Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:56 am BST

PDB ID	:	1W6S
Title	:	The high resolution structure of methanol dehydrogenase from methylobacterium extorquens
Authors	:	Williams, P.A.; Coates, L.; Mohammed, F.; Gill, R.; Erskine, P.T.; Wood, S.P.; Anthony, C.; Cooper, J.B.
Deposited on	:	2004-08-23
Resolution	:	1.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

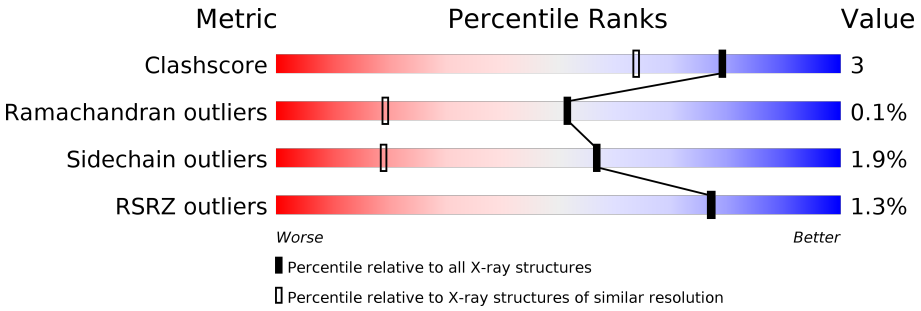
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

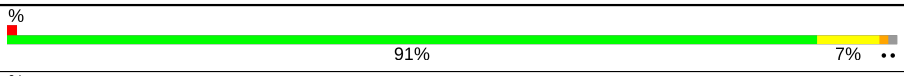
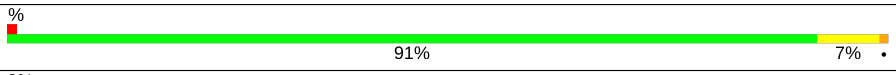
The reported resolution of this entry is 1.20 Å.

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	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 on 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 <=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	599	
1	C	599	
2	B	74	
2	D	74	

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
4	GOL	A	1597	-	X	-	-
4	GOL	A	1598	-	X	-	-
4	GOL	C	3598	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11845 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	596	Total	C	N	O	S	0	0	1
			4607	2938	774	875	20			
1	C	597	Total	C	N	O	S	0	0	1
			4601	2932	772	877	20			

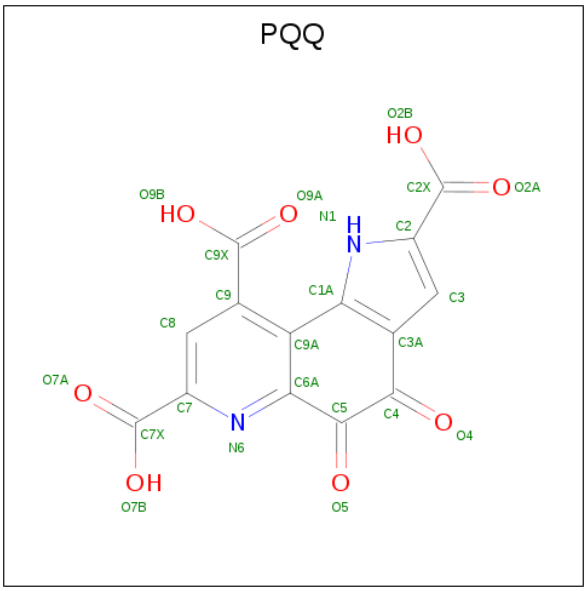
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	LYS	ARG	conflict	UNP P16027
C	2426	LYS	ARG	conflict	UNP P16027

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

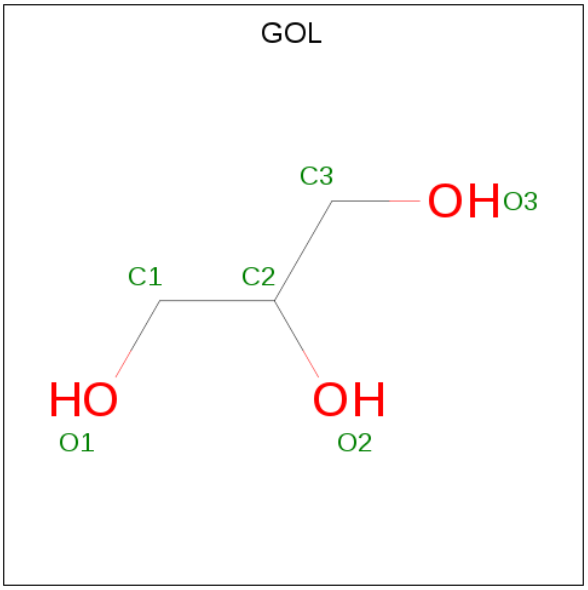
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	1
			574	361	102	108	3			
2	D	73	Total	C	N	O	S	0	0	1
			558	349	98	108	3			

- Molecule 3 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: $C_{14}H_6N_2O_8$).



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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	A	1	Total	C	O		0	0
			6	3	3			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

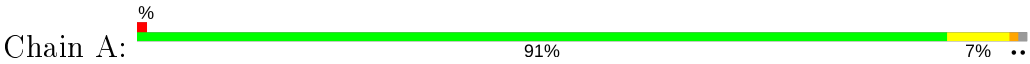
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	605	Total O 605 605	0	0
6	B	133	Total O 133 133	0	0
6	C	610	Total O 610 610	0	0
6	D	89	Total O 89 89	0	0

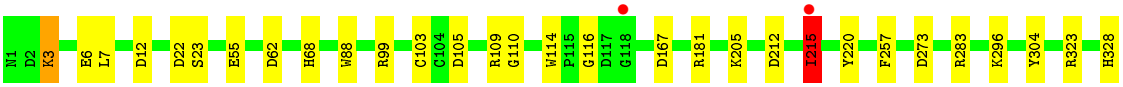
3 Residue-property plots (i)

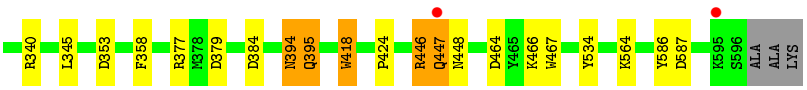
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 SUBUNIT 1

Chain A:

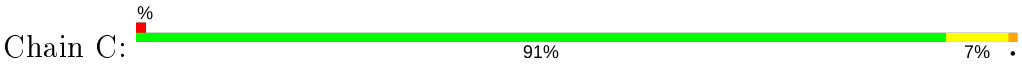


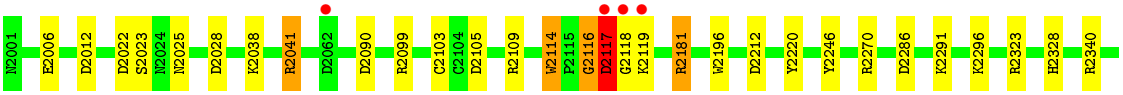


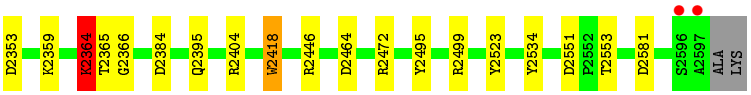


• Molecule 1: METHANOL DEHYDROGENASE SUBUNIT 1

Chain C:

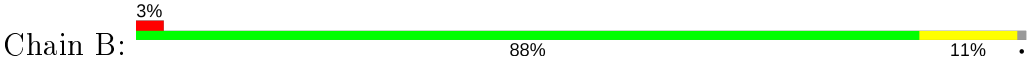


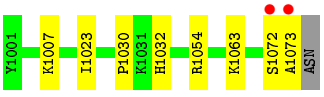




• Molecule 2: METHANOL DEHYDROGENASE SUBUNIT 2

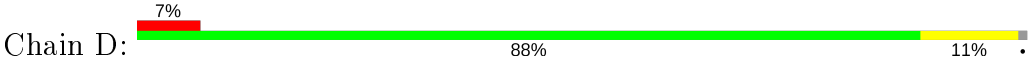
Chain B:

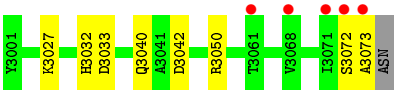




• Molecule 2: METHANOL DEHYDROGENASE SUBUNIT 2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.90Å 73.62Å 88.08Å 86.09° 104.11° 109.68°	Depositor
Resolution (Å)	10.00 – 1.20 10.00 – 1.23	Depositor EDS
% Data completeness (in resolution range)	85.0 (10.00-1.20) 85.0 (10.00-1.23)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 1.23Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.153 , 0.177 0.150 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	11.2	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 96.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	11845	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 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	1.03	2/4737 (0.0%)	1.37	35/6443 (0.5%)
1	C	1.07	4/4731 (0.1%)	1.49	45/6439 (0.7%)
2	B	0.84	0/587	1.27	1/784 (0.1%)
2	D	0.70	0/570	1.28	3/766 (0.4%)
All	All	1.03	6/10625 (0.1%)	1.41	84/14432 (0.6%)

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
1	C	0	3
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2117	ASP	CG-OD2	20.79	1.73	1.25
1	C	2117	ASP	CB-CG	17.39	1.88	1.51
1	C	2364	LYS	CE-NZ	6.45	1.65	1.49
1	C	2117	ASP	CG-OD1	-6.14	1.11	1.25
1	A	215	ILE	CG1-CD1	5.65	1.89	1.50
1	A	55	GLU	CD-OE2	5.21	1.31	1.25

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2117	ASP	CB-CG-OD2	-40.51	81.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2117	ASP	CB-CG-OD1	17.63	134.17	118.30
1	A	215	ILE	CB-CG1-CD1	-13.10	77.22	113.90
1	C	2384	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	A	446	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	A	215	ILE	CG1-CB-CG2	-10.24	88.88	111.40
1	A	446	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	C	2181	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	A	534	TYR	CB-CG-CD1	9.48	126.69	121.00
2	B	1054	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	447	GLN	OE1-CD-NE2	-9.42	100.24	121.90
1	A	99	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	C	2472	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	167	ASP	CB-CG-OD1	9.13	126.52	118.30
1	C	2099	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	C	2551	ASP	CB-CG-OD2	8.80	126.22	118.30
1	C	2109	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	C	2117	ASP	N-CA-CB	8.52	125.94	110.60
1	C	2012	ASP	CB-CG-OD1	8.45	125.91	118.30
1	A	447	GLN	CG-CD-NE2	8.13	136.22	116.70
1	C	2499	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	C	2220	TYR	CB-CG-CD1	8.04	125.82	121.00
1	C	2340	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	C	2384	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	99	ARG	CD-NE-CZ	7.82	134.54	123.60
1	C	2418	TRP	CA-CB-CG	7.78	128.49	113.70
1	A	418	TRP	CA-CB-CG	7.76	128.45	113.70
1	A	446	ARG	CD-NE-CZ	7.70	134.37	123.60
1	C	2384	ASP	N-CA-CB	-7.67	96.79	110.60
1	C	2581	ASP	CB-CG-OD1	7.49	125.04	118.30
1	C	2286	ASP	CB-CG-OD1	7.42	124.97	118.30
1	C	2364	LYS	CD-CE-NZ	7.37	128.66	111.70
1	C	2523	TYR	CB-CG-CD2	7.12	125.27	121.00
1	C	2404	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	C	2117	ASP	CB-CA-C	-6.87	96.67	110.40
1	A	353	ASP	CB-CG-OD1	6.86	124.48	118.30
1	C	2109	ARG	CG-CD-NE	-6.77	97.58	111.80
1	C	2212	ASP	CB-CG-OD1	6.71	124.34	118.30
1	C	2105	ASP	CB-CG-OD1	6.68	124.32	118.30
1	A	109	ARG	CG-CD-NE	-6.68	97.77	111.80
1	A	22	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	105	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	220	TYR	CB-CG-CD1	6.49	124.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	2270	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	467	TRP	CA-CB-CG	6.39	125.85	113.70
1	A	88	TRP	CA-CB-CG	6.39	125.84	113.70
1	C	2022	ASP	CB-CG-OD1	6.12	123.81	118.30
2	D	3050	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	A	377	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	A	304	TYR	CB-CG-CD1	5.98	124.59	121.00
1	C	2109	ARG	CD-NE-CZ	5.95	131.93	123.60
1	C	2446	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	257	PHE	CB-CG-CD2	5.90	124.93	120.80
1	A	273	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	2464	ASP	CB-CG-OD1	5.79	123.52	118.30
1	A	340	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	12	ASP	CB-CG-OD2	5.68	123.42	118.30
1	C	2246	TYR	CB-CG-CD2	5.66	124.40	121.00
1	A	384	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	2366	GLY	O-C-N	-5.60	113.73	122.70
1	A	587	ASP	CB-CG-OD1	5.59	123.33	118.30
2	D	3042	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	2340	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
1	C	2384	ASP	CB-CA-C	5.42	121.24	110.40
1	A	446	ARG	O-C-N	-5.42	114.03	122.70
1	C	2446	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	2041	ARG	CA-CB-CG	5.39	125.25	113.40
1	C	2028	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	2116	GLY	C-N-CA	-5.31	108.42	121.70
1	C	2353	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	323	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	586	TYR	CB-CG-CD2	5.27	124.16	121.00
1	C	2090	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	358	PHE	CB-CG-CD1	5.25	124.48	120.80
1	C	2114	TRP	CE3-CZ3-CH2	-5.25	115.43	121.20
1	A	283	ARG	NE-CZ-NH2	5.23	122.91	120.30
2	D	3033	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	2534	TYR	CB-CG-CD1	5.17	124.11	121.00
1	C	2196	TRP	CA-CB-CG	5.17	123.52	113.70
1	C	2323	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	304	TYR	CG-CD1-CE1	5.10	125.38	121.30
1	A	379	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	2117	ASP	CA-CB-CG	-5.02	102.35	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	CYS	Peptide
1	C	2103	CYS	Peptide
1	C	2117	ASP	Sidechain
1	C	2495	TYR	Peptide

5.2 Too-close contacts (i)

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	4607	0	4406	24	0
1	C	4601	0	4375	19	0
2	B	574	0	561	5	0
2	D	558	0	517	6	0
3	A	24	0	3	0	0
3	C	24	0	5	0	0
4	A	12	0	11	3	0
4	C	6	0	5	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	605	0	0	9	0
6	B	133	0	0	2	0
6	C	610	0	0	5	0
6	D	89	0	0	0	0
All	All	11845	0	9883	57	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 3.

All (57) 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:215:ILE:CD1	1:A:215:ILE:HG21	1.32	1.59
1:A:215:ILE:CG2	1:A:215:ILE:HD13	1.41	1.49
1:A:215:ILE:CD1	1:A:215:ILE:CG1	1.89	1.47
1:C:2117:ASP:CB	1:C:2117:ASP:CG	1.88	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:CD1	1:A:215:ILE:CG2	1.94	1.40
4:C:3598:GOL:O3	4:C:3598:GOL:C3	1.77	1.32
4:A:1597:GOL:C3	4:A:1597:GOL:O3	1.75	1.32
4:A:1598:GOL:O3	4:A:1598:GOL:C3	1.79	1.31
1:A:215:ILE:CB	1:A:215:ILE:CD1	2.10	1.28
1:C:2117:ASP:CG	1:C:2117:ASP:OD2	1.73	1.26
2:D:3072:SER:C	2:D:3073:ALA:N	2.02	1.11
1:C:2364:LYS:HE3	1:C:2365:THR:CG2	2.02	0.89
1:A:447:GLN:HG3	6:A:2489:HOH:O	1.82	0.80
1:C:2364:LYS:HE3	1:C:2365:THR:HG22	1.64	0.80
1:C:2117:ASP:CB	1:C:2117:ASP:OD2	2.36	0.73
1:C:2364:LYS:HE3	1:C:2365:THR:HG23	1.69	0.72
2:D:3072:SER:O	2:D:3073:ALA:N	2.28	0.66
1:A:6:GLU:HG2	6:A:2007:HOH:O	1.99	0.61
1:A:215:ILE:HB	1:A:215:ILE:CD1	2.27	0.60
1:C:2117:ASP:CA	1:C:2117:ASP:CG	2.68	0.59
1:A:215:ILE:CB	1:A:215:ILE:HD12	2.26	0.59
6:C:4456:HOH:O	2:D:3032:HIS:HD2	1.87	0.57
1:C:2181:ARG:H	2:D:3040:GLN:HE22	1.51	0.57
6:A:2454:HOH:O	2:B:1032:HIS:HD2	1.88	0.57
1:A:3:LYS:HE2	1:A:7:LEU:HG	1.88	0.55
1:C:2296:LYS:NZ	1:C:2328:HIS:HE1	2.05	0.55
2:D:3072:SER:CA	2:D:3073:ALA:N	2.72	0.52
1:A:464:ASP:HB3	6:A:2504:HOH:O	2.08	0.52
1:C:2114:TRP:HH2	1:C:2117:ASP:OD1	1.92	0.52
1:C:2114:TRP:CZ3	1:C:2116:GLY:HA2	2.45	0.52
1:A:394:ASN:HD22	1:A:395:GLN:H	1.57	0.52
1:C:2114:TRP:HH2	1:C:2117:ASP:CG	2.13	0.52
2:B:1073:ALA:N	6:B:2133:HOH:O	2.43	0.52
1:A:424:PRO:HD3	6:A:2453:HOH:O	2.09	0.51
1:C:2117:ASP:OD2	1:C:2118:GLY:N	2.44	0.51
1:A:215:ILE:HD13	1:A:215:ILE:HG21	0.54	0.48
1:A:212:ASP:HB2	1:A:215:ILE:HD12	1.95	0.47
1:A:212:ASP:HB2	1:A:215:ILE:CD1	2.45	0.47
1:C:2114:TRP:CH2	1:C:2117:ASP:OD1	2.68	0.47
1:A:448:ASN:OD1	1:A:564:LYS:NZ	2.48	0.47
1:A:114:TRP:CZ3	1:A:116:GLY:HA2	2.50	0.46
2:B:1063:LYS:NZ	6:B:2121:HOH:O	2.48	0.46
2:B:1023:ILE:HD12	2:B:1030:PRO:HD3	1.98	0.45
6:A:2335:HOH:O	2:B:1032:HIS:HE1	2.00	0.44
4:A:1597:GOL:H32	1:C:2041:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLN:NE2	6:A:2487:HOH:O	2.51	0.44
4:C:3598:GOL:C2	4:C:3598:GOL:O3	2.56	0.44
1:C:2038:LYS:HD3	6:C:4543:HOH:O	2.18	0.43
1:A:296:LYS:NZ	1:A:328:HIS:HE1	2.16	0.43
1:C:2359:LYS:NZ	6:C:4397:HOH:O	2.51	0.42
1:A:466:LYS:NZ	6:A:2506:HOH:O	2.52	0.42
1:C:2553:THR:HG22	6:C:4473:HOH:O	2.19	0.42
6:C:4337:HOH:O	2:D:3032:HIS:HE1	2.03	0.41
1:C:2038:LYS:HB2	1:C:2038:LYS:HE2	1.84	0.41
1:A:62:ASP:HB3	6:A:2116:HOH:O	2.20	0.41
1:A:215:ILE:HB	1:A:215:ILE:HD12	2.00	0.40
1:A:68:HIS:CE1	1:A:110:GLY:HA2	2.57	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	594/599 (99%)	562 (95%)	32 (5%)	0	100	100
1	C	595/599 (99%)	568 (96%)	26 (4%)	1 (0%)	47	19
2	B	71/74 (96%)	71 (100%)	0	0	100	100
2	D	70/74 (95%)	70 (100%)	0	0	100	100
All	All	1330/1346 (99%)	1271 (96%)	58 (4%)	1 (0%)	51	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2119	LYS

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	473/478 (99%)	464 (98%)	9 (2%)	57 19
1	C	471/478 (98%)	463 (98%)	8 (2%)	60 24
2	B	60/63 (95%)	58 (97%)	2 (3%)	38 5
2	D	56/63 (89%)	55 (98%)	1 (2%)	59 21
All	All	1060/1082 (98%)	1040 (98%)	20 (2%)	57 19

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	23	SER
1	A	205	LYS
1	A	215	ILE
1	A	345	LEU
1	A	394	ASN
1	A	395	GLN
1	A	418	TRP
1	A	446	ARG
2	B	1007	LYS
2	B	1072	SER
1	C	2006	GLU
1	C	2023	SER
1	C	2025	ASN
1	C	2117	ASP
1	C	2291	LYS
1	C	2364	LYS
1	C	2395	GLN
1	C	2418	TRP
2	D	3027	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	74	ASN
1	A	328	HIS
1	A	394	ASN
1	A	395	GLN
1	A	454	GLN
2	B	1032	HIS
1	C	2025	ASN
1	C	2328	HIS
1	C	2448	ASN
1	C	2454	GLN
2	D	3032	HIS
2	D	3040	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	3597	5	18,26,26	4.71	12 (66%)	14,40,40	3.05	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	1598	-	5,5,5	5.74	4 (80%)	5,5,5	2.25	1 (20%)
4	GOL	A	1597	-	5,5,5	4.81	4 (80%)	5,5,5	1.63	1 (20%)
4	GOL	C	3598	-	5,5,5	5.04	4 (80%)	5,5,5	2.03	1 (20%)
3	PQQ	A	1596	5	18,26,26	4.93	13 (72%)	14,40,40	4.46	9 (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	C	3597	5	-	0/0/28/28	0/3/3/3
4	GOL	A	1598	-	-	2/4/4/4	-
4	GOL	A	1597	-	-	1/4/4/4	-
4	GOL	C	3598	-	-	2/4/4/4	-
3	PQQ	A	1596	5	-	0/0/28/28	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1596	PQQ	C9A-C6A	9.54	1.51	1.40
4	A	1598	GOL	O3-C3	8.71	1.79	1.42
3	C	3597	PQQ	C9A-C6A	8.63	1.50	1.40
3	A	1596	PQQ	O5-C5	8.47	1.41	1.23
4	C	3598	GOL	O3-C3	8.26	1.77	1.42
4	A	1597	GOL	O3-C3	7.85	1.75	1.42
3	C	3597	PQQ	O5-C5	7.61	1.39	1.23
3	C	3597	PQQ	C6A-C5	7.51	1.60	1.50
3	C	3597	PQQ	C9-C9X	7.40	1.54	1.47
4	A	1598	GOL	O1-C1	-7.28	1.11	1.42
3	A	1596	PQQ	C3A-C1A	6.71	1.50	1.40
3	C	3597	PQQ	C8-C7	6.30	1.50	1.39
3	A	1596	PQQ	C5-C4	-6.14	1.33	1.53
3	C	3597	PQQ	C7-N6	6.09	1.44	1.34
3	A	1596	PQQ	C7-N6	5.80	1.43	1.34
3	A	1596	PQQ	C9-C9X	5.67	1.52	1.47
3	A	1596	PQQ	C9-C9A	5.66	1.51	1.41
4	C	3598	GOL	O1-C1	-5.66	1.18	1.42
4	A	1597	GOL	O1-C1	-5.59	1.18	1.42
3	C	3597	PQQ	C8-C9	5.55	1.49	1.39
4	A	1598	GOL	O2-C2	-5.23	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1596	PQQ	O4-C4	4.85	1.33	1.23
4	C	3598	GOL	O2-C2	-4.61	1.29	1.43
3	A	1596	PQQ	C2-N1	4.45	1.51	1.37
4	A	1597	GOL	O2-C2	-4.11	1.31	1.43
3	A	1596	PQQ	C8-C9	3.96	1.46	1.39
3	C	3597	PQQ	O4-C4	3.67	1.31	1.23
3	A	1596	PQQ	C8-C7	3.08	1.44	1.39
3	A	1596	PQQ	C3-C2	3.03	1.45	1.40
3	C	3597	PQQ	C9A-C1A	-2.90	1.43	1.48
4	A	1598	GOL	C3-C2	-2.89	1.39	1.51
3	C	3597	PQQ	C3-C3A	2.83	1.46	1.40
3	A	1596	PQQ	C9A-C1A	-2.61	1.44	1.48
3	C	3597	PQQ	C3A-C4	-2.52	1.43	1.48
3	C	3597	PQQ	C2-N1	2.42	1.45	1.37
4	C	3598	GOL	C3-C2	-2.37	1.42	1.51
4	A	1597	GOL	C3-C2	-2.34	1.42	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1596	PQQ	O5-C5-C6A	-12.04	109.09	121.84
3	C	3597	PQQ	C9-C9A-C1A	6.52	137.37	122.86
3	A	1596	PQQ	O5-C5-C4	4.98	127.96	119.31
3	C	3597	PQQ	C8-C9-C9A	4.90	125.82	118.95
3	A	1596	PQQ	C3-C3A-C1A	4.78	112.94	106.65
4	A	1598	GOL	O2-C2-C3	4.74	130.01	109.12
3	C	3597	PQQ	C9-C8-C7	-4.48	115.21	120.41
3	C	3597	PQQ	C5-C6A-N6	-4.41	107.48	114.96
3	A	1596	PQQ	C9-C8-C7	4.40	125.52	120.41
3	A	1596	PQQ	C9A-C1A-N1	4.11	132.84	124.25
4	C	3598	GOL	O2-C2-C3	3.91	126.36	109.12
3	A	1596	PQQ	C8-C7-N6	-3.90	117.72	122.35
3	A	1596	PQQ	C8-C9-C9A	-3.75	113.69	118.95
4	A	1597	GOL	O2-C2-C3	3.29	123.60	109.12
3	A	1596	PQQ	C6A-N6-C7	3.08	122.79	118.19
3	C	3597	PQQ	C8-C7-N6	-2.52	119.35	122.35
3	C	3597	PQQ	C3-C3A-C1A	2.37	109.77	106.65
3	C	3597	PQQ	O5-C5-C6A	-2.07	119.64	121.84
3	A	1596	PQQ	C3A-C3-C2	-2.01	103.31	105.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1598	GOL	O1-C1-C2-C3
4	C	3598	GOL	C1-C2-C3-O3
4	A	1598	GOL	O2-C2-C3-O3
4	A	1597	GOL	O1-C1-C2-O2
4	C	3598	GOL	O1-C1-C2-O2

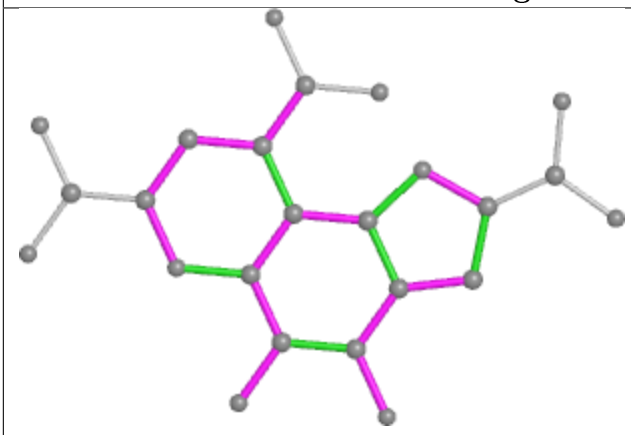
There are no ring outliers.

3 monomers are involved in 5 short contacts:

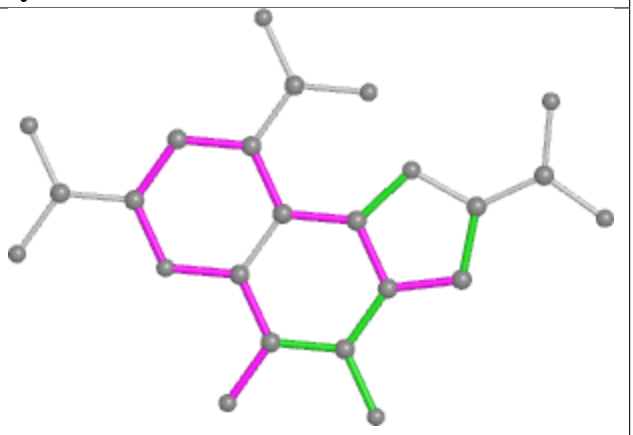
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1598	GOL	1	0
4	A	1597	GOL	2	0
4	C	3598	GOL	2	0

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 then 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.

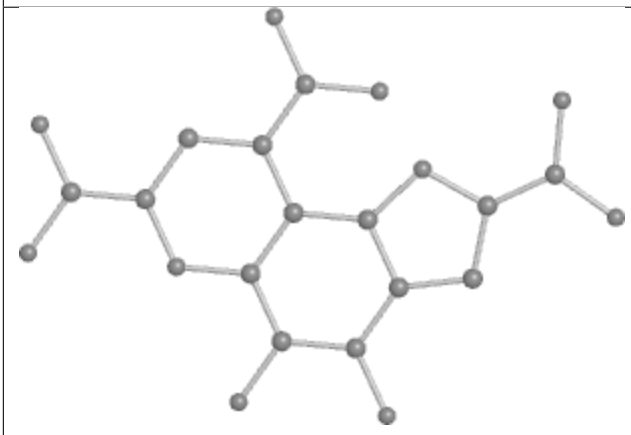
Ligand PQQ C 3597



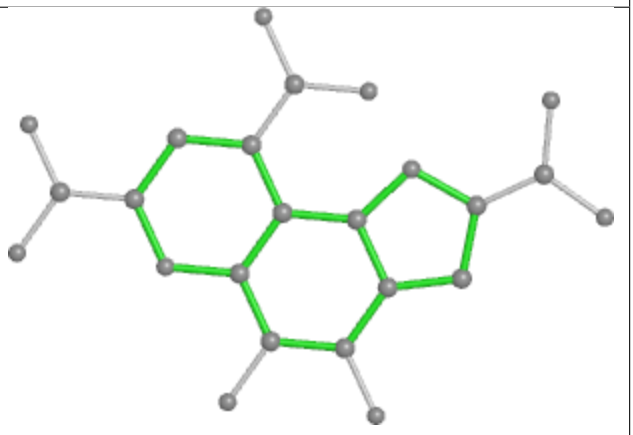
Bond lengths



Bond angles

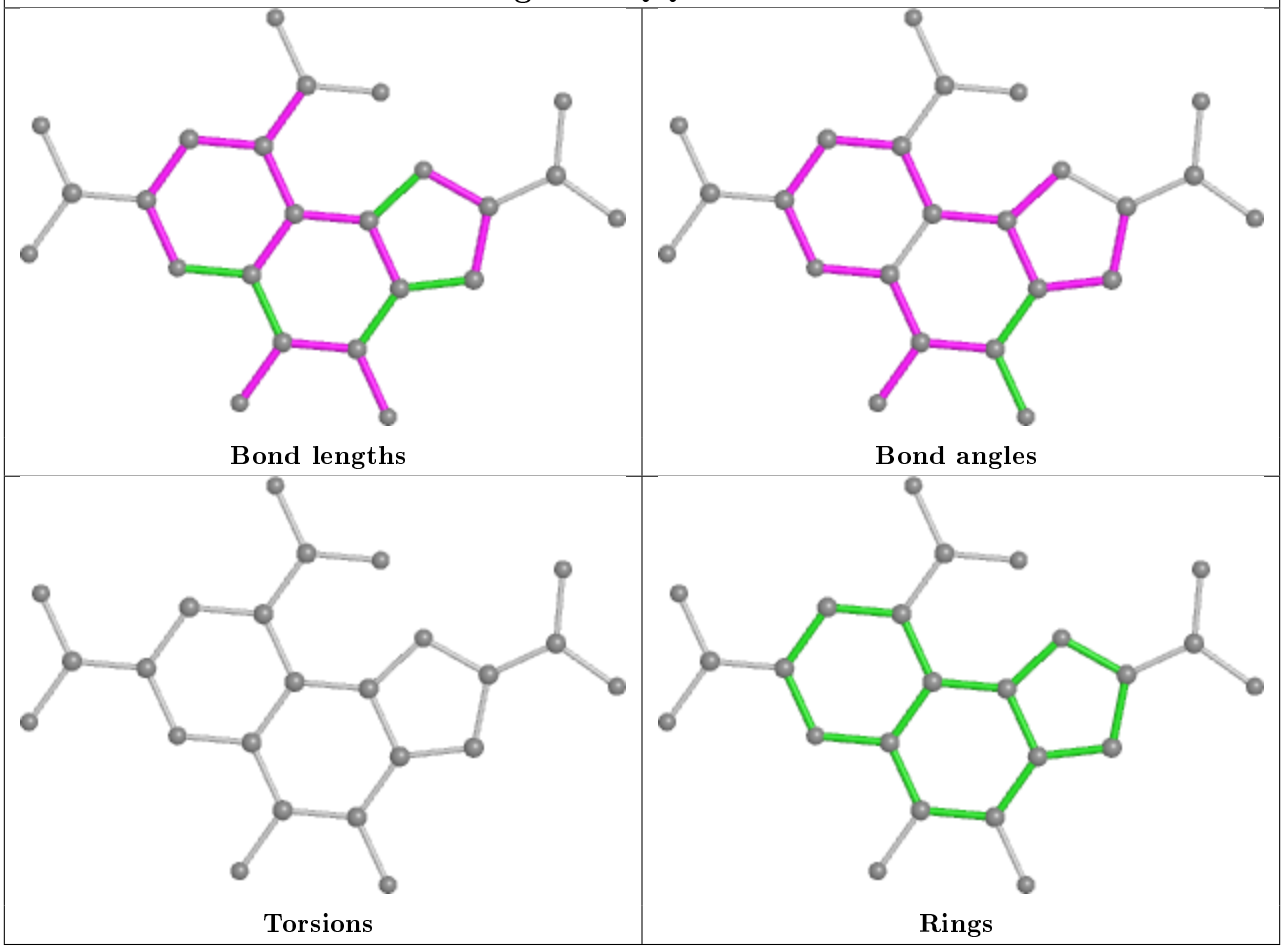


Torsions



Rings

Ligand PQQ A 1596



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3072:SER	C	3073:ALA	N	2.02

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, 95^{th} 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	596/599 (99%)	-0.31	4 (0%)	87	87	9, 13, 26, 43	0
1	C	597/599 (99%)	-0.26	6 (1%)	82	82	9, 14, 26, 76	0
2	B	73/74 (98%)	0.06	2 (2%)	54	53	13, 20, 33, 58	0
2	D	73/74 (98%)	0.26	5 (6%)	17	16	14, 24, 45, 78	0
All	All	1339/1346 (99%)	-0.24	17 (1%)	77	77	9, 14, 30, 78	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2118	GLY	11.8
2	B	1073	ALA	7.1
2	D	3072	SER	6.3
1	C	2597	ALA	6.1
2	B	1072	SER	5.9
2	D	3073	ALA	5.8
1	C	2596	SER	5.6
2	D	3071	ILE	4.1
1	C	2119	LYS	3.7
1	A	447	GLN	3.2
1	C	2117	ASP	3.1
2	D	3068	VAL	3.1
1	A	118	GLY	3.0
1	C	2062	ASP	2.7
1	A	215	ILE	2.2
1	A	595	LYS	2.1
2	D	3061	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

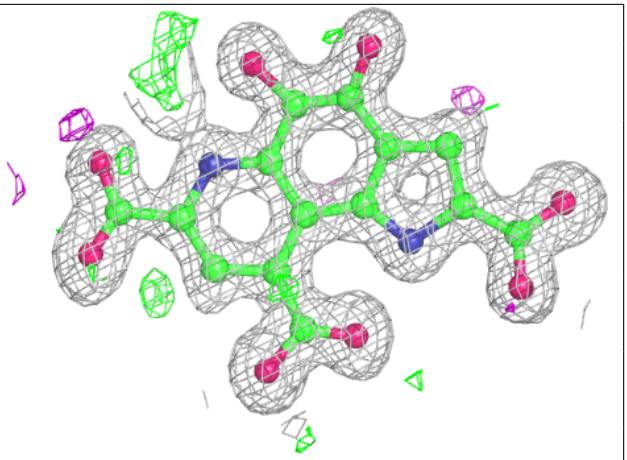
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

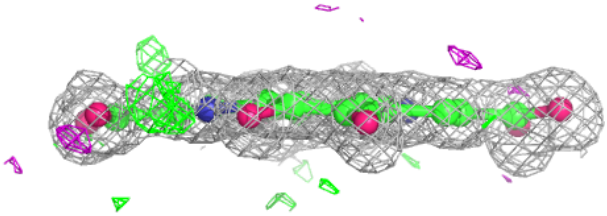
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	1598	6/6	0.93	0.11	17,27,34,45	0
4	GOL	C	3598	6/6	0.93	0.10	14,17,18,22	0
4	GOL	A	1597	6/6	0.94	0.11	12,17,19,20	0
3	PQQ	A	1596	24/24	0.98	0.08	12,14,19,21	0
3	PQQ	C	3597	24/24	0.98	0.07	11,15,19,21	0
5	CA	A	1599	1/1	0.99	0.14	25,25,25,25	1
5	CA	C	3599	1/1	1.00	0.13	25,25,25,25	1

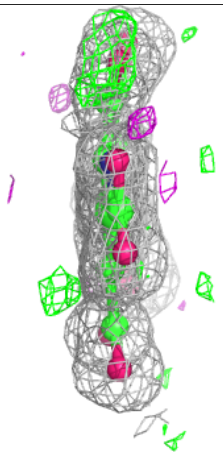
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PQQ A 1596:

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

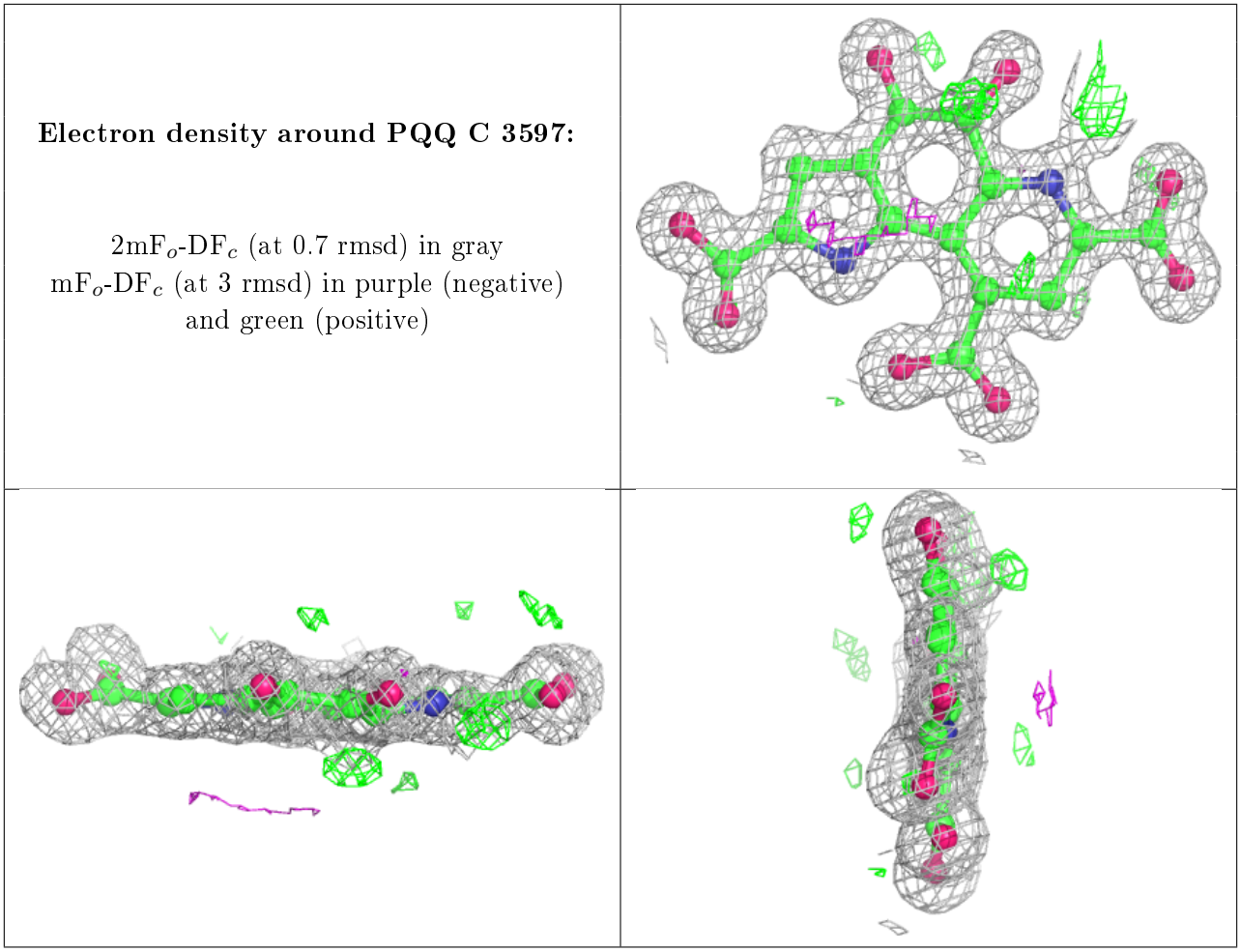






Electron density around PQQ C 3597:

$2mF_o$-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 (i)

There are no such residues in this entry.