



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 6FKW / pdb_00006fkw
Title : Europium-containing methanol dehydrogenase
Authors : Barends, T.; Dietl, A.
Deposited on : 2018-01-24
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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

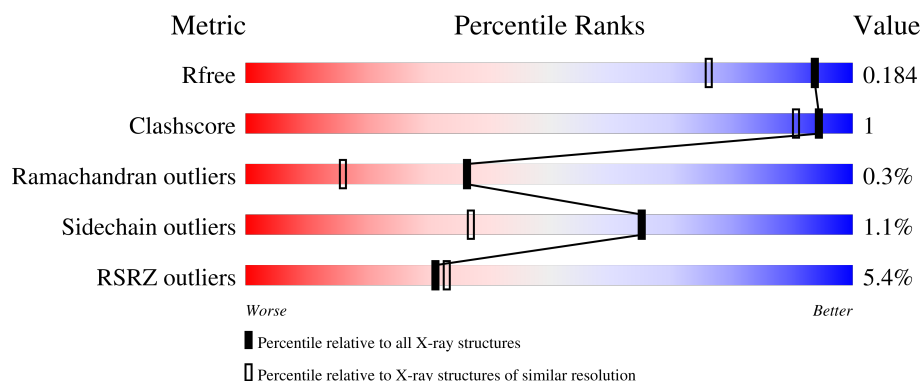
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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))
R_{free}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	577	
1	B	577	
1	C	577	
1	D	577	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19596 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.

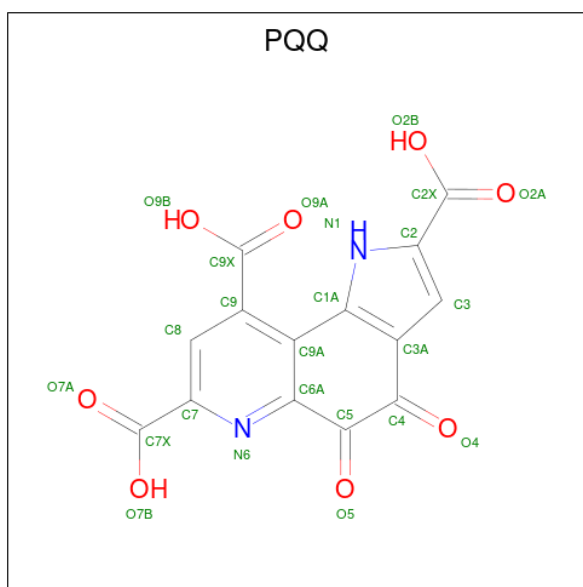
- Molecule 1 is a protein called Methanol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	1	0
			4494	2879	761	836	18			
1	B	576	Total	C	N	O	S	0	2	0
			4494	2881	759	835	19			
1	C	576	Total	C	N	O	S	0	1	0
			4490	2876	760	836	18			
1	D	576	Total	C	N	O	S	0	1	0
			4490	2876	759	837	18			

- Molecule 2 is EUROPIUM ION (CCD ID: EU) (formula: Eu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Eu	0	0
			1	1		
2	B	1	Total	Eu	0	0
			1	1		
2	C	1	Total	Eu	0	0
			1	1		
2	D	1	Total	Eu	0	0
			1	1		

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	509	Total	O	0	0
			509	509		
4	B	427	Total	O	0	0
			427	427		
4	C	443	Total	O	0	0
			443	443		
4	D	149	Total	O	0	0
			149	149		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Methanol dehydrogenase



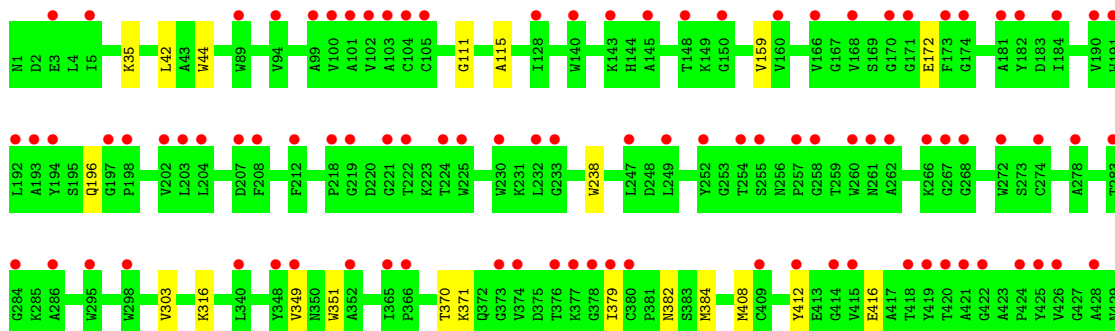
- Molecule 1: Methanol dehydrogenase

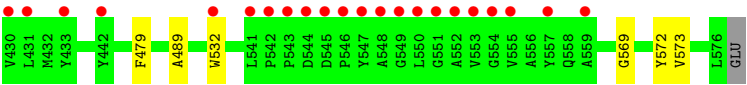


- Molecule 1: Methanol dehydrogenase



- Molecule 1: Methanol dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.08Å 101.18Å 107.79Å 115.21° 97.53° 91.78°	Depositor
Resolution (Å)	96.27 – 1.40 96.27 – 1.40	Depositor EDS
% Data completeness (in resolution range)	90.6 (96.27-1.40) 90.5 (96.27-1.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.169 , 0.185 0.168 , 0.184	Depositor DCC
R_{free} test set	18419 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	19596	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EU, PQQ

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	0.39	0/4625	0.66	1/6295 (0.0%)
1	B	0.38	0/4631	0.64	1/6304 (0.0%)
1	C	0.39	0/4624	0.65	1/6295 (0.0%)
1	D	0.39	0/4624	0.62	1/6295 (0.0%)
All	All	0.39	0/18504	0.64	4/25189 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	111	GLY	N-CA-C	6.53	119.69	111.85
1	C	111	GLY	N-CA-C	5.98	119.36	111.52
1	A	111	GLY	N-CA-C	5.97	119.01	111.85
1	B	111	GLY	N-CA-C	5.56	118.81	111.52

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	4494	0	4337	11	0
1	B	4494	0	4343	12	0
1	C	4490	0	4331	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4490	0	4329	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	3	2	0
3	B	24	0	3	1	0
3	C	24	0	3	2	0
3	D	24	0	3	2	0
4	A	509	0	0	1	0
4	B	427	0	0	0	0
4	C	443	0	0	0	0
4	D	149	0	0	1	0
All	All	19596	0	17352	45	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 1.

All (45) 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:D:382:ASN:HD21	1:D:408:MET:HE3	1.55	0.72
1:B:570:GLU:OE2	1:D:572:TYR:OH	2.12	0.67
1:B:42:LEU:HD22	1:D:42:LEU:HD22	1.81	0.62
1:D:370:THR:HG21	1:D:412:TYR:CD1	2.37	0.59
1:A:42:LEU:HD22	1:C:42:LEU:HD22	1.85	0.57
1:C:426:VAL:HG11	1:C:550:LEU:HD21	1.87	0.56
1:D:384:MET:HG2	1:D:532:TRP:CE3	2.42	0.54
1:A:238:TRP:CZ2	3:A:602:PQQ:C6A	2.92	0.53
1:A:370:THR:HG21	1:A:412:TYR:CD1	2.45	0.52
1:D:44:TRP:CH2	1:D:573:VAL:HG21	2.46	0.50
1:C:370:THR:HG21	1:C:412:TYR:CD1	2.47	0.49
1:A:570:GLU:OE2	1:C:572:TYR:OH	2.30	0.49
1:A:532:TRP:CE3	3:A:602:PQQ:O4	2.66	0.49
1:D:238:TRP:CZ2	1:D:303:VAL:HG21	2.48	0.49
1:D:238:TRP:CE2	1:D:303:VAL:HG21	2.48	0.48
1:B:370:THR:HG21	1:B:412:TYR:CD1	2.48	0.48
1:D:379:ILE:HD13	4:D:751:HOH:O	2.11	0.48
1:B:426:VAL:HG11	1:B:550:LEU:HD21	1.95	0.48
1:D:44:TRP:CZ2	1:D:573:VAL:HG21	2.49	0.48
1:B:238:TRP:CZ2	3:B:602:PQQ:C6A	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:LYS:HE3	1:C:575:ALA:HB1	1.95	0.47
1:C:238:TRP:CZ2	3:C:602:PQQ:C6A	2.97	0.47
1:D:532:TRP:CE3	3:D:602:PQQ:O4	2.67	0.47
1:B:238:TRP:CE2	1:B:303:VAL:HG21	2.51	0.46
1:A:42:LEU:CD2	1:C:42:LEU:HD22	2.46	0.45
1:C:238:TRP:CE2	1:C:303:VAL:HG21	2.52	0.45
1:B:42:LEU:HD22	1:D:42:LEU:CD2	2.46	0.45
1:A:544:ASP:N	1:A:544:ASP:OD1	2.49	0.45
1:D:479:PHE:CE2	1:D:489:ALA:HB2	2.52	0.44
1:A:572:TYR:OH	1:C:570:GLU:OE2	2.34	0.44
1:A:42:LEU:HD22	1:C:42:LEU:CD2	2.48	0.43
1:B:384:MET:HG2	1:B:532:TRP:CE3	2.54	0.43
3:D:602:PQQ:O9A	3:D:602:PQQ:N1	2.48	0.43
1:D:115:ALA:CB	1:D:159:VAL:HG11	2.49	0.43
1:B:7:LEU:HB3	1:B:15:VAL:HG11	2.01	0.42
1:B:44:TRP:CH2	1:B:573:VAL:HG21	2.55	0.42
1:C:44:TRP:CH2	1:C:573:VAL:HG21	2.55	0.42
1:A:493:LYS:NZ	4:A:703:HOH:O	2.53	0.41
1:D:384:MET:SD	1:D:408:MET:HE1	2.60	0.41
1:B:469:GLY:O	1:B:511:PRO:HD2	2.21	0.41
1:B:479:PHE:CE2	1:B:489:ALA:HB2	2.56	0.41
1:D:349:VAL:HG13	1:D:351:TRP:CD1	2.56	0.41
1:C:490:VAL:HG12	1:C:497:VAL:HG22	2.02	0.41
1:C:532:TRP:CE3	3:C:602:PQQ:O4	2.74	0.41
1:A:238:TRP:CE2	1:A:303:VAL:HG21	2.56	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	575/577 (100%)	553 (96%)	20 (4%)	2 (0%)	36 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	576/577 (100%)	558 (97%)	16 (3%)	2 (0%)	36	16
1	C	575/577 (100%)	554 (96%)	19 (3%)	2 (0%)	36	16
1	D	575/577 (100%)	553 (96%)	21 (4%)	1 (0%)	43	19
All	All	2301/2308 (100%)	2218 (96%)	76 (3%)	7 (0%)	36	16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	569	GLY
1	A	107	VAL
1	A	569	GLY
1	B	107	VAL
1	B	569	GLY
1	C	107	VAL
1	D	569	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	462/462 (100%)	456 (99%)	6 (1%)	61	30
1	B	463/462 (100%)	459 (99%)	4 (1%)	70	44
1	C	462/462 (100%)	456 (99%)	6 (1%)	61	30
1	D	462/462 (100%)	456 (99%)	6 (1%)	61	30
All	All	1849/1848 (100%)	1827 (99%)	22 (1%)	65	34

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	314[A]	LYS
1	A	314[B]	LYS
1	A	371	LYS

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Mol	Chain	Res	Type
1	A	412	TYR
1	A	544	ASP
1	B	39	ARG
1	B	83	LYS
1	B	196	GLN
1	B	544	ASP
1	C	35	LYS
1	C	98	GLN
1	C	196	GLN
1	C	358	GLU
1	C	367	GLU
1	C	412	TYR
1	D	35	LYS
1	D	172	GLU
1	D	196	GLN
1	D	316	LYS
1	D	371	LYS
1	D	416	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	429	ASN
1	B	127	GLN
1	B	229	GLN
1	B	429	ASN
1	B	500	GLN
1	B	558	GLN
1	C	98	GLN
1	C	127	GLN
1	C	185	ASN
1	C	229	GLN
1	C	397	GLN
1	C	429	ASN
1	D	95	GLN
1	D	229	GLN
1	D	359	ASN
1	D	429	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 ⓘ

Of 8 ligands modelled in this entry, 4 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	PQQ	C	602	2	26,26,26	2.46	6 (23%)	34,40,40	1.66	10 (29%)
3	PQQ	A	602	2	26,26,26	2.46	5 (19%)	34,40,40	1.55	8 (23%)
3	PQQ	D	602	2	26,26,26	2.43	5 (19%)	34,40,40	1.58	8 (23%)
3	PQQ	B	602	2	26,26,26	2.39	5 (19%)	34,40,40	1.58	8 (23%)

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	C	602	2	-	0/12/28/28	0/3/3/3
3	PQQ	A	602	2	-	3/12/28/28	0/3/3/3
3	PQQ	D	602	2	-	0/12/28/28	0/3/3/3
3	PQQ	B	602	2	-	0/12/28/28	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	PQQ	C9-C9A	6.69	1.51	1.41
3	A	602	PQQ	C9-C9A	6.44	1.50	1.41
3	B	602	PQQ	C9-C9A	6.39	1.50	1.41
3	C	602	PQQ	C9-C9A	6.29	1.50	1.41
3	D	602	PQQ	C9A-C6A	5.77	1.50	1.41
3	A	602	PQQ	C9A-C6A	5.52	1.49	1.41
3	B	602	PQQ	C9A-C6A	5.42	1.49	1.41
3	C	602	PQQ	C9A-C6A	5.34	1.49	1.41
3	C	602	PQQ	C5-C4	-5.33	1.47	1.54
3	A	602	PQQ	C5-C4	-5.30	1.47	1.54
3	B	602	PQQ	C5-C4	-4.92	1.47	1.54
3	D	602	PQQ	C5-C4	-4.85	1.47	1.54
3	C	602	PQQ	C9A-C1A	-4.82	1.40	1.46
3	A	602	PQQ	C9A-C1A	-4.67	1.40	1.46
3	D	602	PQQ	C9A-C1A	-4.52	1.40	1.46
3	B	602	PQQ	C9A-C1A	-4.23	1.41	1.46
3	D	602	PQQ	C3A-C1A	3.68	1.48	1.40
3	C	602	PQQ	C3A-C1A	3.60	1.48	1.40
3	A	602	PQQ	C3A-C1A	3.59	1.48	1.40
3	B	602	PQQ	C3A-C1A	3.56	1.47	1.40
3	C	602	PQQ	O2B-C2X	-2.43	1.24	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	PQQ	C6A-N6-C7	3.32	122.37	118.01
3	B	602	PQQ	O5-C5-C4	3.18	122.29	118.14
3	C	602	PQQ	C3-C2-C2X	-3.14	125.30	132.53
3	A	602	PQQ	C3-C2-C2X	-3.12	125.34	132.53
3	D	602	PQQ	C3-C2-C2X	-3.12	125.35	132.53
3	C	602	PQQ	O5-C5-C4	3.04	122.10	118.14
3	C	602	PQQ	C6A-N6-C7	3.00	121.95	118.01
3	B	602	PQQ	C6A-N6-C7	2.87	121.78	118.01
3	A	602	PQQ	C6A-N6-C7	2.82	121.71	118.01
3	B	602	PQQ	C3-C2-C2X	-2.81	126.05	132.53
3	D	602	PQQ	O2B-C2X-C2	2.79	120.28	114.27
3	A	602	PQQ	C8-C9-C9A	-2.76	116.80	120.33
3	B	602	PQQ	C1A-C3A-C4	-2.52	120.21	122.33
3	C	602	PQQ	C8-C9-C9A	-2.45	117.18	120.33
3	B	602	PQQ	C8-C9-C9A	-2.44	117.20	120.33
3	C	602	PQQ	O2B-C2X-C2	2.43	119.51	114.27
3	D	602	PQQ	C8-C9-C9A	-2.41	117.23	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	PQQ	O5-C5-C4	2.38	121.24	118.14
3	D	602	PQQ	C1A-C3A-C4	-2.36	120.35	122.33
3	A	602	PQQ	C1A-C3A-C4	-2.33	120.37	122.33
3	C	602	PQQ	O9B-C9X-C9	2.32	121.88	115.28
3	C	602	PQQ	C9A-C6A-C5	2.30	123.72	121.59
3	D	602	PQQ	C9A-C6A-N6	-2.28	120.27	123.58
3	A	602	PQQ	C9A-C9-C9X	2.27	126.48	121.49
3	D	602	PQQ	O2A-C2X-C2	-2.25	116.45	121.01
3	C	602	PQQ	C9A-C9-C9X	2.23	126.39	121.49
3	A	602	PQQ	O7A-C7X-C7	-2.21	116.86	121.30
3	B	602	PQQ	O7A-C7X-C7	-2.14	117.00	121.30
3	A	602	PQQ	C9A-C6A-C5	2.10	123.54	121.59
3	C	602	PQQ	O9A-C9X-C9	-2.09	116.98	121.97
3	B	602	PQQ	C9A-C6A-C5	2.07	123.52	121.59
3	C	602	PQQ	C1A-C3A-C4	-2.05	120.61	122.33
3	D	602	PQQ	C9A-C9-C9X	2.04	125.98	121.49
3	B	602	PQQ	C9A-C9-C9X	2.01	125.91	121.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	PQQ	N1-C2-C2X-O2B
3	A	602	PQQ	C3-C2-C2X-O2B
3	A	602	PQQ	C3-C2-C2X-O2A

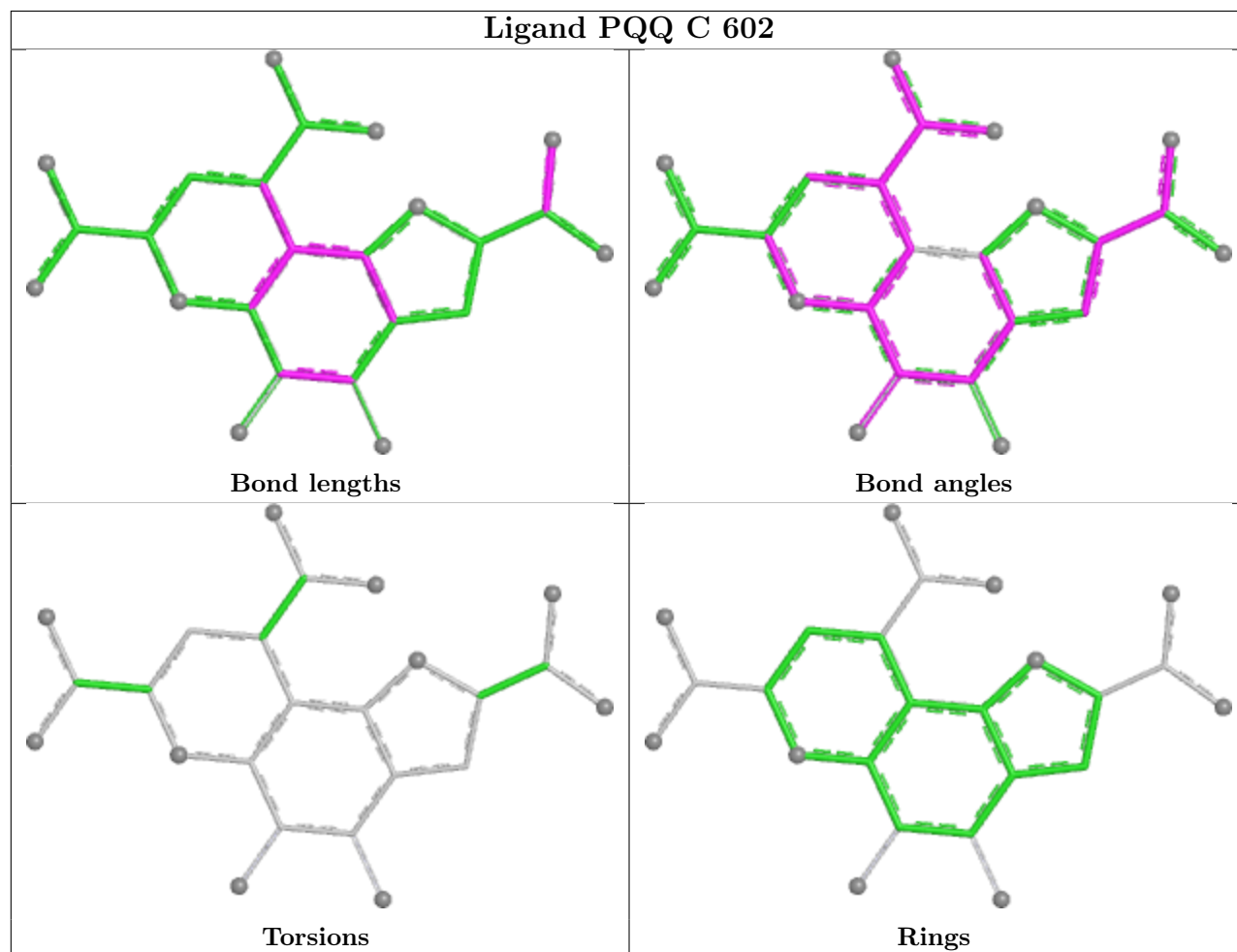
There are no ring outliers.

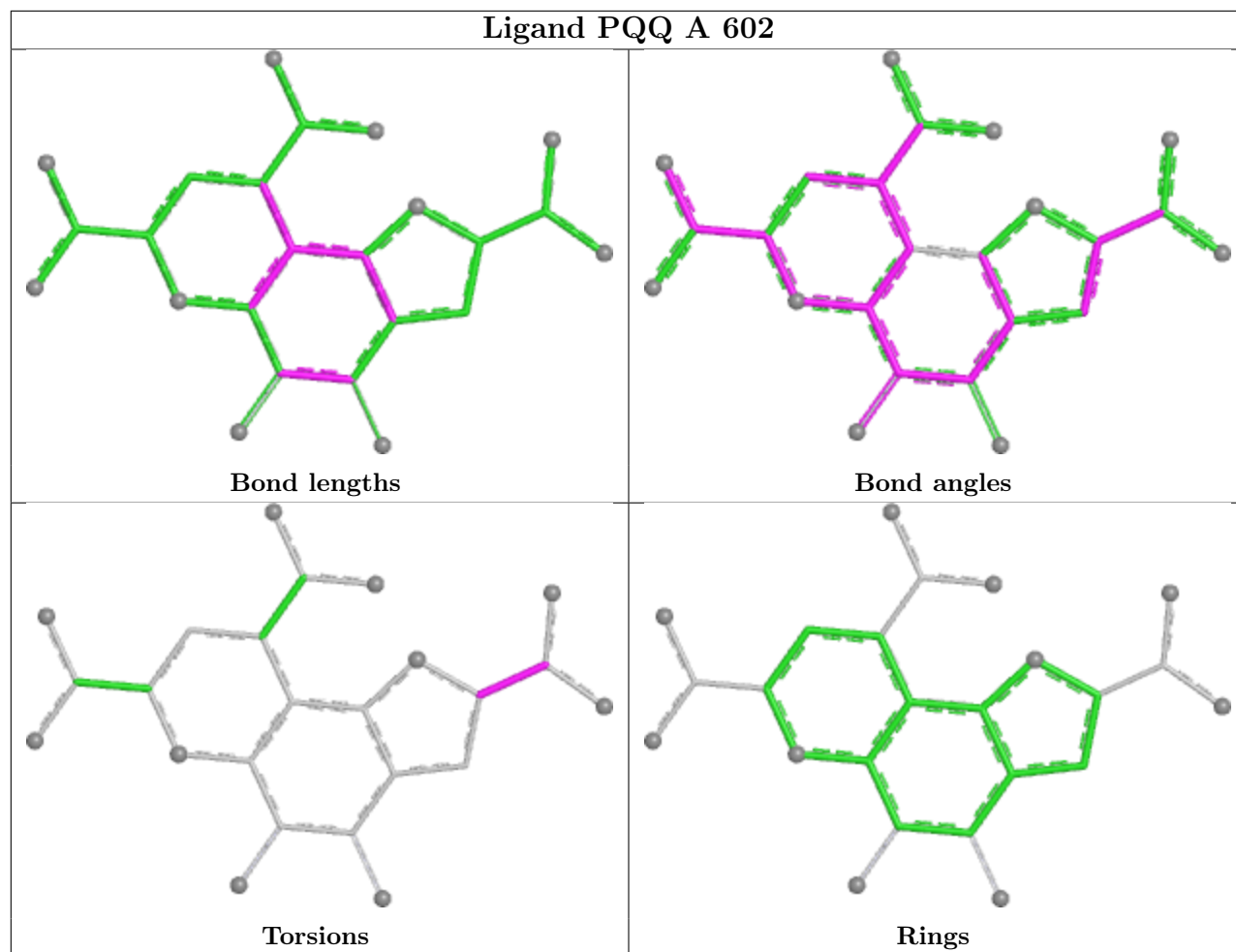
4 monomers are involved in 7 short contacts:

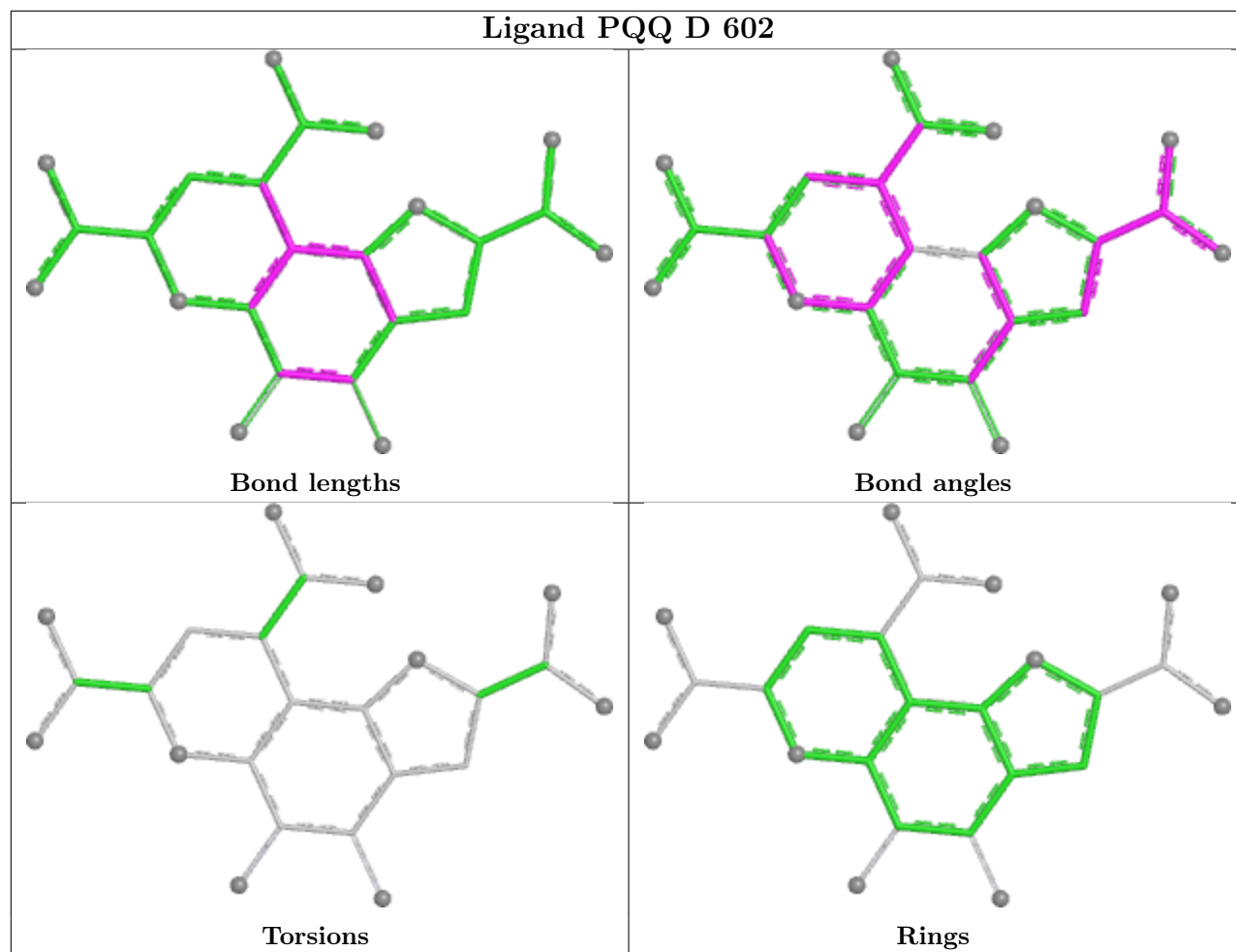
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	PQQ	2	0
3	A	602	PQQ	2	0
3	D	602	PQQ	2	0
3	B	602	PQQ	1	0

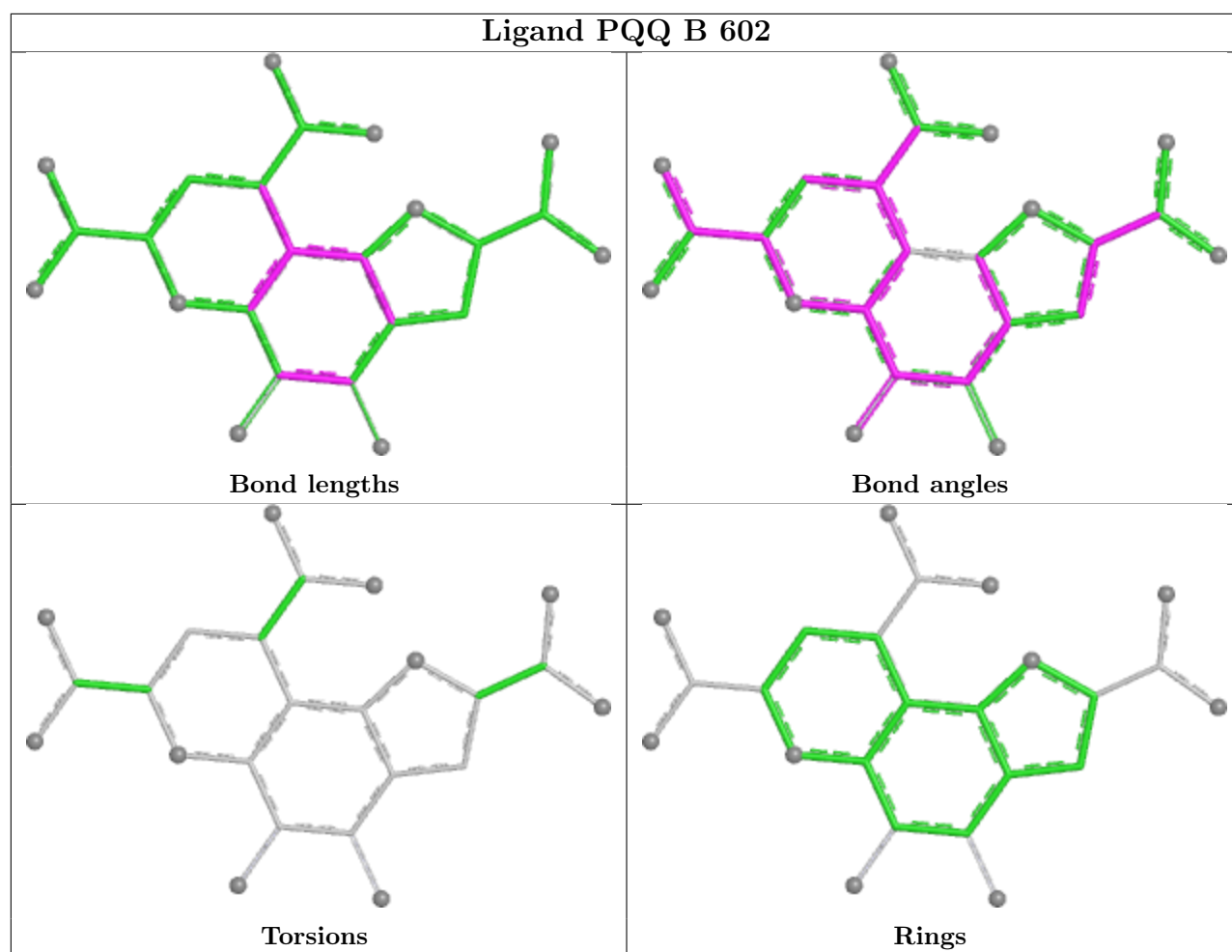
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	576/577 (99%)	-0.16	3 (0%) 87 89	14, 20, 29, 42	1 (0%)
1	B	576/577 (99%)	-0.02	1 (0%) 91 93	13, 23, 34, 45	2 (0%)
1	C	576/577 (99%)	-0.04	2 (0%) 90 92	16, 22, 34, 46	1 (0%)
1	D	576/577 (99%)	1.29	118 (20%) 2 2	23, 40, 63, 77	1 (0%)
All	All	2304/2308 (99%)	0.27	124 (5%) 31 33	13, 24, 52, 77	5 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	ILE	5.3
1	D	547	TYR	4.5
1	D	233	GLY	4.4
1	D	409	CYS	4.2
1	D	546	PRO	4.2
1	B	550	LEU	3.8
1	D	191	TRP	3.8
1	D	295	TRP	3.8
1	D	190	VAL	3.7
1	D	203	LEU	3.7
1	D	225	TRP	3.7
1	D	430	VAL	3.7
1	D	221	GLY	3.7
1	D	204	LEU	3.5
1	D	374	VAL	3.5
1	D	272	TRP	3.4
1	D	202	VAL	3.4
1	D	230	TRP	3.3
1	D	257	PRO	3.3
1	D	379	ILE	3.3
1	D	549	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	551	GLY	3.2
1	D	170	GLY	3.1
1	D	262	ALA	3.1
1	D	421	ALA	3.1
1	D	553	VAL	3.1
1	D	194	TYR	3.1
1	D	222	THR	3.1
1	D	550	LEU	3.1
1	D	340	LEU	3.0
1	D	267	GLY	3.0
1	D	150	GLY	3.0
1	A	357	LYS	3.0
1	D	286	ALA	2.9
1	C	267	GLY	2.9
1	D	378	GLY	2.9
1	D	192	LEU	2.9
1	D	552	ALA	2.9
1	D	414	GLY	2.9
1	D	105	CYS	2.9
1	D	431	LEU	2.8
1	D	544	ASP	2.8
1	D	365	ILE	2.8
1	D	425	TYR	2.8
1	D	145	ALA	2.8
1	D	218	PRO	2.8
1	D	166	VAL	2.7
1	D	373	GLY	2.7
1	D	420	THR	2.7
1	D	366	PRO	2.7
1	D	559	ALA	2.7
1	D	555	VAL	2.7
1	D	380	CYS	2.7
1	D	419	TYR	2.7
1	D	232	LEU	2.7
1	D	298	TRP	2.7
1	D	171	GLY	2.6
1	D	422	GLY	2.6
1	D	255	SER	2.6
1	D	543	PRO	2.6
1	D	548	ALA	2.6
1	D	102	VAL	2.6
1	D	377	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	283	THR	2.5
1	D	249	LEU	2.5
1	D	376	THR	2.5
1	D	428	ALA	2.5
1	D	260	TRP	2.5
1	D	182	TYR	2.5
1	D	219	GLY	2.5
1	D	268	GLY	2.5
1	D	349	VAL	2.5
1	D	208	PHE	2.5
1	D	101	ALA	2.4
1	D	424	PRO	2.4
1	D	557	TYR	2.4
1	D	254	THR	2.4
1	D	415	VAL	2.4
1	D	348	TYR	2.4
1	D	99	ALA	2.4
1	D	198	PRO	2.4
1	D	258	GLY	2.4
1	D	284	GLY	2.4
1	D	168	VAL	2.3
1	D	352	ALA	2.3
1	D	274	CYS	2.3
1	D	224	THR	2.3
1	D	247	LEU	2.3
1	D	104	CYS	2.3
1	D	173	PHE	2.3
1	D	128	ILE	2.3
1	D	442	TYR	2.3
1	D	542	PRO	2.2
1	D	412	TYR	2.2
1	D	197	GLY	2.2
1	D	554	GLY	2.2
1	D	148	THR	2.2
1	D	207	ASP	2.2
1	A	367	GLU	2.1
1	D	100	VAL	2.1
1	C	550	LEU	2.1
1	D	181	ALA	2.1
1	D	433	TYR	2.1
1	D	266	LYS	2.1
1	D	89	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	140	TRP	2.1
1	D	94	VAL	2.1
1	D	160	VAL	2.1
1	D	545	ASP	2.1
1	D	193	ALA	2.1
1	D	3	GLU	2.1
1	D	532	TRP	2.1
1	D	174	GLY	2.1
1	D	143	LYS	2.0
1	D	212	PHE	2.0
1	D	418	THR	2.0
1	D	103	ALA	2.0
1	D	278	ALA	2.0
1	D	541	LEU	2.0
1	D	5	ILE	2.0
1	D	261	ASN	2.0
1	D	426	VAL	2.0
1	A	409	CYS	2.0
1	D	252	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

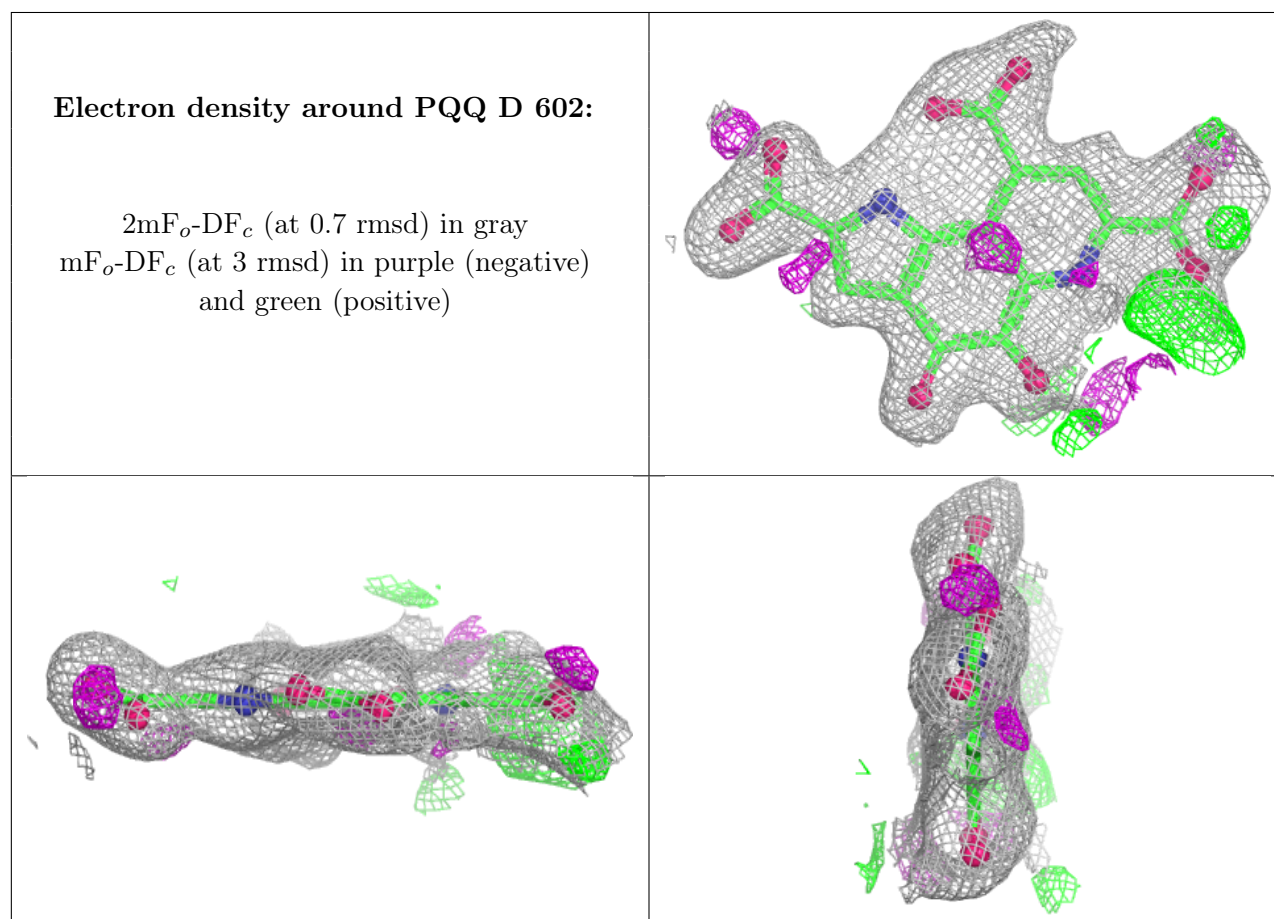
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PQQ	D	602	24/24	0.85	0.11	32,41,45,47	0
3	PQQ	C	602	24/24	0.92	0.08	19,21,22,23	0
3	PQQ	A	602	24/24	0.92	0.08	18,21,23,25	0
3	PQQ	B	602	24/24	0.93	0.08	20,21,23,23	0

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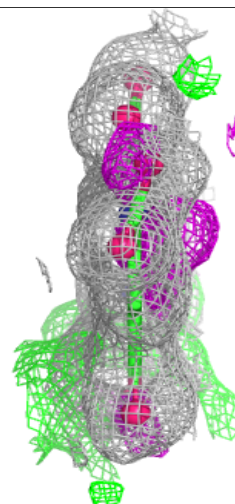
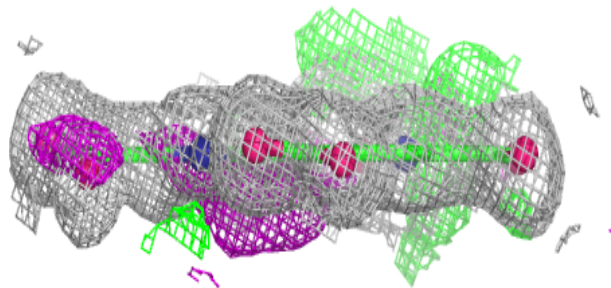
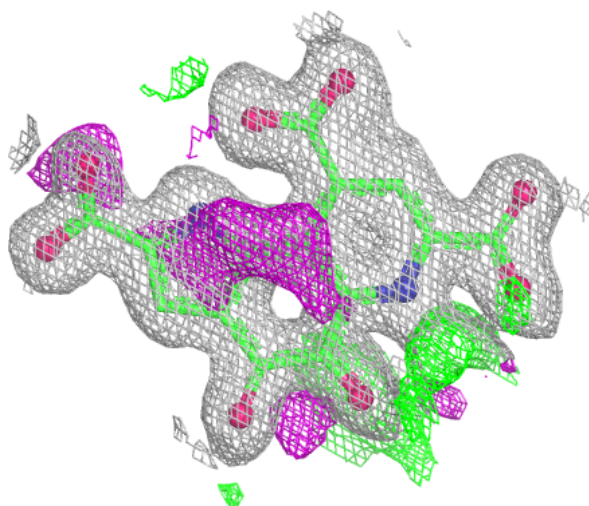
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EU	A	601	1/1	0.97	0.06	24,24,24,24	1
2	EU	D	601	1/1	0.97	0.06	42,42,42,42	1
2	EU	B	601	1/1	0.98	0.04	22,22,22,22	1
2	EU	C	601	1/1	0.99	0.03	20,20,20,20	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



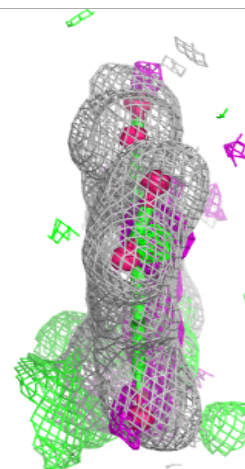
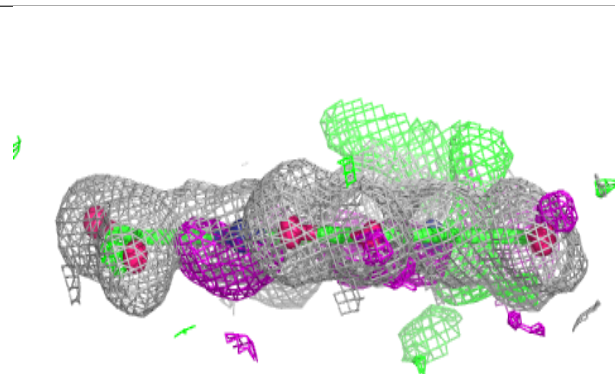
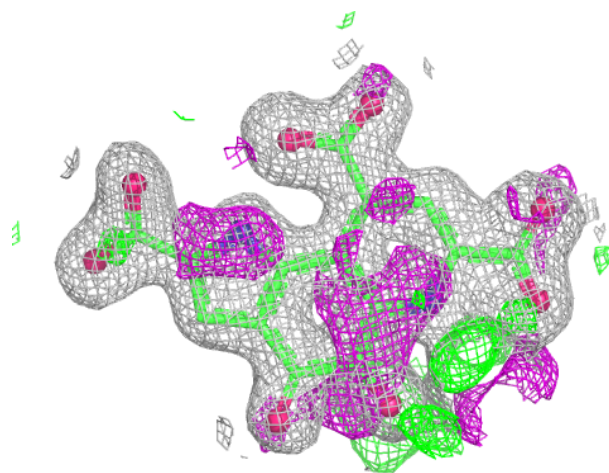
Electron density around PQQ C 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



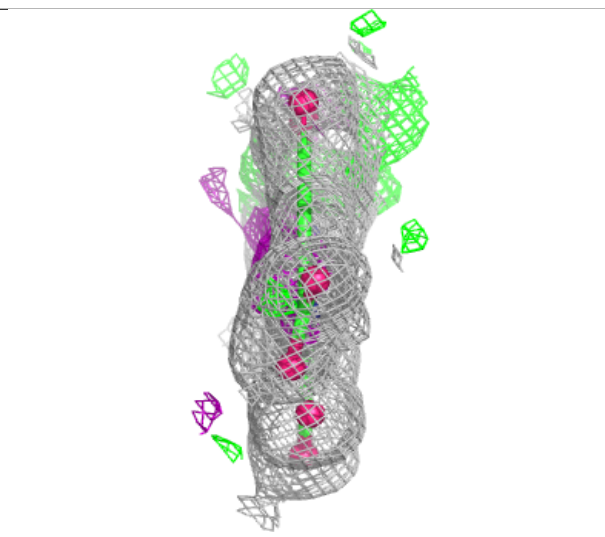
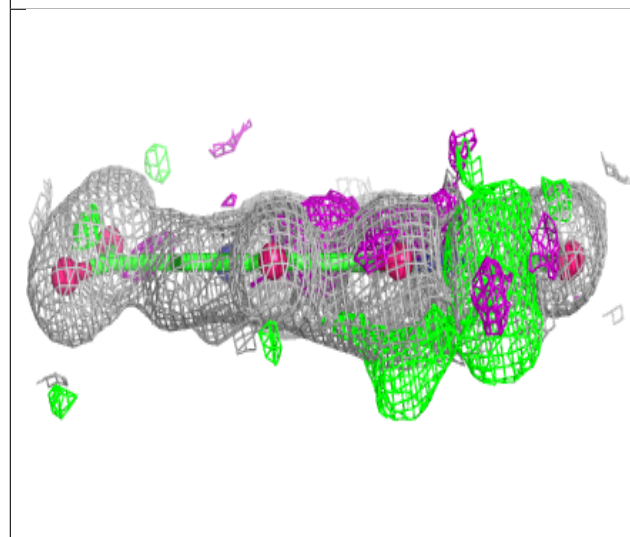
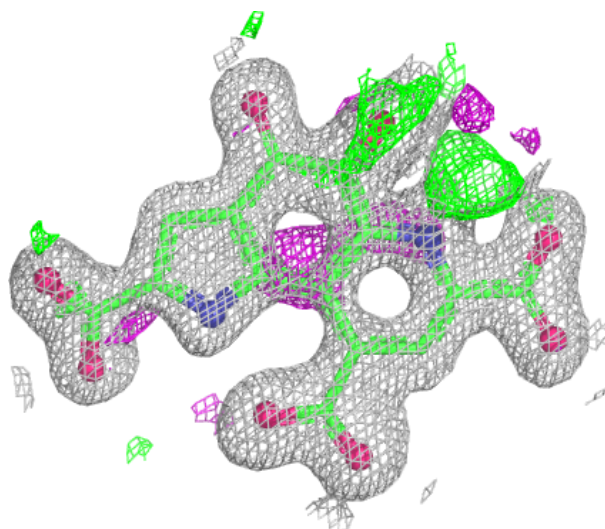
Electron density around PQQ A 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PQQ B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.