



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:30 pm BST

PDB ID : 2JJJ  
Title : Endothiapepsin in complex with a gem-diol inhibitor.  
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Deposited on : 2008-04-09  
Resolution : 1.00 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 : 2.11  
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) : 2.11

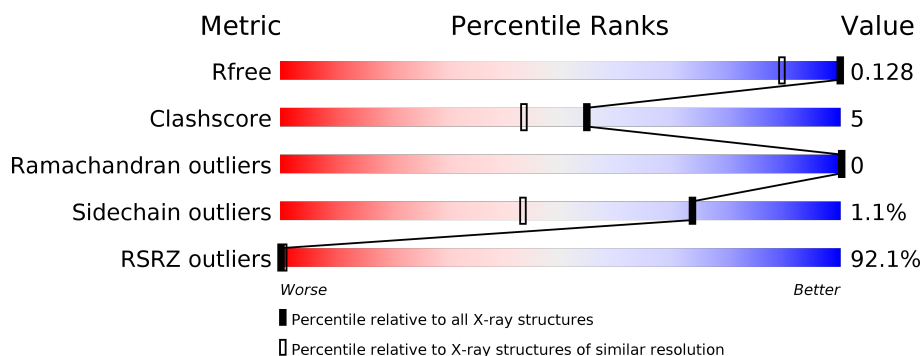
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.00 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	1050 (1.06-0.94)
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	1043 (1.06-0.94)
Sidechain outliers	138945	1045 (1.06-0.94)
RSRZ outliers	127900	1023 (1.06-0.94)

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	329	<div> <div>92%</div> <div>92%8%</div> </div>

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
3	SO4	A	503	-	-	-	X

## 2 Entry composition [i](#)

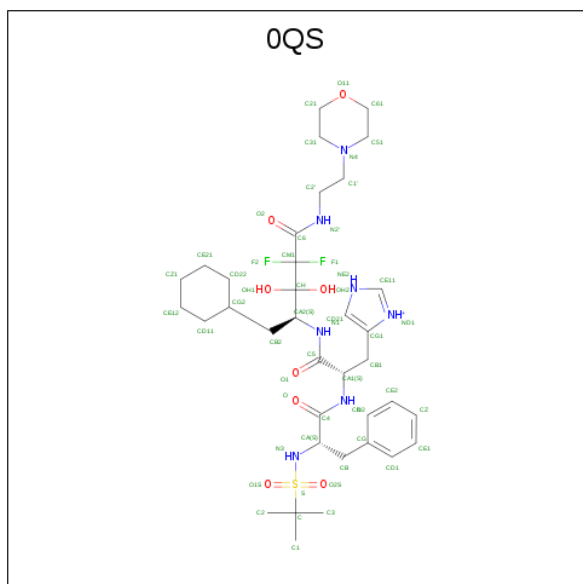
There are 4 unique types of molecules in this entry. The entry contains 5463 atoms, of which 2395 are hydrogens and 0 are deuteriums.

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 ENDOTHIAPEPSIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	329	4861	1573	2388	367	531	2	0	26	0

- Molecule 2 is N 2 -[(2R)-2-benzyl-3-(tert-butylsulfonyl)propanoyl]-N-{(1R)-1-(cyclohexylmethyl)-3,3-difluoro-2,2-dihydroxy-4-[(2-morpholin-4-ylethyl)amino]-4-oxobutyl}-3-(1H-imidazol-3-ium-4-yl)-L-alaninamide (three-letter code: 0QS) (formula: C<sub>36</sub>H<sub>56</sub>F<sub>2</sub>N<sub>7</sub>O<sub>8</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	H	N	O		
2	A	1	61	36	2	7	7	8	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

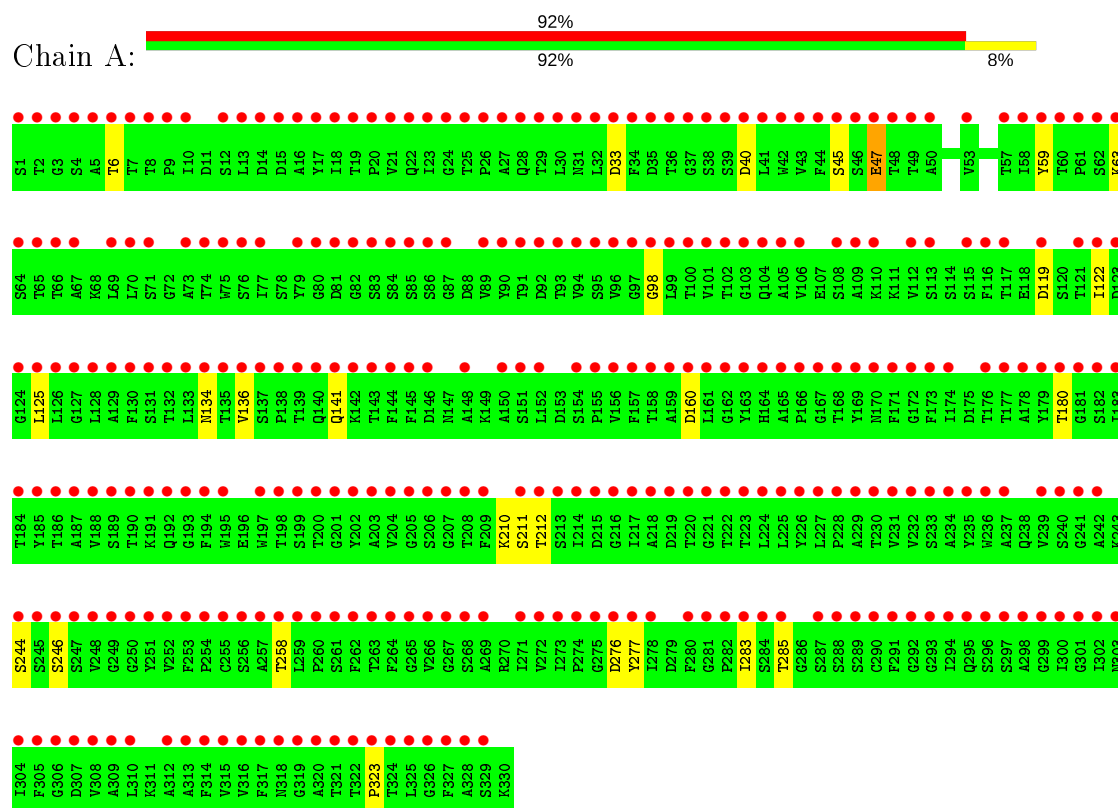
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	521	Total	O	0	0
			521	521		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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: ENDOTHAPEPSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.69Å 74.34Å 42.53Å 90.00° 97.49° 90.00°	Depositor
Resolution (Å)	30.00 – 1.00 42.33 – 1.00	Depositor EDS
% Data completeness (in resolution range)	90.8 (30.00-1.00) 95.6 (42.33-1.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.03 (at 1.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.111 , 0.136 0.108 , 0.128	Depositor DCC
$R_{free}$ test set	6784 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	3.9	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	5463	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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: 0QS, SO4, SUI

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	0.76	2/2606 (0.1%)	1.06	10/3563 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45[A]	SER	CB-OG	-5.37	1.35	1.42
1	A	45[B]	SER	CB-OG	-5.37	1.35	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	TYR	CB-CG-CD1	7.02	125.21	121.00
1	A	33	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	276[A]	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	276[B]	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	47[A]	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	A	47[B]	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	A	160	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	A	59	TYR	CB-CG-CD1	5.10	124.06	121.00
1	A	276[A]	ASP	N-CA-CB	5.00	119.61	110.60
1	A	276[B]	ASP	N-CA-CB	5.00	119.61	110.60

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	A	2473	2388	2401	19	0
2	A	54	7	56	9	0
3	A	20	0	0	0	0
4	A	521	0	0	14	0
All	All	3068	2395	2457	26	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 5.

All (26) 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)
2:A:331:0QS:CE11	2:A:331:0QS:HE11	0.97	1.11
2:A:331:0QS:CD21	2:A:331:0QS:HD21	0.97	1.07
2:A:331:0QS:HD21	2:A:331:0QS:CG1	2.06	0.85
1:A:210:LYS:HE2	4:A:2384:HOH:O	1.85	0.77
2:A:331:0QS:H211	4:A:2520:HOH:O	1.89	0.72
2:A:331:0QS:ND1	2:A:331:0QS:HE11	2.05	0.71
2:A:331:0QS:HE11	2:A:331:0QS:NE2	2.07	0.70
1:A:47[B]:GLU:OE2	4:A:2099:HOH:O	2.09	0.70
2:A:331:0QS:NE2	2:A:331:0QS:HD21	2.10	0.66
1:A:212[A]:THR:HG21	4:A:2388:HOH:O	1.97	0.65
1:A:180[B]:THR:HG21	4:A:2338:HOH:O	1.98	0.64
1:A:180[B]:THR:HG23	4:A:2336:HOH:O	2.03	0.58
1:A:283:ILE:HD11	4:A:2226:HOH:O	2.03	0.57
1:A:6[B]:THR:HG22	4:A:2313:HOH:O	2.07	0.54
1:A:63:LYS:HE3	4:A:2053:HOH:O	2.07	0.53
1:A:134:ASN:ND2	1:A:141:GLN:H	2.07	0.52
1:A:258:THR:HA	4:A:2432:HOH:O	2.10	0.52
1:A:119[A]:ASP:OD2	1:A:122:ILE:HD12	2.10	0.51
1:A:125[A]:LEU:HD21	2:A:331:0QS:HD12	1.93	0.50
1:A:125[B]:LEU:HD11	2:A:331:0QS:HD12	1.96	0.48
1:A:134:ASN:ND2	1:A:136:VAL:H	2.14	0.46
1:A:98:GLY:HA3	4:A:2215:HOH:O	2.17	0.44
1:A:283:ILE:HD11	4:A:2470:HOH:O	2.18	0.43
1:A:323:PRO:HD2	4:A:2353:HOH:O	2.19	0.41
1:A:285:THR:HG23	4:A:2465:HOH:O	2.21	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	352/329 (107%)	349 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	288/262 (110%)	283 (98%)	5 (2%)	60	27

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	244[A]	SER
1	A	244[B]	SER
1	A	246[A]	SER
1	A	246[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	147	ASN
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	303	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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$
1	SUI	A	54	1	10,11,12	1.20	1 (10%)	11,15,17	1.68	3 (27%)

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
1	SUI	A	54	1	-	0/2/19/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	SUI	C1-N2	-2.01	1.35	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	SUI	C1-N2-CG	3.82	115.31	113.04
1	A	54	SUI	C2A-N2-CG	-2.40	121.29	123.46
1	A	54	SUI	O-C-C2A	-2.05	120.19	126.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	SO4	A	503	-	4,4,4	0.58	0	6,6,6	0.96	0
3	SO4	A	500	-	4,4,4	0.29	0	6,6,6	0.25	0
3	SO4	A	501	-	4,4,4	0.40	0	6,6,6	0.74	0
3	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.35	0
2	0QS	A	331	-	51,57,57	2.32	7 (13%)	66,82,82	3.33	18 (27%)

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	0QS	A	331	-	-	6/60/85/85	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	331	0QS	S-N3	12.63	1.90	1.60
2	A	331	0QS	C1-C	5.74	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	331	0QS	O2S-S	3.90	1.50	1.43
2	A	331	0QS	CD11-CG2	-3.25	1.43	1.52
2	A	331	0QS	CA-N3	-2.72	1.41	1.46
2	A	331	0QS	C2-C	2.53	1.57	1.52
2	A	331	0QS	OH2-CH	2.52	1.42	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	331	0QS	O1S-S-C	11.75	117.03	107.60
2	A	331	0QS	CA-N3-S	-11.19	108.08	122.56
2	A	331	0QS	O2S-S-C	11.17	116.57	107.60
2	A	331	0QS	C3-C-S	8.96	121.00	107.86
2	A	331	0QS	C2-C-S	6.28	117.06	107.86
2	A	331	0QS	C-S-N3	-6.17	96.99	107.37
2	A	331	0QS	C3-C-C1	-5.95	99.45	111.04
2	A	331	0QS	C2-C-C1	-4.29	102.68	111.04
2	A	331	0QS	CB1-CA1-N	-3.61	103.19	110.79
2	A	331	0QS	O2S-S-N3	-3.53	101.76	108.92
2	A	331	0QS	O2S-S-O1S	-3.43	113.60	120.57
2	A	331	0QS	O11-C21-C31	-2.98	105.22	111.80
2	A	331	0QS	C3-C-C2	-2.78	105.62	111.04
2	A	331	0QS	O11-C61-C51	-2.77	105.69	111.80
2	A	331	0QS	CZ1-CE12-CD11	-2.54	106.23	111.42
2	A	331	0QS	C4-CA-N3	2.48	117.83	111.17
2	A	331	0QS	C51-N4-C31	-2.40	103.44	108.83
2	A	331	0QS	CB-CA-C4	-2.23	104.48	110.25

There are no chirality outliers.

All (6) torsion outliers are listed below:

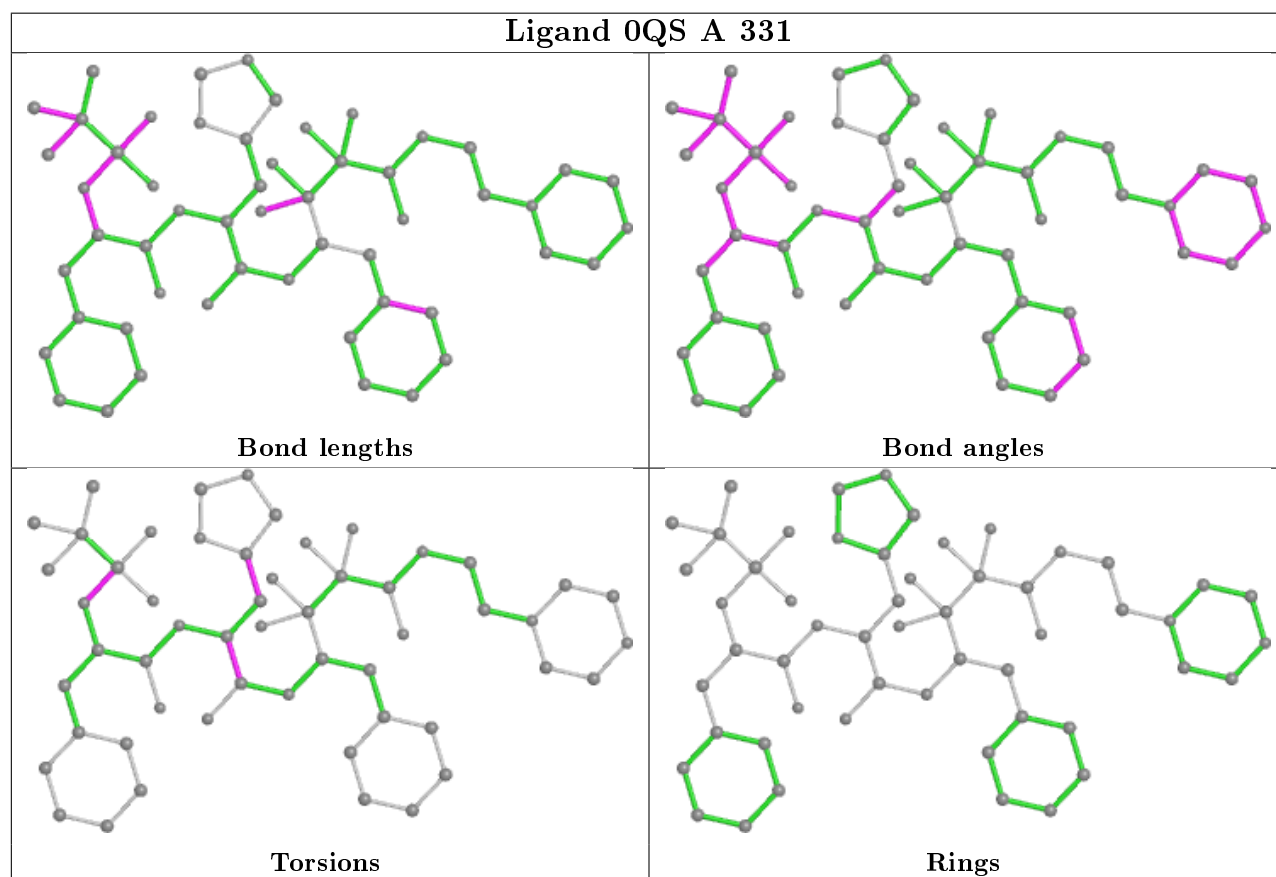
Mol	Chain	Res	Type	Atoms
2	A	331	0QS	CA-N3-S-O1S
2	A	331	0QS	CA-N3-S-O2S
2	A	331	0QS	CA-N3-S-C
2	A	331	0QS	CA1-CB1-CG1-CD21
2	A	331	0QS	N1-C5-CA1-N
2	A	331	0QS	O1-C5-CA1-N

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	331	0QS	9	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 ⓘ

### 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	328/329 (99%)	3.17	302 (92%) 0 0	3, 5, 13, 23	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	ILE	6.6
1	A	283	ILE	5.6
1	A	280	PHE	5.4
1	A	236	TRP	5.4
1	A	258	THR	5.3
1	A	195	TRP	5.3
1	A	246[A]	SER	5.2
1	A	197	TRP	5.2
1	A	284[A]	SER	5.2
1	A	42	TRP	5.0
1	A	18	ILE	4.9
1	A	130	PHE	4.9
1	A	156[A]	VAL	4.9
1	A	75	TRP	4.7
1	A	44	PHE	4.6
1	A	235	TYR	4.6
1	A	255	CYS	4.6
1	A	273	ILE	4.6
1	A	325[A]	LEU	4.5
1	A	239	VAL	4.5
1	A	209	PHE	4.5
1	A	99	LEU	4.5
1	A	231	VAL	4.5
1	A	163	TYR	4.5
1	A	308	VAL	4.4
1	A	144	PHE	4.4
1	A	227	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	217	ILE	4.4
1	A	34	PHE	4.4
1	A	128	LEU	4.3
1	A	226	TYR	4.3
1	A	194	PHE	4.3
1	A	290	CYS	4.3
1	A	21	VAL	4.3
1	A	315	VAL	4.3
1	A	169	TYR	4.3
1	A	122	ILE	4.2
1	A	232	VAL	4.2
1	A	278	ILE	4.2
1	A	6[A]	THR	4.2
1	A	30	LEU	4.2
1	A	314	PHE	4.2
1	A	294	ILE	4.1
1	A	262	PHE	4.1
1	A	302	ILE	4.1
1	A	304	ILE	4.1
1	A	204	VAL	4.1
1	A	13	LEU	4.0
1	A	94	VAL	4.0
1	A	224	LEU	4.0
1	A	225	LEU	4.0
1	A	252	VAL	4.0
1	A	23	ILE	4.0
1	A	106	VAL	4.0
1	A	19	THR	4.0
1	A	212[A]	THR	4.0
1	A	222	THR	4.0
1	A	202	TYR	3.9
1	A	41	LEU	3.9
1	A	126	LEU	3.9
1	A	237	ALA	3.9
1	A	312	ALA	3.9
1	A	145	PHE	3.9
1	A	271	ILE	3.9
1	A	5	ALA	3.9
1	A	129	ALA	3.9
1	A	32	LEU	3.9
1	A	125[A]	LEU	3.9
1	A	133	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	136	VAL	3.9
1	A	264	PHE	3.9
1	A	305	PHE	3.9
1	A	309	ALA	3.9
1	A	230	THR	3.9
1	A	69	LEU	3.9
1	A	266	VAL	3.9
1	A	272	VAL	3.9
1	A	174	ILE	3.8
1	A	43	VAL	3.8
1	A	96	VAL	3.8
1	A	188	VAL	3.8
1	A	316	VAL	3.8
1	A	310	LEU	3.8
1	A	313	ALA	3.8
1	A	328	ALA	3.8
1	A	282	PRO	3.8
1	A	59	TYR	3.8
1	A	251	TYR	3.8
1	A	256[A]	SER	3.8
1	A	214	ILE	3.8
1	A	187	ALA	3.8
1	A	17	TYR	3.7
1	A	90	TYR	3.7
1	A	161	LEU	3.7
1	A	186	THR	3.7
1	A	152	LEU	3.7
1	A	171	PHE	3.7
1	A	229	ALA	3.6
1	A	112	VAL	3.6
1	A	291	PHE	3.6
1	A	181	GLY	3.6
1	A	7	THR	3.6
1	A	173	PHE	3.6
1	A	218	ALA	3.6
1	A	80	GLY	3.6
1	A	277	TYR	3.6
1	A	322	THR	3.6
1	A	168	THR	3.5
1	A	292	GLY	3.5
1	A	306	GLY	3.5
1	A	228	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	317	PHE	3.5
1	A	50	ALA	3.5
1	A	190	THR	3.4
1	A	185	TYR	3.4
1	A	191[A]	LYS	3.4
1	A	203	ALA	3.4
1	A	234	ALA	3.4
1	A	36	THR	3.4
1	A	198	THR	3.4
1	A	321	THR	3.4
1	A	253	PHE	3.4
1	A	327	PHE	3.4
1	A	79	TYR	3.4
1	A	8	THR	3.4
1	A	116	PHE	3.4
1	A	26	PRO	3.3
1	A	139	THR	3.3
1	A	200	THR	3.3
1	A	183	ILE	3.3
1	A	157	PHE	3.3
1	A	166	PRO	3.3
1	A	29	THR	3.3
1	A	220	THR	3.3
1	A	207	GLY	3.3
1	A	298	ALA	3.3
1	A	215	ASP	3.3
1	A	193	GLY	3.3
1	A	216	GLY	3.3
1	A	66	THR	3.3
1	A	184	THR	3.3
1	A	208	THR	3.3
1	A	77	ILE	3.3
1	A	143	THR	3.3
1	A	293	GLY	3.2
1	A	319	GLY	3.2
1	A	45[A]	SER	3.2
1	A	100	THR	3.2
1	A	135	THR	3.2
1	A	263	THR	3.2
1	A	20	PRO	3.2
1	A	89	VAL	3.2
1	A	167	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	276[A]	ASP	3.2
1	A	211[A]	SER	3.2
1	A	269	ALA	3.2
1	A	274	PRO	3.2
1	A	201	GLY	3.2
1	A	165	ALA	3.1
1	A	162	GLY	3.1
1	A	16	ALA	3.1
1	A	70	LEU	3.1
1	A	48	THR	3.1
1	A	158	THR	3.1
1	A	285	THR	3.1
1	A	12	SER	3.1
1	A	296	SER	3.1
1	A	265	GLY	3.1
1	A	289	SER	3.1
1	A	37	GLY	3.1
1	A	60	THR	3.1
1	A	63	LYS	3.1
1	A	137[A]	SER	3.0
1	A	241	GLY	3.0
1	A	299	GLY	3.0
1	A	3	GLY	3.0
1	A	117	THR	3.0
1	A	254	PRO	3.0
1	A	123	ASP	3.0
1	A	179	TYR	3.0
1	A	249	GLY	3.0
1	A	73	ALA	3.0
1	A	148	ALA	3.0
1	A	49	THR	3.0
1	A	31	ASN	3.0
1	A	53	VAL	2.9
1	A	25	THR	2.9
1	A	121	THR	2.9
1	A	221	GLY	2.9
1	A	233[A]	SER	2.9
1	A	119[A]	ASP	2.9
1	A	65	THR	2.9
1	A	67	ALA	2.9
1	A	109	ALA	2.9
1	A	159	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	124	GLY	2.9
1	A	172	GLY	2.9
1	A	240	SER	2.9
1	A	10	ILE	2.9
1	A	324	THR	2.9
1	A	142	LYS	2.9
1	A	132	THR	2.9
1	A	223	THR	2.9
1	A	27	ALA	2.9
1	A	127	GLY	2.8
1	A	58	ILE	2.8
1	A	164	HIS	2.8
1	A	180[A]	THR	2.8
1	A	105	ALA	2.8
1	A	257	ALA	2.8
1	A	261	SER	2.8
1	A	205	GLY	2.8
1	A	91	THR	2.8
1	A	39	SER	2.8
1	A	98	GLY	2.8
1	A	131	SER	2.7
1	A	213[A]	SER	2.7
1	A	178	ALA	2.7
1	A	93	THR	2.7
1	A	138	PRO	2.7
1	A	248	VAL	2.7
1	A	82	GLY	2.7
1	A	297	SER	2.7
1	A	38	SER	2.7
1	A	259	LEU	2.7
1	A	33	ASP	2.7
1	A	9	PRO	2.7
1	A	57	THR	2.7
1	A	74	THR	2.7
1	A	4	SER	2.7
1	A	85[A]	SER	2.7
1	A	134	ASN	2.6
1	A	151[A]	SER	2.6
1	A	154[A]	SER	2.6
1	A	242	ALA	2.6
1	A	281	GLY	2.6
1	A	81	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	182	SER	2.6
1	A	24	GLY	2.6
1	A	87	GLY	2.6
1	A	97	GLY	2.6
1	A	101	VAL	2.6
1	A	303	ASN	2.6
1	A	83	SER	2.6
1	A	189	SER	2.6
1	A	86	SER	2.5
1	A	199	SER	2.5
1	A	320	ALA	2.5
1	A	61	PRO	2.5
1	A	22	GLN	2.5
1	A	40	ASP	2.5
1	A	71[A]	SER	2.5
1	A	108	SER	2.5
1	A	192	GLN	2.5
1	A	275	GLY	2.5
1	A	301	GLY	2.5
1	A	326	GLY	2.5
1	A	307	ASP	2.5
1	A	247	SER	2.4
1	A	150	ALA	2.4
1	A	295	GLN	2.4
1	A	260	PRO	2.4
1	A	46	SER	2.4
1	A	104	GLN	2.4
1	A	35	ASP	2.4
1	A	160	ASP	2.4
1	A	323	PRO	2.4
1	A	28	GLN	2.4
1	A	141	GLN	2.4
1	A	92	ASP	2.4
1	A	47[A]	GLU	2.4
1	A	62	SER	2.4
1	A	176	THR	2.3
1	A	177	THR	2.3
1	A	219	ASP	2.3
1	A	329	SER	2.3
1	A	2	THR	2.3
1	A	95	SER	2.3
1	A	113	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	SER	2.3
1	A	84	SER	2.3
1	A	103	GLY	2.3
1	A	245	SER	2.3
1	A	155	PRO	2.3
1	A	288[A]	SER	2.2
1	A	170	ASN	2.2
1	A	140	GLN	2.2
1	A	14	ASP	2.2
1	A	267	GLY	2.2
1	A	206	SER	2.2
1	A	318	ASN	2.2
1	A	244[A]	SER	2.1
1	A	76	SER	2.1
1	A	102	THR	2.1
1	A	146	ASP	2.1
1	A	1	SER	2.1
1	A	64	SER	2.1
1	A	268[A]	SER	2.1
1	A	250	GLY	2.1
1	A	115[A]	SER	2.0
1	A	110	LYS	2.0
1	A	15	ASP	2.0

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

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
1	SUI	A	54	11/12	0.94	0.17	5,6,8,11	0

## 6.3 Carbohydrates ⓘ

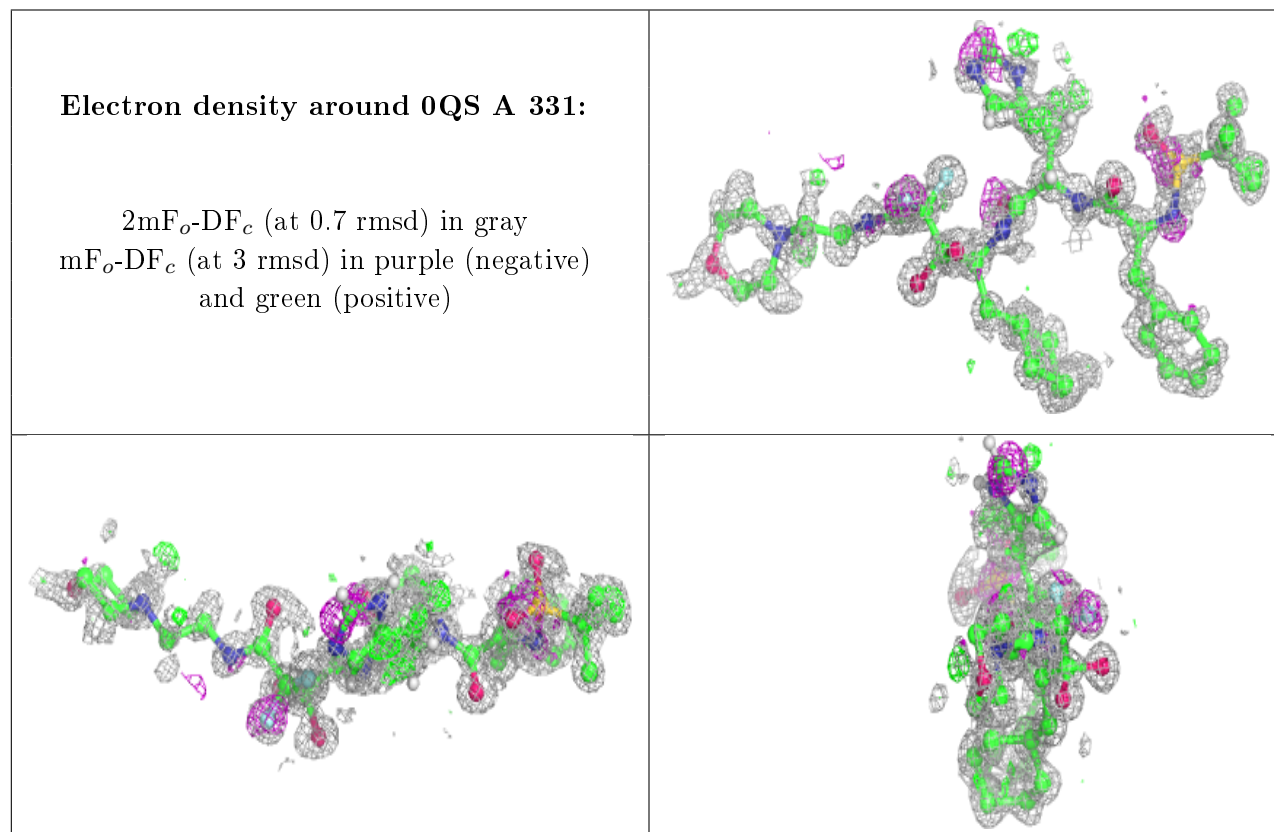
There are no carbohydrates in this entry.

## 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
3	SO4	A	502	5/5	0.47	0.34	24,28,33,37	5
3	SO4	A	503	5/5	0.61	0.43	8,18,29,37	5
3	SO4	A	501	5/5	0.71	0.29	17,17,28,32	5
2	0QS	A	331	54/54	0.89	0.23	5,12,26,31	0
3	SO4	A	500	5/5	0.96	0.22	5,6,9,10	5

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.