



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:30 AM UTC

PDB ID : 1E61 / pdb_00001e61
Title : OXIDIZED DMSO REDUCTASE EXPOSED TO HEPES - Structure II
BUFFER
Authors : Bailey, S.; Bennett, B.; Adams, B.; Smith, A.T.; Bray, R.C.
Deposited on : 2000-08-06
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

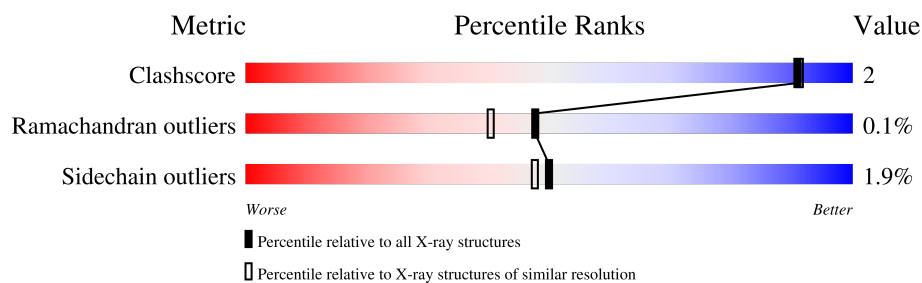
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	823	 85% 7% 7%
1	C	823	 85% 7% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12739 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 Dimethyl sulfoxide/trimethylamine N-oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	766	Total	C	N	O	S	0	0	0
			5880	3737	995	1121	27			
1	C	767	Total	C	N	O	S	0	0	0
			5888	3743	996	1122	27			

There are 26 discrepancies between the modelled and reference sequences:

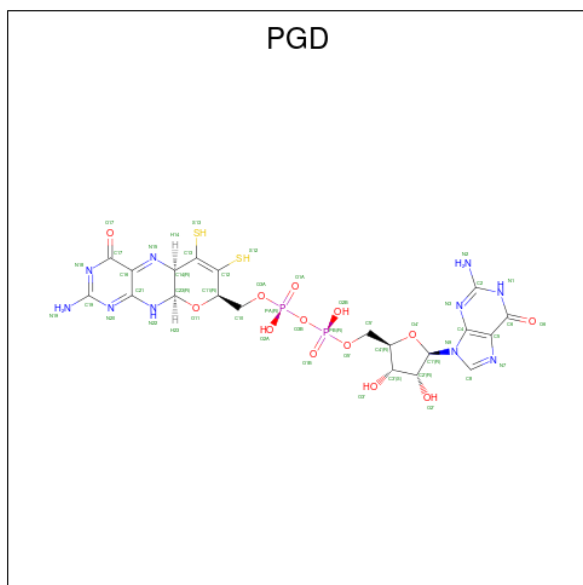
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	SER	THR	conflict	UNP Q52675
A	43	ALA	GLU	conflict	UNP Q52675
A	107	GLU	GLN	conflict	UNP Q52675
A	234	GLU	ASP	conflict	UNP Q52675
A	236	ILE	VAL	conflict	UNP Q52675
A	280	ASP	MET	conflict	UNP Q52675
A	294	GLU	SER	conflict	UNP Q52675
A	295	GLY	ASP	conflict	UNP Q52675
A	312	GLU	ILE	conflict	UNP Q52675
A	374	ALA	SER	conflict	UNP Q52675
A	456	VAL	ILE	conflict	UNP Q52675
A	526	ALA	LYS	conflict	UNP Q52675
A	552	ALA	GLY	conflict	UNP Q52675
C	39	SER	THR	conflict	UNP Q52675
C	43	ALA	GLU	conflict	UNP Q52675
C	107	GLU	GLN	conflict	UNP Q52675
C	234	GLU	ASP	conflict	UNP Q52675
C	236	ILE	VAL	conflict	UNP Q52675
C	280	ASP	MET	conflict	UNP Q52675
C	294	GLU	SER	conflict	UNP Q52675
C	295	GLY	ASP	conflict	UNP Q52675
C	312	GLU	ILE	conflict	UNP Q52675
C	374	ALA	SER	conflict	UNP Q52675
C	456	VAL	ILE	conflict	UNP Q52675
C	526	ALA	LYS	conflict	UNP Q52675

Continued on next page...

Continued from previous page...

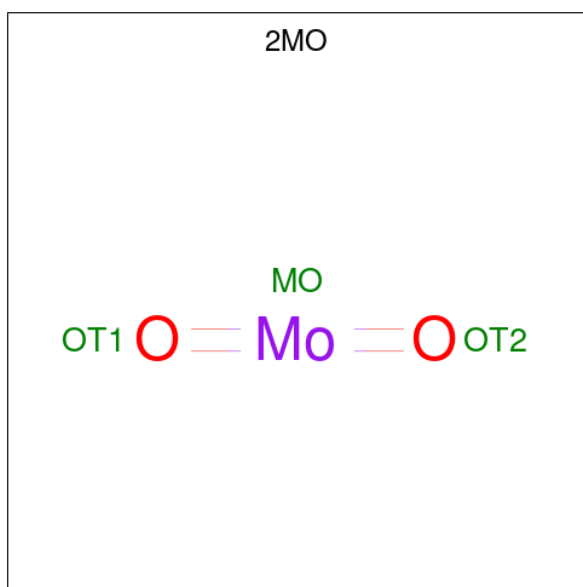
Chain	Residue	Modelled	Actual	Comment	Reference
C	552	ALA	GLY	conflict	UNP Q52675

- Molecule 2 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: PGD) (formula: $C_{20}H_{24}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 3 is MOLYBDENUM (IV)OXIDE (CCD ID: 2MO) (formula: MoO_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Mo	O	0	1
			3	2	1		
3	C	1	Total	Mo	O	0	1
			3	2	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

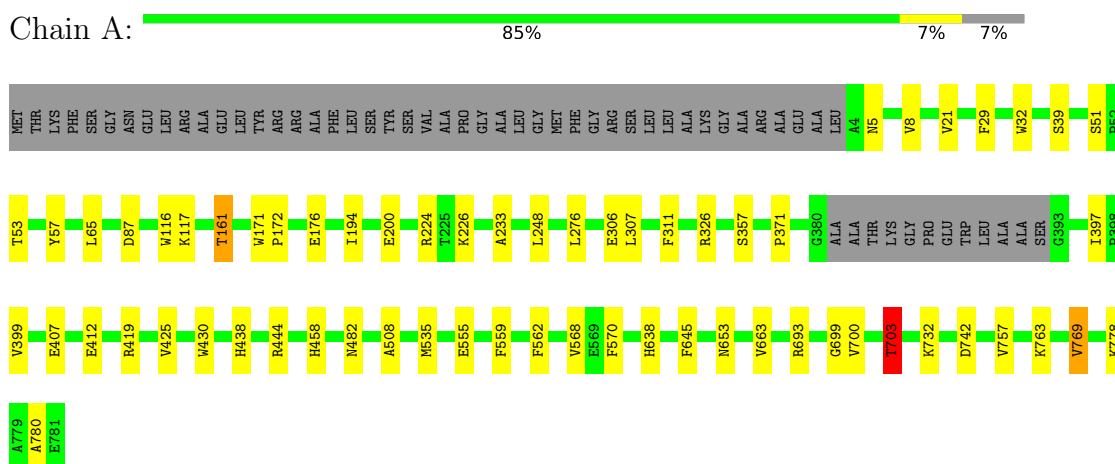
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	428	Total 428	O 428	0	0
5	C	339	Total 339	O 339	0	0

3 Residue-property plots [i](#)

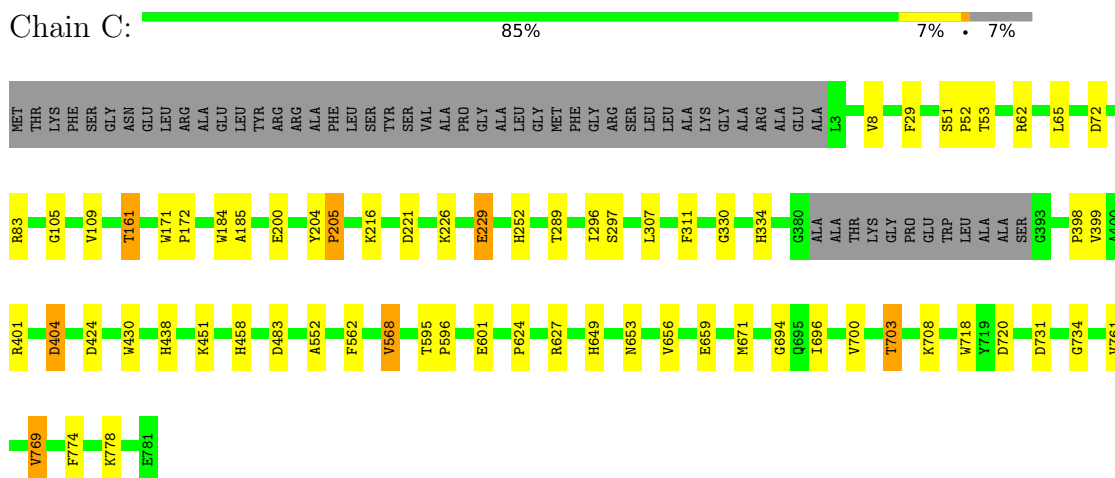
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: Dimethyl sulfoxide/trimethylamine N-oxide reductase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.19Å 118.14Å 235.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	78.2 (20.00-1.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.216	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12739	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: 2MO, SO4, PGD

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	0.69	0/6037	1.45	37/8215 (0.5%)
1	C	0.68	0/6045	1.46	39/8226 (0.5%)
All	All	0.68	0/12082	1.46	76/16441 (0.5%)

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
1	A	0	1

There are no bond length outliers.

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	438	HIS	CA-CB-CG	10.48	124.28	113.80
1	A	438	HIS	CA-CB-CG	10.05	123.86	113.80
1	C	703	THR	CB-CA-C	-9.84	92.15	110.16
1	A	703	THR	CB-CA-C	-9.17	93.38	110.16
1	C	221	ASP	CA-CB-CG	9.08	121.68	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	703	THR	Mainchain

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	5880	0	5680	18	0
1	C	5888	0	5691	18	0
2	A	94	0	41	0	0
2	C	94	0	41	2	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	428	0	0	4	0
5	C	339	0	0	2	0
All	All	12739	0	11453	37	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 2.

The worst 5 of 37 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:C:671:MET:HE1	1:C:761:VAL:HG11	1.72	0.71
1:A:226:LYS:HG2	5:A:2137:HOH:O	1.89	0.71
1:A:226:LYS:HD2	1:A:645:PHE:CZ	2.37	0.58
1:A:562:PHE:HD1	1:A:568:VAL:HG23	1.71	0.55
1:C:552:ALA:HB2	5:C:2214:HOH:O	2.07	0.54

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	762/823 (93%)	740 (97%)	22 (3%)	0	100	100
1	C	763/823 (93%)	742 (97%)	20 (3%)	1 (0%)	48	40
All	All	1525/1646 (93%)	1482 (97%)	42 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	734	GLY

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	609/648 (94%)	598 (98%)	11 (2%)	51	50
1	C	610/648 (94%)	598 (98%)	12 (2%)	48	46
All	All	1219/1296 (94%)	1196 (98%)	23 (2%)	50	47

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	200	GLU
1	C	307	LEU
1	C	229	GLU
1	C	430	TRP
1	A	430	TRP

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	434	ASN
1	A	606	ASN
1	C	241	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	606	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	PGD	A	802	3	46,52,52	3.60	14 (30%)	56,81,81	1.57	11 (19%)
4	SO4	C	901	-	4,4,4	0.61	0	6,6,6	0.43	0
3	2MO	C	803[B]	3,2,1	0,1,2	-	-	-		
4	SO4	A	901	-	4,4,4	0.56	0	6,6,6	0.31	0
2	PGD	A	801	3	46,52,52	3.63	15 (32%)	56,81,81	1.60	9 (16%)
3	2MO	A	803[B]	3,2,1	0,1,2	-	-	-		
3	2MO	C	803[A]	3,2,1	0,1,2	-	-	-		
2	PGD	C	801	3	46,52,52	3.33	13 (28%)	56,81,81	1.71	9 (16%)
2	PGD	C	802	3	46,52,52	3.42	14 (30%)	56,81,81	1.80	13 (23%)
3	2MO	A	803[A]	3,2,1	0,1,2	-	-	-		

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	PGD	A	802	3	-	1/22/82/82	0/6/6/6
2	PGD	C	802	3	-	1/22/82/82	0/6/6/6
2	PGD	A	801	3	-	5/22/82/82	0/6/6/6
2	PGD	C	801	3	-	5/22/82/82	0/6/6/6

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	PGD	C16-N15	18.72	1.46	1.28
2	A	801	PGD	C16-N15	18.07	1.45	1.28
2	C	801	PGD	C16-N15	16.89	1.44	1.28
2	C	802	PGD	C16-N15	15.84	1.43	1.28
2	C	802	PGD	C21-N22	8.21	1.44	1.35

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	PGD	C17-C16-N15	5.66	124.18	118.06
2	A	802	PGD	N20-C19-N18	-5.61	117.56	126.44
2	C	802	PGD	N20-C19-N18	-5.14	118.29	126.44
2	C	802	PGD	C17-C16-N15	5.03	123.50	118.06
2	A	801	PGD	C17-C16-N15	4.52	122.95	118.06

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PGD	C5'-O5'-PB-O1B
2	A	801	PGD	C5'-O5'-PB-O2B
2	A	801	PGD	C5'-O5'-PB-O3B
2	C	801	PGD	C5'-O5'-PB-O1B
2	C	801	PGD	C5'-O5'-PB-O2B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

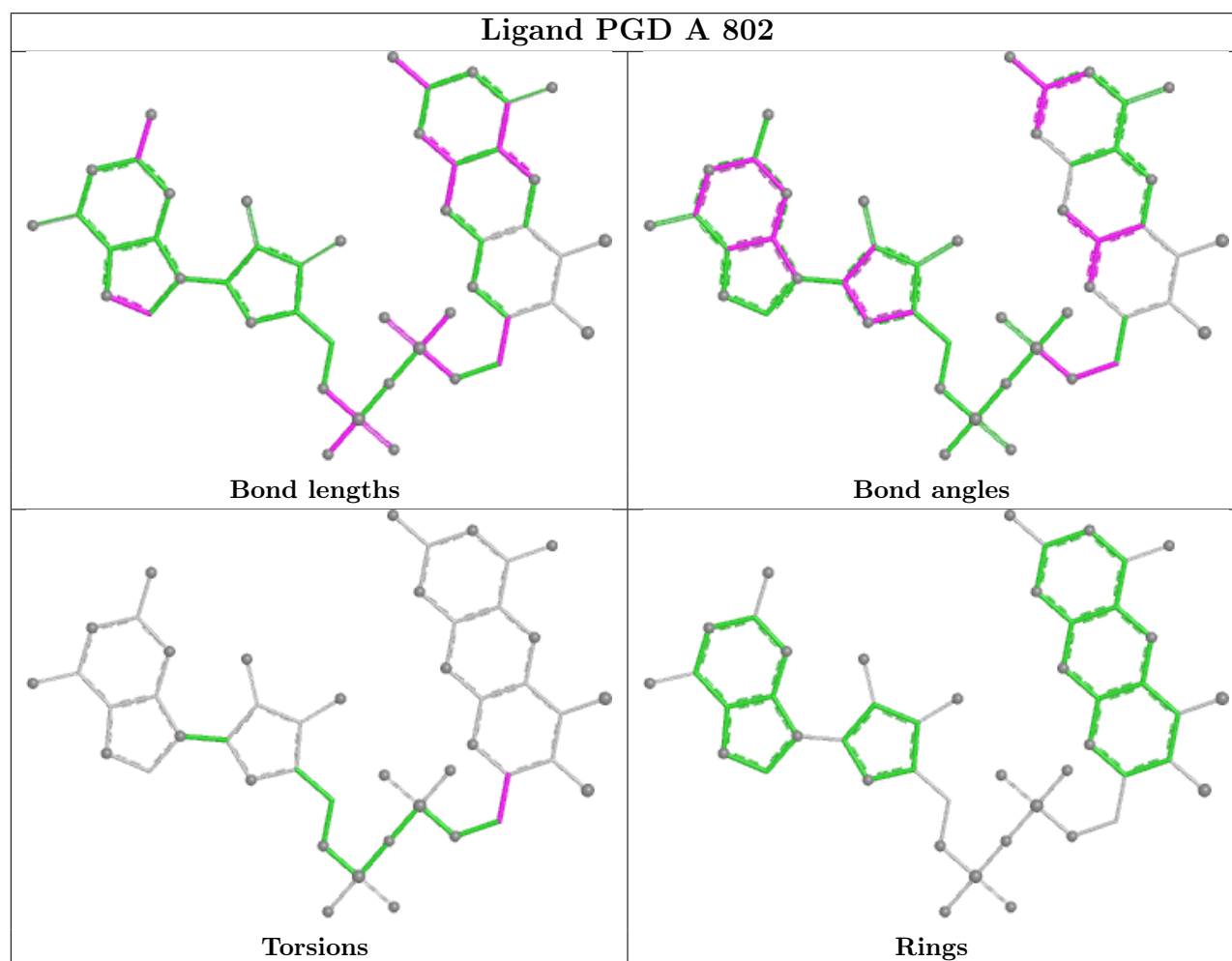
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	PGD	1	0

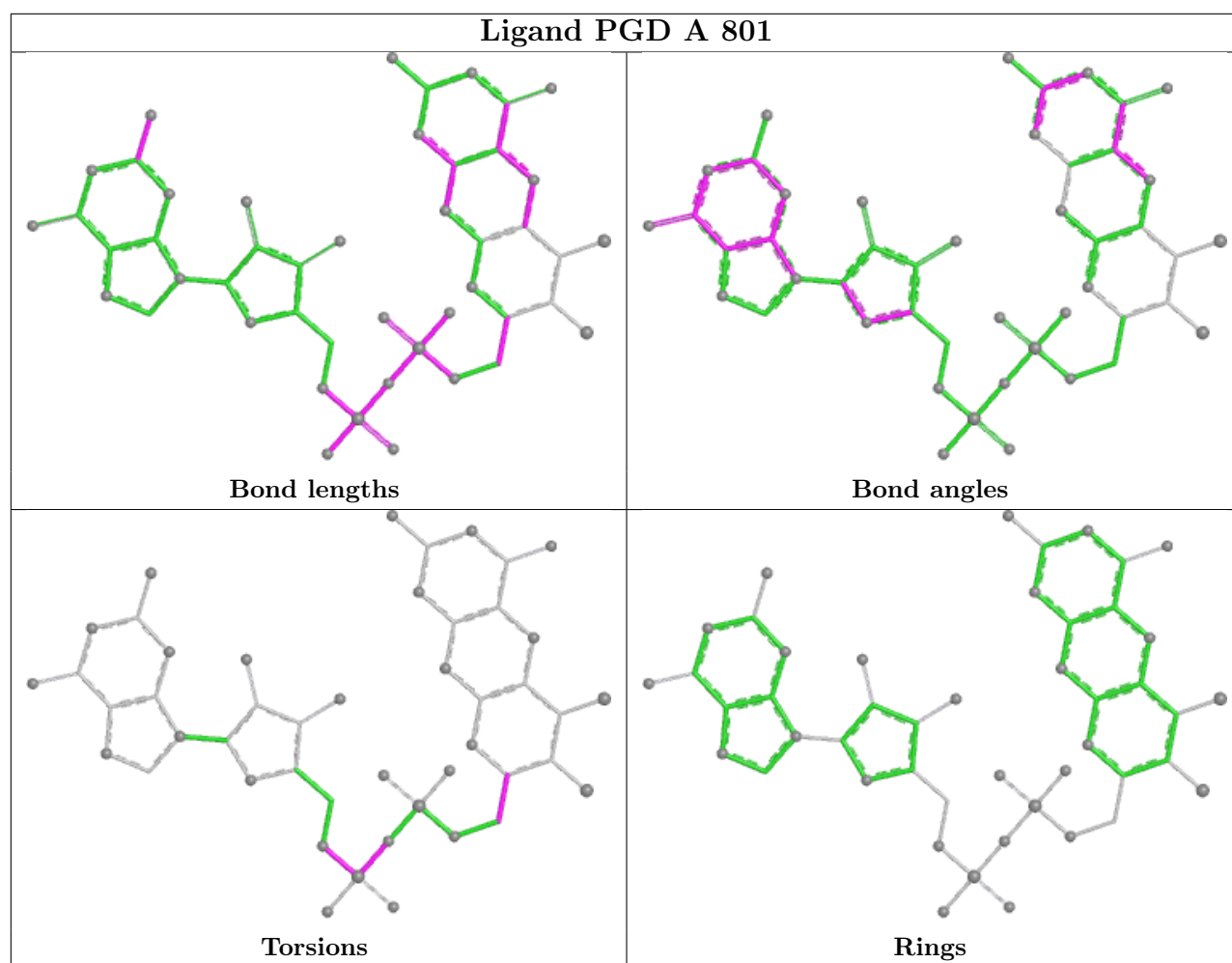
Continued on next page...

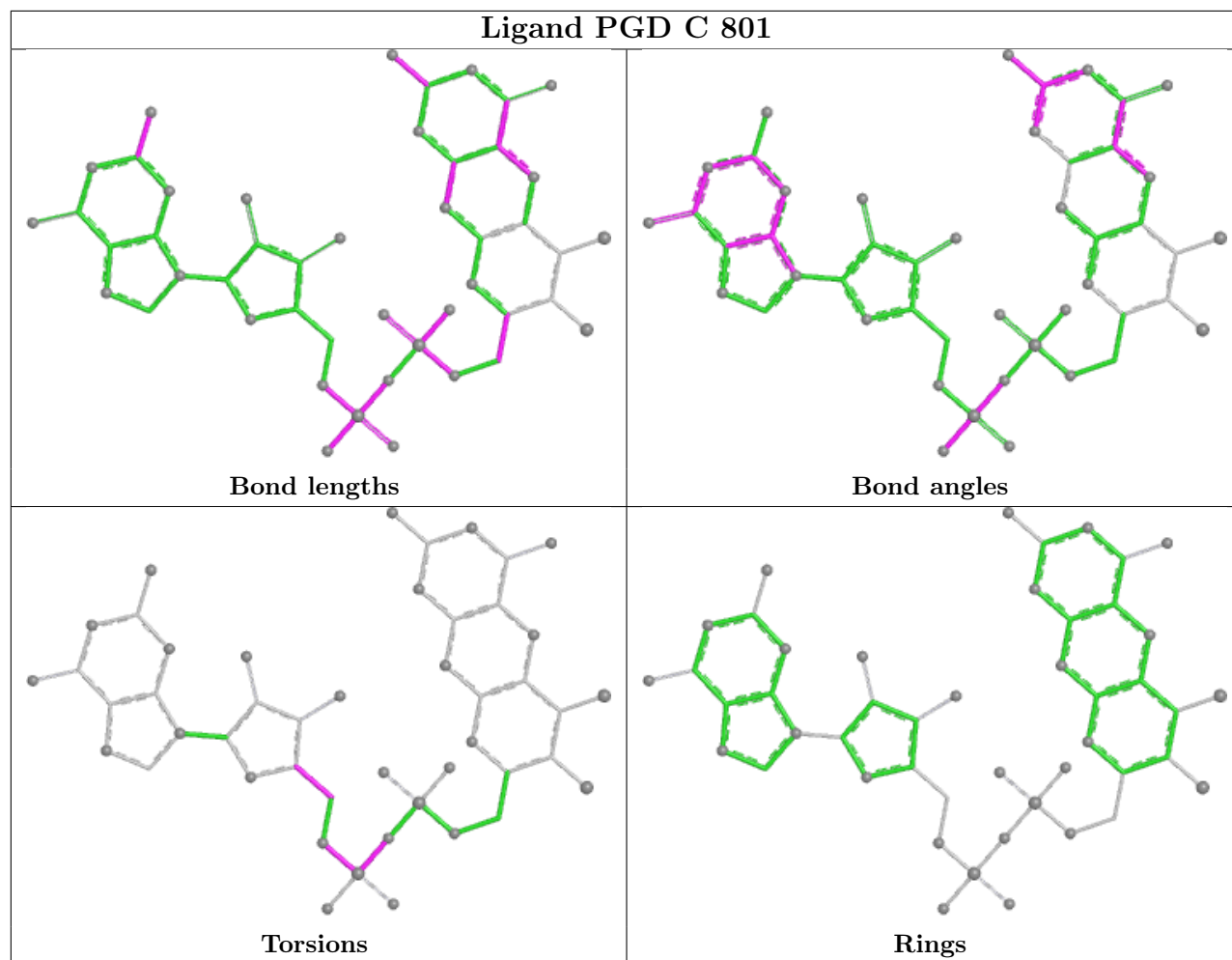
Continued from previous page...

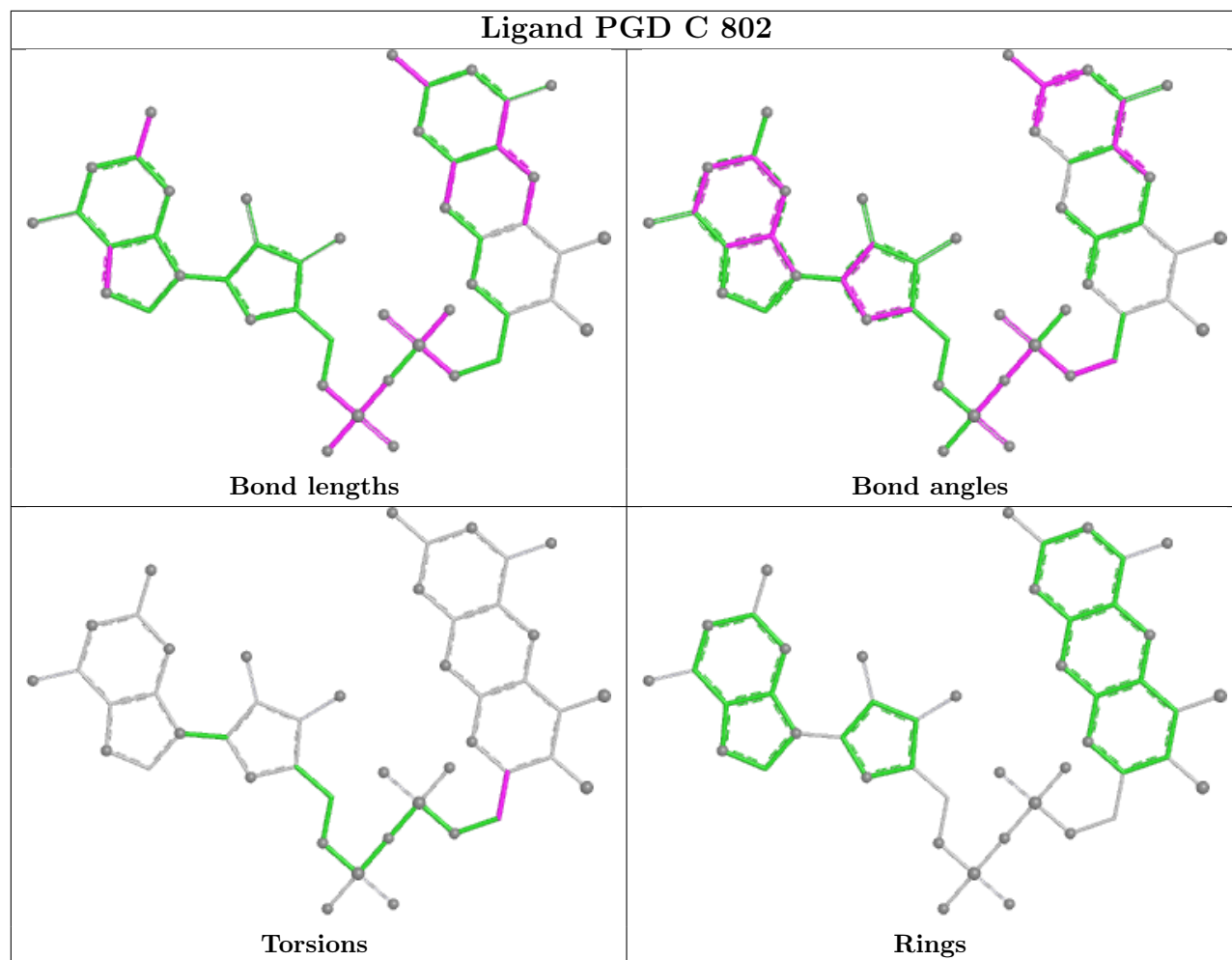
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	PGD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.