



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 07:42 AM EDT

PDB ID : 1LPA  
Title : INTERFACIAL ACTIVATION OF THE LIPASE-PROCOLIPASE COMPLEX BY MIXED MICELLES REVEALED BY X-RAY CRYSTALLOGRAPHY  
Authors : Van Tilbeurgh, H.; Egloff, M.-P.; Cambillau, C.  
Deposited on : 1994-08-19  
Resolution : 3.04 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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

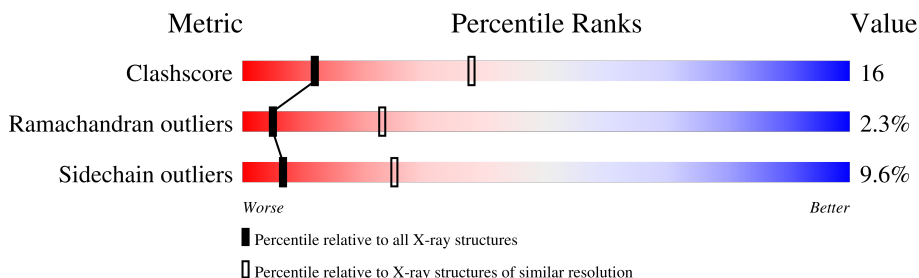
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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	180529	3811 (3.08-3.00)
Ramachandran outliers	177936	3656 (3.08-3.00)
Sidechain outliers	177891	3658 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	95	
2	B	449	

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	BNG	B	450	-	-	X	-
5	PLC	B	452	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4194 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.

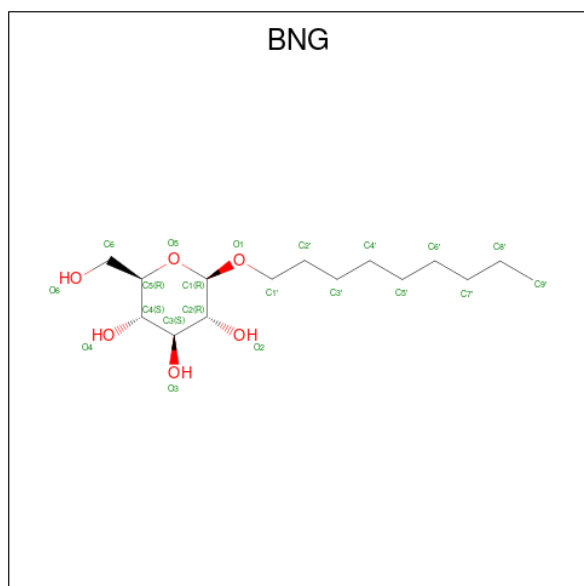
- Molecule 1 is a protein called COLIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			640	392	111	127	10			

- Molecule 2 is a protein called LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	449	Total	C	N	O	S	0	0	0
			3491	2212	600	661	18			

- Molecule 3 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).

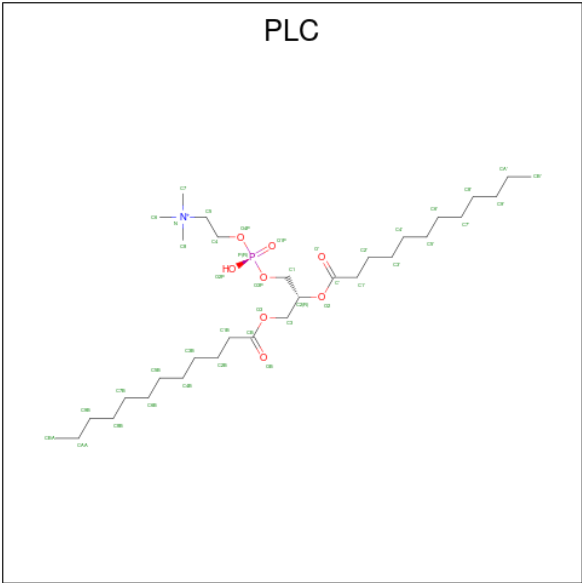


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	Ca			0	0
			1	1				

- Molecule 5 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: C<sub>32</sub>H<sub>65</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			42	32	1	8	1		

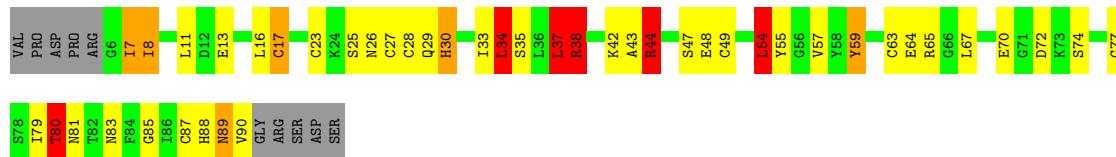
### 3 Residue-property plots

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.

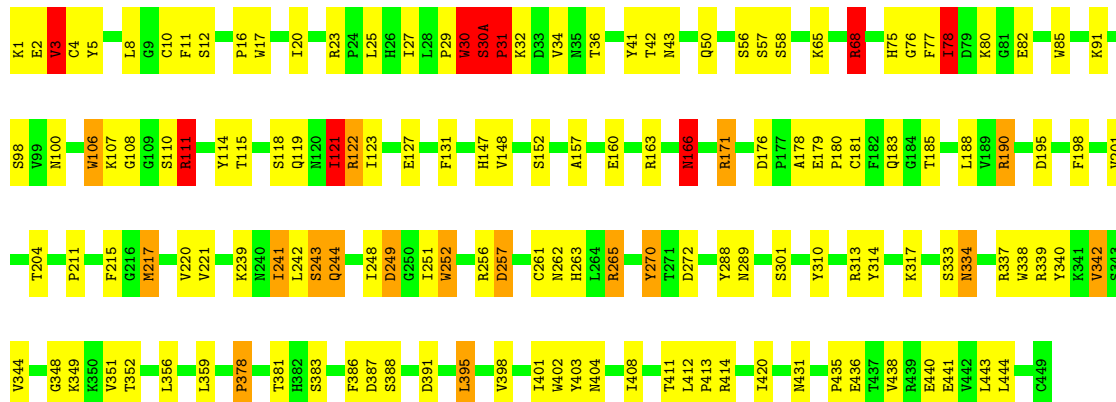
#### • Molecule 1: COLIPASE

Chain A: 



#### • Molecule 2: LIPASE

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.40 Å   133.40 Å   92.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 3.04	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.04)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLC, BNG, CA

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	0.89	0/647	1.91	19/872 (2.2%)
2	B	0.94	1/3583 (0.0%)	1.74	67/4864 (1.4%)
All	All	0.93	1/4230 (0.0%)	1.77	86/5736 (1.5%)

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
2	B	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	30	TRP	CG-CD2	-5.96	1.33	1.43

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	NE-CZ-NH1	12.01	126.31	120.30
2	B	30	TRP	CD1-CG-CD2	11.26	115.31	106.30
2	B	265	ARG	NE-CZ-NH2	-10.62	114.99	120.30
2	B	333	SER	CA-C-N	-10.05	95.09	117.20
1	A	65	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	A	65	ARG	NE-CZ-NH2	-9.78	115.41	120.30
2	B	265	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	B	17	TRP	CD1-CG-CD2	9.32	113.75	106.30
2	B	333	SER	O-C-N	9.24	137.49	122.70
1	A	44	ARG	NE-CZ-NH2	-8.92	115.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	TRP	CD1-CG-CD2	8.88	113.41	106.30
2	B	85	TRP	CD1-CG-CD2	8.57	113.15	106.30
1	A	38	ARG	NE-CZ-NH2	-8.27	116.17	120.30
2	B	338	TRP	CD1-CG-CD2	8.06	112.75	106.30
2	B	252	TRP	CE2-CD2-CG	-8.00	100.90	107.30
2	B	17	TRP	CE2-CD2-CG	-7.98	100.92	107.30
1	A	54	LEU	CA-CB-CG	7.93	133.55	115.30
2	B	338	TRP	CE2-CD2-CG	-7.92	100.96	107.30
2	B	163	ARG	NE-CZ-NH2	-7.89	116.36	120.30
2	B	68	ARG	NE-CZ-NH2	-7.82	116.39	120.30
2	B	166	ASN	CA-C-N	-7.76	100.69	116.20
2	B	106	TRP	CD1-CG-CD2	7.72	112.48	106.30
2	B	106	TRP	CE2-CD2-CG	-7.45	101.34	107.30
2	B	85	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	A	59	TYR	CB-CG-CD1	-7.37	116.58	121.00
2	B	30	TRP	CE2-CD2-CG	-7.34	101.43	107.30
2	B	333	SER	C-N-CA	7.25	139.82	121.70
2	B	30	TRP	CG-CD1-NE1	-7.15	102.95	110.10
2	B	334	ASN	N-CA-CB	7.10	123.38	110.60
2	B	314	TYR	CB-CG-CD1	-7.02	116.79	121.00
2	B	444	LEU	CA-CB-CG	6.93	131.25	115.30
2	B	402	TRP	CD1-CG-CD2	6.86	111.79	106.30
2	B	270	TYR	CB-CG-CD2	-6.86	116.88	121.00
2	B	402	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	72	ASP	CA-C-N	-6.75	102.35	117.20
2	B	244	GLN	N-CA-C	-6.73	92.82	111.00
1	A	17	CYS	N-CA-CB	-6.73	98.48	110.60
2	B	30	TRP	CA-C-N	-6.68	102.49	117.20
2	B	30(A)	SER	N-CA-C	6.65	128.95	111.00
2	B	68	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	B	195	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	37	LEU	CA-CB-CG	6.50	130.26	115.30
2	B	288	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	B	249	ASP	CA-C-N	-6.26	103.68	116.20
1	A	90	VAL	CA-CB-CG2	6.24	120.25	110.90
2	B	248	ILE	CA-C-N	-6.21	103.54	117.20
1	A	25	SER	CA-C-N	6.19	130.82	117.20
2	B	301	SER	N-CA-C	-6.15	94.40	111.00
2	B	3	VAL	CA-CB-CG2	-6.11	101.73	110.90
2	B	8	LEU	CB-CG-CD1	-6.09	100.65	111.00
2	B	148	VAL	CG1-CB-CG2	-6.08	101.17	110.90
2	B	171	ARG	CA-CB-CG	6.01	126.62	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	ILE	CA-C-N	5.99	130.37	117.20
2	B	30(A)	SER	CA-C-O	-5.89	107.73	120.10
2	B	252	TRP	CG-CD1-NE1	-5.89	104.21	110.10
2	B	17	TRP	CG-CD1-NE1	-5.87	104.23	110.10
2	B	431	ASN	CB-CA-C	-5.83	98.74	110.40
1	A	89	ASN	N-CA-C	-5.76	95.44	111.00
2	B	342	VAL	CG1-CB-CG2	-5.75	101.70	110.90
2	B	41	TYR	CB-CG-CD2	-5.70	117.58	121.00
2	B	85	TRP	CG-CD1-NE1	-5.70	104.40	110.10
2	B	391	ASP	N-CA-C	-5.57	95.95	111.00
1	A	90	VAL	CA-CB-CG1	-5.57	102.54	110.90
1	A	49	CYS	CA-CB-SG	-5.49	104.12	114.00
2	B	3	VAL	CB-CA-C	5.48	121.82	111.40
2	B	106	TRP	CG-CD2-CE3	5.46	138.82	133.90
2	B	163	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	B	30	TRP	CB-CG-CD2	-5.44	119.53	126.60
2	B	252	TRP	CG-CD2-CE3	5.41	138.77	133.90
2	B	121	ILE	CA-CB-CG1	-5.38	100.78	111.00
2	B	340	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	A	80	THR	N-CA-C	-5.29	96.72	111.00
2	B	111	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	B	378	PRO	CA-C-N	-5.28	105.58	117.20
1	A	72	ASP	O-C-N	5.27	131.13	122.70
2	B	252	TRP	CB-CG-CD1	-5.26	120.17	127.00
2	B	17	TRP	CB-CG-CD1	-5.20	120.24	127.00
2	B	402	TRP	CB-CG-CD1	-5.18	120.27	127.00
2	B	220	VAL	CB-CA-C	5.16	121.21	111.40
1	A	27	CYS	CA-CB-SG	-5.15	104.72	114.00
2	B	402	TRP	CG-CD1-NE1	-5.11	104.99	110.10
2	B	220	VAL	N-CA-CB	-5.08	100.32	111.50
2	B	217	MET	CA-CB-CG	5.07	121.92	113.30
1	A	34	LEU	CA-CB-CG	5.07	126.95	115.30
2	B	314	TYR	CB-CG-CD2	5.06	124.04	121.00
2	B	338	TRP	CB-CG-CD1	-5.06	120.42	127.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	111	ARG	Sidechain
2	B	30	TRP	Peptide
2	B	30(A)	SER	Peptide

## 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	640	0	616	24	0
2	B	3491	0	3352	80	0
3	B	20	0	27	14	0
4	B	1	0	0	0	0
5	B	42	0	64	33	0
All	All	4194	0	4059	126	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 16.

All (126) 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:B:78:ILE:HD12	5:B:452:PLC:H81	1.29	1.10
3:B:450:BNG:H8'1	5:B:452:PLC:H6'1	1.19	1.09
3:B:450:BNG:H8'1	5:B:452:PLC:C6'	1.88	1.02
3:B:450:BNG:C8'	5:B:452:PLC:H6'1	1.99	0.93
3:B:450:BNG:H7'2	3:B:450:BNG:H3'2	1.61	0.82
3:B:450:BNG:H7'2	3:B:450:BNG:C3'	2.11	0.80
1:A:37:LEU:H	1:A:37:LEU:HD22	1.49	0.77
2:B:65:LYS:HB2	2:B:68:ARG:HD2	1.66	0.77
2:B:3:VAL:HG12	2:B:11:PHE:HB2	1.67	0.76
3:B:450:BNG:H8'1	5:B:452:PLC:C7'	2.15	0.75
3:B:450:BNG:C7'	5:B:452:PLC:H8'2	2.16	0.75
5:B:452:PLC:H83	5:B:452:PLC:H3'1	1.67	0.75
3:B:450:BNG:O5	3:B:450:BNG:C2	2.35	0.74
2:B:121:ILE:HD12	2:B:157:ALA:HB2	1.68	0.74
2:B:152:SER:OG	5:B:452:PLC:H2A2	1.88	0.73
3:B:450:BNG:C2	3:B:450:BNG:O1	2.40	0.69
2:B:80:LYS:HD2	2:B:82:GLU:HB2	1.75	0.68
2:B:80:LYS:HB3	2:B:107:LYS:HD3	1.77	0.66
5:B:452:PLC:H11	5:B:452:PLC:H1'1	1.77	0.65
2:B:78:ILE:HD12	5:B:452:PLC:C8	2.19	0.64
2:B:152:SER:HG	5:B:452:PLC:CB	2.11	0.64
1:A:77:GLY:O	1:A:80:THR:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:GLN:OE1	2:B:217:MET:HB2	1.98	0.64
2:B:107:LYS:HA	2:B:110:SER:OG	1.99	0.62
1:A:17:CYS:HB3	1:A:38:ARG:HA	1.81	0.61
1:A:16:LEU:HG	2:B:243:SER:HB3	1.83	0.61
5:B:452:PLC:H3'1	5:B:452:PLC:C8	2.31	0.60
1:A:33:ILE:HG23	1:A:34:LEU:HD22	1.82	0.60
2:B:204:THR:O	2:B:262:ASN:HB3	2.00	0.60
2:B:403:TYR:HA	2:B:440:GLU:HG3	1.82	0.60
1:A:30:HIS:HB2	1:A:35:SER:HB2	1.82	0.60
3:B:450:BNG:H8'1	5:B:452:PLC:H8'2	1.82	0.60
3:B:450:BNG:H7'2	5:B:452:PLC:H8'2	1.83	0.59
2:B:185:THR:O	2:B:190:ARG:HD3	2.03	0.59
2:B:4:CYS:HA	2:B:10:CYS:HA	1.85	0.59
2:B:78:ILE:O	2:B:111:ARG:HD2	2.03	0.58
3:B:450:BNG:H8'1	5:B:452:PLC:C8'	2.33	0.58
2:B:30(A):SER:HB2	2:B:34:VAL:HG23	1.85	0.58
2:B:78:ILE:HD11	5:B:452:PLC:H61	1.85	0.57
2:B:215:PHE:HB3	5:B:452:PLC:H2A1	1.86	0.57
2:B:43:ASN:OD1	2:B:98:SER:HA	2.03	0.57
2:B:147:HIS:CD2	2:B:171:ARG:HG3	2.40	0.57
2:B:252:TRP:O	2:B:256:ARG:HG3	2.04	0.57
2:B:398:VAL:HG11	2:B:420:ILE:HG21	1.87	0.56
2:B:201:VAL:HG21	2:B:221:VAL:HG23	1.87	0.56
5:B:452:PLC:P	5:B:452:PLC:H82	2.46	0.56
3:B:450:BNG:C8'	5:B:452:PLC:H8'2	2.37	0.55
1:A:17:CYS:SG	1:A:23:CYS:SG	3.05	0.55
1:A:28:CYS:SG	1:A:37:LEU:HB2	2.47	0.55
2:B:252:TRP:HZ3	5:B:452:PLC:H9'2	1.72	0.54
2:B:30:TRP:HZ3	2:B:108:GLY:O	1.90	0.54
2:B:152:SER:OG	5:B:452:PLC:CB	2.56	0.54
2:B:215:PHE:CD1	5:B:452:PLC:H5A2	2.43	0.54
2:B:2:GLU:HG2	2:B:12:SER:HB3	1.90	0.53
2:B:152:SER:HG	5:B:452:PLC:H2A2	1.70	0.53
1:A:33:ILE:HG13	1:A:34:LEU:HD13	1.91	0.53
5:B:452:PLC:H11	5:B:452:PLC:C1'	2.38	0.53
2:B:349:LYS:HD3	2:B:413:PRO:HB3	1.91	0.52
2:B:198:PHE:CE1	2:B:317:LYS:HB2	2.45	0.52
2:B:78:ILE:CD1	5:B:452:PLC:H61	2.41	0.51
2:B:337:ARG:HD3	2:B:388:SER:O	2.10	0.51
2:B:352:THR:O	2:B:404:ASN:HB2	2.11	0.50
2:B:20:ILE:HG13	2:B:23:ARG:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLN:O	2:B:122:ARG:HG3	2.12	0.50
2:B:80:LYS:CB	2:B:107:LYS:HD3	2.41	0.50
5:B:452:PLC:C1'	5:B:452:PLC:C1	2.90	0.50
1:A:43:ALA:O	1:A:64:GLU:HG3	2.12	0.50
2:B:114:TYR:CD1	5:B:452:PLC:H7A1	2.47	0.50
2:B:114:TYR:HE1	5:B:452:PLC:H3A2	1.77	0.49
2:B:339:ARG:HA	2:B:386:PHE:O	2.12	0.49
2:B:178:ALA:HB1	5:B:452:PLC:H3A1	1.95	0.49
1:A:33:ILE:HG23	1:A:34:LEU:H	1.78	0.49
2:B:179:GLU:HB3	2:B:180:PRO:HD3	1.95	0.49
2:B:348:GLY:O	2:B:378:PRO:HG2	2.13	0.48
2:B:356:LEU:HD12	2:B:356:LEU:N	2.28	0.48
2:B:239:LYS:HB3	2:B:243:SER:O	2.13	0.48
2:B:310:TYR:HB3	2:B:313:ARG:HE	1.79	0.48
3:B:450:BNG:O5	3:B:450:BNG:O1	2.32	0.47
1:A:26:ASN:H	1:A:42:LYS:NZ	2.13	0.47
1:A:37:LEU:H	1:A:37:LEU:CD2	2.20	0.47
2:B:401:ILE:HB	2:B:443:LEU:HD13	1.95	0.47
1:A:79:ILE:HG12	1:A:83:ASN:HD21	1.79	0.47
2:B:75:HIS:HD2	2:B:76:GLY:O	1.98	0.47
2:B:5:TYR:CD1	2:B:31:PRO:HD2	2.50	0.47
2:B:3:VAL:HG13	2:B:5:TYR:CE2	2.50	0.47
2:B:342:VAL:O	2:B:383:SER:HA	2.15	0.47
2:B:359:LEU:HB3	2:B:395:LEU:HD21	1.97	0.47
2:B:257:ASP:O	2:B:261:CYS:HB2	2.15	0.46
2:B:152:SER:HA	2:B:176:ASP:O	2.16	0.46
5:B:452:PLC:H1'1	5:B:452:PLC:C1	2.46	0.46
2:B:75:HIS:HE1	2:B:106:TRP:H	1.63	0.46
2:B:337:ARG:HB3	2:B:387:ASP:HB3	1.98	0.46
1:A:70:GLU:HG3	1:A:88:HIS:HB2	1.97	0.45
1:A:59:TYR:HE1	1:A:81:ASN:HB2	1.80	0.45
5:B:452:PLC:H83	5:B:452:PLC:C1'	2.47	0.45
2:B:31:PRO:HG3	2:B:123:ILE:HG23	1.99	0.45
1:A:44:ARG:O	1:A:87:CYS:HB2	2.16	0.45
2:B:344:VAL:O	2:B:381:THR:HA	2.17	0.45
2:B:414:ARG:HA	2:B:438:VAL:O	2.16	0.45
2:B:36:THR:HB	2:B:127:GLU:HG2	1.98	0.44
2:B:16:PRO:CD	2:B:188:LEU:HD23	2.47	0.44
2:B:3:VAL:HG13	2:B:5:TYR:HE2	1.83	0.44
1:A:37:LEU:HD12	1:A:57:VAL:HG21	1.99	0.44
2:B:29:PRO:HB3	2:B:123:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:CE1	1:A:81:ASN:HB2	2.53	0.43
1:A:63:CYS:HB3	1:A:67:LEU:HD23	2.00	0.43
2:B:122:ARG:HH11	2:B:122:ARG:HD2	1.70	0.43
5:B:452:PLC:C8	5:B:452:PLC:H1'2	2.48	0.43
2:B:25:LEU:HD23	2:B:27:ILE:HD11	2.00	0.43
2:B:152:SER:OG	2:B:263:HIS:CE1	2.71	0.43
2:B:152:SER:HG	2:B:263:HIS:CE1	2.36	0.43
2:B:68:ARG:HD3	2:B:100:ASN:OD1	2.19	0.42
2:B:147:HIS:HE1	2:B:270:TYR:OH	2.03	0.42
2:B:251:ILE:HD13	2:B:251:ILE:HA	1.83	0.42
1:A:54:LEU:HD22	1:A:55:TYR:N	2.35	0.42
2:B:252:TRP:CZ3	5:B:452:PLC:H9'2	2.53	0.42
2:B:77:PHE:CD2	2:B:78:ILE:HG13	2.55	0.41
2:B:42:THR:HG22	2:B:100:ASN:HA	2.02	0.41
2:B:180:PRO:O	2:B:181:CYS:HB2	2.21	0.41
2:B:1:LYS:O	2:B:12:SER:HA	2.20	0.41
2:B:30(A):SER:OG	2:B:34:VAL:N	2.49	0.41
1:A:7:ILE:HG23	1:A:8:ILE:N	2.35	0.41
2:B:349:LYS:NZ	2:B:411:THR:HG21	2.37	0.41
2:B:3:VAL:O	2:B:10:CYS:HA	2.21	0.40
1:A:34:LEU:HD22	1:A:34:LEU:H	1.87	0.40
1:A:48:GLU:HA	1:A:85:GLY:O	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	83/95 (87%)	70 (84%)	10 (12%)	3 (4%)	3	14
2	B	447/449 (100%)	413 (92%)	25 (6%)	9 (2%)	6	26
All	All	530/544 (97%)	483 (91%)	35 (7%)	12 (2%)	5	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	THR
2	B	30(A)	SER
2	B	249	ASP
1	A	74	SER
2	B	31	PRO
2	B	166	ASN
2	B	244	GLN
2	B	334	ASN
2	B	78	ILE
2	B	408	ILE
1	A	8	ILE
2	B	241	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	74/83 (89%)	62 (84%)	12 (16%)	2	9
2	B	383/383 (100%)	351 (92%)	32 (8%)	9	31
All	All	457/466 (98%)	413 (90%)	44 (10%)	7	25

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	11	LEU
1	A	13	GLU
1	A	29	GLN
1	A	30	HIS
1	A	34	LEU
1	A	37	LEU
1	A	38	ARG
1	A	44	ARG
1	A	47	SER
1	A	54	LEU

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Mol	Chain	Res	Type
1	A	89	ASN
2	B	3	VAL
2	B	30(A)	SER
2	B	31	PRO
2	B	32	LYS
2	B	50	GLN
2	B	56	SER
2	B	57	SER
2	B	58	SER
2	B	68	ARG
2	B	91	LYS
2	B	115	THR
2	B	118	SER
2	B	121	ILE
2	B	122	ARG
2	B	131	PHE
2	B	160	GLU
2	B	166	ASN
2	B	190	ARG
2	B	211	PRO
2	B	241	ILE
2	B	242	LEU
2	B	243	SER
2	B	257	ASP
2	B	265	ARG
2	B	272	ASP
2	B	289	ASN
2	B	351	VAL
2	B	395	LEU
2	B	412	LEU
2	B	435	PRO
2	B	436	GLU
2	B	441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
2	B	75	HIS
2	B	88	ASN
2	B	166	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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	BNG	B	450	-	18,18,21	0.74	0	19,19,26	1.40	2 (10%)
5	PLC	B	452	-	41,41,41	1.38	5 (12%)	47,49,49	1.86	12 (25%)

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	BNG	B	450	-	-	6/19/19/32	-
5	PLC	B	452	-	-	18/45/45/45	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	452	PLC	O2-C'	4.78	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	452	PLC	O3-CB	3.66	1.44	1.33
5	B	452	PLC	C1'-C'	2.25	1.57	1.50
5	B	452	PLC	O2-C2	-2.16	1.41	1.46
5	B	452	PLC	C1-C2	2.12	1.57	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	452	PLC	O2-C'-C1'	5.70	123.80	111.48
5	B	452	PLC	C3-C2-C1	-4.54	101.20	111.78
5	B	452	PLC	O3-C3-C2	4.39	121.05	108.40
3	B	450	BNG	C5-C4-C3	-4.34	106.35	113.57
5	B	452	PLC	C3B-C2B-C1B	-3.38	100.70	113.13
5	B	452	PLC	C4'-C3'-C2'	-2.96	99.38	114.37
5	B	452	PLC	O2-C2-C3	2.73	118.13	108.34
5	B	452	PLC	C2'-C1'-C'	-2.71	103.78	113.69
3	B	450	BNG	C2-C3-C4	-2.56	106.95	112.17
5	B	452	PLC	O2-C2-C1	2.54	117.45	108.34
5	B	452	PLC	C3-O3-CB	-2.40	108.34	117.12
5	B	452	PLC	O2-C'-O'	-2.30	118.33	123.70
5	B	452	PLC	O3-CB-C1B	2.18	118.48	111.83
5	B	452	PLC	C6'-C5'-C4'	-2.10	103.75	114.37

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	450	BNG	O5-C5-C6-O6
5	B	452	PLC	O'-C'-O2-C2
5	B	452	PLC	C4-O4P-P-O1P
5	B	452	PLC	C4-O4P-P-O2P
5	B	452	PLC	C4-O4P-P-O3P
5	B	452	PLC	OB-CB-O3-C3
5	B	452	PLC	C1'-C'-O2-C2
5	B	452	PLC	C1B-CB-O3-C3
3	B	450	BNG	C4-C5-C6-O6
5	B	452	PLC	CB-C1B-C2B-C3B
5	B	452	PLC	C3'-C4'-C5'-C6'
5	B	452	PLC	C'-C1'-C2'-C3'
3	B	450	BNG	C4'-C5'-C6'-C7'
5	B	452	PLC	C1B-C2B-C3B-C4B
5	B	452	PLC	C1-C2-O2-C'

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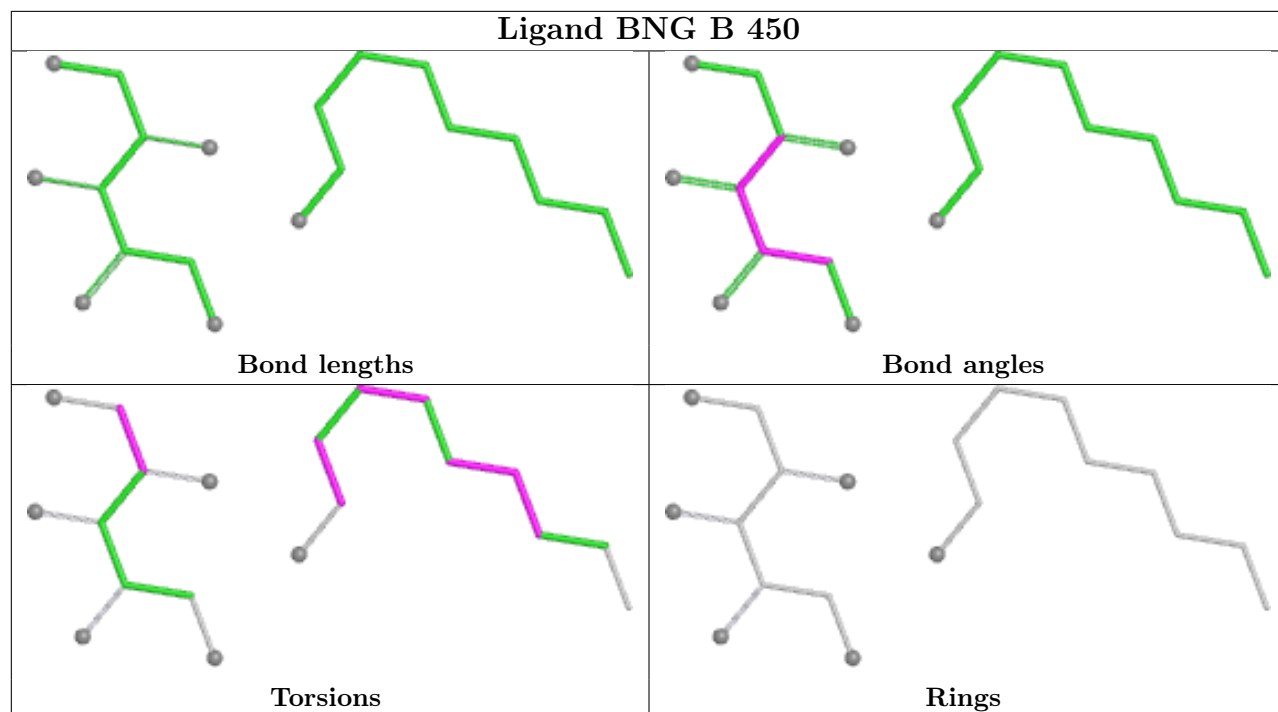
Mol	Chain	Res	Type	Atoms
5	B	452	PLC	C4B-C5B-C6B-C7B
3	B	450	BNG	C5'-C6'-C7'-C8'
5	B	452	PLC	O2-C2-C3-O3
3	B	450	BNG	C2'-C3'-C4'-C5'
3	B	450	BNG	O1-C1'-C2'-C3'
5	B	452	PLC	C7B-C8B-C9B-CAA
5	B	452	PLC	C2B-C3B-C4B-C5B
5	B	452	PLC	C2B-C1B-CB-O3
5	B	452	PLC	C2B-C1B-CB-OB

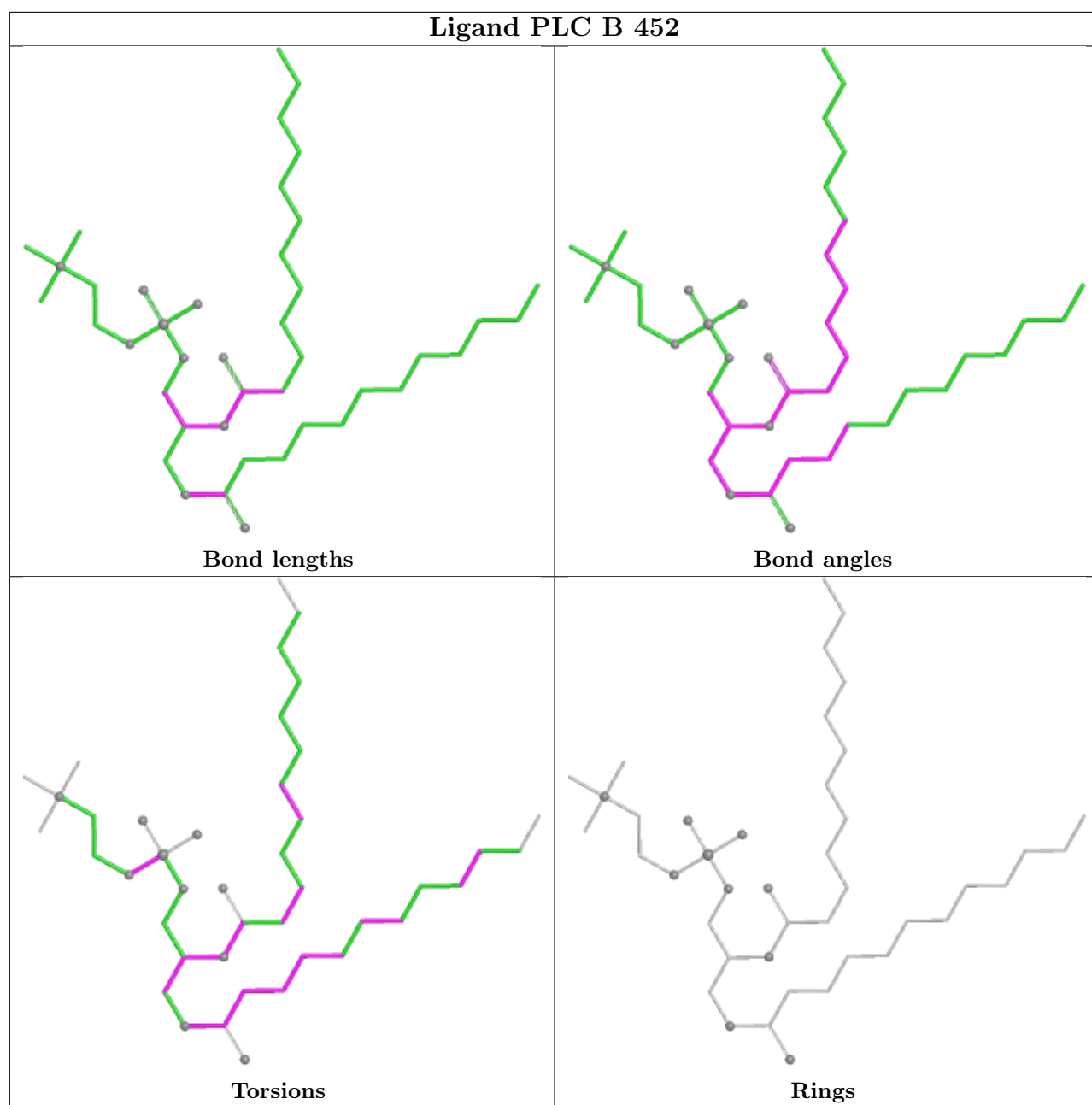
There are no ring outliers.

2 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	450	BNG	14	0
5	B	452	PLC	33	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.