



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:36 PM UTC

PDB ID : 7VCN / pdb_00007vcn
Title : Crystal Structure of PitA fragment from pilus islet-2 of Streptococcus oralis with Tb-Xo4
Authors : Yadav, R.K.; Krishnan, V.
Deposited on : 2021-09-03
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

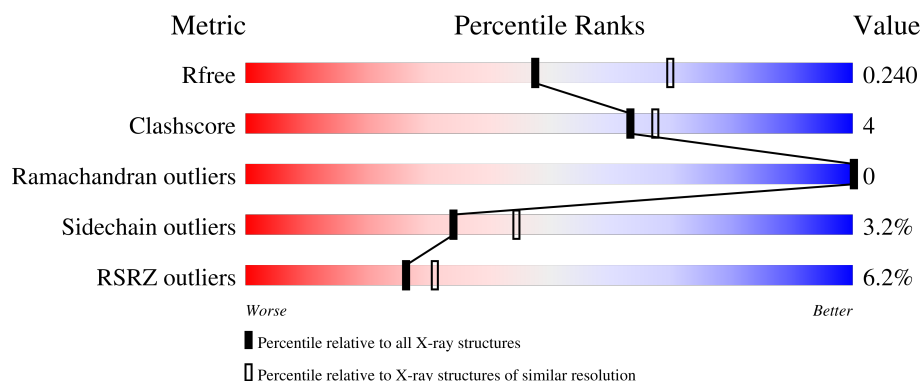
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	C	30	3% 77% 23%
1	D	30	7% 73% 23% .
2	A	471	2% 83% 14% ..
2	B	471	10% 85% 9% ..

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7758 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.

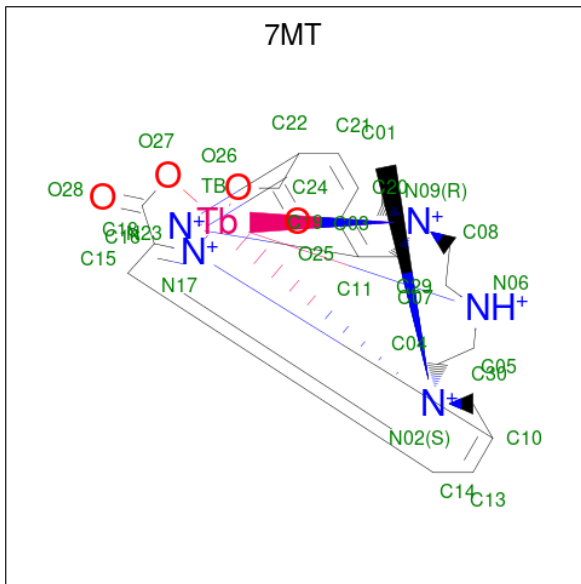
- Molecule 1 is a protein called von Willebrand factor type A domain protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	C	30	Total 236	C 148	N 37	O 51	0	0	0
1	D	30	Total 236	C 148	N 37	O 51	0	0	0

- Molecule 2 is a protein called von Willebrand factor type A domain protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	460	Total 3588	C 2232	N 617	O 739	0	0	0
2	B	450	Total 3521	C 2193	N 603	O 725	0	0	0

- Molecule 3 is Tb-Xo4 (CCD ID: 7MT) (formula: $\text{C}_{20}\text{H}_{23}\text{N}_5\text{O}_4\text{Tb}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	Tb	0	0
			30	20	5	4	1		
3	D	1	Total	C	N	O	Tb	0	0
			30	20	5	4	1		

- Molecule 4 is TERBIUM(III) ION (CCD ID: Tb) (formula: Tb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Tb	0	0
			2	2		
4	B	1	Total	Tb	0	0
			1	1		

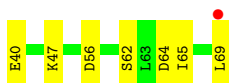
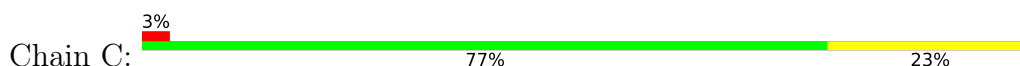
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	13	Total	O	0	0
			13	13		
5	A	74	Total	O	0	0
			74	74		
5	D	8	Total	O	0	0
			8	8		
5	B	19	Total	O	0	0
			19	19		

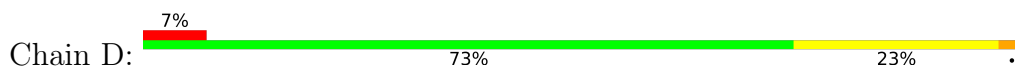
3 Residue-property plots

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.

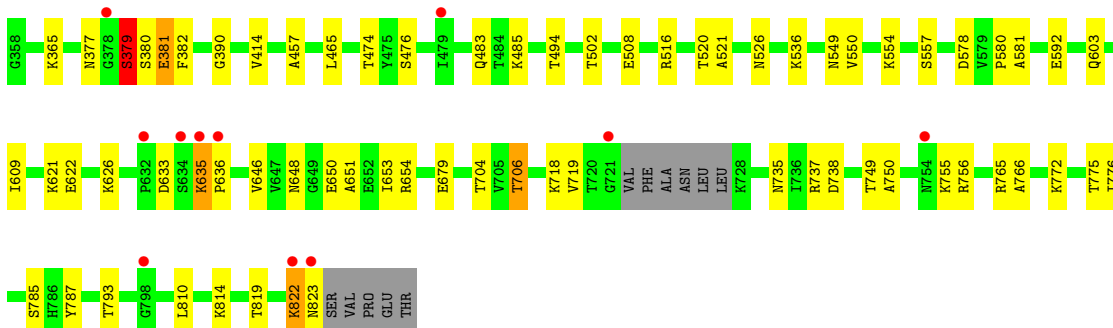
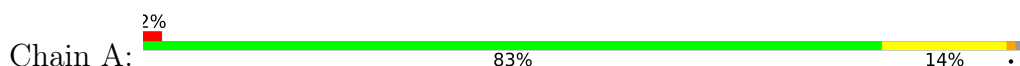
- Molecule 1: von Willebrand factor type A domain protein



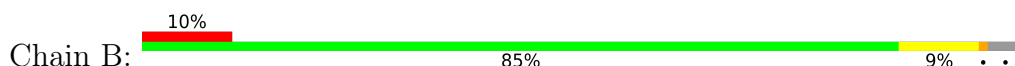
- Molecule 1: von Willebrand factor type A domain protein

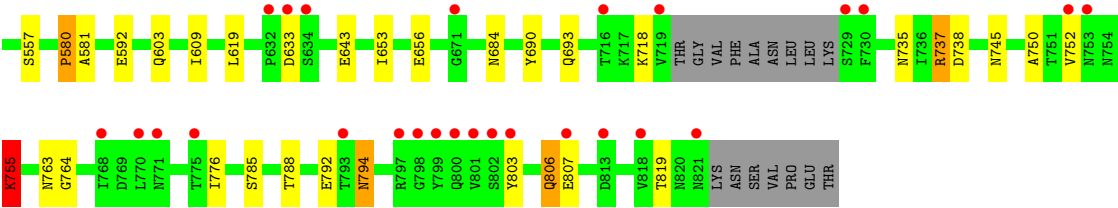


- Molecule 2: von Willebrand factor type A domain protein



- Molecule 2: von Willebrand factor type A domain protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.81Å 70.29Å 82.71Å 79.88° 86.89° 87.19°	Depositor
Resolution (Å)	69.14 – 2.34 69.14 – 2.34	Depositor EDS
% Data completeness (in resolution range)	66.4 (69.14-2.34) 66.4 (69.14-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.240 0.194 , 0.240	Depositor DCC
R_{free} test set	1787 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7758	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TB, 7MT

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	C	0.79	0/239	1.43	1/324 (0.3%)
1	D	0.72	0/239	1.23	0/324
2	A	0.74	0/3645	1.31	20/4931 (0.4%)
2	B	0.62	0/3577	1.14	5/4840 (0.1%)
All	All	0.69	0/7700	1.24	26/10419 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	ASP	CA-CB-CG	9.35	121.95	112.60
2	A	775	THR	CA-CB-OG1	-6.96	99.17	109.60
2	A	549	ASN	CA-CB-CG	-6.61	105.99	112.60
2	A	578	ASP	CA-CB-CG	-6.44	106.16	112.60
2	B	755	LYS	CG-CD-CE	6.26	125.69	111.30
2	A	635	LYS	N-CA-C	6.09	115.14	108.14
2	A	704	THR	CA-CB-OG1	-6.07	100.50	109.60
2	A	650	GLU	CB-CG-CD	5.99	122.78	112.60
2	A	377	ASN	CB-CA-C	-5.96	103.26	111.73
2	B	502	THR	CB-CA-C	5.87	119.87	109.72
2	B	794	ASN	CB-CA-C	-5.80	101.74	110.90
2	A	706	THR	CA-CB-OG1	-5.55	101.27	109.60
2	A	775	THR	CA-C-N	-5.48	116.03	123.10
2	A	775	THR	C-N-CA	-5.48	116.03	123.10
2	B	508	GLU	CB-CG-CD	5.45	121.86	112.60
2	A	379	SER	CA-C-N	5.44	128.32	120.38
2	A	379	SER	C-N-CA	5.44	128.32	120.38
2	A	592	GLU	CB-CG-CD	5.40	121.78	112.60
2	A	474	THR	CA-CB-OG1	-5.30	101.65	109.60
2	A	648	ASN	CA-CB-CG	-5.29	107.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	592	GLU	CB-CG-CD	5.27	121.56	112.60
2	A	381	GLU	CB-CA-C	-5.20	104.89	111.86
2	A	766	ALA	CA-C-N	-5.17	113.75	122.29
2	A	766	ALA	C-N-CA	-5.17	113.75	122.29
2	A	380	SER	CA-C-N	5.15	129.50	122.34
2	A	380	SER	C-N-CA	5.15	129.50	122.34

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	C	236	0	235	3	0
1	D	236	0	236	7	0
2	A	3588	0	3544	29	0
2	B	3521	0	3473	27	0
3	C	30	0	0	0	0
3	D	30	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	74	0	0	0	0
5	B	19	0	0	0	0
5	C	13	0	0	0	0
5	D	8	0	0	0	0
All	All	7758	0	7488	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 4.

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)
2:B:788:THR:HG22	2:B:807:GLU:HG3	1.46	0.96
2:A:718:LYS:HB2	2:A:819:THR:HG22	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:520:THR:H	2:A:603:GLN:HE22	1.22	0.86
2:B:520:THR:H	2:B:603:GLN:HE22	1.37	0.71
2:A:750:ALA:HB1	2:A:776:ILE:HD11	1.75	0.68
2:A:738:ASP:HA	2:A:785:SER:HB3	1.80	0.63
1:D:47:LYS:HD3	2:B:493:PRO:CD	2.29	0.62
2:B:803:TYR:HB3	2:B:806:GLN:HB3	1.83	0.61
2:B:792:GLU:OE1	2:B:794:ASN:HB2	2.01	0.60
1:D:40:GLU:HB3	2:B:477:TYR:CZ	2.37	0.59
2:B:718:LYS:HB2	2:B:819:THR:HG22	1.86	0.58
2:A:526:ASN:HB2	2:A:550:VAL:O	2.02	0.58
2:B:803:TYR:CD2	2:B:806:GLN:OE1	2.57	0.58
2:B:737:ARG:O	2:B:785:SER:HB2	2.05	0.57
2:A:516:ARG:HB2	2:A:516:ARG:NH1	2.23	0.53
2:A:737:ARG:O	2:A:785:SER:HB2	2.09	0.52
2:A:646:VAL:HG22	2:A:651:ALA:HB2	1.91	0.52
2:B:803:TYR:CB	2:B:806:GLN:HB3	2.42	0.50
2:B:609:ILE:HG13	2:B:653:ILE:HD13	1.94	0.49
2:A:822:LYS:O	2:A:823:ASN:HB2	2.12	0.49
2:A:622:GLU:OE1	2:A:654:ARG:NH1	2.43	0.49
2:B:477:TYR:H	2:B:483:GLN:N	2.11	0.48
2:B:360:HIS:HD2	2:B:361:HIS:ND1	2.12	0.48
2:A:382:PHE:HE2	2:A:414:VAL:HG11	1.78	0.48
2:A:520:THR:N	2:A:603:GLN:HE22	2.03	0.48
2:A:508:GLU:HA	2:A:557:SER:O	2.14	0.48
2:B:580:PRO:O	2:B:581:ALA:HB3	2.14	0.47
1:D:65:ILE:HD13	2:B:473:VAL:HG11	1.95	0.47
1:C:64:ASP:C	1:C:64:ASP:OD1	2.57	0.47
2:A:810:LEU:HD23	2:A:814:LYS:HG2	1.96	0.47
2:B:446:ILE:HG12	2:B:500:PRO:HD3	1.96	0.47
2:B:745:ASN:ND2	2:B:763:ASN:H	2.13	0.47
2:A:765:ARG:HB3	2:A:765:ARG:NH1	2.30	0.47
2:A:465:LEU:O	2:A:494:THR:HA	2.15	0.47
1:C:47:LYS:HA	1:C:62:SER:O	2.15	0.47
2:A:735:ASN:O	2:A:787:TYR:HA	2.16	0.46
2:A:390:GLY:HA3	2:B:684:ASN:HD22	1.80	0.46
1:D:40:GLU:HB3	2:B:477:TYR:CE2	2.50	0.46
1:D:64:ASP:OD1	1:D:64:ASP:C	2.60	0.45
1:C:40:GLU:OE2	2:A:485:LYS:HE2	2.16	0.45
2:B:465:LEU:O	2:B:494:THR:HA	2.17	0.45
1:D:47:LYS:HG3	1:D:63:LEU:HG	2.00	0.44
2:B:750:ALA:HB1	2:B:776:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:476:SER:HA	2:A:483:GLN:O	2.17	0.44
2:A:626:LYS:HE2	2:A:626:LYS:HB3	1.78	0.44
2:A:580:PRO:O	2:A:581:ALA:HB3	2.18	0.43
2:B:383:ARG:HG2	2:B:383:ARG:HH11	1.82	0.43
2:B:738:ASP:HA	2:B:785:SER:HB3	1.99	0.43
1:D:43:THR:HA	1:D:66:THR:O	2.19	0.43
2:B:690:TYR:HB3	2:B:693:GLN:HB2	2.01	0.43
2:A:609:ILE:HG13	2:A:653:ILE:CD1	2.49	0.42
2:A:719:VAL:HG21	2:A:772:LYS:HB2	2.01	0.42
2:B:752:VAL:O	2:B:755:LYS:HB2	2.19	0.42
2:A:379:SER:O	2:A:381:GLU:HG3	2.20	0.42
2:B:508:GLU:HA	2:B:557:SER:O	2.20	0.42
2:B:735:ASN:HA	2:B:764:GLY:O	2.19	0.42
2:A:457:ALA:HB2	2:A:465:LEU:HD23	2.02	0.41
2:A:635:LYS:HG2	2:A:636:PRO:HD2	2.01	0.41
2:A:749:THR:HG21	2:A:756:ARG:NH1	2.34	0.41
2:A:521:ALA:H	2:A:603:GLN:NE2	2.20	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	C	28/30 (93%)	28 (100%)	0	0	100	100
1	D	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
2	A	456/471 (97%)	442 (97%)	14 (3%)	0	100	100
2	B	444/471 (94%)	435 (98%)	9 (2%)	0	100	100
All	All	956/1002 (95%)	931 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	29/29 (100%)	27 (93%)	2 (7%)	14	15
1	D	29/29 (100%)	27 (93%)	2 (7%)	14	15
2	A	408/418 (98%)	396 (97%)	12 (3%)	37	48
2	B	401/418 (96%)	389 (97%)	12 (3%)	36	47
All	All	867/894 (97%)	839 (97%)	28 (3%)	34	44

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	65	ILE
1	C	69	LEU
2	A	365	LYS
2	A	379	SER
2	A	502	THR
2	A	536	LYS
2	A	554	LYS
2	A	621	LYS
2	A	633	ASP
2	A	679	GLU
2	A	706	THR
2	A	755	LYS
2	A	793	THR
2	A	822	LYS
1	D	65	ILE
1	D	69	LEU
2	B	451	LYS
2	B	502	THR
2	B	518	VAL
2	B	526	ASN
2	B	580	PRO
2	B	619	LEU
2	B	633	ASP
2	B	643	GLU

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Mol	Chain	Res	Type
2	B	656	GLU
2	B	737	ARG
2	B	755	LYS
2	B	806	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	46	HIS
2	A	373	GLN
2	A	421	ASN
2	A	481	ASN
2	A	492	ASN
2	A	549	ASN
2	A	551	ASN
2	A	558	ASN
2	A	603	GLN
2	A	693	GLN
2	A	740	GLN
2	A	821	ASN
2	B	360	HIS
2	B	373	GLN
2	B	377	ASN
2	B	492	ASN
2	B	526	ASN
2	B	551	ASN
2	B	562	ASN
2	B	594	ASN
2	B	603	GLN
2	B	684	ASN
2	B	693	GLN
2	B	740	GLN
2	B	745	ASN
2	B	754	ASN
2	B	806	GLN

5.3.3 RNA ⓘ

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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	7MT	D	901	1	29,38,38	2.33	3 (10%)	39,76,76	2.07	11 (28%)
3	7MT	C	901	1	29,38,38	2.19	4 (13%)	39,76,76	2.41	13 (33%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	7MT	C11-N23	11.38	1.49	1.34
3	C	901	7MT	C11-N23	9.96	1.47	1.34
3	C	901	7MT	O27-C18	-2.92	1.22	1.28
3	D	901	7MT	C03-N09	-2.73	1.45	1.49
3	C	901	7MT	O26-C24	-2.62	1.23	1.28
3	C	901	7MT	C03-N09	-2.31	1.46	1.49
3	D	901	7MT	O27-C18	-2.09	1.24	1.28

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	7MT	C05-C04-N02	-6.07	108.13	112.88
3	D	901	7MT	C11-C29-N09	-5.63	104.41	112.46
3	C	901	7MT	C16-N17-C10	5.12	122.57	118.70
3	C	901	7MT	C04-N02-C30	-4.87	102.50	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	7MT	C01-C03-N09	-4.67	109.22	112.88
3	C	901	7MT	O27-C18-C16	-4.28	110.16	115.69
3	D	901	7MT	C05-C04-N02	-4.08	109.69	112.88
3	C	901	7MT	C30-C10-N17	4.08	120.88	115.94
3	C	901	7MT	C11-C29-N09	-4.00	106.73	112.46
3	D	901	7MT	C04-N02-C30	-3.90	103.96	109.83
3	C	901	7MT	C19-C11-N23	-3.79	119.04	121.74
3	D	901	7MT	C07-C08-N09	3.50	115.61	112.88
3	C	901	7MT	C13-C10-N17	-3.09	119.54	121.74
3	D	901	7MT	C16-N17-C10	3.05	121.00	118.70
3	C	901	7MT	C03-N09-C29	-2.97	105.37	109.83
3	D	901	7MT	C03-N09-C29	-2.94	105.41	109.83
3	D	901	7MT	C19-C20-C21	2.83	123.89	120.24
3	C	901	7MT	C01-C03-N09	-2.80	110.69	112.88
3	D	901	7MT	C04-N02-C01	-2.77	105.69	109.86
3	C	901	7MT	C22-N23-C11	2.52	120.61	118.70
3	C	901	7MT	C29-C11-C19	2.41	126.57	122.12
3	C	901	7MT	C19-C20-C21	2.39	123.31	120.24
3	D	901	7MT	C30-C10-N17	2.34	118.78	115.94
3	D	901	7MT	O26-C24-C22	-2.05	113.04	115.69

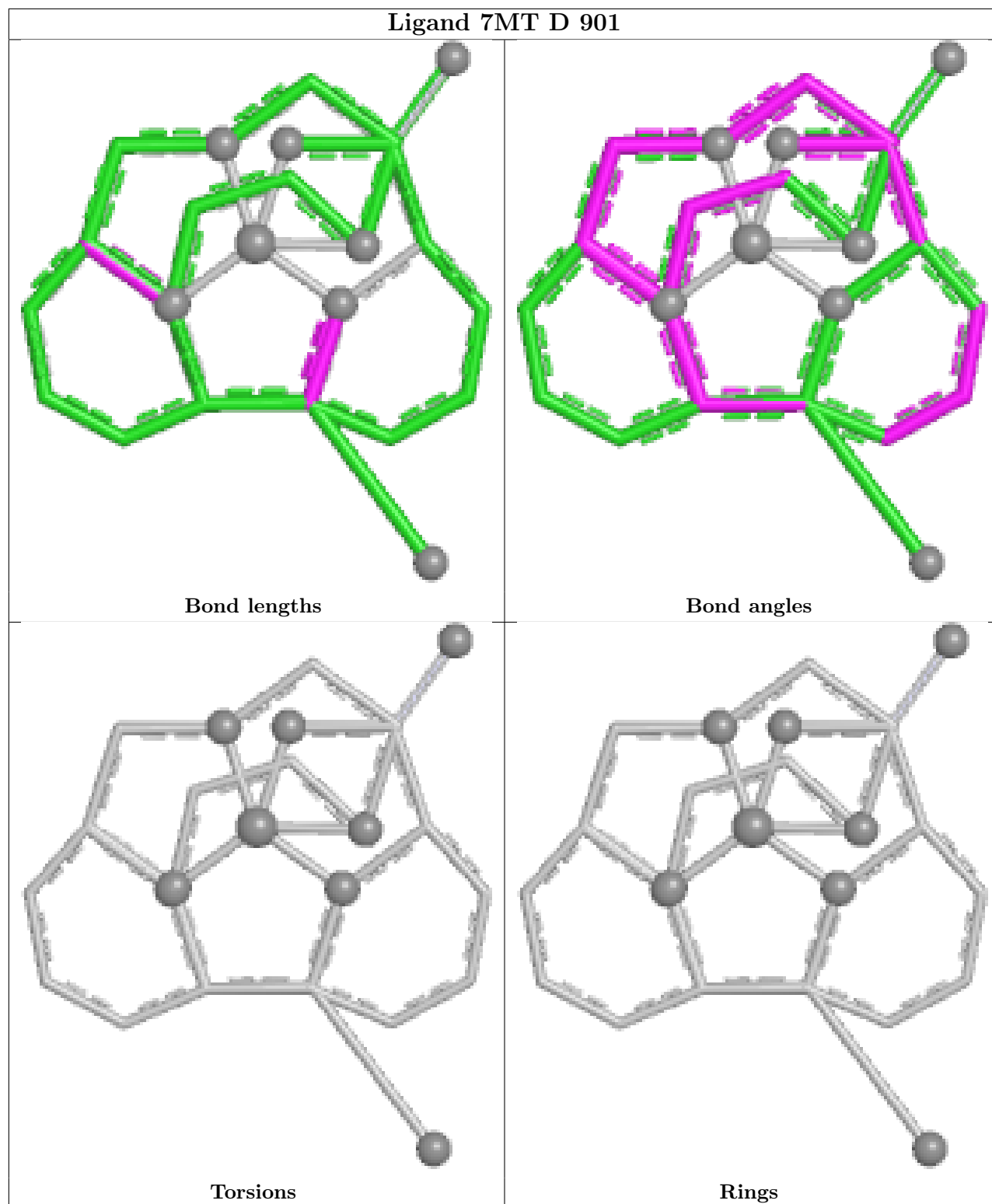
There are no chirality outliers.

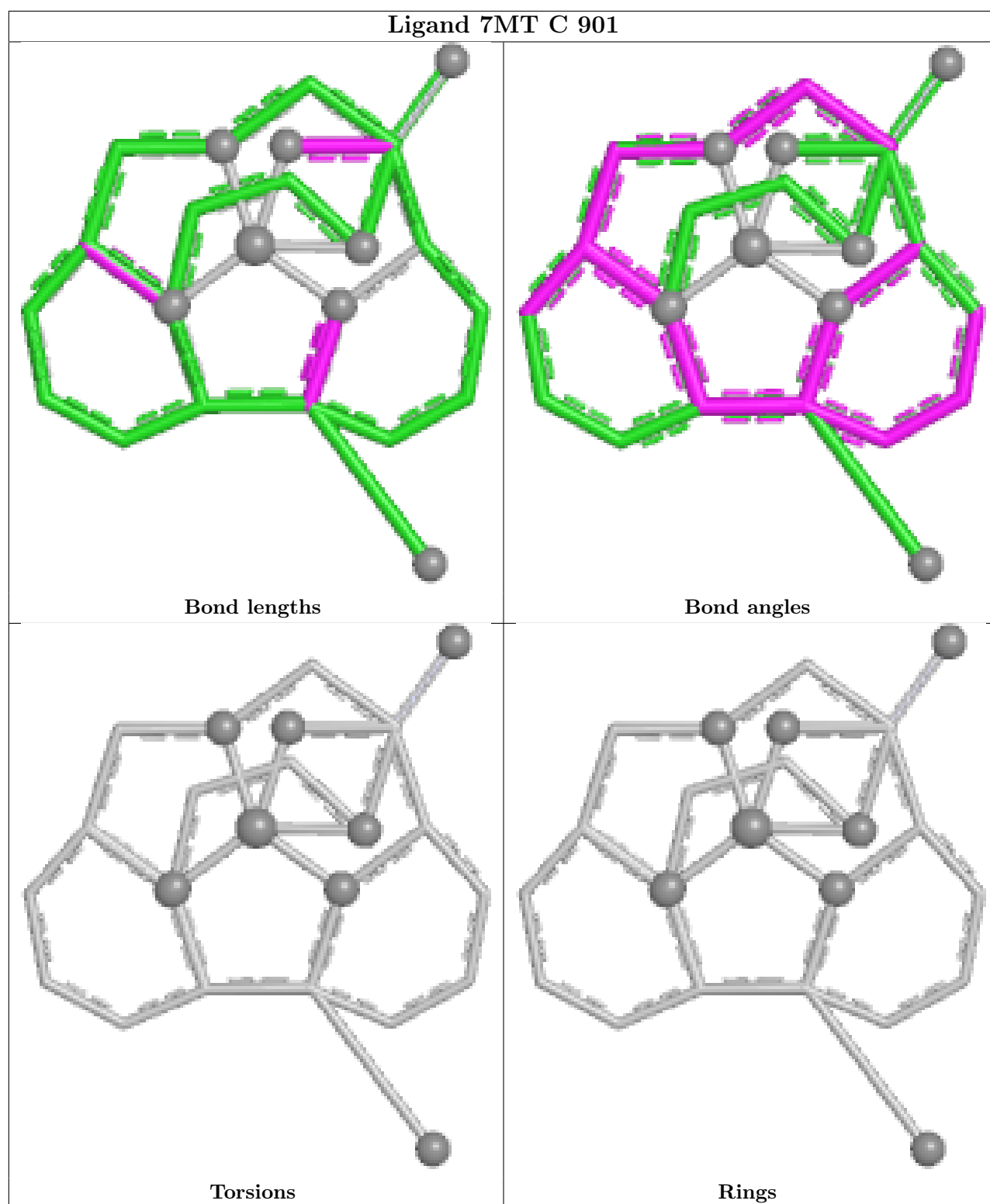
There are no torsion outliers.

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	C	30/30 (100%)	-0.01	1 (3%) 49 55	28, 42, 88, 92	0
1	D	30/30 (100%)	0.46	2 (6%) 24 28	36, 55, 116, 123	0
2	A	460/471 (97%)	-0.15	11 (2%) 59 65	27, 46, 89, 134	0
2	B	450/471 (95%)	0.58	46 (10%) 12 14	36, 68, 143, 190	0
All	All	970/1002 (96%)	0.21	60 (6%) 26 31	27, 57, 121, 190	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	69	LEU	6.3
2	B	770	LEU	4.8
2	B	477	TYR	4.0
2	A	636	PRO	3.9
2	B	719	VAL	3.8
1	C	69	LEU	3.8
2	A	635	LYS	3.7
2	A	634	SER	3.6
2	A	721	GLY	3.6
2	B	378	GLY	3.5
2	B	358	GLY	3.4
2	B	799	TYR	3.3
2	B	793	THR	3.2
2	A	378	GLY	3.1
2	A	823	ASN	3.1
2	B	405	LYS	3.1
2	B	483	GLN	2.9
2	B	821	ASN	2.9
2	B	403	ASP	2.9
2	B	802	SER	2.8
2	B	771	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	420	PRO	2.7
2	B	730	PHE	2.7
2	B	423	SER	2.7
2	B	801	VAL	2.7
2	A	798	GLY	2.7
2	B	379	SER	2.5
2	A	822	LYS	2.5
2	B	798	GLY	2.5
2	B	484	THR	2.5
1	D	41	PRO	2.5
2	B	632	PRO	2.4
2	A	479	ILE	2.4
2	B	752	VAL	2.4
2	B	377	ASN	2.3
2	B	729	SER	2.3
2	B	818	VAL	2.3
2	B	633	ASP	2.3
2	B	361	HIS	2.3
2	B	671	GLY	2.2
2	B	807	GLU	2.2
2	B	775	THR	2.2
2	B	768	ILE	2.2
2	B	753	ASN	2.2
2	B	408	SER	2.2
2	B	411	LEU	2.2
2	B	397	GLU	2.2
2	B	716	THR	2.2
2	B	475	TYR	2.1
2	B	421	ASN	2.1
2	B	634	SER	2.1
2	A	754	ASN	2.1
2	B	803	TYR	2.1
2	B	451	LYS	2.0
2	B	813	ASP	2.0
2	A	632	PRO	2.0
2	B	800	GLN	2.0
2	B	398	ASN	2.0
2	B	359	ILE	2.0
2	B	797	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

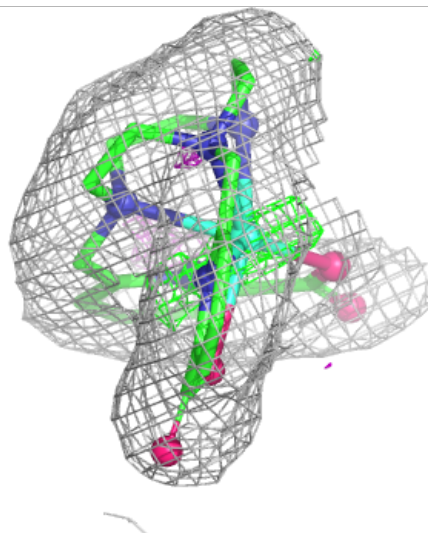
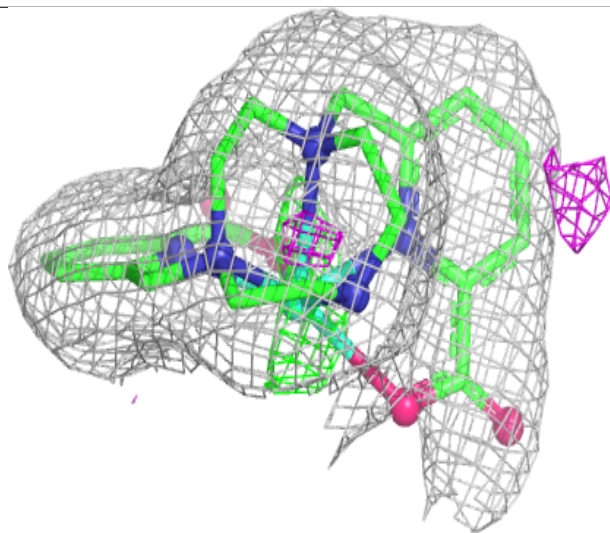
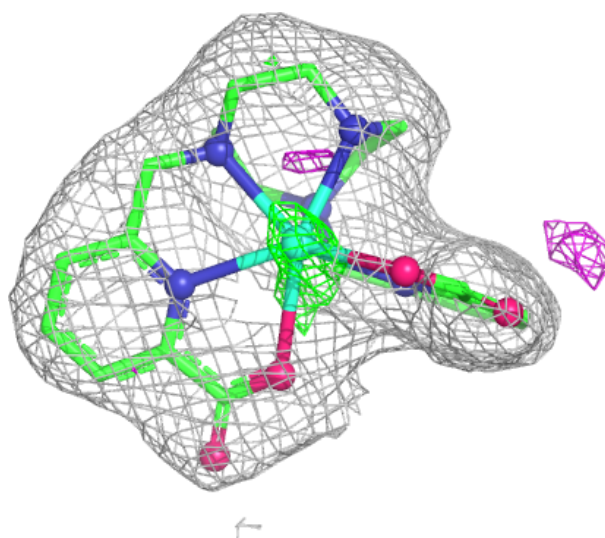
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

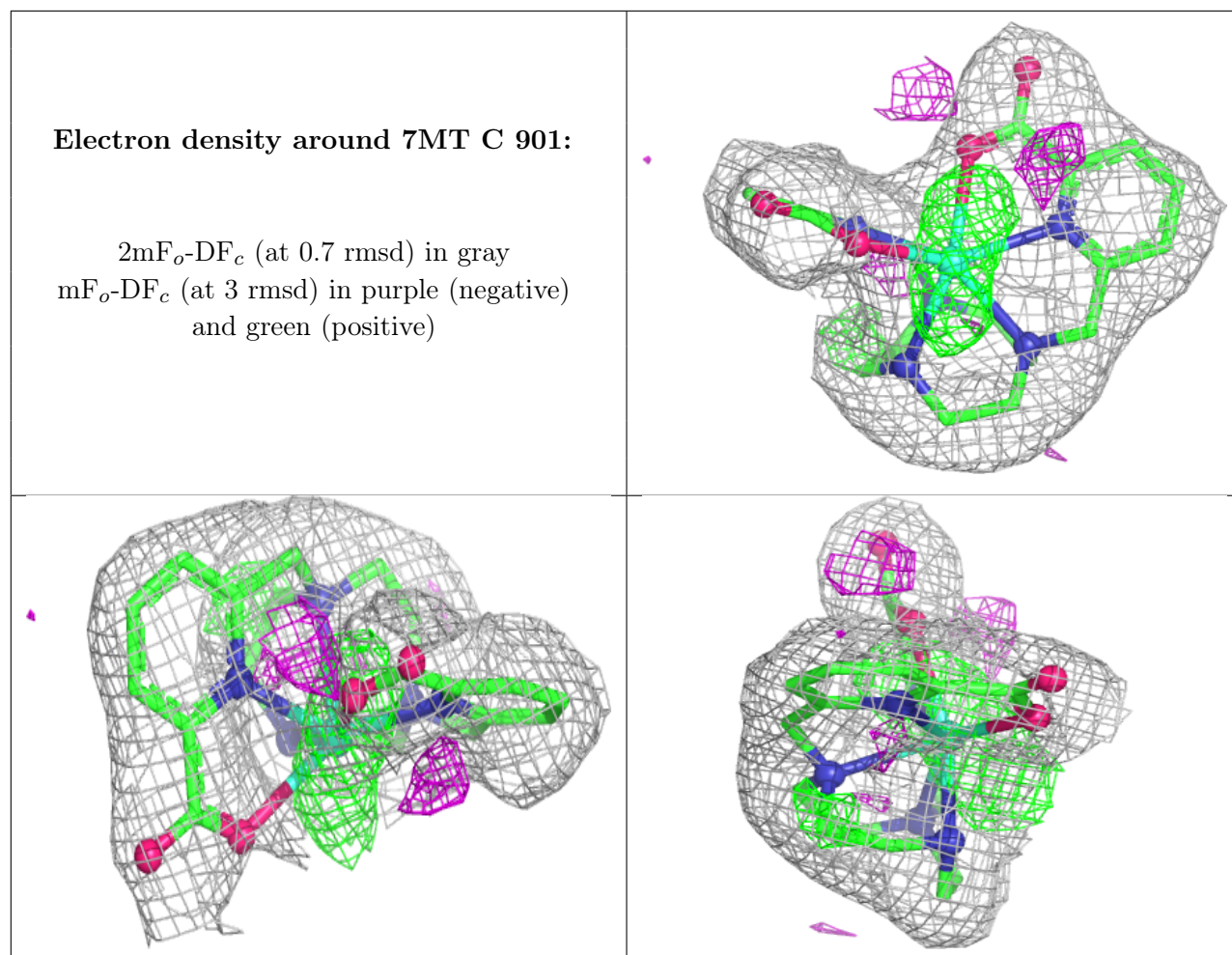
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TB	A	902	1/1	0.93	0.15	101,101,101,101	1
4	TB	A	901	1/1	0.96	0.11	78,78,78,78	1
4	TB	B	901	1/1	0.96	0.12	73,73,73,73	1
3	7MT	D	901	30/30	0.98	0.10	57,74,78,90	0
3	7MT	C	901	30/30	0.99	0.10	51,64,72,81	0

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.

Electron density around 7MT D 901:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.