



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 04:21 PM EDT

PDB ID : 1H4I  
Title : Methylobacterium extorquens methanol dehydrogenase  
Authors : Ghosh, M.; Anthony, C.; Harlos, K.; Goodwin, M.G.; Blake, C.  
Deposited on : 2001-05-11  
Resolution : 1.94 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

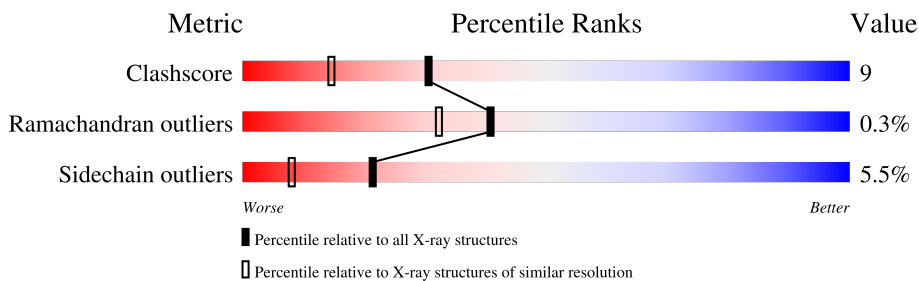
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)

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  $\geq 3$ , 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	599	
1	C	599	
2	B	74	
2	D	74	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10462 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.

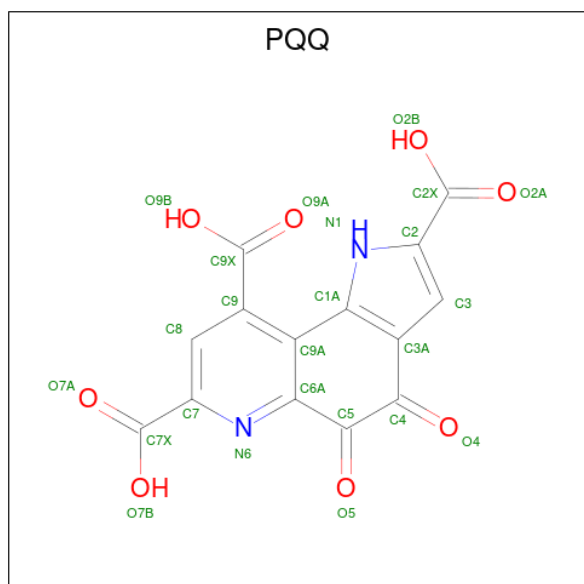
- Molecule 1 is a protein called METHANOL DEHYDROGENASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4620	2947	778	875	20			
1	C	595	Total	C	N	O	S	0	0	0
			4620	2947	778	875	20			

- Molecule 2 is a protein called METHANOL DEHYDROGENASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			586	369	103	111	3			
2	D	73	Total	C	N	O	S	0	0	0
			586	369	103	111	3			

- Molecule 3 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: C<sub>14</sub>H<sub>6</sub>N<sub>2</sub>O<sub>8</sub>).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

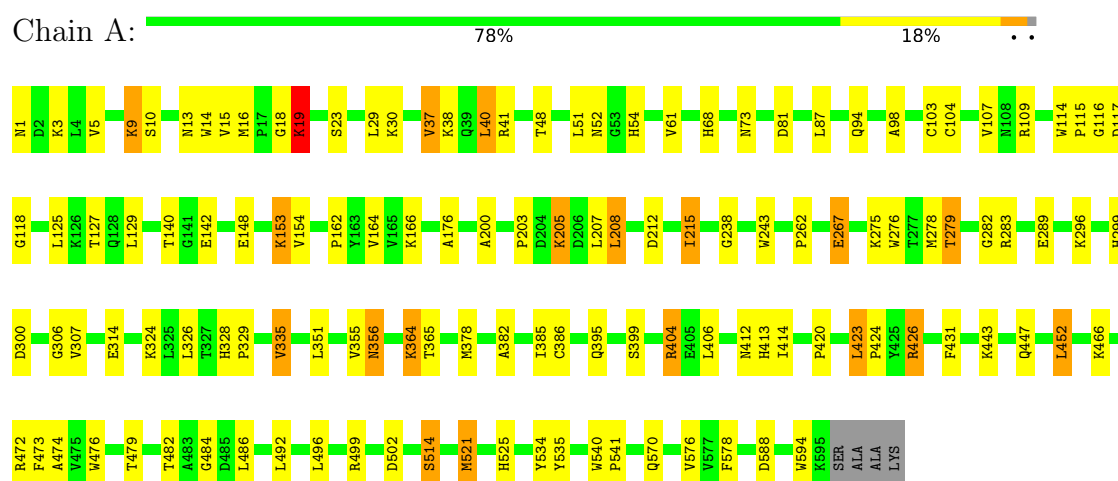
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

### 3 Residue-property plots [i](#)

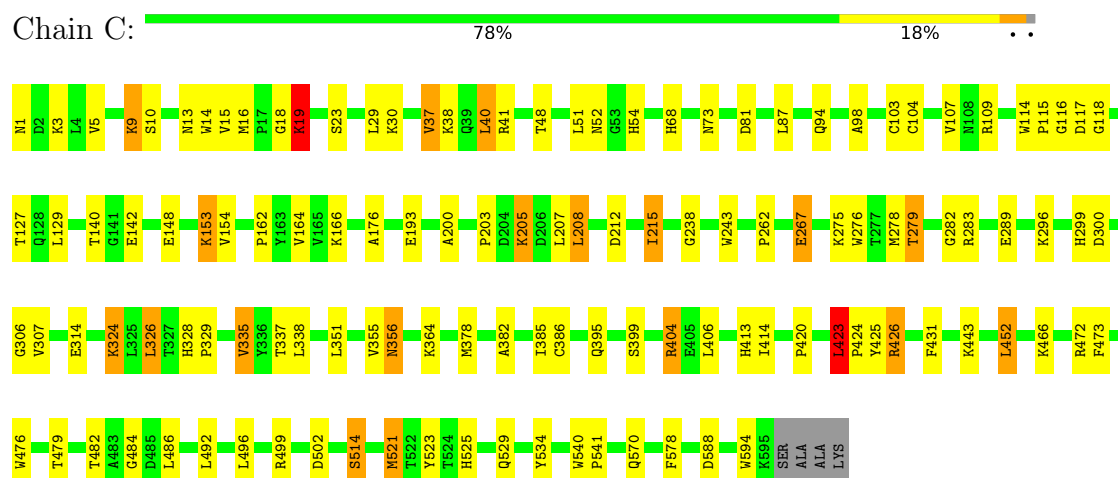
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

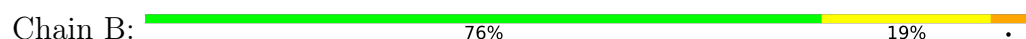
#### • Molecule 1: METHANOL DEHYDROGENASE SUBUNIT 1



#### • Molecule 1: METHANOL DEHYDROGENASE SUBUNIT 1

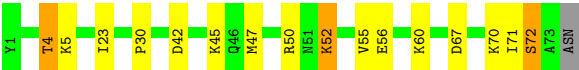
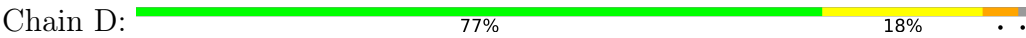


#### • Molecule 2: METHANOL DEHYDROGENASE SUBUNIT 2





● Molecule 2: METHANOL DEHYDROGENASE SUBUNIT 2



## 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, $\alpha$ , $\beta$ , $\gamma$	61.16Å 72.19Å 86.17Å 86.21° 76.09° 70.44°	Depositor
Resolution (Å)	20.00 – 1.94	Depositor
% Data completeness (in resolution range)	87.0 (20.00-1.94)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.199 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10462	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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: CA, 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	0.60	0/4750	0.86	12/6456 (0.2%)
1	C	0.60	0/4750	0.86	15/6456 (0.2%)
2	B	0.51	0/599	0.69	0/798
2	D	0.52	0/599	0.70	0/798
All	All	0.59	0/10698	0.84	27/14508 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	282	GLY	N-CA-C	-5.77	98.68	113.10
1	A	588	ASP	N-CA-C	-5.71	95.58	111.00
1	A	496	LEU	N-CA-C	-5.61	95.86	111.00
1	A	452	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	282	GLY	N-CA-C	-5.52	99.31	113.10
1	A	275	LYS	CA-C-N	-5.45	105.22	117.20
1	C	588	ASP	N-CA-C	-5.44	96.32	111.00
1	C	404	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	335	VAL	CB-CA-C	-5.40	101.15	111.40
1	A	14	TRP	N-CA-C	-5.39	96.44	111.00
1	C	496	LEU	N-CA-C	-5.38	96.47	111.00
1	C	275	LYS	CA-C-N	-5.37	105.38	117.20
1	A	404	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	326	LEU	CA-CB-CG	5.34	127.58	115.30
1	C	14	TRP	N-CA-C	-5.33	96.59	111.00
1	A	335	VAL	CB-CA-C	-5.32	101.29	111.40
1	C	338	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	423	LEU	CA-CB-CG	5.29	127.48	115.30
1	A	499	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASN	N-CA-C	5.21	125.06	111.00
1	C	324	LYS	N-CA-C	-5.14	97.12	111.00
1	A	326	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	356	ASN	N-CA-C	5.09	124.73	111.00
1	A	404	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	499	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	275	LYS	N-CA-C	5.02	124.55	111.00

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	4620	0	4439	88	0
1	C	4620	0	4439	86	0
2	B	586	0	584	10	0
2	D	586	0	584	10	0
3	A	24	0	3	2	0
3	C	24	0	3	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
All	All	10462	0	10052	189	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 9.

All (189) 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:482:THR:HG22	1:C:484:GLY:H	1.35	0.92
1:A:482:THR:HG22	1:A:484:GLY:H	1.33	0.92
1:A:73:ASN:HD22	1:A:94:GLN:HE22	1.22	0.84
1:C:413:HIS:HE1	1:C:443:LYS:H	1.26	0.83
1:C:73:ASN:HD22	1:C:94:GLN:HE22	1.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASP:HB2	1:C:215:ILE:HD12	1.64	0.80
1:A:114:TRP:CZ3	1:A:116:GLY:HA2	2.17	0.80
1:A:413:HIS:HE1	1:A:443:LYS:H	1.26	0.79
1:C:114:TRP:CZ3	1:C:116:GLY:HA2	2.20	0.75
1:C:40:LEU:HD22	1:C:578:PHE:HB3	1.69	0.73
1:A:109:ARG:HE	1:A:395:GLN:HG3	1.54	0.73
1:C:109:ARG:HE	1:C:395:GLN:HG3	1.52	0.73
1:A:203:PRO:HB3	1:A:205:LYS:HE2	1.71	0.72
1:A:212:ASP:HB2	1:A:215:ILE:HD12	1.71	0.71
1:A:40:LEU:HD22	1:A:578:PHE:HB3	1.73	0.69
1:C:203:PRO:HB3	1:C:205:LYS:HE2	1.75	0.69
1:A:98:ALA:HB1	1:A:129:LEU:HD12	1.76	0.68
1:C:98:ALA:HB1	1:C:129:LEU:HD12	1.75	0.68
1:A:140:THR:OG1	1:A:142:GLU:HG3	1.95	0.67
1:C:140:THR:OG1	1:C:142:GLU:HG3	1.95	0.67
1:C:81:ASP:OD2	1:C:525:HIS:HE1	1.78	0.65
1:A:482:THR:HG22	1:A:484:GLY:N	2.09	0.65
1:C:413:HIS:CE1	1:C:443:LYS:H	2.14	0.65
1:C:267:GLU:OE1	1:C:299:HIS:HE1	1.81	0.64
1:C:18:GLY:O	1:C:19:LYS:HB2	1.98	0.63
1:A:81:ASP:OD2	1:A:525:HIS:HE1	1.83	0.62
1:A:18:GLY:O	1:A:19:LYS:HB2	1.99	0.62
1:A:413:HIS:CE1	1:A:443:LYS:H	2.14	0.61
1:C:278:MET:HE2	1:C:300:ASP:HB2	1.82	0.61
2:D:52:LYS:HA	2:D:52:LYS:HE2	1.80	0.61
1:A:267:GLU:OE1	1:A:299:HIS:HE1	1.83	0.61
1:A:355:VAL:O	1:A:386:CYS:O	2.19	0.61
1:A:200:ALA:O	1:A:276:TRP:HB2	2.01	0.61
1:A:10:SER:HB3	1:A:13:ASN:HD22	1.66	0.61
1:C:205:LYS:HD3	1:C:205:LYS:H	1.66	0.61
1:C:382:ALA:HB1	1:C:385:ILE:HD11	1.82	0.60
1:C:16:MET:HE1	1:C:164:VAL:H	1.65	0.60
1:A:404:ARG:HD3	1:A:502:ASP:OD2	2.01	0.60
1:C:404:ARG:HD3	1:C:502:ASP:OD2	2.01	0.60
1:C:482:THR:HG22	1:C:484:GLY:N	2.11	0.60
1:C:355:VAL:O	1:C:386:CYS:O	2.19	0.60
1:C:10:SER:HB3	1:C:13:ASN:HD22	1.67	0.60
1:A:205:LYS:H	1:A:205:LYS:HD3	1.67	0.60
1:C:200:ALA:O	1:C:276:TRP:HB2	2.02	0.60
1:A:16:MET:HE1	1:A:164:VAL:H	1.66	0.60
2:B:52:LYS:HA	2:B:52:LYS:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:CE	1:A:164:VAL:H	2.16	0.58
2:D:71:ILE:O	2:D:72:SER:HB2	2.04	0.58
1:A:382:ALA:HB1	1:A:385:ILE:HD11	1.85	0.58
1:C:276:TRP:HA	1:C:279:THR:HG21	1.86	0.57
1:A:29:LEU:O	1:A:482:THR:HG23	2.04	0.56
1:C:3:LYS:HE3	1:C:115:PRO:HB2	1.85	0.56
2:B:71:ILE:O	2:B:72:SER:HB2	2.05	0.56
1:C:16:MET:CE	1:C:164:VAL:H	2.18	0.56
2:B:42:ASP:HA	2:B:45:LYS:HE3	1.88	0.56
1:A:276:TRP:HA	1:A:279:THR:HG21	1.88	0.56
2:D:4:THR:HG22	2:D:5:LYS:HD3	1.89	0.55
1:A:9:LYS:HA	1:A:9:LYS:HE2	1.89	0.55
1:C:382:ALA:CB	1:C:385:ILE:HD11	2.36	0.55
1:C:109:ARG:NE	1:C:395:GLN:HG3	2.21	0.54
1:C:296:LYS:HZ3	1:C:328:HIS:HE1	1.55	0.54
2:B:4:THR:HG22	2:B:5:LYS:HD3	1.88	0.54
1:C:29:LEU:O	1:C:482:THR:HG23	2.07	0.54
1:A:3:LYS:HE3	1:A:115:PRO:HB2	1.89	0.54
1:A:514:SER:HB3	1:A:570:GLN:O	2.08	0.54
1:A:382:ALA:CB	1:A:385:ILE:HD11	2.38	0.54
1:A:278:MET:HE2	1:A:300:ASP:HB2	1.90	0.53
1:A:296:LYS:NZ	1:A:328:HIS:HE1	2.06	0.53
1:A:205:LYS:HD3	1:A:205:LYS:N	2.24	0.53
1:C:296:LYS:NZ	1:C:328:HIS:HE1	2.06	0.53
1:A:3:LYS:HB3	1:A:115:PRO:HG2	1.91	0.53
1:C:276:TRP:HE3	1:C:279:THR:HG21	1.73	0.53
1:C:9:LYS:HA	1:C:9:LYS:HE2	1.90	0.53
1:A:109:ARG:NE	1:A:395:GLN:HG3	2.23	0.52
1:A:276:TRP:HE3	1:A:279:THR:HG21	1.74	0.52
1:A:521:MET:O	1:A:521:MET:HE2	2.10	0.52
1:C:205:LYS:HD3	1:C:205:LYS:N	2.23	0.52
1:A:176:ALA:HB3	3:A:601:PQQ:O7B	2.09	0.52
1:A:414:ILE:HG12	1:A:452:LEU:HD12	1.92	0.52
1:A:426:ARG:N	1:A:426:ARG:HD3	2.25	0.51
1:C:426:ARG:N	1:C:426:ARG:HD3	2.25	0.51
1:C:314:GLU:HG2	1:C:324:LYS:HD3	1.93	0.51
1:C:514:SER:HB3	1:C:570:GLN:O	2.10	0.51
2:D:42:ASP:HA	2:D:45:LYS:HE3	1.93	0.51
1:A:52:ASN:O	1:A:54:HIS:HD2	1.94	0.50
1:A:296:LYS:HZ1	1:A:306:GLY:HA3	1.76	0.50
1:C:127:THR:HG23	1:C:162:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:O	1:C:283:ARG:NH2	2.45	0.50
1:A:207:LEU:O	1:A:283:ARG:NH2	2.45	0.50
1:C:148:GLU:OE2	2:D:50:ARG:NH1	2.45	0.50
1:A:68:HIS:CE1	1:A:534:TYR:HE1	2.29	0.50
1:C:103:CYS:SG	1:C:104:CYS:N	2.85	0.49
1:C:3:LYS:HB3	1:C:115:PRO:HG2	1.94	0.49
2:D:23:ILE:HD12	2:D:30:PRO:HD3	1.93	0.49
1:A:103:CYS:SG	1:A:104:CYS:N	2.85	0.49
1:C:212:ASP:CB	1:C:215:ILE:HD12	2.39	0.49
1:C:399:SER:OG	1:C:479:THR:HG22	2.12	0.49
1:C:68:HIS:CE1	1:C:534:TYR:HE1	2.30	0.49
1:C:296:LYS:HZ1	1:C:306:GLY:HA3	1.78	0.49
1:C:335:VAL:HG22	1:C:351:LEU:CD2	2.42	0.49
1:A:296:LYS:HZ3	1:A:328:HIS:HE1	1.61	0.48
1:A:594:TRP:HB2	1:C:472:ARG:HB2	1.95	0.48
2:B:23:ILE:HD12	2:B:30:PRO:HD3	1.96	0.48
1:C:37:VAL:O	1:C:40:LEU:HB2	2.13	0.48
1:C:1:ASN:O	1:C:5:VAL:HG23	2.14	0.48
1:A:127:THR:HG23	1:A:162:PRO:HG3	1.95	0.48
1:A:399:SER:OG	1:A:479:THR:HG22	2.13	0.48
1:C:205:LYS:H	1:C:205:LYS:CD	2.23	0.48
1:A:1:ASN:O	1:A:5:VAL:HG23	2.13	0.48
2:D:56:GLU:O	2:D:60:LYS:HG3	2.14	0.48
1:A:314:GLU:HG2	1:A:324:LYS:HD3	1.96	0.47
1:A:335:VAL:HG22	1:A:351:LEU:CD2	2.43	0.47
1:C:52:ASN:O	1:C:54:HIS:HD2	1.98	0.47
1:A:18:GLY:O	1:A:19:LYS:CB	2.63	0.47
1:C:176:ALA:HB3	3:C:601:PQQ:O7B	2.15	0.47
2:B:56:GLU:O	2:B:60:LYS:HG3	2.15	0.47
1:C:521:MET:HE1	1:C:523:TYR:CE2	2.50	0.47
1:A:15:VAL:O	1:A:16:MET:HG2	2.15	0.47
1:C:51:LEU:O	1:C:52:ASN:HB2	2.15	0.46
1:C:15:VAL:O	1:C:16:MET:HG2	2.15	0.46
1:A:148:GLU:OE2	2:B:50:ARG:NH1	2.48	0.46
1:A:208:LEU:CD2	1:A:289:GLU:HG2	2.45	0.46
1:C:18:GLY:O	1:C:19:LYS:CB	2.62	0.46
1:C:414:ILE:HG12	1:C:452:LEU:HD12	1.96	0.46
1:A:243:TRP:CZ2	3:A:601:PQQ:C6A	2.99	0.46
1:A:205:LYS:H	1:A:205:LYS:CD	2.23	0.45
1:A:540:TRP:N	1:A:541:PRO:HD2	2.31	0.45
1:C:424:PRO:O	1:C:426:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HB2	1:A:473:PHE:HA	1.98	0.45
1:C:476:TRP:CZ2	1:C:541:PRO:HD3	2.52	0.45
1:A:37:VAL:O	1:A:40:LEU:HB2	2.17	0.45
1:C:238:GLY:O	1:C:262:PRO:HA	2.17	0.45
1:A:424:PRO:O	1:A:426:ARG:NH1	2.50	0.44
1:A:3:LYS:HB2	1:A:3:LYS:HE2	1.76	0.44
1:A:364:LYS:HD3	1:A:365:THR:N	2.33	0.44
1:C:243:TRP:CZ2	3:C:601:PQQ:C6A	3.00	0.44
1:A:129:LEU:HD13	1:A:129:LEU:O	2.17	0.44
1:C:29:LEU:HD13	1:C:529:GLN:HG3	1.99	0.44
1:C:208:LEU:HD22	1:C:289:GLU:HG2	2.00	0.44
1:A:476:TRP:CZ2	1:A:541:PRO:HD3	2.52	0.44
1:C:243:TRP:CE2	1:C:307:VAL:HG21	2.53	0.44
1:C:521:MET:O	1:C:521:MET:HE2	2.17	0.44
1:C:193:GLU:HB2	2:D:55:VAL:HG11	2.00	0.43
1:A:153:LYS:HA	1:A:153:LYS:HE2	2.00	0.43
1:C:540:TRP:N	1:C:541:PRO:HD2	2.34	0.43
2:B:47:MET:HG2	2:B:50:ARG:HH12	1.84	0.43
1:A:208:LEU:HD22	1:A:289:GLU:HG2	2.00	0.43
1:A:378:MET:HA	1:A:420:PRO:HG2	2.01	0.43
1:A:243:TRP:CE2	1:A:307:VAL:HG21	2.53	0.43
1:C:153:LYS:HA	1:C:153:LYS:HE2	2.00	0.43
1:C:423:LEU:HD21	1:C:431:PHE:HA	2.01	0.43
1:C:117:ASP:OD2	1:C:118:GLY:N	2.52	0.43
1:A:364:LYS:CD	1:A:364:LYS:C	2.87	0.43
1:C:208:LEU:CD2	1:C:289:GLU:HG2	2.49	0.42
1:A:447:GLN:NE2	1:A:447:GLN:H	2.17	0.42
1:C:129:LEU:O	1:C:129:LEU:HD13	2.18	0.42
1:A:212:ASP:CB	1:A:215:ILE:HD12	2.45	0.42
1:C:73:ASN:ND2	1:C:129:LEU:H	2.16	0.42
1:C:278:MET:HE2	1:C:300:ASP:CB	2.49	0.42
1:C:452:LEU:HB2	1:C:473:PHE:HA	2.01	0.42
1:A:117:ASP:OD2	1:A:118:GLY:N	2.52	0.42
1:C:378:MET:HA	1:C:420:PRO:HG2	2.00	0.42
1:A:423:LEU:HD21	1:A:431:PHE:HA	2.01	0.42
1:A:15:VAL:HG12	1:A:61:VAL:HG22	2.02	0.42
1:A:238:GLY:O	1:A:262:PRO:HA	2.19	0.42
1:A:364:LYS:HD3	1:A:364:LYS:C	2.40	0.42
1:A:413:HIS:CE1	1:A:443:LYS:HB2	2.55	0.42
1:A:473:PHE:HB3	1:A:492:LEU:HD12	2.01	0.42
2:B:67:ASP:HB3	2:B:70:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:O	1:A:52:ASN:HB2	2.19	0.42
1:A:329:PRO:HA	1:A:335:VAL:HA	2.02	0.42
1:A:48:THR:OG1	1:A:54:HIS:CE1	2.73	0.42
1:A:412:ASN:ND2	1:A:474:ALA:HB1	2.35	0.42
2:D:47:MET:HG2	2:D:50:ARG:HH12	1.84	0.42
1:C:329:PRO:HA	1:C:335:VAL:HA	2.02	0.41
1:A:73:ASN:ND2	1:A:129:LEU:H	2.19	0.41
1:A:472:ARG:HB2	1:C:594:TRP:HB2	2.03	0.41
1:C:3:LYS:HB2	1:C:3:LYS:HE2	1.75	0.41
1:C:48:THR:OG1	1:C:54:HIS:CE1	2.74	0.41
1:C:425:TYR:C	1:C:426:ARG:HD3	2.41	0.41
1:A:535:TYR:CD2	1:A:576:VAL:HG23	2.56	0.41
1:C:473:PHE:HB3	1:C:492:LEU:HD12	2.03	0.41
2:B:6:CYS:HA	2:B:12:CYS:HA	2.02	0.40
1:C:423:LEU:HA	1:C:424:PRO:HD3	1.91	0.40
2:D:67:ASP:HB3	2:D:70:LYS:NZ	2.36	0.40
1:A:335:VAL:HG22	1:A:351:LEU:HD21	2.04	0.40
1:C:10:SER:HB3	1:C:13:ASN:ND2	2.34	0.40
1:C:326:LEU:O	1:C:337:THR:HA	2.21	0.40
1:A:521:MET:HE2	1:A:521:MET:C	2.41	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	593/599 (99%)	555 (94%)	37 (6%)	1 (0%)	47	39
1	C	593/599 (99%)	555 (94%)	37 (6%)	1 (0%)	47	39
2	B	71/74 (96%)	70 (99%)	0	1 (1%)	11	3
2	D	71/74 (96%)	70 (99%)	0	1 (1%)	11	3
All	All	1328/1346 (99%)	1250 (94%)	74 (6%)	4 (0%)	41	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	72	SER
2	D	72	SER
1	C	19	LYS
1	A	19	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	476/478 (100%)	448 (94%)	28 (6%)	19	7
1	C	476/478 (100%)	449 (94%)	27 (6%)	20	8
2	B	62/63 (98%)	60 (97%)	2 (3%)	39	25
2	D	62/63 (98%)	60 (97%)	2 (3%)	39	25
All	All	1076/1082 (99%)	1017 (94%)	59 (6%)	21	8

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	19	LYS
1	A	23	SER
1	A	30	LYS
1	A	37	VAL
1	A	38	LYS
1	A	40	LEU
1	A	41	ARG
1	A	87	LEU
1	A	107	VAL
1	A	125	LEU
1	A	153	LYS
1	A	154	VAL
1	A	166	LYS
1	A	205	LYS
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	215	ILE
1	A	267	GLU
1	A	279	THR
1	A	356	ASN
1	A	364	LYS
1	A	406	LEU
1	A	423	LEU
1	A	426	ARG
1	A	466	LYS
1	A	486	LEU
1	A	514	SER
1	A	521	MET
2	B	4	THR
2	B	52	LYS
1	C	9	LYS
1	C	19	LYS
1	C	23	SER
1	C	30	LYS
1	C	37	VAL
1	C	38	LYS
1	C	40	LEU
1	C	41	ARG
1	C	87	LEU
1	C	107	VAL
1	C	153	LYS
1	C	154	VAL
1	C	166	LYS
1	C	205	LYS
1	C	208	LEU
1	C	215	ILE
1	C	267	GLU
1	C	279	THR
1	C	356	ASN
1	C	364	LYS
1	C	406	LEU
1	C	423	LEU
1	C	426	ARG
1	C	466	LYS
1	C	486	LEU
1	C	514	SER
1	C	521	MET
2	D	4	THR

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Mol	Chain	Res	Type
2	D	52	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	54	HIS
1	A	73	ASN
1	A	299	HIS
1	A	328	HIS
1	A	367	GLN
1	A	395	GLN
1	A	412	ASN
1	A	413	HIS
1	A	447	GLN
1	A	454	GLN
1	A	525	HIS
1	A	567	ASN
1	C	13	ASN
1	C	54	HIS
1	C	73	ASN
1	C	299	HIS
1	C	328	HIS
1	C	367	GLN
1	C	395	GLN
1	C	412	ASN
1	C	413	HIS
1	C	447	GLN
1	C	454	GLN
1	C	525	HIS
1	C	567	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	C	601	4	23,26,26	2.32	11 (47%)	29,40,40	3.15	14 (48%)
3	PQQ	A	601	4	23,26,26	2.32	11 (47%)	29,40,40	3.15	14 (48%)

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	601	4	-	4/10/28/28	0/3/3/3
3	PQQ	A	601	4	-	4/10/28/28	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	PQQ	O9B-C9X	-4.50	1.16	1.30
3	C	601	PQQ	O9B-C9X	-4.49	1.16	1.30
3	A	601	PQQ	O4-C4	-4.08	1.14	1.23
3	C	601	PQQ	O4-C4	-4.08	1.14	1.23
3	C	601	PQQ	C2-C2X	-3.93	1.45	1.50
3	A	601	PQQ	C2-C2X	-3.91	1.45	1.50
3	C	601	PQQ	O7B-C7X	-3.35	1.20	1.30
3	A	601	PQQ	O7B-C7X	-3.34	1.20	1.30
3	C	601	PQQ	O2A-C2X	3.10	1.31	1.22
3	A	601	PQQ	O2A-C2X	3.10	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	PQQ	O2B-C2X	-2.97	1.21	1.30
3	C	601	PQQ	O2B-C2X	-2.95	1.21	1.30
3	A	601	PQQ	C5-C4	-2.88	1.43	1.53
3	C	601	PQQ	C5-C4	-2.88	1.43	1.53
3	A	601	PQQ	C3A-C4	-2.85	1.43	1.48
3	C	601	PQQ	C3A-C4	-2.82	1.43	1.48
3	C	601	PQQ	O7A-C7X	2.77	1.30	1.22
3	A	601	PQQ	O7A-C7X	2.76	1.30	1.22
3	A	601	PQQ	C6A-C5	2.56	1.53	1.50
3	C	601	PQQ	C3-C2	-2.56	1.35	1.39
3	C	601	PQQ	C6A-C5	2.55	1.53	1.50
3	A	601	PQQ	C3-C2	-2.54	1.35	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	PQQ	C9-C9A-C1A	8.03	129.47	122.88
3	A	601	PQQ	C9-C9A-C1A	8.00	129.44	122.88
3	C	601	PQQ	O5-C5-C6A	5.13	127.27	121.84
3	A	601	PQQ	O5-C5-C6A	5.10	127.24	121.84
3	A	601	PQQ	O7B-C7X-C7	4.59	125.15	114.69
3	C	601	PQQ	O7B-C7X-C7	4.58	125.11	114.69
3	C	601	PQQ	C3A-C4-C5	4.57	120.80	118.14
3	A	601	PQQ	C3A-C4-C5	4.55	120.78	118.14
3	C	601	PQQ	C9-C9A-C6A	-4.40	115.80	121.68
3	A	601	PQQ	C9-C9A-C6A	-4.39	115.81	121.68
3	A	601	PQQ	O9B-C9X-C9	4.33	126.65	114.39
3	C	601	PQQ	O9B-C9X-C9	4.33	126.65	114.39
3	A	601	PQQ	O2A-C2X-C2	-4.12	112.89	121.24
3	C	601	PQQ	O2A-C2X-C2	-4.10	112.92	121.24
3	C	601	PQQ	O4-C4-C5	-3.92	112.51	119.31
3	A	601	PQQ	O4-C4-C5	-3.91	112.52	119.31
3	A	601	PQQ	C2-N1-C1A	3.68	111.45	103.90
3	C	601	PQQ	C2-N1-C1A	3.66	111.42	103.90
3	C	601	PQQ	O7A-C7X-C7	-3.64	113.86	121.24
3	A	601	PQQ	O7A-C7X-C7	-3.63	113.88	121.24
3	C	601	PQQ	O9B-C9X-O9A	-3.61	115.34	123.35
3	A	601	PQQ	O9B-C9X-O9A	-3.60	115.36	123.35
3	A	601	PQQ	O2B-C2X-C2	3.12	121.80	114.69
3	C	601	PQQ	O2B-C2X-C2	3.12	121.79	114.69
3	C	601	PQQ	C3A-C1A-C9A	2.77	125.23	121.54
3	A	601	PQQ	C3A-C1A-C9A	2.75	125.20	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	PQQ	O4-C4-C3A	-2.61	117.20	122.23
3	C	601	PQQ	O4-C4-C3A	-2.60	117.22	122.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

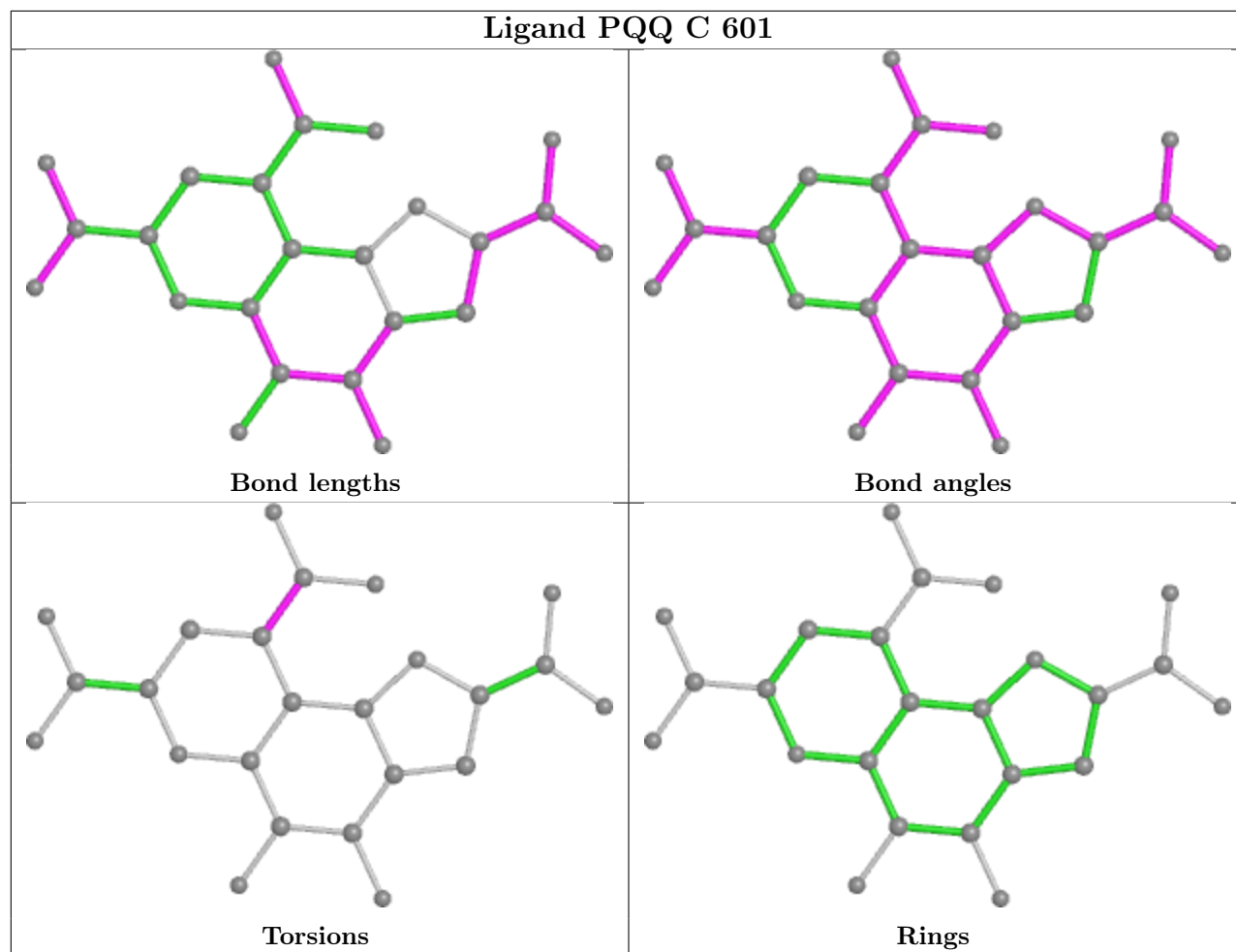
Mol	Chain	Res	Type	Atoms
3	A	601	PQQ	C9A-C9-C9X-O9A
3	A	601	PQQ	C9A-C9-C9X-O9B
3	C	601	PQQ	C9A-C9-C9X-O9A
3	C	601	PQQ	C9A-C9-C9X-O9B
3	A	601	PQQ	C8-C9-C9X-O9A
3	A	601	PQQ	C8-C9-C9X-O9B
3	C	601	PQQ	C8-C9-C9X-O9A
3	C	601	PQQ	C8-C9-C9X-O9B

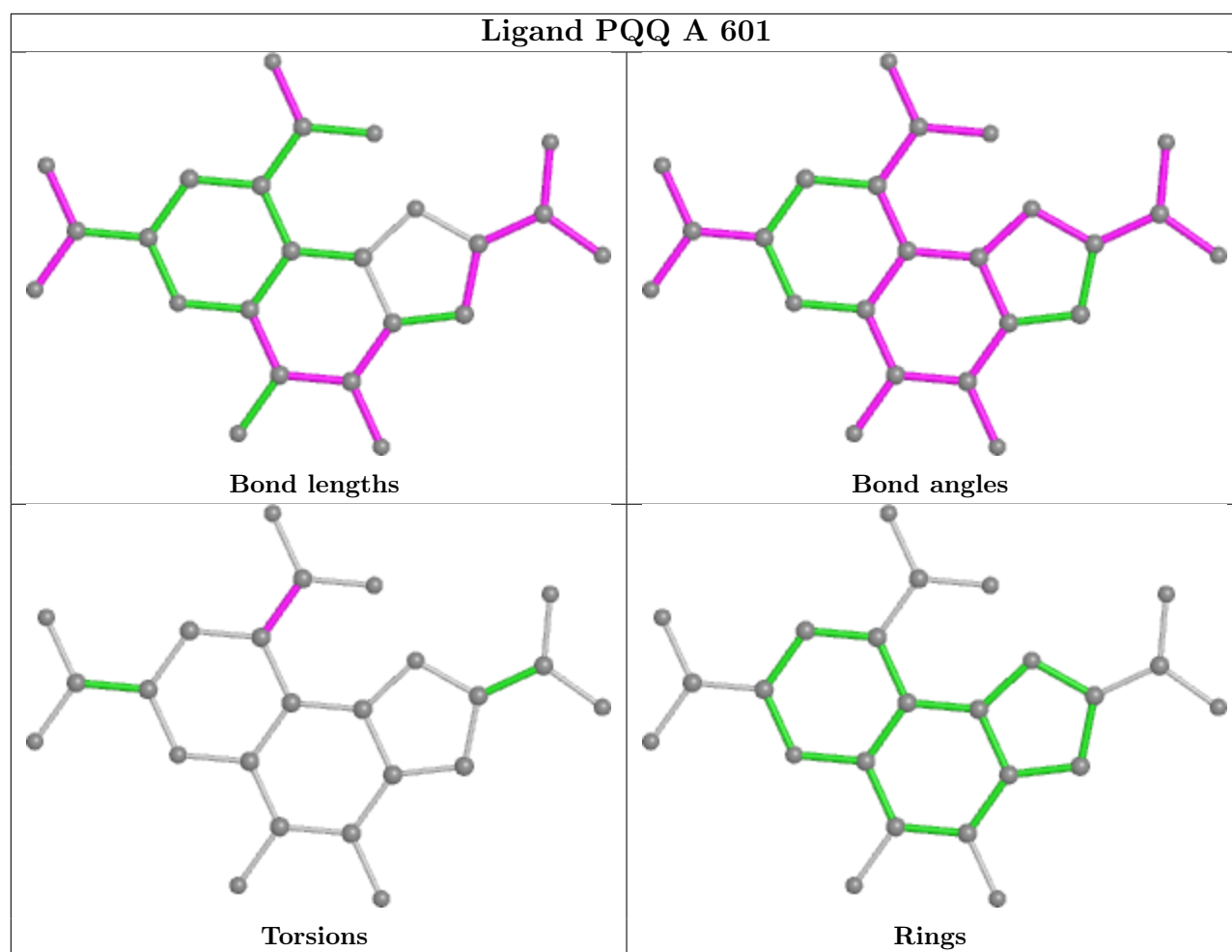
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	PQQ	2	0
3	A	601	PQQ	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.





## 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.