



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:14 AM UTC

PDB ID : 3WT6 / pdb\_00003wt6  
Title : A mixed population of antagonist and agonist binding conformers in a single crystal explains partial agonism against vitamin D receptor: Active vitamin D analogues with 22R-alkyl group  
Authors : Anami, Y.; Itoh, T.; Yamamoto, K.  
Deposited on : 2014-04-08  
Resolution : 2.00 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.

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)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (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

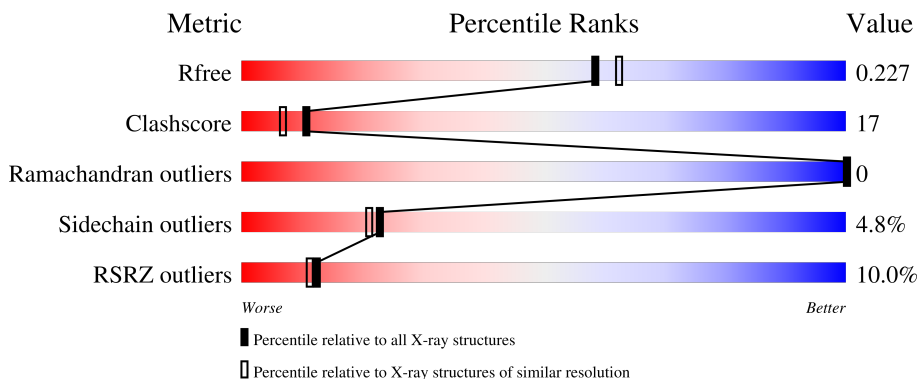
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	271	
2	C	13	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2134 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 Vitamin D3 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1921	1225	327	357	12	0	2	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	expression tag	UNP P13053
A	107	SER	-	expression tag	UNP P13053
A	108	HIS	-	expression tag	UNP P13053
A	109	MET	-	expression tag	UNP P13053
A	110	GLY	-	expression tag	UNP P13053
A	111	SER	-	expression tag	UNP P13053
A	112	PRO	-	expression tag	UNP P13053
A	113	ASN	-	expression tag	UNP P13053
A	114	SER	-	expression tag	UNP P13053
A	115	PRO	-	expression tag	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	TYR	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	PRO	deletion	UNP P13053
A	?	-	ARG	deletion	UNP P13053
A	?	-	PRO	deletion	UNP P13053
A	?	-	THR	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	PHE	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	GLY	deletion	UNP P13053
A	?	-	ASN	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053

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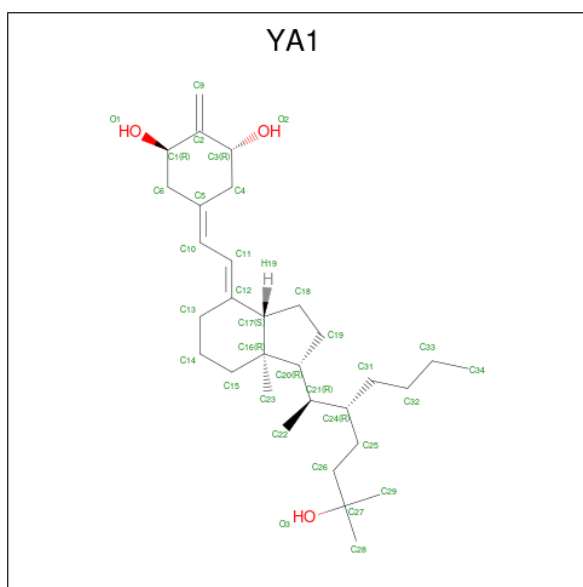
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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	TYR	deletion	UNP P13053
A	?	-	THR	deletion	UNP P13053
A	?	-	THR	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	MET	deletion	UNP P13053
A	?	-	MET	deletion	UNP P13053
A	?	-	GLU	deletion	UNP P13053
A	?	-	PRO	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	GLY	deletion	UNP P13053
A	?	-	PHE	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	ASN	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	ASN	deletion	UNP P13053
A	?	-	GLY	deletion	UNP P13053
A	?	-	GLU	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	PRO	deletion	UNP P13053

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	11	87	56	16	13	2	0	0	0

- Molecule 3 is (1R,3R,7E,17beta)-17-[(2R,3R)-3-butyl-6-hydroxy-6-methylheptan-2-yl]-2-methylidene-9,10-secoestra-5,7-diene-1,3-diol (CCD ID: YA1) (formula: C<sub>31</sub>H<sub>52</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total	C	O	0	1
			68	62	6		

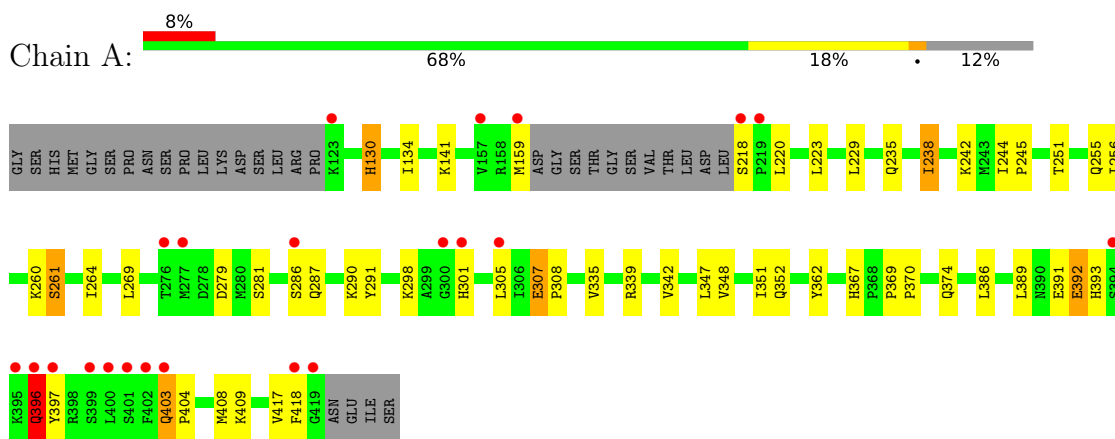
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	C	2	Total	O	0	0
			2	2		

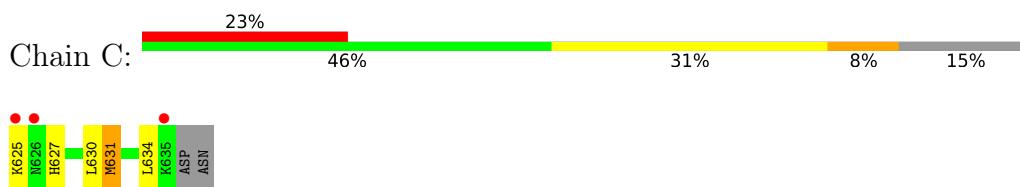
### 3 Residue-property plots [i](#)

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: Vitamin D3 receptor



- Molecule 2: Mediator of RNA polymerase II transcription subunit 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.05Å 44.77Å 45.11Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	44.99 – 2.00 44.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.99-2.00) 98.5 (44.99-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.199 , 0.224 0.206 , 0.227	Depositor DCC
$R_{free}$ test set	870 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtrriage
Anisotropy	0.181	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% 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: YA1

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	1.36	6/1965 (0.3%)	1.13	3/2659 (0.1%)
2	C	0.97	0/88	0.90	0/117
All	All	1.34	6/2053 (0.3%)	1.12	3/2776 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	PRO	CA-C	7.25	1.57	1.52
1	A	130	HIS	C-O	-6.36	1.16	1.24
1	A	238	ILE	C-O	6.24	1.31	1.24
1	A	362	TYR	C-O	6.13	1.31	1.24
1	A	342	VAL	C-O	-5.59	1.18	1.24
1	A	261	SER	C-O	-5.06	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	HIS	CA-C-N	-6.33	113.86	120.38
1	A	367	HIS	C-N-CA	-6.33	113.86	120.38
1	A	396	GLN	N-CA-C	5.32	117.16	111.36

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	1921	0	1932	56	0
2	C	87	0	91	5	0
3	A	68	0	104	25	0
4	A	56	0	0	8	0
4	C	2	0	0	0	0
All	All	2134	0	2127	70	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 17.

All (70) 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:301[B]:HIS:CE1	3:A:501[B]:YA1:H45	1.78	1.16
1:A:301[B]:HIS:HE1	3:A:501[B]:YA1:C26	1.59	1.12
1:A:301[B]:HIS:CE1	3:A:501[B]:YA1:C26	2.33	1.12
1:A:301[B]:HIS:CE1	3:A:501[B]:YA1:H44	2.06	0.90
1:A:301[B]:HIS:HE1	3:A:501[B]:YA1:H44	1.38	0.87
1:A:305[B]:LEU:HD22	1:A:392:GLU:HB3	1.59	0.83
1:A:261:SER:OG	1:A:339:ARG:HD2	1.80	0.81
1:A:260:LYS:HE3	2:C:627:HIS:NE2	1.95	0.80
3:A:501[B]:YA1:H30	3:A:501[B]:YA1:H17	1.64	0.78
1:A:305[B]:LEU:HD11	1:A:389:LEU:HD23	1.64	0.78
1:A:269:LEU:HG	1:A:386:LEU:HD11	1.70	0.72
1:A:301[B]:HIS:HD2	4:A:655:HOH:O	1.76	0.67
3:A:501[B]:YA1:H30	3:A:501[B]:YA1:H22	1.77	0.67
3:A:501[B]:YA1:H44	3:A:501[B]:YA1:H29	1.79	0.65
1:A:264:ILE:HD11	3:A:501[A]:YA1:H38	1.80	0.64
1:A:393:HIS:NE2	1:A:397:TYR:HB2	2.12	0.63
1:A:264:ILE:CD1	3:A:501[A]:YA1:H38	2.28	0.63
1:A:141:LYS:HE2	4:A:604:HOH:O	1.99	0.62
1:A:281:SER:HB2	1:A:291:TYR:O	1.99	0.61
1:A:242:LYS:HD3	2:C:634:LEU:HA	1.83	0.61
3:A:501[B]:YA1:H17	3:A:501[B]:YA1:C22	2.31	0.60
1:A:220:LEU:HA	1:A:298:LYS:O	2.02	0.59
1:A:305[B]:LEU:CD2	1:A:392:GLU:HB3	2.32	0.59
1:A:130:HIS:CE1	1:A:134:ILE:HD11	2.38	0.59
1:A:393:HIS:CE1	1:A:397:TYR:HB2	2.37	0.59
1:A:305[A]:LEU:O	1:A:308:PRO:HD2	2.04	0.58
1:A:335:VAL:HG13	1:A:348:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305[A]:LEU:CD1	4:A:655:HOH:O	2.51	0.57
1:A:396:GLN:HG2	4:A:655:HOH:O	2.05	0.57
1:A:235:GLN:NE2	4:A:635:HOH:O	2.38	0.56
1:A:279:ASP:OD1	1:A:279:ASP:N	2.36	0.56
1:A:260:LYS:CE	2:C:627:HIS:NE2	2.69	0.56
1:A:305[A]:LEU:HD12	4:A:655:HOH:O	2.05	0.55
1:A:335:VAL:HG12	1:A:335:VAL:O	2.05	0.55
1:A:256:ILE:HD11	2:C:631:MET:HG2	1.89	0.55
1:A:335:VAL:HG11	1:A:351:ILE:HB	1.88	0.55
1:A:396:GLN:CG	4:A:655:HOH:O	2.55	0.55
1:A:301[B]:HIS:NE2	3:A:501[B]:YA1:H45	2.16	0.54
1:A:393:HIS:CE1	3:A:501[A]:YA1:H37	2.42	0.54
1:A:305[A]:LEU:C	1:A:308:PRO:HD2	2.34	0.53
3:A:501[B]:YA1:C26	3:A:501[B]:YA1:H29	2.40	0.52
1:A:238:ILE:O	1:A:242:LYS:HG3	2.10	0.51
3:A:501[A]:YA1:H22	3:A:501[A]:YA1:H30	1.93	0.51
1:A:370:PRO:O	1:A:374:GLN:HG3	2.12	0.49
1:A:305[A]:LEU:HD11	1:A:396:GLN:HB2	1.95	0.49
1:A:307:GLU:HB3	1:A:308:PRO:HD3	1.95	0.48
1:A:335:VAL:O	1:A:352:GLN:HB2	2.15	0.47
1:A:251:THR:O	1:A:255:GLN:HG3	2.14	0.47
3:A:501[A]:YA1:H34	3:A:501[A]:YA1:H45	1.54	0.46
1:A:417:VAL:HG12	1:A:418:PHE:CD2	2.50	0.46
1:A:397:TYR:HD2	4:A:601:HOH:O	1.98	0.45
1:A:286:SER:O	1:A:290:LYS:HB2	2.16	0.45
1:A:418:PHE:CE1	3:A:501[A]:YA1:C34	3.00	0.45
3:A:501[B]:YA1:C22	3:A:501[B]:YA1:C15	2.93	0.44
1:A:393:HIS:O	1:A:396:GLN:N	2.51	0.44
1:A:409:LYS:HA	1:A:409:LYS:HD2	1.90	0.44
1:A:223:LEU:CD1	3:A:501[B]:YA1:H46	2.48	0.44
1:A:305[B]:LEU:HA	1:A:308:PRO:HD2	2.00	0.43
1:A:264:ILE:HD13	3:A:501[A]:YA1:H38	2.01	0.43
3:A:501[B]:YA1:H22	3:A:501[B]:YA1:C22	2.40	0.43
3:A:501[B]:YA1:H30	3:A:501[B]:YA1:C23	2.44	0.42
3:A:501[A]:YA1:H30	3:A:501[A]:YA1:H17	2.01	0.42
3:A:501[B]:YA1:H33	3:A:501[B]:YA1:C19	2.50	0.42
1:A:305[B]:LEU:C	1:A:308:PRO:HD2	2.44	0.42
1:A:403:GLN:HE21	1:A:404:PRO:HD2	1.84	0.42
1:A:159:MET:HG3	1:A:218:SER:CB	2.50	0.41
1:A:397:TYR:CD1	1:A:397:TYR:O	2.73	0.40
2:C:625:LYS:O	2:C:627:HIS:CE1	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:O	1:A:245:PRO:C	2.63	0.40
3:A:501[A]:YA1:H33	3:A:501[A]:YA1:H29	1.72	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	A	237/271 (88%)	228 (96%)	9 (4%)	0	100	100
2	C	9/13 (69%)	9 (100%)	0	0	100	100
All	All	246/284 (87%)	237 (96%)	9 (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	219/247 (89%)	210 (96%)	9 (4%)	27	26
2	C	10/13 (77%)	8 (80%)	2 (20%)	1	0
All	All	229/260 (88%)	218 (95%)	11 (5%)	23	21

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	A	287	GLN
1	A	307	GLU
1	A	347	LEU
1	A	391	GLU
1	A	392	GLU
1	A	396	GLN
1	A	403	GLN
1	A	408	MET
2	C	630	LEU
2	C	631	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	272	ASN
1	A	273	GLN
1	A	287	GLN
1	A	320	ASN
1	A	357	ASN
1	A	373	HIS
1	A	403	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](#)

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
3	YA1	A	501[B]	-	34,36,36	0.95	2 (5%)	44,53,53	2.60	12 (27%)
3	YA1	A	501[A]	-	34,36,36	1.00	1 (2%)	44,53,53	1.81	9 (20%)

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	YA1	A	501[B]	-	-	9/23/67/67	0/3/3/3
3	YA1	A	501[A]	-	-	7/23/67/67	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501[A]	YA1	C16-C17	-3.12	1.50	1.56
3	A	501[B]	YA1	C16-C17	-3.04	1.51	1.56
3	A	501[B]	YA1	C3-C2	-2.08	1.48	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[B]	YA1	C22-C21-C24	-7.30	99.63	112.76
3	A	501[B]	YA1	C16-C20-C21	-7.11	108.75	118.99
3	A	501[B]	YA1	C4-C5-C6	5.62	121.43	113.20
3	A	501[A]	YA1	C16-C20-C21	-5.55	110.99	118.99
3	A	501[B]	YA1	C19-C20-C21	5.07	120.11	112.64
3	A	501[A]	YA1	C4-C5-C6	4.84	120.28	113.20
3	A	501[B]	YA1	C11-C10-C5	-4.60	120.95	127.20
3	A	501[B]	YA1	C24-C21-C20	4.60	121.82	112.66
3	A	501[B]	YA1	C17-C16-C20	4.39	104.31	99.72
3	A	501[A]	YA1	C11-C10-C5	-3.75	122.11	127.20
3	A	501[A]	YA1	C4-C5-C10	-3.48	115.93	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[B]	YA1	C25-C26-C27	3.29	122.37	116.24
3	A	501[B]	YA1	C22-C21-C20	-2.76	107.78	112.78
3	A	501[A]	YA1	C25-C24-C21	2.73	121.35	112.65
3	A	501[B]	YA1	C4-C5-C10	-2.63	117.76	123.44
3	A	501[B]	YA1	C28-C27-C29	-2.53	104.97	110.63
3	A	501[A]	YA1	C28-C27-C29	2.34	115.87	110.63
3	A	501[A]	YA1	C19-C18-C17	-2.28	101.53	105.25
3	A	501[A]	YA1	C17-C12-C11	-2.21	120.07	123.56
3	A	501[A]	YA1	C31-C24-C21	-2.15	105.79	112.65
3	A	501[B]	YA1	C10-C11-C12	-2.08	123.05	126.13

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501[A]	YA1	C20-C21-C24-C25
3	A	501[B]	YA1	C20-C21-C24-C31
3	A	501[B]	YA1	C25-C26-C27-C29
3	A	501[B]	YA1	C25-C26-C27-O3
3	A	501[B]	YA1	C25-C26-C27-C28
3	A	501[B]	YA1	C24-C31-C32-C33
3	A	501[A]	YA1	C5-C10-C11-C12
3	A	501[A]	YA1	C25-C26-C27-C29
3	A	501[A]	YA1	C25-C26-C27-O3
3	A	501[A]	YA1	C22-C21-C24-C25
3	A	501[A]	YA1	C24-C31-C32-C33
3	A	501[A]	YA1	C22-C21-C24-C31
3	A	501[B]	YA1	C31-C32-C33-C34
3	A	501[B]	YA1	C21-C24-C25-C26
3	A	501[B]	YA1	C5-C10-C11-C12
3	A	501[B]	YA1	C31-C24-C25-C26

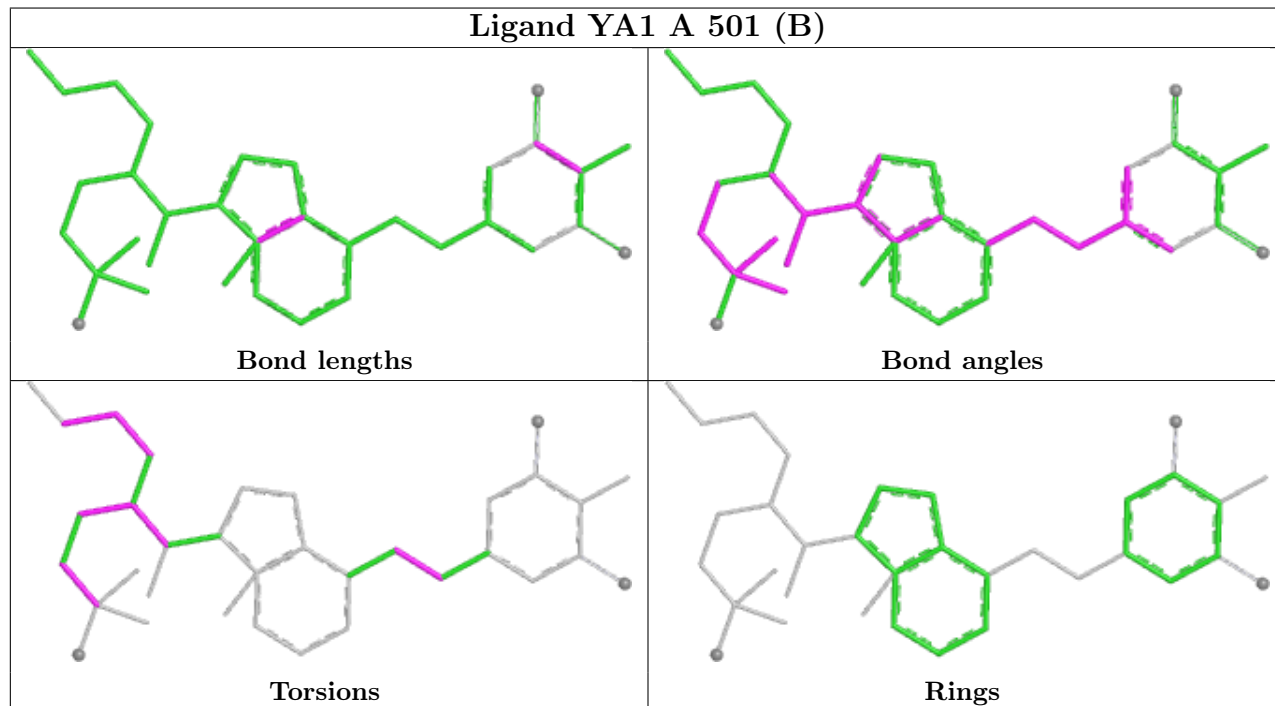
There are no ring outliers.

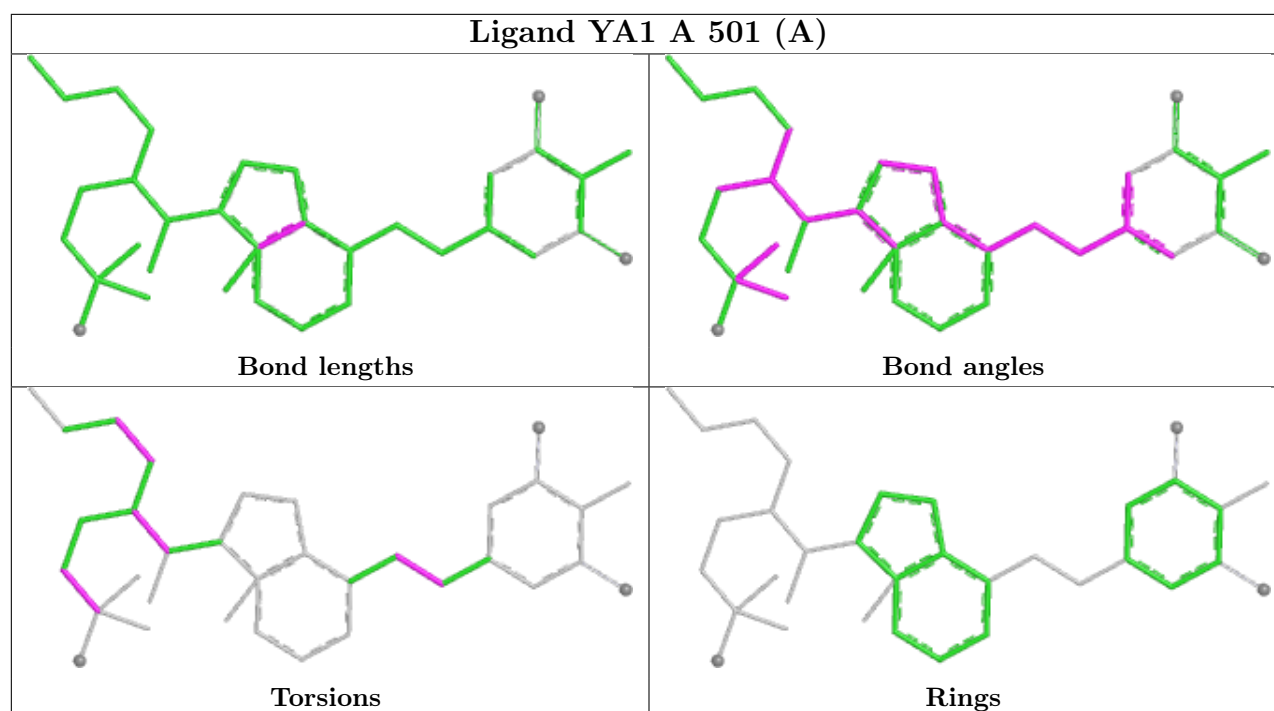
2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501[B]	YA1	16	0
3	A	501[A]	YA1	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 [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

### 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	239/271 (88%)	0.38	22 (9%) 14 13	17, 31, 67, 94	3 (1%)
2	C	11/13 (84%)	1.65	3 (27%) 1 1	40, 45, 71, 77	0
All	All	250/284 (88%)	0.44	25 (10%) 12 11	17, 32, 67, 94	3 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	625	LYS	6.1
1	A	402	PHE	4.7
1	A	219	PRO	4.7
1	A	397	TYR	4.5
1	A	400	LEU	4.3
1	A	419	GLY	4.1
1	A	396	GLN	4.0
1	A	305[A]	LEU	3.7
1	A	401	SER	3.2
1	A	403	GLN	3.0
1	A	395	LYS	3.0
1	A	418	PHE	3.0
1	A	123	LYS	2.9
1	A	300	GLY	2.8
1	A	218	SER	2.6
1	A	157	VAL	2.5
2	C	626	ASN	2.5
1	A	301[A]	HIS	2.4
1	A	394	SER	2.3
1	A	399	SER	2.3
2	C	635	LYS	2.2
1	A	159	MET	2.2
1	A	277	MET	2.2
1	A	276	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	286	SER	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

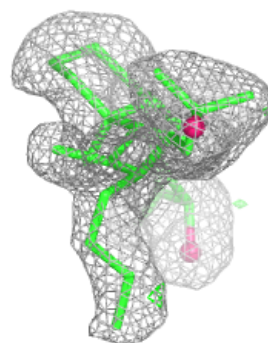
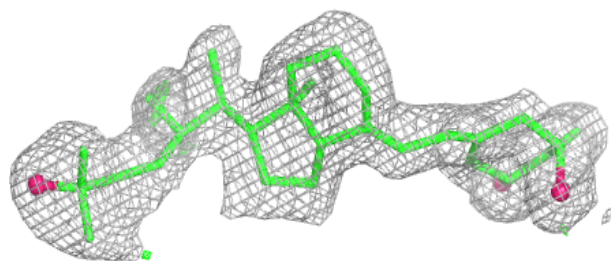
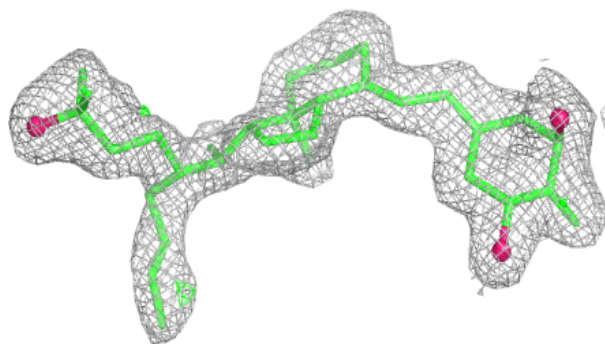
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	YA1	A	501[A]	34/34	0.91	0.12	25,31,48,49	34
3	YA1	A	501[B]	34/34	0.91	0.12	27,33,45,46	34

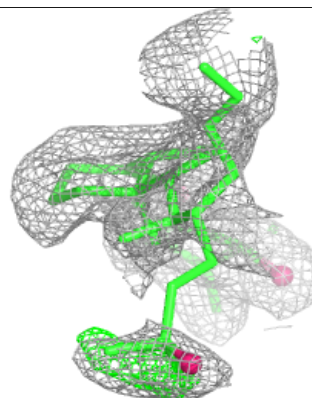
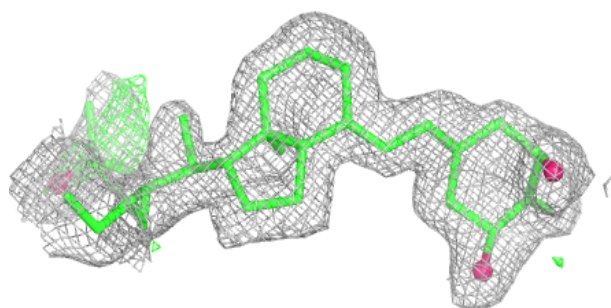
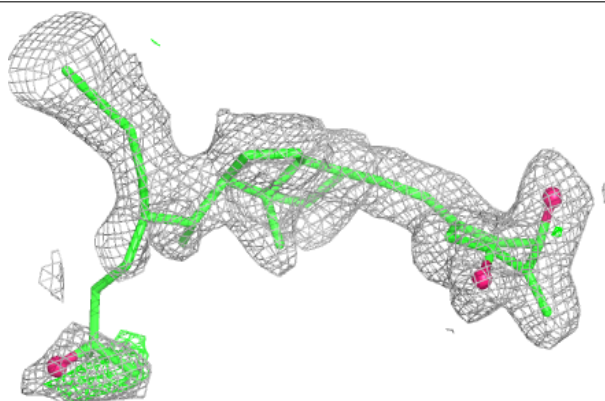
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around YA1 A 501 (A):**

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

**Electron density around YA1 A 501 (B):**

$2mF_o-DF_c$  (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.