wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 12:21 am GMT

PDB ID	:	6YR2
Title	:	TetR(D) soaked with Tigecycline P4(1)2(1)2
Authors	:	Hinrichs, W.; Stary, K.
Deposited on	:	2020-04-19
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

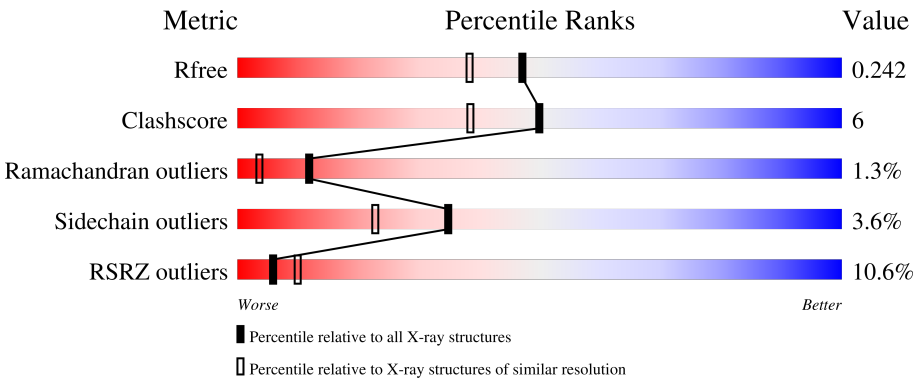
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	AAA	207	12% 85% 13% •
1	BBB	207	9% 81% 14% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3436 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.

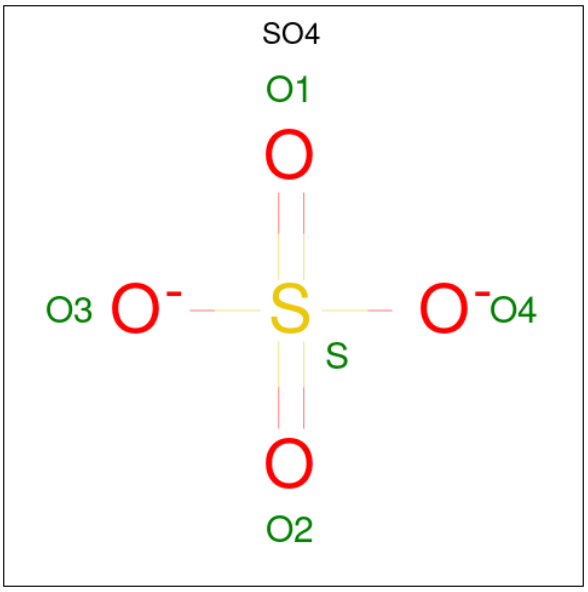
- Molecule 1 is a protein called Tetracycline repressor protein class D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	207	1643	1034	293	313	3	0	1	0
1	BBB	197	1567	989	283	292	3	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	SER	ALA	engineered mutation	UNP P0ACT4
BBB	2	SER	ALA	engineered mutation	UNP P0ACT4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	AAA	1	5	4	1	0	0

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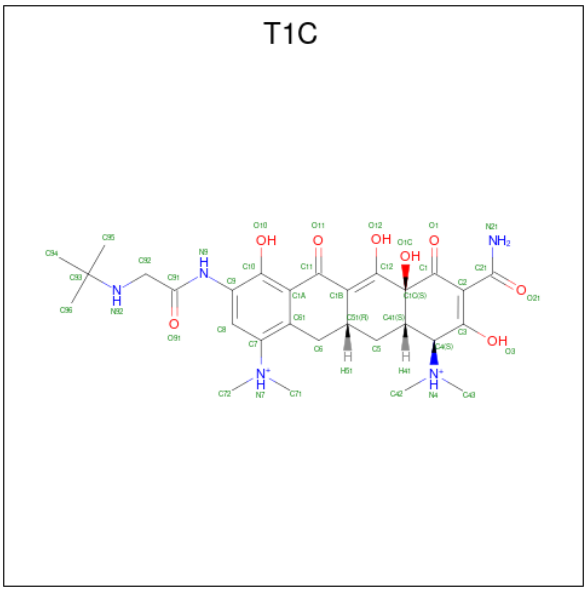
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	BBB	1	5	4	1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	AAA	4	4	4	0	0
			Total	Cl		
3	BBB	4	4	4	0	0

- Molecule 4 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	BBB	1	42	29	5	8	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	BBB	1	1	1	0	0

- Molecule 6 is water.

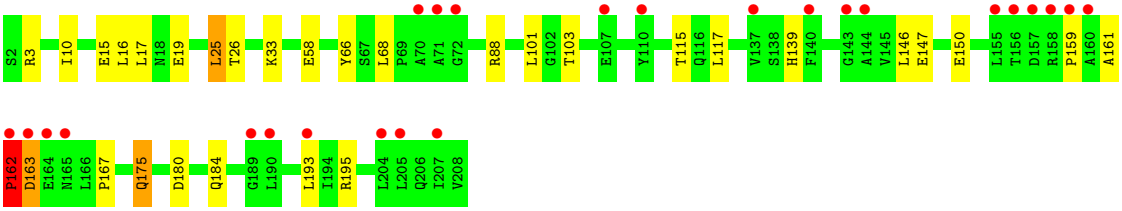
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	AAA	73	73	73	0	0
			Total	O		
6	BBB	92	92	92	0	0

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.

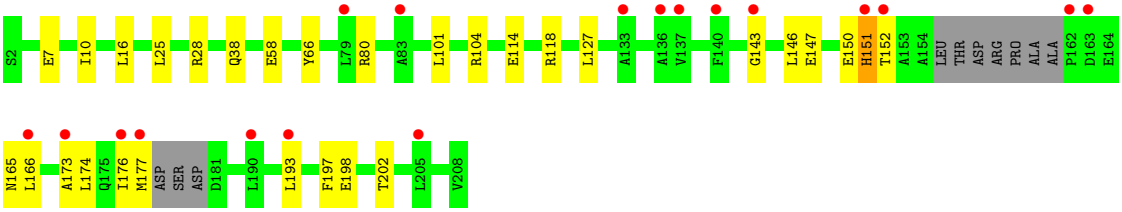
• Molecule 1: Tetracycline repressor protein class D

Chain AAA:



• Molecule 1: Tetracycline repressor protein class D

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	68.34Å 68.34Å 178.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.53 – 1.95 37.50 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.53-1.95) 98.1 (37.50-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.237 0.218 , 0.242	Depositor DCC
R_{free} test set	1573 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3436	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4458e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, CL, MG, T1C

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	AAA	0.85	2/1672 (0.1%)	0.99	3/2265 (0.1%)
1	BBB	0.88	0/1593	0.98	3/2151 (0.1%)
All	All	0.87	2/3265 (0.1%)	0.99	6/4416 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	147	GLU	CD-OE1	-6.33	1.18	1.25
1	AAA	150	GLU	CD-OE1	-5.26	1.19	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	88	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	BBB	118	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	BBB	118	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	AAA	88	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	AAA	162	PRO	N-CA-C	5.28	125.81	112.10

There are no chirality outliers.

There are no planarity outliers.

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	AAA	1643	0	1632	28	0
1	BBB	1567	0	1565	19	0
2	AAA	5	0	0	0	0
2	BBB	5	0	0	0	0
3	AAA	4	0	0	0	0
3	BBB	4	0	0	0	0
4	BBB	42	0	37	0	0
5	BBB	1	0	0	0	0
6	AAA	73	0	0	2	0
6	BBB	92	0	0	2	0
All	All	3436	0	3234	38	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 6.

The worst 5 of 38 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:AAA:25[A]:LEU:C	1:AAA:25[A]:LEU:CD1	2.43	0.87
1:AAA:180:ASP:OD2	1:AAA:184:GLN:HB2	1.85	0.77
1:AAA:161:ALA:HB1	1:AAA:162:PRO:HD2	1.65	0.76
1:AAA:25[A]:LEU:HD13	1:AAA:26:THR:N	2.02	0.73
1:AAA:161:ALA:HB1	1:AAA:162:PRO:CD	2.18	0.73

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	AAA	206/207 (100%)	196 (95%)	7 (3%)	3 (2%)	10 3
1	BBB	192/207 (93%)	184 (96%)	6 (3%)	2 (1%)	15 6
All	All	398/414 (96%)	380 (96%)	13 (3%)	5 (1%)	12 3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	151	HIS
1	AAA	162	PRO
1	BBB	176	ILE
1	AAA	163	ASP
1	AAA	159	PRO

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	AAA	173/173 (100%)	166 (96%)	7 (4%)	31	19
1	BBB	164/173 (95%)	158 (96%)	6 (4%)	34	22
All	All	337/346 (97%)	324 (96%)	13 (4%)	35	19

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	66	TYR
1	BBB	104	ARG
1	BBB	174	LEU
1	BBB	165	ASN
1	BBB	166	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	T1C	BBB	1001	5	44,45,45	1.73	9 (20%)	53,72,72	2.07	16 (30%)
2	SO4	AAA	301	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	BBB	1003	-	4,4,4	0.51	0	6,6,6	0.09	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
4	T1C	BBB	1001	5	-	4/22/80/80	0/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	1001	T1C	C91-N9	-4.03	1.26	1.35
4	BBB	1001	T1C	C2-C3	-3.92	1.30	1.40
4	BBB	1001	T1C	C9-N9	-3.85	1.34	1.41
4	BBB	1001	T1C	C1B-C11	-3.77	1.38	1.47
4	BBB	1001	T1C	C2-C1	-3.43	1.37	1.45

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	1001	T1C	O11-C11-C1A	-4.61	113.28	121.99
4	BBB	1001	T1C	C11-C1B-C12	4.41	122.29	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	1001	T1C	C71-N7-C7	-4.32	101.78	115.17
4	BBB	1001	T1C	O11-C11-C1B	4.13	127.12	120.78
4	BBB	1001	T1C	C72-N7-C71	-3.58	104.59	116.12

There are no chirality outliers.

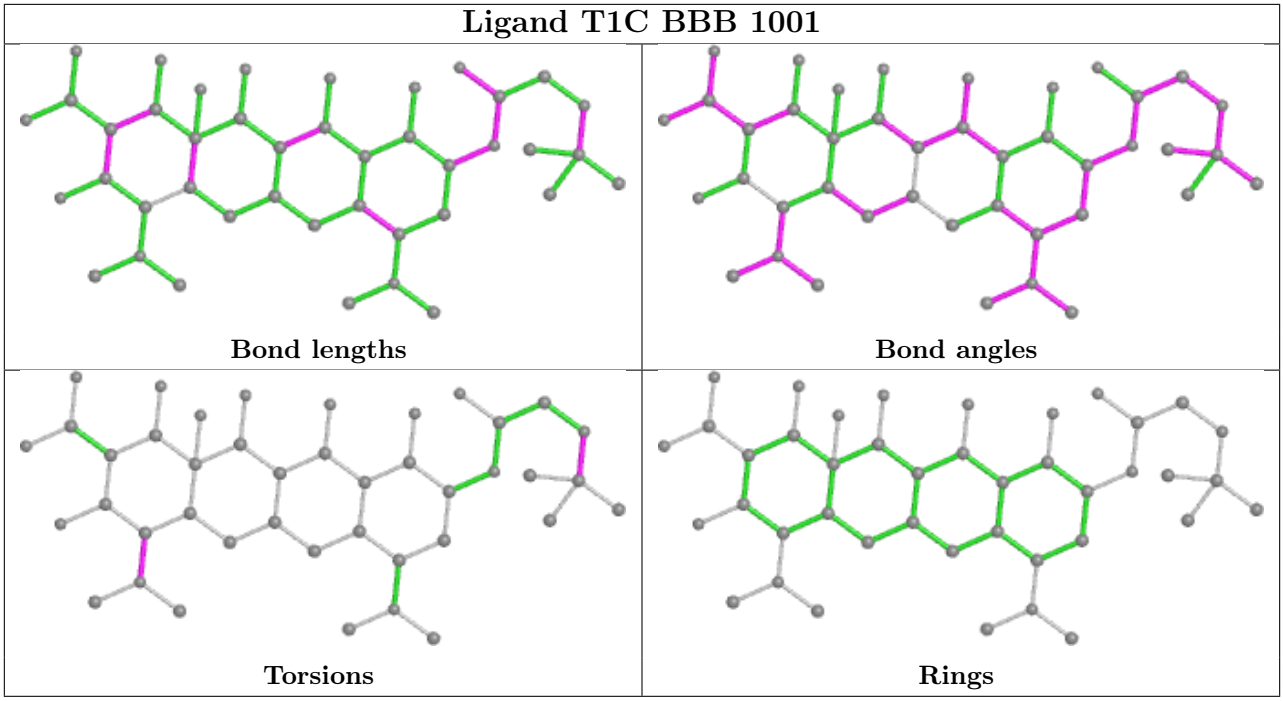
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	1001	T1C	C41-C4-N4-C43
4	BBB	1001	T1C	C95-C93-N92-C92
4	BBB	1001	T1C	C96-C93-N92-C92
4	BBB	1001	T1C	C94-C93-N92-C92

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 then 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	AAA	207/207 (100%)	0.59	25 (12%)	4	7	23, 36, 66, 121	0
1	BBB	197/207 (95%)	0.41	18 (9%)	9	15	21, 31, 65, 107	0
All	All	404/414 (97%)	0.50	43 (10%)	6	10	21, 33, 65, 121	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	162	PRO	8.5
1	AAA	159	PRO	6.9
1	AAA	205	LEU	5.2
1	AAA	163	ASP	4.4
1	BBB	152	THR	4.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

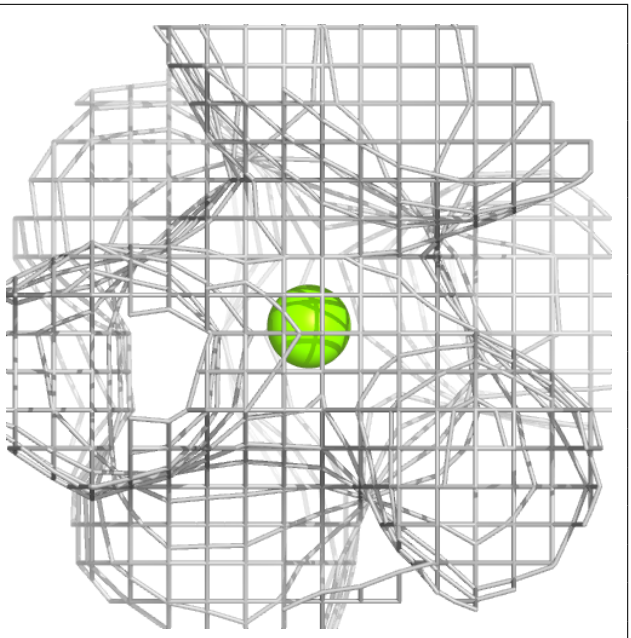
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

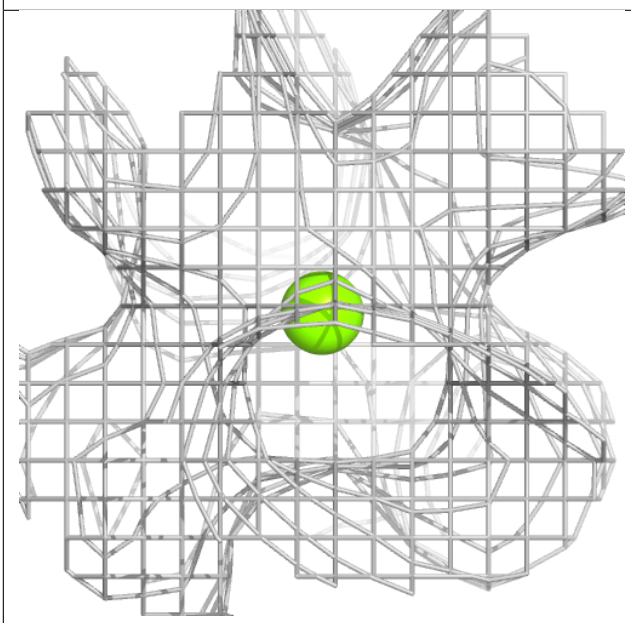
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	BBB	1007	1/1	0.79	0.10	72,72,72,72	0
3	CL	BBB	1006	1/1	0.88	0.05	65,65,65,65	0
3	CL	AAA	303	1/1	0.91	0.09	56,56,56,56	0
3	CL	BBB	1005	1/1	0.91	0.07	59,59,59,59	0
5	MG	BBB	1002	1/1	0.92	0.09	22,22,22,22	0
3	CL	AAA	304	1/1	0.93	0.06	63,63,63,63	0
3	CL	AAA	305	1/1	0.94	0.10	50,50,50,50	0
2	SO4	BBB	1003	5/5	0.95	0.23	49,54,67,70	0
4	T1C	BBB	1001	42/42	0.96	0.09	21,23,44,45	0
2	SO4	AAA	301	5/5	0.96	0.15	55,59,71,75	0
3	CL	BBB	1004	1/1	0.98	0.05	34,34,34,34	0
3	CL	AAA	302	1/1	0.98	0.09	40,40,40,40	0

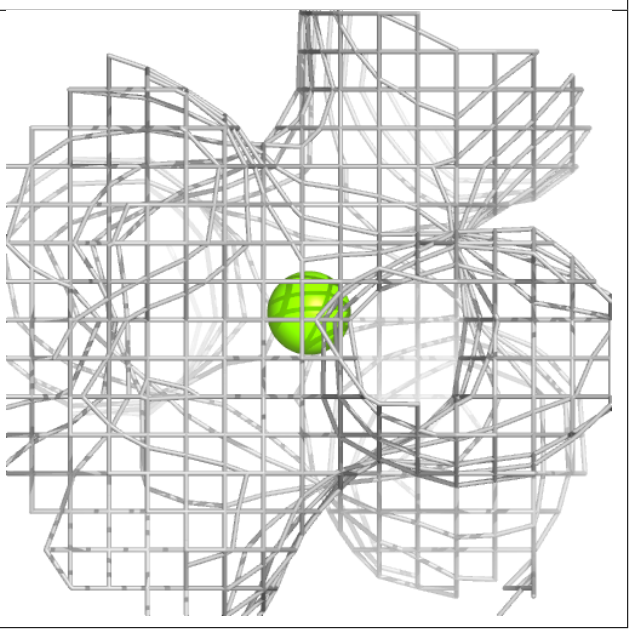
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MG BBB 1002:

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

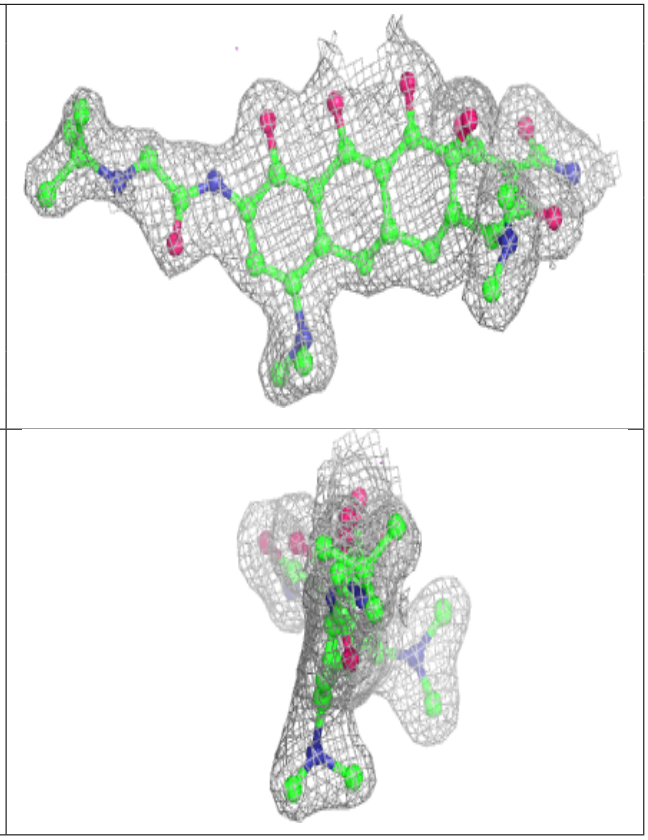






Electron density around T1C BBB 1001:

$2mF_o$-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 (i)

There are no such residues in this entry.