



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:14 PM UTC

PDB ID : 1FLG / pdb_00001flg
Title : CRYSTAL STRUCTURE OF THE QUINOPROTEIN ETHANOL DEHYDROGENASE FROM PSEUDOMONAS AERUGINOSA
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Deposited on : 2000-08-14
Resolution : 2.60 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

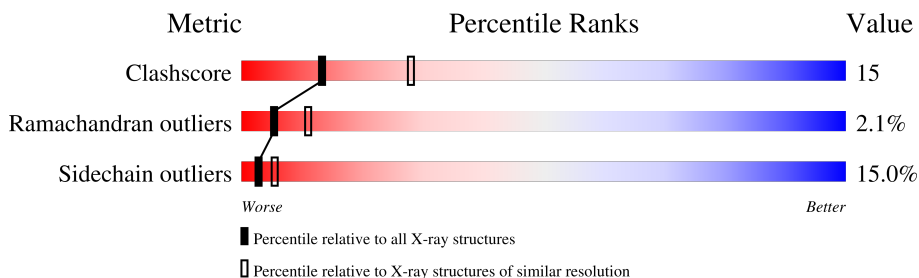
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	582	
1	B	582	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9232 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.

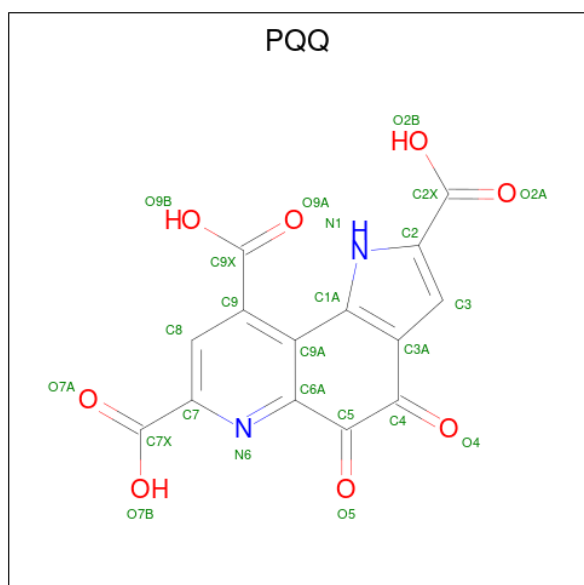
- Molecule 1 is a protein called PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4537	2891	783	852	11			
1	B	582	Total	C	N	O	S	0	0	0
			4537	2891	783	852	11			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is PYRROLOQUINOLINE QUINONE (CCD ID: PQQ) (formula: C₁₄H₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 24	C 14	N 2	O 8	0	0
3	B	1	Total 24	C 14	N 2	O 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total 73	O 73	0	0
4	B	33	Total 33	O 33	0	0

L564	T565	R566	P567	G572	W575	V576	F577	K578	L579	W582	L493	A494	T495	A496	G497	W498	L499	V500	F501	T502	G503	T504	G507	Y508	F509	K510	A511	F512	D513	A514	G517	L520	W521	K522	F523	Q524	S527	S531	P532	P533	G536	D539	G540	E541	Q542	Y543	L544	T547	Y550	G551	G552	A553	V554	P555	L556	W557	D560	M561	A562	D563																																					
Y419	S420	Q421	D422	Y427	V428	P429	A430	N431	H432	W433	K434	P362	D366	R367	I368	T369	W370	A371	S372	H373	I374	D375	L376	K377	T378	G379	R380	E383	R384	E385	G386	Q387	R388	P389	P390	L391	F392	E393	P394	G395	Q396	K397	H398	V402	S405	P406	P407	K412	N413	W414	R415	P416	Y465	G466	S467	L468	R469	A470	W471	D472	G476	K477	V478	V479	W480	E481	H482	K483	E484	H485	L488	W489	A490																								
G346	F347	F348	Y349	V350	V351	D352	R353	G356	K357	A361	F362	P363	D366	R367	I368	T369	W370	A371	S372	H373	I374	D375	L376	K377	T378	G379	R380	E383	R384	E385	G386	Q387	R388	P389	P390	L391	F392	E393	P394	G395	Q396	K397	H398	V402	S405	P406	P407	K412	N413	W414	R415	P416	Y465	G466	S467	L468	R469	A470	W471	D472	G476	K477	V478	V479	W480	E481	H482	K483	E484	H485	L488	W489	A490																								
N281	P282	H283	D284	Y285	D286	S287	L288	Y289	G292	Q293	V294	G295	S299	S300	P301	E302	F306	Y307	Q308	H309	T310	P311	D312	D313	A314	W315	D316	F317	S318	G319	N320	N321	E322	L323	V324	L325	F326	D327	Y328	K329	A330	D332	G333	K334	I335	V336	K337	A338	T339	A340	H341	A342	D343	R344	N345																																										
D214	S215	T216	V217	T218	G219	D220	V221	K222	A223	P224	S225	W226	R230	N231	S232	P233	T234	G235	K236	V237	S241	H242	G243	G244	G245	A246	P247	W248	Q249	S250	A251	S252	F253	E256	T257	N258	T259	I260	D261	V262	G263	A264	G265	G268	F269	W270	N271	T272	W273	A274	A277	K278	G279	G280																																											
K138	K142	K143	K144	F145	A146	D147	H148	Y152	Y153	M154	A157	P158	T159	I160	Y161	K162	D163	K165	T166	V169	I172	H173	S176	G177	D178	V182	R185	L186	F187	A188	R189	D190	P191	E195	M199	R200	P201	F202	V203	H206	G208	R209	L210	M211	G212	K213	D683	I71	Y72	V73	T74	Y77	S78	R79	L80	F81	A82	L83	K86	T87	G88	K89	R90	T93	Y94	N95	H96	R97	D101	I102	R103	P104	C105	D106	D107	V108	V109	N110	R111	G112	A113	A114	I115	Y116	G117	D118	V119	F121	L125	D126	A127	S128	M133	K134	N135	T136	G137
K1	D2	V3	T4	W5	E6	D7	I8	A9	N10	D11	T14	T15	G16	D17	V18	L19	G22	P23	G24	Q28	R29	K30	S31	P32	L33	K34	Q35	A38	D39	N40	V41	F42	K43	L44	T45	P46	A47	W48	S49	Y50	S51	F52	G53	D54	E55	K56	Q57	R58	G59	Q60	E61	S62	Q63	A64	I65																																										

4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	159.40 Å 159.40 Å 130.95 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.50 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (12.50-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9232	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: PQQ, 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	1.36	25/4679 (0.5%)	3.11	612/6366 (9.6%)
1	B	1.07	8/4679 (0.2%)	2.69	394/6366 (6.2%)
All	All	1.22	33/9358 (0.4%)	2.91	1006/12732 (7.9%)

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
1	A	0	36
1	B	0	21
All	All	0	57

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ASN	N-CA	16.12	1.69	1.46
1	A	312	ASN	N-CA	8.54	1.58	1.46
1	A	386	GLY	N-CA	8.51	1.57	1.45
1	A	414	TRP	CA-CB	7.37	1.65	1.53
1	A	295	GLY	CA-C	7.37	1.57	1.51

The worst 5 of 1006 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	LEU	CA-C-N	30.53	176.66	121.70
1	A	288	LEU	C-N-CA	30.53	176.66	121.70
1	A	29	ARG	CD-NE-CZ	26.56	161.58	124.40
1	B	288	LEU	CA-C-N	25.25	169.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	LEU	C-N-CA	25.25	169.76	121.54

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASP	Mainchain
1	A	13	LYS	Mainchain
1	A	14	THR	Mainchain
1	A	58	ARG	Mainchain
1	A	6	GLU	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	4537	0	4312	125	6
1	B	4537	0	4312	149	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	24	0	3	1	0
3	B	24	0	3	0	0
4	A	73	0	0	4	0
4	B	33	0	0	1	0
All	All	9232	0	8630	263	6

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 15.

The worst 5 of 263 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:A:367:ASN:N	1:A:367:ASN:CA	1.69	1.51
1:A:366:ASP:O	1:A:367:ASN:HA	1.37	1.21
1:A:293:GLN:HE22	1:A:339:THR:HG21	0.95	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASP:O	1:A:367:ASN:CA	2.02	1.02
1:A:293:GLN:NE2	1:A:339:THR:HG21	1.77	0.98

The worst 5 of 6 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)
1:A:373:HIS:CD2	1:A:456:ARG:NH2[2_665]	1.57	0.63
1:A:372:SER:OG	1:A:456:ARG:NH2[2_665]	1.92	0.28
1:A:372:SER:OG	1:A:456:ARG:NH1[2_665]	2.04	0.16
1:A:373:HIS:CG	1:A:456:ARG:NH2[2_665]	2.08	0.12
1:A:373:HIS:CD2	1:A:456:ARG:CZ[2_665]	2.13	0.07

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	580/582 (100%)	530 (91%)	45 (8%)	5 (1%)	14	30
1	B	580/582 (100%)	514 (89%)	47 (8%)	19 (3%)	3	5
All	All	1160/1164 (100%)	1044 (90%)	92 (8%)	24 (2%)	5	11

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ALA
1	A	385	GLU
1	B	217	VAL
1	B	289	TYR
1	B	330	ALA

5.3.2 Protein sidechains [i](#)

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	469/469 (100%)	404 (86%)	65 (14%)	3	7
1	B	469/469 (100%)	393 (84%)	76 (16%)	2	4
All	All	938/938 (100%)	797 (85%)	141 (15%)	3	5

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	378	THR
1	B	433	TRP
1	B	500	VAL
1	A	439	THR
1	A	433	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	249	GLN
1	B	421	GLN
1	B	258	ASN
1	B	320	ASN
1	B	464	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](#)

Of 6 ligands modelled in this entry, 4 are 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	PQQ	A	701	2	26,26,26	3.88	10 (38%)	34,40,40	4.73	20 (58%)
3	PQQ	B	702	2	26,26,26	3.59	12 (46%)	34,40,40	4.54	22 (64%)

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	PQQ	A	701	2	-	4/12/28/28	0/3/3/3
3	PQQ	B	702	2	-	1/12/28/28	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	PQQ	C5-C4	-9.84	1.40	1.54
3	A	701	PQQ	C5-C4	-9.15	1.41	1.54
3	A	701	PQQ	C6A-C5	-9.12	1.39	1.50
3	B	702	PQQ	O5-C5	8.46	1.40	1.23
3	A	701	PQQ	O4-C4	8.35	1.42	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PQQ	C9-C8-C7	13.40	130.93	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PQQ	C8-C7-N6	-10.00	106.05	123.41
3	B	702	PQQ	O7B-C7X-O7A	-9.88	102.12	123.35
3	B	702	PQQ	O5-C5-C4	-9.66	105.53	118.14
3	A	701	PQQ	O4-C4-C5	-8.44	107.97	118.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

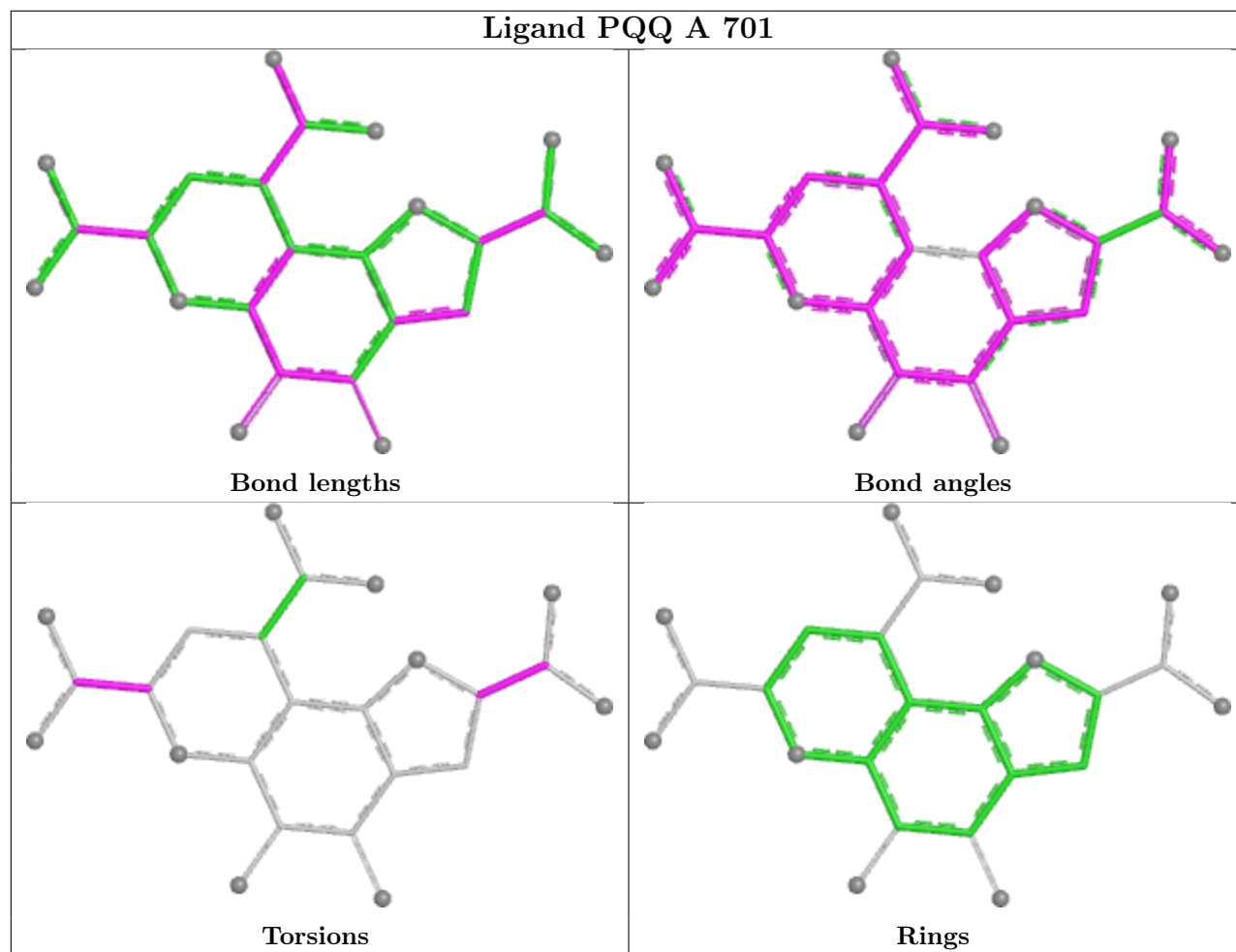
Mol	Chain	Res	Type	Atoms
3	A	701	PQQ	N1-C2-C2X-O2B
3	A	701	PQQ	C3-C2-C2X-O2B
3	B	702	PQQ	C8-C7-C7X-O7A
3	A	701	PQQ	C8-C7-C7X-O7A
3	A	701	PQQ	C8-C7-C7X-O7B

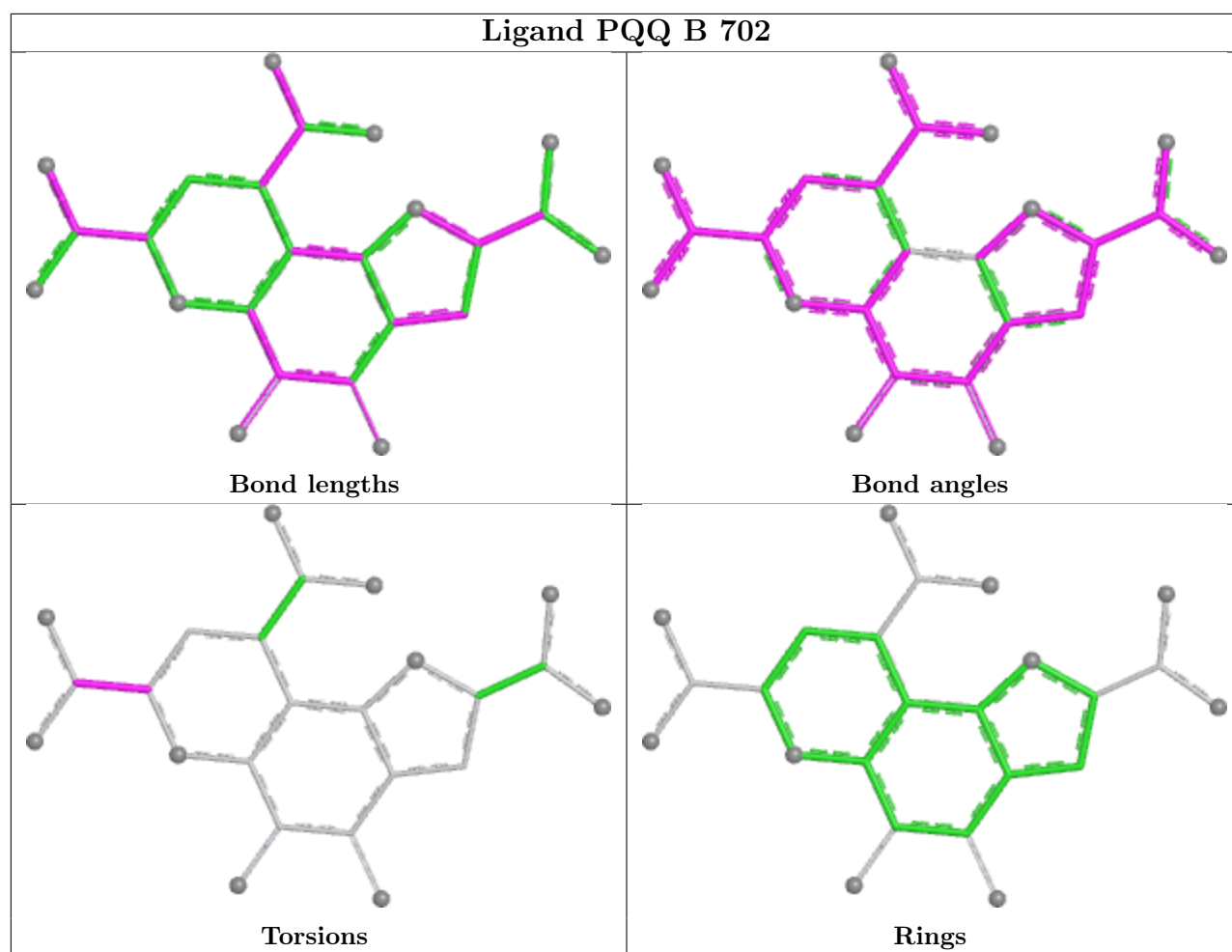
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	PQQ	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.