



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:50 PM EDT

PDB ID : 2FNW / pdb_00002fnw
Title : Pseudomonas aeruginosa E2Q/H83Q/M109H-azurin RE(PHEN)(CO)₃
Authors : Gradinaru, C.; Crane, B.R.
Deposited on : 2006-01-11
Resolution : 1.40 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)	:	2.50

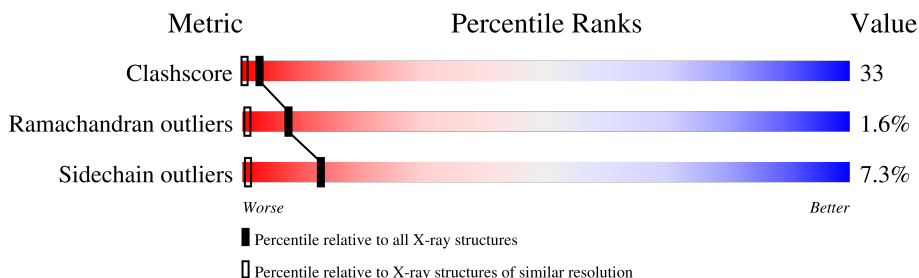
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)

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	128	
1	B	128	

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	REP	A	801[B]	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2262 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 Azurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	1	0
			981	611	168	194	8			
1	B	128	Total	C	N	O	S	0	3	0
			980	611	168	193	8			

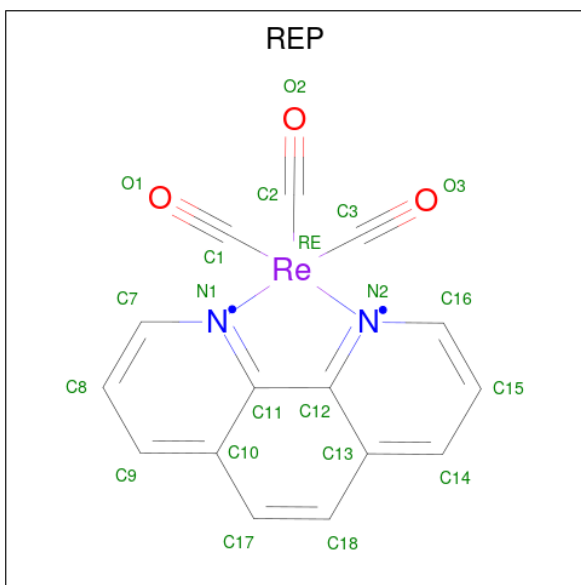
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLN	GLU	engineered mutation	UNP P00282
A	83	GLN	HIS	engineered mutation	UNP P00282
A	109	HIS	MET	engineered mutation	UNP P00282
B	202	GLN	GLU	engineered mutation	UNP P00282
B	283	GLN	HIS	engineered mutation	UNP P00282
B	309	HIS	MET	engineered mutation	UNP P00282

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is (1,10 PHENANTHROLINE)-(TRI-CARBON MONOXIDE) RHENIUM (I) (CCD ID: REP) (formula: C₁₅H₈N₂O₃Re).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	Re	0	1
			42	30	4	6	2		
3	B	1	Total	C	N	O	Re	0	1
			42	30	4	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	107	Total	O	0	0
			107	107		

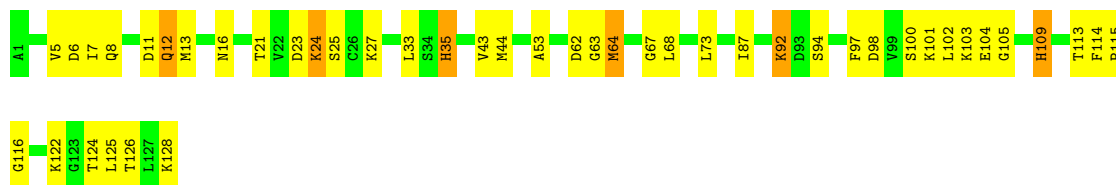
3 Residue-property plots

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.

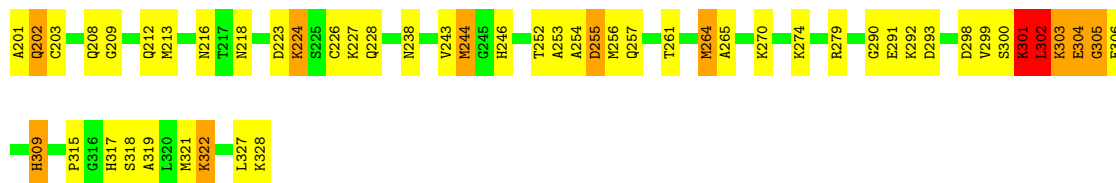
• Molecule 1: Azurin

Chain A: 



• Molecule 1: Azurin

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 1	Depositor
Cell constants a, b, c, α , β , γ	30.93Å 38.33Å 48.84Å 100.50° 106.25° 109.43°	Depositor
Resolution (Å)	30.00 – 1.40	Depositor
% Data completeness (in resolution range)	80.1 (30.00-1.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.196 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2262	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: CU, REP

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	0.74	0/1003	1.78	17/1352 (1.3%)
1	B	0.82	1/1013 (0.1%)	1.89	27/1366 (2.0%)
All	All	0.78	1/2016 (0.0%)	1.84	44/2718 (1.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	LYS	C-OXT	5.55	1.34	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109[A]	HIS	CA-CB-CG	8.38	122.18	113.80
1	A	109[B]	HIS	CA-CB-CG	8.38	122.18	113.80
1	B	227	LYS	O-C-N	7.95	133.65	122.36
1	B	238	ASN	OD1-CG-ND2	7.74	130.34	122.60
1	A	5	VAL	CA-C-O	-7.55	113.28	121.28
1	B	279	ARG	CA-C-N	-7.24	111.67	121.80
1	B	279	ARG	C-N-CA	-7.24	111.67	121.80
1	B	290	GLY	CA-C-O	6.98	126.77	119.02
1	A	23	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	256	MET	CA-C-O	6.15	127.48	120.90
1	A	105	GLY	CA-C-N	6.00	131.98	122.62
1	A	105	GLY	C-N-CA	6.00	131.98	122.62
1	A	109[A]	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
1	A	109[B]	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
1	A	73	LEU	CA-C-N	-5.94	112.05	120.49
1	A	73	LEU	C-N-CA	-5.94	112.05	120.49
1	B	261	THR	O-C-N	-5.84	116.06	122.07
1	A	35	HIS	CB-CG-CD2	-5.81	123.64	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	GLY	CA-C-N	-5.73	111.45	123.20
1	B	209	GLY	C-N-CA	-5.73	111.45	123.20
1	B	293	ASP	CA-CB-CG	-5.72	106.88	112.60
1	B	256	MET	CA-C-N	-5.67	112.68	120.28
1	B	256	MET	C-N-CA	-5.67	112.68	120.28
1	A	62	ASP	CA-C-N	-5.64	113.79	120.00
1	A	62	ASP	C-N-CA	-5.64	113.79	120.00
1	B	309[A]	HIS	CA-CB-CG	5.54	119.33	113.80
1	B	309[B]	HIS	CA-CB-CG	5.54	119.33	113.80
1	A	67	GLY	CA-C-O	5.43	127.44	122.39
1	B	302	LEU	CA-C-N	-5.37	114.65	122.65
1	B	302	LEU	C-N-CA	-5.37	114.65	122.65
1	B	279	ARG	O-C-N	5.36	129.85	122.46
1	B	244	MET	N-CA-CB	-5.32	105.41	111.79
1	B	291	GLU	CA-C-N	-5.32	113.59	122.21
1	B	291	GLU	C-N-CA	-5.32	113.59	122.21
1	B	209	GLY	O-C-N	5.25	129.52	122.70
1	A	63	GLY	O-C-N	-5.22	117.12	122.19
1	A	33	LEU	O-C-N	-5.21	117.38	123.27
1	B	265	ALA	CA-C-O	5.18	125.93	119.97
1	B	301	LYS	CA-C-N	-5.17	113.47	122.37
1	B	301	LYS	C-N-CA	-5.17	113.47	122.37
1	B	212	GLN	CA-C-O	5.08	125.59	119.59
1	B	223	ASP	CA-C-O	5.04	126.66	120.92
1	A	103	LYS	CA-C-O	5.03	126.38	120.80
1	B	319	ALA	CA-C-O	5.02	125.74	119.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	981	0	956	60	0
1	B	980	0	941	65	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	42	0	16	17	0
3	B	42	0	16	3	0
4	A	108	0	0	21	1
4	B	107	0	0	16	1
All	All	2262	0	1929	131	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (131) 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:213[B]:MET:HE2	1:B:317:HIS:CD2	1.59	1.34
1:A:109[A]:HIS:HE1	4:A:1148:HOH:O	0.96	1.26
1:A:24:LYS:HD2	1:A:24:LYS:C	1.61	1.20
1:B:302:LEU:HD23	1:B:327:LEU:HD11	1.25	1.18
1:A:98:ASP:OD2	1:A:101:LYS:CD	1.92	1.16
1:B:208[B]:GLN:NE2	4:B:1152:HOH:O	1.79	1.14
1:A:98:ASP:OD2	1:A:101:LYS:CE	1.97	1.13
1:A:12:GLN:HG2	4:A:1197:HOH:O	1.47	1.13
1:B:318:SER:O	1:B:322:LYS:HD2	1.50	1.12
3:A:801[B]:REP:C14	4:A:1042:HOH:O	2.03	1.06
1:B:302:LEU:HD23	1:B:327:LEU:CD1	1.86	1.05
1:B:301:LYS:O	1:B:302:LEU:CD1	2.06	1.04
1:A:98:ASP:OD1	1:A:100:SER:OG	1.75	1.01
1:B:202:GLN:N	4:B:1203:HOH:O	1.95	0.99
1:B:301:LYS:O	1:B:302:LEU:HD12	1.62	0.99
1:B:252:THR:OG1	1:B:255:ASP:OD1	1.80	0.98
1:A:109[B]:HIS:CE1	4:A:1148:HOH:O	2.17	0.95
1:B:213[B]:MET:CE	1:B:317:HIS:CD2	2.49	0.94
1:A:122:LYS:HE2	3:A:801[B]:REP:H171	1.50	0.94
3:B:802[B]:REP:H151	4:B:1032:HOH:O	1.68	0.94
1:B:228:GLN:NE2	1:B:298:ASP:OD1	2.00	0.93
1:B:254:ALA:O	4:B:1170:HOH:O	1.85	0.92
1:A:53:ALA:HB1	3:A:801[B]:REP:C3	1.99	0.92
1:B:303:LYS:O	1:B:304:GLU:O	1.89	0.90
1:B:322:LYS:NZ	3:B:802[A]:REP:O2	2.04	0.90
1:B:257:GLN:HA	1:B:257:GLN:OE1	1.71	0.89
1:A:98:ASP:OD2	1:A:101:LYS:HD2	1.73	0.87
1:A:24:LYS:HD2	1:A:25:SER:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HE3	4:A:1147:HOH:O	1.75	0.85
1:B:301:LYS:O	1:B:302:LEU:HD13	1.77	0.83
3:A:801[B]:REP:C2	4:A:1148:HOH:O	2.25	0.83
1:A:98:ASP:OD2	1:A:101:LYS:CG	2.27	0.81
1:B:213[B]:MET:HE2	1:B:317:HIS:HD2	1.10	0.81
1:B:201:ALA:C	4:B:1203:HOH:O	2.22	0.80
1:A:98:ASP:OD2	1:A:101:LYS:HE3	1.81	0.79
1:B:304:GLU:O	1:B:306:GLU:N	2.14	0.79
1:B:318:SER:O	1:B:322:LYS:CD	2.30	0.79
1:A:122:LYS:CE	3:A:801[B]:REP:H171	2.14	0.77
1:A:24:LYS:C	1:A:24:LYS:CD	2.46	0.77
1:B:202:GLN:OE1	1:B:202:GLN:HA	1.84	0.77
1:A:98:ASP:OD2	1:A:101:LYS:HG3	1.86	0.75
1:B:253:ALA:CB	1:B:309[B]:HIS:HD2	1.99	0.75
1:B:224:LYS:NZ	4:B:1195:HOH:O	2.13	0.75
1:A:53:ALA:HB1	3:A:801[B]:REP:O3	1.87	0.74
1:A:24:LYS:HD2	1:A:24:LYS:O	1.88	0.74
1:B:203:CYS:N	4:B:1090:HOH:O	2.03	0.72
1:A:8:GLN:NE2	4:A:1020:HOH:O	2.09	0.72
1:B:304:GLU:O	4:B:1044:HOH:O	2.09	0.71
1:B:302:LEU:CD2	1:B:327:LEU:HD11	2.15	0.70
1:A:122:LYS:HG3	3:A:801[B]:REP:H91	1.74	0.70
1:A:109[B]:HIS:HE1	4:A:1148:HOH:O	1.62	0.69
3:A:801[B]:REP:H141	4:A:1042:HOH:O	1.79	0.68
1:A:64:MET:HE3	1:A:115:PRO:HA	1.77	0.67
1:B:208[B]:GLN:HE21	1:B:216:ASN:HB3	1.60	0.66
1:B:306:GLU:OE2	4:B:1085:HOH:O	2.12	0.66
1:B:299:VAL:HG13	1:B:327:LEU:HD21	1.78	0.66
1:B:301:LYS:C	1:B:302:LEU:HD13	2.21	0.65
1:A:124:THR:HG23	4:A:1030:HOH:O	1.96	0.65
1:B:253:ALA:HB1	3:B:802[B]:REP:C7	2.27	0.64
1:A:98:ASP:CG	1:A:101:LYS:HG3	2.23	0.62
1:A:122:LYS:HG2	3:A:801[B]:REP:C17	2.30	0.61
1:B:302:LEU:HB3	1:B:327:LEU:HD22	1.82	0.61
1:A:122:LYS:HG3	3:A:801[B]:REP:C9	2.31	0.60
1:B:208[B]:GLN:NE2	1:B:216:ASN:HB3	2.15	0.60
1:A:13:MET:HE3	1:B:243:VAL:HG13	1.82	0.60
1:A:24:LYS:HZ2	1:A:25:SER:HA	1.67	0.59
1:B:274:LYS:CB	4:B:1095:HOH:O	2.49	0.59
3:A:801[A]:REP:H171	4:A:1076:HOH:O	2.02	0.59
1:A:21:THR:OG1	1:A:128:LYS:HE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ALA:HB1	1:B:309[B]:HIS:HD2	1.68	0.58
1:A:122:LYS:CG	3:A:801[B]:REP:H171	2.33	0.58
1:A:6:ASP:OD1	4:A:1202:HOH:O	2.17	0.57
1:A:92:LYS:NZ	1:A:94:SER:OG	2.34	0.57
1:A:44:MET:HG3	1:A:44:MET:O	2.04	0.57
1:B:301:LYS:C	1:B:302:LEU:CD1	2.79	0.55
1:A:122:LYS:HG2	3:A:801[B]:REP:H171	1.90	0.54
1:B:201:ALA:O	1:B:202:GLN:O	2.25	0.54
1:B:201:ALA:O	1:B:202:GLN:C	2.52	0.53
1:B:305:GLY:HA3	4:B:1111:HOH:O	2.10	0.52
1:B:213[B]:MET:CE	1:B:317:HIS:HD2	2.01	0.52
1:A:98:ASP:OD2	1:A:101:LYS:HE2	2.02	0.51
1:B:302:LEU:HD23	1:B:327:LEU:HD13	1.88	0.50
1:B:303:LYS:O	1:B:304:GLU:C	2.54	0.50
3:A:801[B]:REP:C16	4:A:1148:HOH:O	2.60	0.50
1:A:8:GLN:NE2	4:A:1089:HOH:O	2.43	0.50
1:A:12:GLN:CG	4:A:1197:HOH:O	2.26	0.49
1:A:92:LYS:CE	1:A:94:SER:OG	2.61	0.48
1:A:109[A]:HIS:CE1	4:A:1148:HOH:O	1.89	0.48
1:A:53:ALA:CB	1:A:109[B]:HIS:CD2	2.97	0.48
3:A:801[B]:REP:O1	4:A:1215:HOH:O	2.20	0.48
1:B:246:HIS:CG	1:B:321:MET:HE1	2.49	0.47
1:A:126:THR:HG23	4:A:1030:HOH:O	2.14	0.47
1:A:13:MET:CE	1:B:243:VAL:HA	2.46	0.46
1:A:122:LYS:CG	3:A:801[B]:REP:C17	2.93	0.46
1:A:97:PHE:HE2	1:A:102:LEU:HD11	1.81	0.46
1:B:264:MET:HG3	1:B:315:PRO:HG3	1.97	0.45
1:A:64:MET:HE3	1:A:116:GLY:H	1.81	0.45
1:A:125:LEU:C	1:A:125:LEU:HD23	2.42	0.45
1:A:53:ALA:HB2	1:A:109[B]:HIS:CD2	2.52	0.45
1:A:11:ASP:OD1	1:A:35:HIS:HE1	1.99	0.45
1:B:264:MET:HE2	4:B:1123:HOH:O	2.17	0.45
1:B:257:GLN:OE1	1:B:257:GLN:CA	2.51	0.45
1:B:226:CYS:O	1:B:299:VAL:HG11	2.18	0.44
1:B:252:THR:OG1	1:B:255:ASP:CG	2.58	0.44
1:B:253:ALA:CB	1:B:309[B]:HIS:CD2	2.90	0.44
1:A:24:LYS:HD2	1:A:25:SER:CA	2.47	0.44
1:B:306:GLU:CD	4:B:1085:HOH:O	2.57	0.43
1:B:202:GLN:HB3	1:B:203:CYS:H	1.64	0.43
1:B:246:HIS:ND1	1:B:321:MET:HE1	2.34	0.43
1:A:8:GLN:CB	4:A:1089:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LEU:HB3	1:B:327:LEU:CD2	2.49	0.43
1:B:201:ALA:HA	4:B:1177:HOH:O	2.20	0.42
1:B:255:ASP:HA	4:B:1170:HOH:O	2.18	0.42
1:B:302:LEU:HD12	1:B:302:LEU:HA	1.78	0.42
1:B:300:SER:C	1:B:302:LEU:H	2.27	0.42
1:B:270:LYS:HA	1:B:270:LYS:HD2	1.81	0.41
1:B:244:MET:O	1:B:244:MET:HG3	2.19	0.41
1:B:264:MET:HB2	4:B:1061:HOH:O	2.20	0.41
1:A:8:GLN:HG3	1:A:16:ASN:ND2	2.35	0.41
1:A:64:MET:SD	1:A:113:THR:O	2.79	0.41
1:A:24:LYS:NZ	1:A:25:SER:HA	2.35	0.41
1:A:98:ASP:OD1	1:A:101:LYS:HG3	2.21	0.41
1:A:128:LYS:HB2	4:A:1151:HOH:O	2.19	0.41
3:A:801[B]:REP:H161	4:A:1148:HOH:O	2.19	0.41
1:B:253:ALA:HB2	1:B:309[B]:HIS:HD2	1.84	0.41
1:A:35:HIS:HD2	1:A:87:ILE:O	2.02	0.41
1:B:304:GLU:C	1:B:306:GLU:H	2.25	0.41
1:A:7:ILE:HD13	1:A:7:ILE:HG21	1.94	0.40
1:A:114:PHE:CD1	1:A:115:PRO:HD2	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1042:HOH:O	4:B:1074:HOH:O[1_545]	1.96	0.24

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	127/128 (99%)	126 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	129/128 (101%)	120 (93%)	5 (4%)	4 (3%)	3	0
All	All	256/256 (100%)	246 (96%)	6 (2%)	4 (2%)	7	1

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	GLN
1	B	304	GLU
1	B	305	GLY
1	B	301	LYS

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	111/110 (101%)	104 (94%)	7 (6%)	16	1
1	B	111/110 (101%)	102 (92%)	9 (8%)	11	0
All	All	222/220 (101%)	206 (93%)	16 (7%)	13	1

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	24	LYS
1	A	27	LYS
1	A	64	MET
1	A	68	LEU
1	A	92	LYS
1	A	104	GLU
1	B	218	ASN
1	B	224	LYS
1	B	255	ASP
1	B	264	MET
1	B	292	LYS

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Mol	Chain	Res	Type
1	B	301	LYS
1	B	302	LEU
1	B	303	LYS
1	B	322	LYS

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	2	GLN
1	A	8	GLN
1	A	12	GLN
1	A	107	GLN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	REP	B	802[A]	1	11,24,24	1.53	2 (18%)	6,39,39	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	REP	A	801[A]	1	11,24,24	1.53	2 (18%)	6,39,39	0.59	0
3	REP	A	801[B]	1	11,24,24	1.51	2 (18%)	6,39,39	0.60	0
3	REP	B	802[B]	1	11,24,24	1.52	2 (18%)	6,39,39	0.59	0

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	REP	B	802[A]	1	-	-	0/4/4/4
3	REP	A	801[A]	1	-	-	0/4/4/4
3	REP	A	801[B]	1	-	-	0/4/4/4
3	REP	B	802[B]	1	-	-	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801[A]	REP	C8-C9	-2.74	1.33	1.41
3	B	802[A]	REP	C8-C9	-2.73	1.33	1.41
3	A	801[B]	REP	C8-C9	-2.68	1.34	1.41
3	B	802[A]	REP	C17-C18	-2.67	1.34	1.38
3	B	802[B]	REP	C8-C9	-2.67	1.34	1.41
3	A	801[B]	REP	C17-C18	-2.65	1.34	1.38
3	B	802[B]	REP	C17-C18	-2.63	1.34	1.38
3	A	801[A]	REP	C17-C18	-2.58	1.34	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

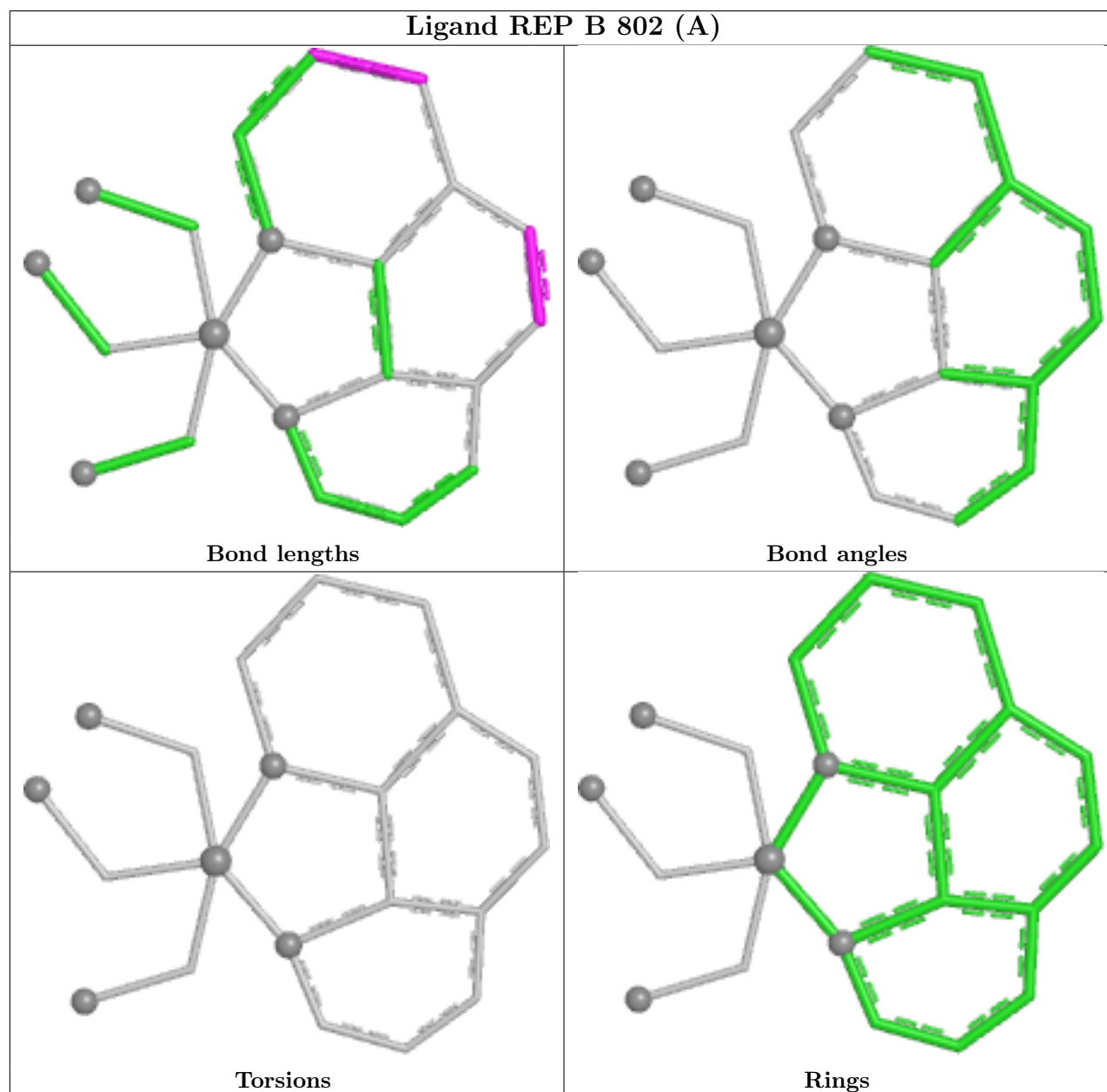
There are no ring outliers.

4 monomers are involved in 20 short contacts:

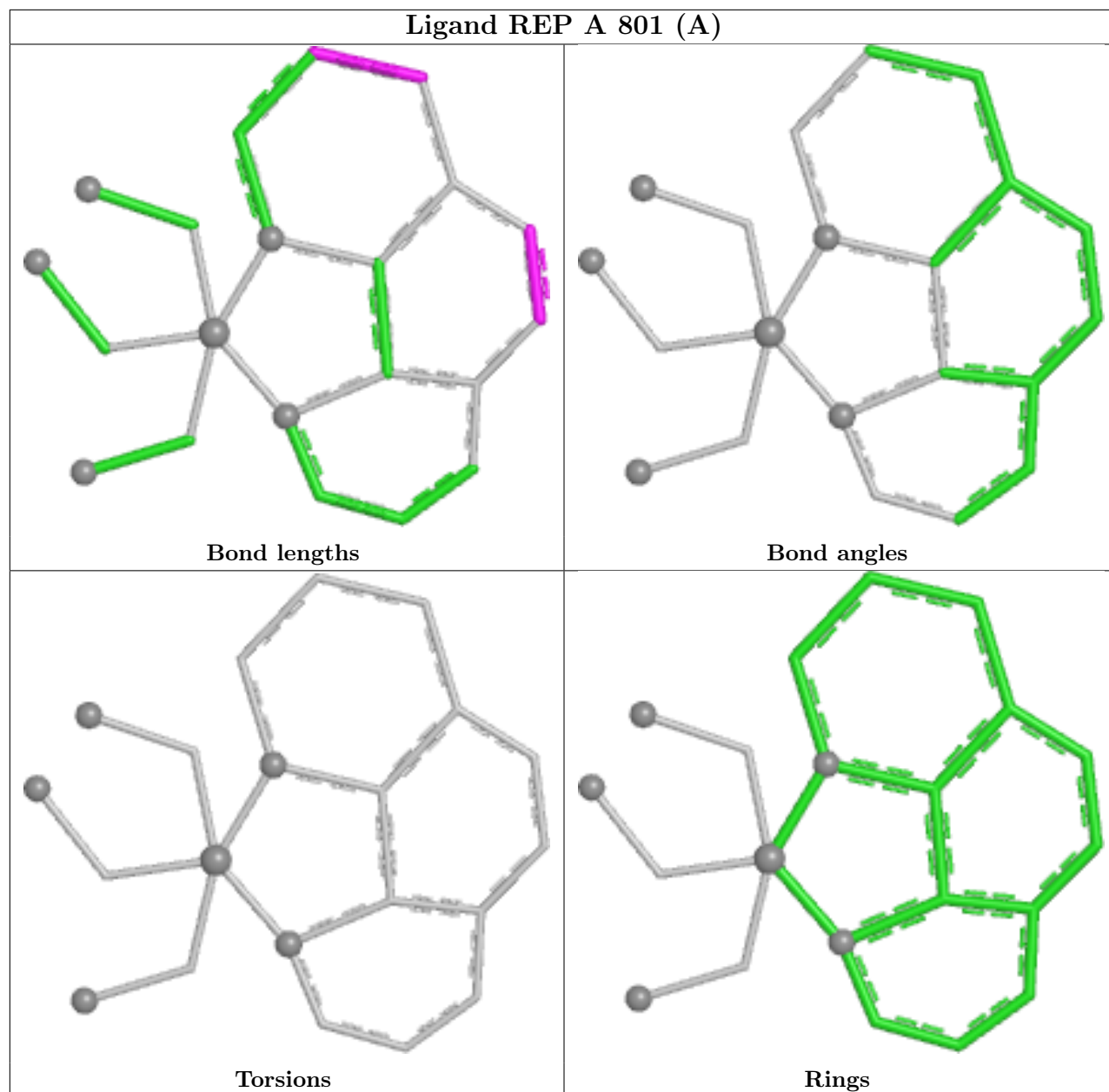
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802[A]	REP	1	0
3	A	801[A]	REP	1	0
3	A	801[B]	REP	16	0
3	B	802[B]	REP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

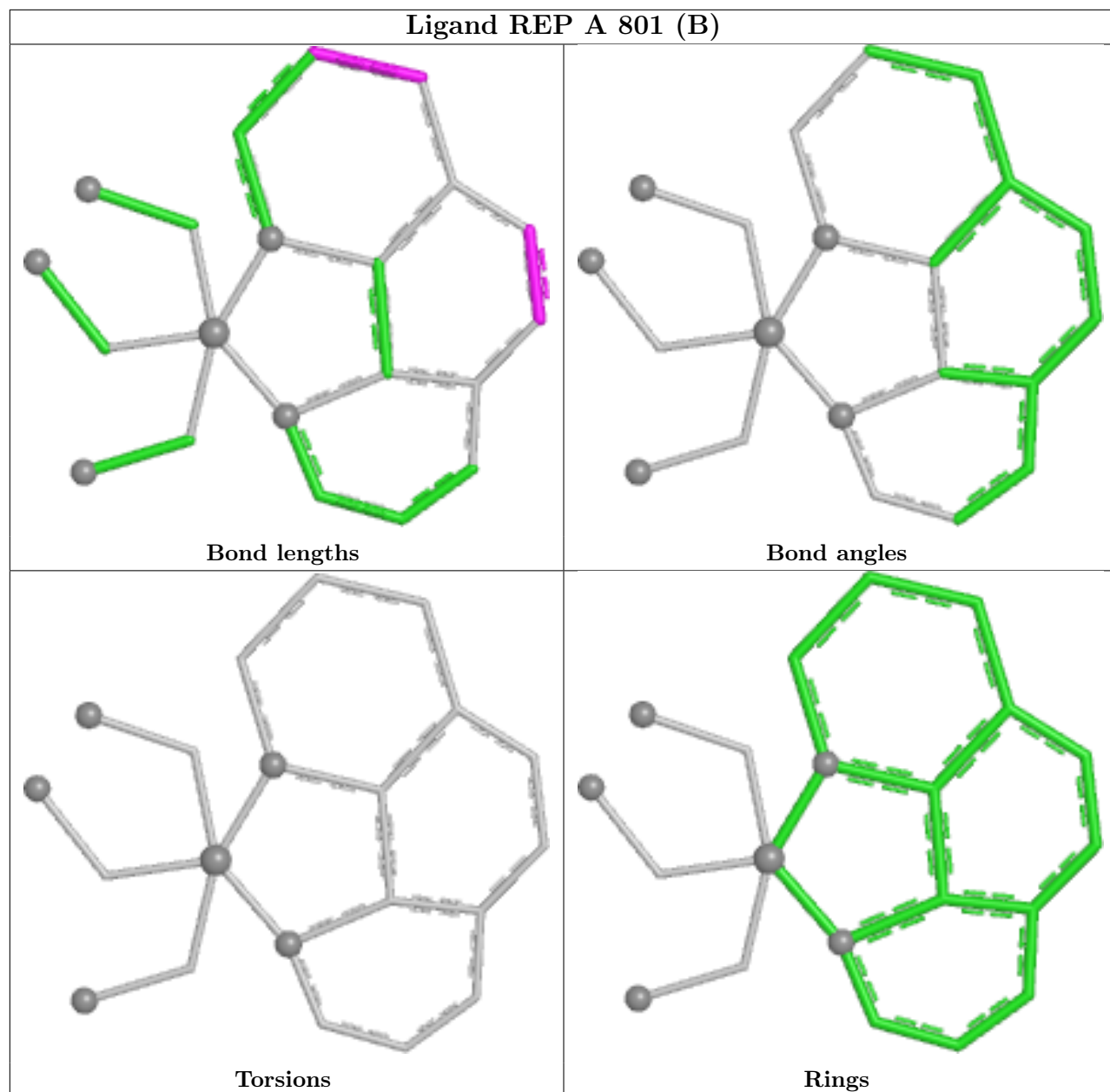
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

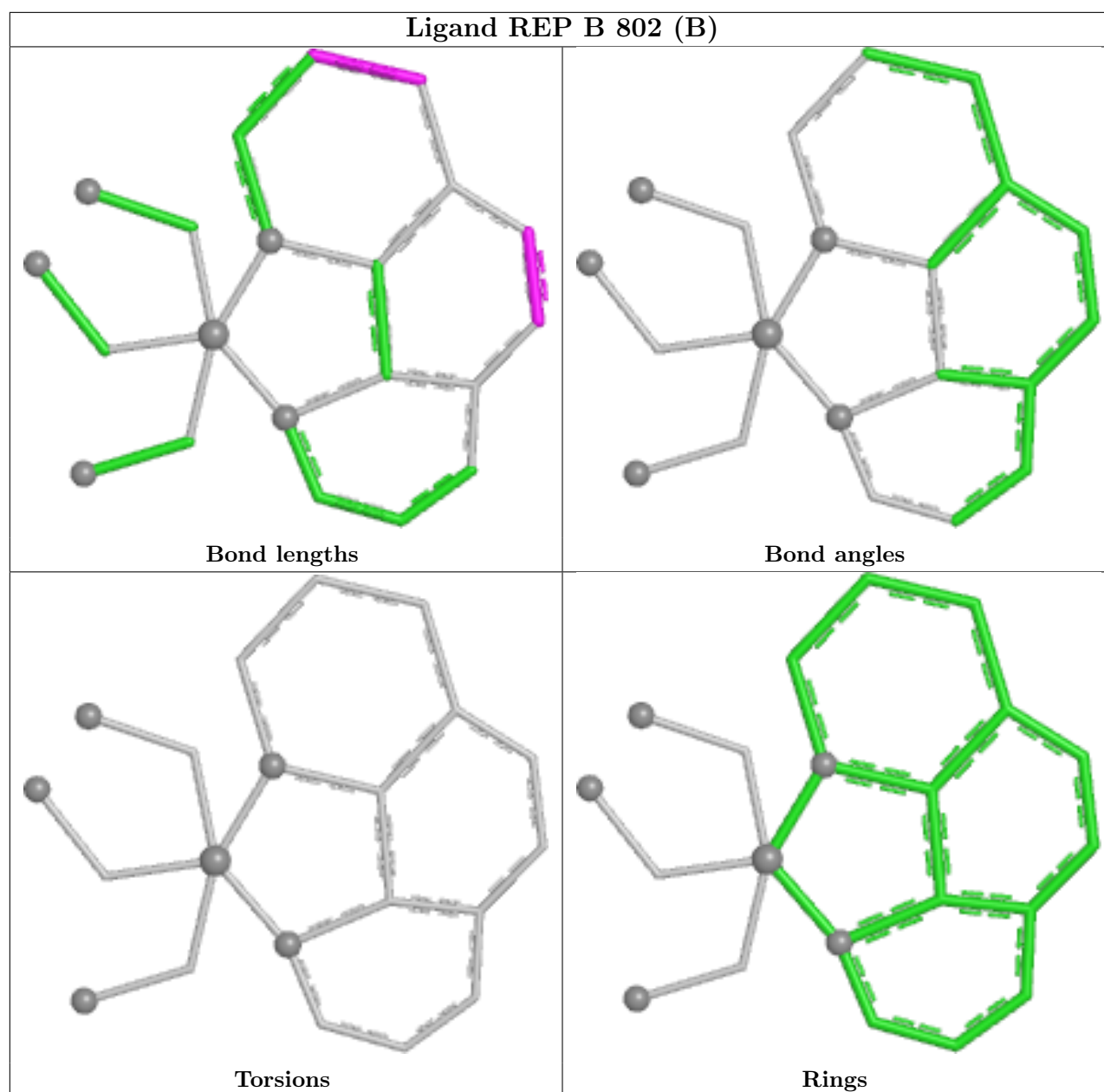


Ligand REP A 801 (A)



Ligand REP A 801 (B)





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.