



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:53 AM UTC

PDB ID : 4HLE / pdb_00004hle
Title : Compound 21 (1-alkyl-substituted 1,2,4-triazoles)
Authors : Murray, J.M.; Rouge, L.; Wu, P.
Deposited on : 2012-10-16
Resolution : 2.78 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

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>.

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

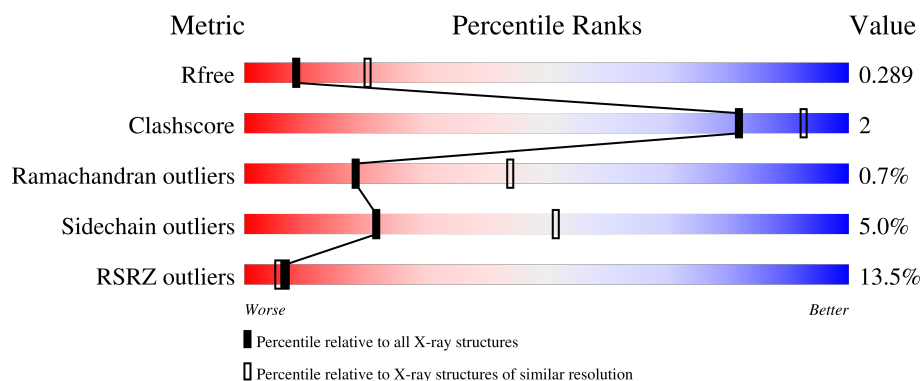
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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 ≥ 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	966	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6737 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.

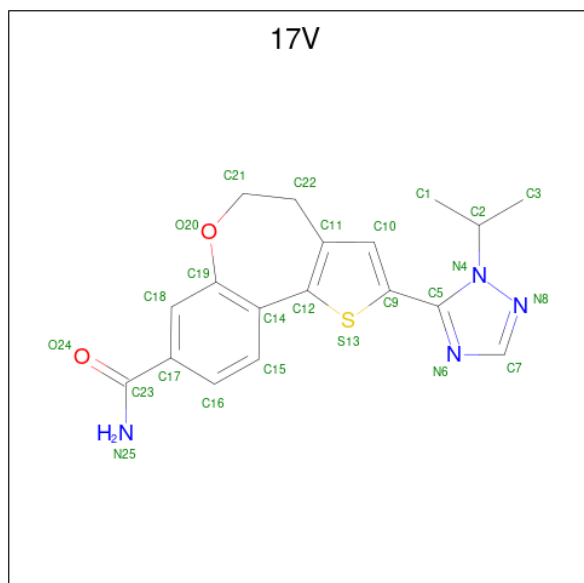
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	828	Total	C	N	O	S	29	0	0
			6712	4319	1144	1215	34			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is 2-[1-(propan-2-yl)-1H-1,2,4-triazol-5-yl]-4,5-dihydrothieno[3,2-d][1]benzoxepine-8-carboxamide (CCD ID: 17V) (formula: C₁₈H₁₈N₄O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	18	4	2	1		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.38Å 67.79Å 106.76Å 90.00° 95.44° 90.00°	Depositor
Resolution (Å)	61.31 – 2.78 61.31 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.6 (61.31-2.78) 99.6 (61.31-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.77Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.11.2	Depositor
R, R_{free}	0.254 , 0.274 0.268 , 0.289	Depositor DCC
R_{free} test set	1314 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6737	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 17V

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	0.73	0/6857	1.31	6/9281 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	MET	N-CA-C	6.70	117.30	109.60
1	A	411	ASN	CA-C-N	6.04	128.66	120.63
1	A	411	ASN	C-N-CA	6.04	128.66	120.63
1	A	503	THR	N-CA-C	5.53	118.35	110.10
1	A	470	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	484	MET	N-CA-C	5.24	118.35	109.76

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	6712	0	6758	32	0
2	A	25	0	18	1	0
All	All	6737	0	6776	33	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 (33) 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:834:HIS:HB2	1:A:876:ILE:HD12	1.81	0.61
1:A:887:THR:HG22	1:A:890:LYS:H	1.66	0.60
1:A:662:GLN:HE22	1:A:847:ILE:HD11	1.72	0.54
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.92	0.51
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.93	0.51
1:A:224:ILE:HD12	1:A:233:ILE:HD12	1.93	0.50
1:A:547:MET:HB2	1:A:552:ARG:HH21	1.77	0.50
1:A:750:LYS:HA	1:A:809:LYS:HD2	1.93	0.50
2:A:1201:17V:H4	2:A:1201:17V:S13	2.51	0.49
1:A:628:MET:HE1	1:A:662:GLN:HB3	1.93	0.49
1:A:464:VAL:HB	1:A:484:MET:HG2	1.94	0.49
1:A:151:GLN:HA	1:A:154:LEU:HD12	1.95	0.48
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.50	0.46
1:A:1041:GLN:HG2	1:A:1042:LEU:HD12	1.97	0.46
1:A:726:THR:HA	1:A:729:LEU:HB2	1.98	0.46
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.97	0.46
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.99	0.45
1:A:798:ILE:H	1:A:798:ILE:HG13	1.57	0.45
1:A:1069:LEU:HA	1:A:1072:ILE:HD12	1.99	0.45
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.99	0.45
1:A:429:LEU:HB2	1:A:468:LEU:HD21	2.00	0.44
1:A:1008:LYS:HG2	1:A:1012:ILE:HD11	1.99	0.44
1:A:207:LEU:HD13	1:A:288:LYS:HB2	2.00	0.43
1:A:983:VAL:HG22	1:A:1082:VAL:HG21	2.00	0.43
1:A:192:ASP:HB3	1:A:195:LEU:HB2	2.01	0.43
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.99	0.43
1:A:149:ALA:HA	1:A:152:ARG:HD2	2.01	0.43
1:A:384:GLU:HG3	1:A:398:ARG:HG2	2.02	0.42
1:A:623:ASP:HB3	1:A:626:LEU:HB3	2.01	0.42
1:A:424:PRO:HD2	1:A:427:ALA:HB2	2.02	0.41
1:A:949:ASN:HA	1:A:952:ILE:HD12	2.03	0.41
1:A:1018:LEU:HD23	1:A:1021:ARG:HD3	2.02	0.41
1:A:1039:MET:HE3	1:A:1042:LEU:HD13	2.02	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	810/966 (84%)	764 (94%)	40 (5%)	6 (1%)	18	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ALA
1	A	227	SER
1	A	916	PRO
1	A	949	ASN
1	A	778	GLN
1	A	897	GLY

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	744/864 (86%)	707 (95%)	37 (5%)	22	51

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	LEU
1	A	282	VAL
1	A	307	LEU
1	A	357	CYS
1	A	370	ILE

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	402	LYS
1	A	419	LYS
1	A	461	LEU
1	A	464	VAL
1	A	518	ILE
1	A	521	ASP
1	A	529	LEU
1	A	610	LEU
1	A	615	GLU
1	A	662	GLN
1	A	729	LEU
1	A	739	ILE
1	A	779	LEU
1	A	796	LEU
1	A	798	ILE
1	A	799	GLU
1	A	823	LEU
1	A	865	LEU
1	A	879	ILE
1	A	887	THR
1	A	939	THR
1	A	946	ASP
1	A	955	THR
1	A	957	THR
1	A	959	ASN
1	A	968	ILE
1	A	1026	LEU
1	A	1027	LEU
1	A	1042	LEU
1	A	1051	ILE
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	GLN
1	A	299	ASN
1	A	389	HIS
1	A	391	GLN
1	A	483	HIS
1	A	512	ASN

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Mol	Chain	Res	Type
1	A	600	GLN
1	A	639	ASN
1	A	662	GLN
1	A	705	GLN
1	A	834	HIS
1	A	892	GLN
1	A	898	ASN
1	A	959	ASN
1	A	1022	HIS
1	A	1085	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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	$\# Z > 2$
2	17V	A	1201	-	28,28,28	1.28	4 (14%)	30,41,41	3.04	12 (40%)

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	17V	A	1201	-	-	0/12/22/22	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	17V	C5-N4	2.60	1.38	1.35
2	A	1201	17V	C14-C12	2.15	1.49	1.47
2	A	1201	17V	N4-N8	2.12	1.41	1.37
2	A	1201	17V	C9-C5	2.12	1.48	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	17V	C7-N6-C5	9.40	110.22	101.80
2	A	1201	17V	C7-N8-N4	8.25	107.57	101.28
2	A	1201	17V	C2-N4-N8	5.70	125.51	119.62
2	A	1201	17V	N8-C7-N6	-4.62	109.45	116.78
2	A	1201	17V	C9-C5-N4	3.27	129.44	125.14
2	A	1201	17V	C5-C9-S13	3.11	126.97	117.24
2	A	1201	17V	C11-C12-S13	-2.63	109.34	111.36
2	A	1201	17V	O24-C23-N25	-2.45	119.07	122.62
2	A	1201	17V	C17-C23-N25	2.42	120.72	117.74
2	A	1201	17V	O20-C19-C18	2.40	120.73	116.83
2	A	1201	17V	C10-C9-S13	-2.17	107.90	111.55
2	A	1201	17V	C22-C11-C12	2.13	128.86	125.01

There are no chirality outliers.

There are no torsion outliers.

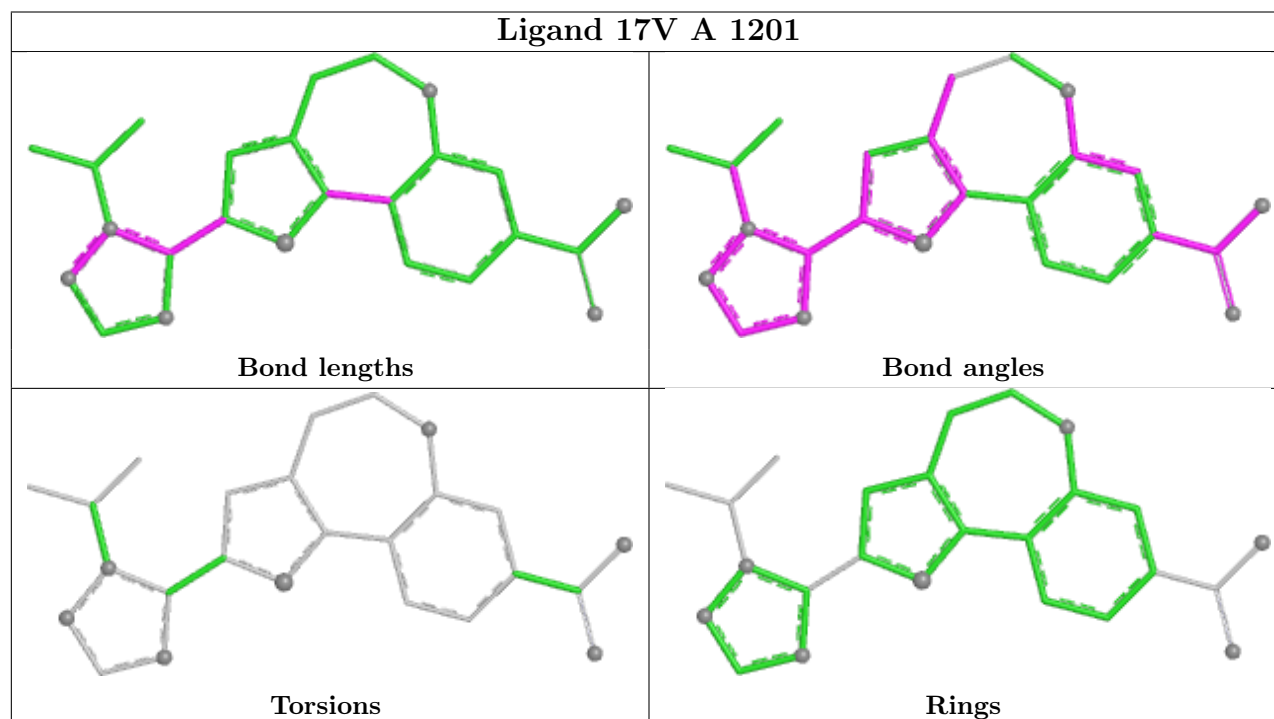
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	17V	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 95th 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 ²)	Q<0.9
1	A	825/966 (85%)	0.99	111 (13%) 7 5	39, 82, 127, 149	1 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1042	LEU	7.0
1	A	968	ILE	5.8
1	A	435	CYS	4.6
1	A	757	TYR	4.3
1	A	749	ILE	4.2
1	A	1090	LEU	4.1
1	A	379	LEU	3.8
1	A	986	VAL	3.7
1	A	394	LEU	3.6
1	A	303	ILE	3.6
1	A	518	ILE	3.5
1	A	895	THR	3.4
1	A	894	SER	3.4
1	A	823	LEU	3.3
1	A	1002	THR	3.3
1	A	249	PHE	3.2
1	A	497	PHE	3.2
1	A	1092	LEU	3.2
1	A	380	THR	3.1
1	A	248	PHE	3.1
1	A	746	THR	3.1
1	A	1084	PHE	3.1
1	A	404	PHE	3.1
1	A	862	LEU	3.0
1	A	811	LEU	3.0
1	A	481	VAL	2.9
1	A	519	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1082	VAL	2.9
1	A	496	SER	2.9
1	A	413	TRP	2.9
1	A	985	PHE	2.9
1	A	1041	GLN	2.8
1	A	878	MET	2.8
1	A	233	ILE	2.8
1	A	898	ASN	2.8
1	A	402	LYS	2.7
1	A	924	ALA	2.7
1	A	280	TYR	2.7
1	A	395	CYS	2.6
1	A	358	ASP	2.6
1	A	595	SER	2.6
1	A	401	PRO	2.6
1	A	995	MET	2.5
1	A	283	GLY	2.5
1	A	393	VAL	2.5
1	A	250	THR	2.5
1	A	224	ILE	2.5
1	A	419	LYS	2.5
1	A	414	LEU	2.5
1	A	520	LEU	2.5
1	A	987	LEU	2.5
1	A	530	PRO	2.5
1	A	305	VAL	2.5
1	A	1091	VAL	2.4
1	A	901	ALA	2.4
1	A	211	LEU	2.4
1	A	752	LEU	2.4
1	A	767	LEU	2.4
1	A	779	LEU	2.4
1	A	907	LEU	2.4
1	A	863	CYS	2.4
1	A	832	PHE	2.4
1	A	403	PRO	2.4
1	A	925	VAL	2.4
1	A	1014	VAL	2.4
1	A	416	PHE	2.4
1	A	1069	LEU	2.3
1	A	1000	LYS	2.3
1	A	383	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	361	PHE	2.3
1	A	1055	LEU	2.3
1	A	601	GLN	2.3
1	A	237	PRO	2.3
1	A	1079	GLY	2.3
1	A	285	THR	2.3
1	A	639	ASN	2.3
1	A	398	ARG	2.3
1	A	994	VAL	2.3
1	A	1088	LEU	2.3
1	A	469	ILE	2.2
1	A	989	PRO	2.2
1	A	354	LEU	2.2
1	A	528	ALA	2.2
1	A	409	LEU	2.2
1	A	223	VAL	2.2
1	A	844	ILE	2.2
1	A	1006	PHE	2.2
1	A	385	ALA	2.2
1	A	529	LEU	2.2
1	A	245	LEU	2.2
1	A	599	GLY	2.2
1	A	374	PRO	2.1
1	A	316	ASP	2.1
1	A	891	ILE	2.1
1	A	272	LEU	2.1
1	A	368	ILE	2.1
1	A	410	TRP	2.1
1	A	198	MET	2.1
1	A	188	VAL	2.1
1	A	270	PHE	2.1
1	A	216	ALA	2.1
1	A	229	THR	2.1
1	A	771	LEU	2.1
1	A	1075	CYS	2.1
1	A	1048	ILE	2.1
1	A	274	VAL	2.1
1	A	189	ALA	2.0
1	A	418	ILE	2.0
1	A	952	ILE	2.0
1	A	271	VAL	2.0
1	A	477	ARG	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](#)

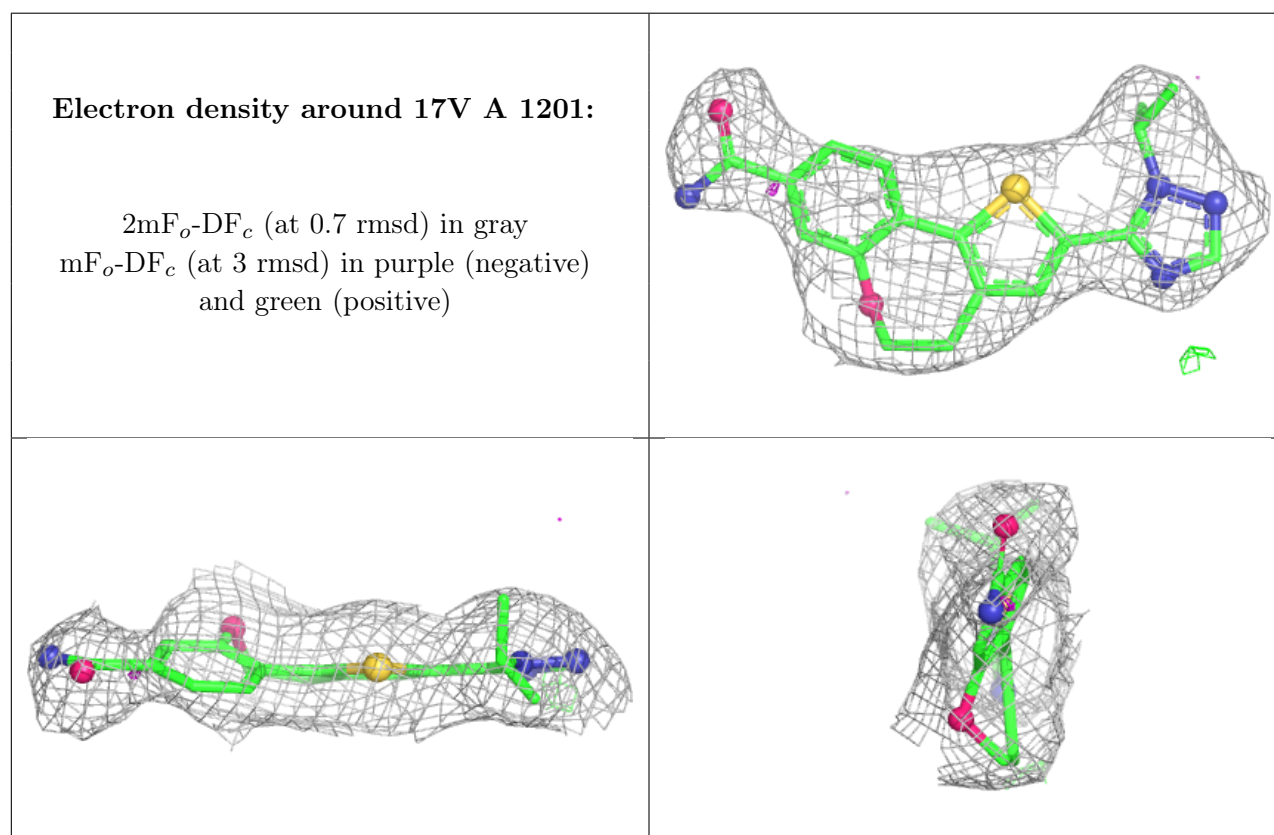
There are no oligosaccharides in this entry.

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, 95th 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
2	17V	A	1201	25/25	0.92	0.12	71,75,79,80	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.