



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 AM UTC

PDB ID : 4NY7 / pdb_00004ny7
Title : Bond length analysis of the PqqC Y175F mutant structure shows evidence for bound PQQ in the reduced form
Authors : Fisher, S.J.; Puehringer, S.
Deposited on : 2013-12-10
Resolution : 1.44 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

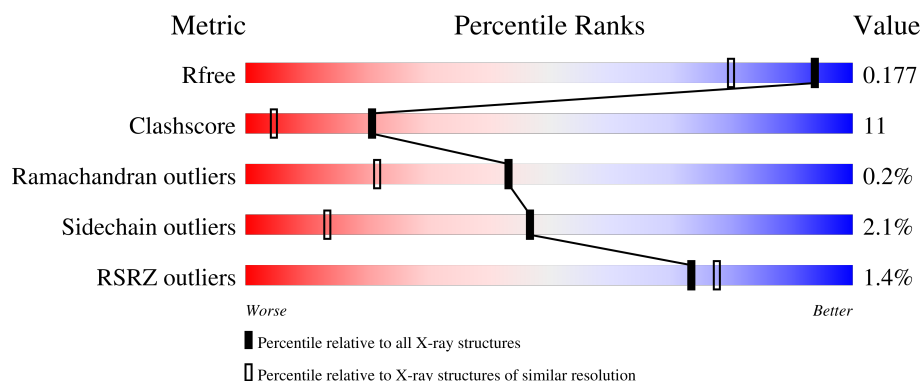
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.44 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	258	2% 72% 22% ...
1	B	258	% 77% 18% ...

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
3	GOL	A	302	-	-	X	-
3	GOL	A	303	-	-	X	-
3	GOL	A	306	-	X	X	-
3	GOL	A	307	-	X	X	-
3	GOL	B	303	-	X	X	-
3	GOL	B	305	-	X	X	-
3	GOL	B	306	-	X	-	-
3	GOL	B	307	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5137 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.

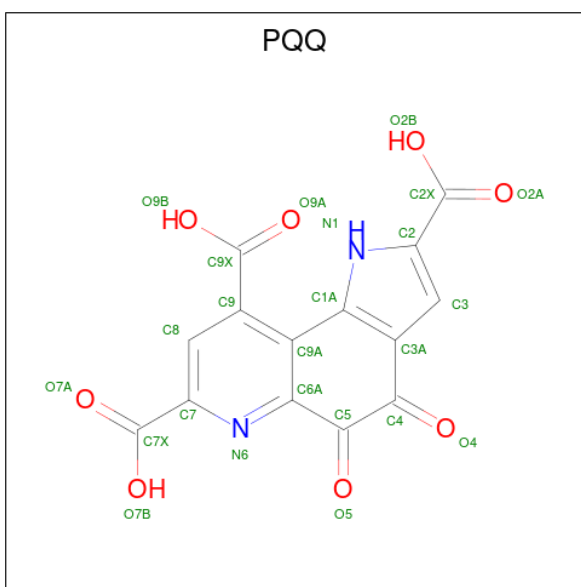
- Molecule 1 is a protein called Pyrroloquinoline-quinone synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	19	0
			2195	1396	398	388	13			
1	B	254	Total	C	N	O	S	0	30	0
			2264	1437	407	406	14			

There are 16 discrepancies between the modelled and reference sequences:

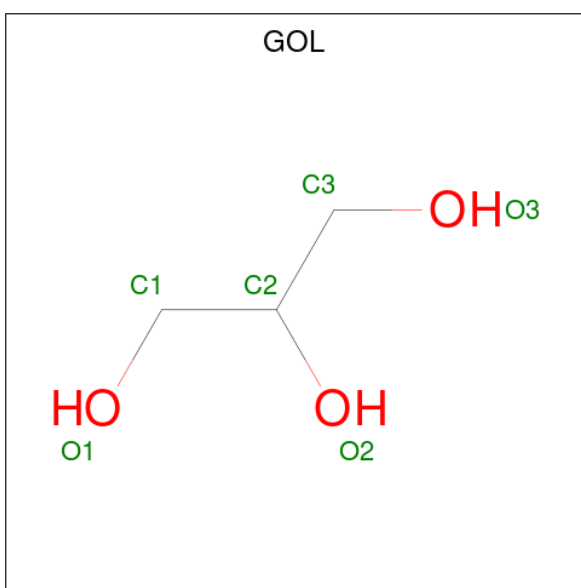
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	PHE	TYR	engineered mutation	UNP A6T9H1
A	252	LEU	-	expression tag	UNP A6T9H1
A	253	GLU	-	expression tag	UNP A6T9H1
A	254	HIS	-	expression tag	UNP A6T9H1
A	255	HIS	-	expression tag	UNP A6T9H1
A	256	HIS	-	expression tag	UNP A6T9H1
A	257	HIS	-	expression tag	UNP A6T9H1
A	258	HIS	-	expression tag	UNP A6T9H1
B	175	PHE	TYR	engineered mutation	UNP A6T9H1
B	252	LEU	-	expression tag	UNP A6T9H1
B	253	GLU	-	expression tag	UNP A6T9H1
B	254	HIS	-	expression tag	UNP A6T9H1
B	255	HIS	-	expression tag	UNP A6T9H1
B	256	HIS	-	expression tag	UNP A6T9H1
B	257	HIS	-	expression tag	UNP A6T9H1
B	258	HIS	-	expression tag	UNP A6T9H1

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



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

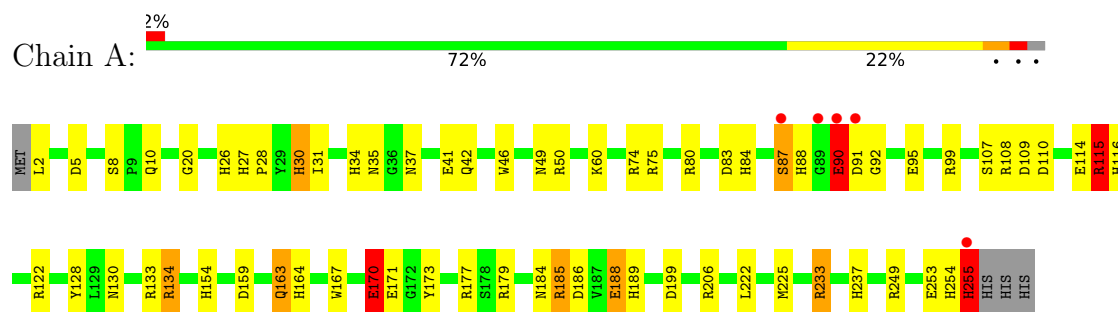
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	280	Total O 280 280	0	0
5	B	288	Total O 288 288	0	0

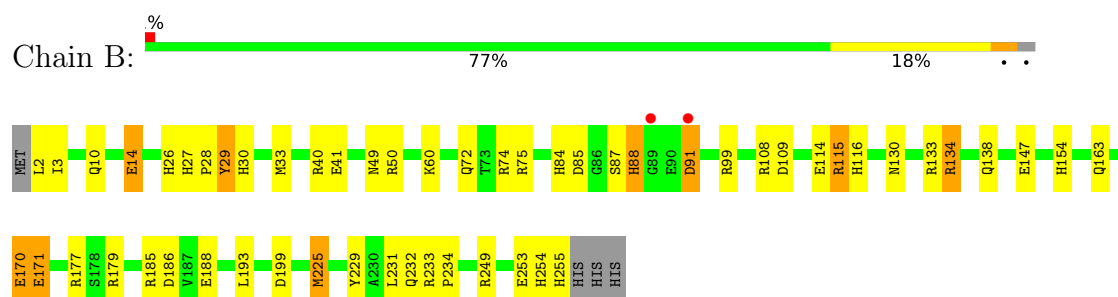
3 Residue-property plots

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: Pyrroloquinoline-quinone synthase



• Molecule 1: Pyrroloquinoline-quinone synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.00Å 116.02Å 67.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.44 10.00 – 1.44	Depositor EDS
% Data completeness (in resolution range)	97.8 (10.00-1.44) 97.9 (10.00-1.44)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.44Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.125 , 0.182 0.133 , 0.177	Depositor DCC
R_{free} test set	4998 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5137	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 6.57% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	2.06	64/2299 (2.8%)	2.01	62/3116 (2.0%)
1	B	2.13	47/2376 (2.0%)	1.91	40/3219 (1.2%)
All	All	2.09	111/4675 (2.4%)	1.96	102/6335 (1.6%)

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

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	GLU	CD-OE2	32.93	1.88	1.25
1	A	115	ARG	CZ-NH1	32.90	1.78	1.32
1	B	115	ARG	CZ-NH2	30.21	1.72	1.33
1	A	115	ARG	NE-CZ	-29.86	1.00	1.33
1	B	115	ARG	NE-CZ	-26.33	1.04	1.33
1	B	134[A]	ARG	CZ-NH1	-25.44	0.97	1.32
1	B	134[B]	ARG	CZ-NH1	-25.44	0.97	1.32
1	A	30[A]	HIS	CE1-NE2	-22.23	1.10	1.32
1	A	30[B]	HIS	CE1-NE2	-22.23	1.10	1.32
1	B	254	HIS	ND1-CE1	-21.06	1.11	1.32
1	B	254	HIS	CE1-NE2	18.91	1.51	1.32
1	A	185[A]	ARG	CZ-NH1	18.49	1.58	1.32
1	A	185[B]	ARG	CZ-NH1	18.49	1.58	1.32
1	B	30	HIS	CE1-NE2	-17.96	1.14	1.32
1	B	14	GLU	CD-OE2	17.79	1.59	1.25
1	A	171	GLU	CD-OE2	17.60	1.58	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	HIS	CE1-NE2	17.24	1.49	1.32
1	B	177	ARG	CZ-NH2	17.23	1.55	1.33
1	B	171	GLU	CD-OE1	-17.19	0.92	1.25
1	A	171	GLU	CD-OE1	-15.26	0.96	1.25
1	B	177	ARG	CZ-NH1	-14.52	1.12	1.32
1	B	116	HIS	CE1-NE2	14.40	1.47	1.32
1	A	75	ARG	CZ-NH1	13.76	1.52	1.32
1	B	255	HIS	CE1-NE2	13.53	1.46	1.32
1	A	30[A]	HIS	CD2-NE2	13.44	1.52	1.37
1	A	30[B]	HIS	CD2-NE2	13.44	1.52	1.37
1	B	134[A]	ARG	NE-CZ	13.03	1.47	1.33
1	B	134[B]	ARG	NE-CZ	13.03	1.47	1.33
1	A	255	HIS	ND1-CE1	-12.83	1.19	1.32
1	B	108	ARG	CZ-NH1	12.26	1.50	1.32
1	A	185[A]	ARG	NE-CZ	-11.44	1.20	1.33
1	A	185[B]	ARG	NE-CZ	-11.44	1.20	1.33
1	A	88	HIS	CE1-NE2	-10.98	1.21	1.32
1	A	75	ARG	NE-CZ	-10.89	1.21	1.33
1	A	116	HIS	CE1-NE2	-10.23	1.22	1.32
1	A	249	ARG	CZ-NH1	-9.93	1.18	1.32
1	B	108	ARG	NE-CZ	-9.86	1.22	1.33
1	B	116	HIS	CD2-NE2	-9.56	1.27	1.37
1	A	88	HIS	CD2-NE2	9.49	1.48	1.37
1	B	50	ARG	CZ-NH1	9.41	1.46	1.32
1	B	255	HIS	ND1-CE1	-9.29	1.23	1.32
1	A	109[A]	ASP	CG-OD1	-9.21	1.07	1.25
1	A	109[B]	ASP	CG-OD1	-9.21	1.07	1.25
1	B	154	HIS	CD2-NE2	-9.19	1.27	1.37
1	A	164	HIS	CE1-NE2	9.10	1.41	1.32
1	B	14	GLU	CD-OE1	-9.09	1.08	1.25
1	B	116	HIS	ND1-CE1	-8.95	1.23	1.32
1	B	27	HIS	CG-ND1	-8.91	1.28	1.38
1	B	154	HIS	CE1-NE2	8.83	1.41	1.32
1	A	254	HIS	CE1-NE2	8.79	1.41	1.32
1	A	199	ASP	CG-OD1	-8.70	1.08	1.25
1	B	114	GLU	CD-OE2	8.60	1.41	1.25
1	B	50	ARG	NE-CZ	-8.12	1.24	1.33
1	A	133	ARG	NE-CZ	8.10	1.42	1.33
1	A	254	HIS	ND1-CE1	-8.08	1.24	1.32
1	A	90	GLU	CD-OE2	8.00	1.40	1.25
1	A	5	ASP	CG-OD2	7.89	1.40	1.25
1	B	75	ARG	NE-CZ	-7.79	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	ARG	NE-CZ	7.65	1.41	1.33
1	A	206	ARG	CZ-NH1	7.62	1.43	1.32
1	A	109[A]	ASP	CG-OD2	-7.62	1.10	1.25
1	A	109[B]	ASP	CG-OD2	-7.62	1.10	1.25
1	B	134[A]	ARG	CZ-NH2	-7.56	1.23	1.33
1	B	134[B]	ARG	CZ-NH2	-7.56	1.23	1.33
1	A	237	HIS	ND1-CE1	7.47	1.40	1.32
1	A	26	HIS	CE1-NE2	7.43	1.40	1.32
1	A	27	HIS	CG-ND1	-7.43	1.30	1.38
1	A	206	ARG	NE-CZ	-7.31	1.25	1.33
1	A	95	GLU	CD-OE1	7.15	1.39	1.25
1	A	27	HIS	CE1-NE2	7.13	1.39	1.32
1	A	199	ASP	CG-OD2	7.06	1.38	1.25
1	A	84	HIS	ND1-CE1	7.05	1.39	1.32
1	B	109	ASP	CG-OD1	7.01	1.38	1.25
1	A	154	HIS	CE1-NE2	6.79	1.39	1.32
1	A	88	HIS	ND1-CE1	6.46	1.39	1.32
1	B	75	ARG	CZ-NH2	6.29	1.41	1.33
1	A	91[A]	ASP	CG-OD2	6.11	1.36	1.25
1	A	91[B]	ASP	CG-OD2	6.11	1.36	1.25
1	B	41	GLU	CD-OE1	6.05	1.36	1.25
1	A	90	GLU	CD-OE1	-5.89	1.14	1.25
1	B	199	ASP	CG-OD1	-5.77	1.14	1.25
1	A	30[A]	HIS	ND1-CE1	5.74	1.38	1.32
1	A	30[B]	HIS	ND1-CE1	5.74	1.38	1.32
1	A	134[A]	ARG	CZ-NH1	-5.70	1.24	1.32
1	A	134[B]	ARG	CZ-NH1	-5.70	1.24	1.32
1	A	50	ARG	NE-CZ	-5.67	1.26	1.33
1	B	26	HIS	CG-ND1	-5.61	1.32	1.38
1	B	199	ASP	CG-OD2	5.59	1.35	1.25
1	A	154	HIS	CD2-NE2	-5.53	1.31	1.37
1	A	164	HIS	ND1-CE1	-5.51	1.27	1.32
1	A	159	ASP	CG-OD2	5.49	1.35	1.25
1	B	84	HIS	CD2-NE2	5.46	1.43	1.37
1	B	170[A]	GLU	CD-OE1	5.42	1.35	1.25
1	B	170[B]	GLU	CD-OE1	5.42	1.35	1.25
1	B	75	ARG	CZ-NH1	5.42	1.40	1.32
1	A	114	GLU	CD-OE1	-5.40	1.15	1.25
1	A	91[A]	ASP	CG-OD1	-5.30	1.15	1.25
1	A	91[B]	ASP	CG-OD1	-5.30	1.15	1.25
1	B	74	ARG	NE-CZ	5.29	1.38	1.33
1	B	85	ASP	CG-OD2	5.28	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	GLU	CD-OE1	-5.28	1.15	1.25
1	A	26	HIS	CD2-NE2	-5.27	1.32	1.37
1	A	249	ARG	NE-CZ	5.27	1.38	1.33
1	B	179	ARG	CZ-NH1	5.26	1.40	1.32
1	A	114	GLU	CD-OE2	5.25	1.35	1.25
1	A	253	GLU	CD-OE2	5.22	1.35	1.25
1	A	99	ARG	CZ-NH2	5.16	1.40	1.33
1	A	108	ARG	CZ-NH2	5.15	1.40	1.33
1	B	109	ASP	CG-OD2	-5.11	1.15	1.25
1	A	189	HIS	ND1-CE1	5.11	1.37	1.32
1	A	34	HIS	CE1-NE2	5.10	1.37	1.32

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	CD-NE-CZ	36.38	175.33	124.40
1	A	115	ARG	NE-CZ-NH2	35.93	151.53	119.20
1	B	115	ARG	CD-NE-CZ	33.39	171.15	124.40
1	B	171	GLU	CG-CD-OE1	24.07	173.76	118.40
1	B	134[A]	ARG	NE-CZ-NH2	-22.86	98.63	119.20
1	B	134[B]	ARG	NE-CZ-NH2	-22.86	98.63	119.20
1	A	185[A]	ARG	NE-CZ-NH2	22.46	139.42	119.20
1	A	185[B]	ARG	NE-CZ-NH2	22.46	139.42	119.20
1	B	115	ARG	NE-CZ-NH1	19.23	140.73	121.50
1	B	134[A]	ARG	NE-CZ-NH1	-18.91	102.59	121.50
1	B	134[B]	ARG	NE-CZ-NH1	-18.91	102.59	121.50
1	A	75	ARG	NE-CZ-NH2	17.91	135.32	119.20
1	B	177	ARG	NE-CZ-NH2	-16.63	104.23	119.20
1	A	115	ARG	NH1-CZ-NH2	-16.32	98.08	119.30
1	B	115	ARG	NH1-CZ-NH2	-14.84	100.01	119.30
1	B	177	ARG	NE-CZ-NH1	14.21	135.72	121.50
1	B	171	GLU	CG-CD-OE2	-13.18	88.08	118.40
1	B	108	ARG	NE-CZ-NH2	13.08	130.97	119.20
1	A	28	PRO	CA-C-N	12.52	137.45	120.54
1	A	28	PRO	C-N-CA	12.52	137.45	120.54
1	A	28	PRO	O-C-N	-11.12	109.45	122.24
1	A	115	ARG	NE-CZ-NH1	-11.12	110.38	121.50
1	B	28	PRO	CA-C-N	10.95	135.32	120.54
1	B	28	PRO	C-N-CA	10.95	135.32	120.54
1	B	14	GLU	CG-CD-OE1	10.40	142.33	118.40
1	A	41	GLU	CA-C-N	10.40	135.06	120.29
1	A	41	GLU	C-N-CA	10.40	135.06	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	GLU	OE1-CD-OE2	-10.31	98.16	122.90
1	A	27	HIS	ND1-CE1-NE2	-10.26	98.14	108.40
1	A	185[A]	ARG	CD-NE-CZ	10.25	138.75	124.40
1	A	185[B]	ARG	CD-NE-CZ	10.25	138.75	124.40
1	B	28	PRO	O-C-N	-10.23	110.48	122.24
1	A	171	GLU	CG-CD-OE1	10.00	141.40	118.40
1	A	10	GLN	CA-C-N	9.31	132.76	120.28
1	A	10	GLN	C-N-CA	9.31	132.76	120.28
1	A	27	HIS	CG-ND1-CE1	9.10	124.76	109.30
1	B	41	GLU	O-C-N	-9.08	112.50	122.12
1	B	41	GLU	CA-C-N	8.92	132.96	120.29
1	B	41	GLU	C-N-CA	8.92	132.96	120.29
1	A	185[A]	ARG	NE-CZ-NH1	-8.82	112.68	121.50
1	A	185[B]	ARG	NE-CZ-NH1	-8.82	112.68	121.50
1	A	185[A]	ARG	NH1-CZ-NH2	-8.64	108.07	119.30
1	A	185[B]	ARG	NH1-CZ-NH2	-8.64	108.07	119.30
1	A	249	ARG	NE-CZ-NH2	-8.62	111.44	119.20
1	A	41	GLU	O-C-N	-8.60	113.00	122.12
1	A	75	ARG	CD-NE-CZ	8.51	136.31	124.40
1	A	91[A]	ASP	CA-C-N	8.51	136.42	122.21
1	A	91[A]	ASP	C-N-CA	8.51	136.42	122.21
1	A	91[B]	ASP	CA-C-N	8.51	136.42	122.21
1	A	91[B]	ASP	C-N-CA	8.51	136.42	122.21
1	B	27	HIS	ND1-CE1-NE2	-8.42	99.98	108.40
1	A	75	ARG	NH1-CZ-NH2	-8.17	108.68	119.30
1	A	27	HIS	ND1-CG-CD2	-7.99	98.11	106.10
1	A	170	GLU	CB-CG-CD	7.96	126.14	112.60
1	A	171	GLU	CG-CD-OE2	-7.92	100.18	118.40
1	B	75	ARG	NE-CZ-NH2	7.41	125.86	119.20
1	A	206	ARG	NE-CZ-NH2	7.37	125.84	119.20
1	A	163	GLN	CA-C-O	7.01	127.85	120.42
1	B	49	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	B	254	HIS	CE1-NE2-CD2	-6.93	102.07	109.00
1	A	179	ARG	NE-CZ-NH2	6.88	125.39	119.20
1	A	249	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	B	27	HIS	CG-ND1-CE1	6.65	120.61	109.30
1	A	10	GLN	O-C-N	-6.56	114.67	122.15
1	A	88	HIS	CA-CB-CG	6.42	120.22	113.80
1	A	92	GLY	O-C-N	-6.37	118.05	123.59
1	B	49	ASN	CB-CG-OD1	6.17	133.15	120.80
1	A	74	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	A	134[A]	ARG	NE-CZ-NH2	-6.12	113.70	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134[B]	ARG	NE-CZ-NH2	-6.12	113.70	119.20
1	A	99	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	B	84	HIS	CA-CB-CG	-5.94	107.86	113.80
1	A	199	ASP	CA-CB-CG	-5.75	106.85	112.60
1	B	114	GLU	CG-CD-OE1	5.74	131.60	118.40
1	B	108	ARG	NH1-CZ-NH2	-5.62	112.00	119.30
1	A	42	GLN	N-CA-C	-5.60	105.25	111.36
1	A	83	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	109[A]	ASP	CB-CG-OD2	5.52	131.09	118.40
1	A	109[B]	ASP	CB-CG-OD2	5.52	131.09	118.40
1	B	249	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	A	75	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	A	206	ARG	CD-NE-CZ	5.46	132.04	124.40
1	A	30[A]	HIS	CG-CD2-NE2	-5.38	101.82	107.20
1	A	30[B]	HIS	CG-CD2-NE2	-5.38	101.82	107.20
1	A	133	ARG	NE-CZ-NH2	-5.35	114.38	119.20
1	A	122	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	A	37	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	114	GLU	O-C-N	-5.30	114.61	122.04
1	B	14	GLU	CG-CD-OE2	-5.30	106.22	118.40
1	B	29	TYR	CA-C-O	-5.28	115.25	120.90
1	B	49	ASN	CA-CB-CG	-5.28	107.32	112.60
1	A	49	ASN	CB-CG-OD1	5.27	131.35	120.80
1	B	75	ARG	NH1-CZ-NH2	-5.26	112.46	119.30
1	B	134[A]	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	B	134[B]	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	A	233	ARG	CD-NE-CZ	5.19	131.66	124.40
1	B	40	ARG	NE-CZ-NH2	-5.17	114.54	119.20
1	B	27	HIS	ND1-CG-CD2	-5.10	101.00	106.10
1	A	99	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	B	75	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	90	GLU	CG-CD-OE1	5.05	130.01	118.40
1	B	60	LYS	CA-CB-CG	5.03	124.15	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	GLU	Peptide

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	2195	0	2139	32	0
1	B	2264	0	2208	46	0
2	A	24	0	4	0	0
2	B	24	0	3	0	0
3	A	30	0	40	18	0
3	B	30	0	40	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	280	0	0	14	0
5	B	288	0	0	12	0
All	All	5137	0	4434	100	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 11.

All (100) 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:185[A]:ARG:NH1	1:A:185[A]:ARG:CZ	1.69	1.55
1:B:115:ARG:CZ	1:B:115:ARG:NH2	1.72	1.50
1:A:115:ARG:CZ	1:A:115:ARG:NH1	1.78	1.46
1:B:134[B]:ARG:NH1	1:B:134[B]:ARG:CZ	1.83	1.39
1:B:253[B]:GLU:OE1	1:B:253[B]:GLU:CD	1.74	1.30
1:B:188[A]:GLU:CD	1:B:188[A]:GLU:OE2	1.80	1.23
1:B:170[B]:GLU:CD	1:B:170[B]:GLU:OE2	1.81	1.22
1:B:171:GLU:OE2	1:B:171:GLU:CD	1.87	1.16
3:B:305:GOL:C1	3:B:305:GOL:C2	2.39	1.00
3:A:306:GOL:C2	3:A:306:GOL:C3	2.41	0.99
3:B:305:GOL:C1	3:B:305:GOL:O1	2.11	0.99
3:B:306:GOL:C1	3:B:306:GOL:C2	2.40	0.99
3:A:306:GOL:C2	3:A:306:GOL:O2	2.11	0.99
3:A:307:GOL:C2	3:A:307:GOL:O2	2.11	0.99
3:B:307:GOL:C2	3:B:307:GOL:C3	2.41	0.98
3:B:303:GOL:C1	3:B:303:GOL:O1	2.11	0.98
3:B:306:GOL:C1	3:B:306:GOL:O1	2.11	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:302:GOL:C2	3:B:302:GOL:C3	2.41	0.97
3:A:307:GOL:O1	3:A:307:GOL:C1	2.12	0.97
3:B:307:GOL:C2	3:B:307:GOL:O2	2.12	0.97
3:A:302:GOL:O3	3:A:302:GOL:C3	2.12	0.96
3:B:305:GOL:C2	3:B:305:GOL:O2	2.13	0.95
1:B:138:GLN:HE22	3:B:306:GOL:H32	1.37	0.90
5:A:606:HOH:O	3:B:303:GOL:H11	1.86	0.76
1:B:134[B]:ARG:NH1	1:B:134[B]:ARG:NE	2.31	0.75
1:B:170[B]:GLU:OE2	1:B:170[B]:GLU:CG	2.36	0.73
5:A:654:HOH:O	1:B:130[B]:ASN:HB3	1.88	0.73
1:B:115:ARG:NH2	1:B:115:ARG:NH1	2.37	0.73
1:B:253[B]:GLU:OE1	1:B:253[B]:GLU:CG	2.37	0.72
1:A:185[A]:ARG:NH1	1:A:185[A]:ARG:NH2	2.36	0.72
1:B:134[B]:ARG:NH1	1:B:134[B]:ARG:NH2	2.36	0.71
1:B:171:GLU:OE2	1:B:171:GLU:CG	2.37	0.71
5:A:654:HOH:O	1:B:130[A]:ASN:HB3	1.91	0.71
1:A:115:ARG:NH1	1:A:115:ARG:NH2	2.39	0.69
1:B:233:ARG:HH22	3:B:303:GOL:H12	1.56	0.69
1:A:185[A]:ARG:NH1	1:A:185[A]:ARG:NE	2.31	0.68
1:A:233:ARG:HH22	3:A:303:GOL:H12	1.59	0.68
1:B:188[A]:GLU:OE2	1:B:188[A]:GLU:CG	2.42	0.67
3:A:303:GOL:H11	5:A:661:HOH:O	1.95	0.66
3:A:306:GOL:H2	5:A:452:HOH:O	1.96	0.66
1:A:115:ARG:NH1	1:A:115:ARG:NE	2.33	0.65
1:B:233:ARG:NH2	3:B:303:GOL:H12	2.13	0.63
1:A:8:SER:HA	3:A:307:GOL:H31	1.81	0.63
1:A:46:TRP:HA	1:A:225[A]:MET:SD	2.40	0.62
1:A:233:ARG:NH2	3:A:303:GOL:H12	2.17	0.59
1:B:133[B]:ARG:NH2	3:B:305:GOL:O1	2.35	0.58
1:B:171:GLU:OE2	1:B:171:GLU:HG3	2.03	0.58
1:B:170[B]:GLU:OE2	1:B:170[B]:GLU:HG3	2.03	0.57
1:B:234:PRO:CB	3:B:307:GOL:H12	2.35	0.57
1:A:60[A]:LYS:HE2	1:A:128:TYR:CZ	2.40	0.56
1:A:233:ARG:HD2	5:A:566:HOH:O	2.06	0.56
3:B:307:GOL:H31	5:B:537:HOH:O	2.05	0.55
1:B:170[B]:GLU:CD	1:B:170[B]:GLU:H	2.14	0.53
3:A:306:GOL:H12	5:A:677:HOH:O	2.10	0.52
1:B:253[B]:GLU:OE1	1:B:253[B]:GLU:HG3	2.10	0.51
1:A:186:ASP:HA	3:A:302:GOL:H2	1.93	0.51
1:B:234:PRO:HB3	3:B:307:GOL:H12	1.93	0.51
1:A:170:GLU:H	1:A:170:GLU:CD	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87[B]:SER:O	1:A:90:GLU:OE1	2.29	0.50
1:B:87[B]:SER:O	1:B:91[B]:ASP:OD2	2.30	0.50
1:B:193[A]:LEU:HD21	5:B:483:HOH:O	2.11	0.50
5:A:606:HOH:O	3:B:303:GOL:H31	2.10	0.50
1:B:115:ARG:NH2	1:B:115:ARG:HE	2.05	0.50
1:A:80:ARG:HG3	3:A:302:GOL:H32	1.92	0.49
1:B:163[B]:GLN:HB3	5:B:617:HOH:O	2.11	0.49
1:A:87[A]:SER:O	1:A:90:GLU:OE1	2.30	0.49
3:B:307:GOL:O2	3:B:307:GOL:O3	2.29	0.49
1:B:231:LEU:O	1:B:232[A]:GLN:HB2	2.13	0.48
1:A:184:ASN:O	1:A:188[B]:GLU:HG3	2.15	0.47
1:A:233:ARG:HH12	3:A:303:GOL:C1	2.28	0.47
1:B:185[B]:ARG:NH1	5:B:621:HOH:O	2.49	0.46
1:B:134[B]:ARG:NH2	5:B:661:HOH:O	2.49	0.46
1:B:10[A]:GLN:HG3	5:B:667:HOH:O	2.15	0.45
1:B:29:TYR:O	1:B:33[A]:MET:HG3	2.17	0.45
1:A:31:ILE:O	1:A:35[B]:ASN:ND2	2.49	0.45
1:A:134[A]:ARG:NH1	5:A:673:HOH:O	2.49	0.45
3:A:305:GOL:H12	5:A:501:HOH:O	2.16	0.45
1:A:130[A]:ASN:ND2	5:A:488:HOH:O	2.48	0.44
1:A:173:TYR:O	1:A:177[B]:ARG:HG3	2.18	0.44
1:B:88[B]:HIS:N	5:B:605:HOH:O	2.49	0.44
1:B:91[B]:ASP:HB3	5:B:608:HOH:O	2.17	0.44
1:B:225[A]:MET:HB3	1:B:229:TYR:CE2	2.53	0.44
1:A:8:SER:CB	3:A:307:GOL:H31	2.48	0.43
1:A:255:HIS:HB2	5:A:549:HOH:O	2.18	0.43
3:A:302:GOL:O3	3:A:302:GOL:O1	2.29	0.43
1:B:233:ARG:HH22	3:B:303:GOL:C1	2.29	0.43
1:B:72:GLN:NE2	5:B:602:HOH:O	2.50	0.43
1:A:107:SER:O	1:A:110:ASP:HB2	2.19	0.43
1:A:134[B]:ARG:HD2	1:B:133[B]:ARG:CZ	2.49	0.43
1:A:30[B]:HIS:CE1	1:A:222:LEU:HD11	2.54	0.42
1:B:171:GLU:OE2	1:B:171:GLU:OE1	2.20	0.42
1:B:147:GLU:OE2	1:B:186:ASP:OD2	2.37	0.42
1:B:233:ARG:HD2	5:B:582:HOH:O	2.20	0.42
1:B:2:LEU:HD23	1:B:3:ILE:O	2.20	0.42
1:A:35[B]:ASN:ND2	5:A:467:HOH:O	2.48	0.41
1:A:130[B]:ASN:ND2	5:A:659:HOH:O	2.50	0.41
1:B:14:GLU:HG2	5:B:594:HOH:O	2.21	0.41
1:A:20:GLY:HA3	3:A:305:GOL:H12	2.02	0.41
1:A:167:TRP:CD1	1:A:167:TRP:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185[B]:ARG:HG3	5:B:628:HOH:O	2.22	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	271/258 (105%)	270 (100%)	1 (0%)	0	100	100
1	B	282/258 (109%)	280 (99%)	0	2 (1%)	18	4
All	All	553/516 (107%)	550 (100%)	1 (0%)	2 (0%)	43	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	88[A]	HIS
1	B	88[B]	HIS

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	231/217 (106%)	222 (96%)	9 (4%)	28	3
1	B	241/217 (111%)	237 (98%)	4 (2%)	53	20
All	All	472/434 (109%)	459 (97%)	13 (3%)	47	7

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	87[A]	SER
1	A	87[B]	SER
1	A	115	ARG
1	A	163	GLN
1	A	170	GLU
1	A	188[A]	GLU
1	A	188[B]	GLU
1	A	255	HIS
1	B	91[A]	ASP
1	B	91[B]	ASP
1	B	225[A]	MET
1	B	225[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	164	HIS
1	B	37	ASN

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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	GOL	A	303	-	5,5,5	0.27	0	5,5,5	0.53	0
3	GOL	B	305	-	5,5,5	16.70	3 (60%)	5,5,5	5.57	3 (60%)
2	PQQ	A	301	-	26,26,26	3.49	11 (42%)	34,40,40	3.29	23 (67%)
3	GOL	B	303	-	5,5,5	7.38	1 (20%)	5,5,5	1.69	1 (20%)
3	GOL	A	307	-	5,5,5	12.87	2 (40%)	5,5,5	2.63	3 (60%)
3	GOL	B	302	-	5,5,5	10.49	1 (20%)	5,5,5	3.69	3 (60%)
3	GOL	A	302	-	5,5,5	7.47	1 (20%)	5,5,5	1.78	1 (20%)
2	PQQ	B	301	-	26,26,26	4.53	15 (57%)	34,40,40	2.95	18 (52%)
3	GOL	B	307	-	5,5,5	14.92	2 (40%)	5,5,5	4.88	4 (80%)
3	GOL	A	306	-	5,5,5	14.81	2 (40%)	5,5,5	4.85	4 (80%)
3	GOL	B	306	-	5,5,5	12.78	2 (40%)	5,5,5	4.46	2 (40%)
3	GOL	A	305	-	5,5,5	0.21	0	5,5,5	0.87	0

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	GOL	A	303	-	-	0/4/4/4	-
3	GOL	B	305	-	-	3/4/4/4	-
2	PQQ	A	301	-	-	2/12/28/28	0/3/3/3
3	GOL	B	303	-	-	4/4/4/4	-
3	GOL	A	307	-	-	1/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	A	302	-	-	2/4/4/4	-
2	PQQ	B	301	-	-	2/12/28/28	0/3/3/3
3	GOL	B	307	-	-	1/4/4/4	-
3	GOL	A	306	-	-	2/4/4/4	-
3	GOL	B	306	-	-	2/4/4/4	-
3	GOL	A	305	-	-	3/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	305	GOL	O2-C2	24.28	2.13	1.43
3	B	307	GOL	O2-C2	23.67	2.12	1.43
3	A	307	GOL	O2-C2	23.52	2.11	1.43
3	B	307	GOL	C3-C2	23.51	2.41	1.51
3	B	302	GOL	C3-C2	23.46	2.41	1.51
3	A	306	GOL	C3-C2	23.43	2.41	1.51
3	A	306	GOL	O2-C2	23.39	2.11	1.43
3	B	306	GOL	C1-C2	23.31	2.40	1.51
3	B	305	GOL	C1-C2	23.12	2.39	1.51
3	A	302	GOL	O3-C3	16.71	2.12	1.42
3	A	307	GOL	O1-C1	16.58	2.12	1.42
3	B	306	GOL	O1-C1	16.53	2.11	1.42
3	B	303	GOL	O1-C1	16.50	2.11	1.42
3	B	305	GOL	O1-C1	16.42	2.11	1.42
2	B	301	PQQ	C5-C4	-15.69	1.32	1.54
2	A	301	PQQ	C9A-C1A	-9.39	1.34	1.46
2	B	301	PQQ	O5-C5	7.46	1.38	1.23
2	B	301	PQQ	C9A-C1A	-6.56	1.38	1.46
2	A	301	PQQ	O5-C5	6.55	1.36	1.23
2	A	301	PQQ	O4-C4	6.12	1.37	1.23
2	A	301	PQQ	C5-C4	-5.65	1.46	1.54
2	B	301	PQQ	C7-C7X	-5.55	1.40	1.50
2	A	301	PQQ	C2-C2X	-5.52	1.35	1.48
2	B	301	PQQ	C2-N1	5.50	1.47	1.37
2	B	301	PQQ	C9A-C6A	4.63	1.48	1.41
2	B	301	PQQ	C3A-C4	-4.51	1.33	1.46
2	B	301	PQQ	C8-C9	3.96	1.46	1.39
2	B	301	PQQ	O2A-C2X	3.84	1.32	1.22
2	A	301	PQQ	C9A-C6A	3.72	1.46	1.41
2	A	301	PQQ	O7A-C7X	3.49	1.32	1.22
2	A	301	PQQ	C7-C7X	-3.36	1.44	1.50
2	B	301	PQQ	O9A-C9X	3.32	1.32	1.22
2	A	301	PQQ	O2A-C2X	3.00	1.30	1.22
2	A	301	PQQ	C3A-C4	-2.98	1.37	1.46
2	B	301	PQQ	C7-N6	2.83	1.38	1.34
2	B	301	PQQ	O2B-C2X	-2.75	1.23	1.30
2	B	301	PQQ	C9-C9X	-2.39	1.44	1.49
2	B	301	PQQ	C6A-N6	2.34	1.39	1.34
2	B	301	PQQ	O4-C4	2.21	1.28	1.23
2	A	301	PQQ	O9B-C9X	2.19	1.37	1.30

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	PQQ	O5-C5-C6A	-8.91	111.57	121.76
3	B	305	GOL	O2-C2-C1	-8.68	73.24	109.18
3	B	307	GOL	O2-C2-C3	-8.64	73.42	109.18
3	A	306	GOL	O2-C2-C3	-8.63	73.46	109.18
3	B	306	GOL	O1-C1-C2	-8.10	73.92	110.38
3	B	305	GOL	O1-C1-C2	-8.06	74.09	110.38
2	A	301	PQQ	C3A-C3-C2	-7.34	100.39	107.94
2	B	301	PQQ	O5-C5-C4	7.19	127.52	118.14
2	A	301	PQQ	O2B-C2X-O2A	-7.06	107.10	123.90
2	A	301	PQQ	O5-C5-C4	5.87	125.80	118.14
3	B	302	GOL	O2-C2-C3	-5.60	85.99	109.18
3	B	302	GOL	O3-C3-C2	-5.49	85.68	110.38
3	B	306	GOL	O2-C2-C1	-5.38	86.89	109.18
3	B	307	GOL	O3-C3-C2	-5.33	86.38	110.38
3	A	306	GOL	O3-C3-C2	-5.23	86.84	110.38
2	A	301	PQQ	O2B-C2X-C2	5.07	125.21	114.27
2	A	301	PQQ	C3A-C4-C5	4.45	122.07	117.03
2	A	301	PQQ	C9-C8-C7	-4.45	116.28	119.93
2	B	301	PQQ	C3A-C4-C5	4.32	121.92	117.03
2	B	301	PQQ	O2B-C2X-C2	4.28	123.49	114.27
2	A	301	PQQ	C3-C2-N1	4.16	114.67	107.74
2	A	301	PQQ	C9A-C6A-N6	3.95	129.31	123.58
2	B	301	PQQ	C1A-N1-C2	-3.78	104.10	110.20
2	A	301	PQQ	C1A-C3A-C4	-3.73	119.19	122.33
3	B	305	GOL	O2-C2-C3	-3.65	94.08	109.18
2	A	301	PQQ	O7B-C7X-O7A	-3.58	115.66	123.35
3	A	307	GOL	O1-C1-C2	-3.41	95.04	110.38
2	A	301	PQQ	O9B-C9X-O9A	-3.36	116.13	123.35
3	B	307	GOL	O2-C2-C1	-3.35	95.30	109.18
3	A	302	GOL	O3-C3-C2	-3.34	95.34	110.38
3	A	307	GOL	O2-C2-C1	-3.34	95.36	109.18
3	A	307	GOL	O2-C2-C3	-3.32	95.42	109.18
2	B	301	PQQ	O4-C4-C5	-3.28	114.33	118.37
3	B	303	GOL	O1-C1-C2	-3.26	95.71	110.38
3	A	306	GOL	O2-C2-C1	-3.25	95.73	109.18
2	B	301	PQQ	O9A-C9X-C9	-3.23	114.25	121.97
2	A	301	PQQ	O7B-C7X-C7	3.21	122.32	114.71
2	B	301	PQQ	C9A-C6A-C5	-3.17	118.64	121.59
2	A	301	PQQ	O2A-C2X-C2	3.08	127.26	121.01
2	A	301	PQQ	O4-C4-C5	-3.06	114.59	118.37
2	B	301	PQQ	C3A-C1A-N1	3.03	111.22	107.23
2	B	301	PQQ	O9B-C9X-C9	2.90	123.53	115.28
2	B	301	PQQ	C1A-C3A-C4	-2.79	119.98	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	PQQ	C3-C3A-C1A	2.79	111.47	107.09
2	B	301	PQQ	C8-C7-C7X	2.59	125.35	119.61
2	A	301	PQQ	C8-C9-C9A	2.57	123.63	120.33
2	A	301	PQQ	O5-C5-C6A	-2.53	118.86	121.76
2	B	301	PQQ	C7X-C7-N6	-2.52	112.69	116.46
2	A	301	PQQ	C7X-C7-N6	-2.52	112.70	116.46
2	B	301	PQQ	O7B-C7X-O7A	-2.51	117.95	123.35
2	A	301	PQQ	C9A-C6A-C5	-2.30	119.45	121.59
2	B	301	PQQ	C3-C3A-C4	2.29	134.49	128.02
2	A	301	PQQ	C5-C6A-N6	-2.29	111.24	115.06
2	A	301	PQQ	C6A-N6-C7	-2.23	115.08	118.01
2	B	301	PQQ	C9-C8-C7	-2.21	118.12	119.93
3	A	306	GOL	C3-C2-C1	-2.21	103.70	111.80
2	B	301	PQQ	O2B-C2X-O2A	-2.20	118.66	123.90
3	B	302	GOL	C3-C2-C1	-2.15	103.91	111.80
2	B	301	PQQ	O2A-C2X-C2	-2.12	116.71	121.01
3	B	307	GOL	C3-C2-C1	-2.12	104.03	111.80
2	A	301	PQQ	C1A-N1-C2	-2.09	106.82	110.20
2	A	301	PQQ	C8-C7-N6	2.01	126.89	123.41

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	O1-C1-C2-C3
3	A	305	GOL	O1-C1-C2-C3
3	A	306	GOL	C1-C2-C3-O3
3	B	303	GOL	O1-C1-C2-C3
3	B	303	GOL	C1-C2-C3-O3
3	B	305	GOL	C1-C2-C3-O3
3	B	306	GOL	O2-C2-C3-O3
3	A	306	GOL	O1-C1-C2-O2
3	B	303	GOL	O2-C2-C3-O3
3	B	305	GOL	O1-C1-C2-O2
3	A	302	GOL	O1-C1-C2-O2
3	A	305	GOL	O1-C1-C2-O2
3	B	303	GOL	O1-C1-C2-O2
3	B	307	GOL	O1-C1-C2-O2
3	A	305	GOL	C1-C2-C3-O3
3	B	306	GOL	C1-C2-C3-O3
3	A	307	GOL	O2-C2-C3-O3
2	A	301	PQQ	C8-C9-C9X-O9B

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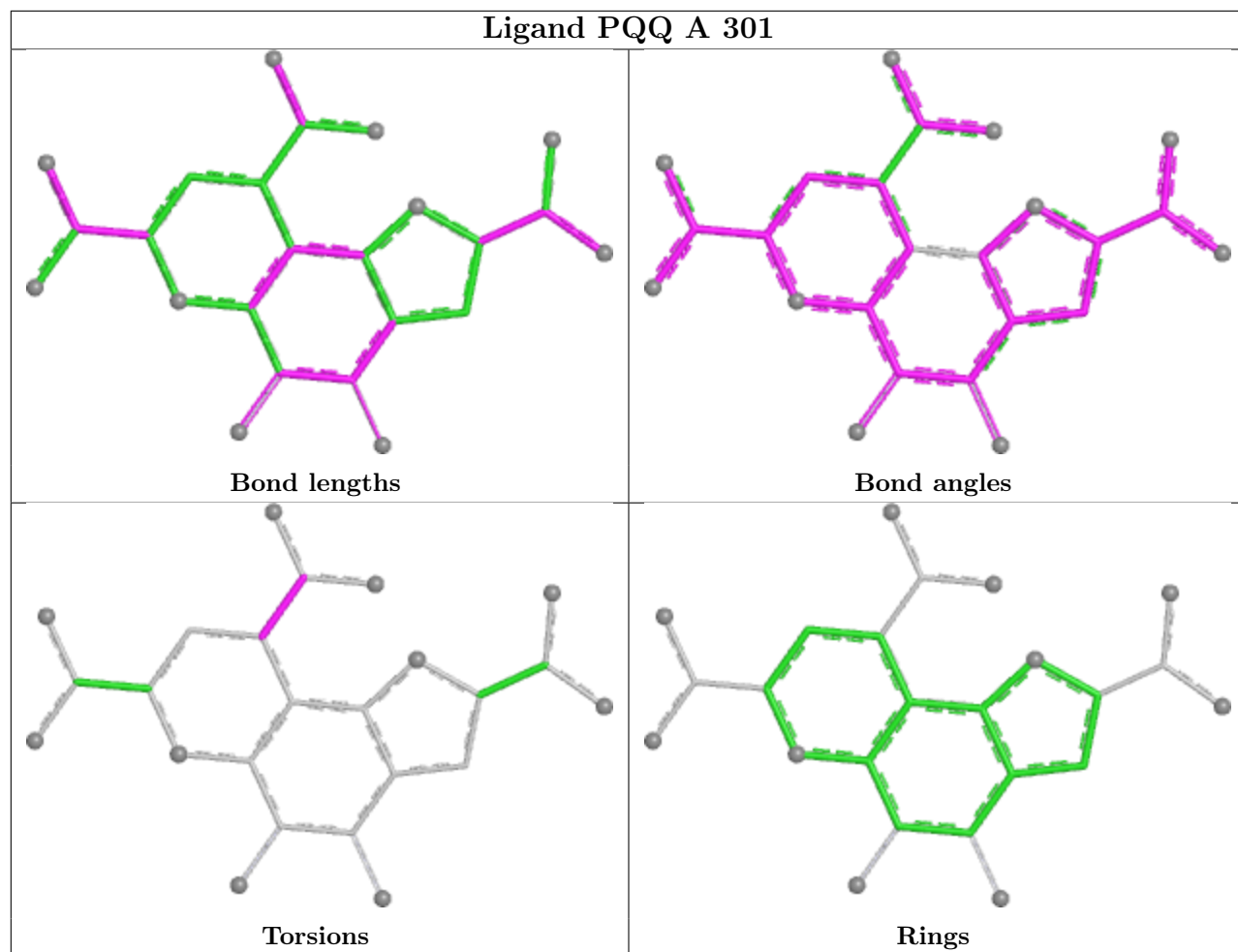
Mol	Chain	Res	Type	Atoms
2	B	301	PQQ	C8-C9-C9X-O9A
2	B	301	PQQ	C8-C9-C9X-O9B
2	A	301	PQQ	C8-C9-C9X-O9A
3	B	305	GOL	O2-C2-C3-O3

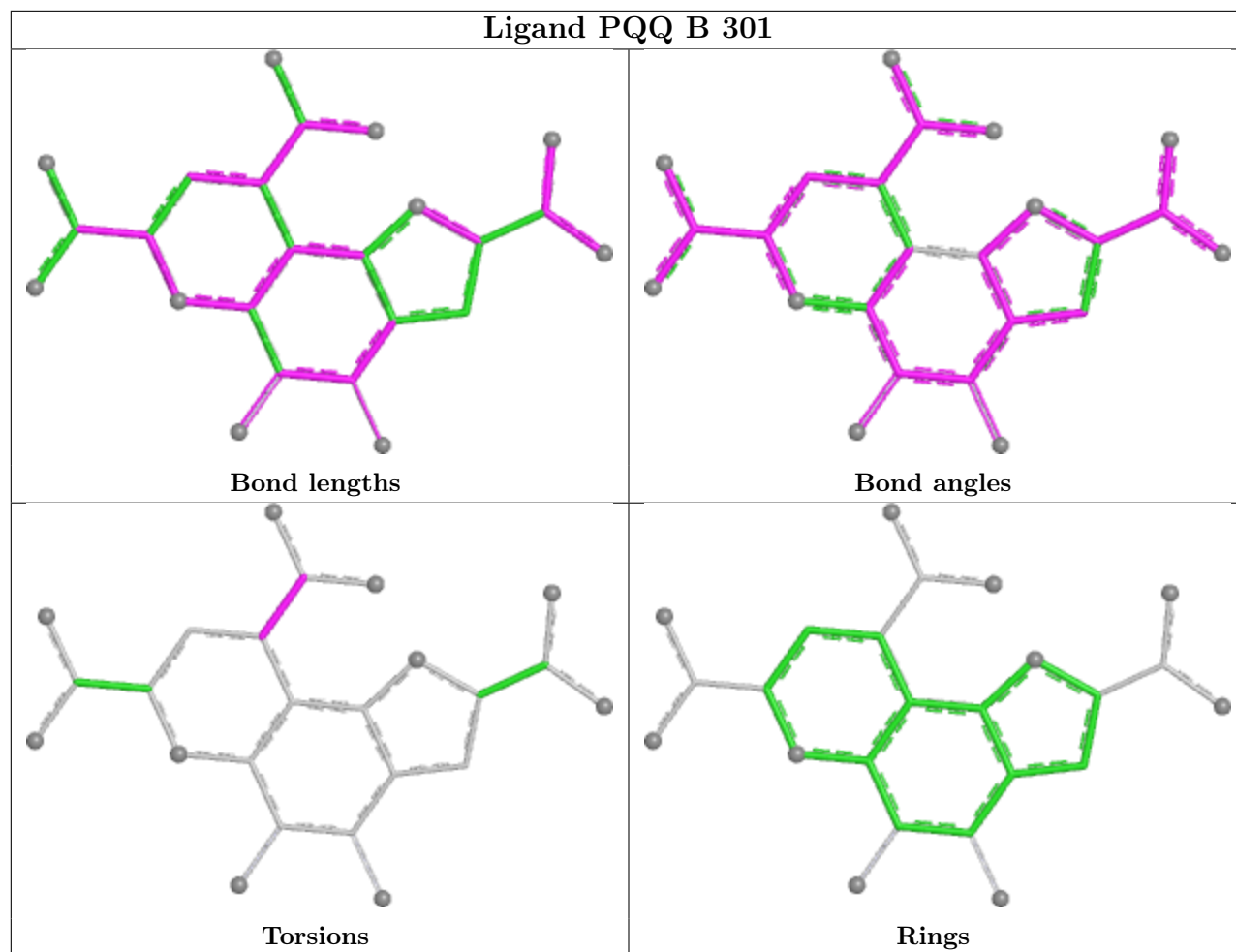
There are no ring outliers.

10 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	GOL	4	0
3	B	305	GOL	4	0
3	B	303	GOL	6	0
3	A	307	GOL	4	0
3	B	302	GOL	1	0
3	A	302	GOL	4	0
3	B	307	GOL	6	0
3	A	306	GOL	4	0
3	B	306	GOL	3	0
3	A	305	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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	254/258 (98%)	-0.66	5 (1%) 65 68	5, 12, 28, 52	22 (8%)
1	B	254/258 (98%)	-0.66	2 (0%) 82 86	5, 13, 24, 50	34 (13%)
All	All	508/516 (98%)	-0.66	7 (1%) 73 77	5, 13, 26, 52	56 (11%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	GLY	3.7
1	B	89[A]	GLY	3.2
1	A	87[A]	SER	2.7
1	A	91[A]	ASP	2.7
1	A	90	GLU	2.5
1	B	91[A]	ASP	2.5
1	A	255	HIS	2.3

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](#)

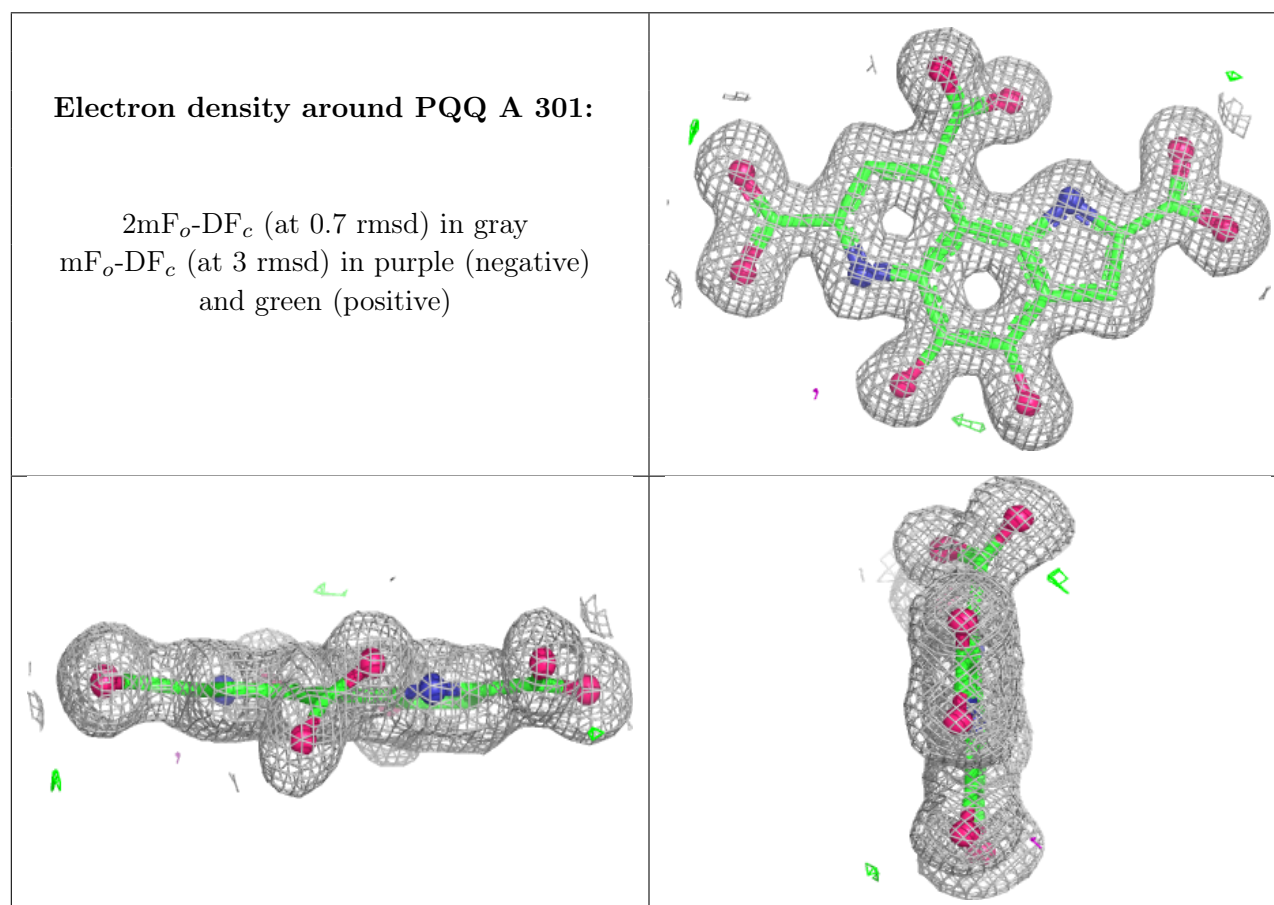
There are no oligosaccharides in this entry.

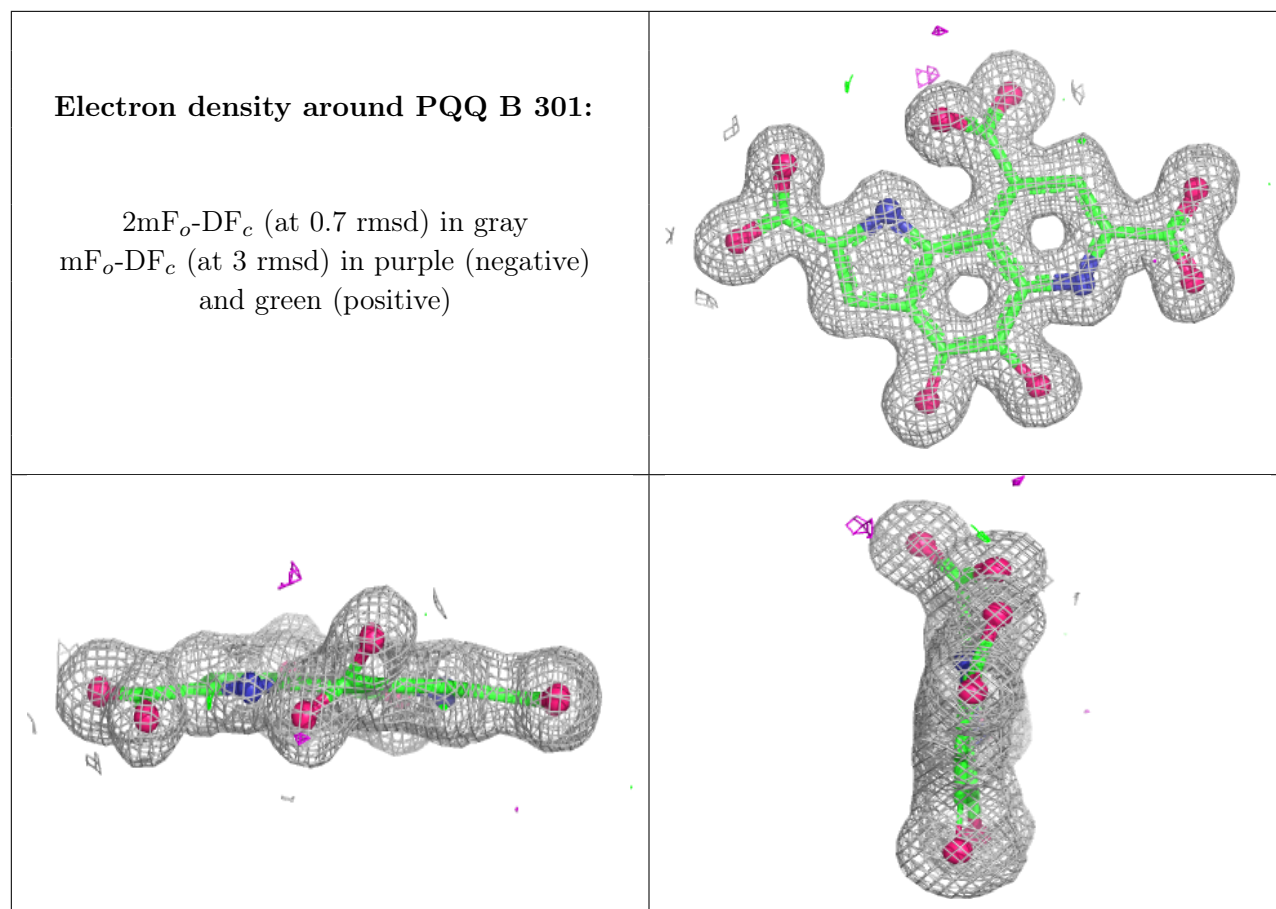
6.4 Ligands [i](#)

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	GOL	A	306	6/6	0.75	0.21	54,67,107,108	0
3	GOL	A	307	6/6	0.76	0.20	75,109,111,136	0
3	GOL	B	306	6/6	0.78	0.12	49,57,67,70	0
3	GOL	B	307	6/6	0.82	0.12	50,54,61,113	0
3	GOL	B	305	6/6	0.84	0.28	44,75,81,105	6
3	GOL	A	305	6/6	0.86	0.12	45,46,51,59	6
3	GOL	B	303	6/6	0.88	0.10	34,43,45,50	0
3	GOL	A	303	6/6	0.88	0.11	24,38,42,59	0
3	GOL	A	302	6/6	0.93	0.11	14,39,46,54	0
3	GOL	B	302	6/6	0.93	0.11	15,36,38,48	0
2	PQQ	A	301	24/24	0.98	0.03	8,10,13,15	0
2	PQQ	B	301	24/24	0.99	0.02	9,11,13,16	0
4	CL	A	304	1/1	1.00	0.04	13,13,13,13	0
4	CL	B	304	1/1	1.00	0.04	14,14,14,14	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 ⓘ

There are no such residues in this entry.