



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:50 AM UTC

PDB ID : 1LPA / pdb_00001lpa
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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

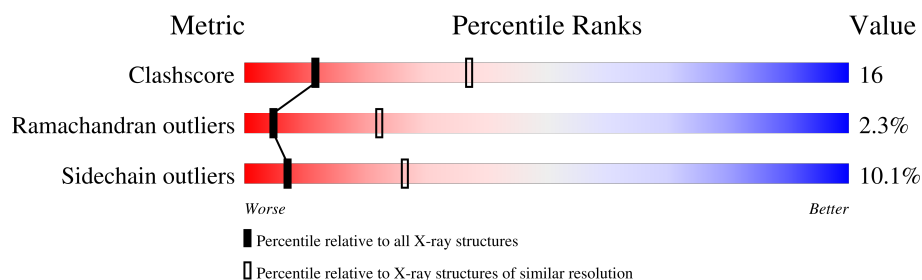
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (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 ≥ 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.

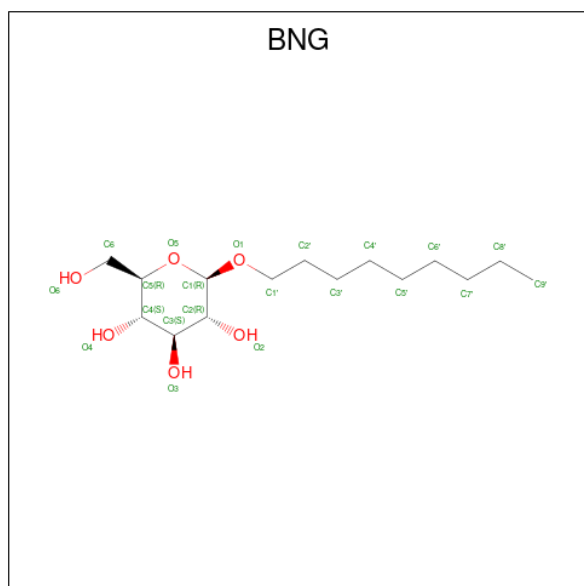
- Molecule 1 is a protein called COLIPASE.

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 (CCD ID: BNG) (formula: C₁₅H₃₀O₆).

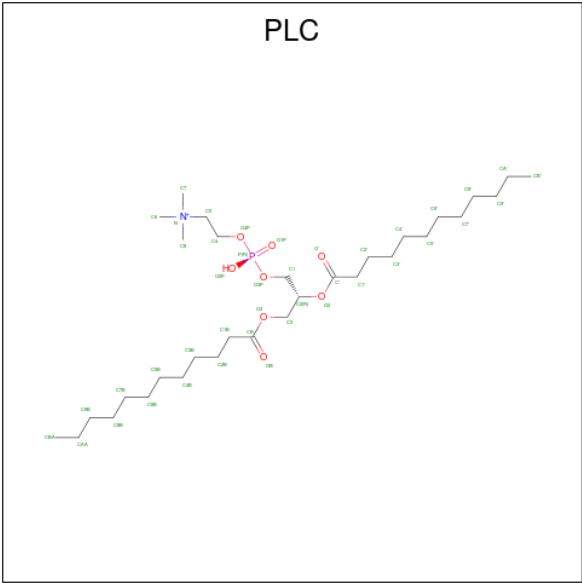


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



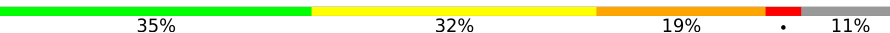
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	42	32	1	8	1	0	0

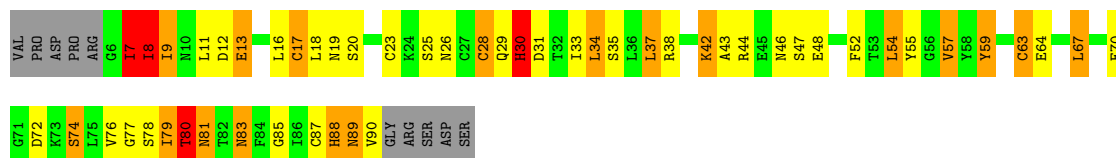
3 Residue-property plots

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.

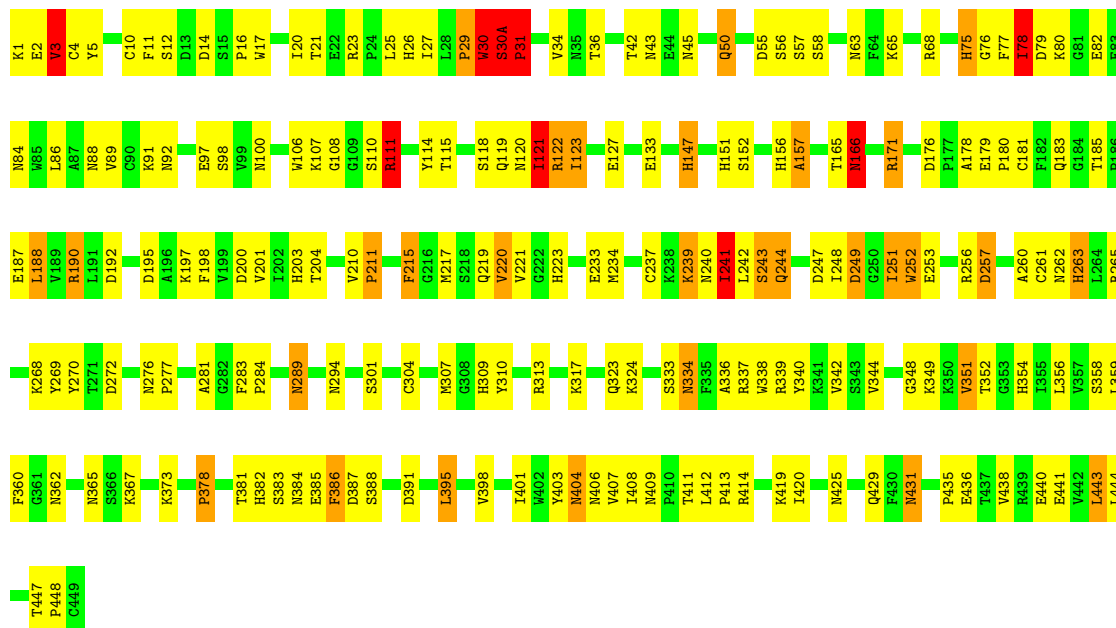
• Molecule 1: COLIPASE

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, α , β , γ	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 ²)	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: BNG, PLC, 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	1.17	3/647 (0.5%)	2.25	39/872 (4.5%)
2	B	1.21	20/3583 (0.6%)	2.08	128/4864 (2.6%)
All	All	1.20	23/4230 (0.5%)	2.11	167/5736 (2.9%)

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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	75	HIS	CD2-NE2	-9.53	1.27	1.37
2	B	156	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	30	HIS	CD2-NE2	-6.97	1.30	1.37
2	B	309	HIS	CD2-NE2	-6.77	1.30	1.37
2	B	263	HIS	CD2-NE2	-6.69	1.30	1.37
2	B	354	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	88	HIS	CD2-NE2	-6.62	1.30	1.37
2	B	382	HIS	CD2-NE2	-6.58	1.30	1.37
2	B	26	HIS	CD2-NE2	-6.43	1.30	1.37
2	B	223	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	30	HIS	CG-ND1	-6.05	1.31	1.38
2	B	203	HIS	CD2-NE2	-5.83	1.31	1.37
2	B	151	HIS	CD2-NE2	-5.70	1.31	1.37
2	B	30	TRP	CG-CD2	-5.68	1.33	1.43
2	B	75	HIS	CG-ND1	-5.52	1.32	1.38
2	B	263	HIS	CG-ND1	-5.49	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	HIS	CG-ND1	-5.44	1.32	1.38
2	B	29	PRO	CA-CB	-5.37	1.46	1.53
2	B	147	HIS	CD2-NE2	-5.23	1.32	1.37
2	B	187	GLU	C-O	5.16	1.30	1.24
2	B	151	HIS	CG-ND1	-5.13	1.32	1.38
2	B	354	HIS	CG-ND1	-5.11	1.32	1.38
2	B	190	ARG	C-O	5.11	1.30	1.23

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	333	SER	O-C-N	11.94	137.49	122.81
2	B	406	ASN	CA-CB-CG	11.25	123.85	112.60
2	B	365	ASN	CA-CB-CG	11.14	123.74	112.60
1	A	7	ILE	N-CA-C	10.56	121.41	111.48
2	B	301	SER	N-CA-C	-10.24	94.40	109.15
2	B	89	VAL	N-CA-C	-9.69	101.42	110.53
2	B	333	SER	CA-C-N	9.57	139.82	121.54
2	B	333	SER	C-N-CA	9.57	139.82	121.54
2	B	79	ASP	CA-CB-CG	9.56	122.17	112.60
2	B	190	ARG	N-CA-C	9.55	122.75	109.18
2	B	220	VAL	N-CA-CB	-9.31	100.32	111.21
2	B	334	ASN	CA-CB-CG	-9.08	103.52	112.60
2	B	30(A)	SER	CA-C-O	-9.07	107.73	120.16
2	B	30(A)	SER	N-CA-C	8.66	128.95	109.81
1	A	59	TYR	N-CA-C	-8.57	102.95	113.41
2	B	362	ASN	CA-CB-CG	8.53	121.12	112.60
2	B	244	GLN	N-CA-C	-8.44	92.82	110.80
1	A	78	SER	N-CA-C	-8.39	101.37	111.69
2	B	251	ILE	N-CA-C	-8.28	102.36	110.72
2	B	166	ASN	CA-CB-CG	8.24	120.84	112.60
2	B	45	ASN	CA-CB-CG	8.23	120.83	112.60
1	A	89	ASN	N-CA-C	-8.05	95.44	108.41
2	B	334	ASN	OD1-CG-ND2	-7.95	114.65	122.60
1	A	89	ASN	CA-CB-CG	7.93	120.53	112.60
2	B	237	CYS	N-CA-C	7.89	122.73	113.18
2	B	147	HIS	CA-CB-CG	7.83	121.62	113.80
2	B	55	ASP	CA-CB-CG	7.80	120.40	112.60
2	B	334	ASN	N-CA-CB	7.62	123.38	110.49
2	B	240	ASN	CA-CB-CG	7.59	120.19	112.60
1	A	25	SER	N-CA-C	-7.58	97.70	109.76
2	B	220	VAL	CB-CA-C	7.46	121.21	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	309	HIS	CA-CB-CG	-7.44	106.36	113.80
2	B	50	GLN	CG-CD-NE2	7.44	127.56	116.40
2	B	30(A)	SER	CA-C-N	7.27	128.93	119.84
2	B	30(A)	SER	C-N-CA	7.27	128.93	119.84
2	B	187	GLU	N-CA-C	7.22	121.73	112.34
2	B	404	ASN	CA-CB-CG	7.22	119.82	112.60
2	B	50	GLN	OE1-CD-NE2	-7.21	115.39	122.60
1	A	42	LYS	N-CA-C	-7.21	98.86	110.32
2	B	391	ASP	N-CA-C	-7.16	95.95	108.20
1	A	17	CYS	N-CA-CB	-7.12	98.48	110.80
2	B	283	PHE	CA-CB-CG	-7.03	106.77	113.80
2	B	92	ASN	OD1-CG-ND2	-7.02	115.58	122.60
2	B	133	GLU	N-CA-C	-6.92	103.66	111.14
2	B	249	ASP	CA-C-O	6.87	130.34	120.51
2	B	188	LEU	O-C-N	6.87	129.45	122.03
1	A	83	ASN	OD1-CG-ND2	-6.79	115.81	122.60
2	B	447	THR	CA-C-N	6.76	126.79	119.90
2	B	447	THR	C-N-CA	6.76	126.79	119.90
2	B	425	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	72	ASP	O-C-N	6.72	131.13	122.87
2	B	304	CYS	N-CA-C	-6.71	99.88	109.62
2	B	30	TRP	CA-C-N	-6.68	102.49	117.20
1	A	63	CYS	N-CA-C	6.65	119.11	110.53
1	A	80	THR	N-CA-C	-6.61	96.72	110.80
1	A	7	ILE	CB-CG1-CD1	6.60	127.66	113.80
2	B	192	ASP	N-CA-C	-6.58	102.30	108.22
1	A	29	GLN	OE1-CD-NE2	-6.56	116.04	122.60
2	B	386	PHE	CA-CB-CG	6.55	120.35	113.80
1	A	28	CYS	N-CA-C	-6.49	99.12	109.76
2	B	200	ASP	CA-CB-CG	6.47	119.07	112.60
2	B	3	VAL	N-CA-CB	-6.47	100.56	111.23
1	A	25	SER	O-C-N	-6.42	115.52	123.04
1	A	19	ASN	OD1-CG-ND2	-6.42	116.18	122.60
2	B	3	VAL	CB-CA-C	6.42	121.82	111.29
2	B	431	ASN	CB-CA-C	-6.37	98.74	109.50
2	B	223	HIS	N-CA-C	-6.36	104.27	111.14
2	B	429	GLN	OE1-CD-NE2	-6.36	116.24	122.60
2	B	86	LEU	N-CA-C	-6.30	103.72	111.40
2	B	171	ARG	CA-CB-CG	6.26	126.62	114.10
2	B	30	TRP	CA-C-O	6.22	128.55	122.01
2	B	260	ALA	N-CA-CB	-6.22	104.33	111.79
1	A	25	SER	CA-C-O	-6.17	113.65	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ASP	CA-CB-CG	6.17	118.77	112.60
2	B	88	ASN	OD1-CG-ND2	-6.11	116.49	122.60
2	B	443	LEU	N-CA-CB	-6.07	100.55	110.21
2	B	14	ASP	CA-CB-CG	6.05	118.66	112.60
2	B	409	ASN	CA-C-N	6.01	125.71	119.82
2	B	409	ASN	C-N-CA	6.01	125.71	119.82
2	B	223	HIS	CB-CG-CD2	-5.97	123.44	131.20
2	B	334	ASN	N-CA-C	-5.96	98.11	110.80
2	B	215	PHE	N-CA-C	5.93	118.53	111.71
2	B	166	ASN	CA-C-O	5.91	128.96	120.51
2	B	166	ASN	N-CA-C	5.91	123.39	110.80
1	A	30	HIS	CA-CB-CG	5.87	119.67	113.80
1	A	81	ASN	CA-CB-CG	5.83	118.43	112.60
2	B	448	PRO	N-CA-C	5.82	120.34	111.15
1	A	90	VAL	CA-CB-CG2	5.80	120.25	110.40
2	B	378	PRO	O-C-N	5.75	130.14	123.06
2	B	248	ILE	N-CA-C	-5.74	99.21	107.37
2	B	351	VAL	N-CA-CB	-5.71	105.75	112.32
1	A	13	GLU	CB-CG-CD	5.71	122.31	112.60
2	B	276	ASN	O-C-N	-5.69	116.24	121.42
2	B	241	ILE	N-CA-CB	-5.69	101.85	111.23
2	B	340	TYR	CA-C-O	-5.68	114.82	121.46
2	B	324	LYS	N-CA-C	5.67	118.88	109.46
2	B	121	ILE	CA-CB-CG1	-5.66	100.78	110.40
1	A	12	ASP	N-CA-C	-5.65	102.92	110.55
2	B	123	ILE	N-CA-C	-5.65	105.02	110.72
2	B	30	TRP	CD1-CG-CD2	5.63	115.31	106.30
2	B	97	GLU	N-CA-C	5.62	116.69	108.14
2	B	78	ILE	O-C-N	-5.62	115.55	122.57
2	B	195	ASP	CA-CB-CG	5.59	118.19	112.60
2	B	30	TRP	CG-CD1-NE1	-5.58	102.95	110.20
2	B	276	ASN	CA-C-N	5.57	126.30	120.12
2	B	276	ASN	C-N-CA	5.57	126.30	120.12
1	A	88	HIS	CB-CG-CD2	-5.53	124.01	131.20
2	B	384	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	74	SER	N-CA-C	5.50	122.53	110.80
2	B	354	HIS	CB-CG-CD2	-5.48	124.08	131.20
2	B	121	ILE	CA-CB-CG2	5.46	119.79	110.50
2	B	156	HIS	CB-CG-CD2	-5.46	124.10	131.20
2	B	203	HIS	CB-CG-CD2	-5.46	124.10	131.20
2	B	406	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	52	PHE	CA-CB-CG	5.45	119.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	B	157	ALA	N-CA-C	-5.44	105.35	111.28
2	B	260	ALA	N-CA-C	5.43	116.82	110.41
2	B	281	ALA	N-CA-C	5.43	118.23	110.24
2	B	277	PRO	N-CA-C	5.42	120.71	114.20
1	A	76	VAL	N-CA-C	-5.41	102.53	109.30
2	B	409	ASN	OD1-CG-ND2	-5.41	117.19	122.60
2	B	268	LYS	N-CA-C	-5.38	105.07	111.69
2	B	30	TRP	CE2-CD2-CE3	5.37	124.17	118.80
2	B	78	ILE	CA-C-O	-5.37	114.07	120.78
2	B	253	GLU	CB-CG-CD	5.35	121.70	112.60
2	B	45	ASN	CA-C-N	5.33	125.42	119.87
2	B	45	ASN	C-N-CA	5.33	125.42	119.87
1	A	19	ASN	CB-CG-ND2	5.32	124.38	116.40
2	B	63	ASN	OD1-CG-ND2	-5.30	117.30	122.60
2	B	211	PRO	N-CD-CG	-5.30	97.44	103.80
2	B	165	THR	N-CA-C	-5.26	107.04	112.93
2	B	284	PRO	CA-C-O	-5.25	115.61	121.23
2	B	190	ARG	CA-C-O	5.25	127.58	121.49
2	B	252	TRP	CE2-CD2-CG	-5.25	100.90	107.20
2	B	294	ASN	OD1-CG-ND2	-5.25	117.35	122.60
2	B	365	ASN	OD1-CG-ND2	-5.24	117.36	122.60
2	B	17	TRP	CE2-CD2-CG	-5.24	100.92	107.20
2	B	338	TRP	CE2-CD2-CG	-5.20	100.96	107.20
2	B	30	TRP	CB-CG-CD2	-5.20	119.53	126.80
1	A	79	ILE	CA-C-N	5.19	131.46	121.54
1	A	79	ILE	C-N-CA	5.19	131.46	121.54
2	B	120	ASN	OD1-CG-ND2	-5.17	117.43	122.60
2	B	247	ASP	CA-CB-CG	5.16	117.76	112.60
2	B	233	GLU	N-CA-CB	-5.16	102.67	110.77
1	A	7	ILE	N-CA-CB	-5.15	106.47	111.57
1	A	9	ILE	N-CA-C	-5.15	100.35	108.90
2	B	373	LYS	N-CA-C	-5.14	99.58	108.69
2	B	323	GLN	CG-CD-NE2	5.14	124.11	116.40
1	A	72	ASP	CA-CB-CG	-5.13	107.47	112.60
1	A	46	ASN	OD1-CG-ND2	-5.13	117.47	122.60
2	B	407	VAL	CA-C-O	5.12	125.44	120.27
1	A	20	SER	N-CA-C	5.12	117.60	111.71
1	A	83	ASN	CA-CB-CG	5.11	117.71	112.60
2	B	3	VAL	CA-CB-CG2	-5.10	101.73	110.40
2	B	26	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	18	LEU	CA-C-O	5.09	124.42	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	336	ALA	O-C-N	5.09	129.10	122.89
2	B	195	ASP	O-C-N	-5.06	115.04	122.43
1	A	72	ASP	CA-C-O	5.04	126.29	120.84
2	B	187	GLU	CB-CG-CD	5.03	121.15	112.60
2	B	197	LYS	O-C-N	-5.03	116.79	122.12
2	B	367	LYS	CA-CB-CG	5.03	124.15	114.10
2	B	358	SER	CA-CB-OG	-5.01	101.08	111.10
2	B	84	ASN	CA-CB-CG	-5.01	107.59	112.60
2	B	289	ASN	CA-CB-CG	5.01	117.61	112.60
2	B	360	PHE	CA-CB-CG	-5.00	108.80	113.80

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	83	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	129	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 (129) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:419:LYS:HZ2	2:B:431:ASN:HB3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:HIS:HD2	2:B:76:GLY:O	1.98	0.47
2:B:204:THR:HA	2:B:234:MET:HE3	1.96	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
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:269:TYR:HB3	2:B:307:MET:HE3	2.02	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	2	13
2	B	447/449 (100%)	413 (92%)	25 (6%)	9 (2%)	6	25
All	All	530/544 (97%)	483 (91%)	35 (7%)	12 (2%)	5	22

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%)	61 (82%)	13 (18%)	2	9
2	B	383/383 (100%)	350 (91%)	33 (9%)	10	33
All	All	457/466 (98%)	411 (90%)	46 (10%)	7	26

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	8	ILE
1	A	9	ILE
1	A	11	LEU
1	A	13	GLU
1	A	30	HIS
1	A	34	LEU
1	A	37	LEU
1	A	47	SER
1	A	54	LEU
1	A	57	VAL
1	A	67	LEU
1	A	89	ASN
2	B	3	VAL
2	B	21	THR
2	B	31	PRO
2	B	50	GLN
2	B	56	SER
2	B	57	SER
2	B	58	SER
2	B	91	LYS
2	B	111	ARG
2	B	115	THR
2	B	118	SER
2	B	121	ILE
2	B	122	ARG
2	B	166	ASN

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Mol	Chain	Res	Type
2	B	210	VAL
2	B	211	PRO
2	B	220	VAL
2	B	239	LYS
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	385	GLU
2	B	395	LEU
2	B	412	LEU
2	B	435	PRO
2	B	436	GLU
2	B	441	GLU
2	B	444	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
2	B	26	HIS
2	B	35	ASN
2	B	63	ASN
2	B	75	HIS
2	B	88	ASN
2	B	136	GLN
2	B	145	ASN
2	B	166	ASN
2	B	365	ASN
2	B	404	ASN

5.3.3 RNA ⓘ

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
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'
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

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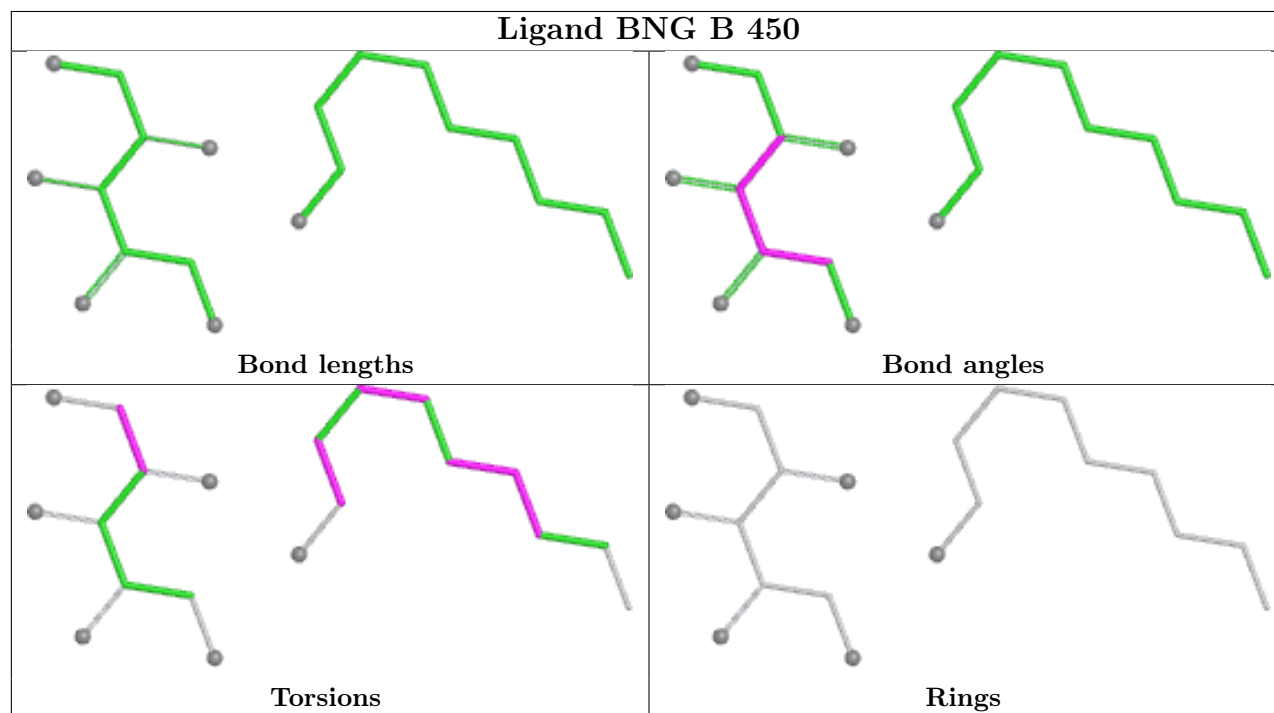
Mol	Chain	Res	Type	Atoms
5	B	452	PLC	C2B-C1B-CB-O3
5	B	452	PLC	C2B-C1B-CB-OB

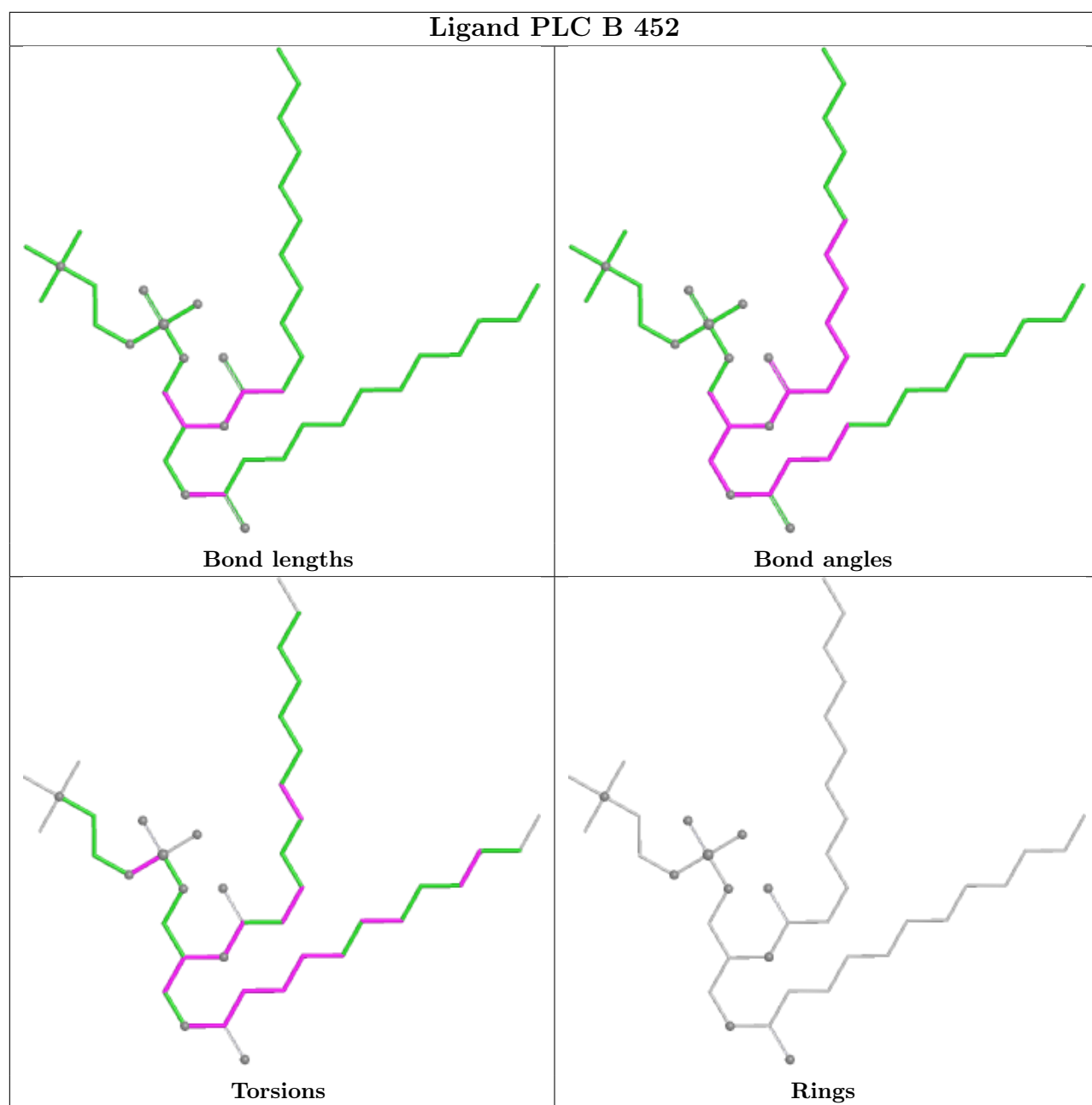
There are no ring outliers.

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.