



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:34 PM UTC

PDB ID : 4MH1 / pdb_00004mh1
Title : Crystal structure and functional studies of quinoprotein L-sorbose dehydrogenase from *Ketogulonicigenium vulgare* Y25
Authors : Han, X.; Liu, X.
Deposited on : 2013-08-29
Resolution : 2.70 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

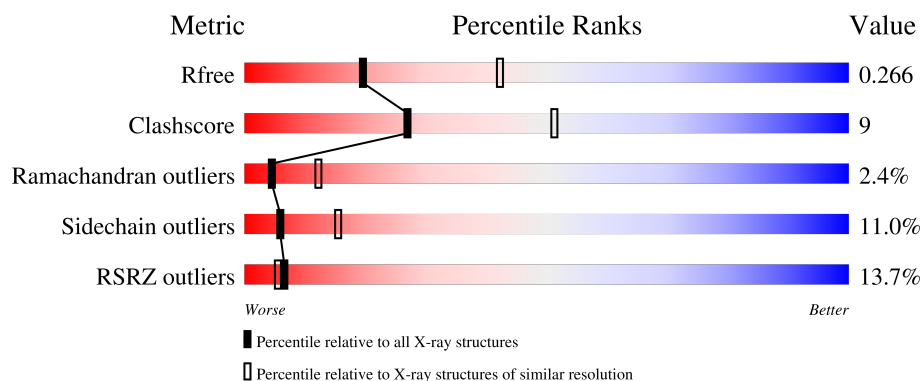
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	560	10% 71% 16% • 9%
1	B	560	15% 65% 19% 7% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7710 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.

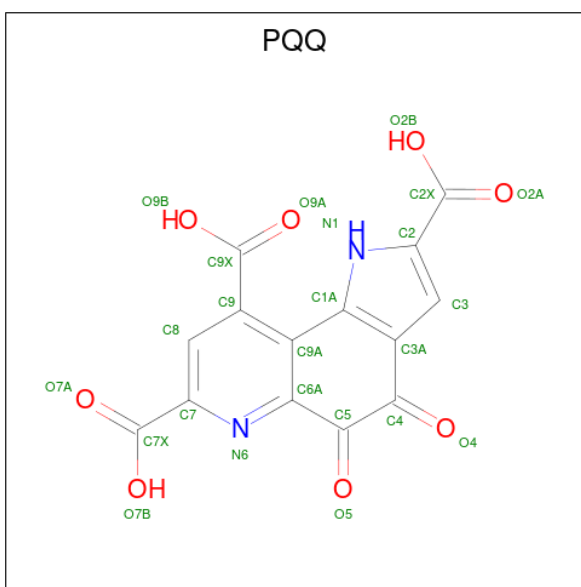
- Molecule 1 is a protein called Sorbose dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			3818	2392	655	753	18			
1	B	514	Total	C	N	O	S	0	0	0
			3867	2420	660	768	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	expression tag	UNP E3F069
A	-3	PHE	-	expression tag	UNP E3F069
A	-2	GLN	-	expression tag	UNP E3F069
A	-1	SER	-	expression tag	UNP E3F069
B	-4	TYR	-	expression tag	UNP E3F069
B	-3	PHE	-	expression tag	UNP E3F069
B	-2	GLN	-	expression tag	UNP E3F069
B	-1	SER	-	expression tag	UNP E3F069

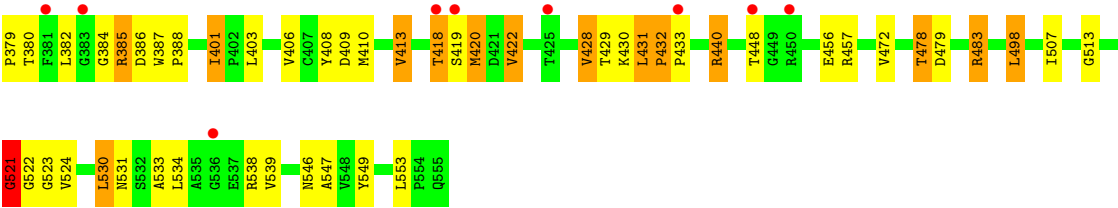
- Molecule 2 is PYRROLOQUINOLINE QUINONE (CCD ID: PQQ) (formula: C₁₄H₆N₂O₈).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	201.53Å 201.53Å 201.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.14 – 2.70 41.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.14-2.70) 99.0 (41.14-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.16 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.226 , 0.232 0.217 , 0.266	Depositor DCC
R_{free} test set	1943 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7710	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: 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	0.61	1/3903 (0.0%)	0.98	12/5333 (0.2%)
1	B	0.57	0/3951	0.99	18/5399 (0.3%)
All	All	0.59	1/7854 (0.0%)	0.98	30/10732 (0.3%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	ALA	N-CA	-7.33	1.36	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	522	GLY	N-CA-C	10.55	125.37	110.38
1	A	236	ALA	N-CA-C	-9.34	90.91	110.80
1	B	99	THR	N-CA-C	-7.84	104.32	114.04
1	B	6	ASP	N-CA-C	-6.78	100.00	110.10
1	B	432	PRO	CA-C-N	6.74	128.26	119.84
1	B	432	PRO	C-N-CA	6.74	128.26	119.84
1	A	0	ALA	CA-C-N	6.55	133.49	121.70
1	A	0	ALA	C-N-CA	6.55	133.49	121.70
1	B	315	GLU	CA-C-N	6.05	132.59	121.70
1	B	315	GLU	C-N-CA	6.05	132.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	431	LEU	CA-C-N	6.04	126.60	120.38
1	B	431	LEU	C-N-CA	6.04	126.60	120.38
1	A	94	LEU	CA-C-N	5.97	141.34	127.00
1	A	94	LEU	C-N-CA	5.97	141.34	127.00
1	A	94	LEU	C-N-CD	-5.91	107.60	120.60
1	B	359	ILE	CA-C-N	5.68	131.93	121.70
1	B	359	ILE	C-N-CA	5.68	131.93	121.70
1	B	341	TRP	N-CA-C	5.68	116.89	108.60
1	A	384	GLY	N-CA-C	-5.55	100.03	113.18
1	A	104	GLY	N-CA-C	5.28	120.76	111.57
1	A	97	ILE	N-CA-C	5.27	115.65	107.28
1	B	382	LEU	N-CA-C	-5.25	106.26	113.30
1	B	521	GLY	CA-C-N	-5.24	115.02	121.83
1	B	521	GLY	C-N-CA	-5.24	115.02	121.83
1	A	334	ALA	N-CA-C	5.24	116.99	111.28
1	A	382	LEU	N-CA-C	-5.22	106.14	112.88
1	B	105	GLU	CA-C-N	-5.16	114.67	120.14
1	B	105	GLU	C-N-CA	-5.16	114.67	120.14
1	B	413	VAL	N-CA-C	5.16	115.33	108.11
1	A	333	ASP	O-C-N	-5.02	116.75	122.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	GLY	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	3818	0	3541	53	0
1	B	3867	0	3604	84	0
2	B	24	0	3	0	0
3	B	1	0	0	0	0
All	All	7710	0	7148	137	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 (137) 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:B:359:ILE:HB	1:B:360:VAL:HA	1.50	0.93
1:A:235:THR:C	1:A:236:ALA:O	2.09	0.88
1:B:305:GLN:HG3	1:B:354:ILE:HB	1.62	0.81
1:B:308:ASN:HB3	1:B:311:ALA:HB2	1.63	0.79
1:A:142:ARG:HH21	1:A:178:SER:HB3	1.49	0.78
1:B:315:GLU:HA	1:B:316:ARG:HB2	1.64	0.77
1:B:306:SER:HB3	1:B:354:ILE:HG22	1.68	0.75
1:A:403:LEU:HB2	1:A:440:ARG:HG2	1.70	0.72
1:A:343:ARG:NH1	1:A:344:ASP:O	2.24	0.71
1:A:105:GLU:HG2	1:A:106:PRO:HD2	1.73	0.71
1:A:381:PHE:H	1:A:381:PHE:HD2	1.40	0.70
1:B:354:ILE:HA	1:B:359:ILE:HG21	1.75	0.69
1:A:105:GLU:HB2	1:A:122:TRP:CZ2	2.30	0.67
1:B:316:ARG:HH11	1:B:333:ASP:HB2	1.59	0.67
1:A:252:LEU:O	1:A:255:THR:HB	1.95	0.66
1:B:403:LEU:HB2	1:B:440:ARG:HG2	1.78	0.66
1:B:315:GLU:HA	1:B:316:ARG:CB	2.25	0.66
1:B:318:VAL:HG21	1:B:331:GLN:HE21	1.59	0.66
1:B:359:ILE:CB	1:B:360:VAL:HA	2.25	0.65
1:B:287:GLU:OE2	1:B:385:ARG:NH2	2.19	0.65
1:A:270:TRP:NE1	1:A:334:ALA:O	2.28	0.65
1:B:358:GLY:C	1:B:359:ILE:HD12	2.23	0.63
1:A:478:THR:CG2	1:A:531:ASN:HD21	2.11	0.63
1:A:63:HIS:HD2	1:A:131:MET:HE1	1.65	0.62
1:B:355:ASP:N	1:B:359:ILE:HG12	2.15	0.62
1:A:475:ASN:O	1:A:483:ARG:HG3	2.01	0.61
1:B:380:THR:HG23	1:B:406:VAL:HG13	1.83	0.61
1:B:368:LEU:HB2	1:B:410:MET:HE3	1.83	0.61
1:B:233:GLY:HA3	1:B:285:THR:HA	1.84	0.59
1:B:376:ASP:OD2	1:B:430:LYS:NZ	2.25	0.59
1:A:440:ARG:HD2	1:A:442:ASP:OD1	2.02	0.59
1:B:213:TRP:N	1:B:256:ASN:OD1	2.36	0.59
1:B:385:ARG:HG3	1:B:401:ILE:HD11	1.85	0.58
1:B:355:ASP:H	1:B:359:ILE:CG2	2.17	0.58
1:A:28:ARG:HD3	1:A:505:GLN:OE1	2.04	0.58
1:B:440:ARG:HB2	1:B:456:GLU:HG2	1.86	0.58
1:B:354:ILE:HG12	1:B:359:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLY:O	1:A:546:ASN:HA	2.05	0.56
1:B:369:LYS:O	1:B:375:TYR:OH	2.23	0.56
1:B:316:ARG:NH1	1:B:333:ASP:HB2	2.21	0.56
1:B:409:ASP:HB2	1:B:428:VAL:HG13	1.88	0.56
1:B:521:GLY:HA3	1:B:547:ALA:O	2.06	0.55
1:B:418:THR:HG22	1:B:419:SER:HA	1.88	0.55
1:A:478:THR:HG21	1:A:531:ASN:HD21	1.72	0.55
1:B:420:MET:HB3	1:B:422:VAL:HG12	1.88	0.54
1:B:184:THR:HG22	1:B:186:GLU:H	1.72	0.54
1:A:236:ALA:HA	1:A:255:THR:HG23	1.88	0.54
1:B:429:THR:HG22	1:B:533:ALA:HB2	1.90	0.54
1:A:120:VAL:HG23	1:A:155:PRO:HD3	1.91	0.53
1:A:254:GLY:HA3	1:A:271:ARG:HH22	1.72	0.53
1:B:270:TRP:CE3	1:B:337:GLY:HA3	2.44	0.53
1:B:478:THR:HG21	1:B:531:ASN:HD21	1.74	0.52
1:B:478:THR:CG2	1:B:531:ASN:HD21	2.22	0.52
1:A:47:TRP:CZ2	1:A:550:VAL:HG21	2.46	0.51
1:B:312:ALA:O	1:B:313:THR:HB	2.11	0.51
1:A:-4:TYR:HB3	1:A:87:ILE:O	2.10	0.51
1:A:460:ALA:O	1:A:478:THR:HB	2.11	0.51
1:B:310:ASN:HA	1:B:311:ALA:HB3	1.93	0.51
1:B:284:CYS:HA	1:B:323:PRO:O	2.11	0.50
1:B:301:MET:HE1	1:B:341:TRP:CD2	2.46	0.50
1:A:26:ASN:OD1	1:A:28:ARG:NH2	2.45	0.50
1:A:108:ARG:HH22	1:A:218:TRP:HZ3	1.59	0.50
1:B:305:GLN:HG2	1:B:354:ILE:HD12	1.93	0.50
1:B:406:VAL:HG21	1:B:530:LEU:HG	1.92	0.50
1:B:341:TRP:HZ3	1:B:343:ARG:HG2	1.77	0.50
1:B:355:ASP:H	1:B:359:ILE:HG21	1.77	0.50
1:B:62:ILE:HD13	1:B:507:ILE:HD11	1.94	0.49
1:A:26:ASN:O	1:A:28:ARG:N	2.44	0.49
1:A:220:GLN:HB2	1:A:287:GLU:HB3	1.93	0.49
1:B:61:LEU:HD13	1:B:112:LEU:HG	1.95	0.49
1:A:219:GLY:HA3	1:A:285:THR:O	2.13	0.49
1:B:521:GLY:O	1:B:546:ASN:HA	2.13	0.48
1:A:1:GLN:HG3	1:A:2:THR:HA	1.95	0.48
1:A:392:LEU:HD12	1:A:398:ILE:O	2.12	0.48
1:B:371:LEU:HD13	1:B:372:ASP:N	2.29	0.48
1:B:272:HIS:HE1	1:B:358:GLY:O	1.97	0.48
1:A:301:MET:HE2	1:A:449:GLY:HA3	1.96	0.47
1:B:322:VAL:HG22	1:B:385:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ASP:OD1	1:B:483:ARG:NH2	2.47	0.47
1:A:430:LYS:HG2	1:A:431:LEU:N	2.30	0.47
1:B:331:GLN:HG2	1:B:340:LEU:HD23	1.96	0.46
1:B:354:ILE:HG23	1:B:359:ILE:CD1	2.45	0.46
1:A:28:ARG:HH11	1:A:28:ARG:HB2	1.80	0.46
1:A:477:GLY:H	1:A:502:ALA:HB3	1.81	0.46
1:B:301:MET:HE1	1:B:341:TRP:CG	2.51	0.46
1:B:61:LEU:C	1:B:62:ILE:HD12	2.41	0.45
1:A:437:MET:HB3	1:A:457:ARG:C	2.41	0.45
1:B:55:LYS:HA	1:B:523:GLY:HA3	1.98	0.45
1:B:290:VAL:HA	1:B:318:VAL:O	2.16	0.45
1:A:254:GLY:HA3	1:A:271:ARG:NH2	2.31	0.45
1:B:179:GLY:HA3	1:B:189:TRP:NE1	2.32	0.44
1:A:437:MET:HB3	1:A:457:ARG:O	2.17	0.44
1:B:224:ASP:HB2	1:B:290:VAL:HG21	1.99	0.44
1:A:108:ARG:HG3	1:A:152:SER:O	2.18	0.44
1:B:23:ASN:ND2	1:B:25:GLU:HB2	2.33	0.44
1:B:431:LEU:HA	1:B:432:PRO:HD3	1.79	0.44
1:B:22:GLN:HG2	1:B:29:HIS:O	2.18	0.44
1:B:299:THR:HA	1:B:307:ILE:HD11	1.99	0.44
1:B:386:ASP:HB3	1:B:388:PRO:HD2	1.99	0.44
1:A:0:ALA:HB1	1:A:1:GLN:C	2.43	0.43
1:B:345:THR:OG1	1:B:346:ASN:N	2.50	0.43
1:B:354:ILE:CG1	1:B:359:ILE:HD13	2.48	0.43
1:A:71:ASN:HB2	1:A:75:VAL:HB	2.00	0.43
1:B:498:LEU:HG	1:B:549:TYR:CE2	2.53	0.43
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.90	0.43
1:A:383:GLY:HA3	1:A:385:ARG:O	2.19	0.43
1:B:8:MET:HE2	1:B:8:MET:HB3	1.79	0.43
1:B:354:ILE:C	1:B:359:ILE:HG12	2.44	0.43
1:A:20:TYR:HE2	1:A:28:ARG:HH21	1.64	0.42
1:B:293:VAL:O	1:B:315:GLU:CB	2.67	0.42
1:B:387:TRP:CG	1:B:388:PRO:HD3	2.54	0.42
1:A:235:THR:O	1:A:236:ALA:O	2.34	0.42
1:A:282:GLN:HB3	1:A:326:THR:HG22	2.01	0.42
1:B:162:ILE:H	1:B:162:ILE:HG12	1.65	0.42
1:B:377:VAL:HB	1:B:408:TYR:CE1	2.55	0.42
1:B:231:HIS:HA	1:B:259:PHE:O	2.20	0.41
1:B:272:HIS:NE2	1:B:358:GLY:HA3	2.35	0.41
1:A:478:THR:HG23	1:A:531:ASN:HD21	1.82	0.41
1:A:484:ALA:HB3	1:A:494:TRP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ALA:CB	1:B:316:ARG:HH21	2.32	0.41
1:A:302:GLU:HG2	1:A:343:ARG:NH2	2.36	0.41
1:A:387:TRP:CD1	1:A:388:PRO:HD3	2.54	0.41
1:A:520:ALA:HB1	1:A:521:GLY:HA3	2.02	0.41
1:B:303:GLY:HA3	1:B:344:ASP:HB2	2.02	0.41
1:A:193:PHE:HE2	1:A:216:GLY:HA2	1.85	0.41
1:A:302:GLU:O	1:A:343:ARG:HG3	2.19	0.41
1:A:32:LEU:HD11	1:A:510:GLU:HB2	2.03	0.41
1:A:280:TRP:CZ3	1:A:350:MET:HB3	2.55	0.41
1:B:34:GLN:NE2	1:B:513:GLY:O	2.52	0.41
1:B:374:GLU:OE1	1:B:409:ASP:HB3	2.21	0.41
1:B:380:THR:CG2	1:B:406:VAL:HG13	2.50	0.41
1:A:482:PHE:HB3	1:A:496:THR:HG22	2.03	0.41
1:B:6:ASP:O	1:B:7:GLU:HB2	2.20	0.40
1:B:19:SER:O	1:B:20:TYR:C	2.63	0.40
1:B:125:HIS:ND1	1:B:139:ASP:OD2	2.47	0.40
1:B:384:GLY:O	1:B:403:LEU:HA	2.20	0.40
1:B:35:ILE:HD13	1:B:43:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/560 (88%)	451 (91%)	35 (7%)	9 (2%)	6	18
1	B	504/560 (90%)	446 (88%)	43 (8%)	15 (3%)	3	8
All	All	999/1120 (89%)	897 (90%)	78 (8%)	24 (2%)	4	12

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	B	7	GLU
1	B	276	PRO
1	B	316	ARG
1	B	370	GLU
1	A	26	ASN
1	A	96	ASN
1	A	103	PHE
1	A	175	CYS
1	A	236	ALA
1	B	307	ILE
1	B	420	MET
1	B	309	PRO
1	B	313	THR
1	B	359	ILE
1	B	433	PRO
1	A	95	PRO
1	B	176	PHE
1	B	294	ASP
1	B	312	ALA
1	A	276	PRO
1	B	379	PRO
1	B	521	GLY
1	A	379	PRO

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	390/458 (85%)	356 (91%)	34 (9%)	9	24
1	B	401/458 (88%)	348 (87%)	53 (13%)	4	10
All	All	791/916 (86%)	704 (89%)	87 (11%)	6	15

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	TYR
1	A	-2	GLN
1	A	-1	SER
1	A	1	GLN
1	A	22	GLN
1	A	28	ARG
1	A	38	GLU
1	A	43	LEU
1	A	105	GLU
1	A	107	THR
1	A	108	ARG
1	A	140	VAL
1	A	255	THR
1	A	274	THR
1	A	296	GLN
1	A	299	THR
1	A	302	GLU
1	A	313	THR
1	A	318	VAL
1	A	326	THR
1	A	328	THR
1	A	340	LEU
1	A	343	ARG
1	A	362	VAL
1	A	376	ASP
1	A	381	PHE
1	A	430	LYS
1	A	436	ASP
1	A	440	ARG
1	A	472	VAL
1	A	478	THR
1	A	483	ARG
1	A	530	LEU
1	A	553	LEU
1	B	-1	SER
1	B	7	GLU
1	B	22	GLN
1	B	26	ASN
1	B	28	ARG
1	B	43	LEU
1	B	99	THR
1	B	102	SER
1	B	105	GLU

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Mol	Chain	Res	Type
1	B	135	GLN
1	B	162	ILE
1	B	176	PHE
1	B	186	GLU
1	B	255	THR
1	B	257	THR
1	B	267	GLU
1	B	280	TRP
1	B	287	GLU
1	B	289	MET
1	B	293	VAL
1	B	295	VAL
1	B	296	GLN
1	B	300	GLU
1	B	305	GLN
1	B	306	SER
1	B	308	ASN
1	B	318	VAL
1	B	322	VAL
1	B	328	THR
1	B	340	LEU
1	B	354	ILE
1	B	357	ASN
1	B	359	ILE
1	B	362	VAL
1	B	385	ARG
1	B	401	ILE
1	B	413	VAL
1	B	418	THR
1	B	422	VAL
1	B	428	VAL
1	B	440	ARG
1	B	448	THR
1	B	457	ARG
1	B	472	VAL
1	B	478	THR
1	B	483	ARG
1	B	498	LEU
1	B	524	VAL
1	B	530	LEU
1	B	534	LEU
1	B	538	ARG

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Mol	Chain	Res	Type
1	B	539	VAL
1	B	553	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	279	ASN
1	A	296	GLN
1	A	305	GLN
1	A	531	ASN
1	B	273	GLN
1	B	282	GLN
1	B	296	GLN
1	B	331	GLN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
2	PQQ	B	601	3	26,26,26	3.59	8 (30%)	34,40,40	2.79	11 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PQQ	B	601	3	-	7/12/28/28	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PQQ	C9A-C1A	12.64	1.61	1.46
2	B	601	PQQ	C5-C4	-7.20	1.44	1.54
2	B	601	PQQ	C1A-N1	5.72	1.47	1.37
2	B	601	PQQ	C2-N1	4.95	1.46	1.37
2	B	601	PQQ	C3A-C1A	4.18	1.49	1.40
2	B	601	PQQ	C3A-C4	3.84	1.57	1.46
2	B	601	PQQ	C3-C2	3.45	1.46	1.38
2	B	601	PQQ	C3-C3A	2.07	1.47	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	PQQ	C1A-C3A-C4	-11.27	112.84	122.33
2	B	601	PQQ	O4-C4-C5	4.38	123.77	118.37
2	B	601	PQQ	C1A-N1-C2	-4.14	103.51	110.20
2	B	601	PQQ	C3-C2-C2X	-3.66	124.10	132.53
2	B	601	PQQ	C3A-C1A-N1	-3.27	102.92	107.23
2	B	601	PQQ	C6A-N6-C7	3.09	122.07	118.01
2	B	601	PQQ	C3A-C3-C2	-3.03	104.82	107.94
2	B	601	PQQ	O5-C5-C4	2.99	122.04	118.14
2	B	601	PQQ	O2B-C2X-C2	2.71	120.11	114.27
2	B	601	PQQ	O9B-C9X-O9A	-2.17	118.69	123.35
2	B	601	PQQ	C3A-C4-C5	-2.09	114.67	117.03

There are no chirality outliers.

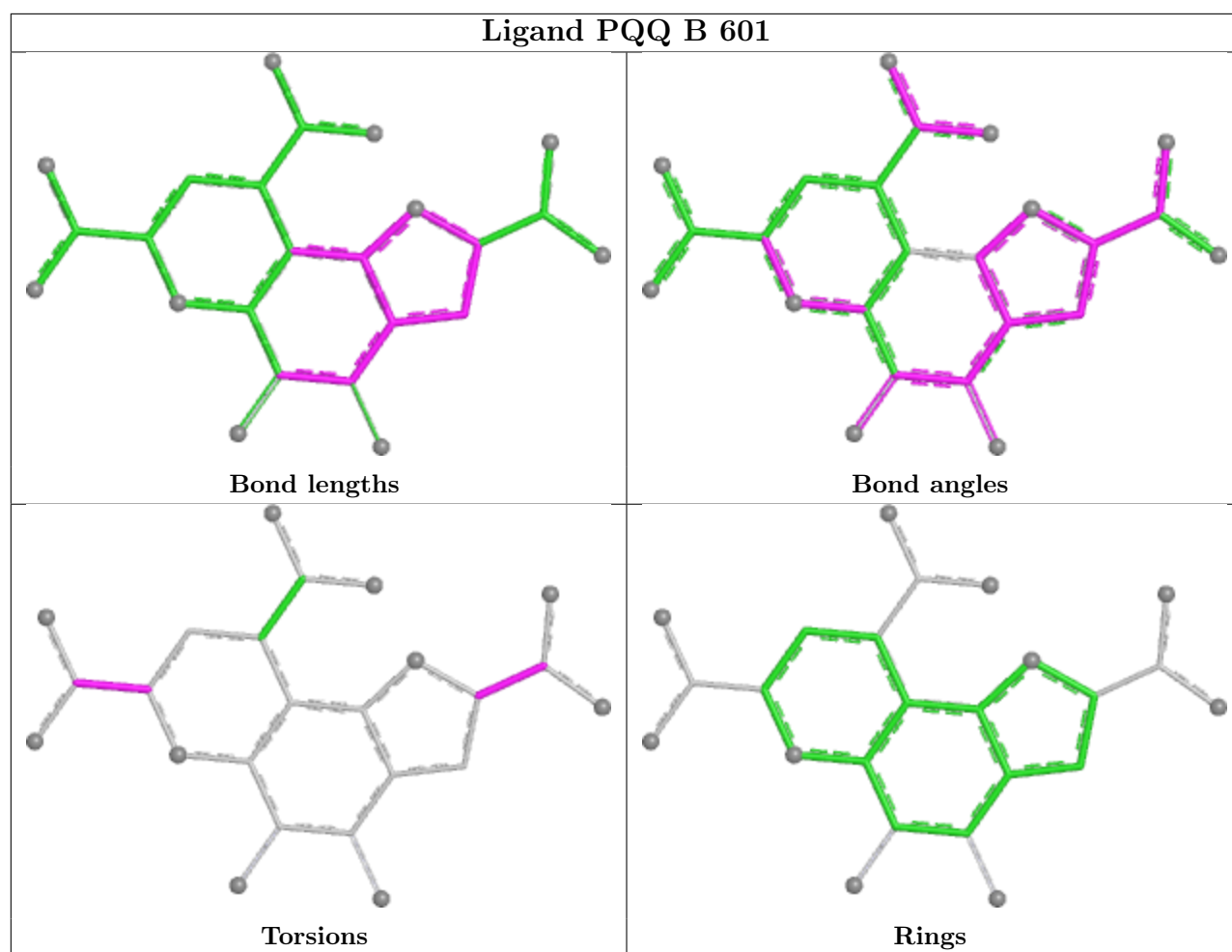
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	PQQ	N1-C2-C2X-O2B
2	B	601	PQQ	C3-C2-C2X-O2A
2	B	601	PQQ	C3-C2-C2X-O2B
2	B	601	PQQ	N1-C2-C2X-O2A
2	B	601	PQQ	N6-C7-C7X-O7B
2	B	601	PQQ	N6-C7-C7X-O7A
2	B	601	PQQ	C8-C7-C7X-O7B

There are no ring outliers.

No monomer is involved in short contacts.

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	509/560 (90%)	0.22	56 (11%)	10 9	10, 25, 83, 125	0
1	B	514/560 (91%)	0.68	84 (16%)	4 4	9, 39, 94, 137	0
All	All	1023/1120 (91%)	0.45	140 (13%)	6 5	9, 30, 89, 137	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	THR	8.5
1	A	102	SER	6.9
1	B	213	TRP	6.3
1	B	176	PHE	6.1
1	B	277	ARG	6.0
1	B	146	ASP	6.0
1	A	0	ALA	5.9
1	A	426	SER	5.6
1	A	98	ALA	5.5
1	B	311	ALA	5.3
1	A	2	THR	5.3
1	A	216	GLY	5.2
1	B	175	CYS	5.2
1	B	194	ILE	5.2
1	A	237	VAL	5.1
1	A	217	ALA	4.8
1	A	167	THR	4.8
1	A	108	ARG	4.8
1	A	95	PRO	4.7
1	B	174	GLY	4.7
1	A	107	THR	4.7
1	A	375	TYR	4.7
1	A	424	ASN	4.7
1	B	419	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	373	VAL	4.6
1	A	146	ASP	4.5
1	B	358	GLY	4.5
1	A	213	TRP	4.4
1	A	144	GLN	4.4
1	A	555	GLN	4.4
1	B	370	GLU	4.3
1	B	143	GLY	4.3
1	A	236	ALA	4.1
1	A	212	ARG	4.1
1	B	418	THR	4.1
1	B	192	TYR	4.1
1	A	197	ALA	4.0
1	A	103	PHE	4.0
1	B	-2	GLN	3.9
1	A	174	GLY	3.9
1	A	100	LEU	3.9
1	A	109	GLY	3.9
1	B	99	THR	3.9
1	B	359	ILE	3.9
1	A	1	GLN	3.8
1	B	307	ILE	3.8
1	B	360	VAL	3.8
1	B	254	GLY	3.8
1	B	193	PHE	3.7
1	B	299	THR	3.7
1	A	215	THR	3.7
1	B	309	PRO	3.6
1	B	310	ASN	3.6
1	B	216	GLY	3.6
1	A	175	CYS	3.5
1	A	214	MET	3.5
1	A	410	MET	3.5
1	A	-4	TYR	3.5
1	A	97	ILE	3.5
1	B	97	ILE	3.5
1	A	99	THR	3.4
1	B	425	THR	3.4
1	A	145	GLY	3.3
1	B	536	GLY	3.3
1	A	252	LEU	3.3
1	B	144	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	411	MET	3.3
1	B	354	ILE	3.2
1	A	94	LEU	3.1
1	B	186	GLU	3.1
1	B	103	PHE	3.1
1	B	95	PRO	3.1
1	A	253	TYR	3.1
1	A	427	ASN	3.1
1	A	367	ILE	3.1
1	A	151	ASN	3.0
1	B	187	GLU	3.0
1	B	312	ALA	3.0
1	B	7	GLU	3.0
1	B	96	ASN	3.0
1	A	408	TYR	2.9
1	A	409	ASP	2.9
1	B	292	ASN	2.9
1	B	264	ASP	2.9
1	B	217	ALA	2.9
1	A	277	ARG	2.8
1	B	98	ALA	2.8
1	B	183	ALA	2.8
1	B	371	LEU	2.8
1	B	255	THR	2.8
1	A	376	ASP	2.8
1	B	293	VAL	2.8
1	B	149	VAL	2.7
1	B	433	PRO	2.7
1	B	-1	SER	2.7
1	B	102	SER	2.7
1	B	383	GLY	2.7
1	A	374	GLU	2.7
1	B	167	THR	2.7
1	B	259	PHE	2.7
1	B	263	PRO	2.7
1	B	280	TRP	2.6
1	B	448	THR	2.6
1	B	316	ARG	2.6
1	B	283	GLU	2.6
1	B	214	MET	2.6
1	A	425	THR	2.6
1	B	372	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	143	GLY	2.5
1	B	276	PRO	2.5
1	B	184	THR	2.5
1	B	341	TRP	2.5
1	B	365	ASP	2.4
1	B	188	LEU	2.4
1	B	332	PHE	2.4
1	B	366	ALA	2.4
1	B	374	GLU	2.4
1	B	294	ASP	2.4
1	B	369	LYS	2.4
1	B	257	THR	2.3
1	B	270	TRP	2.3
1	B	177	VAL	2.3
1	A	148	ARG	2.3
1	A	152	SER	2.3
1	A	37	THR	2.2
1	A	122	TRP	2.2
1	B	330	TRP	2.2
1	A	149	VAL	2.2
1	B	147	GLU	2.2
1	A	428	VAL	2.2
1	B	295	VAL	2.2
1	A	105	GLU	2.1
1	B	281	ASP	2.1
1	B	381	PHE	2.1
1	B	189	TRP	2.1
1	B	180	HIS	2.1
1	A	364	GLU	2.1
1	B	222	THR	2.0
1	B	296	GLN	2.0
1	B	450	ARG	2.0

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 ⓘ

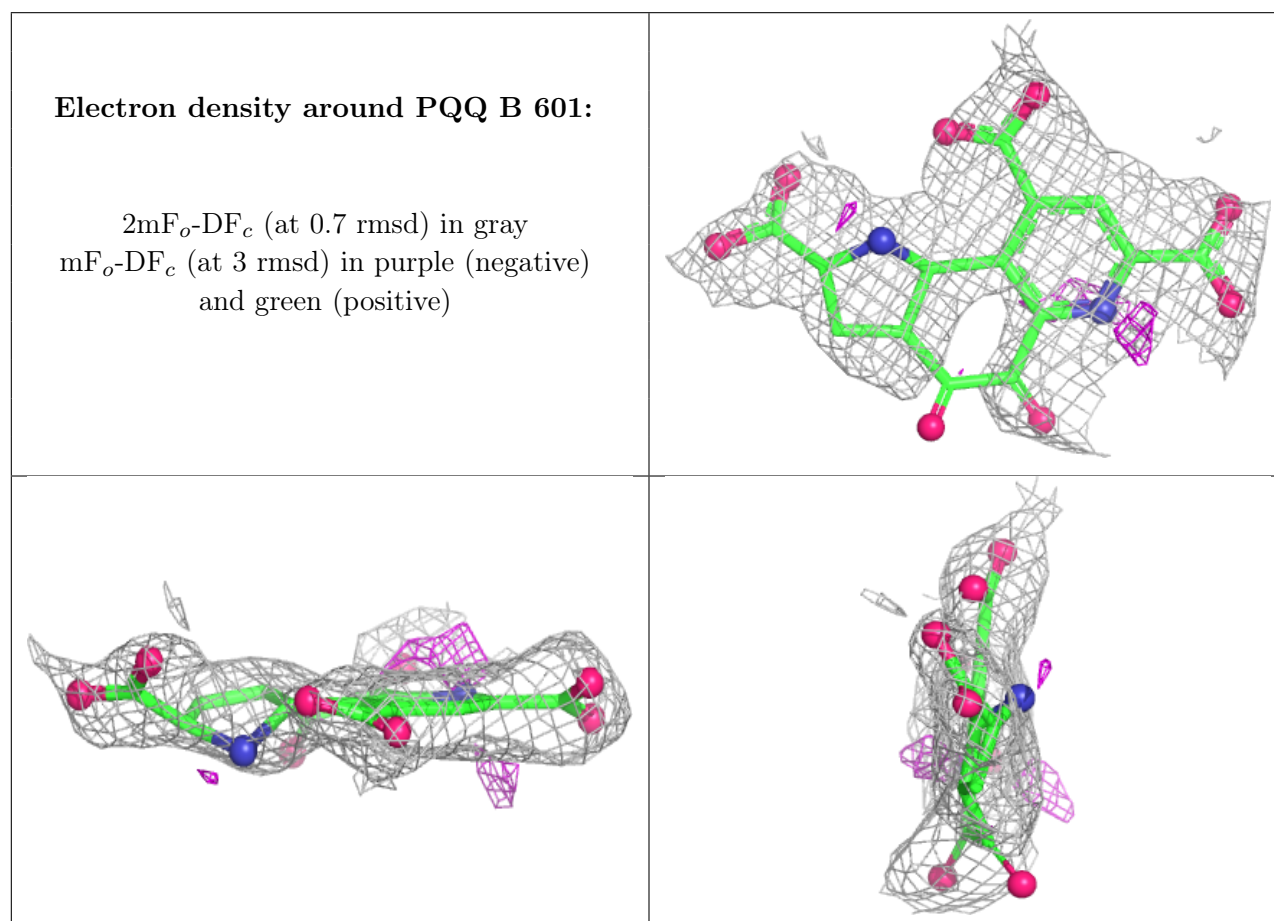
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	CA	B	602	1/1	0.71	0.18	107,107,107,107	0
2	PQQ	B	601	24/24	0.76	0.18	62,77,86,86	0

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.