



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:17 AM UTC

PDB ID : 1EIN / pdb_00001ein
Title : THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors : Brozozowski, A.M.; Savage, H.
Deposited on : 2000-02-26
Resolution : 3.00 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)	:	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

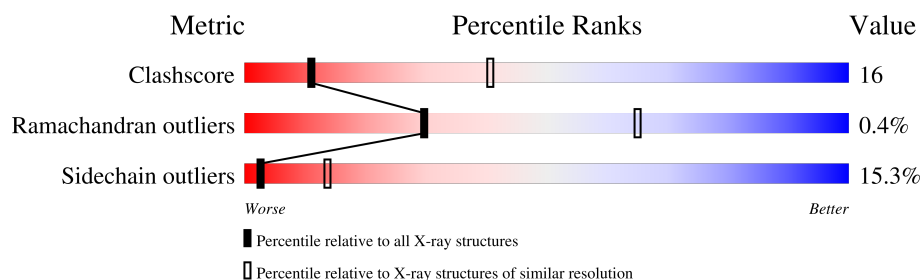
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	269	 63% 31% 5% •
1	B	269	 56% 35% 7% •
1	C	269	 55% 37% 6% •

2 Entry composition i

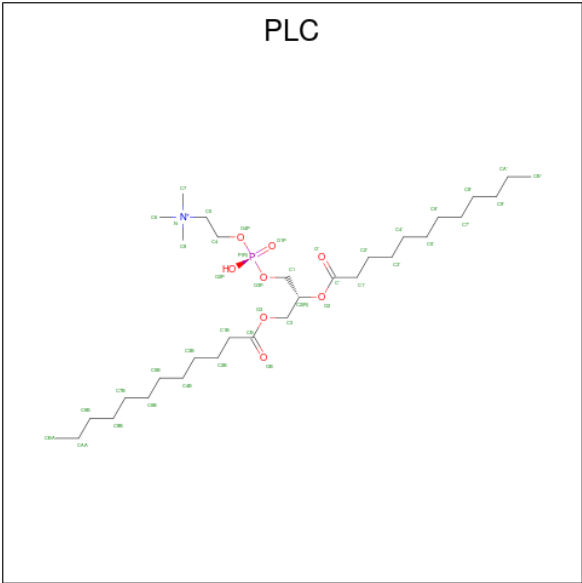
There are 3 unique types of molecules in this entry. The entry contains 6499 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			
1	B	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			
1	C	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			

- Molecule 2 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total 68	O 68	0	0
3	B	57	Total 57	O 57	0	0
3	C	59	Total 59	O 59	0	0

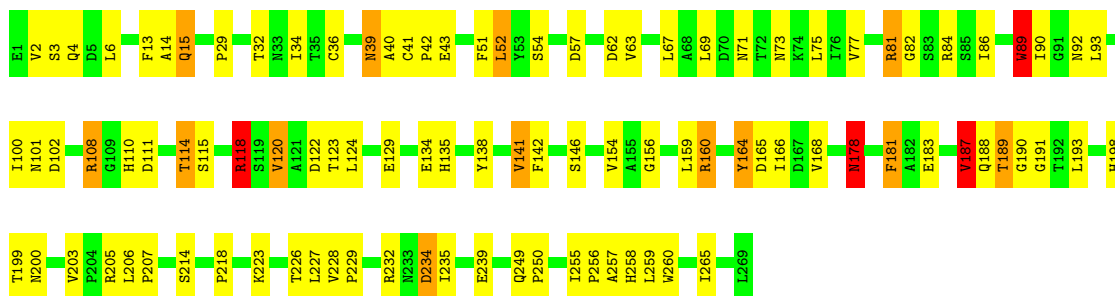
3 Residue-property plots

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.

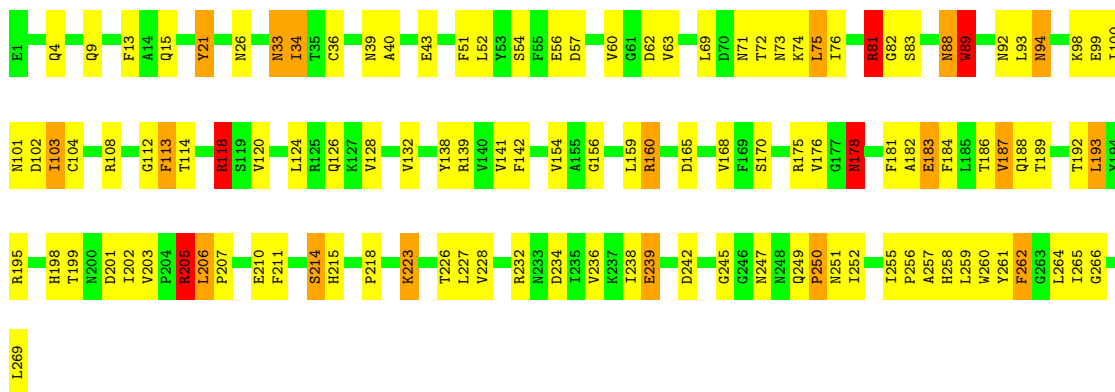
• Molecule 1: LIPASE

Chain A: 



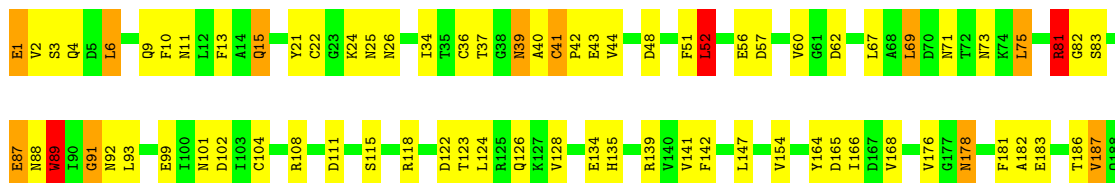
• Molecule 1: LIPASE

Chain B: 



• Molecule 1: LIPASE

Chain C: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	135.95Å 135.95Å 149.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.40 – 3.00	Depositor
% Data completeness (in resolution range)	99.8 (27.40-3.00)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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

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	0.55	0/2113	1.56	22/2878 (0.8%)
1	B	0.54	0/2113	1.57	23/2878 (0.8%)
1	C	0.51	0/2113	1.58	23/2878 (0.8%)
All	All	0.53	0/6339	1.57	68/8634 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	7
1	C	0	10
All	All	0	28

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	ARG	CD-NE-CZ	10.38	138.93	124.40
1	A	81	ARG	CG-CD-NE	8.45	130.59	112.00
1	C	195	ARG	CD-NE-CZ	8.09	135.73	124.40
1	B	203	VAL	N-CA-CB	7.72	115.36	110.50
1	C	203	VAL	N-CA-CB	7.23	115.05	110.50
1	A	118	ARG	CD-NE-CZ	7.13	134.38	124.40
1	C	205	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	B	81	ARG	CD-NE-CZ	7.11	134.35	124.40
1	A	110	HIS	CA-CB-CG	7.09	120.89	113.80
1	B	205	ARG	NE-CZ-NH2	7.02	125.52	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASP	CA-C-O	-7.01	114.12	121.55
1	C	71	ASN	OD1-CG-ND2	7.00	129.60	122.60
1	A	111	ASP	CA-C-N	6.95	127.84	119.99
1	A	111	ASP	C-N-CA	6.95	127.84	119.99
1	A	89	TRP	CA-CB-CG	-6.91	100.47	113.60
1	B	118	ARG	CD-NE-CZ	6.79	133.90	124.40
1	B	89	TRP	CA-CB-CG	-6.72	100.83	113.60
1	A	187	VAL	N-CA-CB	-6.68	103.11	112.12
1	B	160	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	B	113	PHE	N-CA-C	-6.63	103.97	111.14
1	C	52	LEU	N-CA-C	-6.49	105.01	113.12
1	C	91	GLY	O-C-N	-6.42	114.36	122.70
1	C	89	TRP	CA-CB-CG	-6.38	101.48	113.60
1	B	205	ARG	CD-NE-CZ	6.04	132.86	124.40
1	B	88	ASN	CA-C-O	5.97	127.08	120.82
1	A	135	HIS	CA-C-N	5.94	125.64	119.82
1	A	135	HIS	C-N-CA	5.94	125.64	119.82
1	A	14	ALA	N-CA-C	-5.89	104.81	112.23
1	C	15	GLN	OE1-CD-NE2	-5.87	116.73	122.60
1	B	142	PHE	CA-C-O	-5.80	114.56	120.71
1	A	189	THR	CA-CB-OG1	-5.73	101.00	109.60
1	A	89	TRP	N-CA-C	5.73	117.53	111.28
1	B	126	GLN	N-CA-C	5.67	117.14	111.07
1	B	178	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	108	ARG	CA-C-N	-5.65	117.13	122.66
1	A	108	ARG	C-N-CA	-5.65	117.13	122.66
1	B	264	LEU	N-CA-CB	5.59	118.24	109.69
1	B	94	ASN	CA-C-O	-5.57	115.68	122.64
1	A	81	ARG	CA-CB-CG	5.56	125.22	114.10
1	B	262	PHE	CA-C-N	5.55	129.75	121.04
1	B	262	PHE	C-N-CA	5.55	129.75	121.04
1	A	191	GLY	CA-C-O	-5.53	116.11	121.86
1	B	72	THR	CA-C-O	-5.52	115.01	120.70
1	A	101	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	111	ASP	CA-CB-CG	-5.49	107.11	112.60
1	C	126	GLN	OE1-CD-NE2	5.45	128.05	122.60
1	B	202	ILE	CA-C-N	5.41	123.65	120.24
1	B	202	ILE	C-N-CA	5.41	123.65	120.24
1	A	15	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	C	201	ASP	N-CA-C	-5.26	102.26	110.10
1	B	184	PHE	N-CA-C	5.21	117.64	111.33
1	C	135	HIS	CA-C-N	5.16	124.82	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	HIS	C-N-CA	5.16	124.82	119.56
1	B	195	ARG	CA-CB-CG	5.15	124.40	114.10
1	C	187	VAL	N-CA-CB	-5.15	102.45	112.75
1	C	189	THR	N-CA-CB	-5.14	101.88	110.83
1	C	186	THR	CA-C-N	5.14	127.65	121.84
1	C	186	THR	C-N-CA	5.14	127.65	121.84
1	C	48	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	234	ASP	CA-CB-CG	-5.12	107.48	112.60
1	C	111	ASP	N-CA-CB	-5.08	102.57	110.04
1	C	89	TRP	N-CA-C	5.08	116.50	111.07
1	B	112	GLY	CA-C-O	-5.08	113.76	120.36
1	A	160	ARG	CB-CG-CD	5.07	122.96	111.30
1	B	187	VAL	N-CA-CB	-5.02	105.34	112.12
1	A	52	LEU	N-CA-C	-5.01	106.86	113.12
1	C	254	ASP	CA-C-O	-5.01	115.25	121.11
1	C	242	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	GLU	Mainchain
1	A	134	GLU	Mainchain
1	A	141	VAL	Mainchain
1	A	164	TYR	Mainchain
1	A	178	ASN	Mainchain
1	A	214	SER	Mainchain
1	A	235	ILE	Mainchain
1	A	265	ILE	Mainchain
1	A	3	SER	Mainchain
1	A	41	CYS	Mainchain
1	A	92	ASN	Mainchain
1	B	113	PHE	Mainchain
1	B	165	ASP	Mainchain
1	B	21	TYR	Mainchain
1	B	250	PRO	Mainchain
1	B	33	ASN	Mainchain
1	B	76	ILE	Mainchain
1	B	94	ASN	Mainchain
1	C	134	GLU	Mainchain
1	C	203	VAL	Mainchain
1	C	262	PHE	Mainchain

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Mol	Chain	Res	Type	Group
1	C	3	SER	Mainchain
1	C	41	CYS	Mainchain
1	C	51	PHE	Mainchain
1	C	67	LEU	Mainchain
1	C	69	LEU	Mainchain
1	C	87	GLU	Mainchain
1	C	91	GLY	Mainchain

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	2063	0	1956	51	0
1	B	2063	0	1956	65	0
1	C	2063	0	1956	66	0
2	A	42	0	64	15	0
2	B	42	0	64	12	0
2	C	42	0	64	16	0
3	A	68	0	0	1	0
3	B	57	0	0	1	0
3	C	59	0	0	0	0
All	All	6499	0	6060	203	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 (203) 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:15:GLN:HE22	1:B:43:GLU:H	1.09	0.97
1:A:15:GLN:HE22	1:A:43:GLU:H	1.18	0.91
2:A:601:PLC:H5'2	1:C:89:TRP:HZ3	1.39	0.87
1:B:81:ARG:HG2	1:B:81:ARG:HH21	1.39	0.87
1:C:36:CYS:HB3	1:C:40:ALA:HB3	1.56	0.86
1:C:118:ARG:HH11	1:C:118:ARG:HG3	1.43	0.84
2:C:801:PLC:O'	2:C:801:PLC:H11	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:CYS:HB3	1:B:40:ALA:HB3	1.65	0.79
2:B:701:PLC:HE'1	2:C:801:PLC:HT'1	1.66	0.78
1:A:178:ASN:ND2	1:A:181:PHE:H	1.82	0.76
1:A:118:ARG:HG3	1:A:118:ARG:HH11	1.52	0.75
1:A:15:GLN:HE22	1:A:43:GLU:N	1.84	0.73
1:B:118:ARG:HH11	1:B:118:ARG:HG3	1.54	0.72
1:A:73:ASN:HB2	1:A:75:LEU:HD22	1.70	0.72
2:A:601:PLC:H52	2:C:801:PLC:H72	1.72	0.71
1:B:261:TYR:HB2	1:B:265:ILE:HG21	1.74	0.70
1:C:202:ILE:HB	1:C:253:PRO:HB2	1.75	0.68
2:B:701:PLC:H81	2:C:801:PLC:O1P	1.93	0.68
1:B:15:GLN:HE22	1:B:43:GLU:N	1.89	0.67
1:A:218:PRO:HB3	1:A:239:GLU:HG3	1.77	0.67
1:A:100:ILE:HG21	1:A:114:THR:HG21	1.77	0.66
1:C:178:ASN:ND2	1:C:181:PHE:H	1.94	0.65
1:C:73:ASN:HB2	1:C:75:LEU:HD22	1.79	0.65
2:B:701:PLC:H11	2:B:701:PLC:O'	1.98	0.64
1:C:99:GLU:HA	1:C:108:ARG:HG2	1.81	0.63
1:B:252:ILE:H	1:B:252:ILE:HD12	1.63	0.63
1:A:36:CYS:HB3	1:A:40:ALA:HB3	1.81	0.63
1:A:226:THR:HG23	1:A:260:TRP:HB2	1.82	0.62
1:B:73:ASN:HB2	1:B:75:LEU:HD22	1.81	0.61
1:A:39:ASN:O	1:A:42:PRO:HD3	2.01	0.61
1:B:223:LYS:HG2	1:B:234:ASP:O	2.00	0.61
2:A:601:PLC:P	2:C:801:PLC:H61	2.40	0.60
1:C:15:GLN:HE22	1:C:43:GLU:H	1.49	0.60
1:A:100:ILE:CG2	1:A:114:THR:HG21	2.32	0.59
1:C:4:GLN:NE2	1:C:232:ARG:HD3	2.18	0.59
1:C:261:TYR:HB2	1:C:265:ILE:HG21	1.85	0.59
1:C:226:THR:O	1:C:227:LEU:HB2	2.03	0.58
1:B:176:VAL:HG12	3:B:738:HOH:O	2.03	0.58
1:C:81:ARG:HH21	1:C:81:ARG:HG2	1.69	0.58
1:C:223:LYS:HG2	1:C:234:ASP:O	2.04	0.57
1:C:10:PHE:HD2	1:C:235:ILE:HD13	1.69	0.57
2:C:801:PLC:O'	2:C:801:PLC:C1	2.46	0.57
1:B:99:GLU:HA	1:B:108:ARG:HG2	1.87	0.56
1:C:21:TYR:OH	1:C:82:GLY:HA3	2.05	0.56
1:A:156:GLY:O	1:A:160:ARG:HG3	2.05	0.56
1:C:124:LEU:O	1:C:128:VAL:HG23	2.05	0.56
1:C:183:GLU:HG3	1:C:241:ILE:HD12	1.88	0.56
1:A:81:ARG:HD2	1:A:82:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HG13	1:A:51:PHE:CZ	2.41	0.56
1:A:146:SER:HB2	1:A:258:HIS:CE1	2.41	0.56
1:C:24:LYS:HE2	1:C:37:THR:HG23	1.87	0.56
1:B:4:GLN:HA	1:B:232:ARG:HD2	1.87	0.55
1:A:249:GLN:HB3	1:A:250:PRO:HD2	1.87	0.55
1:C:252:ILE:N	1:C:252:ILE:HD12	2.21	0.55
2:A:601:PLC:H51	2:C:801:PLC:H63	1.89	0.54
1:B:255:ILE:H	1:B:256:PRO:HD2	1.73	0.54
2:A:601:PLC:HT'1	2:C:801:PLC:HE'1	1.90	0.54
1:C:34:ILE:HG21	1:C:44:VAL:HG11	1.90	0.54
2:B:701:PLC:H61	2:C:801:PLC:P	2.48	0.53
1:B:108:ARG:H	1:B:178:ASN:ND2	2.06	0.53
1:B:255:ILE:N	1:B:256:PRO:HD2	2.24	0.53
1:A:203:VAL:HG22	2:A:601:PLC:H2	1.90	0.53
1:B:81:ARG:HG2	1:B:81:ARG:NH2	2.15	0.53
1:C:26:ASN:HB3	1:C:56:GLU:HB3	1.91	0.52
1:B:178:ASN:ND2	1:B:181:PHE:H	2.07	0.52
1:C:198:HIS:HD2	1:C:257:ALA:O	1.93	0.52
1:C:252:ILE:HD12	1:C:252:ILE:H	1.73	0.52
1:B:15:GLN:NE2	1:B:43:GLU:H	1.93	0.52
1:B:128:VAL:O	1:B:132:VAL:HG23	2.09	0.52
1:A:187:VAL:O	1:A:188:GLN:C	2.54	0.51
1:B:226:THR:O	1:B:227:LEU:HB2	2.10	0.51
1:B:250:PRO:O	1:B:251:ASN:HB3	2.10	0.51
2:B:701:PLC:C8	1:C:255:ILE:HG13	2.41	0.51
1:C:142:PHE:HB2	1:C:168:VAL:HG22	1.91	0.51
2:A:601:PLC:CA'	2:C:801:PLC:HE'1	2.41	0.51
1:C:198:HIS:HE1	1:C:224:SER:O	1.94	0.51
1:C:13:PHE:CE2	1:C:141:VAL:HG11	2.46	0.51
1:A:73:ASN:CB	1:A:75:LEU:HD22	2.40	0.51
2:B:701:PLC:H71	2:C:801:PLC:O4P	2.11	0.51
1:C:164:TYR:HE2	1:C:166:ILE:HD11	1.76	0.50
1:B:26:ASN:HB3	1:B:56:GLU:HB3	1.92	0.50
1:C:236:VAL:HG12	1:C:238:ILE:HD12	1.92	0.50
1:A:226:THR:O	1:A:227:LEU:HB2	2.11	0.50
1:C:122:ASP:O	1:C:123:THR:C	2.54	0.50
2:B:701:PLC:CB'	2:C:801:PLC:HT'1	2.38	0.50
1:B:57:ASP:HA	1:B:62:ASP:OD1	2.11	0.49
1:C:87:GLU:O	1:C:88:ASN:C	2.54	0.49
1:A:255:ILE:N	1:A:256:PRO:HD2	2.28	0.49
1:B:4:GLN:NE2	1:B:232:ARG:HD3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ARG:HG3	1:C:118:ARG:NH1	2.15	0.49
1:C:57:ASP:HA	1:C:62:ASP:OD1	2.12	0.49
1:C:81:ARG:HG2	1:C:82:GLY:O	2.13	0.49
1:A:164:TYR:HE2	1:A:166:ILE:HD11	1.79	0.48
1:A:84:ARG:HD3	3:A:659:HOH:O	2.12	0.48
1:A:206:LEU:HA	1:A:207:PRO:C	2.36	0.48
1:C:166:ILE:O	1:C:191:GLY:HA3	2.13	0.48
1:C:220:TYR:CE2	1:C:237:LYS:HG3	2.47	0.48
1:C:165:ASP:HA	1:C:190:GLY:O	2.14	0.48
1:B:21:TYR:OH	1:B:82:GLY:HA3	2.13	0.48
1:C:92:ASN:HB3	2:C:801:PLC:H3A1	1.94	0.48
1:C:39:ASN:O	1:C:42:PRO:HD3	2.14	0.48
2:A:601:PLC:O4P	2:C:801:PLC:H61	2.14	0.48
1:A:2:VAL:HG13	1:A:6:LEU:HB3	1.95	0.48
1:B:226:THR:HG23	1:B:260:TRP:HB2	1.96	0.48
1:C:101:ASN:HA	1:C:104:CYS:O	2.14	0.47
1:A:71:ASN:ND2	1:A:138:TYR:OH	2.44	0.47
1:A:57:ASP:HA	1:A:62:ASP:OD1	2.14	0.47
1:B:156:GLY:O	1:B:160:ARG:HG3	2.14	0.47
1:B:206:LEU:HA	1:B:207:PRO:C	2.40	0.47
2:A:601:PLC:HE'1	2:B:701:PLC:HT'1	1.95	0.47
1:B:201:ASP:OD1	1:B:258:HIS:HB2	2.15	0.47
1:A:89:TRP:CZ3	1:A:93:LEU:HD11	2.49	0.47
1:B:34:ILE:HD12	1:B:51:PHE:CE2	2.49	0.47
1:B:92:ASN:HB3	2:B:701:PLC:H3A2	1.96	0.47
1:B:210:GLU:H	1:B:210:GLU:CD	2.23	0.47
1:C:108:ARG:H	1:C:178:ASN:ND2	2.13	0.47
1:B:102:ASP:OD1	1:B:118:ARG:NH2	2.48	0.46
1:C:102:ASP:OD1	1:C:118:ARG:NH2	2.46	0.46
1:A:108:ARG:H	1:A:178:ASN:ND2	2.14	0.46
2:A:601:PLC:O'	2:A:601:PLC:C1	2.55	0.46
1:C:154:VAL:HG12	1:C:176:VAL:HG21	1.97	0.46
1:B:13:PHE:CZ	1:B:141:VAL:HG21	2.50	0.46
1:B:175:ARG:HG2	1:B:215:HIS:CD2	2.50	0.46
1:B:178:ASN:N	1:B:178:ASN:HD22	2.13	0.46
1:B:211:PHE:HB3	1:C:227:LEU:HD12	1.97	0.46
1:A:165:ASP:HA	1:A:190:GLY:O	2.15	0.46
1:C:102:ASP:OD2	1:C:102:ASP:N	2.48	0.46
1:A:146:SER:HB2	1:A:258:HIS:NE2	2.31	0.46
2:A:601:PLC:C'	2:A:601:PLC:O3P	2.63	0.46
2:B:701:PLC:H73	2:B:701:PLC:H42	1.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HD2	1:A:32:THR:HG21	1.97	0.46
1:A:39:ASN:HD22	1:A:39:ASN:HA	1.48	0.45
1:A:67:LEU:HD12	1:A:77:VAL:O	2.16	0.45
1:C:73:ASN:CB	1:C:75:LEU:HD22	2.45	0.45
1:C:250:PRO:O	1:C:251:ASN:HB3	2.16	0.45
2:B:701:PLC:H4'2	2:B:701:PLC:H1'2	1.82	0.45
1:C:232:ARG:NH2	1:C:232:ARG:HG3	2.32	0.45
1:B:9:GLN:OE1	1:B:139:ARG:NH1	2.49	0.45
1:C:206:LEU:HA	1:C:207:PRO:C	2.41	0.45
1:B:261:TYR:O	1:B:262:PHE:HB2	2.17	0.45
1:A:4:GLN:NE2	1:A:232:ARG:HD3	2.31	0.45
1:B:89:TRP:HZ3	2:C:801:PLC:H4'1	1.82	0.45
1:C:182:ALA:HB2	1:C:214:SER:HB3	1.98	0.45
1:B:249:GLN:HB3	1:B:250:PRO:HD2	1.99	0.44
1:B:21:TYR:CD2	1:B:266:GLY:HA2	2.52	0.44
1:B:187:VAL:O	1:B:188:GLN:C	2.60	0.44
1:B:198:HIS:HD2	1:B:257:ALA:O	1.99	0.44
1:C:22:CYS:HB2	1:C:25:ASN:ND2	2.33	0.44
1:C:75:LEU:HD12	1:C:139:ARG:HB3	1.99	0.44
1:C:101:ASN:O	1:C:102:ASP:C	2.58	0.44
1:B:101:ASN:HA	1:B:104:CYS:O	2.18	0.44
2:C:801:PLC:H4'2	2:C:801:PLC:H1'2	1.55	0.44
1:B:98:LYS:HE2	1:B:114:THR:HG21	1.99	0.44
1:A:84:ARG:O	2:A:601:PLC:H8'2	2.18	0.44
1:C:1:GLU:HB3	1:C:235:ILE:O	2.18	0.43
1:A:200:ASN:OD1	1:A:200:ASN:N	2.50	0.43
1:B:73:ASN:O	1:B:74:LYS:C	2.60	0.43
1:B:182:ALA:HB2	1:B:214:SER:HB3	2.00	0.43
1:A:15:GLN:NE2	1:A:43:GLU:HB2	2.34	0.43
1:A:102:ASP:OD1	1:A:118:ARG:NH2	2.51	0.43
1:A:13:PHE:CZ	1:A:141:VAL:HG21	2.54	0.43
1:C:92:ASN:ND2	1:C:147:LEU:HD13	2.33	0.43
1:A:198:HIS:HD2	1:A:257:ALA:O	2.01	0.43
1:B:21:TYR:HA	1:B:81:ARG:HD3	1.99	0.43
2:A:601:PLC:H5'2	1:C:89:TRP:CZ3	2.32	0.43
1:B:218:PRO:HB3	1:B:239:GLU:HG3	2.01	0.43
1:A:223:LYS:NZ	1:A:234:ASP:HA	2.34	0.43
1:B:33:ASN:O	1:B:34:ILE:C	2.60	0.43
2:B:701:PLC:H1A2	2:B:701:PLC:H32	1.63	0.43
1:A:228:VAL:HG23	1:A:229:PRO:HD2	2.01	0.43
1:B:98:LYS:HG2	1:B:99:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:SER:OG	1:B:242:ASP:OD1	2.37	0.43
1:B:245:GLY:H	1:B:249:GLN:HG2	1.84	0.43
2:A:601:PLC:H41	2:A:601:PLC:H82	1.85	0.43
1:B:88:ASN:HD22	1:B:88:ASN:HA	1.65	0.43
1:C:255:ILE:HB	1:C:256:PRO:HD3	2.01	0.43
1:B:100:ILE:HB	1:B:103:ILE:HG13	2.00	0.42
1:C:255:ILE:N	1:C:256:PRO:HD2	2.34	0.42
1:A:255:ILE:H	1:A:256:PRO:HD2	1.85	0.42
1:C:52:LEU:HD22	1:C:69:LEU:HB2	2.02	0.42
1:A:122:ASP:O	1:A:123:THR:C	2.61	0.42
1:C:10:PHE:CD2	1:C:235:ILE:HD13	2.52	0.42
1:B:75:LEU:HD12	1:B:139:ARG:HB3	2.02	0.42
1:B:183:GLU:O	1:B:186:THR:HB	2.20	0.42
1:B:108:ARG:H	1:B:178:ASN:HD21	1.66	0.42
1:C:255:ILE:H	1:C:256:PRO:HD2	1.85	0.42
1:C:232:ARG:HG3	1:C:232:ARG:HH21	1.83	0.42
1:C:6:LEU:HD23	1:C:6:LEU:HA	1.83	0.42
1:B:236:VAL:HG12	1:B:238:ILE:CD1	2.49	0.41
1:C:9:GLN:OE1	1:C:139:ARG:NH1	2.50	0.41
2:A:601:PLC:H1A1	2:A:601:PLC:H32	1.21	0.41
1:B:71:ASN:ND2	1:B:138:TYR:OH	2.53	0.41
1:A:142:PHE:O	1:A:168:VAL:HA	2.21	0.41
1:A:259:LEU:HD21	1:C:93:LEU:HD22	2.02	0.41
1:B:93:LEU:HD23	1:B:93:LEU:HA	1.88	0.41
1:C:15:GLN:NE2	1:C:41:CYS:HA	2.36	0.41
1:B:205:ARG:HG2	1:B:247:ASN:HD21	1.86	0.41
1:A:86:ILE:O	1:A:90:ILE:HG12	2.20	0.40
1:A:226:THR:HG23	1:A:260:TRP:CB	2.49	0.40
1:B:168:VAL:CG1	1:B:193:LEU:HD23	2.51	0.40
1:A:4:GLN:HA	1:A:232:ARG:HD2	2.03	0.40
1:A:63:VAL:HG11	1:A:120:VAL:HG11	2.03	0.40
1:B:118:ARG:HG3	1:B:118:ARG:NH1	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	267/269 (99%)	246 (92%)	20 (8%)	1 (0%)	30	65
1	B	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	65
1	C	267/269 (99%)	246 (92%)	20 (8%)	1 (0%)	30	65
All	All	801/807 (99%)	742 (93%)	56 (7%)	3 (0%)	30	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	THR
1	C	199	THR
1	B	199	THR

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	112/220 (51%)	93 (83%)	19 (17%)	2	11
1	B	196/220 (89%)	165 (84%)	31 (16%)	2	13
1	C	189/220 (86%)	163 (86%)	26 (14%)	3	17
All	All	497/660 (75%)	421 (85%)	76 (15%)	3	14

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	52	LEU
1	A	54	SER
1	A	69	LEU
1	A	89	TRP
1	A	114	THR

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Mol	Chain	Res	Type
1	A	115	SER
1	A	118	ARG
1	A	120	VAL
1	A	124	LEU
1	A	154	VAL
1	A	159	LEU
1	A	178	ASN
1	A	181	PHE
1	A	183	GLU
1	A	187	VAL
1	A	189	THR
1	A	193	LEU
1	A	205	ARG
1	B	34	ILE
1	B	39	ASN
1	B	52	LEU
1	B	54	SER
1	B	60	VAL
1	B	63	VAL
1	B	69	LEU
1	B	75	LEU
1	B	81	ARG
1	B	83	SER
1	B	89	TRP
1	B	103	ILE
1	B	118	ARG
1	B	120	VAL
1	B	124	LEU
1	B	154	VAL
1	B	159	LEU
1	B	170	SER
1	B	178	ASN
1	B	183	GLU
1	B	189	THR
1	B	192	THR
1	B	193	LEU
1	B	205	ARG
1	B	206	LEU
1	B	214	SER
1	B	223	LYS
1	B	228	VAL
1	B	239	GLU

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Mol	Chain	Res	Type
1	B	259	LEU
1	B	269	LEU
1	C	1	GLU
1	C	2	VAL
1	C	6	LEU
1	C	11	ASN
1	C	39	ASN
1	C	52	LEU
1	C	60	VAL
1	C	75	LEU
1	C	81	ARG
1	C	83	SER
1	C	89	TRP
1	C	115	SER
1	C	178	ASN
1	C	187	VAL
1	C	189	THR
1	C	193	LEU
1	C	205	ARG
1	C	206	LEU
1	C	214	SER
1	C	215	HIS
1	C	219	GLU
1	C	228	VAL
1	C	232	ARG
1	C	239	GLU
1	C	259	LEU
1	C	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	71	ASN
1	A	73	ASN
1	A	92	ASN
1	A	135	HIS
1	A	178	ASN
1	A	198	HIS
1	B	39	ASN
1	B	71	ASN
1	B	73	ASN

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Mol	Chain	Res	Type
1	B	92	ASN
1	B	126	GLN
1	B	178	ASN
1	B	198	HIS
1	B	247	ASN
1	C	4	GLN
1	C	11	ASN
1	C	15	GLN
1	C	39	ASN
1	C	71	ASN
1	C	73	ASN
1	C	92	ASN
1	C	178	ASN
1	C	198	HIS

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](#)

3 ligands are modelled in this entry.

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
2	PLC	C	801	-	41,41,41	0.71	0	47,49,49	1.03	4 (8%)
2	PLC	A	601	-	41,41,41	0.74	0	47,49,49	1.17	6 (12%)
2	PLC	B	701	-	41,41,41	0.74	0	47,49,49	1.20	5 (10%)

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
2	PLC	C	801	-	-	24/45/45/45	-
2	PLC	A	601	-	-	22/45/45/45	-
2	PLC	B	701	-	-	21/45/45/45	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	PLC	C4-C5-N	-3.67	104.03	115.82
2	A	601	PLC	C2-O2-C'	-3.08	110.42	117.80
2	A	601	PLC	O2P-P-O4P	-2.74	95.15	107.57
2	C	801	PLC	C2B-C1B-CB	-2.61	104.14	113.69
2	A	601	PLC	C7-N-C6	2.47	115.48	108.98
2	A	601	PLC	O2-C2-C3	2.35	116.79	108.34
2	B	701	PLC	C2B-C1B-CB	-2.30	105.28	113.69
2	A	601	PLC	C8-N-C7	-2.29	102.95	108.98
2	A	601	PLC	O4P-P-O1P	2.23	117.79	108.94
2	B	701	PLC	P-O3P-C1	-2.20	108.73	121.35
2	B	701	PLC	C8-N-C7	-2.18	103.24	108.98
2	B	701	PLC	OB-CB-C1B	-2.09	115.59	123.78
2	C	801	PLC	C4-C5-N	-2.07	109.19	115.82
2	C	801	PLC	O3-CB-OB	2.06	128.79	123.63
2	C	801	PLC	O2P-P-O4P	-2.05	98.29	107.57

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PLC	O4P-C4-C5-N
2	A	601	PLC	C1B-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
2	A	601	PLC	C1-O3P-P-O4P
2	B	701	PLC	C1B-CB-O3-C3
2	B	701	PLC	OB-CB-O3-C3
2	B	701	PLC	C1-O3P-P-O1P
2	B	701	PLC	C1-O3P-P-O2P
2	B	701	PLC	C1-O3P-P-O4P
2	B	701	PLC	C4-O4P-P-O3P
2	C	801	PLC	O4P-C4-C5-N
2	C	801	PLC	C1B-CB-O3-C3
2	C	801	PLC	OB-CB-O3-C3
2	C	801	PLC	C1-O3P-P-O2P
2	C	801	PLC	C4-O4P-P-O1P
2	C	801	PLC	C4-O4P-P-O2P
2	C	801	PLC	C4-O4P-P-O3P
2	A	601	PLC	OB-CB-O3-C3
2	B	701	PLC	C1'-C2'-C3'-C4'
2	C	801	PLC	C1'-C2'-C3'-C4'
2	B	701	PLC	CB-C1B-C2B-C3B
2	A	601	PLC	CB-C1B-C2B-C3B
2	C	801	PLC	CB-C1B-C2B-C3B
2	B	701	PLC	C'-C1'-C2'-C3'
2	B	701	PLC	C2B-C3B-C4B-C5B
2	B	701	PLC	C6B-C7B-C8B-C9B
2	C	801	PLC	C4'-C5'-C6'-C7'
2	B	701	PLC	C5'-C6'-C7'-C8'
2	A	601	PLC	C2'-C3'-C4'-C5'
2	B	701	PLC	C3'-C4'-C5'-C6'
2	C	801	PLC	C5'-C6'-C7'-C8'
2	B	701	PLC	C4'-C5'-C6'-C7'
2	C	801	PLC	C1B-C2B-C3B-C4B
2	C	801	PLC	C5B-C6B-C7B-C8B
2	C	801	PLC	C3'-C4'-C5'-C6'
2	C	801	PLC	C4B-C5B-C6B-C7B
2	A	601	PLC	O3P-C1-C2-O2
2	C	801	PLC	C3B-C4B-C5B-C6B
2	A	601	PLC	C3B-C4B-C5B-C6B
2	A	601	PLC	C3'-C4'-C5'-C6'
2	A	601	PLC	O3P-C1-C2-C3
2	B	701	PLC	C1B-C2B-C3B-C4B
2	C	801	PLC	C8B-C9B-CAA-CBA
2	A	601	PLC	C8B-C9B-CAA-CBA
2	C	801	PLC	C'-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	A	601	PLC	C1B-C2B-C3B-C4B
2	A	601	PLC	C4B-C5B-C6B-C7B
2	A	601	PLC	C7B-C8B-C9B-CAA
2	A	601	PLC	C2B-C3B-C4B-C5B
2	B	701	PLC	C1-C2-O2-C'
2	C	801	PLC	C1-C2-O2-C'
2	C	801	PLC	C6B-C7B-C8B-C9B
2	B	701	PLC	O4P-C4-C5-N
2	A	601	PLC	C1'-C2'-C3'-C4'
2	A	601	PLC	C1-O3P-P-O1P
2	A	601	PLC	C4-O4P-P-O1P
2	B	701	PLC	C4-C5-N-C7
2	B	701	PLC	C4-O4P-P-O1P
2	C	801	PLC	C2B-C3B-C4B-C5B
2	C	801	PLC	C2'-C3'-C4'-C5'
2	A	601	PLC	O2-C2-C3-O3
2	A	601	PLC	C1-C2-O2-C'
2	C	801	PLC	O2-C2-C3-O3
2	A	601	PLC	C2B-C1B-CB-O3
2	C	801	PLC	O'-C'-C1'-C2'
2	A	601	PLC	O2-C'-C1'-C2'
2	B	701	PLC	O2-C'-C1'-C2'
2	B	701	PLC	O'-C'-C1'-C2'

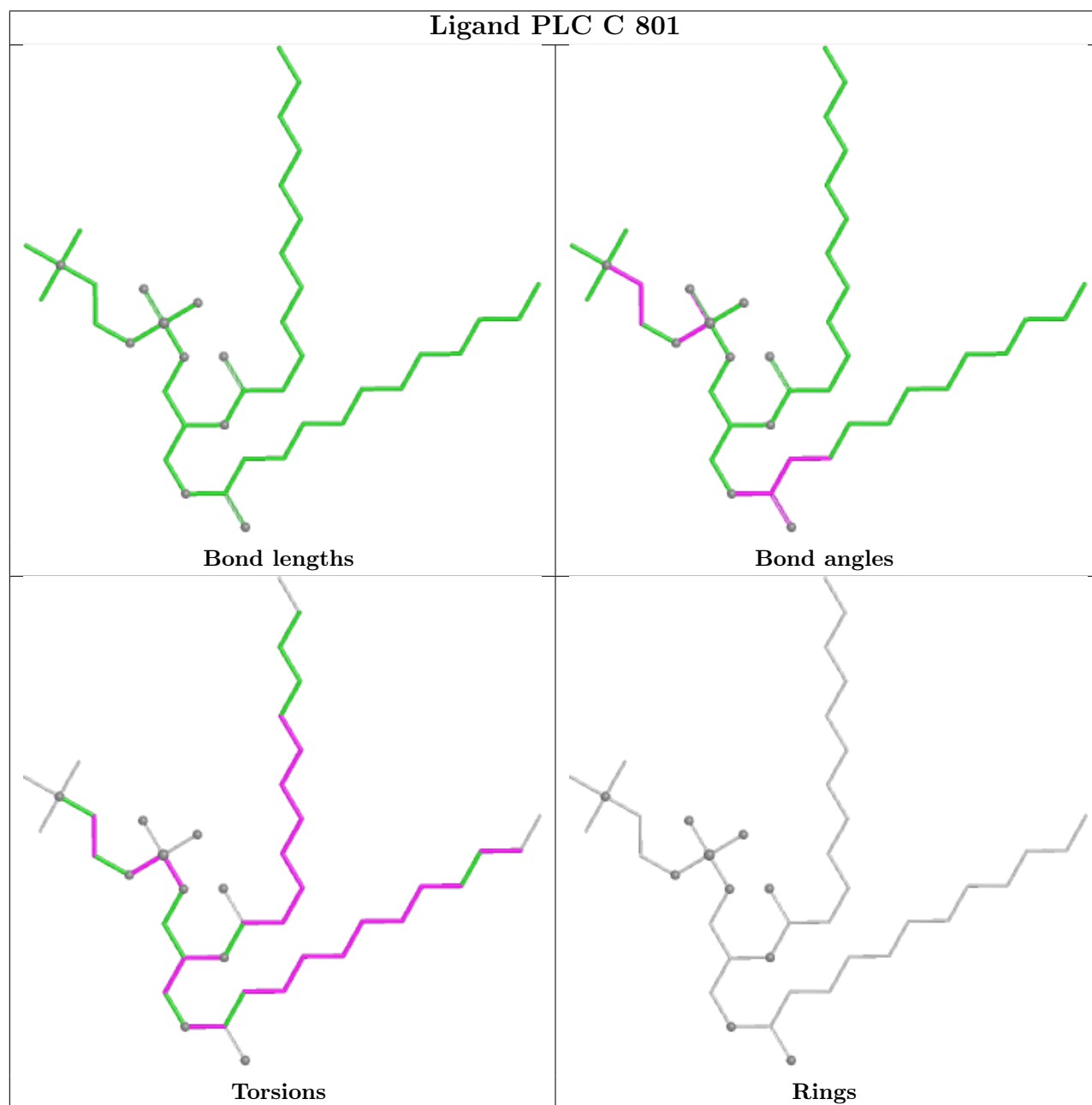
There are no ring outliers.

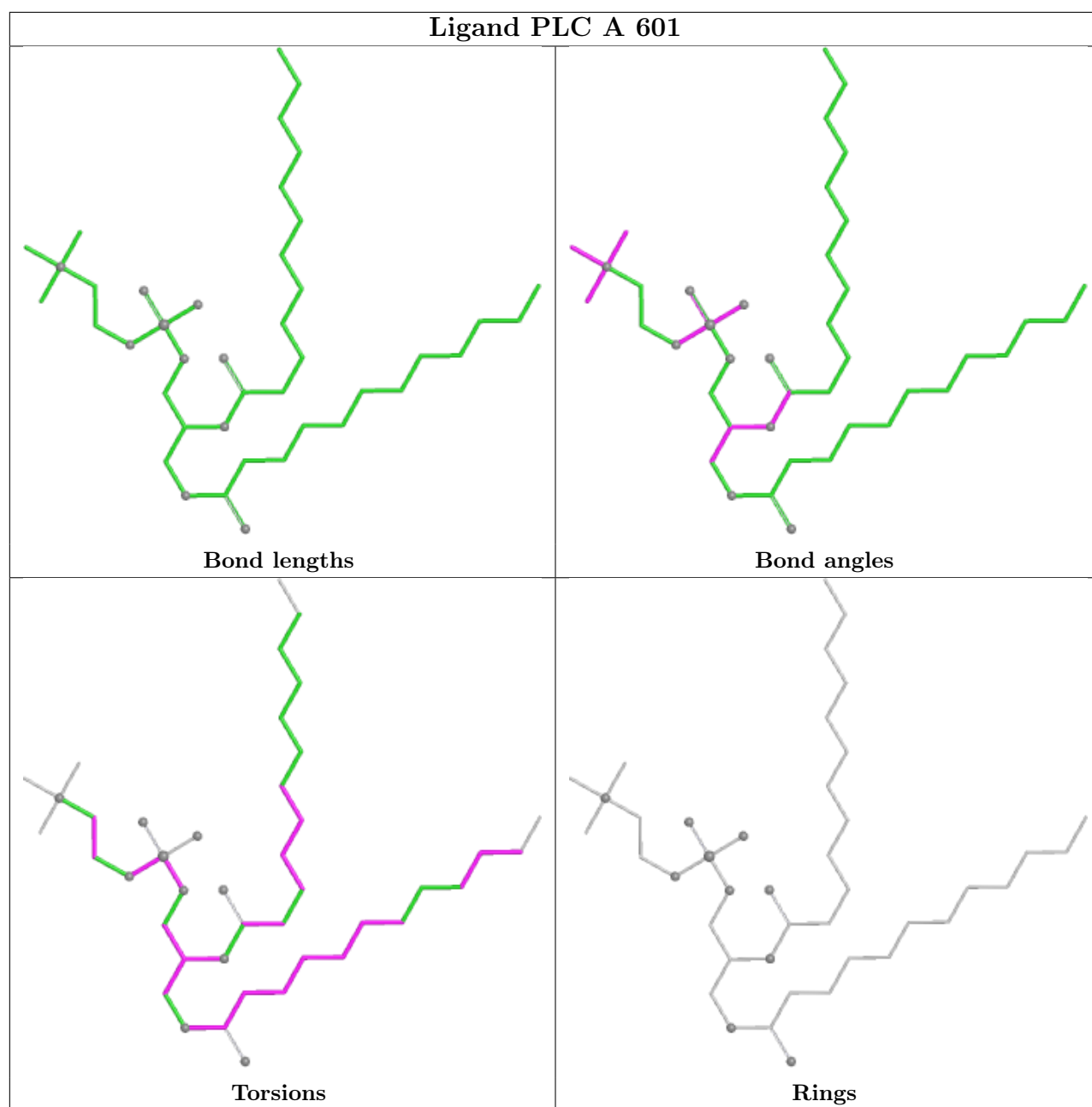
3 monomers are involved in 31 short contacts:

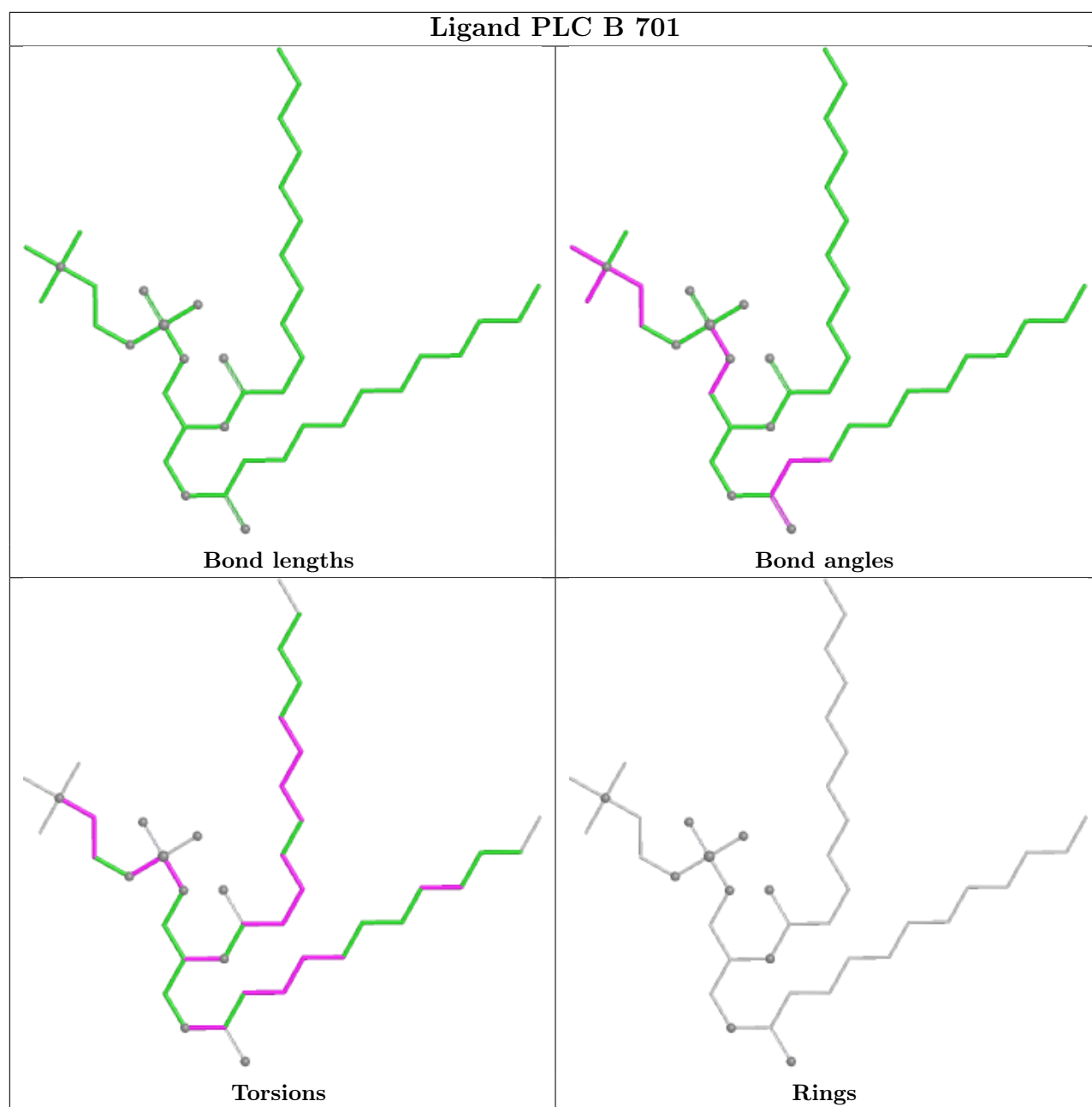
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	PLC	16	0
2	A	601	PLC	15	0
2	B	701	PLC	12	0

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.