



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 09:38 PM EDT

PDB ID : 4NY7
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

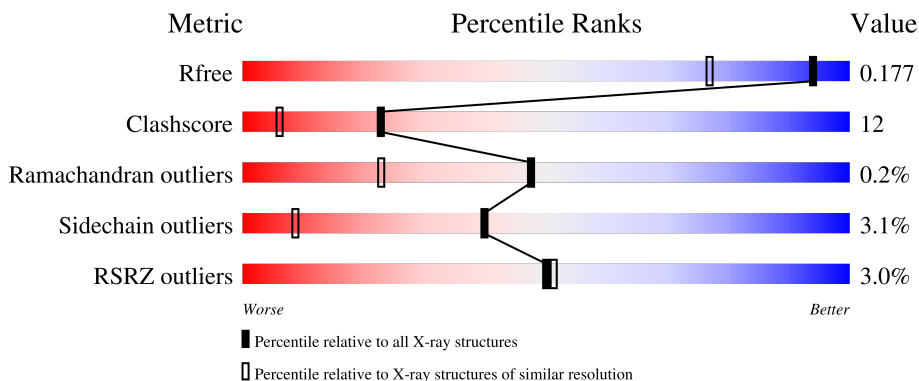
1 Overall quality at a glance

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}	130704	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (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	 3% 76% 19% ...
1	B	258	 3% 74% 19% 5% ..

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	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 [i](#)

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.

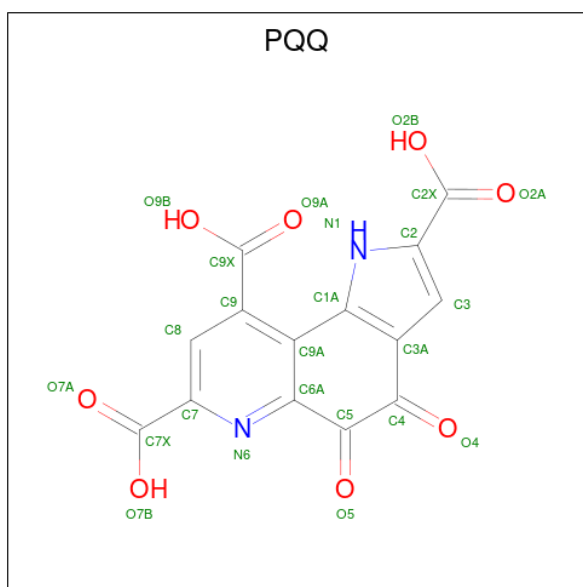
- Molecule 1 is a protein called Pyrroloquinoline-quinone synthase.

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

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 (three-letter code: PQQ) (formula: C₁₄H₆N₂O₈).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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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 (three-letter code: 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

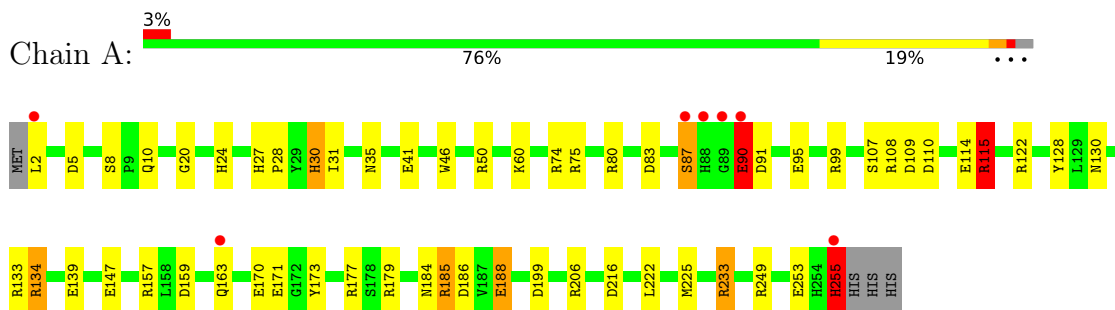
- Molecule 5 is water.

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

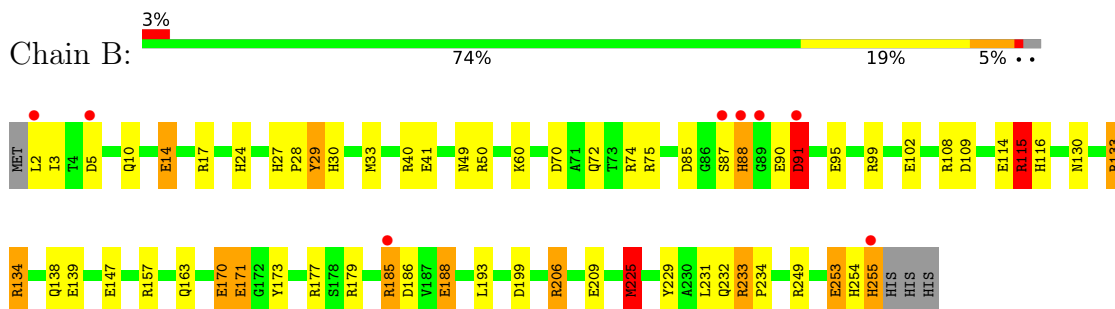
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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 19.45 – 1.44	Depositor EDS
% Data completeness (in resolution range)	97.8 (10.00-1.44) 97.8 (19.45-1.44)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.44Å)	Xtrriage
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	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for l,-k,h	Xtrriage
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

Xtrriage'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: GOL, CL, 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	2.32	53/2299 (2.3%)	2.95	78/3116 (2.5%)
1	B	2.96	59/2376 (2.5%)	2.81	85/3219 (2.6%)
All	All	2.66	112/4675 (2.4%)	2.88	163/6335 (2.6%)

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 (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	GLU	CD-OE2	56.60	1.88	1.25
1	B	188[A]	GLU	CD-OE2	49.53	1.80	1.25
1	B	188[B]	GLU	CD-OE2	49.53	1.80	1.25
1	A	115	ARG	CZ-NH1	35.20	1.78	1.33
1	B	115	ARG	CZ-NH2	30.52	1.72	1.33
1	B	14	GLU	CD-OE2	30.45	1.59	1.25
1	A	171	GLU	CD-OE2	30.13	1.58	1.25
1	B	171	GLU	CD-OE1	-29.97	0.92	1.25
1	B	188[A]	GLU	CD-OE1	-29.92	0.92	1.25
1	B	188[B]	GLU	CD-OE1	-29.92	0.92	1.25
1	A	185[A]	ARG	CZ-NH1	28.05	1.69	1.33
1	A	185[B]	ARG	CZ-NH1	28.05	1.69	1.33
1	B	134[A]	ARG	CZ-NH1	-27.62	0.97	1.33
1	B	134[B]	ARG	CZ-NH1	-27.62	0.97	1.33
1	A	171	GLU	CD-OE1	-26.63	0.96	1.25
1	A	115	ARG	NE-CZ	-25.27	1.00	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134[A]	ARG	CZ-NH2	23.96	1.64	1.33
1	B	134[B]	ARG	CZ-NH2	23.96	1.64	1.33
1	A	188[A]	GLU	CD-OE1	23.91	1.51	1.25
1	A	188[B]	GLU	CD-OE1	23.91	1.51	1.25
1	B	115	ARG	NE-CZ	-22.28	1.04	1.33
1	A	185[A]	ARG	NE-CZ	-20.78	1.06	1.33
1	A	185[B]	ARG	NE-CZ	-20.78	1.06	1.33
1	A	188[A]	GLU	CD-OE2	-17.98	1.05	1.25
1	A	188[B]	GLU	CD-OE2	-17.98	1.05	1.25
1	B	177	ARG	CZ-NH2	17.54	1.55	1.33
1	B	14	GLU	CD-OE1	-15.98	1.08	1.25
1	B	177	ARG	CZ-NH1	-15.87	1.12	1.33
1	A	134[A]	ARG	CZ-NH1	14.60	1.52	1.33
1	A	134[B]	ARG	CZ-NH1	14.60	1.52	1.33
1	A	75	ARG	CZ-NH1	14.59	1.52	1.33
1	B	114	GLU	CD-OE2	14.57	1.41	1.25
1	A	90	GLU	CD-OE2	13.55	1.40	1.25
1	B	108	ARG	CZ-NH1	12.97	1.50	1.33
1	A	95	GLU	CD-OE1	12.07	1.39	1.25
1	A	91[A]	ASP	CG-OD2	-11.51	0.98	1.25
1	A	91[B]	ASP	CG-OD2	-11.51	0.98	1.25
1	B	134[A]	ARG	NE-CZ	11.03	1.47	1.33
1	B	134[B]	ARG	NE-CZ	11.03	1.47	1.33
1	A	249	ARG	CZ-NH1	-10.93	1.18	1.33
1	A	91[A]	ASP	CG-OD1	10.80	1.50	1.25
1	A	91[B]	ASP	CG-OD1	10.80	1.50	1.25
1	A	90	GLU	CD-OE1	-10.45	1.14	1.25
1	B	41	GLU	CD-OE1	10.19	1.36	1.25
1	B	50	ARG	CZ-NH1	9.90	1.46	1.33
1	A	30[A]	HIS	CE1-NE2	-9.71	1.10	1.32
1	A	30[B]	HIS	CE1-NE2	-9.71	1.10	1.32
1	A	114	GLU	CD-OE1	-9.60	1.15	1.25
1	B	114	GLU	CD-OE1	-9.38	1.15	1.25
1	B	254	HIS	ND1-CE1	-9.30	1.11	1.34
1	A	75	ARG	NE-CZ	-9.21	1.21	1.33
1	B	170[A]	GLU	CD-OE1	9.10	1.35	1.25
1	B	170[B]	GLU	CD-OE1	9.10	1.35	1.25
1	A	114	GLU	CD-OE2	8.79	1.35	1.25
1	A	253	GLU	CD-OE2	8.75	1.35	1.25
1	B	139	GLU	CD-OE2	-8.49	1.16	1.25
1	B	170[A]	GLU	CD-OE2	-8.38	1.16	1.25
1	B	170[B]	GLU	CD-OE2	-8.38	1.16	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	ARG	NE-CZ	-8.35	1.22	1.33
1	B	139	GLU	CD-OE1	8.28	1.34	1.25
1	A	109[A]	ASP	CG-OD1	8.26	1.44	1.25
1	A	109[B]	ASP	CG-OD1	8.26	1.44	1.25
1	B	254	HIS	CE1-NE2	8.18	1.51	1.32
1	A	206	ARG	CZ-NH1	7.98	1.43	1.33
1	A	134[A]	ARG	CZ-NH2	-7.93	1.22	1.33
1	A	134[B]	ARG	CZ-NH2	-7.93	1.22	1.33
1	B	30	HIS	CE1-NE2	-7.85	1.14	1.32
1	B	253[A]	GLU	CD-OE2	7.83	1.34	1.25
1	B	253[B]	GLU	CD-OE2	7.83	1.34	1.25
1	B	95	GLU	CD-OE2	7.47	1.33	1.25
1	A	255	HIS	CE1-NE2	7.45	1.49	1.32
1	B	133[A]	ARG	CZ-NH1	-7.20	1.23	1.33
1	B	133[B]	ARG	CZ-NH1	-7.20	1.23	1.33
1	A	199	ASP	CG-OD1	-7.19	1.08	1.25
1	B	91[A]	ASP	CG-OD1	6.99	1.41	1.25
1	B	91[B]	ASP	CG-OD1	6.99	1.41	1.25
1	A	139	GLU	CD-OE2	-6.94	1.18	1.25
1	B	50	ARG	NE-CZ	-6.87	1.24	1.33
1	A	133	ARG	NE-CZ	6.86	1.42	1.33
1	A	95	GLU	CD-OE2	-6.85	1.18	1.25
1	B	75	ARG	CZ-NH2	6.59	1.41	1.33
1	B	75	ARG	NE-CZ	-6.59	1.24	1.33
1	A	5	ASP	CG-OD2	6.52	1.40	1.25
1	B	99	ARG	NE-CZ	6.47	1.41	1.33
1	B	133[A]	ARG	NE-CZ	6.32	1.41	1.33
1	B	133[B]	ARG	NE-CZ	6.32	1.41	1.33
1	B	133[A]	ARG	CZ-NH2	6.32	1.41	1.33
1	B	133[B]	ARG	CZ-NH2	6.32	1.41	1.33
1	A	109[A]	ASP	CG-OD2	-6.29	1.10	1.25
1	A	109[B]	ASP	CG-OD2	-6.29	1.10	1.25
1	B	116	HIS	CE1-NE2	6.22	1.47	1.32
1	A	206	ARG	NE-CZ	-6.18	1.25	1.33
1	B	91[A]	ASP	CG-OD2	-6.10	1.11	1.25
1	B	91[B]	ASP	CG-OD2	-6.10	1.11	1.25
1	A	255	HIS	ND1-CE1	-6.01	1.19	1.34
1	A	147	GLU	CD-OE2	5.88	1.32	1.25
1	A	30[A]	HIS	CD2-NE2	5.87	1.54	1.42
1	A	30[B]	HIS	CD2-NE2	5.87	1.54	1.42
1	B	255	HIS	CE1-NE2	5.84	1.46	1.32
1	A	199	ASP	CG-OD2	5.83	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	ASP	CG-OD1	5.79	1.38	1.25
1	B	102	GLU	CD-OE1	-5.66	1.19	1.25
1	B	75	ARG	CZ-NH1	5.60	1.40	1.33
1	B	185[A]	ARG	CZ-NH2	5.48	1.40	1.33
1	B	185[B]	ARG	CZ-NH2	5.48	1.40	1.33
1	A	99	ARG	CZ-NH2	5.47	1.40	1.33
1	A	108	ARG	CZ-NH2	5.45	1.40	1.33
1	B	179	ARG	CZ-NH1	5.44	1.40	1.33
1	A	74	ARG	CZ-NH1	-5.18	1.26	1.33
1	B	209	GLU	CD-OE1	5.07	1.31	1.25
1	A	74	ARG	CZ-NH2	5.06	1.39	1.33
1	A	99	ARG	CZ-NH1	-5.01	1.26	1.33

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	NE-CZ-NH2	62.47	151.53	120.30
1	A	185[A]	ARG	NE-CZ-NH2	52.15	146.38	120.30
1	A	185[B]	ARG	NE-CZ-NH2	52.15	146.38	120.30
1	B	134[A]	ARG	NE-CZ-NH1	43.49	142.04	120.30
1	B	134[B]	ARG	NE-CZ-NH1	43.49	142.04	120.30
1	B	134[A]	ARG	NE-CZ-NH2	-43.35	98.63	120.30
1	B	134[B]	ARG	NE-CZ-NH2	-43.35	98.63	120.30
1	B	115	ARG	NE-CZ-NH1	40.86	140.73	120.30
1	A	115	ARG	CD-NE-CZ	36.95	175.33	123.60
1	B	115	ARG	CD-NE-CZ	33.96	171.15	123.60
1	B	177	ARG	NE-CZ-NH2	-32.14	104.23	120.30
1	A	134[A]	ARG	NE-CZ-NH2	31.27	135.94	120.30
1	A	134[B]	ARG	NE-CZ-NH2	31.27	135.94	120.30
1	B	177	ARG	NE-CZ-NH1	30.83	135.72	120.30
1	A	75	ARG	NE-CZ-NH2	30.03	135.32	120.30
1	B	171	GLU	CG-CD-OE1	27.73	173.76	118.30
1	A	185[A]	ARG	CD-NE-CZ	26.05	160.08	123.60
1	A	185[B]	ARG	CD-NE-CZ	26.05	160.08	123.60
1	B	188[A]	GLU	CG-CD-OE1	22.75	163.79	118.30
1	B	188[B]	GLU	CG-CD-OE1	22.75	163.79	118.30
1	B	108	ARG	NE-CZ-NH2	21.34	130.97	120.30
1	B	171	GLU	OE1-CD-OE2	-20.95	98.16	123.30
1	B	133[A]	ARG	NE-CZ-NH2	-20.74	109.93	120.30
1	B	133[B]	ARG	NE-CZ-NH2	-20.74	109.93	120.30
1	A	134[A]	ARG	NE-CZ-NH1	-19.87	110.37	120.30
1	A	134[B]	ARG	NE-CZ-NH1	-19.87	110.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	NE-CZ-NH1	-19.84	110.38	120.30
1	A	115	ARG	NH1-CZ-NH2	-19.38	98.08	119.40
1	A	249	ARG	NE-CZ-NH2	-17.71	111.44	120.30
1	B	115	ARG	NH1-CZ-NH2	-17.63	100.01	119.40
1	B	188[A]	GLU	OE1-CD-OE2	-17.48	102.33	123.30
1	B	188[B]	GLU	OE1-CD-OE2	-17.48	102.33	123.30
1	A	185[A]	ARG	NH1-CZ-NH2	-16.78	100.94	119.40
1	A	185[B]	ARG	NH1-CZ-NH2	-16.78	100.94	119.40
1	A	91[A]	ASP	CB-CG-OD2	16.12	132.80	118.30
1	A	91[B]	ASP	CB-CG-OD2	16.12	132.80	118.30
1	A	249	ARG	NE-CZ-NH1	15.86	128.23	120.30
1	A	185[A]	ARG	NE-CZ-NH1	-15.24	112.68	120.30
1	A	185[B]	ARG	NE-CZ-NH1	-15.24	112.68	120.30
1	B	171	GLU	CG-CD-OE2	-15.11	88.08	118.30
1	A	91[A]	ASP	CB-CG-OD1	-14.57	105.19	118.30
1	A	91[B]	ASP	CB-CG-OD1	-14.57	105.19	118.30
1	A	109[A]	ASP	CB-CG-OD2	14.21	131.09	118.30
1	A	109[B]	ASP	CB-CG-OD2	14.21	131.09	118.30
1	B	249	ARG	NE-CZ-NH1	13.42	127.01	120.30
1	A	74	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	A	99	ARG	NE-CZ-NH2	-13.10	113.75	120.30
1	A	99	ARG	NE-CZ-NH1	12.60	126.60	120.30
1	B	188[A]	GLU	CG-CD-OE2	-12.21	93.88	118.30
1	B	188[B]	GLU	CG-CD-OE2	-12.21	93.88	118.30
1	B	14	GLU	CG-CD-OE1	12.01	142.33	118.30
1	A	133	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	A	27	HIS	CG-ND1-CE1	11.83	124.76	108.20
1	A	122	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	B	40	ARG	NE-CZ-NH1	11.75	126.17	120.30
1	A	171	GLU	CG-CD-OE1	11.55	141.40	118.30
1	B	40	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	A	5	ASP	CB-CG-OD1	11.48	128.63	118.30
1	A	157	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	B	75	ARG	NE-CZ-NH2	11.13	125.86	120.30
1	A	206	ARG	NE-CZ-NH2	11.07	125.84	120.30
1	B	91[A]	ASP	CB-CG-OD2	11.03	128.23	118.30
1	B	91[B]	ASP	CB-CG-OD2	11.03	128.23	118.30
1	B	199	ASP	CB-CG-OD1	10.91	128.12	118.30
1	B	91[A]	ASP	CB-CG-OD1	-10.83	108.56	118.30
1	B	91[B]	ASP	CB-CG-OD1	-10.83	108.56	118.30
1	B	206	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	A	109[A]	ASP	CB-CG-OD1	-10.76	108.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109[B]	ASP	CB-CG-OD1	-10.76	108.61	118.30
1	B	199	ASP	CB-CG-OD2	-10.75	108.62	118.30
1	A	179	ARG	NE-CZ-NH2	10.19	125.39	120.30
1	A	199	ASP	CB-CG-OD1	10.02	127.32	118.30
1	B	109	ASP	CB-CG-OD2	9.89	127.20	118.30
1	B	14	GLU	OE1-CD-OE2	-9.87	111.45	123.30
1	A	75	ARG	NH1-CZ-NH2	-9.74	108.68	119.40
1	B	206	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	B	85	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	A	74	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	75	ARG	CD-NE-CZ	9.08	136.31	123.60
1	A	171	GLU	CG-CD-OE2	-9.06	100.18	118.30
1	A	50	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	5	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	A	199	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	B	27	HIS	CG-ND1-CE1	8.86	120.61	108.20
1	A	75	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	B	233	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	B	185[A]	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	B	185[B]	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	A	28	PRO	O-C-N	-8.28	109.45	122.70
1	A	188[A]	GLU	CG-CD-OE2	8.28	134.86	118.30
1	A	188[B]	GLU	CG-CD-OE2	8.28	134.86	118.30
1	B	133[A]	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	B	133[B]	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	91[A]	ASP	CA-C-N	7.82	131.83	116.20
1	A	91[B]	ASP	CA-C-N	7.82	131.83	116.20
1	B	28	PRO	O-C-N	-7.64	110.48	122.70
1	A	157	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	B	109	ASP	CB-CG-OD1	-7.42	111.62	118.30
1	B	70	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	91[A]	ASP	CA-C-N	7.27	130.73	116.20
1	B	91[B]	ASP	CA-C-N	7.27	130.73	116.20
1	B	17	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	122	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	225[A]	MET	CA-CB-CG	6.98	125.17	113.30
1	B	225[B]	MET	CA-CB-CG	6.98	125.17	113.30
1	A	233	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	B	70	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	B	74	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	185[A]	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	185[B]	ARG	NE-CZ-NH1	6.78	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ARG	NH1-CZ-NH2	-6.73	112.00	119.40
1	B	157	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	91[A]	ASP	C-N-CA	6.72	136.42	122.30
1	A	91[B]	ASP	C-N-CA	6.72	136.42	122.30
1	B	114	GLU	CG-CD-OE1	6.65	131.60	118.30
1	B	249	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	254	HIS	CG-ND1-CE1	6.60	117.44	108.20
1	B	108	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	90	GLU	O-C-N	-6.50	112.30	122.70
1	A	108	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	B	41	GLU	O-C-N	-6.38	112.50	122.70
1	B	75	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
1	A	28	PRO	C-N-CA	6.30	137.45	121.70
1	B	255	HIS	CG-ND1-CE1	6.30	117.02	108.20
1	B	90[A]	GLU	O-C-N	-6.24	112.72	122.70
1	B	90[B]	GLU	O-C-N	-6.24	112.72	122.70
1	A	188[A]	GLU	CG-CD-OE1	-6.15	106.01	118.30
1	A	188[B]	GLU	CG-CD-OE1	-6.15	106.01	118.30
1	A	41	GLU	O-C-N	-6.06	113.00	122.70
1	B	157	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	14	GLU	CG-CD-OE2	-6.04	106.22	118.30
1	A	206	ARG	CD-NE-CZ	6.03	132.04	123.60
1	B	99	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	29	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	A	90	GLU	CG-CD-OE1	5.86	130.01	118.30
1	B	133[A]	ARG	NH1-CZ-NH2	5.79	125.77	119.40
1	B	133[B]	ARG	NH1-CZ-NH2	5.79	125.77	119.40
1	B	5	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	49	ASN	CB-CG-OD1	5.77	133.15	121.60
1	A	233	ARG	CD-NE-CZ	5.76	131.66	123.60
1	B	75	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	27	HIS	ND1-CG-CD2	-5.64	98.11	106.00
1	B	29	TYR	CB-CG-CD2	5.55	124.33	121.00
1	A	255	HIS	CG-ND1-CE1	5.54	115.96	108.20
1	B	91[A]	ASP	O-C-N	-5.53	113.80	123.20
1	B	91[B]	ASP	O-C-N	-5.53	113.80	123.20
1	B	114	GLU	CG-CD-OE2	-5.49	107.33	118.30
1	B	74	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	28	PRO	C-N-CA	5.45	135.32	121.70
1	B	108	ARG	CD-NE-CZ	5.45	131.22	123.60
1	B	5	ASP	CB-CG-OD1	-5.42	113.43	118.30
1	B	173	TYR	CB-CG-CD2	5.42	124.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	HIS	ND1-CE1-NE2	-5.35	98.14	109.90
1	A	41	GLU	C-N-CA	5.34	135.06	121.70
1	A	206	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	A	216	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	134[A]	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	A	134[B]	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	B	50	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	159	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	114	GLU	O-C-N	-5.05	114.61	122.70
1	A	83	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	10	GLN	O-C-N	-5.02	114.67	122.70

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 [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	2195	0	2139	31	0
1	B	2264	0	2208	49	0
2	A	24	0	4	0	0
2	B	24	0	3	0	0
3	A	30	0	40	20	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	104	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 12.

All (104) 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	1.23
1:B:188[A]:GLU:CD	1:B:188[A]:GLU:OE2	1.80	1.19
1:B:170[B]:GLU:CD	1:B:170[B]:GLU:OE2	1.81	1.17
1:B:171:GLU:OE2	1:B:171:GLU:CD	1.87	1.11
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:188[A]:GLU:OE2	1:B:188[A]:GLU:OE1	2.19	0.51
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:B:170[B]:GLU:CD	1:B:170[B]:GLU:H	2.14	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:170:GLU:H	1:A:170:GLU:CD	2.17	0.47
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:29:TYR:CZ	1:B:225[A]:MET:HE3	2.49	0.46
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:B:170[B]:GLU:OE2	1:B:170[B]:GLU:OE1	2.19	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
3:A:306:GOL:O2	3:A:306:GOL:O3	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	22	4
All	All	553/516 (107%)	550 (100%)	1 (0%)	2 (0%)	47	13

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%)	224 (97%)	7 (3%)	41 9
1	B	241/217 (111%)	232 (96%)	9 (4%)	34 5
All	All	472/434 (109%)	456 (97%)	16 (3%)	40 6

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	24	HIS
1	A	87[A]	SER
1	A	87[B]	SER
1	A	115	ARG
1	A	163	GLN
1	A	255	HIS
1	B	24	HIS
1	B	60	LYS
1	B	91[A]	ASP
1	B	91[B]	ASP
1	B	115	ARG
1	B	206	ARG
1	B	225[A]	MET
1	B	225[B]	MET
1	B	255	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS

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 monosaccharides 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	$\# Z > 2$
2	PQQ	B	301	-	23,26,26	4.33	15 (65%)	29,40,40	3.74	16 (55%)
3	GOL	A	302	-	5,5,5	7.44	1 (20%)	5,5,5	1.65	1 (20%)
3	GOL	B	307	-	5,5,5	14.18	2 (40%)	5,5,5	4.57	3 (60%)
3	GOL	A	307	-	5,5,5	12.62	2 (40%)	5,5,5	2.46	3 (60%)
3	GOL	B	305	-	5,5,5	16.03	3 (60%)	5,5,5	5.22	3 (60%)
3	GOL	B	306	-	5,5,5	12.15	2 (40%)	5,5,5	4.17	2 (40%)
3	GOL	A	306	-	5,5,5	14.07	2 (40%)	5,5,5	4.54	4 (80%)
3	GOL	B	303	-	5,5,5	7.35	1 (20%)	5,5,5	1.56	1 (20%)
2	PQQ	A	301	-	23,26,26	3.86	13 (56%)	29,40,40	4.32	18 (62%)
3	GOL	A	305	-	5,5,5	0.21	0	5,5,5	0.79	0
3	GOL	B	302	-	5,5,5	9.73	1 (20%)	5,5,5	3.45	3 (60%)
3	GOL	A	303	-	5,5,5	0.26	0	5,5,5	0.48	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
2	PQQ	B	301	-	-	0/10/28/28	0/3/3/3
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	B	307	-	-	1/4/4/4	-
3	GOL	A	307	-	-	1/4/4/4	-
3	GOL	B	305	-	-	2/4/4/4	-
3	GOL	B	306	-	-	2/4/4/4	-
3	GOL	A	306	-	-	2/4/4/4	-
3	GOL	B	303	-	-	4/4/4/4	-
2	PQQ	A	301	-	-	0/10/28/28	0/3/3/3
3	GOL	A	305	-	-	3/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	A	303	-	-	0/4/4/4	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	305	GOL	O2-C2	23.63	2.13	1.43
3	B	307	GOL	O2-C2	23.04	2.12	1.43
3	A	307	GOL	O2-C2	22.88	2.11	1.43
3	A	306	GOL	O2-C2	22.76	2.11	1.43
3	B	307	GOL	C3-C2	21.80	2.41	1.51
3	B	302	GOL	C3-C2	21.75	2.41	1.51
3	A	306	GOL	C3-C2	21.73	2.41	1.51
3	B	306	GOL	C1-C2	21.61	2.40	1.51
3	B	305	GOL	C1-C2	21.44	2.39	1.51
3	A	302	GOL	O3-C3	16.62	2.12	1.42
3	A	307	GOL	O1-C1	16.50	2.12	1.42
3	B	306	GOL	O1-C1	16.45	2.11	1.42
3	B	303	GOL	O1-C1	16.42	2.11	1.42
3	B	305	GOL	O1-C1	16.33	2.11	1.42
2	A	301	PQQ	C2-C2X	-10.94	1.35	1.50
2	B	301	PQQ	C3A-C4	-8.89	1.33	1.48
2	B	301	PQQ	C6A-N6	8.78	1.39	1.32
2	B	301	PQQ	O5-C5	7.36	1.38	1.23
2	B	301	PQQ	C7-C7X	-7.22	1.40	1.50
2	A	301	PQQ	O4-C4	6.55	1.37	1.23
2	A	301	PQQ	O5-C5	6.47	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	PQQ	C5-C4	-6.34	1.32	1.53
2	A	301	PQQ	C3A-C4	-6.25	1.37	1.48
2	B	301	PQQ	C6A-C9A	4.80	1.48	1.42
2	B	301	PQQ	C2-C2X	-4.59	1.44	1.50
2	A	301	PQQ	C7-C7X	-4.42	1.44	1.50
2	B	301	PQQ	C8-C9	4.19	1.46	1.37
2	A	301	PQQ	C6A-C9A	3.68	1.46	1.42
2	B	301	PQQ	C9-C9X	-3.63	1.44	1.50
2	A	301	PQQ	O7A-C7X	3.42	1.32	1.22
2	A	301	PQQ	C9A-C1A	-3.33	1.34	1.42
2	B	301	PQQ	O9A-C9X	3.26	1.32	1.22
2	B	301	PQQ	O2A-C2X	3.15	1.32	1.22
2	B	301	PQQ	C7-N6	2.90	1.38	1.34
2	A	301	PQQ	C3-C3A	2.73	1.46	1.40
2	A	301	PQQ	C9-C9X	-2.51	1.46	1.50
2	B	301	PQQ	C3-C2	-2.50	1.35	1.39
2	B	301	PQQ	O2B-C2X	-2.44	1.23	1.30
2	A	301	PQQ	O2A-C2X	2.44	1.30	1.22
2	B	301	PQQ	O4-C4	2.42	1.28	1.23
2	A	301	PQQ	O9B-C9X	2.15	1.37	1.30
2	A	301	PQQ	C8-C9	2.03	1.41	1.37

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	PQQ	C9-C9A-C1A	13.18	133.69	122.88
2	B	301	PQQ	C9-C9A-C1A	10.73	131.68	122.88
2	A	301	PQQ	C9-C9A-C6A	-9.73	108.67	121.68
2	B	301	PQQ	O5-C5-C6A	-9.70	111.57	121.84
3	B	305	GOL	O2-C2-C1	-8.15	73.24	109.12
3	B	307	GOL	O2-C2-C3	-8.11	73.42	109.12
3	A	306	GOL	O2-C2-C3	-8.10	73.46	109.12
3	B	306	GOL	O1-C1-C2	-7.57	73.92	110.20
3	B	305	GOL	O1-C1-C2	-7.53	74.09	110.20
2	A	301	PQQ	O2B-C2X-O2A	-7.32	107.10	123.35
2	A	301	PQQ	C3A-C4-C5	6.76	122.07	118.14
2	B	301	PQQ	C3A-C4-C5	6.50	121.92	118.14
2	B	301	PQQ	C9-C9A-C6A	-5.39	114.47	121.68
3	B	302	GOL	O2-C2-C3	-5.25	85.99	109.12
3	B	302	GOL	O3-C3-C2	-5.11	85.68	110.20
3	B	306	GOL	O2-C2-C1	-5.05	86.89	109.12
3	B	307	GOL	O3-C3-C2	-4.97	86.38	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	306	GOL	O3-C3-C2	-4.87	86.84	110.20
2	B	301	PQQ	O5-C5-C4	4.73	127.52	119.31
2	A	301	PQQ	O2B-C2X-C2	4.62	125.21	114.69
2	A	301	PQQ	C2-C3-C3A	-4.22	100.39	105.98
2	A	301	PQQ	C8-C9-C9X	-3.98	113.78	118.27
2	B	301	PQQ	O2B-C2X-C2	3.87	123.49	114.69
2	A	301	PQQ	O5-C5-C4	3.74	125.80	119.31
2	A	301	PQQ	O7B-C7X-O7A	-3.47	115.66	123.35
3	B	305	GOL	O2-C2-C3	-3.41	94.08	109.12
2	A	301	PQQ	O7B-C7X-C7	3.35	122.32	114.69
2	A	301	PQQ	C3A-C1A-C9A	3.32	125.95	121.54
2	A	301	PQQ	O9B-C9X-O9A	-3.25	116.13	123.35
2	B	301	PQQ	O9B-C9X-C9	3.23	123.53	114.39
3	A	307	GOL	O1-C1-C2	-3.16	95.04	110.20
3	B	307	GOL	O2-C2-C1	-3.14	95.30	109.12
3	A	307	GOL	O2-C2-C1	-3.13	95.36	109.12
3	A	307	GOL	O2-C2-C3	-3.11	95.42	109.12
3	A	302	GOL	O3-C3-C2	-3.10	95.34	110.20
3	A	306	GOL	O2-C2-C1	-3.04	95.73	109.12
3	B	303	GOL	O1-C1-C2	-3.02	95.71	110.20
2	B	301	PQQ	O9A-C9X-C9	-2.99	114.25	122.23
2	A	301	PQQ	O2A-C2X-C2	2.97	127.26	121.24
2	B	301	PQQ	O4-C4-C5	-2.87	114.33	119.31
2	A	301	PQQ	O5-C5-C6A	-2.81	118.86	121.84
2	A	301	PQQ	O4-C4-C5	-2.72	114.59	119.31
2	B	301	PQQ	C8-C7-C7X	2.68	125.35	119.57
2	A	301	PQQ	C8-C9-C9A	2.63	123.63	120.06
2	B	301	PQQ	C7X-C7-N6	-2.56	112.69	116.48
2	A	301	PQQ	C7X-C7-N6	-2.56	112.70	116.48
2	A	301	PQQ	C9-C8-C7	-2.55	116.28	120.33
2	B	301	PQQ	O7B-C7X-O7A	-2.43	117.95	123.35
2	B	301	PQQ	O2A-C2X-C2	-2.23	116.71	121.24
2	B	301	PQQ	C2-C3-C3A	2.18	108.86	105.98
2	B	301	PQQ	O2B-C2X-O2A	-2.11	118.66	123.35
3	A	306	GOL	C3-C2-C1	-2.06	103.70	111.70
2	B	301	PQQ	C8-C9-C9X	-2.03	115.98	118.27
3	B	302	GOL	C3-C2-C1	-2.00	103.91	111.70

There are no chirality outliers.

All (17) 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	306	GOL	C1-C2-C3-O3
3	B	307	GOL	O1-C1-C2-O2
3	A	305	GOL	C1-C2-C3-O3
3	A	307	GOL	O2-C2-C3-O3

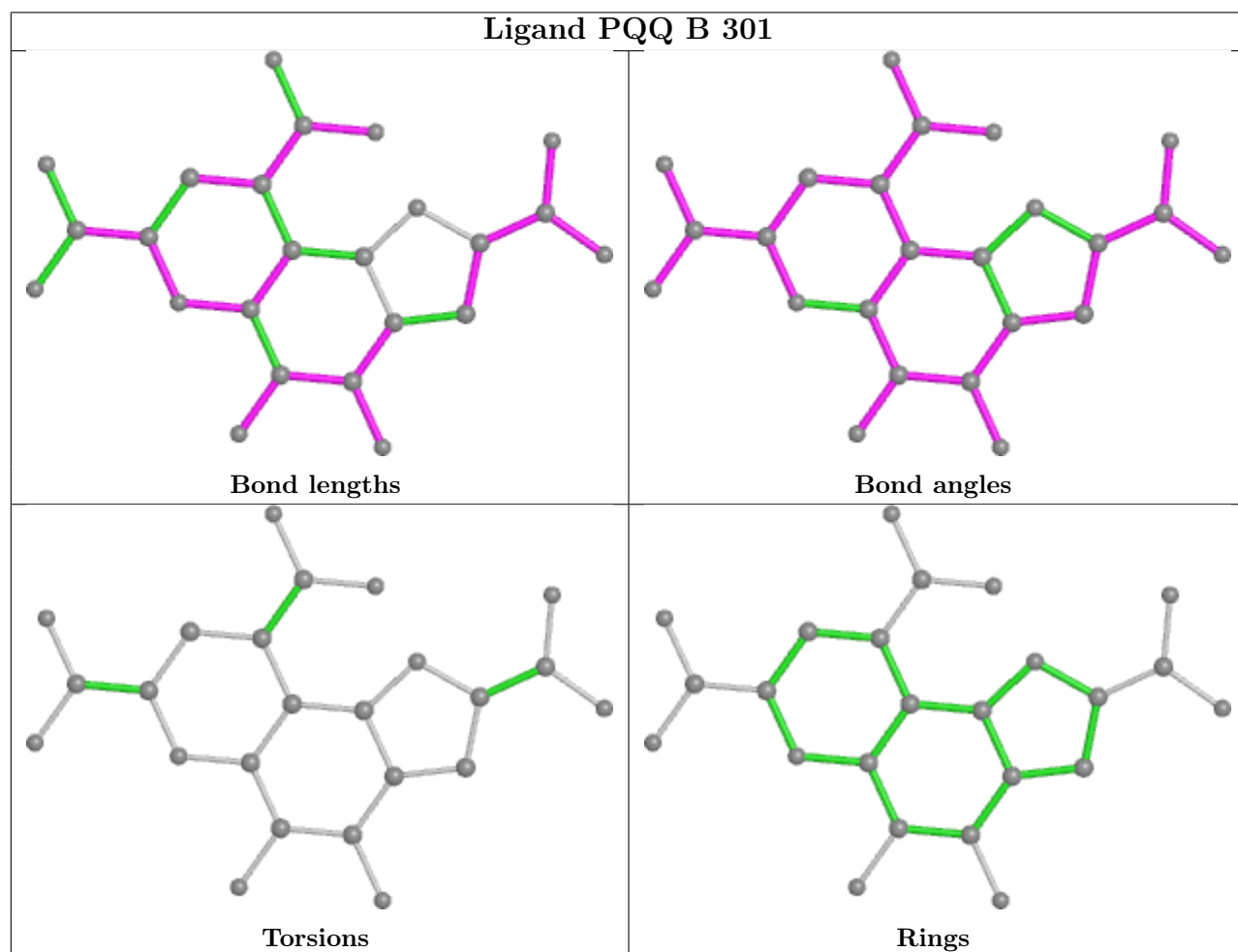
There are no ring outliers.

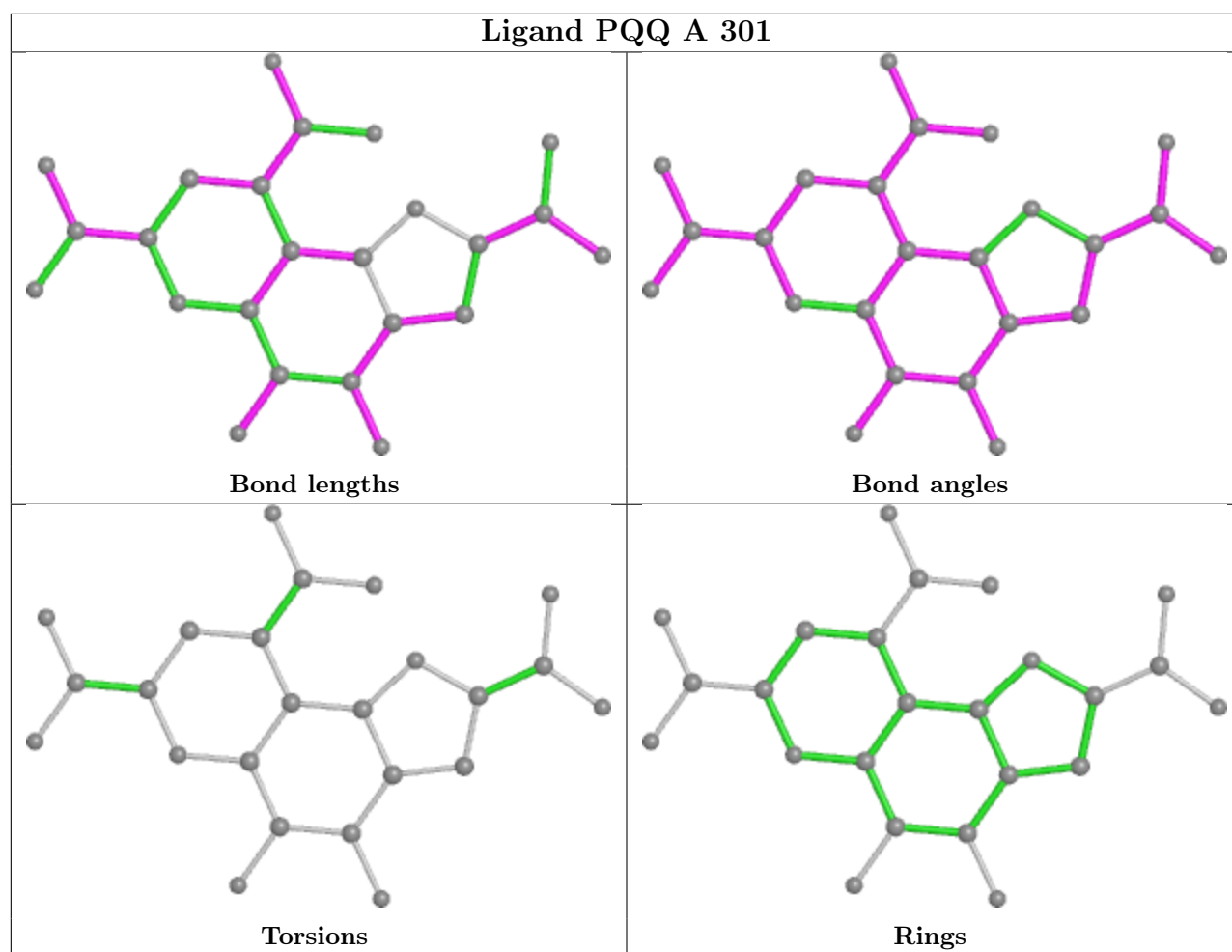
10 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	GOL	4	0
3	B	307	GOL	6	0
3	A	307	GOL	4	0
3	B	305	GOL	4	0
3	B	306	GOL	3	0
3	A	306	GOL	6	0
3	B	303	GOL	6	0
3	A	305	GOL	2	0
3	B	302	GOL	1	0
3	A	303	GOL	4	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%)	-0.34	7 (2%) 53 53	8, 12, 32, 52	3 (1%)
1	B	254/258 (98%)	-0.31	8 (3%) 49 50	8, 14, 28, 50	4 (1%)
All	All	508/516 (98%)	-0.33	15 (2%) 50 51	8, 13, 28, 52	7 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88[A]	HIS	4.5
1	A	90	GLU	4.4
1	A	89	GLY	4.4
1	B	2	LEU	4.3
1	A	88	HIS	4.2
1	B	89[A]	GLY	3.8
1	A	87[A]	SER	3.5
1	A	255	HIS	3.3
1	B	91[A]	ASP	2.4
1	A	2	LEU	2.2
1	B	87[A]	SER	2.2
1	B	255	HIS	2.1
1	B	5	ASP	2.1
1	A	163	GLN	2.1
1	B	185[A]	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

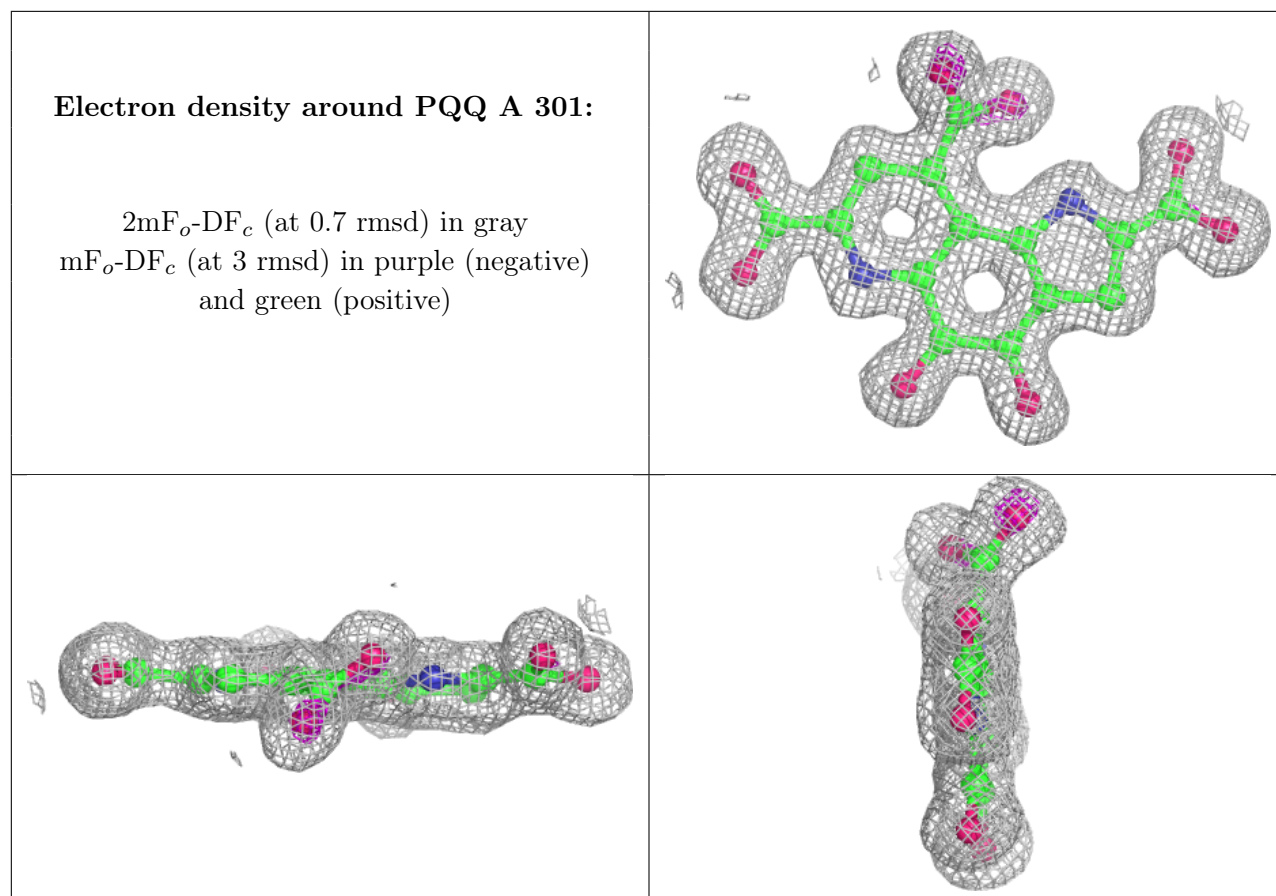
There are no monosaccharides in this entry.

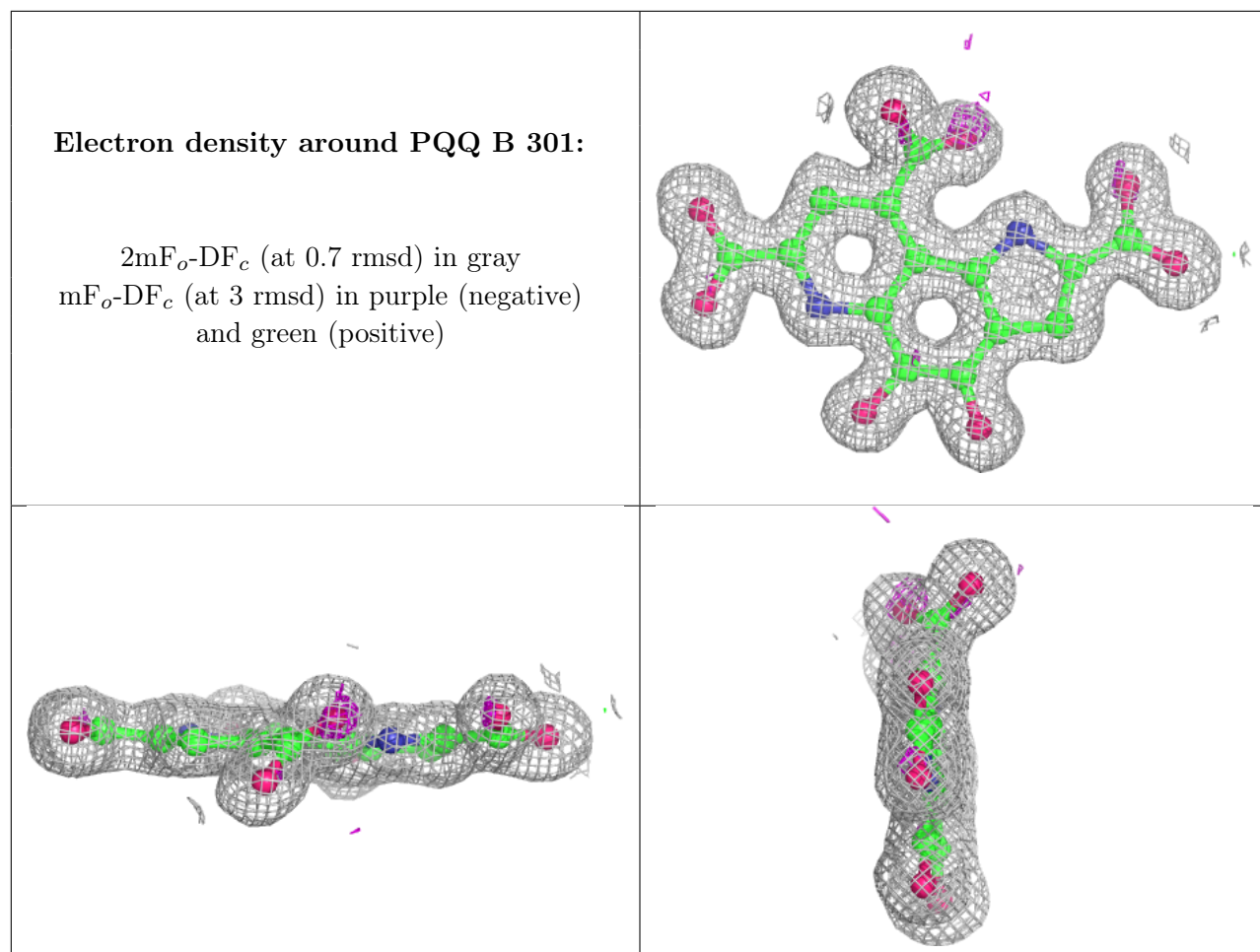
6.4 Ligands

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	GOL	A	307	6/6	0.73	0.36	75,109,111,136	0
3	GOL	A	306	6/6	0.74	0.46	54,67,107,108	0
3	GOL	B	306	6/6	0.77	0.26	49,57,67,70	0
3	GOL	A	303	6/6	0.81	0.22	24,38,42,59	0
3	GOL	A	305	6/6	0.82	0.34	45,46,51,59	6
3	GOL	B	305	6/6	0.84	0.41	44,75,81,105	6
3	GOL	B	307	6/6	0.86	0.34	50,54,61,113	0
3	GOL	B	303	6/6	0.88	0.17	34,43,45,50	0
3	GOL	A	302	6/6	0.93	0.14	14,39,46,54	0
3	GOL	B	302	6/6	0.94	0.13	15,36,38,48	0
2	PQQ	A	301	24/24	0.98	0.04	8,10,13,15	0
2	PQQ	B	301	24/24	0.98	0.05	9,11,13,16	0
4	CL	A	304	1/1	1.00	0.03	13,13,13,13	0
4	CL	B	304	1/1	1.00	0.02	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 [i](#)

There are no such residues in this entry.