



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 02:26 PM EDT

PDB ID : 37ZR / pdb_000037zr
Title : Crystal structure of TP53 (89-293, Y220C) bound to compound 3
Authors : Setser, J.W.
Deposited on : 2026-08-16
Resolution : 2.39 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

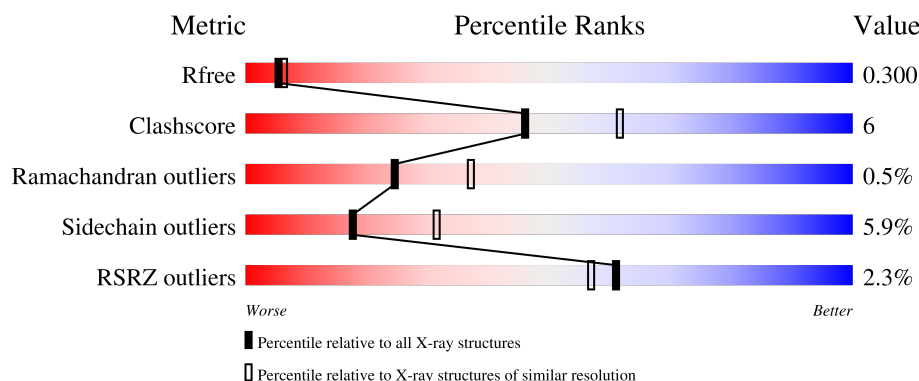
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	AAA	206	% 80% 15% • •
1	BBB	206	3% 83% 11% • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3235 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.

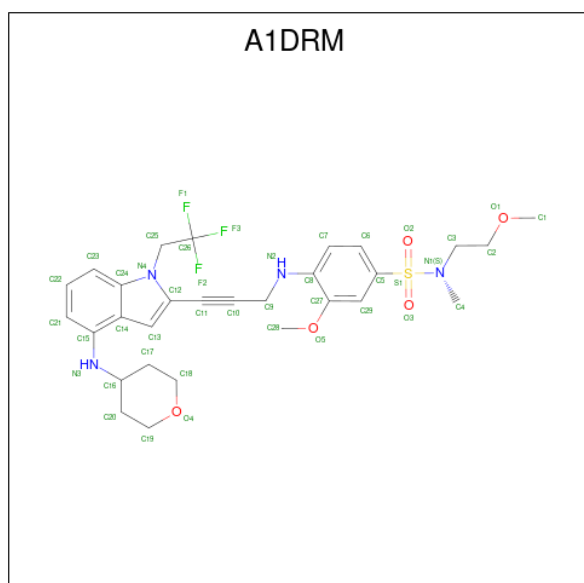
- Molecule 1 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	200	Total	C	N	O	S	0	3	0
			1583	976	292	295	20			
1	BBB	197	Total	C	N	O	S	0	0	0
			1542	953	282	290	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	88	GLY	-	expression tag	UNP P04637
AAA	220	CYS	TYR	conflict	UNP P04637
BBB	88	GLY	-	expression tag	UNP P04637
BBB	220	CYS	TYR	conflict	UNP P04637

- Molecule 2 is 3-methoxy-N-(2-methoxyethyl)-N-methyl-4-[(3-{4-[(oxan-4-yl)amino]-1-(2,2,2-trifluoroethyl)-1H-indol-2-yl}prop-2-yn-1-yl)amino]benzene-1-sulfonamide (CCD ID: A1DRM) (formula: C₂₉H₃₅F₃N₄O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	S	0	0
			42	29	3	4	5	1		
2	BBB	1	Total	C	F	N	O	S	0	0
			42	29	3	4	5	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Zn	0	0
			1	1		
3	BBB	1	Total	Zn	0	0
			1	1		

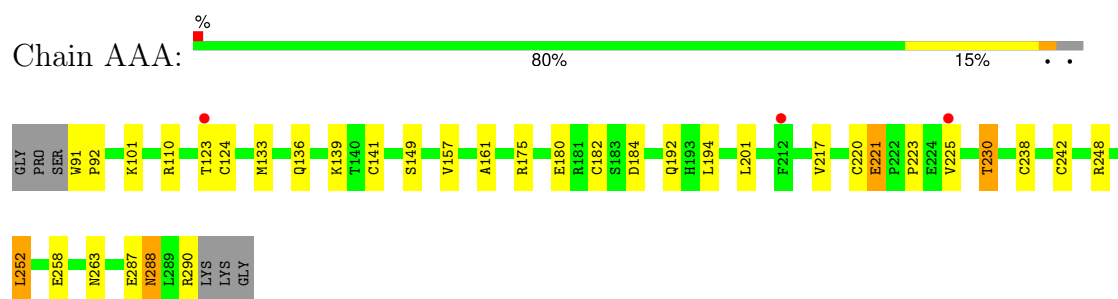
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	12	Total	O	0	0
			12	12		
4	BBB	12	Total	O	0	0
			12	12		

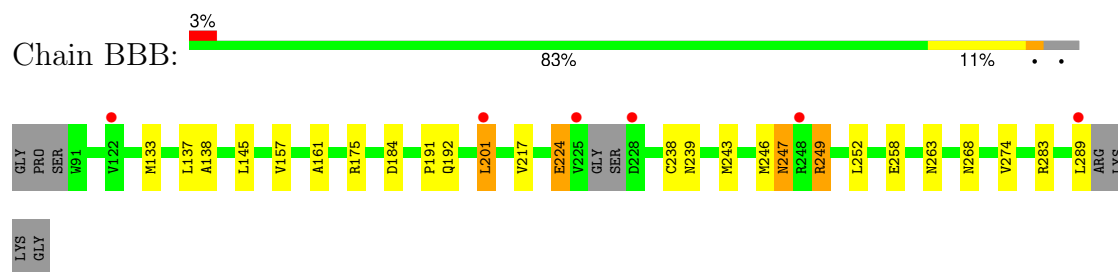
3 Residue-property plots

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: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.49Å 68.54Å 59.60Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	44.66 – 2.39 44.66 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.66-2.39) 99.9 (44.66-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.220 , 0.299 0.225 , 0.300	Depositor DCC
R_{free} test set	816 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.2	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	0.94	EDS
Total number of atoms	3235	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.72% 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: ZN, A1DRM

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	1.02	0/1626	1.29	0/2207
1	BBB	1.01	0/1578	1.29	0/2142
All	All	1.01	0/3204	1.29	0/4349

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	1583	0	1546	20	0
1	BBB	1542	0	1494	16	0
2	AAA	42	0	0	1	0
2	BBB	42	0	0	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
4	AAA	12	0	0	0	0
4	BBB	12	0	0	0	0
All	All	3235	0	3040	36	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.

All (36) 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:BBB:246:MET:O	1:BBB:249:ARG:HB2	1.78	0.83
1:BBB:243:MET:HG3	1:BBB:247:ASN:HD21	1.56	0.70
1:AAA:123:THR:HA	1:AAA:136:GLN:NE2	2.10	0.66
1:BBB:243:MET:HA	1:BBB:247:ASN:OD1	1.97	0.64
1:AAA:136:GLN:HB2	1:AAA:139:LYS:HG3	1.83	0.60
1:BBB:243:MET:HA	1:BBB:247:ASN:CG	2.26	0.59
1:BBB:175:ARG:NH2	1:BBB:184:ASP:OD2	2.34	0.56
1:BBB:201:LEU:HD22	1:BBB:201:LEU:H	1.71	0.56
1:BBB:239:ASN:ND2	1:BBB:274:VAL:HG12	2.22	0.54
1:AAA:220:CYS:SG	2:AAA:301:A1DRM:F2	2.60	0.50
1:BBB:201:LEU:H	1:BBB:201:LEU:HD13	1.76	0.49
1:AAA:123:THR:HA	1:AAA:136:GLN:HE22	1.76	0.49
1:AAA:133[A]:MET:HE3	1:AAA:133[A]:MET:HB2	1.72	0.49
1:AAA:175:ARG:NH2	1:AAA:184:ASP:OD2	2.43	0.49
1:AAA:221:GLU:O	1:AAA:230:THR:HG21	2.13	0.49
1:AAA:133[B]:MET:HE3	1:AAA:141[B]:CYS:SG	2.53	0.49
1:BBB:145:LEU:HD11	1:BBB:157:VAL:HG11	1.93	0.48
1:AAA:91:TRP:HE3	1:AAA:92:PRO:HD2	1.77	0.48
1:AAA:180:GLU:OE2	1:AAA:192:GLN:NE2	2.47	0.47
1:BBB:137:LEU:HD23	1:BBB:138:ALA:HB2	1.97	0.45
1:BBB:224:GLU:H	1:BBB:224:GLU:HG2	1.61	0.45
1:AAA:288:ASN:N	1:AAA:288:ASN:HD22	2.13	0.45
1:BBB:201:LEU:HD13	1:BBB:201:LEU:N	2.32	0.45
1:AAA:161:ALA:HA	1:AAA:252:LEU:O	2.18	0.44
1:AAA:223:PRO:HA	1:AAA:230:THR:HG22	2.00	0.44
1:AAA:157:VAL:O	1:AAA:217:VAL:HA	2.19	0.42
1:BBB:157:VAL:O	1:BBB:217:VAL:HA	2.19	0.42
1:AAA:194:LEU:CD1	1:AAA:238:CYS:HB2	2.49	0.42
1:AAA:258:GLU:HA	1:AAA:263:ASN:O	2.20	0.42
1:AAA:223:PRO:CA	1:AAA:230:THR:HG22	2.49	0.42
1:AAA:201:LEU:HD23	1:AAA:201:LEU:HA	1.97	0.41
1:AAA:223:PRO:N	1:AAA:230:THR:HG22	2.35	0.41
1:BBB:161:ALA:HA	1:BBB:252:LEU:O	2.21	0.41
1:BBB:175:ARG:HD3	1:BBB:191:PRO:O	2.21	0.41
1:AAA:124:CYS:SG	1:AAA:133[B]:MET:SD	3.16	0.41
1:BBB:258:GLU:HA	1:BBB:263:ASN:O	2.21	0.41

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	AAA	201/206 (98%)	191 (95%)	8 (4%)	2 (1%)	12	20
1	BBB	193/206 (94%)	189 (98%)	4 (2%)	0	100	100
All	All	394/412 (96%)	380 (96%)	12 (3%)	2 (0%)	24	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	242	CYS
1	AAA	225	VAL

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	AAA	183/184 (100%)	172 (94%)	11 (6%)	17	31
1	BBB	177/184 (96%)	167 (94%)	10 (6%)	19	33
All	All	360/368 (98%)	339 (94%)	21 (6%)	18	32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	101	LYS
1	AAA	110	ARG
1	AAA	149	SER
1	AAA	182	CYS

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Mol	Chain	Res	Type
1	AAA	221	GLU
1	AAA	230	THR
1	AAA	248	ARG
1	AAA	252	LEU
1	AAA	287	GLU
1	AAA	288	ASN
1	AAA	290	ARG
1	BBB	133	MET
1	BBB	192	GLN
1	BBB	201	LEU
1	BBB	224	GLU
1	BBB	238	CYS
1	BBB	247	ASN
1	BBB	249	ARG
1	BBB	268	ASN
1	BBB	283	ARG
1	BBB	289	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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
2	A1DRM	AAA	301	-	44,45,45	0.77	1 (2%)	57,64,64	0.66	0
2	A1DRM	BBB	301	-	44,45,45	0.85	3 (6%)	57,64,64	0.89	3 (5%)

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	A1DRM	AAA	301	-	-	8/30/42/42	0/4/4/4
2	A1DRM	BBB	301	-	-	5/30/42/42	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	301	A1DRM	C3-N1	3.13	1.49	1.47
2	AAA	301	A1DRM	C11-C10	3.03	1.22	1.19
2	BBB	301	A1DRM	C11-C10	2.43	1.21	1.19
2	BBB	301	A1DRM	C25-C26	2.04	1.54	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	301	A1DRM	C15-N3-C16	3.01	129.54	124.60
2	BBB	301	A1DRM	C20-C16-N3	2.38	114.61	110.77
2	BBB	301	A1DRM	C14-C15-N3	-2.24	118.66	120.91

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	A1DRM	C4-N1-S1-O2
2	AAA	301	A1DRM	C4-N1-S1-C5
2	BBB	301	A1DRM	O1-C2-C3-N1
2	BBB	301	A1DRM	C2-C3-N1-C4

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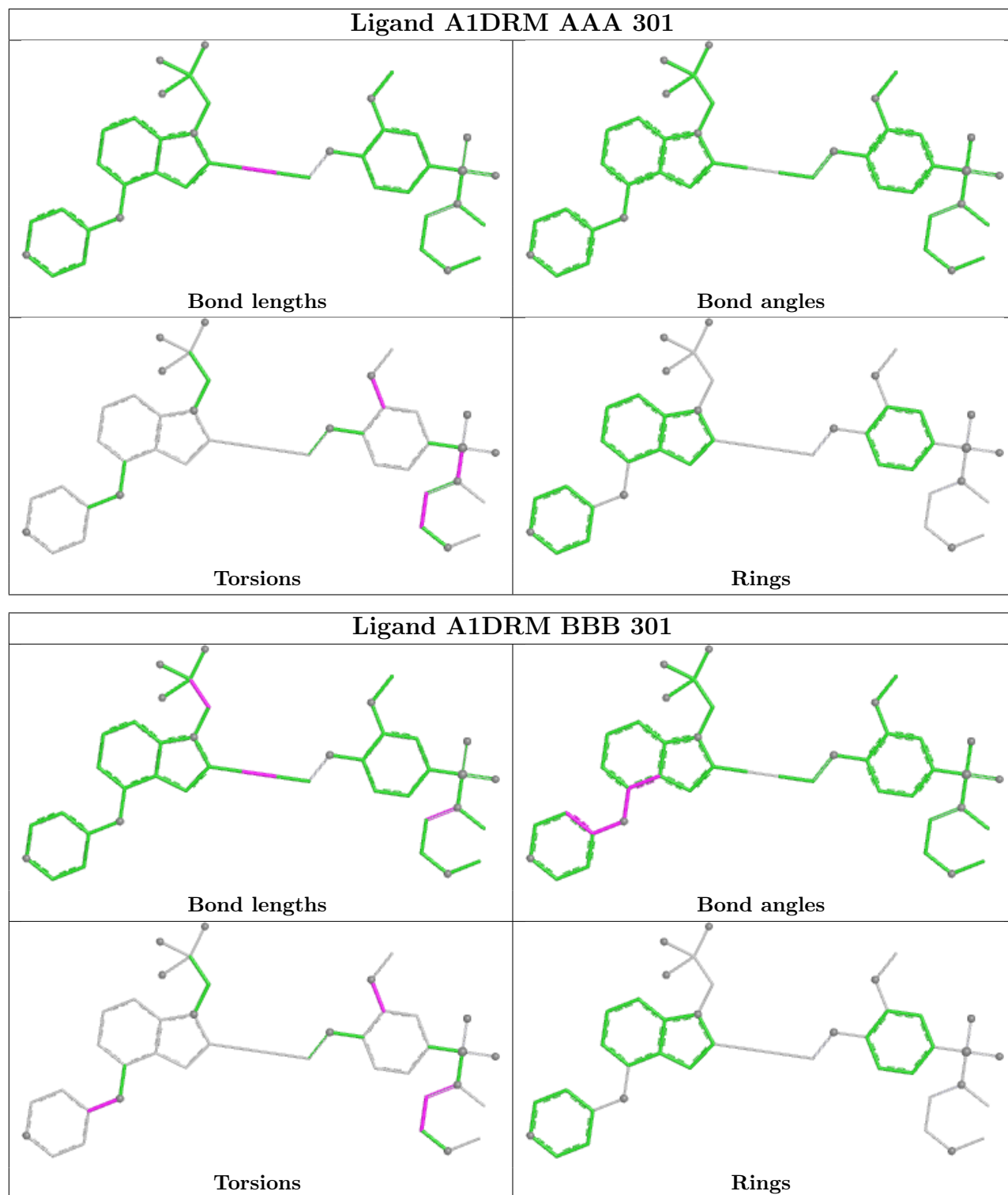
Mol	Chain	Res	Type	Atoms
2	BBB	301	A1DRM	C20-C16-N3-C15
2	BBB	301	A1DRM	C8-C27-O5-C28
2	AAA	301	A1DRM	C3-N1-S1-O2
2	BBB	301	A1DRM	C29-C27-O5-C28
2	AAA	301	A1DRM	O1-C2-C3-N1
2	AAA	301	A1DRM	C8-C27-O5-C28
2	AAA	301	A1DRM	C3-N1-S1-C5
2	AAA	301	A1DRM	C29-C27-O5-C28
2	AAA	301	A1DRM	C3-N1-S1-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	301	A1DRM	1	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 ⓘ

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 [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	200/206 (97%)	0.33	3 (1%) 72 68	26, 56, 87, 106	3 (1%)
1	BBB	197/206 (95%)	0.46	6 (3%) 52 48	43, 60, 88, 101	0
All	All	397/412 (96%)	0.39	9 (2%) 61 57	26, 58, 88, 106	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	201	LEU	3.7
1	BBB	225	VAL	3.0
1	AAA	225	VAL	2.8
1	BBB	122	VAL	2.6
1	AAA	212	PHE	2.5
1	BBB	289	LEU	2.4
1	AAA	123	THR	2.3
1	BBB	248	ARG	2.2
1	BBB	228	ASP	2.1

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.

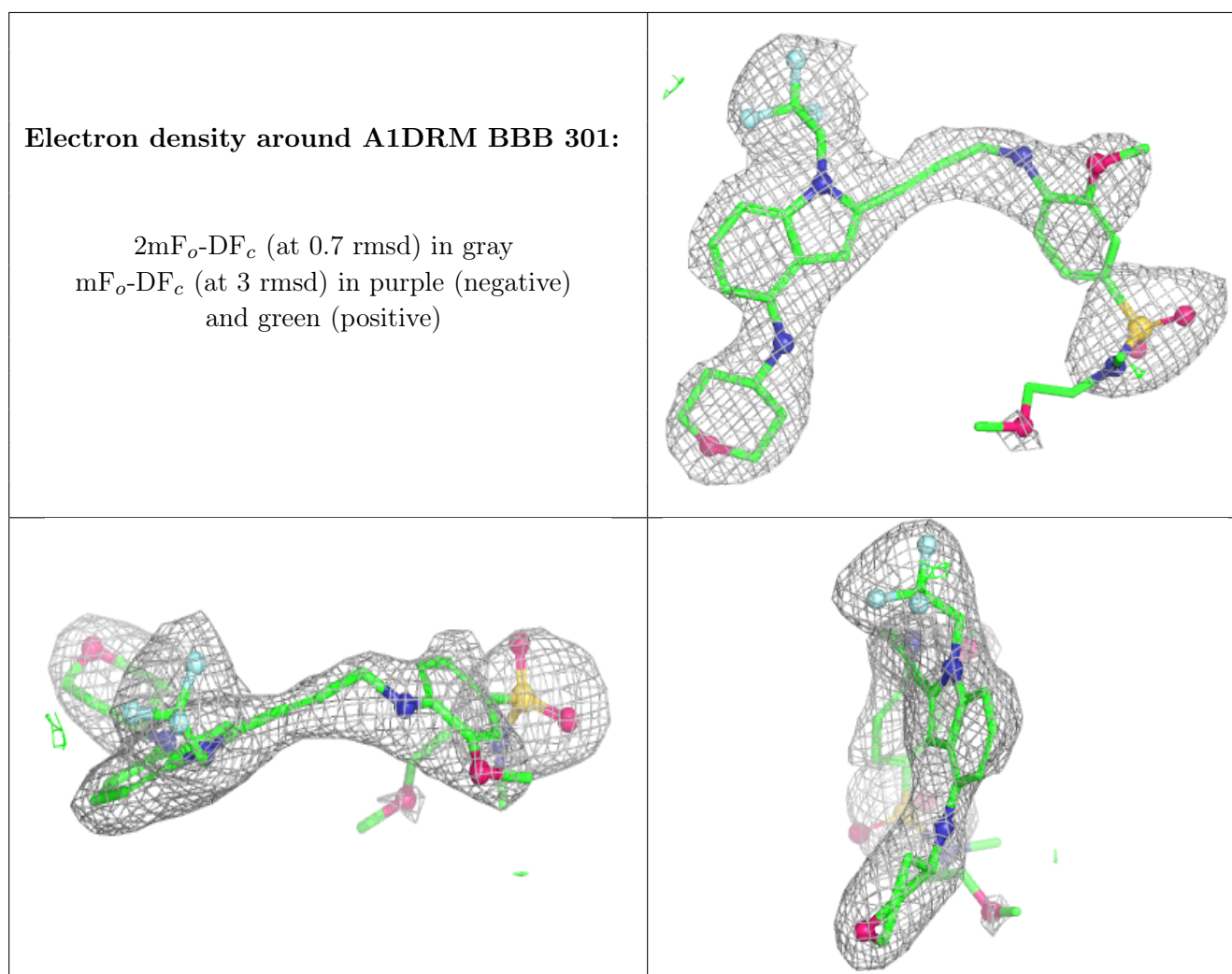
6.4 Ligands [i](#)

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.

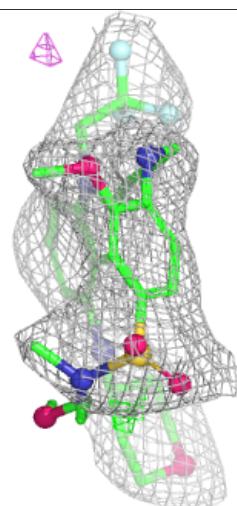
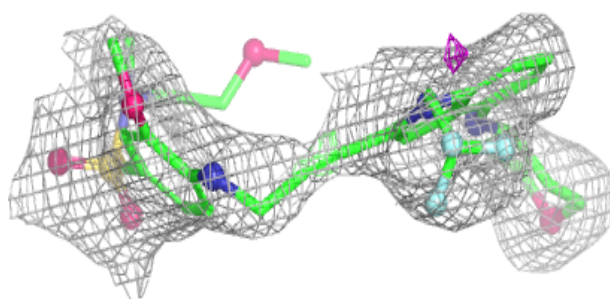
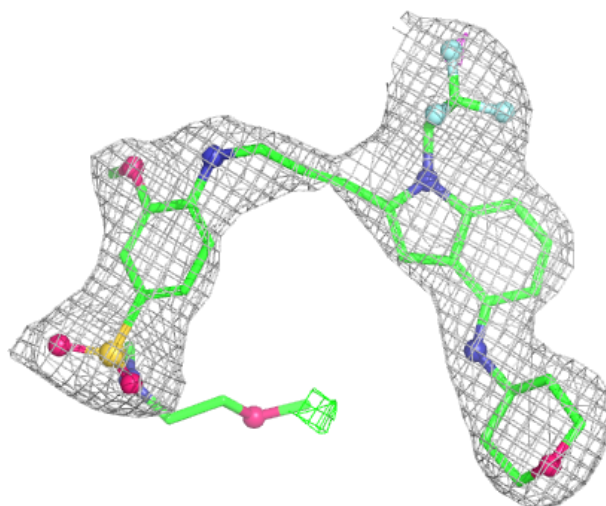
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1DRM	BBB	301	42/42	0.86	0.13	53,75,111,120	0
2	A1DRM	AAA	301	42/42	0.89	0.11	59,70,97,114	0
3	ZN	AAA	302	1/1	0.99	0.02	71,71,71,71	0
3	ZN	BBB	302	1/1	0.99	0.03	63,63,63,63	0

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 A1DRM AAA 301:

$2mF_o-DF_c$ (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.