



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2021 – 02:05 am GMT

PDB ID : 7A6W  
Title : Structure of the FKBP51FK1 domain in complex with the macrocyclic SAFit analogue 33-(Z)  
Authors : Bauder, M.; Meyners, C.; Purder, P.; Merz, S.; Voll, A.; Heymann, T.; Hausch, F.  
Deposited on : 2020-08-27  
Resolution : 1.85 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 : 2.17.1  
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) : 2.17.1

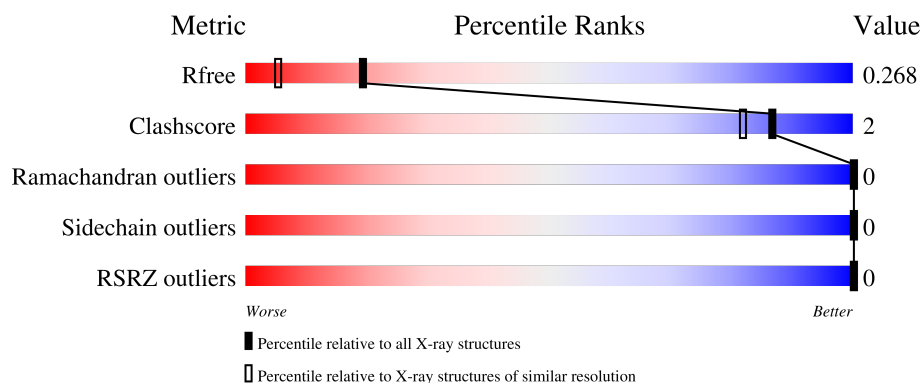
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


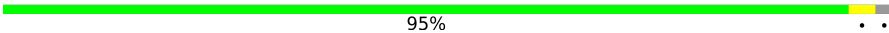
The reported resolution of this entry is 1.85 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	AAA	130	 88% 8% .
1	BBB	130	 95% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4038 atoms, of which 2006 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.

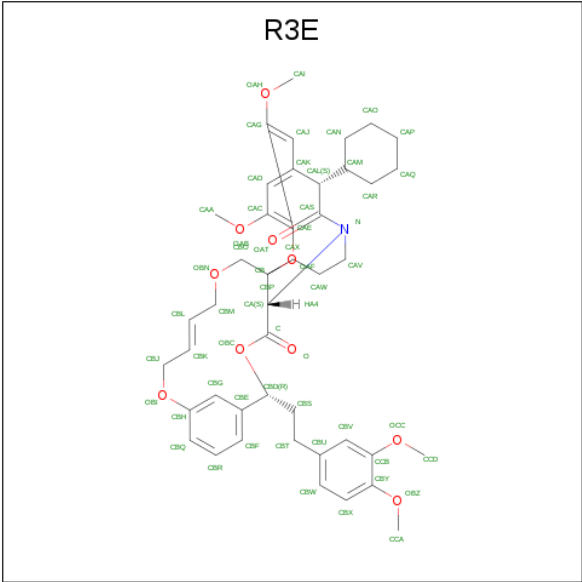
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	126	Total	C	H	N	O	S	34	0	0
			1896	607	958	157	172	2			
1	BBB	128	Total	C	H	N	O	S	35	0	0
			1874	605	934	153	180	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	11	HIS	-	expression tag	UNP Q13451
AAA	12	MET	-	expression tag	UNP Q13451
AAA	13	GLY	-	expression tag	UNP Q13451
AAA	14	ALA	-	expression tag	UNP Q13451
AAA	15	PRO	-	expression tag	UNP Q13451
AAA	19	THR	ALA	engineered mutation	UNP Q13451
AAA	103	ALA	CYS	engineered mutation	UNP Q13451
AAA	107	ILE	CYS	engineered mutation	UNP Q13451
BBB	11	HIS	-	expression tag	UNP Q13451
BBB	12	MET	-	expression tag	UNP Q13451
BBB	13	GLY	-	expression tag	UNP Q13451
BBB	14	ALA	-	expression tag	UNP Q13451
BBB	15	PRO	-	expression tag	UNP Q13451
BBB	19	THR	ALA	engineered mutation	UNP Q13451
BBB	103	ALA	CYS	engineered mutation	UNP Q13451
BBB	107	ILE	CYS	engineered mutation	UNP Q13451

- Molecule 2 is (2S,9S,12R,20Z)-2-cyclohexyl-12-[2-(3,4-dimethoxyphenyl)ethyl]-28,31-dimethoxy-11,18,23,26-tetraoxa-4-azatetracyclo[25.2.2.113,17.04,9]dotriaconta-1(29),13(32),14,16,20,27,30-heptaene-3,10-dione (three-letter code: R3E) (formula: C<sub>45</sub>H<sub>57</sub>NO<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	0	0
			113	45	57	1	10		
2	BBB	1	Total	C	H	N	O	0	0
			113	45	57	1	10		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	16	Total	O	0	0
			16	16		
3	BBB	26	Total	O	0	0
			26	26		

### 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: Peptidyl-prolyl cis-trans isomerase FKBP5

Chain AAA:  88% 8% .



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP5

Chain BBB:  95% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.80Å 47.87Å 61.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.27 – 1.85 32.27 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (32.27-1.85) 95.9 (32.27-1.50)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, $R_{free}$	0.183 , 0.267 0.190 , 0.268	Depositor DCC
$R_{free}$ test set	1689 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.4	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 14.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
Reported twinning fraction	0.524 for H, K, L 0.476 for -h,-k,l	Depositor
Outliers	0 of 34135 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: R3E

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	0.78	0/958	0.79	0/1291
1	BBB	0.77	0/960	0.79	0/1299
All	All	0.78	0/1918	0.79	0/2590

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	938	958	935	6	0
1	BBB	940	934	908	2	0
2	AAA	56	57	0	0	0
2	BBB	56	57	0	0	0
3	AAA	16	0	0	0	0
3	BBB	26	0	0	0	0
All	All	2032	2006	1843	8	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 (8) 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:80:SER:N	1:AAA:85:GLN:OE1	2.38	0.54
1:AAA:113:TYR:CD2	1:AAA:122:ILE:HG21	2.47	0.49
1:BBB:47:PRO:HD2	1:BBB:97:MET:O	2.13	0.47
1:BBB:81:LEU:HD11	1:BBB:95:ALA:HB2	1.97	0.46
1:AAA:62:SER:HB3	1:AAA:127:THR:HG22	1.98	0.45
1:AAA:53:VAL:HG11	1:AAA:94:VAL:HG11	1.97	0.45
1:AAA:35:LYS:HA	1:AAA:104:HIS:O	2.18	0.43
1:AAA:128:LEU:N	1:AAA:128:LEU:HD23	2.35	0.40

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	124/130 (95%)	118 (95%)	6 (5%)	0	100	100
1	BBB	126/130 (97%)	120 (95%)	6 (5%)	0	100	100
All	All	250/260 (96%)	238 (95%)	12 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	95/107 (89%)	95 (100%)	0	100	100
1	BBB	94/107 (88%)	94 (100%)	0	100	100
All	All	189/214 (88%)	189 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are 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
2	R3E	AAA	201	-	60,61,61	2.15	8 (13%)	80,82,82	1.20	10 (12%)
2	R3E	BBB	201	-	60,61,61	1.92	8 (13%)	80,82,82	1.26	10 (12%)

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	R3E	AAA	201	-	-	12/53/72/72	0/5/6/6
2	R3E	BBB	201	-	-	11/53/72/72	0/5/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	201	R3E	CAL-CAS	-9.01	1.42	1.53
2	BBB	201	R3E	CAL-CAS	-8.17	1.43	1.53
2	AAA	201	R3E	CAK-CAL	-6.77	1.42	1.52
2	AAA	201	R3E	CBE-CBD	-6.70	1.40	1.51
2	BBB	201	R3E	CAK-CAL	-5.23	1.44	1.52
2	AAA	201	R3E	CA-C	-4.97	1.42	1.52
2	BBB	201	R3E	CA-N	4.81	1.52	1.47
2	BBB	201	R3E	CA-C	-4.27	1.44	1.52
2	BBB	201	R3E	CBT-CBU	-3.68	1.41	1.51
2	BBB	201	R3E	CBE-CBD	-3.64	1.45	1.51
2	AAA	201	R3E	CA-N	3.11	1.50	1.47
2	AAA	201	R3E	CBT-CBU	-2.86	1.43	1.51
2	BBB	201	R3E	OBZ-CBY	2.19	1.40	1.37
2	AAA	201	R3E	CBQ-CBH	2.16	1.43	1.38
2	BBB	201	R3E	CAD-CAC	2.03	1.42	1.38
2	AAA	201	R3E	CAJ-CAG	2.00	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	201	R3E	CCA-OBZ-CBY	-3.59	112.11	117.53
2	AAA	201	R3E	CBP-OAF-CAE	3.43	124.61	114.23
2	BBB	201	R3E	CBS-CBD-CBE	3.26	118.52	112.62
2	BBB	201	R3E	CAW-CAV-N	-3.25	105.57	110.67
2	BBB	201	R3E	CAP-CAO-CAN	-3.21	104.87	111.42
2	AAA	201	R3E	CAP-CAO-CAN	-3.00	105.29	111.42
2	BBB	201	R3E	CAK-CAL-CAS	2.93	113.72	108.39
2	AAA	201	R3E	CAQ-CAR-CAM	-2.84	107.09	111.93
2	BBB	201	R3E	OAB-CAC-CAD	2.56	128.52	124.12
2	AAA	201	R3E	OBC-CBD-CBS	2.47	108.87	105.34
2	AAA	201	R3E	CB-CA-N	2.45	113.94	110.53
2	BBB	201	R3E	CAG-CAE-CAC	2.40	122.03	119.57
2	BBB	201	R3E	CBH-CBG-CBE	2.39	123.31	119.95
2	BBB	201	R3E	OAT-CAS-N	-2.35	117.20	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	201	R3E	OCC-CCB-CBY	2.27	118.57	115.41
2	BBB	201	R3E	CBQ-CBH-CBG	-2.25	117.45	120.53
2	AAA	201	R3E	OCC-CCB-CBV	-2.14	120.43	124.12
2	AAA	201	R3E	OBC-C-CA	2.13	115.48	110.78
2	AAA	201	R3E	OAT-CAS-N	-2.10	117.64	121.38
2	AAA	201	R3E	CAD-CAK-CAL	-2.06	117.21	120.31

There are no chirality outliers.

All (23) torsion outliers are listed below:

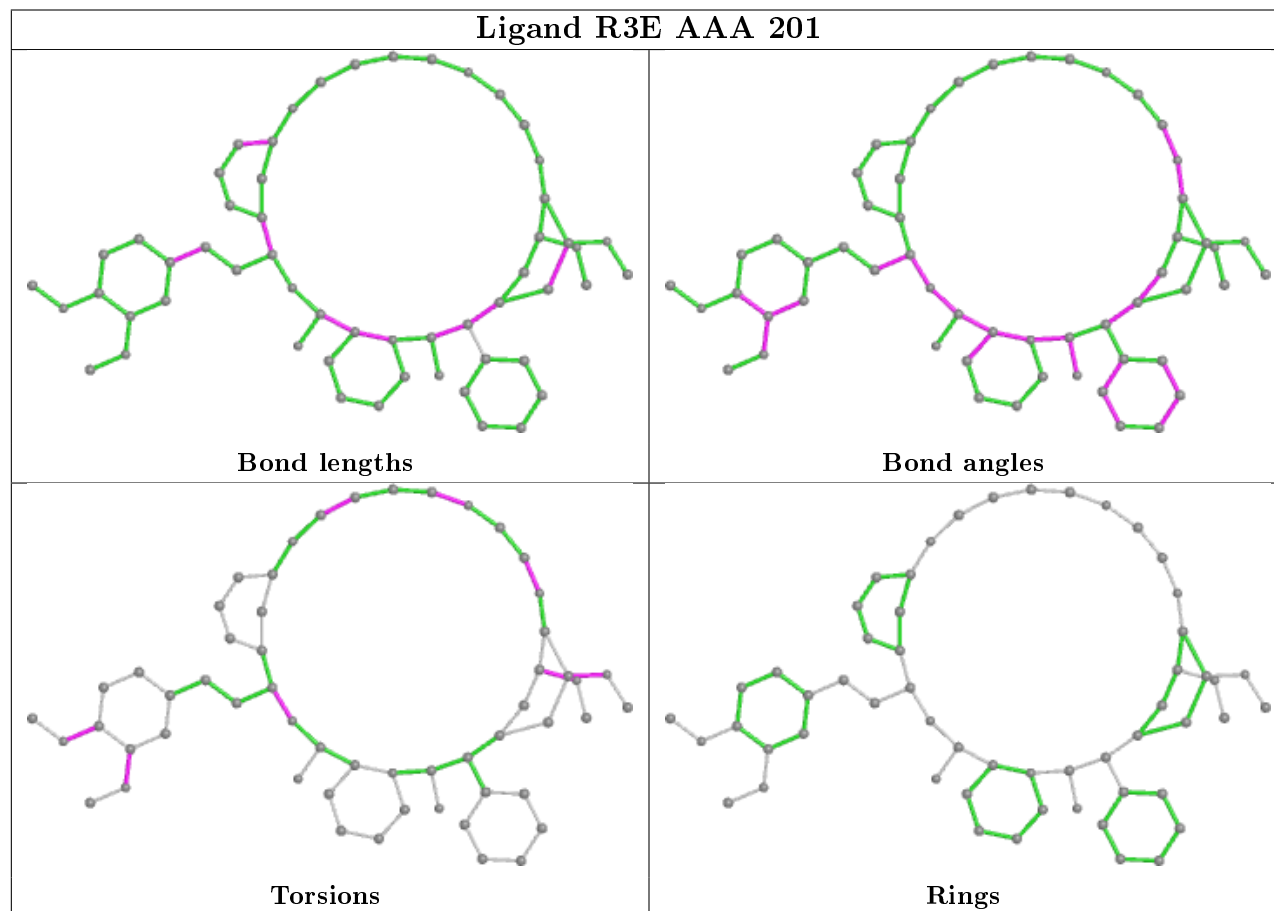
Mol	Chain	Res	Type	Atoms
2	BBB	201	R3E	CCB-CBY-OBZ-CCA
2	BBB	201	R3E	CBX-CBY-OBZ-CCA
2	AAA	201	R3E	CAE-CAG-OAH-CAI
2	AAA	201	R3E	CAJ-CAG-OAH-CAI
2	AAA	201	R3E	CBV-CCB-OCC-CCD
2	BBB	201	R3E	CBY-CCB-OCC-CCD
2	AAA	201	R3E	CAE-CAC-OAB-CAA
2	AAA	201	R3E	CBY-CCB-OCC-CCD
2	AAA	201	R3E	CAD-CAC-OAB-CAA
2	BBB	201	R3E	CBV-CCB-OCC-CCD
2	BBB	201	R3E	CAE-CAG-OAH-CAI
2	AAA	201	R3E	CBS-CBD-OBC-C
2	BBB	201	R3E	CAJ-CAG-OAH-CAI
2	AAA	201	R3E	CBL-CBM-OBN-CBO
2	AAA	201	R3E	CBE-CBD-OBC-C
2	BBB	201	R3E	CBG-CBH-OBI-CBJ
2	BBB	201	R3E	CBQ-CBH-OBI-CBJ
2	AAA	201	R3E	CBO-CBP-OAF-CAE
2	BBB	201	R3E	CBD-CBS-CBT-CBU
2	AAA	201	R3E	OBI-CBJ-CBK-CBL
2	AAA	201	R3E	CCB-CBY-OBZ-CCA
2	BBB	201	R3E	CBS-CBD-OBC-C
2	BBB	201	R3E	CBO-CBP-OAF-CAE

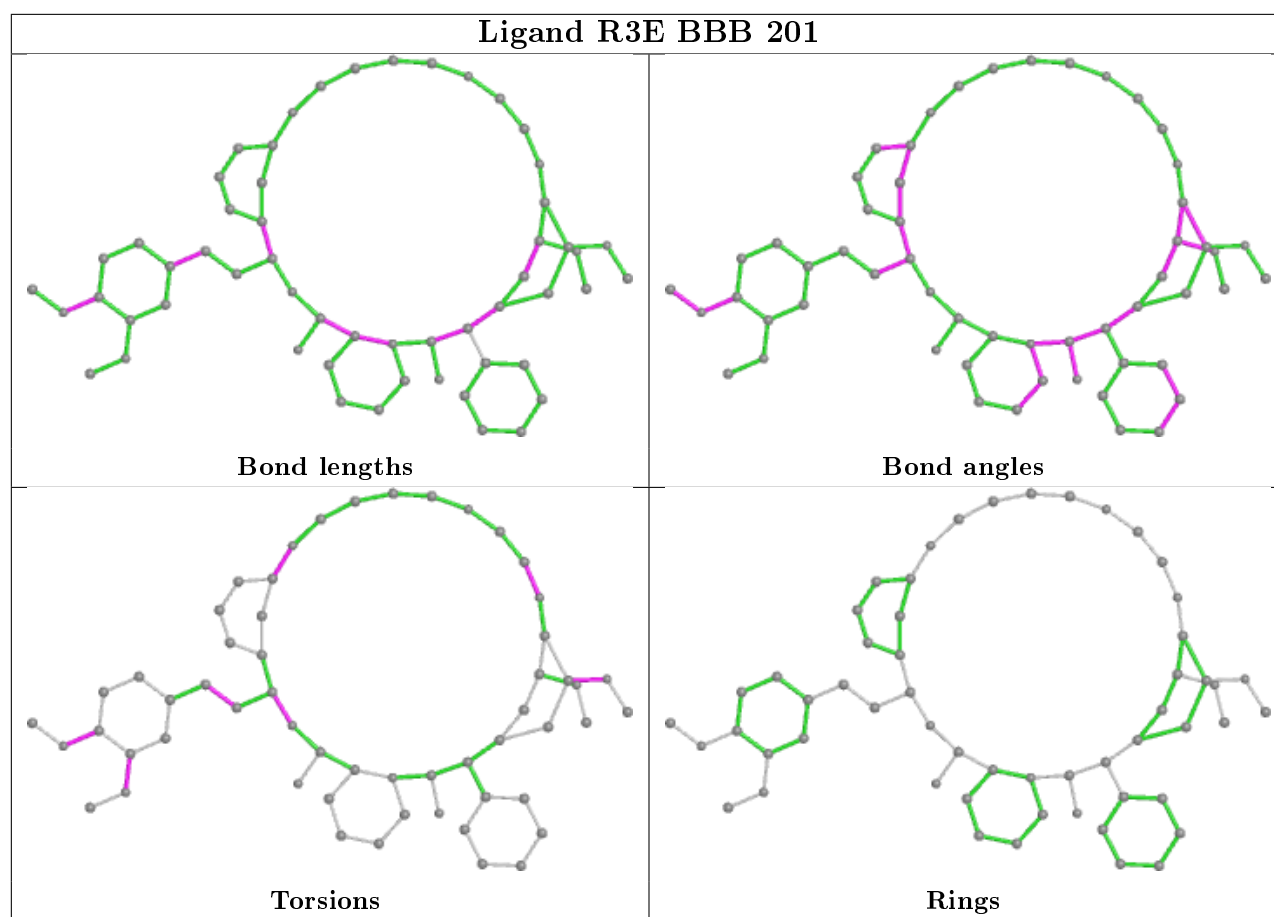
There are no ring outliers.

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 [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, 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(Å <sup>2</sup> )	Q<0.9
1	AAA	126/130 (96%)	-0.94	0 100 100	10, 17, 29, 35	0
1	BBB	128/130 (98%)	-0.88	0 100 100	8, 18, 32, 36	0
All	All	254/260 (97%)	-0.91	0 100 100	8, 18, 32, 36	0

There are no RSRZ outliers to report.

### 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](#)

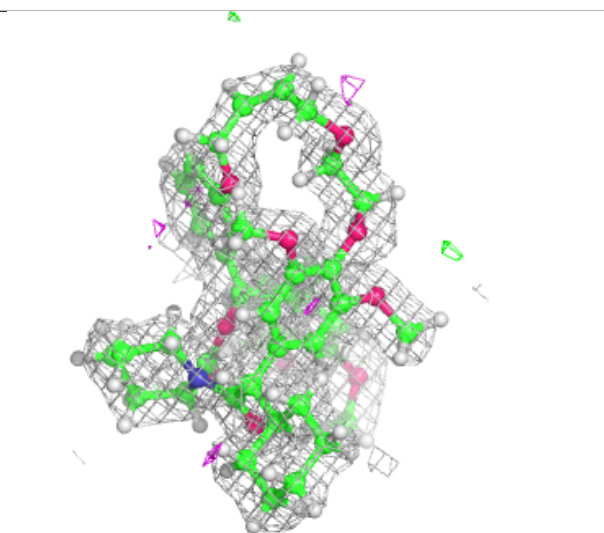
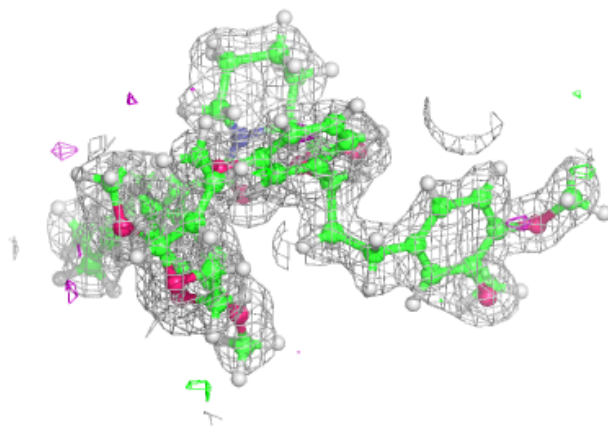
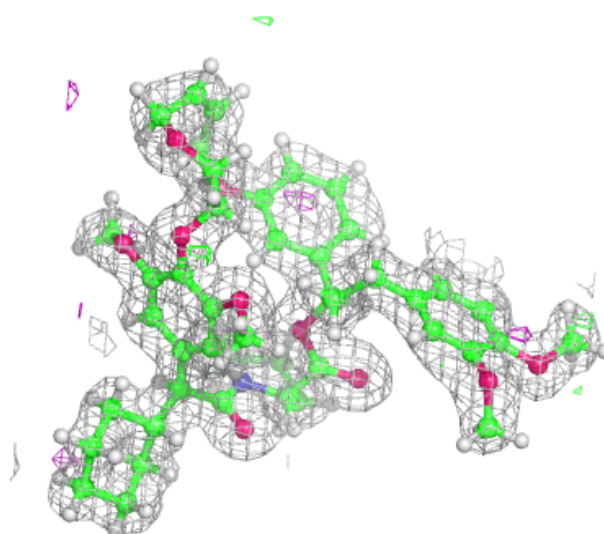
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	R3E	AAA	201	56/56	0.97	0.07	10,14,23,24	0
2	R3E	BBB	201	56/56	0.97	0.07	13,17,23,25	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.

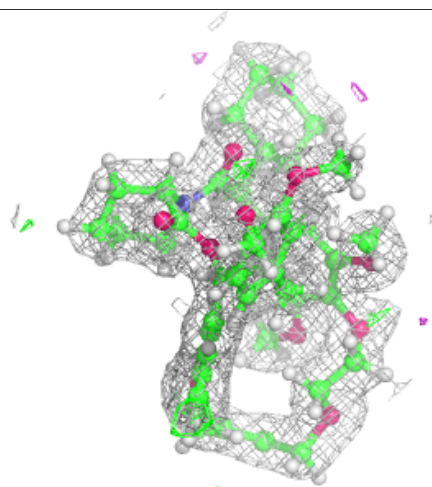
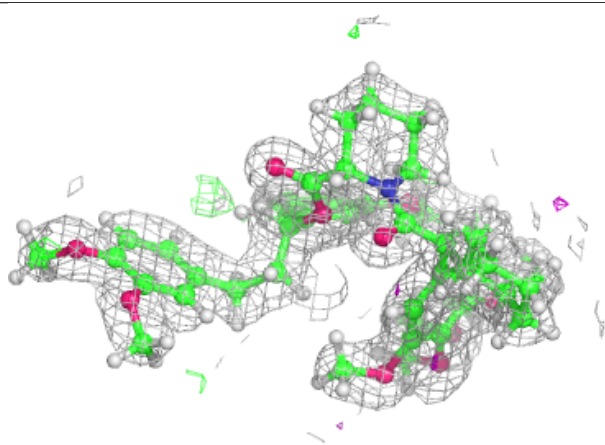
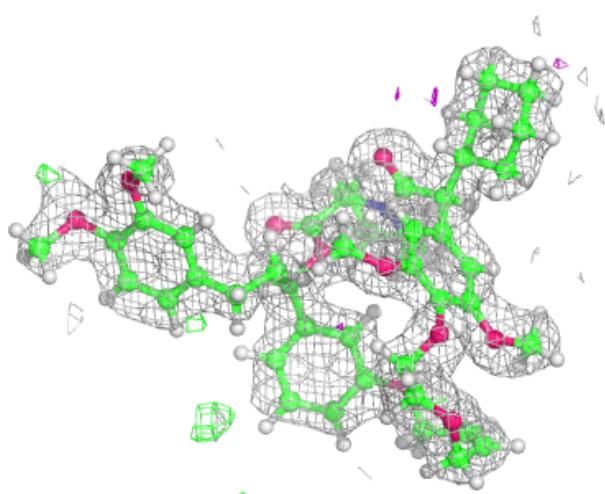
**Electron density around R3E AAA 201:**

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



**Electron density around R3E BBB 201:**

$2mF_o-DF_c$  (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.