	B	196	LEU	4.0
1	B	120	TYR	4.0
1	B	176	PHE	3.9
1	B	278	ASP	3.9
1	B	192	VAL	3.8
1	B	200	TYR	3.8
1	A	97	ILE	3.7
1	B	126	GLY	3.7
1	B	228	PHE	3.6
1	B	268	HIS	3.6
1	B	135	ILE	3.6
1	B	283	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	145	GLY	3.6
1	A	279	VAL	3.5
1	B	131	GLY	3.5
1	B	182	ILE	3.5
1	B	141	PHE	3.5
1	A	99	ASN	3.5
1	B	147	PRO	3.4
1	B	284	ALA	3.4
1	B	124	ASP	3.4
1	B	167	PHE	3.4
1	B	187	ASN	3.4
1	B	129	PRO	3.4
1	B	163	PHE	3.4
1	B	265	ALA	3.3
1	B	261	LEU	3.3
1	B	281	GLY	3.2
1	A	276	ALA	3.2
1	B	94	ALA	3.2
1	A	187	ASN	3.2
1	B	148	LEU	3.2
1	B	277	ASN	3.2
1	B	244	ALA	3.2
1	B	225	ILE	3.2
1	B	291	LYS	3.2
1	B	153	VAL	3.1
1	A	272	GLU	3.1
1	A	100	ALA	3.1
1	B	287	VAL	3.1
1	A	8	THR	3.1
1	A	296	VAL	3.1
1	B	3	VAL	3.1
1	B	107	GLY	3.1
1	B	98	GLU	3.1
1	B	118	VAL	3.1
1	B	227	TYR	3.0
1	B	270	ASP	3.0
1	B	288	PHE	3.0
1	A	277	ASN	3.0
1	B	280	GLU	3.0
1	B	166	HIS	3.0
1	A	64	GLN	2.9
1	A	11	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	258	ARG	2.9
1	B	127	SER	2.9
1	B	150	ASN	2.9
1	B	224	HIS	2.9
1	A	21	LEU	2.8
1	B	155	ILE	2.8
1	B	144	ASP	2.8
1	B	171	GLY	2.8
1	B	172	GLU	2.8
1	B	177	ASN	2.8
1	B	96	GLY	2.8
1	B	199	GLY	2.8
1	B	198	ALA	2.8
1	B	242	ASN	2.7
1	A	15	LEU	2.7
1	B	164	TYR	2.7
1	A	3	VAL	2.7
1	B	189	GLN	2.7
1	A	205	GLU	2.7
1	A	199	GLY	2.7
1	B	162	GLY	2.7
1	B	136	LEU	2.6
1	B	140	ILE	2.6
1	B	262	VAL	2.6
1	B	101	THR	2.6
1	B	237	LEU	2.6
1	B	183	ILE	2.6
1	A	23	GLN	2.6
1	A	273	ALA	2.6
1	A	169	PRO	2.6
1	B	271	PRO	2.6
1	B	117	SER	2.6
1	B	294	ARG	2.6
1	B	241	ILE	2.6
1	A	170	THR	2.6
1	B	67	ALA	2.6
1	B	158	ALA	2.6
1	B	170	THR	2.6
1	B	191	ARG	2.6
1	B	215	LEU	2.6
1	A	200	TYR	2.5
1	B	190	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	282	PRO	2.5
1	B	251	ASP	2.5
1	B	139	THR	2.5
1	B	197	PRO	2.5
1	B	95	LEU	2.5
1	A	270	ASP	2.5
1	B	132	HIS	2.5
1	B	210	GLN	2.4
1	B	229	VAL	2.4
1	B	204	PRO	2.4
1	B	99	ASN	2.4
1	B	186	GLU	2.4
1	A	278	ASP	2.4
1	B	169	PRO	2.4
1	B	121	ALA	2.4
1	B	130	ASN	2.4
1	B	156	TRP	2.4
1	A	94	ALA	2.3
1	A	113	GLY	2.3
1	B	245	GLY	2.3
1	A	91	GLU	2.3
1	B	247	PRO	2.3
1	B	289	ASP	2.3
1	B	275	LYS	2.3
1	B	157	HIS	2.3
1	A	9	GLN	2.3
1	B	97	ILE	2.3
1	B	243	VAL	2.3
1	B	125	ASP	2.3
1	B	137	HIS	2.2
1	A	294	ARG	2.2
1	A	7	ASN	2.2
1	B	128	ASP	2.2
1	B	119	GLY	2.2
1	A	176	PHE	2.2
1	B	178	MET	2.2
1	A	280	GLU	2.2
1	B	90	ALA	2.2
1	B	151	ALA	2.2
1	A	48	LEU	2.2
1	B	185	ASP	2.2
1	A	173	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	265	ALA	2.1
1	B	149	PRO	2.1
1	B	249	THR	2.1
1	A	4	LYS	2.1
1	A	207	PRO	2.1
1	B	122	ARG	2.1
1	B	195	ILE	2.1
1	B	116	GLU	2.1
1	A	297	ASP	2.1
1	B	142	ASP	2.1
1	B	248	TYR	2.1
1	B	255	TYR	2.1
1	B	11	VAL	2.1
1	A	22	GLU	2.0
1	B	181	SER	2.1
1	B	230	SER	2.1
1	B	69	GLN	2.0
1	A	161	LYS	2.0
1	B	223	ALA	2.0
1	B	239	THR	2.0
1	A	25	GLY	2.0
1	B	110	TYR	2.0
1	B	250	TYR	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.

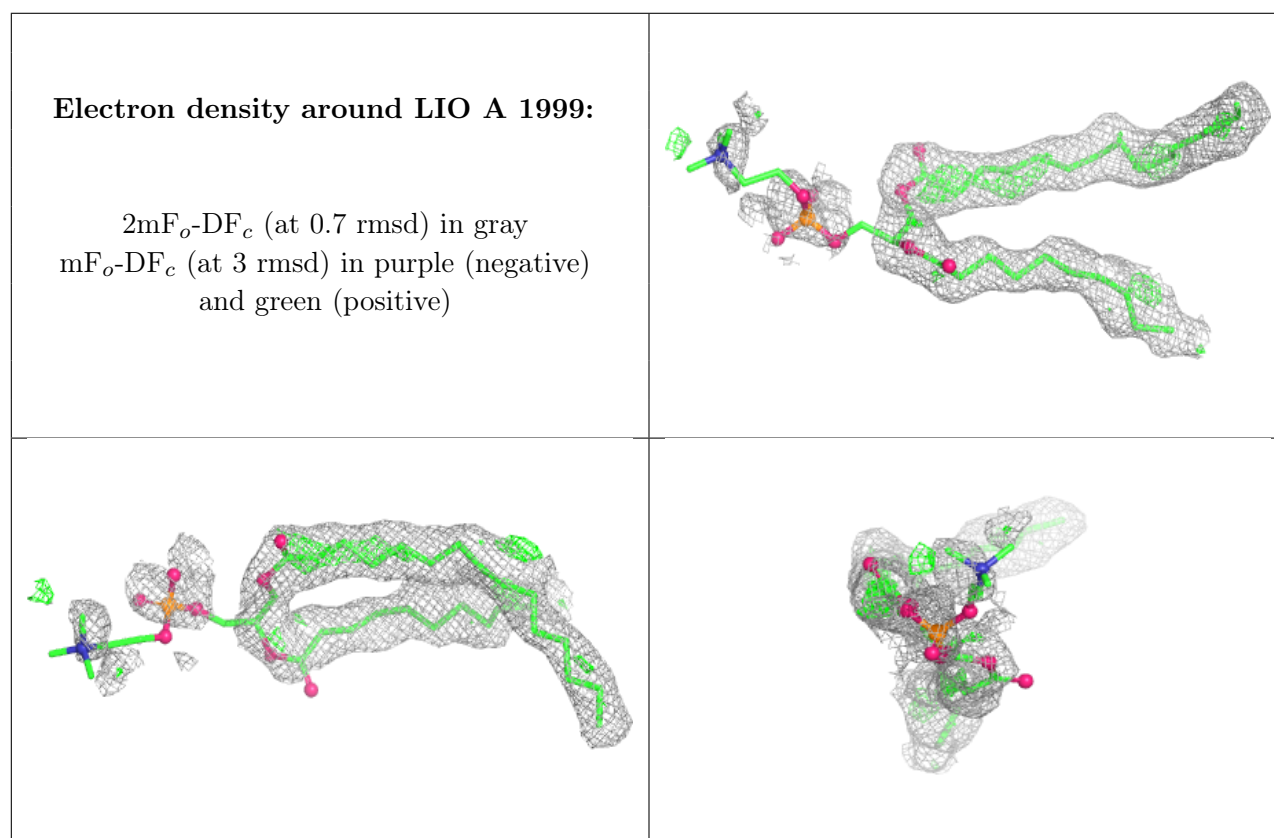
Continued on next page...

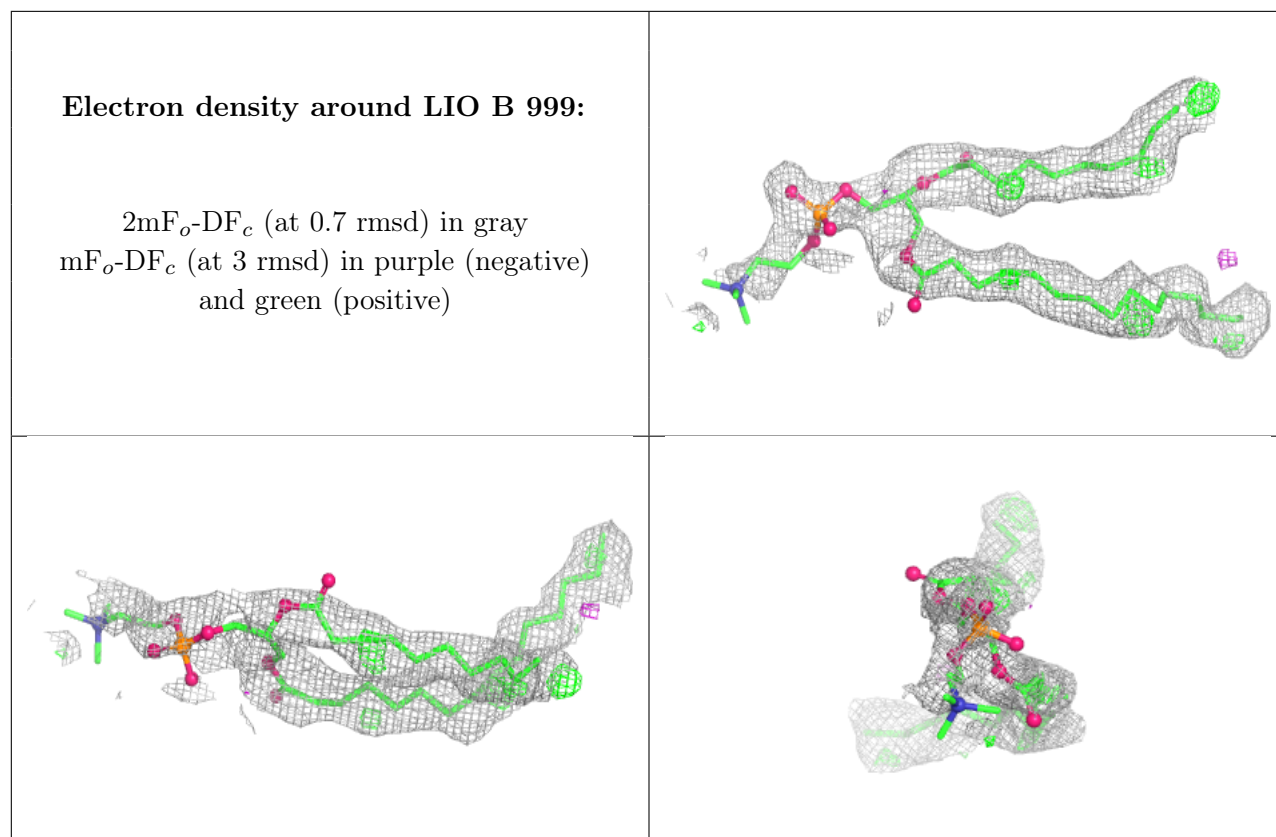
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LIO	A	1999	43/43	0.69	0.28	6,22,51,52	43
3	LIO	B	999	43/43	0.70	0.25	12,22,50,50	43
2	FE	B	400	1/1	0.79	0.10	17,17,17,17	0
2	FE	A	400	1/1	0.91	0.08	21,21,21,21	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.