



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:04 PM UTC

PDB ID : 6BEC / pdb\_00006bec  
Title : Crystal structure of VACV D13 in complex with Rifabutin  
Authors : Garriga, D.; Accurso, C.; Coulibaly, F.  
Deposited on : 2017-10-25  
Resolution : 2.91 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.

The types of validation reports are described at

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

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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)  
Xtrriage (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

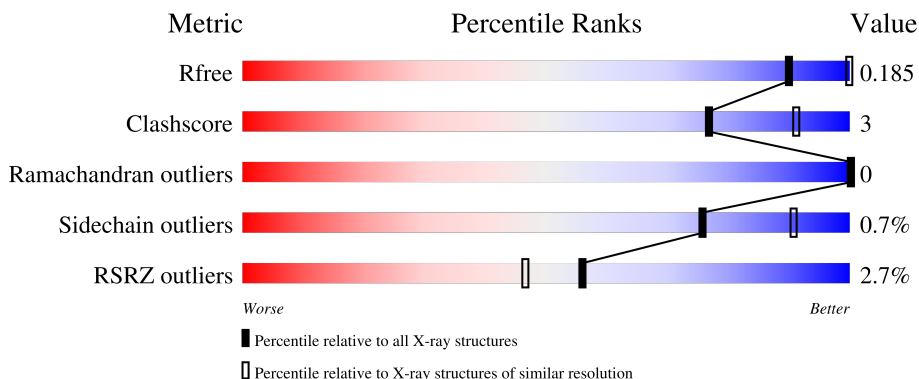
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

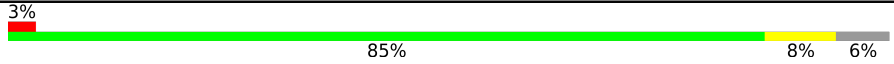
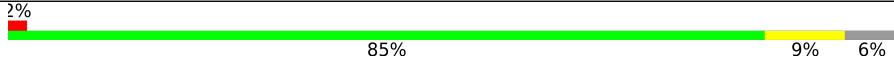

The reported resolution of this entry is 2.91 Å.

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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	A	576	 3% 85% 9% 6%
1	B	576	 2% 85% 9% 6%
1	C	576	 3% 85% 9% 6%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13191 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 Scaffold protein D13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	540	4268	2730	696	829	13	0	3	0
1	B	541	4260	2721	696	831	12	0	3	0
1	C	541	4252	2725	686	829	12	0	0	0

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P68440
A	-23	SER	-	expression tag	UNP P68440
A	-22	TYR	-	expression tag	UNP P68440
A	-21	TYR	-	expression tag	UNP P68440
A	-20	HIS	-	expression tag	UNP P68440
A	-19	HIS	-	expression tag	UNP P68440
A	-18	HIS	-	expression tag	UNP P68440
A	-17	HIS	-	expression tag	UNP P68440
A	-16	HIS	-	expression tag	UNP P68440
A	-15	HIS	-	expression tag	UNP P68440
A	-14	ASP	-	expression tag	UNP P68440
A	-13	TYR	-	expression tag	UNP P68440
A	-12	ASP	-	expression tag	UNP P68440
A	-11	ILE	-	expression tag	UNP P68440
A	-10	PRO	-	expression tag	UNP P68440
A	-9	THR	-	expression tag	UNP P68440
A	-8	THR	-	expression tag	UNP P68440
A	-7	GLU	-	expression tag	UNP P68440
A	-6	ASN	-	expression tag	UNP P68440
A	-5	LEU	-	expression tag	UNP P68440
A	-4	TYR	-	expression tag	UNP P68440
A	-3	PHE	-	expression tag	UNP P68440
A	-2	GLN	-	expression tag	UNP P68440

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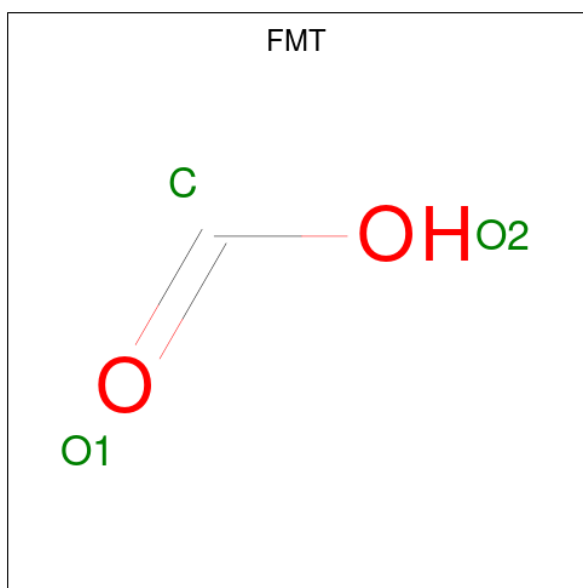
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P68440
A	0	ALA	-	expression tag	UNP P68440
B	-24	MET	-	initiating methionine	UNP P68440
B	-23	SER	-	expression tag	UNP P68440
B	-22	TYR	-	expression tag	UNP P68440
B	-21	TYR	-	expression tag	UNP P68440
B	-20	HIS	-	expression tag	UNP P68440
B	-19	HIS	-	expression tag	UNP P68440
B	-18	HIS	-	expression tag	UNP P68440
B	-17	HIS	-	expression tag	UNP P68440
B	-16	HIS	-	expression tag	UNP P68440
B	-15	HIS	-	expression tag	UNP P68440
B	-14	ASP	-	expression tag	UNP P68440
B	-13	TYR	-	expression tag	UNP P68440
B	-12	ASP	-	expression tag	UNP P68440
B	-11	ILE	-	expression tag	UNP P68440
B	-10	PRO	-	expression tag	UNP P68440
B	-9	THR	-	expression tag	UNP P68440
B	-8	THR	-	expression tag	UNP P68440
B	-7	GLU	-	expression tag	UNP P68440
B	-6	ASN	-	expression tag	UNP P68440
B	-5	LEU	-	expression tag	UNP P68440
B	-4	TYR	-	expression tag	UNP P68440
B	-3	PHE	-	expression tag	UNP P68440
B	-2	GLN	-	expression tag	UNP P68440
B	-1	GLY	-	expression tag	UNP P68440
B	0	ALA	-	expression tag	UNP P68440
C	-24	MET	-	initiating methionine	UNP P68440
C	-23	SER	-	expression tag	UNP P68440
C	-22	TYR	-	expression tag	UNP P68440
C	-21	TYR	-	expression tag	UNP P68440
C	-20	HIS	-	expression tag	UNP P68440
C	-19	HIS	-	expression tag	UNP P68440
C	-18	HIS	-	expression tag	UNP P68440
C	-17	HIS	-	expression tag	UNP P68440
C	-16	HIS	-	expression tag	UNP P68440
C	-15	HIS	-	expression tag	UNP P68440
C	-14	ASP	-	expression tag	UNP P68440
C	-13	TYR	-	expression tag	UNP P68440
C	-12	ASP	-	expression tag	UNP P68440
C	-11	ILE	-	expression tag	UNP P68440
C	-10	PRO	-	expression tag	UNP P68440

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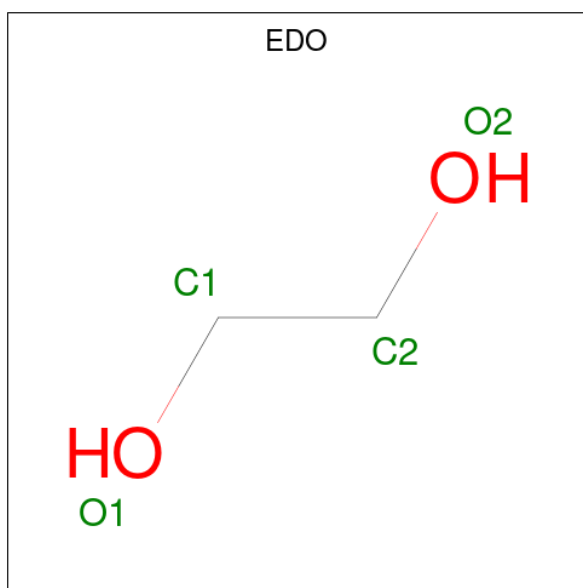
Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	THR	-	expression tag	UNP P68440
C	-8	THR	-	expression tag	UNP P68440
C	-7	GLU	-	expression tag	UNP P68440
C	-6	ASN	-	expression tag	UNP P68440
C	-5	LEU	-	expression tag	UNP P68440
C	-4	TYR	-	expression tag	UNP P68440
C	-3	PHE	-	expression tag	UNP P68440
C	-2	GLN	-	expression tag	UNP P68440
C	-1	GLY	-	expression tag	UNP P68440
C	0	ALA	-	expression tag	UNP P68440

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



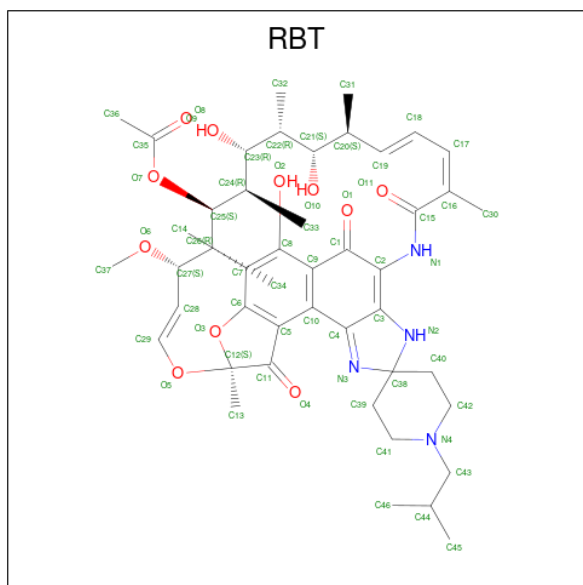
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 1 2	0	0
2	B	1	Total C O 3 1 2	0	0
2	B	1	Total C O 3 1 2	0	0
2	C	1	Total C O 3 1 2	0	0
2	C	1	Total C O 3 1 2	0	0
2	C	1	Total C O 3 1 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is RIFABUTIN (CCD ID: RBT) (formula:  $C_{46}H_{62}N_4O_{11}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			61	46	4	11		

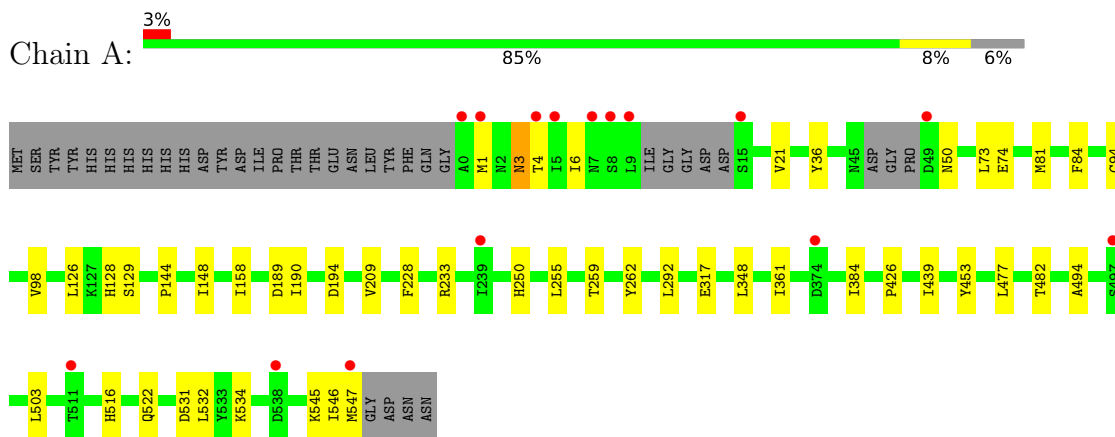
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	B	88	Total	O	0	0
			88	88		
5	C	104	Total	O	0	0
			104	104		

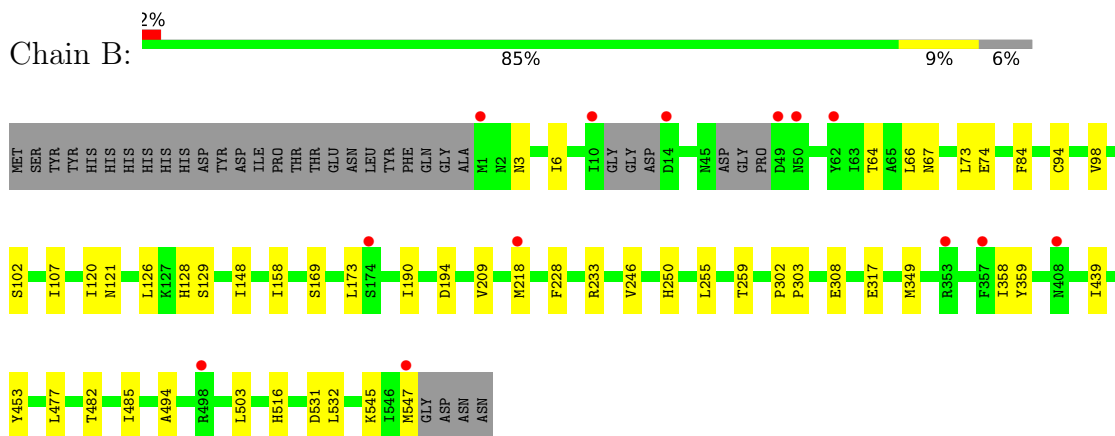
### 3 Residue-property plots [i](#)

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.

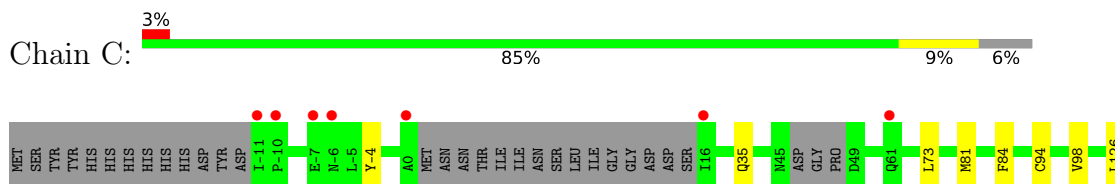
- Molecule 1: Scaffold protein D13

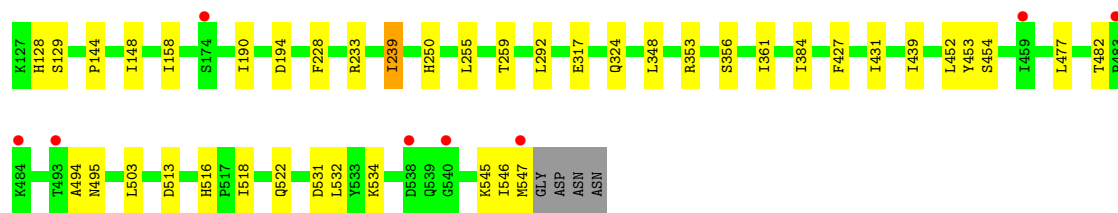


- Molecule 1: Scaffold protein D13



- Molecule 1: Scaffold protein D13





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.62Å 188.62Å 261.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.91 19.99 – 2.91	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.91) 99.6 (19.99-2.91)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.93Å)	Xtrriage
Refinement program	BUSTER, BUSTER	Depositor
R, $R_{free}$	0.195 , 0.226 (Not available) , 0.185	Depositor DCC
$R_{free}$ test set	3001 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtrriage
Anisotropy	0.160	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: EDO, RBT, FMT

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	0.70	0/4362	1.14	7/5938 (0.1%)
1	B	0.71	0/4353	1.13	9/5930 (0.2%)
1	C	0.70	0/4346	1.11	11/5921 (0.2%)
All	All	0.70	0/13061	1.13	27/17789 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	317	GLU	CA-C-N	5.91	128.20	120.28
1	C	317	GLU	C-N-CA	5.91	128.20	120.28
1	A	317	GLU	CA-C-N	5.91	128.20	120.28
1	A	317	GLU	C-N-CA	5.91	128.20	120.28
1	B	317	GLU	CA-C-N	5.87	128.14	120.28
1	B	317	GLU	C-N-CA	5.87	128.14	120.28
1	B	128	HIS	CA-C-N	5.65	128.41	120.28
1	B	128	HIS	C-N-CA	5.65	128.41	120.28
1	C	128	HIS	CA-C-N	5.59	128.33	120.28
1	C	128	HIS	C-N-CA	5.59	128.33	120.28
1	A	128	HIS	CA-C-N	5.57	128.30	120.28
1	A	128	HIS	C-N-CA	5.57	128.30	120.28
1	A	50	ASN	CA-C-N	5.44	128.57	120.95
1	A	50	ASN	C-N-CA	5.44	128.57	120.95
1	C	194	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	-4	TYR	CA-C-N	5.38	130.00	122.36
1	C	-4	TYR	C-N-CA	5.38	130.00	122.36
1	C	513	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	194	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	194	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	495	ASN	CA-C-N	5.12	127.20	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	495	ASN	C-N-CA	5.12	127.20	120.60
1	B	308	GLU	CA-C-N	5.11	127.63	120.28
1	B	308	GLU	C-N-CA	5.11	127.63	120.28
1	B	121	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	67	ASN	CA-CB-CG	5.04	117.64	112.60
1	C	427	PHE	CA-CB-CG	5.00	118.80	113.80

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	4268	0	4193	25	0
1	B	4260	0	4168	23	0
1	C	4252	0	4164	25	0
2	A	3	0	1	0	0
2	B	6	0	2	1	0
2	C	9	0	5	0	0
3	A	12	0	18	3	0
3	B	4	0	6	2	0
3	C	12	0	18	5	0
4	C	61	0	61	3	0
5	A	112	0	0	0	0
5	B	88	0	0	0	0
5	C	104	0	0	0	0
All	All	13191	0	12636	73	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 3.

All (73) 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:36:TYR:H	3:A:604:EDO:H12	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:HIS:ND1	3:A:602:EDO:H21	2.13	0.64
4:C:601:RBT:H18	4:C:601:RBT:HN1	1.64	0.63
1:B:259:THR:HG21	1:B:439:ILE:HD11	1.80	0.63
1:C:353:ARG:HB2	1:C:356:SER:HB3	1.82	0.62
1:C:259:THR:HG21	1:C:439:ILE:HD11	1.82	0.61
1:A:259:THR:HG21	1:A:439:ILE:HD11	1.84	0.59
1:A:21:VAL:HG11	1:C:482:THR:HG22	1.86	0.58
1:C:81:MET:HE2	1:C:144:PRO:HG3	1.86	0.58
1:C:324:GLN:HE22	3:C:606:EDO:H21	1.70	0.57
1:A:81:MET:HE2	1:A:144:PRO:HG3	1.85	0.57
1:A:1:MET:HE2	1:B:218:MET:HB2	1.88	0.55
1:A:94:CYS:HB3	1:A:190:ILE:HG21	1.87	0.55
1:A:262:TYR:HB3	1:A:522:GLN:HB2	1.89	0.54
1:C:94:CYS:HB3	1:C:190:ILE:HG21	1.91	0.53
3:A:604:EDO:H11	1:B:477:LEU:HD22	1.93	0.51
1:C:516:HIS:ND1	3:C:605:EDO:H12	2.25	0.51
1:A:84:PHE:HB3	1:A:148:ILE:HG21	1.93	0.51
1:C:84:PHE:HB3	1:C:148:ILE:HG21	1.93	0.51
1:B:84:PHE:HB3	1:B:148:ILE:HG21	1.93	0.50
4:C:601:RBT:H332	4:C:601:RBT:H342	1.91	0.50
1:C:35:GLN:HA	3:C:607:EDO:H12	1.94	0.50
1:B:233:ARG:HD3	1:B:531:ASP:OD1	2.11	0.50
1:B:74:GLU:HB2	1:B:209:VAL:HB	1.94	0.49
1:A:477:LEU:HB3	3:C:607:EDO:H21	1.95	0.49
1:B:102:SER:HB3	1:B:107:ILE:HD11	1.96	0.48
1:B:66:LEU:HD23	1:B:173:LEU:HD11	1.95	0.48
1:B:98:VAL:HG11	1:B:158:ILE:HG21	1.97	0.47
1:C:239:ILE:HD11	1:C:522:GLN:CD	2.40	0.47
1:A:250:HIS:HA	1:A:494:ALA:HB2	1.97	0.47
1:C:255:LEU:HD13	1:C:503:LEU:HD13	1.97	0.47
1:A:74:GLU:HB2	1:A:209:VAL:HB	1.97	0.47
1:B:545:LYS:HB3	1:B:547:MET:HE2	1.97	0.47
1:B:250:HIS:HA	1:B:494:ALA:HB2	1.97	0.47
1:B:255:LEU:HD13	1:B:503:LEU:HD13	1.96	0.47
1:A:233:ARG:HD3	1:A:531:ASP:OD1	2.16	0.46
1:B:94:CYS:HB3	1:B:190:ILE:HG21	1.97	0.46
1:C:98:VAL:HG11	1:C:158:ILE:HG21	1.98	0.46
1:C:545:LYS:HB3	1:C:547:MET:HE2	1.97	0.46
4:C:601:RBT:H18	4:C:601:RBT:N1	2.31	0.46
1:A:545:LYS:HB3	1:A:547:MET:HE2	1.98	0.45
1:A:98:VAL:HG11	1:A:158:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:LEU:HD11	1:C:384:ILE:HG13	1.96	0.45
1:A:255:LEU:HD13	1:A:503:LEU:HD13	1.98	0.45
1:A:453:TYR:CD2	1:A:477:LEU:HD21	2.52	0.45
1:B:349:MET:HE3	1:B:358:ILE:HG21	1.99	0.45
1:C:233:ARG:HD3	1:C:531:ASP:OD1	2.17	0.44
1:A:4:THR:HG21	1:C:452:LEU:HA	2.00	0.44
1:C:250:HIS:HA	1:C:494:ALA:HB2	1.98	0.44
1:A:126:LEU:O	1:A:129:SER:HB3	2.18	0.43
1:B:228:PHE:HB3	1:B:532:LEU:HD11	2.01	0.43
1:B:126:LEU:O	1:B:129:SER:HB3	2.18	0.43
1:B:453:TYR:CD2	1:B:477:LEU:HD21	2.54	0.43
1:C:126:LEU:O	1:C:129:SER:HB3	2.18	0.43
1:A:228:PHE:HB3	1:A:532:LEU:HD11	2.00	0.43
1:B:516:HIS:ND1	3:B:603:EDO:H12	2.34	0.43
1:C:228:PHE:HB3	1:C:532:LEU:HD11	2.00	0.42
1:B:246:VAL:HA	2:B:602:FMT:H	2.01	0.42
1:C:453:TYR:CD2	1:C:477:LEU:HD21	2.54	0.42
1:C:348:LEU:HD12	1:C:361:ILE:HG21	2.01	0.42
1:A:348:LEU:HD12	1:A:361:ILE:HG21	2.01	0.42
1:A:534:LYS:HB2	1:A:546:ILE:HD11	2.02	0.42
1:B:3:ASN:HA	1:B:6:ILE:HD12	2.02	0.42
1:B:302:PRO:HA	1:B:303:PRO:HD3	1.98	0.42
1:C:534:LYS:HB2	1:C:546:ILE:HD11	2.01	0.42
1:A:292:LEU:HD11	1:A:384:ILE:HG13	2.01	0.42
1:C:324:GLN:NE2	3:C:606:EDO:H21	2.35	0.42
1:C:431:ILE:HD13	1:C:518:ILE:HG12	2.01	0.42
1:A:189:ASP:HB3	1:A:426:PRO:HD3	2.01	0.41
1:B:169:SER:HB3	1:B:485:ILE:HG13	2.00	0.41
1:A:3:ASN:HA	1:A:6:ILE:HD12	2.02	0.41
1:C:431:ILE:HG12	1:C:439:ILE:HG21	2.03	0.41
1:B:359:TYR:OH	3:B:603:EDO:H21	2.20	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	A	537/576 (93%)	516 (96%)	21 (4%)	0	100	100
1	B	538/576 (93%)	512 (95%)	26 (5%)	0	100	100
1	C	535/576 (93%)	513 (96%)	22 (4%)	0	100	100
All	All	1610/1728 (93%)	1541 (96%)	69 (4%)	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	A	486/528 (92%)	483 (99%)	3 (1%)	78	92
1	B	485/528 (92%)	481 (99%)	4 (1%)	73	89
1	C	484/528 (92%)	481 (99%)	3 (1%)	78	92
All	All	1455/1584 (92%)	1445 (99%)	10 (1%)	76	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	73	LEU
1	A	482	THR
1	B	64	THR
1	B	73	LEU
1	B	120	ILE
1	B	482	THR
1	C	73	LEU
1	C	239	ILE
1	C	454	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	96	ASN
1	A	408	ASN
1	A	411	ASN
1	A	435	ASN
1	A	480	ASN
1	B	96	ASN
1	B	203	ASN
1	B	408	ASN
1	B	411	ASN
1	B	435	ASN
1	B	472	ASN
1	C	96	ASN
1	C	203	ASN
1	C	408	ASN
1	C	411	ASN
1	C	435	ASN
1	C	456	ASN
1	C	472	ASN
1	C	522	GLN
1	C	524	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

14 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
3	EDO	C	607	-	3,3,3	0.53	0	2,2,2	0.23	0
3	EDO	A	602	-	3,3,3	0.56	0	2,2,2	0.14	0
2	FMT	C	604	-	2,2,2	1.22	0	1,1,1	1.09	0
2	FMT	C	603	-	2,2,2	1.18	0	1,1,1	1.10	0
3	EDO	A	604	-	3,3,3	0.59	0	2,2,2	0.26	0
2	FMT	B	601	-	2,2,2	1.12	0	1,1,1	1.01	0
3	EDO	C	605	-	3,3,3	0.55	0	2,2,2	0.10	0
3	EDO	A	603	-	3,3,3	0.54	0	2,2,2	0.29	0
2	FMT	B	602	-	2,2,2	1.13	0	1,1,1	1.00	0
3	EDO	B	603	-	3,3,3	0.49	0	2,2,2	0.22	0
3	EDO	C	606	-	3,3,3	0.53	0	2,2,2	0.14	0
4	RBT	C	601	-	61,66,66	0.68	1 (1%)	87,101,101	1.15	4 (4%)
2	FMT	C	602	-	2,2,2	1.12	0	1,1,1	1.07	0
2	FMT	A	601	-	2,2,2	1.11	0	1,1,1	1.08	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
3	EDO	C	607	-	-	1/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	C	605	-	-	1/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	C	606	-	-	0/1/1/1	-
4	RBT	C	601	-	-	25/59/116/116	0/5/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	RBT	C22-C21	2.08	1.59	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	C	601	RBT	C40-C38-N3	-5.54	106.61	111.44
4	C	601	RBT	C39-C38-N3	-3.81	108.12	111.44
4	C	601	RBT	C1-C2-N1	3.48	122.82	115.21
4	C	601	RBT	O5-C12-C11	2.08	117.71	111.99

There are no chirality outliers.

All (28) torsion outliers are listed below:

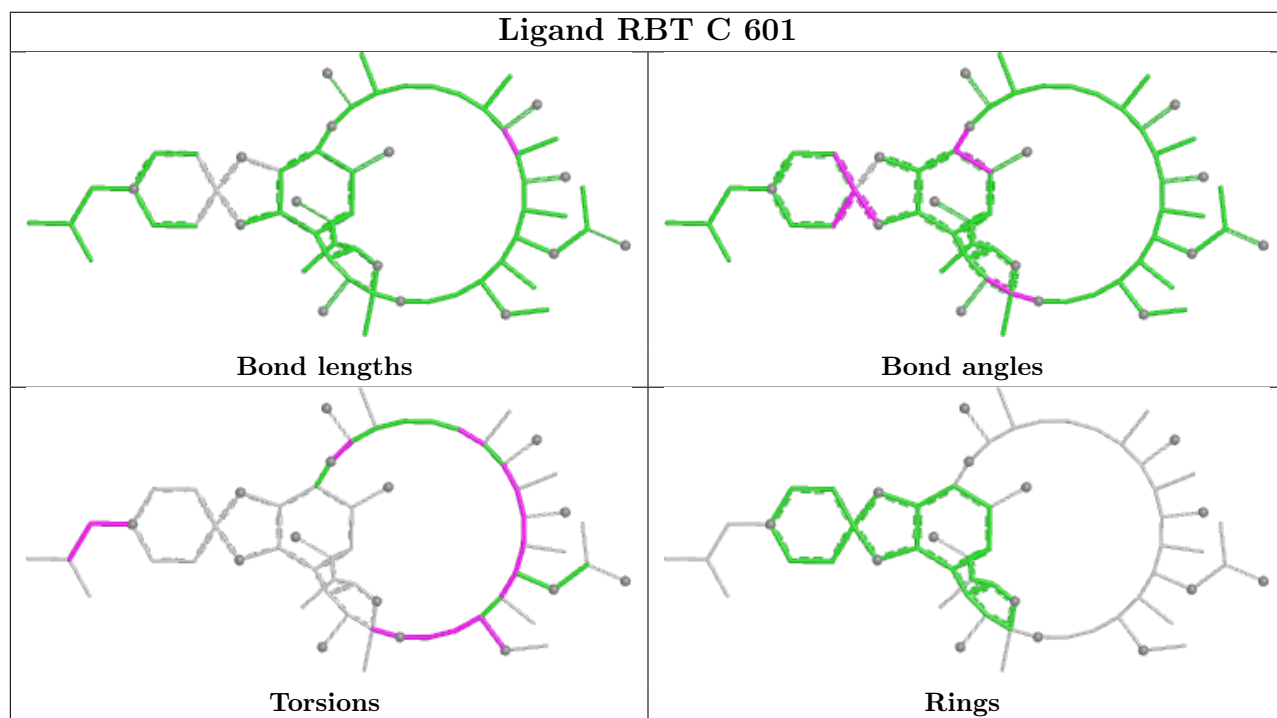
Mol	Chain	Res	Type	Atoms
4	C	601	RBT	C13-C12-O5-C29
4	C	601	RBT	O3-C12-O5-C29
4	C	601	RBT	C16-C15-N1-C2
4	C	601	RBT	O11-C15-N1-C2
4	C	601	RBT	C21-C22-C23-O9
4	C	601	RBT	C26-C27-C28-C29
4	C	601	RBT	C27-C28-C29-O5
4	C	601	RBT	C44-C43-N4-C41
4	C	601	RBT	O10-C21-C22-C23
4	C	601	RBT	C21-C22-C23-C24
4	C	601	RBT	C32-C22-C23-O9
4	C	601	RBT	C20-C21-C22-C23
4	C	601	RBT	N4-C43-C44-C45
4	C	601	RBT	O10-C21-C22-C32
4	C	601	RBT	C28-C27-O6-C37
4	C	601	RBT	C20-C21-C22-C32
4	C	601	RBT	O7-C25-C26-C27
4	C	601	RBT	C32-C22-C23-C24
4	C	601	RBT	C26-C27-O6-C37
4	C	601	RBT	O6-C27-C28-C29
3	C	605	EDO	O1-C1-C2-O2
4	C	601	RBT	C18-C19-C20-C31
4	C	601	RBT	O9-C23-C24-C25
4	C	601	RBT	C23-C24-C25-C26
4	C	601	RBT	O7-C25-C26-C34
3	A	602	EDO	O1-C1-C2-O2
3	C	607	EDO	O1-C1-C2-O2
4	C	601	RBT	C28-C29-O5-C12

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	607	EDO	2	0
3	A	602	EDO	1	0
3	A	604	EDO	2	0
3	C	605	EDO	1	0
2	B	602	FMT	1	0
3	B	603	EDO	2	0
3	C	606	EDO	2	0
4	C	601	RBT	3	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

### 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, 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	A	540/576 (93%)	-0.04	15 (2%) 55 45	20, 45, 68, 127	3 (0%)
1	B	541/576 (93%)	-0.02	13 (2%) 59 50	25, 48, 72, 106	4 (0%)
1	C	541/576 (93%)	-0.02	15 (2%) 55 45	33, 48, 75, 103	0
All	All	1622/1728 (93%)	-0.03	43 (2%) 56 46	20, 47, 71, 127	7 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	ALA	5.0
1	B	10	ILE	4.3
1	C	0	ALA	4.0
1	B	1	MET	3.8
1	A	511	THR	3.6
1	B	218	MET	3.6
1	A	9	LEU	3.4
1	A	5	ILE	3.4
1	B	62	TYR	3.4
1	A	49	ASP	3.3
1	C	538	ASP	3.3
1	B	14	ASP	3.2
1	C	483	PRO	3.2
1	C	-10	PRO	3.1
1	A	8	SER	3.1
1	A	538	ASP	3.0
1	A	7	ASN	2.9
1	C	-6	ASN	2.8
1	A	1	MET	2.7
1	A	4	THR	2.7
1	B	498	ARG	2.6
1	B	353	ARG	2.5
1	B	174	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	-11	ILE	2.5
1	B	49	ASP	2.4
1	B	357	PHE	2.4
1	C	61	GLN	2.3
1	A	497	SER	2.3
1	C	484	LYS	2.3
1	A	239	ILE	2.3
1	A	547	MET	2.2
1	B	547	MET	2.2
1	C	547	MET	2.2
1	C	459	ILE	2.1
1	B	50	ASN	2.1
1	C	493	THR	2.1
1	C	540	GLY	2.1
1	C	16	ILE	2.1
1	C	174	SER	2.0
1	B	408	ASN	2.0
1	A	15	SER	2.0
1	A	374	ASP	2.0
1	C	-7	GLU	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, 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.

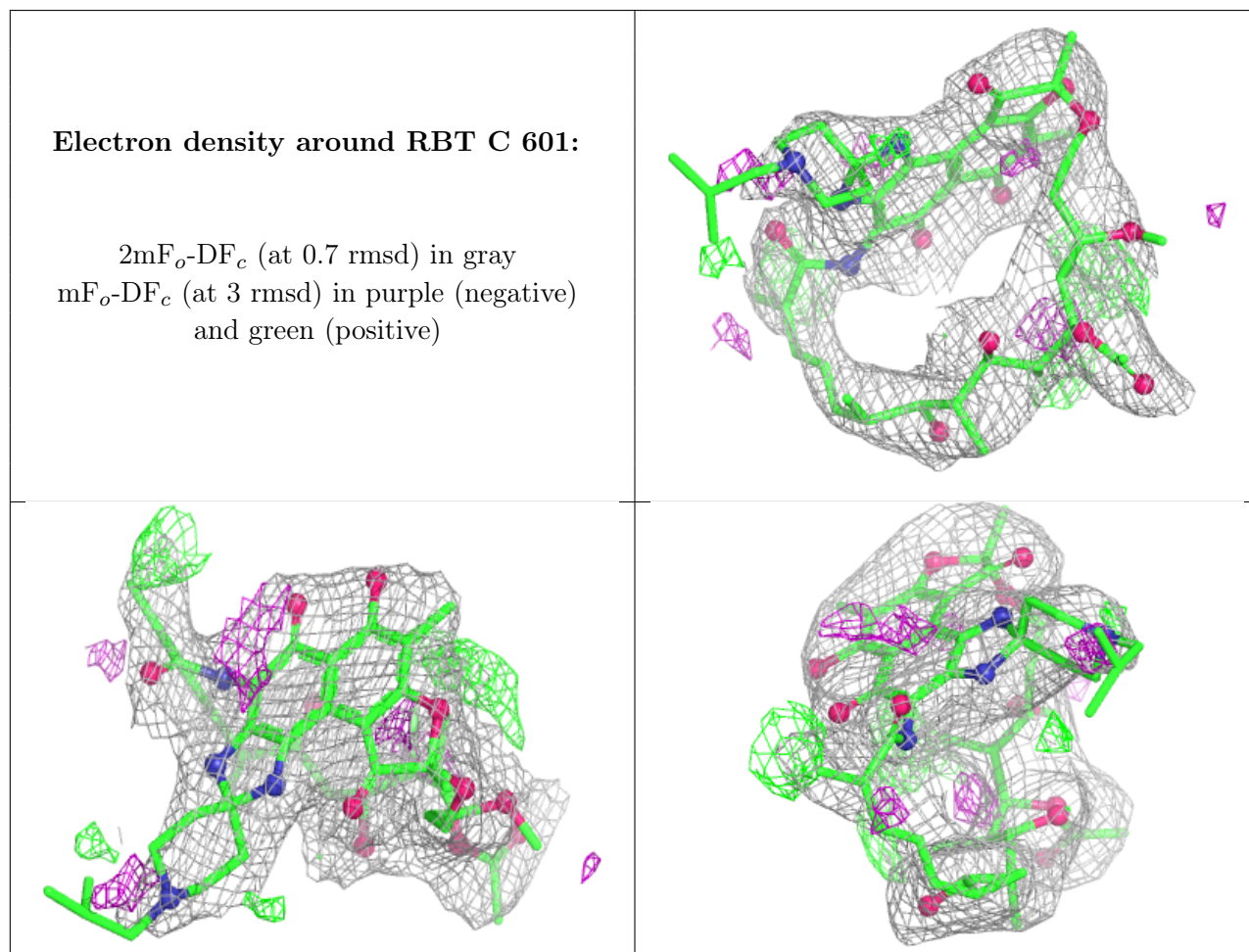
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FMT	B	602	3/3	0.78	0.20	63,63,63,63	0
3	EDO	A	604	4/4	0.80	0.20	57,59,60,60	0
3	EDO	C	605	4/4	0.80	0.16	40,42,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	RBT	C	601	61/61	0.81	0.17	75,80,88,89	0
3	EDO	A	602	4/4	0.83	0.15	50,51,51,52	0
3	EDO	B	603	4/4	0.83	0.13	46,46,47,47	0
3	EDO	C	607	4/4	0.85	0.18	69,69,69,70	0
2	FMT	C	604	3/3	0.86	0.16	69,69,70,70	0
3	EDO	A	603	4/4	0.91	0.12	51,51,52,52	0
2	FMT	B	601	3/3	0.93	0.14	71,71,72,72	0
2	FMT	C	603	3/3	0.93	0.11	48,48,49,50	0
2	FMT	A	601	3/3	0.94	0.09	47,47,48,50	0
3	EDO	C	606	4/4	0.95	0.11	46,46,46,46	0
2	FMT	C	602	3/3	0.96	0.06	52,52,53,53	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.