



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 10:36 pm GMT

PDB ID : 2BMK  
Title : Fab fragment of PLP-dependent catalytic antibody 15A9 in complex with phosphopyridoxyl-D-alanine  
Authors : Golinelli-Pimpaneau, B.; Christen, P.  
Deposited on : 2005-03-14  
Resolution : 2.30 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 : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

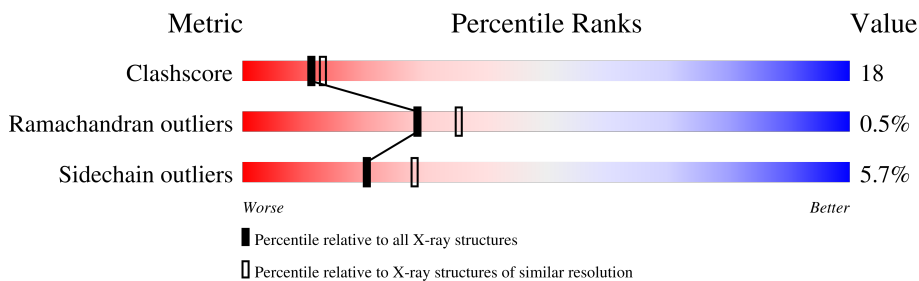
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	213	
1	L	213	
2	B	226	
2	H	226	

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	IOD	B	1215	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6967 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 FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	Total 1610	C 1003	N 264	O 334	S 9	0	0	0
1	L	213	Total 1629	C 1016	N 271	O 333	S 9	0	0	0

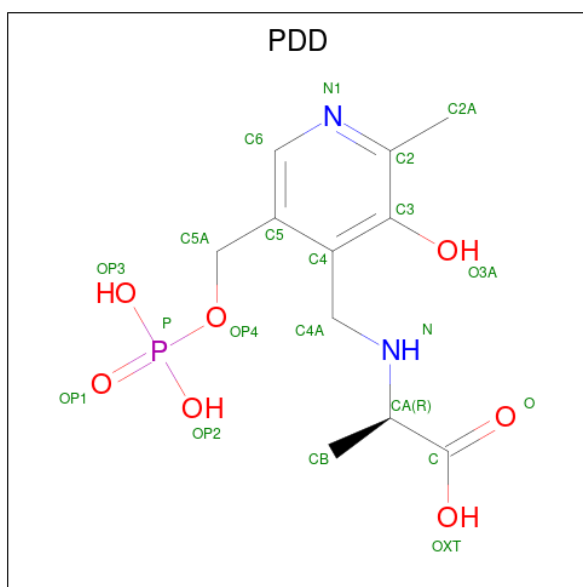
- Molecule 2 is a protein called FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	224	Total 1658	C 1053	N 276	O 322	S 7	0	0	1
2	H	222	Total 1668	C 1059	N 282	O 320	S 7	0	0	1

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total 3 I 3	0	0
3	H	3	Total 3 I 3	0	0

- Molecule 4 is N-(5'-PHOSPHOPYRIDOXYL)-D-ALANINE (three-letter code: PDD) (formula: C<sub>11</sub>H<sub>17</sub>N<sub>2</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	21	11	2	7	1	0	0
4	L	1	21	11	2	7	1	0	0

- Molecule 5 is water.

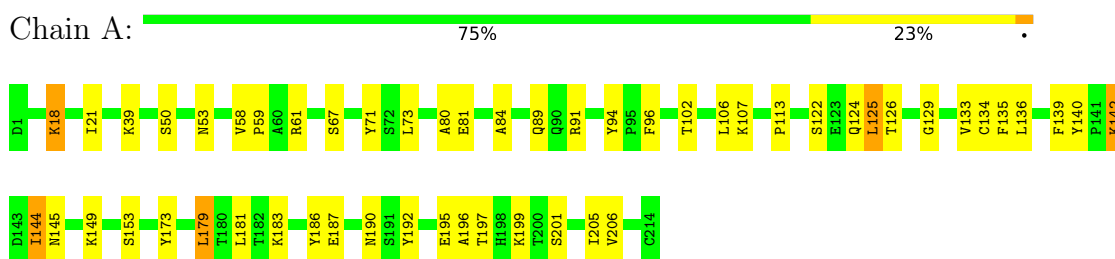
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	81	81	81	0	0
5	B	82	82	82	0	0
5	H	94	94	94	0	0
5	L	97	97	97	0	0

### 3 Residue-property plots

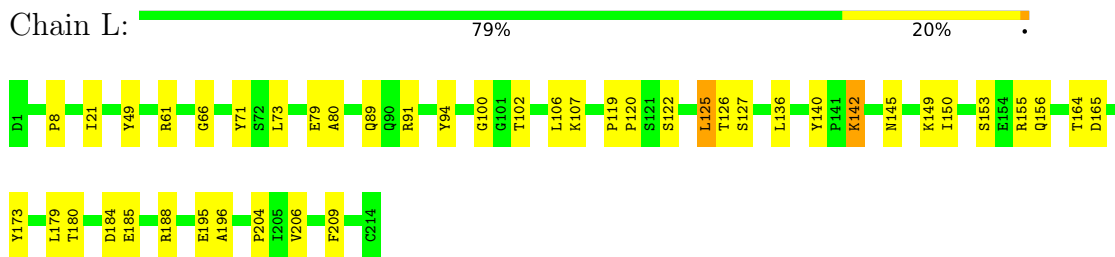
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

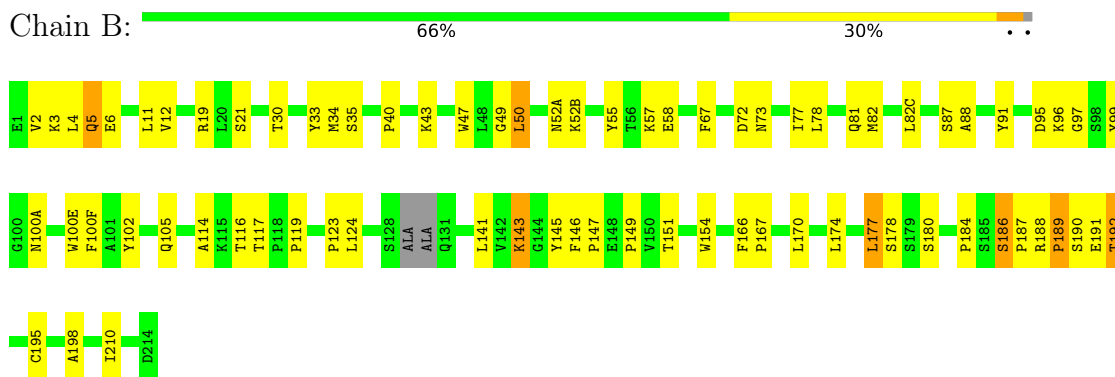
- Molecule 1: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN



- Molecule 1: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN

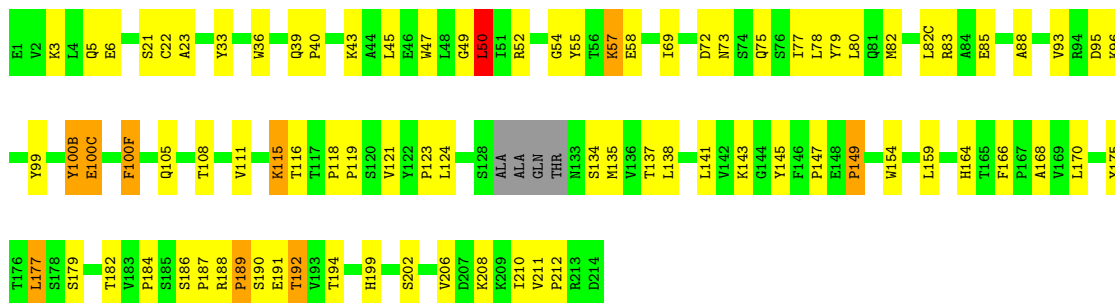


- Molecule 2: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN



- Molecule 2: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.15Å 81.15Å 79.33Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	90.2 (40.00-2.30)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6967	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP



## 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: PDD, IOD

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	0.37	0/1649	0.62	0/2247
1	L	0.39	0/1668	0.65	0/2267
2	B	0.38	0/1703	0.66	0/2333
2	H	0.39	0/1713	0.68	1/2341 (0.0%)
All	All	0.38	0/6733	0.65	1/9188 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	50	LEU	CA-CB-CG	5.42	127.77	115.30

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	1610	0	1499	40	0
1	L	1629	0	1547	38	0
2	B	1658	0	1571	82	0
2	H	1668	0	1611	91	0
3	B	3	0	0	3	0
3	H	3	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	13	0	0
4	L	21	0	13	1	0
5	A	81	0	0	3	0
5	B	82	0	0	6	0
5	H	94	0	0	3	0
5	L	97	0	0	4	0
All	All	6967	0	6254	229	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 18.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:ARG:CZ	1:L:79:GLU:HG3	2.00	0.91
2:H:186:SER:HB2	2:H:187:PRO:HD3	1.58	0.85
2:H:191:GLU:O	2:H:192:THR:HB	1.78	0.84
1:L:142:LYS:HD3	1:L:173:TYR:CE1	2.14	0.83
1:L:195:GLU:HG3	1:L:204:PRO:HB3	1.63	0.81
2:B:19:ARG:HD2	2:H:75:GLN:OE1	1.81	0.81
2:B:191:GLU:O	2:B:192:THR:HB	1.82	0.80
2:H:184:PRO:O	2:H:187:PRO:HD2	1.85	0.76
1:L:61:ARG:NE	1:L:79:GLU:HG3	2.02	0.74
1:A:89:GLN:NE2	1:A:91:ARG:HE	1.86	0.73
1:L:100:GLY:HA3	5:L:2052:HOH:O	1.87	0.72
2:B:50:LEU:C	2:B:50:LEU:HD23	2.10	0.72
2:H:184:PRO:HG2	2:H:187:PRO:HG2	1.71	0.71
1:A:94:TYR:CD2	2:B:58:GLU:HG2	2.27	0.70
2:B:184:PRO:HG2	2:B:187:PRO:HG2	1.73	0.70
2:B:124:LEU:HD11	2:B:141:LEU:HB2	1.74	0.70
2:B:184:PRO:HG2	2:B:187:PRO:CD	2.22	0.70
2:H:40:PRO:HG2	2:H:43:LYS:CB	2.24	0.68
1:L:21:ILE:HD12	1:L:102:THR:HG21	1.75	0.68
1:L:142:LYS:HD3	1:L:173:TYR:CD1	2.29	0.68
2:B:184:PRO:O	2:B:187:PRO:HD2	1.95	0.67
1:L:120:PRO:HB2	1:L:125:LEU:HD21	1.78	0.65
1:A:125:LEU:HG	1:A:183:LYS:HZ3	1.61	0.65
2:B:186:SER:CB	2:B:187:PRO:HD3	2.27	0.65
2:B:105:GLN:CD	2:B:105:GLN:H	2.00	0.64
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.79	0.64
2:B:184:PRO:HG2	2:B:187:PRO:HD2	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TYR:HB2	2:B:95:ASP:HB3	1.80	0.63
2:B:184:PRO:HG2	2:B:187:PRO:CG	2.29	0.63
2:B:33:TYR:CB	2:B:95:ASP:HB3	2.29	0.62
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.33	0.62
1:A:106:LEU:HD13	1:A:107:LYS:O	1.99	0.62
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.35	0.62
2:B:97:GLY:HA3	3:B:1215:IOD:I	2.69	0.62
2:B:143:LYS:NZ	2:B:143:LYS:HB2	2.15	0.62
2:H:83:ARG:HG3	2:H:85:GLU:HG2	1.81	0.62
1:A:80:ALA:HA	1:A:106:LEU:HG	1.82	0.61
1:A:149:LYS:HA	1:A:153:SER:O	2.01	0.61
2:B:81:GLN:NE2	2:H:75:GLN:HE22	1.98	0.61
2:H:177:LEU:C	2:H:177:LEU:HD12	2.21	0.61
2:H:23:ALA:HA	2:H:77:ILE:HD13	1.83	0.60
2:H:100(C):GLU:HB3	1:L:49:TYR:CZ	2.36	0.60
1:A:124:GLN:HG2	1:A:129:GLY:O	2.01	0.60
2:B:177:LEU:HD12	2:B:177:LEU:C	2.21	0.60
1:A:21:ILE:HD12	1:A:102:THR:HG21	1.83	0.60
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.84	0.60
1:L:122:SER:O	1:L:126:THR:HG23	2.02	0.60
2:H:33:TYR:HB2	2:H:95:ASP:HB3	1.84	0.59
2:H:100(B):TYR:HB2	5:H:2058:HOH:O	2.03	0.58
2:H:108:THR:CG2	2:H:149:PRO:HD3	2.33	0.58
2:B:143:LYS:HB2	2:B:143:LYS:HZ3	1.69	0.58
2:B:6:GLU:H	2:B:105:GLN:HE22	1.51	0.58
2:B:100(A):ASN:ND2	5:B:2048:HOH:O	2.36	0.57
1:A:18:LYS:HB2	1:A:18:LYS:NZ	2.19	0.56
1:A:67:SER:HA	1:A:71:TYR:CZ	2.39	0.56
2:B:154:TRP:CZ3	2:B:195:CYS:HB3	2.39	0.56
2:H:99:TYR:HB2	3:H:1216:IOD:I	2.75	0.56
2:H:123:PRO:O	2:H:124:LEU:HD12	2.05	0.56
2:B:5:GLN:HA	2:B:105:GLN:HE22	1.70	0.56
1:A:122:SER:O	1:A:126:THR:HG23	2.06	0.56
2:H:188:ARG:HA	2:H:190:SER:H	1.69	0.56
1:A:50:SER:HB2	1:A:53:ASN:HD22	1.71	0.56
1:L:150:ILE:HD12	1:L:155:ARG:HE	1.70	0.55
2:B:188:ARG:HA	2:B:190:SER:H	1.71	0.55
2:B:177:LEU:HD12	2:B:178:SER:N	2.22	0.55
2:H:184:PRO:HG2	2:H:187:PRO:CG	2.35	0.55
1:A:195:GLU:HA	1:A:206:VAL:HG12	1.87	0.55
1:A:107:LYS:HA	1:A:140:TYR:OH	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:GLN:NE2	1:L:91:ARG:HE	2.05	0.54
1:A:205:ILE:HD12	1:A:205:ILE:N	2.23	0.54
1:L:80:ALA:HA	1:L:106:LEU:HD22	1.89	0.54
2:H:199:HIS:ND1	2:H:202:SER:HB2	2.22	0.54
1:A:201:SER:HB3	1:A:205:ILE:HD11	1.90	0.54
1:L:188:ARG:NH2	5:L:2086:HOH:O	2.40	0.54
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.90	0.54
1:A:179:LEU:HD22	1:A:181:LEU:HG	1.91	0.53
2:H:83:ARG:HE	2:H:85:GLU:CD	2.11	0.53
1:A:183:LYS:O	1:A:187:GLU:HG3	2.07	0.53
2:B:186:SER:HB3	2:B:187:PRO:HD3	1.90	0.53
2:H:50:LEU:C	2:H:50:LEU:HD23	2.29	0.53
1:A:67:SER:HB3	5:A:2039:HOH:O	2.08	0.53
2:H:137:THR:O	2:H:138:LEU:HD23	2.09	0.53
2:B:33:TYR:CZ	2:B:96:LYS:HD3	2.44	0.53
1:A:142:LYS:HG2	1:A:173:TYR:CE2	2.44	0.52
2:H:170:LEU:HB2	2:H:175:TYR:CE1	2.44	0.52
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.92	0.52
1:A:142:LYS:HD3	1:A:173:TYR:CD1	2.44	0.52
1:L:195:GLU:CG	1:L:204:PRO:HB3	2.37	0.52
2:H:33:TYR:CB	2:H:95:ASP:HB3	2.40	0.52
2:H:121:VAL:HG21	2:H:206:VAL:CG2	2.40	0.51
2:B:6:GLU:H	2:B:105:GLN:NE2	2.08	0.51
2:H:211:VAL:HG13	2:H:212:PRO:HD2	1.92	0.51
1:A:61:ARG:NH2	1:A:81:GLU:HG3	2.26	0.51
2:H:93:VAL:HG11	2:H:100(F):PHE:CD2	2.46	0.51
2:B:188:ARG:HA	2:B:190:SER:N	2.26	0.51
2:B:40:PRO:HG2	2:B:43:LYS:CB	2.41	0.50
2:H:33:TYR:CZ	2:H:96:LYS:HD3	2.46	0.50
2:H:52:ARG:O	2:H:55:TYR:HA	2.11	0.50
2:H:154:TRP:CZ3	2:H:210:ILE:HD11	2.46	0.50
1:L:142:LYS:HD3	1:L:173:TYR:CZ	2.45	0.50
2:B:77:ILE:HD13	5:B:2035:HOH:O	2.10	0.50
1:A:89:GLN:HE22	1:A:91:ARG:HH21	1.59	0.50
2:B:50:LEU:C	2:B:50:LEU:CD2	2.79	0.50
2:H:118:PRO:HB3	2:H:202:SER:OG	2.11	0.50
2:B:151:THR:CG2	2:B:198:ALA:HB3	2.42	0.49
2:H:184:PRO:HG2	2:H:187:PRO:CD	2.43	0.49
2:B:170:LEU:HD12	2:B:174:LEU:O	2.13	0.49
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.94	0.49
2:H:47:TRP:HZ2	2:H:50:LEU:HD13	1.78	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:C	1:A:73:LEU:HD23	2.33	0.49
2:B:123:PRO:C	2:B:124:LEU:HD12	2.33	0.49
2:B:188:ARG:HG2	2:B:189:PRO:HA	1.95	0.49
2:H:57:LYS:HD2	2:H:57:LYS:N	2.28	0.49
1:L:184:ASP:HA	5:L:2084:HOH:O	2.13	0.49
2:B:5:GLN:NE2	5:B:2004:HOH:O	2.37	0.49
2:B:154:TRP:CZ3	2:B:210:ILE:HD11	2.48	0.48
2:B:188:ARG:C	2:B:188:ARG:HD3	2.34	0.48
2:B:191:GLU:O	2:B:192:THR:CB	2.55	0.48
2:B:19:ARG:HH12	2:H:72:ASP:HB3	1.77	0.48
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.48	0.48
2:H:188:ARG:HH22	2:H:212:PRO:HA	1.78	0.48
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.95	0.48
2:H:199:HIS:ND1	2:H:202:SER:CB	2.77	0.48
1:L:120:PRO:HB2	1:L:125:LEU:CD2	2.42	0.48
2:B:100(A):ASN:ND2	5:B:2050:HOH:O	2.41	0.48
2:B:114:ALA:HB3	2:B:146:PHE:CE2	2.49	0.48
2:H:115:LYS:HG2	2:H:116:THR:N	2.28	0.47
1:A:106:LEU:HD13	1:A:106:LEU:C	2.35	0.47
2:B:30:THR:O	2:B:52(A):ASN:HB2	2.14	0.47
2:H:40:PRO:HG2	2:H:43:LYS:HB3	1.97	0.47
2:H:168:ALA:HA	2:H:177:LEU:HB3	1.97	0.47
2:H:188:ARG:HG2	2:H:189:PRO:HA	1.97	0.47
2:B:151:THR:HG23	5:B:2068:HOH:O	2.13	0.47
2:B:19:ARG:NH2	2:H:72:ASP:HB2	2.30	0.47
2:B:97:GLY:CA	3:B:1215:IOD:I	3.32	0.47
2:H:58:GLU:HG2	1:L:94:TYR:CE2	2.48	0.47
1:A:89:GLN:HE22	1:A:91:ARG:HE	1.61	0.47
2:H:188:ARG:HD3	2:H:188:ARG:C	2.34	0.47
2:B:6:GLU:N	2:B:105:GLN:HE22	2.12	0.47
2:H:57:LYS:NZ	2:H:69:ILE:O	2.48	0.47
2:B:19:ARG:NH1	2:H:72:ASP:CB	2.79	0.46
1:L:73:LEU:C	1:L:73:LEU:HD23	2.36	0.46
1:L:106:LEU:HG	1:L:107:LYS:N	2.30	0.46
1:L:80:ALA:CB	1:L:106:LEU:HD22	2.45	0.46
2:H:100(C):GLU:HA	1:L:49:TYR:CD1	2.51	0.46
1:A:135:PHE:CE2	2:B:180:SER:HB3	2.51	0.46
2:B:99:TYR:HB2	3:B:1215:IOD:I	2.86	0.46
1:L:145:ASN:O	1:L:196:ALA:HA	2.16	0.46
1:A:94:TYR:CE2	2:B:58:GLU:HG2	2.51	0.46
1:A:186:TYR:HA	1:A:192:TYR:OH	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:MET:HB3	2:B:82(C):LEU:HD21	1.98	0.46
2:B:2:VAL:HB	2:B:102:TYR:CE1	2.51	0.46
2:B:19:ARG:HH12	2:H:72:ASP:CB	2.29	0.45
2:B:19:ARG:HH22	2:H:72:ASP:HB2	1.81	0.45
2:B:81:GLN:NE2	2:H:75:GLN:NE2	2.64	0.45
2:H:164:HIS:O	2:H:179:SER:HA	2.17	0.45
2:H:108:THR:HG21	2:H:149:PRO:HD3	1.97	0.45
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.98	0.45
1:A:197:THR:HG23	5:A:2081:HOH:O	2.16	0.45
2:H:100(C):GLU:HA	1:L:49:TYR:CE1	2.52	0.45
1:L:195:GLU:HA	1:L:206:VAL:HG12	1.98	0.45
2:B:6:GLU:OE2	2:B:91:TYR:HA	2.17	0.45
2:H:187:PRO:O	2:H:191:GLU:N	2.46	0.45
2:B:12:VAL:HG11	2:B:82(C):LEU:HD13	2.00	0.44
2:H:100(C):GLU:CB	1:L:49:TYR:CZ	2.99	0.44
2:B:6:GLU:HA	2:B:21:SER:O	2.17	0.44
2:B:19:ARG:NH2	2:H:79:TYR:HE2	2.15	0.44
2:H:115:LYS:HD2	2:H:116:THR:O	2.17	0.44
2:H:184:PRO:C	2:H:187:PRO:HD2	2.38	0.44
2:B:188:ARG:HD3	2:B:189:PRO:N	2.33	0.44
2:H:95:ASP:OD1	4:L:1215:PDD:N1	2.50	0.44
2:H:208:LYS:HD2	2:H:208:LYS:HA	1.90	0.44
1:L:150:ILE:HD12	1:L:155:ARG:HH21	1.83	0.44
1:A:91:ARG:HA	1:A:96:PHE:CD2	2.53	0.44
1:A:142:LYS:HG2	1:A:173:TYR:CD2	2.53	0.44
2:H:21:SER:HG	2:H:79:TYR:HE1	1.63	0.44
2:H:188:ARG:HA	2:H:190:SER:N	2.33	0.44
2:H:23:ALA:HA	2:H:77:ILE:CD1	2.49	0.43
2:B:81:GLN:HE21	2:H:75:GLN:NE2	2.17	0.43
1:L:195:GLU:HG3	1:L:204:PRO:CB	2.41	0.43
2:H:54:GLY:HA2	5:H:2034:HOH:O	2.17	0.43
2:H:194:THR:HG23	2:H:208:LYS:C	2.39	0.43
1:L:107:LYS:HA	1:L:140:TYR:OH	2.19	0.43
2:H:6:GLU:H	2:H:105:GLN:HE22	1.66	0.43
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	2.01	0.43
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.00	0.42
2:H:100(B):TYR:HD1	2:H:100(C):GLU:N	2.17	0.42
2:H:6:GLU:HA	2:H:21:SER:O	2.19	0.42
2:H:58:GLU:HG2	1:L:94:TYR:CD2	2.53	0.42
2:B:34:MET:HB3	2:B:78:LEU:HD22	2.01	0.42
2:B:143:LYS:NZ	2:B:143:LYS:CB	2.82	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HG13	1:A:145:ASN:N	2.33	0.42
2:H:138:LEU:HD11	2:H:188:ARG:HD2	2.01	0.42
1:L:136:LEU:HD21	1:L:196:ALA:HB2	2.01	0.42
1:A:106:LEU:HD11	5:A:2056:HOH:O	2.19	0.42
2:H:72:ASP:OD2	2:H:72:ASP:C	2.59	0.42
2:B:146:PHE:HA	2:B:147:PRO:HA	1.79	0.41
2:H:119:PRO:CB	2:H:145:TYR:HB3	2.48	0.41
2:H:166:PHE:CD2	1:L:164:THR:HG23	2.55	0.41
1:L:100:GLY:CA	5:L:2052:HOH:O	2.60	0.41
1:L:149:LYS:HA	1:L:153:SER:O	2.21	0.41
2:B:151:THR:HG22	2:B:198:ALA:HB3	2.03	0.41
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.85	0.41
2:B:19:ARG:NH1	2:H:79:TYR:OH	2.53	0.41
2:B:50:LEU:HD23	2:B:50:LEU:O	2.20	0.41
2:B:100(E):TRP:HB2	5:B:2049:HOH:O	2.20	0.41
1:A:18:LYS:HB2	1:A:18:LYS:HZ3	1.86	0.41
2:B:67:PHE:HA	2:B:81:GLN:O	2.20	0.41
2:H:39:GLN:C	2:H:88:ALA:HB1	2.41	0.41
2:H:50:LEU:C	2:H:50:LEU:CD2	2.88	0.41
2:H:168:ALA:HB2	2:H:177:LEU:HD23	2.03	0.41
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.56	0.41
2:H:3:LYS:HA	5:H:2002:HOH:O	2.21	0.41
2:H:135:MET:CE	2:H:182:THR:HG22	2.51	0.41
2:B:87:SER:O	2:B:88:ALA:HB2	2.21	0.41
2:H:83:ARG:C	2:H:111:VAL:HG11	2.41	0.41
1:A:133:VAL:HG12	1:A:134:CYS:N	2.36	0.41
2:B:5:GLN:HE21	2:B:5:GLN:HB3	1.47	0.41
2:B:11:LEU:HB2	2:B:147:PRO:HG3	2.03	0.41
2:B:116:THR:HG22	2:B:117:THR:N	2.35	0.41
1:A:39:LYS:HG2	1:A:84:ALA:HB2	2.03	0.41
2:B:55:TYR:CZ	2:B:73:ASN:ND2	2.89	0.41
2:B:67:PHE:N	2:B:67:PHE:CD1	2.88	0.41
2:B:99:TYR:HB2	2:B:100(A):ASN:HD22	1.86	0.41
2:H:55:TYR:CZ	2:H:73:ASN:ND2	2.88	0.41
2:B:166:PHE:HA	2:B:167:PRO:HD3	1.96	0.40
2:H:57:LYS:N	2:H:57:LYS:CD	2.85	0.40
1:L:8:PRO:O	1:L:102:THR:HG23	2.20	0.40
2:B:72:ASP:OD1	2:H:73:ASN:HB2	2.21	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	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
1	L	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
2	B	220/226 (97%)	202 (92%)	16 (7%)	2 (1%)	17	20
2	H	218/226 (96%)	205 (94%)	11 (5%)	2 (1%)	17	20
All	All	860/878 (98%)	817 (95%)	39 (4%)	4 (0%)	29	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	192	THR
2	H	192	THR
2	H	189	PRO
2	B	189	PRO

### 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	178/185 (96%)	171 (96%)	7 (4%)	32	46
1	L	182/185 (98%)	174 (96%)	8 (4%)	28	39
2	B	178/192 (93%)	166 (93%)	12 (7%)	16	21
2	H	182/192 (95%)	168 (92%)	14 (8%)	13	16
All	All	720/754 (96%)	679 (94%)	41 (6%)	20	28



All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	125	LEU
1	A	142	LYS
1	A	144	ILE
1	A	179	LEU
1	A	190	ASN
1	A	199	LYS
2	B	3	LYS
2	B	4	LEU
2	B	5	GLN
2	B	35	SER
2	B	50	LEU
2	B	52(B)	LYS
2	B	57	LYS
2	B	100(F)	PHE
2	B	143	LYS
2	B	149	PRO
2	B	177	LEU
2	B	186	SER
2	H	5	GLN
2	H	50	LEU
2	H	57	LYS
2	H	100(B)	TYR
2	H	100(C)	GLU
2	H	100(F)	PHE
2	H	115	LYS
2	H	134	SER
2	H	141	LEU
2	H	143	LYS
2	H	147	PRO
2	H	149	PRO
2	H	159	LEU
2	H	177	LEU
1	L	125	LEU
1	L	127	SER
1	L	142	LYS
1	L	156	GLN
1	L	165	ASP
1	L	179	LEU
1	L	180	THR
1	L	185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	89	GLN
1	A	137	ASN
1	A	212	ASN
2	B	81	GLN
2	B	100(A)	ASN
2	B	105	GLN
2	B	164	HIS
2	H	5	GLN
2	H	81	GLN
2	H	82(A)	ASN
2	H	164	HIS
1	L	31	ASN
1	L	89	GLN
1	L	137	ASN
1	L	190	ASN
1	L	212	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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$
4	PDD	B	1217	-	20,21,21	1.97	5 (25%)	26,30,30	1.64	7 (26%)
4	PDD	L	1215	-	20,21,21	2.03	5 (25%)	26,30,30	1.57	6 (23%)

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
4	PDD	B	1217	-	-	9/15/15/15	0/1/1/1
4	PDD	L	1215	-	-	9/15/15/15	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1215	PDD	O-C	4.75	1.36	1.22
4	B	1217	PDD	O-C	4.73	1.36	1.22
4	L	1215	PDD	C3-C4	4.22	1.46	1.40
4	B	1217	PDD	C3-C2	3.65	1.44	1.40
4	L	1215	PDD	C5-C4	3.63	1.45	1.40
4	B	1217	PDD	C3-C4	3.62	1.45	1.40
4	B	1217	PDD	C5-C4	3.50	1.45	1.40
4	L	1215	PDD	C3-C2	3.24	1.44	1.40
4	B	1217	PDD	CA-C	2.20	1.55	1.52
4	L	1215	PDD	CA-C	2.20	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1217	PDD	C4A-C4-C5	3.29	123.37	119.71
4	B	1217	PDD	O-C-CA	-3.22	111.36	121.83
4	L	1215	PDD	O-C-CA	-3.18	111.50	121.83
4	L	1215	PDD	C6-N1-C2	3.14	124.98	119.17
4	B	1217	PDD	C6-N1-C2	3.01	124.74	119.17
4	B	1217	PDD	OXT-C-CA	2.96	124.27	114.13
4	L	1215	PDD	OXT-C-CA	2.92	124.13	114.13
4	L	1215	PDD	C4A-C4-C5	2.80	122.83	119.71
4	B	1217	PDD	C2A-C2-C3	2.59	124.09	120.89

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1215	PDD	C3-C2-N1	-2.54	117.49	120.77
4	B	1217	PDD	C3-C2-N1	-2.53	117.50	120.77
4	L	1215	PDD	C2A-C2-C3	2.47	123.94	120.89
4	B	1217	PDD	C4A-C4-C3	-2.24	117.65	120.04

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1217	PDD	CB-CA-N-C4A
4	B	1217	PDD	C5-C4-C4A-N
4	B	1217	PDD	O-C-CA-N
4	B	1217	PDD	OXT-C-CA-N
4	L	1215	PDD	CB-CA-N-C4A
4	L	1215	PDD	O-C-CA-CB
4	L	1215	PDD	OXT-C-CA-CB
4	L	1215	PDD	C5-C4-C4A-N
4	L	1215	PDD	C4-C4A-N-CA
4	B	1217	PDD	O-C-CA-CB
4	L	1215	PDD	OXT-C-CA-N
4	B	1217	PDD	C3-C4-C4A-N
4	L	1215	PDD	C3-C4-C4A-N
4	B	1217	PDD	OXT-C-CA-CB
4	B	1217	PDD	C-CA-N-C4A
4	L	1215	PDD	C-CA-N-C4A
4	L	1215	PDD	O-C-CA-N
4	B	1217	PDD	C4-C4A-N-CA

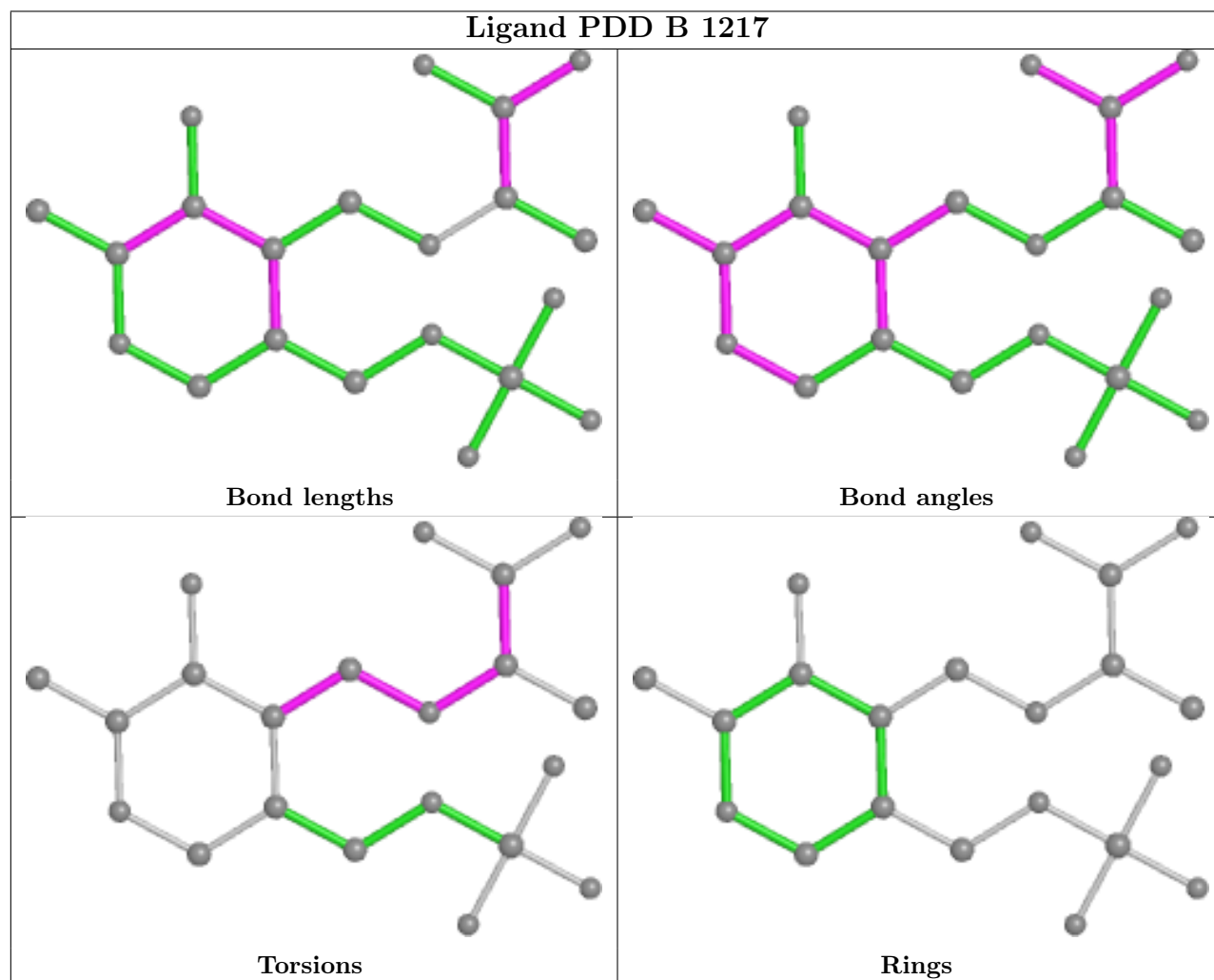
There are no ring outliers.

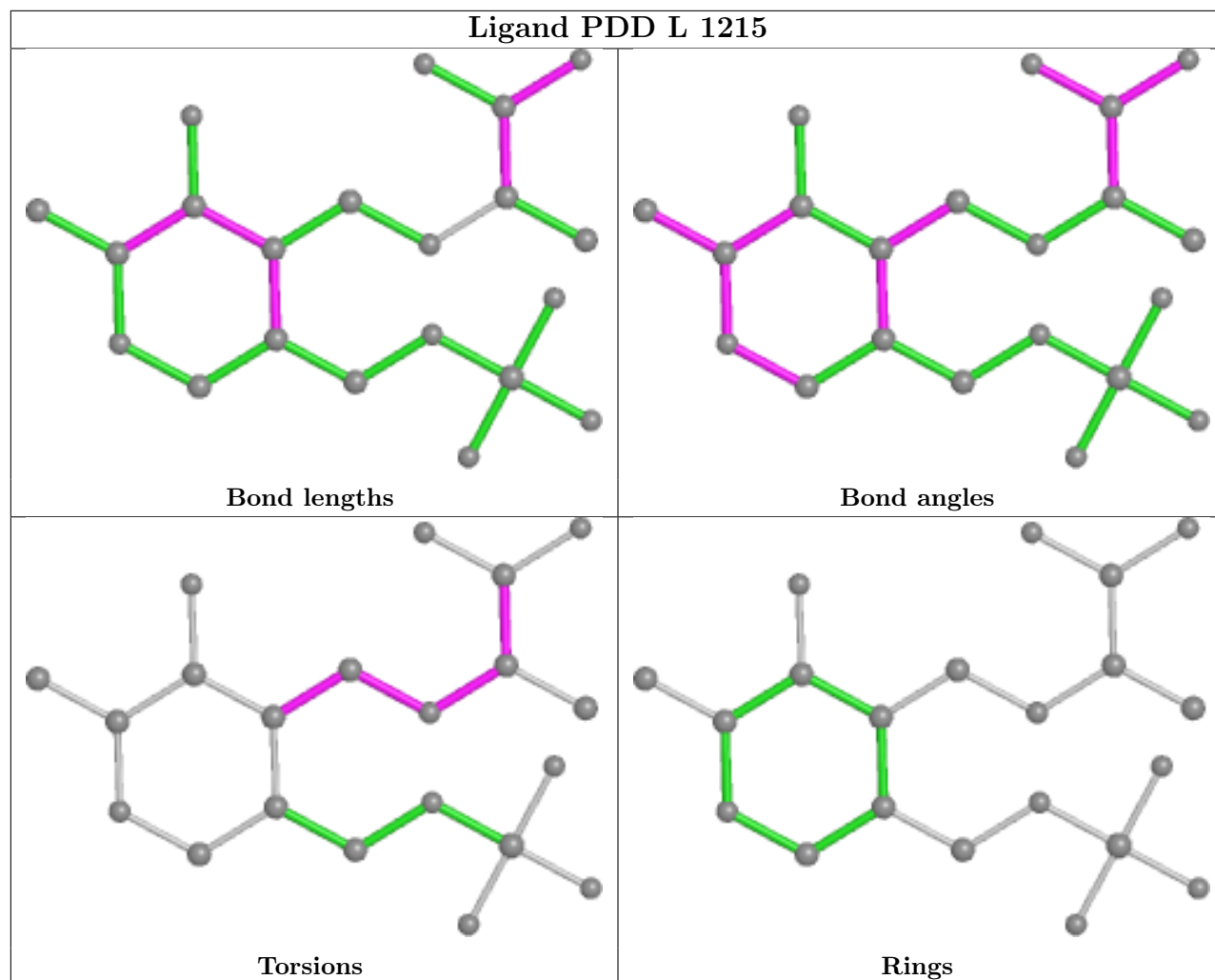
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1215	PDD	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.