



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2020 – 06:26 PM EST

PDB ID : 6VGG  
Title : Crystal structure of the DNA binding domains of human transcription factor ERG, human Runx2 bound to core binding factor beta (Cbfb), and mithramycin, in complex with 16mer DNA CAGAGGATGTGGCTTC  
Authors : Hou, C.; Rohr, J.; Tsodikov, O.V.  
Deposited on : 2020-01-08  
Resolution : 4.31 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](mailto: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.

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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 : 2.14.6  
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) : 2.14.6

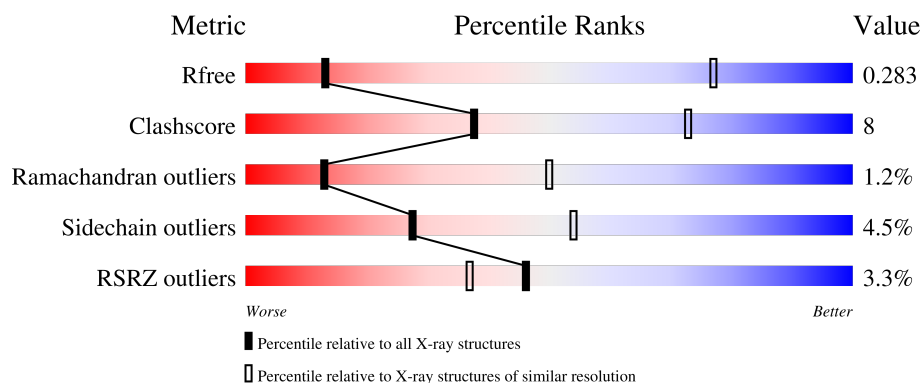
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


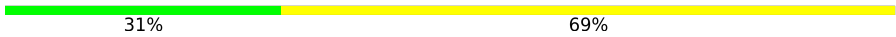


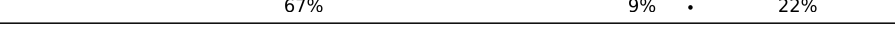
The reported resolution of this entry is 4.31 Å.

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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	128	
2	B	16	
3	C	16	
4	D	177	
5	G	156	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	QWP	C	101	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3515 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 Transcriptional regulator ERG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			806	512	143	146	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	GLY	-	expression tag	UNP P11308
A	303	PRO	-	expression tag	UNP P11308
A	304	HIS	-	expression tag	UNP P11308
A	305	MET	-	expression tag	UNP P11308
A	420	SER	-	expression tag	UNP P11308
A	421	TYR	-	expression tag	UNP P11308
A	422	HIS	-	expression tag	UNP P11308
A	423	ALA	-	expression tag	UNP P11308
A	424	HIS	-	expression tag	UNP P11308
A	425	PRO	-	expression tag	UNP P11308
A	426	GLN	-	expression tag	UNP P11308
A	427	LYS	-	expression tag	UNP P11308
A	428	MET	-	expression tag	UNP P11308
A	429	ASN	-	expression tag	UNP P11308

- Molecule 2 is a DNA chain called DNA (5'-D(P\*CP\*AP\*GP\*AP\*GP\*GP\*AP\*TP\*GP\*TP\*GP\*GP\*CP\*TP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	P	0	0	0
			332	157	62	97	16			

- Molecule 3 is a DNA chain called DNA (5'-D(P\*GP\*AP\*AP\*GP\*CP\*CP\*AP\*CP\*AP\*TP\*CP\*CP\*TP\*CP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	P	0	0	0
			324	154	59	95	16			

- Molecule 4 is a protein called Runt-related transcription factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	117	Total	C	N	O	S	0	0	0
			901	567	164	166	4			

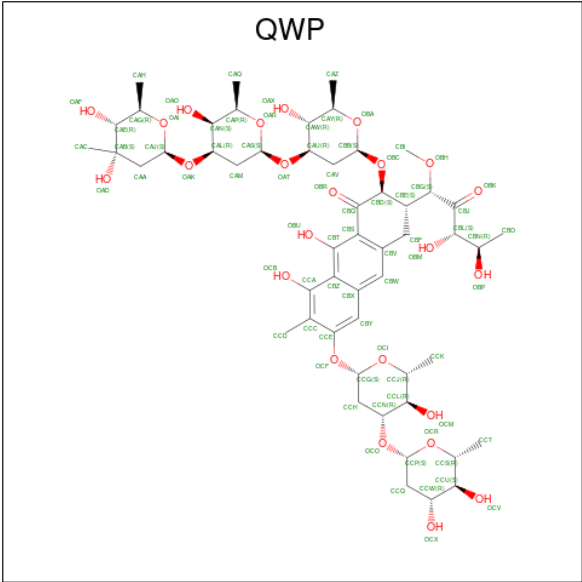
- Molecule 5 is a protein called Core-binding factor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	121	Total	C	N	O	S	0	0	0
			998	622	181	189	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	MET	-	expression tag	UNP Q13951
G	-12	GLY	-	expression tag	UNP Q13951
G	-11	SER	-	expression tag	UNP Q13951
G	-10	SER	-	expression tag	UNP Q13951
G	-9	HIS	-	expression tag	UNP Q13951
G	-8	HIS	-	expression tag	UNP Q13951
G	-7	HIS	-	expression tag	UNP Q13951
G	-6	HIS	-	expression tag	UNP Q13951
G	-5	HIS	-	expression tag	UNP Q13951
G	-4	HIS	-	expression tag	UNP Q13951
G	-3	SER	-	expression tag	UNP Q13951
G	-2	GLN	-	expression tag	UNP Q13951
G	-1	ASP	-	expression tag	UNP Q13951
G	0	PRO	-	expression tag	UNP Q13951

- Molecule 6 is mithramycin (three-letter code: QWP) (formula:  $C_{52}H_{76}O_{24}$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			76	52	24		
6	C	1	Total	C	O	0	0
			75	52	23		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		

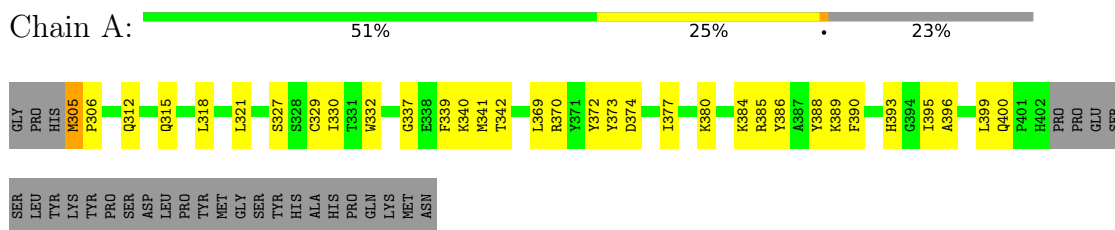
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	O	0	0
			1	1		
8	C	1	Total	O	0	0
			1	1		

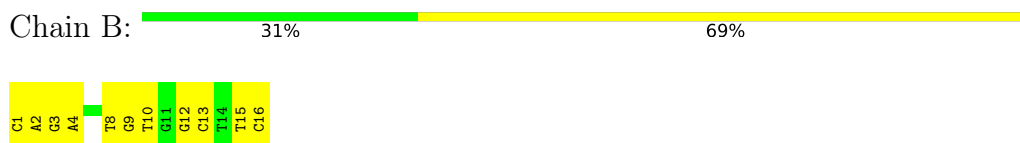
### 3 Residue-property plots

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.

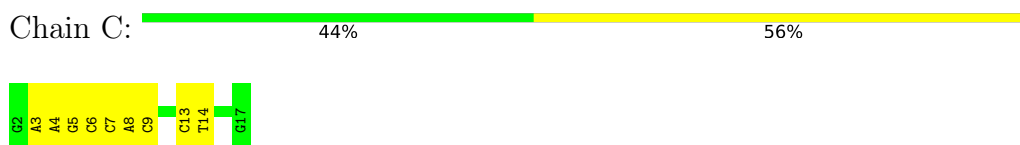
- Molecule 1: Transcriptional regulator ERG



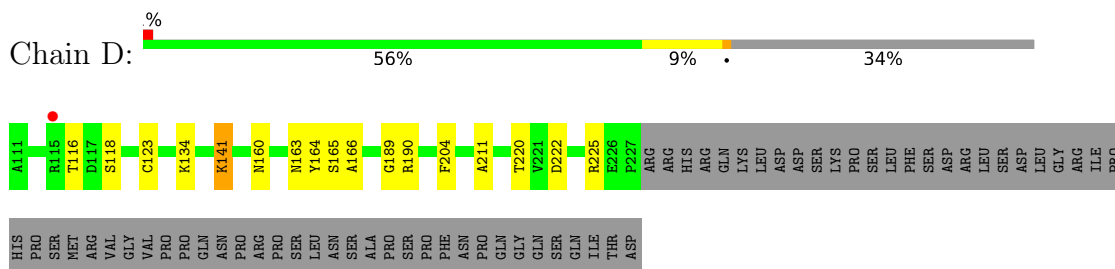
- Molecule 2: DNA (5'-D(P\*CP\*AP\*GP\*AP\*GP\*GP\*AP\*TP\*GP\*TP\*GP\*GP\*CP\*TP\*TP\*C)-3')



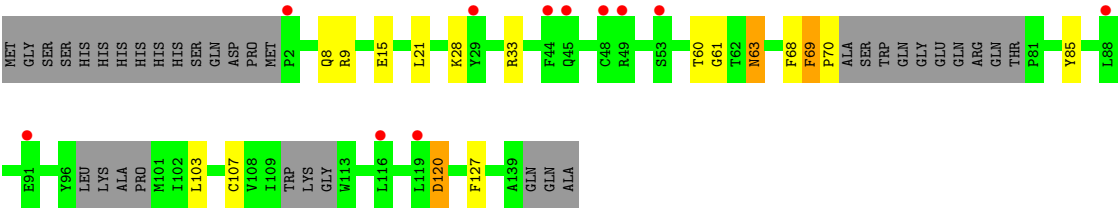
- Molecule 3: DNA (5'-D(P\*GP\*AP\*AP\*GP\*CP\*CP\*AP\*CP\*AP\*TP\*CP\*CP\*TP\*CP\*TP\*G)-3')



- Molecule 4: Runt-related transcription factor 2



- Molecule 5: Core-binding factor subunit beta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.68Å 104.68Å 322.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 4.31 41.11 – 4.31	Depositor EDS
% Data completeness (in resolution range)	98.1 (35.00-4.31) 98.4 (41.11-4.31)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.251 , 0.285 0.253 , 0.283	Depositor DCC
$R_{free}$ test set	377 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	195.7	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 234.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, QWP

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	0.65	0/828	0.74	0/1114
2	B	0.25	0/372	0.78	0/573
3	C	0.27	0/362	0.80	0/555
4	D	0.66	0/920	0.75	0/1253
5	G	0.66	0/1014	0.72	0/1355
All	All	0.59	0/3496	0.75	0/4850

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	806	0	777	21	0
2	B	332	0	181	8	0
3	C	324	0	180	6	0
4	D	901	0	905	8	0
5	G	998	0	956	9	0
6	B	76	0	0	0	0
6	C	75	0	0	1	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	0	0	0	0
8	C	1	0	0	0	0
All	All	3515	0	2999	49	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 8.

All (49) 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:337:GLY:O	1:A:389:LYS:HB2	1.78	0.83
1:A:318:LEU:HD21	1:A:390:PHE:CZ	2.22	0.74
3:C:13:DC:H2''	3:C:14:DT:OP2	2.00	0.62
2:B:12:DG:N2	3:C:7:DC:O2	2.38	0.57
5:G:68:PHE:HB3	5:G:85:TYR:HB3	1.86	0.57
1:A:305:MET:HG3	1:A:306:PRO:HD2	1.89	0.55
1:A:318:LEU:HD21	1:A:390:PHE:CE1	2.41	0.54
4:D:116:THR:OG1	4:D:118:SER:O	2.26	0.54
5:G:28:LYS:HG2	5:G:120:ASP:HB2	1.89	0.54
4:D:165:SER:O	5:G:33:ARG:NH1	2.41	0.53
1:A:321:LEU:HD23	1:A:332:TRP:CE2	2.44	0.53
1:A:396:ALA:O	1:A:400:GLN:N	2.41	0.52
2:B:1:DC:H2''	2:B:2:DA:C8	2.46	0.50
1:A:372:TYR:HA	1:A:377:ILE:HD12	1.93	0.49
2:B:15:DT:H2''	2:B:16:DC:C6	2.47	0.49
1:A:339:PHE:CZ	1:A:388:TYR:HB2	2.48	0.49
4:D:160:ASN:O	4:D:164:TYR:HA	2.13	0.49
1:A:380:LYS:NZ	1:A:384:LYS:O	2.46	0.49
2:B:2:DA:C6	2:B:3:DG:C6	3.00	0.48
1:A:395:ILE:O	1:A:399:LEU:HB2	2.12	0.48
1:A:329:CYS:HA	1:A:342:THR:HB	1.96	0.48
5:G:61:GLY:O	5:G:63:ASN:ND2	2.47	0.48
1:A:321:LEU:HD23	1:A:332:TRP:NE1	2.29	0.47
2:B:8:DT:H1'	2:B:9:DG:C8	2.49	0.47
1:A:330:ILE:HG13	1:A:340:LYS:O	2.14	0.47
4:D:118:SER:HB3	4:D:211:ALA:HB2	1.96	0.47
3:C:3:DA:H4'	3:C:4:DA:OP1	2.15	0.46
5:G:63:ASN:N	5:G:63:ASN:HD22	2.13	0.46
3:C:8:DA:H2''	3:C:9:DC:O5'	2.16	0.46
5:G:8:GLN:HE21	5:G:107:CYS:H	1.62	0.46
4:D:166:ALA:HB1	4:D:189:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:DT:H73	4:D:225:ARG:HD3	1.97	0.45
5:G:21:LEU:HD21	5:G:60:THR:HG21	1.99	0.45
5:G:9:ARG:HD3	5:G:127:PHE:CE1	2.53	0.44
6:C:101:QWP:OAX	6:C:101:QWP:OAR	2.36	0.44
5:G:69:PHE:HB3	5:G:70:PRO:HD2	1.99	0.44
1:A:327:SER:HA	1:A:330:ILE:O	2.18	0.43
1:A:370:ARG:HA	1:A:373:TYR:CE1	2.52	0.43
1:A:332:TRP:HZ3	1:A:337:GLY:HA2	1.84	0.43
4:D:220:THR:OG1	4:D:222:ASP:O	2.37	0.43
4:D:123:CYS:HA	4:D:141:LYS:O	2.19	0.42
1:A:399:LEU:HA	1:A:399:LEU:HD12	1.87	0.42
3:C:5:DG:C4	3:C:6:DC:C6	3.07	0.42
1:A:305:MET:CG	1:A:306:PRO:HD2	2.50	0.41
1:A:370:ARG:HD2	2:B:4:DA:C8	2.55	0.41
3:C:4:DA:C6	3:C:5:DG:C6	3.08	0.41
2:B:12:DG:C2	2:B:13:DC:C2	3.09	0.41
1:A:369:LEU:O	1:A:372:TYR:HB2	2.21	0.41
1:A:340:LYS:HG3	1:A:341:MET:N	2.36	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	96/128 (75%)	80 (83%)	14 (15%)	2 (2%)	7	39
4	D	115/177 (65%)	98 (85%)	15 (13%)	2 (2%)	9	43
5	G	113/156 (72%)	105 (93%)	8 (7%)	0	100	100
All	All	324/461 (70%)	283 (87%)	37 (11%)	4 (1%)	13	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ARG
4	D	163	ASN
4	D	204	PHE
1	A	386	TYR

### 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	85/113 (75%)	80 (94%)	5 (6%)	19	47
4	D	100/156 (64%)	97 (97%)	3 (3%)	41	64
5	G	106/135 (78%)	101 (95%)	5 (5%)	26	53
All	All	291/404 (72%)	278 (96%)	13 (4%)	27	54

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	MET
1	A	312	GLN
1	A	315	GLN
1	A	374	ASP
1	A	393	HIS
4	D	134	LYS
4	D	141	LYS
4	D	190	ARG
5	G	15	GLU
5	G	63	ASN
5	G	69	PHE
5	G	103	LEU
5	G	120	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	GLN

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Mol	Chain	Res	Type
1	A	315	GLN
1	A	376	ASN
5	G	8	GLN
5	G	67	GLN

### 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 3 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
6	QWP	B	101	7	81,83,83	1.29	4 (4%)	112,127,127	1.04	5 (4%)
6	QWP	C	101	7	80,82,83	1.32	4 (5%)	110,125,127	1.12	8 (7%)

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
6	QWP	B	101	7	-	3/38/137/137	0/8/8/8
6	QWP	C	101	7	-	12/38/134/137	0/8/8/8

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	101	QWP	CBF-CBV	-5.78	1.40	1.51
6	C	101	QWP	CBF-CBV	-5.68	1.40	1.51
6	B	101	QWP	CCD-CCC	-5.49	1.40	1.51
6	C	101	QWP	CCD-CCC	-5.49	1.40	1.51
6	C	101	QWP	CBD-CBQ	-3.68	1.40	1.50
6	B	101	QWP	CBD-CBQ	-3.65	1.40	1.50
6	B	101	QWP	CBS-CBQ	-2.80	1.40	1.46
6	C	101	QWP	CBS-CBQ	-2.78	1.40	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	101	QWP	OCF-CCE-CCC	3.52	117.56	114.19
6	B	101	QWP	CAB-CAA-CAJ	-3.37	108.35	114.82
6	C	101	QWP	OCF-CCE-CCC	3.04	117.10	114.19
6	C	101	QWP	CAB-CAA-CAJ	-2.95	109.17	114.82
6	C	101	QWP	CAH-CAG-CAE	-2.79	107.81	112.57
6	C	101	QWP	OAK-CAJ-CAA	-2.57	104.58	109.01
6	C	101	QWP	OAI-CAG-CAH	2.52	112.14	106.70
6	B	101	QWP	CBF-CBV-CBS	2.43	122.17	118.03
6	C	101	QWP	CBS-CBQ-CBD	2.25	120.56	116.00
6	C	101	QWP	CBT-CBS-CBV	-2.21	118.42	119.77
6	B	101	QWP	CBY-CCE-CCC	-2.15	119.92	122.52
6	C	101	QWP	OBR-CBQ-CBS	-2.11	119.53	122.78
6	B	101	QWP	OCI-CCG-OCF	2.10	112.41	108.45

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	101	QWP	OBK-CBJ-CBL-OBM
6	C	101	QWP	CBE-CBG-OBH-CBI
6	C	101	QWP	CBJ-CBG-OBH-CBI
6	C	101	QWP	CBG-CBJ-CBL-OBM
6	C	101	QWP	CBG-CBJ-CBL-CBN
6	C	101	QWP	OBK-CBJ-CBL-OBM

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
6	C	101	QWP	OBK-CBJ-CBL-CBN
6	C	101	QWP	CCH-CCG-OCF-CCE
6	C	101	QWP	CBE-CBG-CBJ-CBL
6	C	101	QWP	CBF-CBE-CBG-OBH
6	B	101	QWP	CBG-CBJ-CBL-OBM
6	B	101	QWP	OBK-CBJ-CBL-CBN
6	C	101	QWP	OBH-CBG-CBJ-CBL
6	C	101	QWP	CBF-CBE-CBG-CBJ
6	C	101	QWP	CBE-CBG-CBJ-OBK

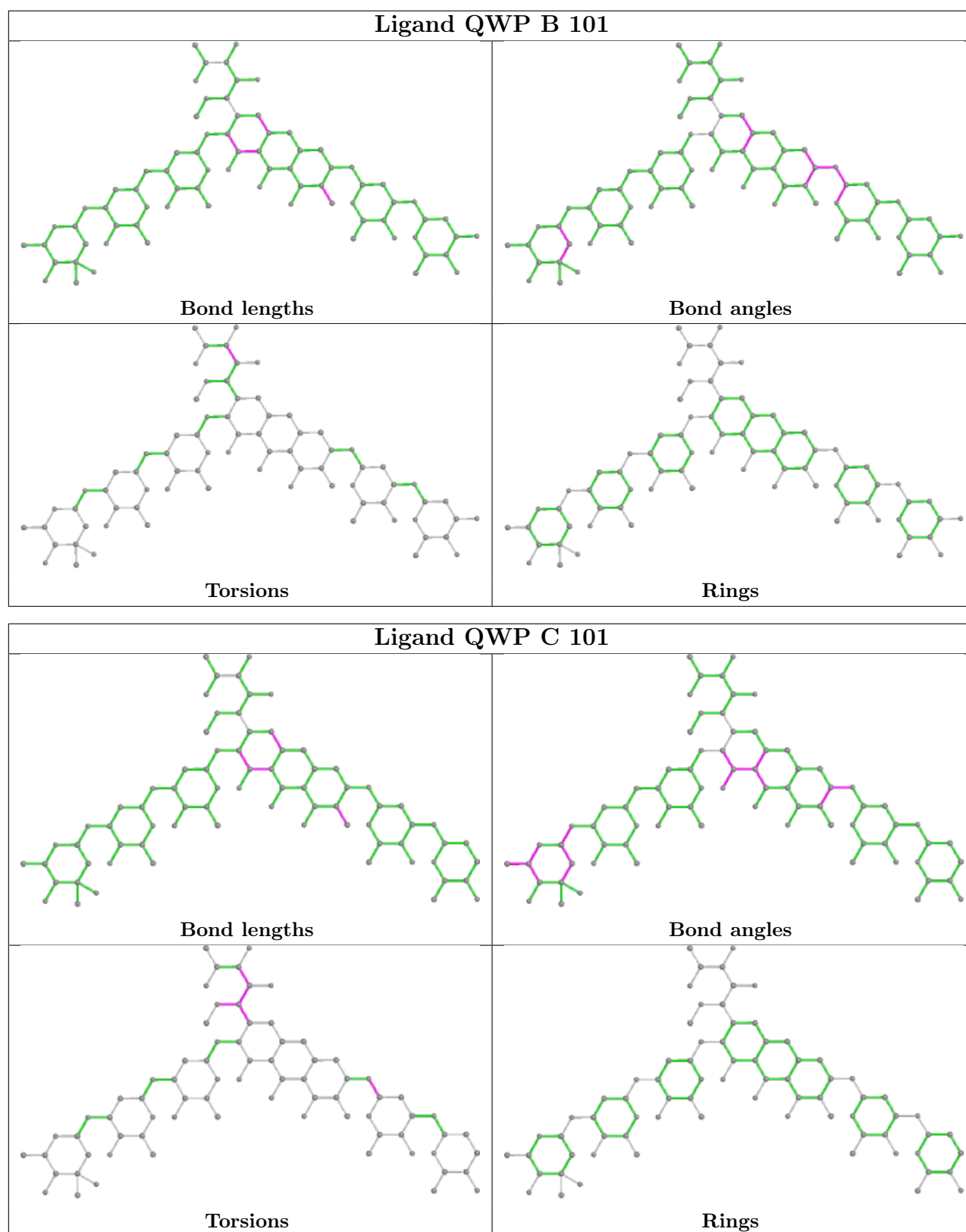
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	101	QWP	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 [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 [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, 95<sup>th</sup> 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(Å²)	Q<0.9
1	A	98/128 (76%)	-0.47	0	100	100	199, 260, 312, 348	0
2	B	16/16 (100%)	-0.54	0	100	100	224, 271, 291, 310	0
3	C	16/16 (100%)	-0.21	0	100	100	227, 266, 337, 363	0
4	D	117/177 (66%)	-0.14	1 (0%)	84	77	232, 279, 331, 370	0
5	G	121/156 (77%)	0.64	11 (9%)	9	8	325, 398, 443, 459	0
All	All	368/493 (74%)	0.01	12 (3%)	46	37	199, 290, 429, 459	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	115	ARG	3.7
5	G	53	SER	3.3
5	G	45	GLN	3.1
5	G	119	LEU	3.1
5	G	48	CYS	2.9
5	G	116	LEU	2.8
5	G	49	ARG	2.6
5	G	29	TYR	2.4
5	G	88	LEU	2.4
5	G	44	PHE	2.3
5	G	2	PRO	2.2
5	G	91	GLU	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](#)

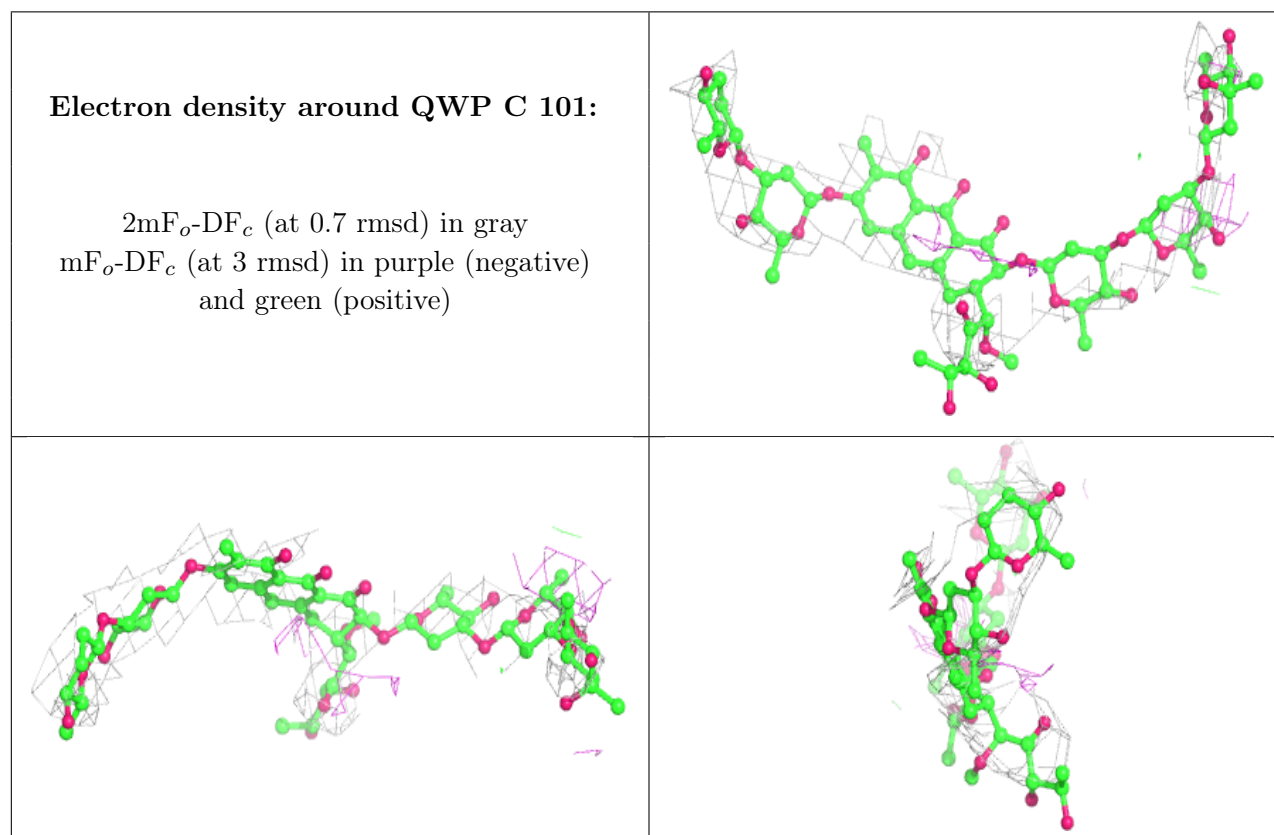
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

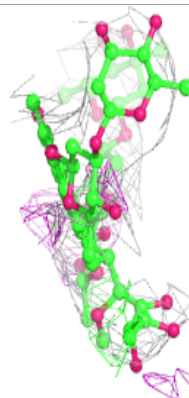
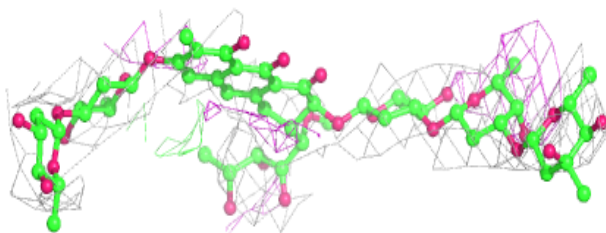
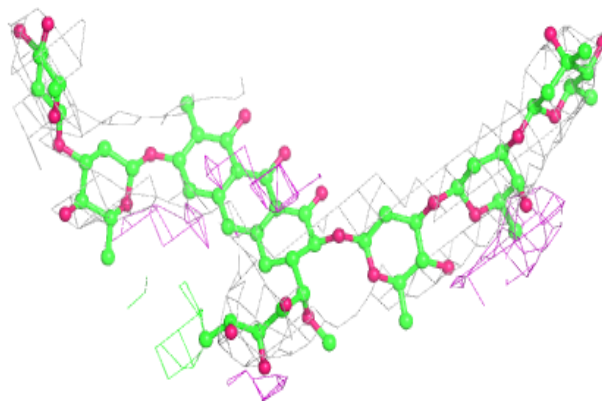
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	QWP	C	101	75/76	0.79	0.43	227,284,322,326	0
6	QWP	B	101	76/76	0.85	0.37	195,236,295,305	0
7	MG	B	102	1/1	0.95	0.07	216,216,216,216	0

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.



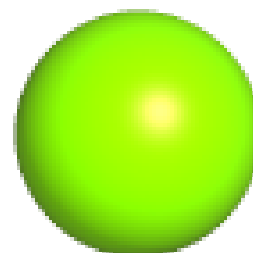
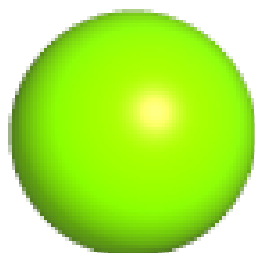
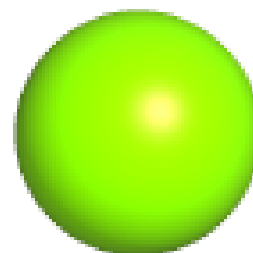
**Electron density around QWP B 101:**

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



**Electron density around MG B 102:**

$2mF_o-DF_c$  (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.