



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 01:49 PM EDT

PDB ID : 5ENP
Title : MBX2931 bound structure of bacterial efflux pump.
Authors : Sjuts, H.; Ornik, A.R.; Pos, K.M.
Deposited on : 2015-11-09
Resolution : 1.90 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	:	2.37.1
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)	:	2.37.1

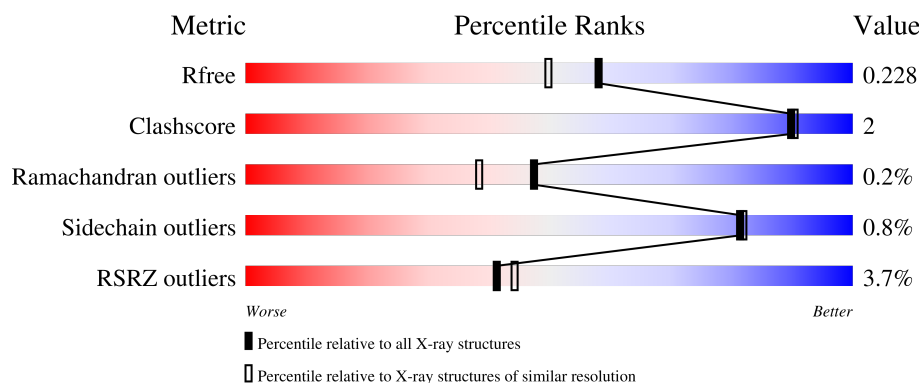
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	609	 4% 90% 5% 5%
1	B	609	 2% 89% 5% 5%
1	C	609	 3% 88% 6% 5%
2	D	169	 4% 92% 5% 5%
2	E	169	 7% 90% 8% 5%

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Mol	Chain	Length	Quality of chain
2	F	169	<div><div></div><div>7%</div><div>87%</div><div>9%</div><div>.</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18206 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 Multidrug efflux pump subunit AcrB, Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	3	0
			4431	2783	749	877	22			
1	B	578	Total	C	N	O	S	0	2	0
			4411	2770	746	873	22			
1	C	578	Total	C	N	O	S	0	1	0
			4404	2766	745	871	22			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLY	-	linker	UNP P31224
A	553	GLY	-	linker	UNP P31224
A	554	SER	-	linker	UNP P31224
A	555	GLY	-	linker	UNP P31224
A	556	GLY	-	linker	UNP P31224
A	557	SER	-	linker	UNP P31224
A	558	GLY	-	linker	UNP P31224
A	559	GLY	-	linker	UNP P31224
A	560	SER	-	linker	UNP P31224
B	552	GLY	-	linker	UNP P31224
B	553	GLY	-	linker	UNP P31224
B	554	SER	-	linker	UNP P31224
B	555	GLY	-	linker	UNP P31224
B	556	GLY	-	linker	UNP P31224
B	557	SER	-	linker	UNP P31224
B	558	GLY	-	linker	UNP P31224
B	559	GLY	-	linker	UNP P31224
B	560	SER	-	linker	UNP P31224
C	552	GLY	-	linker	UNP P31224
C	553	GLY	-	linker	UNP P31224
C	554	SER	-	linker	UNP P31224
C	555	GLY	-	linker	UNP P31224

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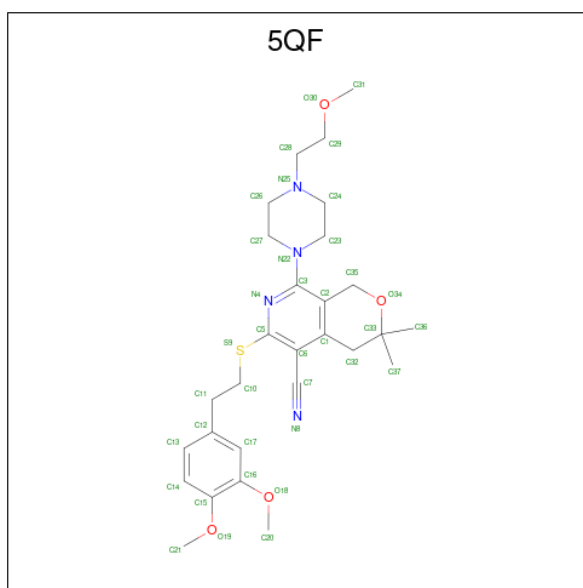
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Chain	Residue	Modelled	Actual	Comment	Reference
C	556	GLY	-	linker	UNP P31224
C	557	SER	-	linker	UNP P31224
C	558	GLY	-	linker	UNP P31224
C	559	GLY	-	linker	UNP P31224
C	560	SER	-	linker	UNP P31224

- Molecule 2 is a protein called DARPin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	161	Total	C	N	O	S	0	0	0
			1227	771	221	234	1			
2	E	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	F	162	Total	C	N	O	S	0	0	0
			1237	777	224	235	1			

- Molecule 3 is 6-[2-(3,4-dimethoxyphenyl)ethylsulfanyl]-8-[4-(2-methoxyethyl)piperazin-1-yl]-3,3-dimethyl-1,4-dihydropyrano[3,4-c]pyridine-5-carbonitrile (three-letter code: 5QF) (formula: C₂₈H₃₈N₄O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			37	28	4	4	1		

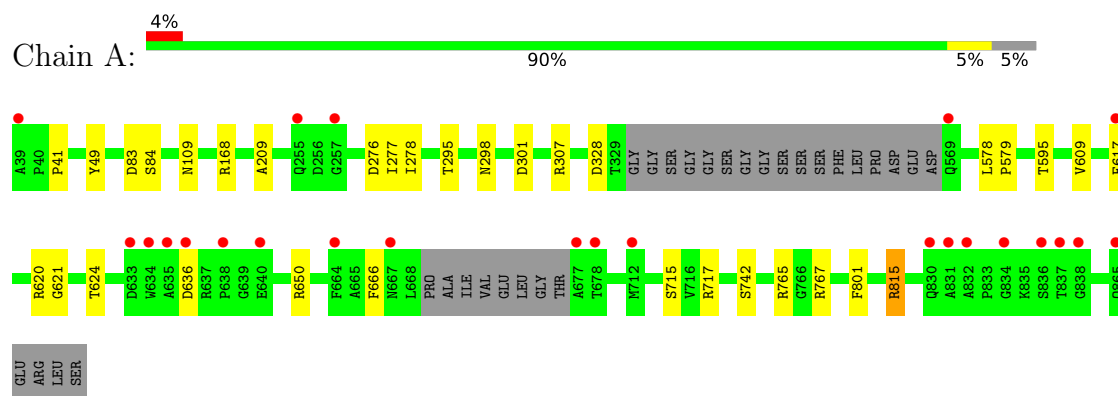
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	385	Total 385	O 385	0	0
4	B	385	Total 385	O 385	0	0
4	C	354	Total 354	O 354	0	0
4	D	64	Total 64	O 64	0	0
4	E	45	Total 45	O 45	0	0
4	F	49	Total 49	O 49	0	0

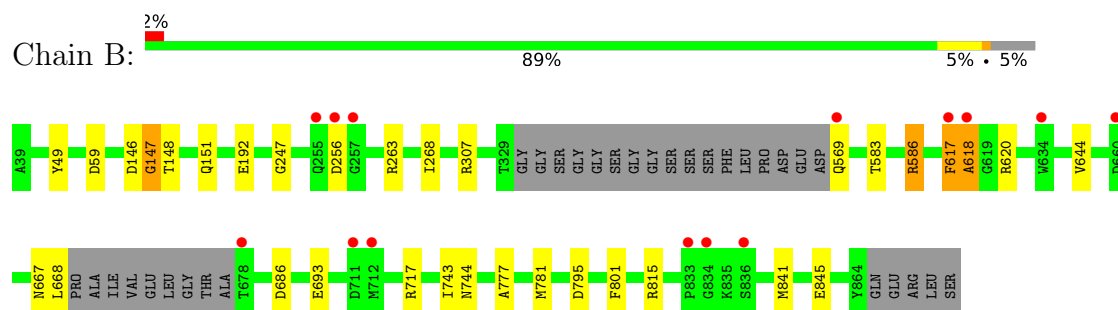
3 Residue-property plots [i](#)

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.

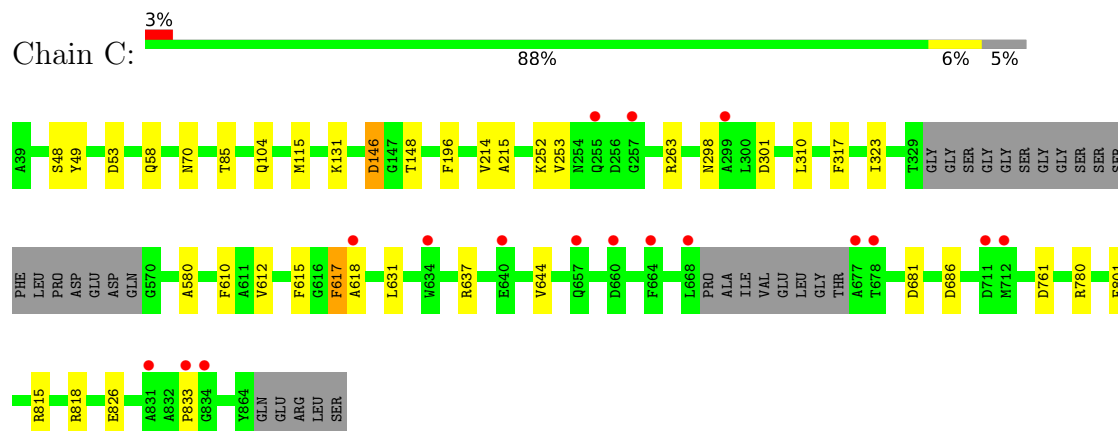
- Molecule 1: Multidrug efflux pump subunit AcrB, Multidrug efflux pump subunit AcrB



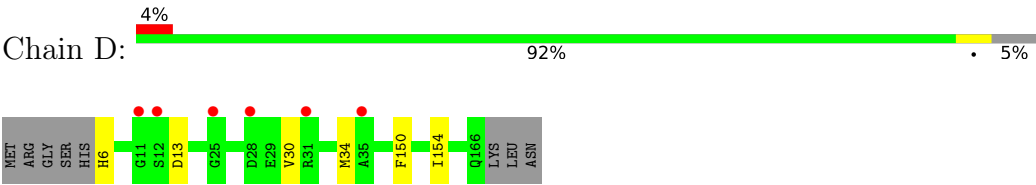
- Molecule 1: Multidrug efflux pump subunit AcrB, Multidrug efflux pump subunit AcrB



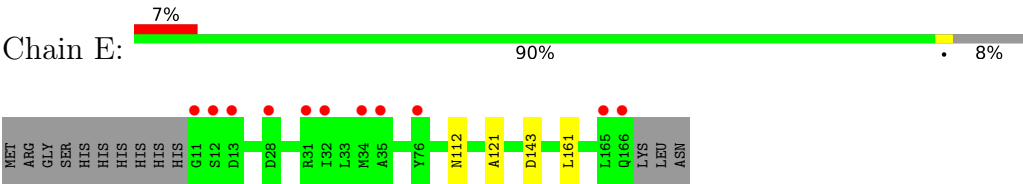
- Molecule 1: Multidrug efflux pump subunit AcrB, Multidrug efflux pump subunit AcrB



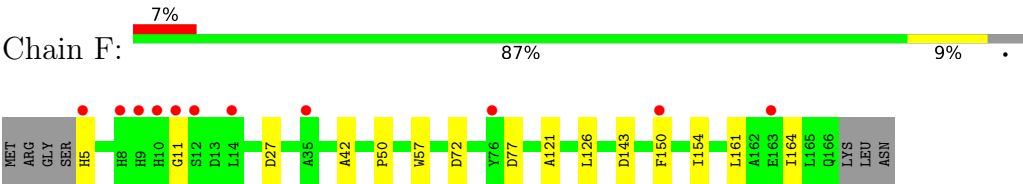
● Molecule 2: DARPin



● Molecule 2: DARPin



● Molecule 2: DARPin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.65Å 145.34Å 174.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 49.64 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.90) 99.8 (49.64-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.182 , 0.222 0.191 , 0.228	Depositor DCC
R_{free} test set	10661 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18206	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: 5QF

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	0.96	2/4515 (0.0%)	0.93	10/6119 (0.2%)
1	B	0.93	0/4492	0.96	10/6086 (0.2%)
1	C	0.90	1/4482 (0.0%)	0.94	15/6073 (0.2%)
2	D	0.88	0/1251	0.89	1/1701 (0.1%)
2	E	0.79	0/1196	0.90	2/1626 (0.1%)
2	F	0.83	1/1262 (0.1%)	0.88	2/1716 (0.1%)
All	All	0.91	4/17198 (0.0%)	0.93	40/23321 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	SER	CB-OG	8.54	1.53	1.42
1	C	48	SER	CB-OG	-5.42	1.35	1.42
1	A	765	ARG	CZ-NH2	5.26	1.39	1.33
2	F	57	TRP	CB-CG	5.08	1.59	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	815	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	717	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	761	ASP	CB-CG-OD1	7.69	125.22	118.30
1	C	263	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	767	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	E	143	ASP	CB-CG-OD1	6.65	124.29	118.30
1	C	637	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	307	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	A	765	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	C	686	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	795	ASP	CB-CG-OD1	6.32	123.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	77	ASP	CB-CG-OD1	6.32	123.98	118.30
1	C	780	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	815	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	E	143	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	307	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	115	MET	CG-SD-CE	6.18	110.09	100.20
1	B	717	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	586	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	780	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	168	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	586	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	650	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	276	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	168	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	263	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	815	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	761	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	818	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	815	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	146	ASP	CB-CA-C	-5.37	99.65	110.40
1	B	686	ASP	CB-CG-OD1	5.35	123.11	118.30
1	C	146	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	53	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	815	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	F	143	ASP	CB-CG-OD1	5.13	122.92	118.30
2	D	13	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	637	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	617	PHE	CB-CA-C	5.05	120.51	110.40
1	B	59	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4431	0	4377	14	0
1	B	4411	0	4353	17	0
1	C	4404	0	4345	19	0
2	D	1227	0	1194	4	0
2	E	1177	0	1159	2	0
2	F	1237	0	1201	5	0
3	C	37	0	0	0	0
4	A	385	0	0	4	0
4	B	385	0	0	6	0
4	C	354	0	0	5	0
4	D	64	0	0	1	0
4	E	45	0	0	1	0
4	F	49	0	0	0	0
All	All	18206	0	16629	60	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 2.

All (60) 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:298:ASN:HD22	1:A:301:ASP:H	1.37	0.73
2:D:150:PHE:CE2	2:D:154:ILE:HD11	2.24	0.72
1:A:620:ARG:HD3	4:A:902:HOH:O	1.90	0.71
1:C:58:GLN:OE1	4:C:1001:HOH:O	2.10	0.70
1:B:620:ARG:HD3	4:B:902:HOH:O	1.91	0.70
1:B:644:VAL:CG1	1:B:667:ASN:HD21	2.10	0.63
2:D:6:HIS:N	4:D:202:HOH:O	2.31	0.62
1:B:192:GLU:HG3	4:B:1237:HOH:O	2.03	0.58
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.85	0.58
4:A:920:HOH:O	1:C:214:VAL:HG13	2.03	0.58
1:A:209:ALA:HB1	1:B:743:ILE:HG21	1.85	0.57
1:A:109:ASN:HB3	4:C:1309:HOH:O	2.05	0.56
1:B:644:VAL:HG11	1:B:667:ASN:HD21	1.71	0.56
1:B:744:ASN:CG	4:B:1033:HOH:O	2.44	0.55
1:C:298:ASN:HD22	1:C:301:ASP:H	1.53	0.55
1:C:644:VAL:HG23	4:C:1033:HOH:O	2.06	0.55
1:B:583:THR:HG23	1:B:586:ARG:H	1.71	0.55
1:C:580:ALA:HA	4:C:1076:HOH:O	2.07	0.54
1:B:693:GLU:OE2	4:B:901:HOH:O	2.19	0.53
1:B:617:PHE:O	1:B:618:ALA:CB	2.58	0.52
1:B:247:GLY:HA2	1:B:268:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:914:HOH:O	1:C:70:ASN:HB3	2.10	0.51
1:B:841:MET:O	1:B:845:GLU:HG3	2.11	0.51
1:A:595[B]:THR:HG22	1:A:609:VAL:HG11	1.92	0.51
1:A:621:GLY:O	1:A:624:THR:HG22	2.11	0.51
1:B:569:GLN:O	1:B:644:VAL:HG21	2.11	0.50
1:B:617:PHE:O	1:B:618:ALA:HB3	2.11	0.50
1:C:631:LEU:CD1	1:C:644:VAL:HG22	2.42	0.50
1:A:298:ASN:ND2	1:A:301:ASP:H	2.09	0.48
1:C:104:GLN:OE1	1:C:131:LYS:HG3	2.13	0.48
1:C:681:ASP:OD1	1:C:826:GLU:OE1	2.31	0.48
1:A:277:ILE:O	1:A:278:ILE:HD13	2.14	0.48
1:C:580:ALA:CA	4:C:1076:HOH:O	2.61	0.47
2:F:150:PHE:CZ	2:F:154:ILE:HD11	2.49	0.47
1:C:317:PHE:HZ	1:C:323:ILE:HD11	1.80	0.46
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.98	0.46
2:F:126:LEU:HD22	2:F:164:ILE:HD12	1.98	0.46
4:A:984:HOH:O	1:C:253:VAL:HG21	2.16	0.46
2:D:30:VAL:O	2:D:34:MET:HG2	2.17	0.45
2:D:34:MET:HA	2:D:34:MET:CE	2.47	0.45
1:B:777:ALA:O	1:B:781:MET:HG2	2.16	0.45
1:C:617:PHE:O	1:C:618:ALA:HB3	2.16	0.45
1:C:146:ASP:HB3	1:C:148:THR:HG23	2.00	0.44
2:F:5:HIS:HD2	2:F:72:ASP:OD2	2.01	0.43
1:A:617:PHE:CZ	1:A:666:PHE:HZ	2.36	0.43
1:A:595[B]:THR:HG21	4:A:1144:HOH:O	2.18	0.43
2:F:121:ALA:HB1	2:F:161:LEU:HD21	2.00	0.43
1:C:214:VAL:CG1	1:C:215:ALA:N	2.83	0.42
1:C:310:LEU:HB3	1:C:323:ILE:HD13	2.01	0.42
1:B:146:ASP:HB2	1:B:148:THR:OG1	2.19	0.42
4:B:1173:HOH:O	1:C:85:THR:HG22	2.20	0.41
1:B:667:ASN:O	1:B:668:LEU:HB2	2.20	0.41
2:E:112:ASN:OD1	4:E:201:HOH:O	2.22	0.41
1:C:612:VAL:HG11	1:C:615:PHE:CE2	2.56	0.41
2:E:121:ALA:HB1	2:E:161:LEU:HD21	2.03	0.41
1:A:578:LEU:HD12	1:A:578:LEU:N	2.36	0.41
1:C:196:PHE:O	1:C:252:LYS:HE2	2.21	0.41
1:A:83:ASP:OD1	1:A:815:ARG:HD3	2.20	0.40
1:B:146:ASP:O	1:B:147:GLY:C	2.59	0.40
2:F:42:ALA:O	2:F:50:PRO:HD3	2.22	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	577/609 (95%)	562 (97%)	15 (3%)	0	100	100
1	B	574/609 (94%)	561 (98%)	11 (2%)	2 (0%)	41	31
1	C	573/609 (94%)	555 (97%)	17 (3%)	1 (0%)	47	38
2	D	159/169 (94%)	155 (98%)	4 (2%)	0	100	100
2	E	154/169 (91%)	150 (97%)	4 (3%)	0	100	100
2	F	160/169 (95%)	156 (98%)	3 (2%)	1 (1%)	25	15
All	All	2197/2334 (94%)	2139 (97%)	54 (2%)	4 (0%)	47	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	11	GLY
1	B	618	ALA
1	C	833	PRO
1	B	147	GLY

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	474/492 (96%)	468 (99%)	6 (1%)	69	68
1	B	472/492 (96%)	467 (99%)	5 (1%)	73	73
1	C	470/492 (96%)	467 (99%)	3 (1%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	125/132 (95%)	125 (100%)	0	100	100
2	E	120/132 (91%)	120 (100%)	0	100	100
2	F	126/132 (96%)	125 (99%)	1 (1%)	81	82
All	All	1787/1872 (96%)	1772 (99%)	15 (1%)	81	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TYR
1	A	328	ASP
1	A	636	ASP
1	A	715	SER
1	A	742	SER
1	A	801	PHE
1	B	49	TYR
1	B	151	GLN
1	B	256	ASP
1	B	617	PHE
1	B	801	PHE
1	C	49	TYR
1	C	610	PHE
1	C	801	PHE
2	F	27	ASP

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

Mol	Chain	Res	Type
1	A	298	ASN
1	A	577	GLN
1	A	687	GLN
1	B	70	ASN
1	B	112	GLN
1	B	231	ASN
1	B	255	GLN
1	B	667	ASN
1	C	58	GLN
1	C	284	GLN
1	C	298	ASN
1	C	744	ASN
2	F	5	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](#)

1 ligand is modelled in this entry.

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	5QF	C	901	-	40,40,40	1.87	7 (17%)	49,56,56	2.29	16 (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
3	5QF	C	901	-	-	7/19/41/41	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	5QF	C6-C7	-7.50	1.30	1.44
3	C	901	5QF	C5-S9	-4.88	1.70	1.76
3	C	901	5QF	O34-C33	-3.59	1.42	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	5QF	O34-C35	-2.63	1.40	1.43
3	C	901	5QF	C6-C5	-2.62	1.38	1.41
3	C	901	5QF	C5-N4	2.53	1.36	1.33
3	C	901	5QF	C14-C13	2.09	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	5QF	C21-O19-C15	7.39	128.68	117.53
3	C	901	5QF	O19-C15-C16	6.09	123.89	115.41
3	C	901	5QF	C10-S9-C5	4.51	108.92	101.82
3	C	901	5QF	C27-C26-N25	3.91	118.66	110.64
3	C	901	5QF	C2-C3-N4	-3.45	117.29	122.61
3	C	901	5QF	O18-C16-C17	-3.21	118.59	124.12
3	C	901	5QF	C6-C5-S9	3.07	121.18	117.75
3	C	901	5QF	C6-C5-N4	-3.06	120.80	123.12
3	C	901	5QF	C1-C6-C7	3.02	123.51	119.57
3	C	901	5QF	O19-C15-C14	-2.99	119.24	124.37
3	C	901	5QF	C3-N4-C5	2.82	123.93	116.30
3	C	901	5QF	O18-C16-C15	2.74	119.23	115.41
3	C	901	5QF	C10-C11-C12	2.46	118.38	113.97
3	C	901	5QF	C26-C27-N22	-2.38	106.08	110.70
3	C	901	5QF	C6-C7-N8	-2.32	172.15	177.40
3	C	901	5QF	C14-C15-C16	-2.14	116.82	119.70

There are no chirality outliers.

All (7) torsion outliers are listed below:

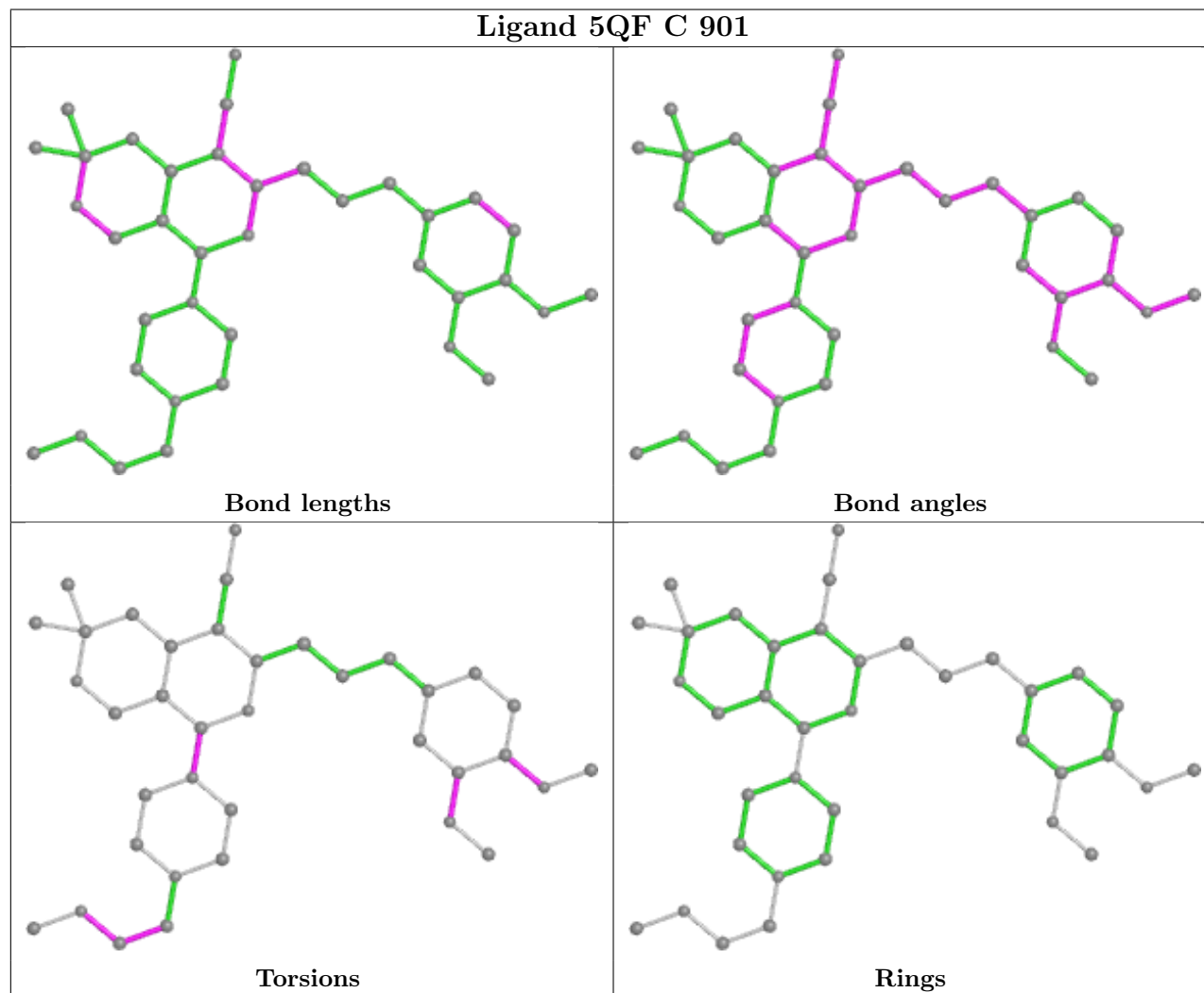
Mol	Chain	Res	Type	Atoms
3	C	901	5QF	C15-C16-O18-C20
3	C	901	5QF	C17-C16-O18-C20
3	C	901	5QF	C14-C15-O19-C21
3	C	901	5QF	N25-C28-C29-O30
3	C	901	5QF	C16-C15-O19-C21
3	C	901	5QF	N4-C3-N22-C27
3	C	901	5QF	C28-C29-O30-C31

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 ⓘ

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	580/609 (95%)	0.17	24 (4%) 37 40	18, 29, 56, 92	0
1	B	578/609 (94%)	0.04	14 (2%) 59 62	18, 28, 53, 104	0
1	C	578/609 (94%)	0.14	17 (2%) 51 54	17, 31, 61, 98	0
2	D	161/169 (95%)	0.11	6 (3%) 41 44	24, 34, 61, 79	0
2	E	156/169 (92%)	0.37	11 (7%) 16 17	27, 40, 70, 125	0
2	F	162/169 (95%)	0.26	11 (6%) 17 19	26, 37, 71, 104	0
All	All	2215/2334 (94%)	0.14	83 (3%) 41 44	17, 31, 61, 125	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	11	GLY	16.0
1	A	677	ALA	6.1
1	C	677	ALA	5.9
2	E	12	SER	5.8
1	A	634	TRP	4.7
1	A	865	GLN	4.6
1	A	678	THR	4.3
1	C	668	LEU	4.2
1	C	634	TRP	4.0
2	E	31	ARG	4.0
2	F	11	GLY	4.0
1	C	618	ALA	3.9
2	F	8	HIS	3.9
1	A	831	ALA	3.8
1	A	837	THR	3.8
2	E	166	GLN	3.6
2	E	28	ASP	3.6
1	A	834	GLY	3.6
1	C	257	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	834	GLY	3.3
2	D	11	GLY	3.3
2	D	12	SER	3.3
1	A	617	PHE	3.2
1	A	569	GLN	3.2
2	F	5	HIS	3.1
2	E	32	ILE	3.1
1	B	617	PHE	3.1
2	F	150	PHE	3.0
1	C	255	GLN	3.0
1	B	834	GLY	3.0
1	B	255	GLN	2.9
2	D	31	ARG	2.9
1	A	640	GLU	2.8
2	F	10	HIS	2.8
1	B	618	ALA	2.8
2	D	28	ASP	2.8
1	B	569	GLN	2.8
1	B	833	PRO	2.8
1	A	255	GLN	2.7
2	E	13	ASP	2.7
1	C	299	ALA	2.7
1	A	633	ASP	2.7
1	A	836	SER	2.7
1	B	634	TRP	2.6
1	A	635	ALA	2.6
1	C	833	PRO	2.6
2	E	76	TYR	2.5
1	A	636	ASP	2.5
1	A	39	ALA	2.5
2	D	35	ALA	2.5
1	C	660	ASP	2.4
1	C	664	PHE	2.4
2	E	165	LEU	2.4
1	B	257	GLY	2.4
1	B	712	MET	2.4
2	E	35	ALA	2.4
1	A	838	GLY	2.4
1	A	664	PHE	2.3
1	C	678	THR	2.3
2	F	9	HIS	2.3
1	B	256	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	35	ALA	2.2
2	F	14	LEU	2.2
1	A	832	ALA	2.2
1	C	831	ALA	2.2
1	B	660	ASP	2.2
1	B	836	SER	2.1
2	E	34	MET	2.1
2	F	12	SER	2.1
1	C	711	ASP	2.1
2	D	25	GLY	2.1
1	A	667	ASN	2.1
2	F	163	GLU	2.1
1	A	638	PRO	2.1
1	B	711	ASP	2.1
1	C	657	GLN	2.1
1	B	678	THR	2.0
1	A	257	GLY	2.0
1	A	712	MET	2.0
1	A	830	GLN	2.0
2	F	76	TYR	2.0
1	C	712	MET	2.0
1	C	640	GLU	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 [\(i\)](#)

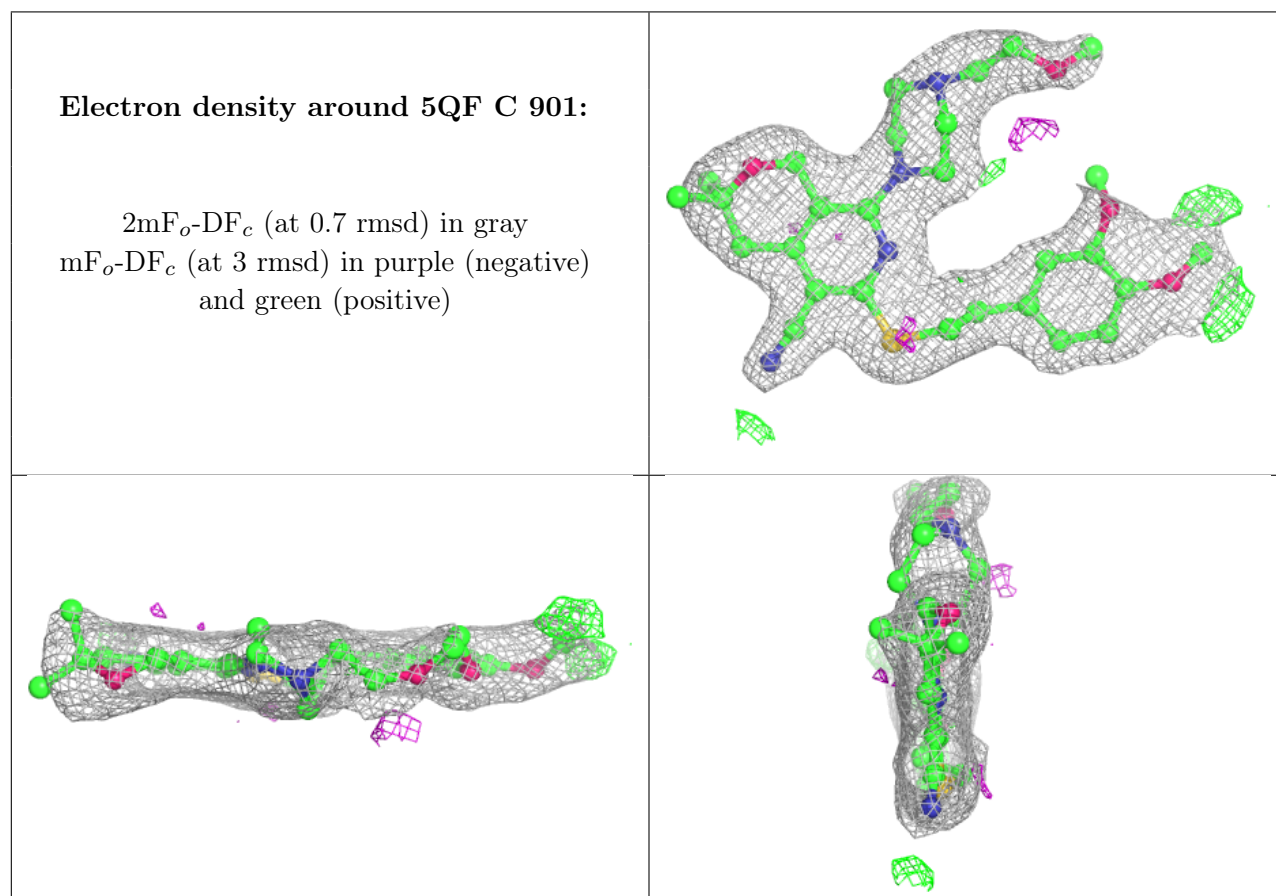
There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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(\AA^2)	Q<0.9
3	5QF	C	901	37/37	0.93	0.13	37,47,69,71	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.