



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:29 am BST

PDB ID : 4HLE
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 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

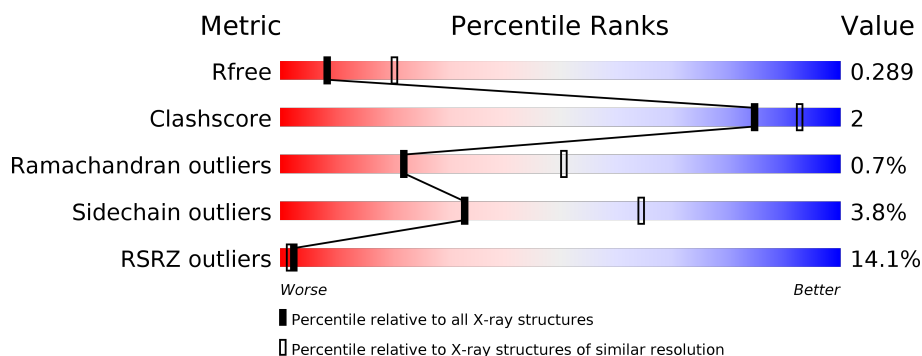
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (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 on 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.

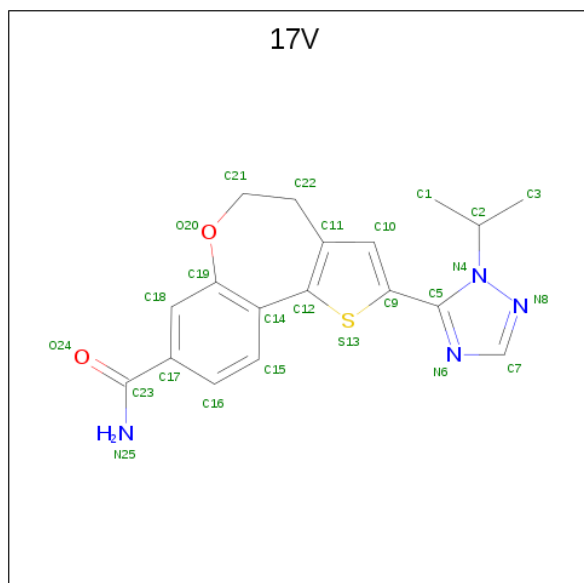
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

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 (three-letter code: 17V) (formula: C₁₈H₁₈N₄O₂S).

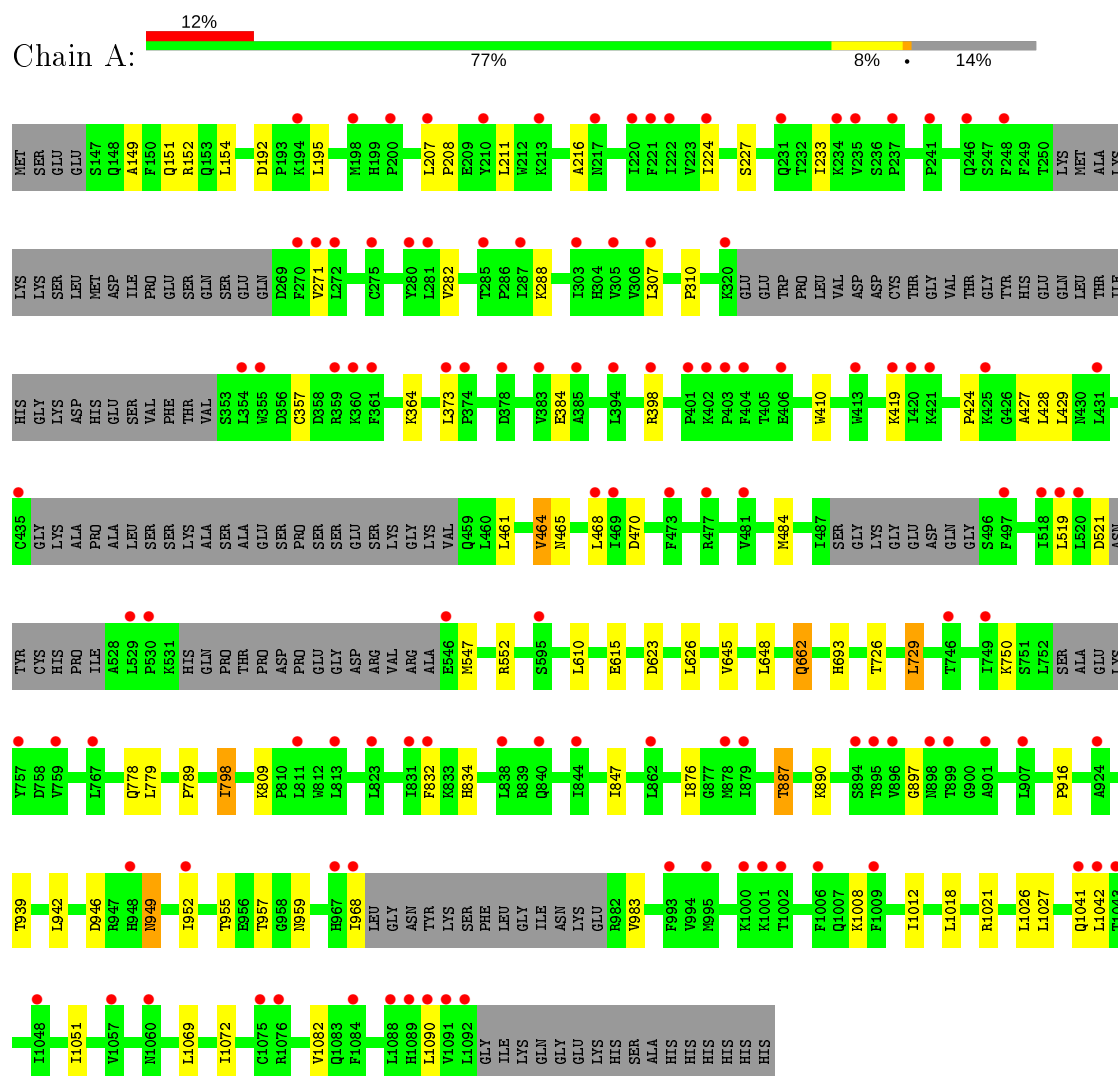


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	18	4	2	1		

3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.38 Å 67.79 Å 106.76 Å 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 2.77 Å)	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)	0.30 , 56.0	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	0.40	0/6857	0.59	0/9281

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	30	0
2	A	25	0	18	1	0
All	All	6737	0	6776	31	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 (31) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S13	2:A:1201:17V:H4	2.51	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:1041:GLN:HG2	1:A:1042:LEU:HD12	1.97	0.46
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.50	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:HG13	1:A:798:ILE:H	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:983:VAL:HG22	1:A:1082:VAL:HG21	2.00	0.43
1:A:207:LEU:HD13	1:A:288:LYS:HB2	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:1018:LEU:HD23	1:A:1021:ARG:HD3	2.02	0.41
1:A:949:ASN:HA	1:A:952:ILE:HD12	2.03	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	810/966 (84%)	764 (94%)	40 (5%)	6 (1%)	22 50

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%)	716 (96%)	28 (4%)	33 64

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	VAL
1	A	307	LEU
1	A	357	CYS
1	A	373	LEU
1	A	410	TRP
1	A	419	LYS
1	A	461	LEU
1	A	464	VAL
1	A	470	ASP
1	A	521	ASP
1	A	610	LEU
1	A	615	GLU
1	A	662	GLN
1	A	729	LEU
1	A	779	LEU

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Mol	Chain	Res	Type
1	A	798	ILE
1	A	832	PHE
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	1051	ILE
1	A	1090	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	HIS
1	A	391	GLN
1	A	483	HIS
1	A	600	GLN
1	A	662	GLN
1	A	705	GLN
1	A	834	HIS

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 carbohydrates 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	-	21,28,28	1.07	1 (4%)	20,41,41	1.26	3 (15%)

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	-	-	0/8/22/22	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	17V	N8-N4	2.55	1.41	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	17V	O20-C19-C18	2.61	120.73	116.95
2	A	1201	17V	C17-C23-N25	2.48	120.72	117.75
2	A	1201	17V	O24-C23-N25	-2.47	119.07	122.58

There are no chirality outliers.

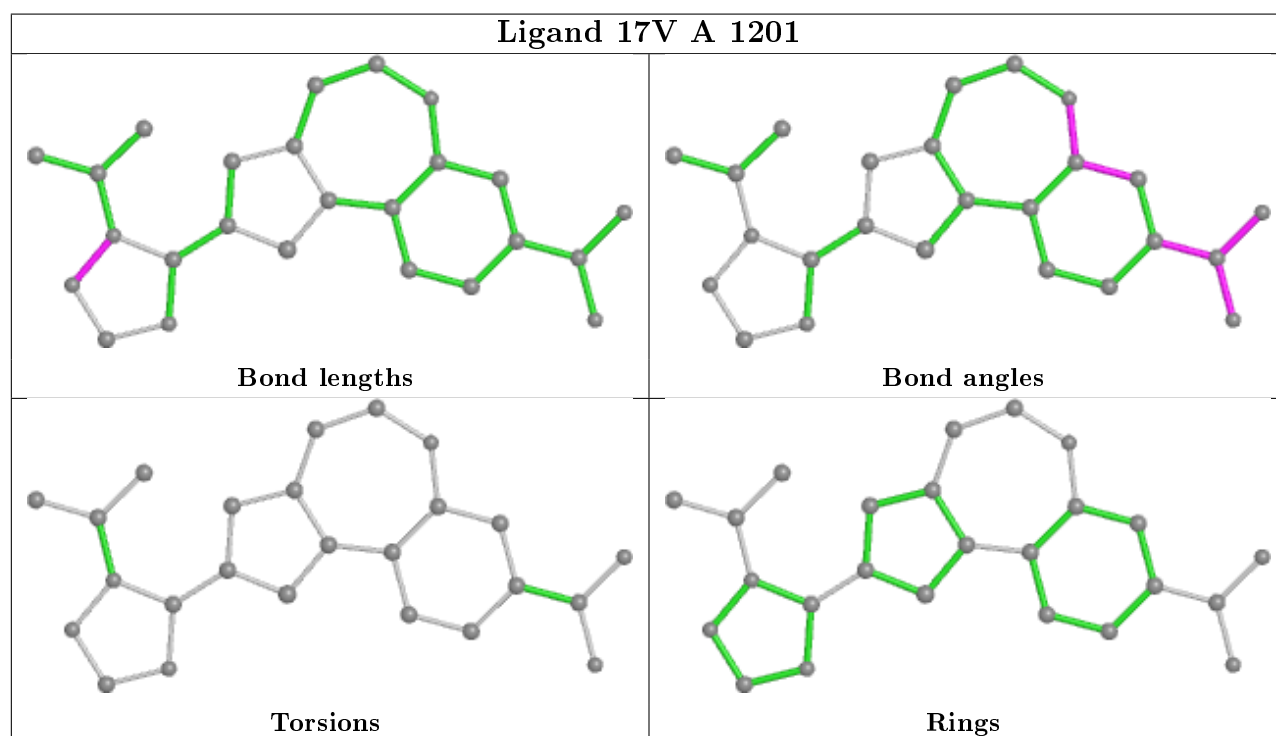
There are no torsion outliers.

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 ⓘ

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, 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%)	0.92	116 (14%) 2 2	39, 82, 127, 149	1 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1042	LEU	16.7
1	A	1041	GLN	7.3
1	A	895	THR	6.0
1	A	378	ASP	5.6
1	A	404	PHE	5.3
1	A	749	ILE	4.9
1	A	235	VAL	4.7
1	A	497	PHE	4.6
1	A	823	LEU	4.4
1	A	374	PRO	4.3
1	A	270	PHE	4.3
1	A	529	LEU	4.2
1	A	898	ASN	4.2
1	A	995	MET	4.1
1	A	907	LEU	3.9
1	A	303	ILE	3.9
1	A	477	ARG	3.8
1	A	287	ILE	3.8
1	A	221	PHE	3.7
1	A	272	LEU	3.6
1	A	217	ASN	3.5
1	A	1090	LEU	3.5
1	A	354	LEU	3.4
1	A	1075	CYS	3.4
1	A	767	LEU	3.4
1	A	220	ILE	3.3
1	A	813	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	194	LYS	3.3
1	A	373	LEU	3.3
1	A	1092	LEU	3.3
1	A	271	VAL	3.2
1	A	307	LEU	3.1
1	A	811	LEU	3.1
1	A	530	PRO	3.1
1	A	280	TYR	3.0
1	A	1000	LYS	3.0
1	A	419	LYS	3.0
1	A	1002	THR	3.0
1	A	281	LEU	3.0
1	A	518	ILE	3.0
1	A	385	ALA	3.0
1	A	248	PHE	3.0
1	A	398	ARG	2.9
1	A	359	ARG	2.9
1	A	967	HIS	2.8
1	A	894	SER	2.8
1	A	595	SER	2.8
1	A	320	LYS	2.8
1	A	403	PRO	2.8
1	A	394	LEU	2.8
1	A	207	LEU	2.8
1	A	832	PHE	2.8
1	A	468	LEU	2.8
1	A	1091	VAL	2.7
1	A	1043	THR	2.7
1	A	305	VAL	2.7
1	A	879	ILE	2.7
1	A	757	TYR	2.7
1	A	224	ILE	2.7
1	A	401	PRO	2.6
1	A	1084	PHE	2.6
1	A	383	VAL	2.6
1	A	481	VAL	2.6
1	A	844	ILE	2.6
1	A	435	CYS	2.6
1	A	425	LYS	2.6
1	A	1009	PHE	2.6
1	A	1089	HIS	2.5
1	A	469	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	896	VAL	2.5
1	A	222	ILE	2.5
1	A	901	ALA	2.5
1	A	360	LYS	2.5
1	A	924	ALA	2.4
1	A	862	LEU	2.4
1	A	948	HIS	2.4
1	A	993	PHE	2.4
1	A	355	TRP	2.3
1	A	231	GLN	2.3
1	A	413	TRP	2.3
1	A	421	LYS	2.3
1	A	275	CYS	2.3
1	A	285	THR	2.3
1	A	473	PHE	2.3
1	A	968	ILE	2.3
1	A	878	MET	2.3
1	A	237	PRO	2.3
1	A	519	LEU	2.3
1	A	831	ILE	2.3
1	A	1048	ILE	2.3
1	A	241	PRO	2.3
1	A	838	LEU	2.2
1	A	952	ILE	2.2
1	A	759	VAL	2.2
1	A	200	PRO	2.2
1	A	840	GLN	2.2
1	A	546	GLU	2.2
1	A	213	LYS	2.2
1	A	198	MET	2.2
1	A	210	TYR	2.1
1	A	402	LYS	2.1
1	A	1057	VAL	2.1
1	A	246	GLN	2.1
1	A	1001	LYS	2.1
1	A	1088	LEU	2.1
1	A	899	THR	2.1
1	A	420	ILE	2.1
1	A	520	LEU	2.1
1	A	234	LYS	2.1
1	A	1076	ARG	2.0
1	A	431	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	406	GLU	2.0
1	A	1060	ASN	2.0
1	A	1006	PHE	2.0
1	A	746	THR	2.0
1	A	361	PHE	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](#)

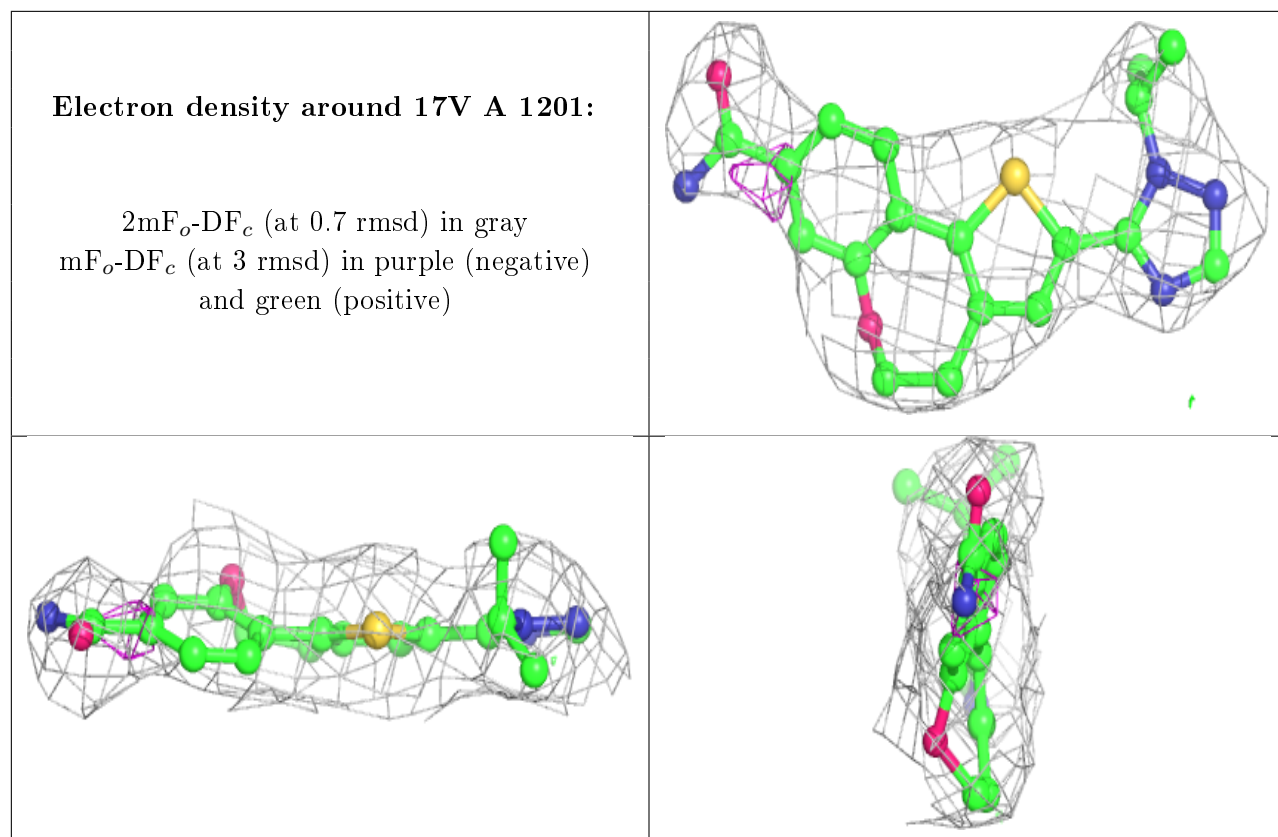
There are no carbohydrates in this entry.

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, 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(\AA^2)	Q<0.9
2	17V	A	1201	25/25	0.93	0.25	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.