



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:35 AM UTC

PDB ID : 3ZSO / pdb_00003zso
Title : Small molecule inhibitors of the LEDGF site of HIV type 1 integrase identified by fragment screening and structure based design
Authors : Peat, T.S.; Newman, J.; Rhodes, D.I.; Deadman, J.J.; Vandergraaff, N.; Le, G.; Jones, E.D.; Smith, J.A.; Coates, J.A.V.; Thienthong, N.; Dolezal, O.; Ryan, J.H.; Savage, G.P.; Francis, C.L.
Deposited on : 2011-06-30
Resolution : 1.75 Å(reported)

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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](#) ①) 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

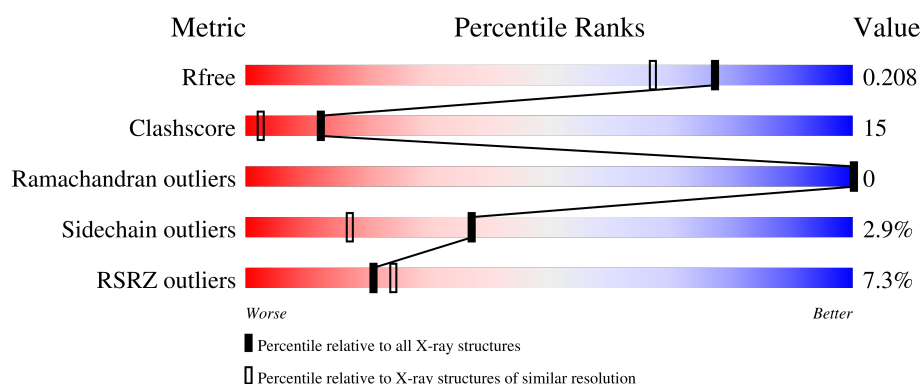
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	167	
1	B	167	

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:

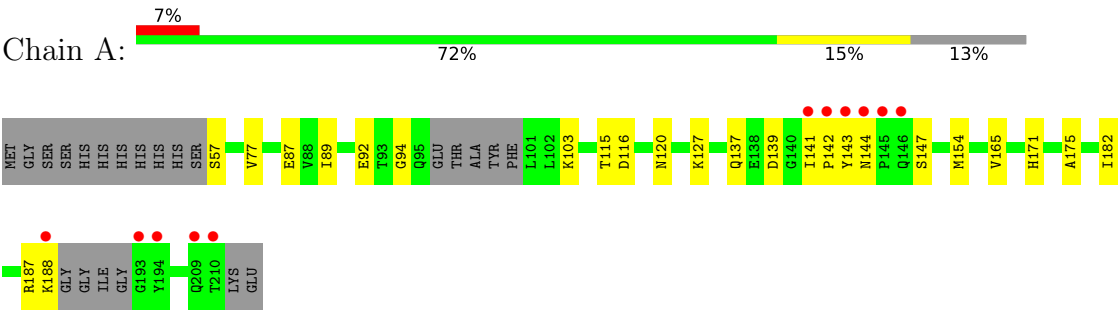
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	A	1215	-	-	X	-
3	ACY	A	1216	-	-	X	-
3	ACY	A	1217	-	-	X	-
3	ACY	B	1215	-	-	X	-
4	NA	B	1216	-	-	X	-

ENTRY-COMPOSITION INFOmissingINFO

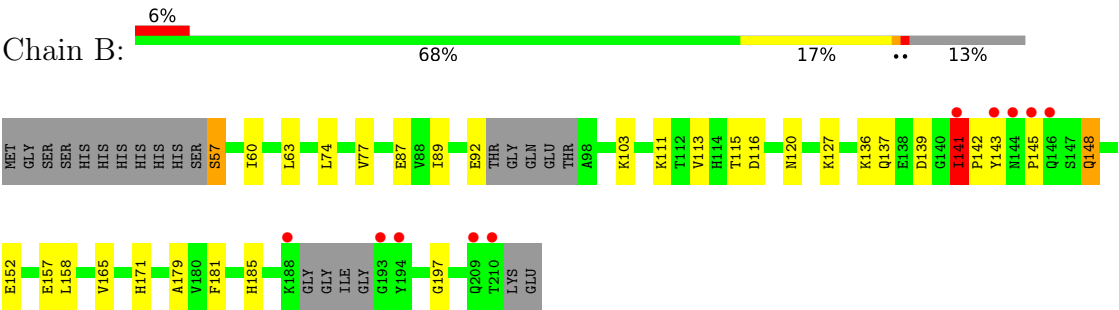
2 Residue-property plots i

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: INTEGRASE



• Molecule 1: INTEGRASE



GLOBAL-STATISTICS INFOmissingINFO

3 Model quality

3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: O2N, NA, ACY, SO4

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	1.37	4/1276 (0.3%)	1.24	1/1732 (0.1%)
1	B	1.44	6/1291 (0.5%)	1.22	1/1750 (0.1%)
All	All	1.41	10/2567 (0.4%)	1.23	2/3482 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	ILE	N-CA	6.20	1.52	1.46
1	A	89	ILE	N-CA	6.10	1.52	1.46
1	B	165	VAL	CA-CB	5.49	1.60	1.54
1	A	175	ALA	CA-CB	5.39	1.61	1.53
1	A	165	VAL	CA-CB	5.38	1.60	1.54
1	B	60	ILE	CA-CB	5.32	1.60	1.54
1	B	77	VAL	CA-CB	5.21	1.60	1.54
1	B	113[A]	VAL	C-O	-5.07	1.18	1.24
1	B	113[B]	VAL	C-O	-5.07	1.18	1.24
1	A	182	ILE	N-CA	5.03	1.52	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	GLY	N-CA-C	-6.52	104.43	112.77
1	B	141	ILE	N-CA-CB	5.76	115.44	110.08

There are no chirality outliers.

There are no planarity outliers.

CLOSE-CONTACTS INFOmissingINFO

3.2 Torsion angles

3.2.1 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	157/167 (94%)	154 (98%)	3 (2%)	0	100	100
1	B	157/167 (94%)	155 (99%)	2 (1%)	0	100	100
All	All	314/334 (94%)	309 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

3.2.2 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	136/137 (99%)	134 (98%)	2 (2%)	57	41
1	B	137/137 (100%)	132 (96%)	5 (4%)	31	11
All	All	273/274 (100%)	266 (97%)	7 (3%)	37	20

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	188	LYS
1	B	57	SER
1	B	141	ILE
1	B	148	GLN
1	B	152	GLU
1	B	157	GLU

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	137	GLN
1	A	148	GLN
1	A	171	HIS
1	A	209	GLN
1	B	137	GLN
1	B	148	GLN
1	B	171	HIS
1	B	185	HIS

3.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

3.4 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.5 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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	SO4	A	1213	-	4,4,4	0.62	0	6,6,6	0.65	0
3	ACY	A	1215	-	3,3,3	1.73	1 (33%)	3,3,3	1.21	0
2	SO4	B	1211	-	4,4,4	0.28	0	6,6,6	1.28	1 (16%)
2	SO4	B	1213	-	4,4,4	0.92	0	6,6,6	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1211	-	4,4,4	0.25	0	6,6,6	1.56	2 (33%)
5	O2N	B	1217	-	48,48,48	1.27	4 (8%)	64,66,66	1.86	18 (28%)
3	ACY	A	1216	-	3,3,3	1.63	1 (33%)	3,3,3	1.26	0
3	ACY	B	1215	-	3,3,3	0.96	0	3,3,3	0.92	0
2	SO4	A	1214	4	4,4,4	0.46	0	6,6,6	0.61	0
2	SO4	B	1212	-	4,4,4	0.21	0	6,6,6	0.98	0
2	SO4	B	1214	4	4,4,4	0.23	0	6,6,6	0.61	0
2	SO4	A	1212	-	4,4,4	0.43	0	6,6,6	0.98	0
3	ACY	A	1217	-	3,3,3	0.62	0	3,3,3	1.73	1 (33%)
5	O2N	A	1219	-	48,48,48	1.34	5 (10%)	64,66,66	1.81	18 (28%)

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
5	O2N	A	1219	-	-	8/35/41/41	0/5/5/5
5	O2N	B	1217	-	-	6/35/41/41	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1219	O2N	C33-N37	4.95	1.57	1.47
5	B	1217	O2N	C33-N37	4.44	1.56	1.47
5	A	1219	O2N	C10-C5	2.96	1.43	1.38
5	B	1217	O2N	C14-C9	2.84	1.43	1.38
3	A	1215	ACY	O-C	2.83	1.34	1.22
3	A	1216	ACY	O-C	2.72	1.34	1.22
5	A	1219	O2N	C32-N37	2.62	1.52	1.47
5	A	1219	O2N	C27-N36	2.48	1.40	1.34
5	B	1217	O2N	C10-C5	2.46	1.42	1.38
5	B	1217	O2N	C15-C27	-2.22	1.45	1.50
5	A	1219	O2N	C14-C9	2.01	1.42	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1217	O2N	C9-C14-C24	-4.72	114.34	119.73
5	B	1217	O2N	C9-C18-C35	4.68	128.62	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1217	O2N	C14-C9-C18	4.62	125.80	121.18
5	A	1219	O2N	C9-C14-C24	-4.20	114.93	119.73
5	A	1219	O2N	C14-C9-C18	4.06	125.24	121.18
5	A	1219	O2N	O42-C22-C16	-3.96	123.91	128.33
5	A	1219	O2N	C29-O42-C22	-3.90	100.40	105.05
5	B	1217	O2N	C8-C18-C35	-3.63	114.63	120.75
5	B	1217	O2N	O38-C28-C16	3.17	123.58	114.67
5	B	1217	O2N	C29-O42-C22	-3.17	101.28	105.05
5	A	1219	O2N	O42-C29-O41	3.12	112.98	108.09
5	B	1217	O2N	C6-C11-C23	-3.11	116.18	119.73
5	A	1219	O2N	C33-N37-C32	3.01	116.60	110.64
5	B	1217	O2N	O42-C29-O41	2.96	112.73	108.09
5	B	1217	O2N	O42-C22-C16	-2.94	125.04	128.33
5	A	1219	O2N	C9-C18-C35	2.93	125.67	120.75
2	A	1211	SO4	O3-S-O1	-2.64	95.78	109.56
5	B	1217	O2N	C20-C33-N37	-2.60	108.13	112.75
5	B	1217	O2N	O40-C28-C16	-2.59	114.98	121.18
5	B	1217	O2N	C33-N37-C32	2.46	115.52	110.64
5	A	1219	O2N	C5-C10-C21	-2.43	115.46	120.06
5	B	1217	O2N	C18-C35-N36	-2.42	106.89	111.23
5	A	1219	O2N	C31-O44-C24	-2.40	112.34	117.50
5	A	1219	O2N	C26-C34-N37	2.38	117.39	112.86
5	A	1219	O2N	O42-C22-C21	2.36	112.45	109.82
5	A	1219	O2N	C20-C16-C28	2.32	125.35	120.86
5	A	1219	O2N	C18-C35-C17	2.31	116.96	112.33
2	B	1211	SO4	O3-S-O1	2.30	121.59	109.56
5	A	1219	O2N	C6-C11-C23	-2.30	117.10	119.73
5	A	1219	O2N	C8-C18-C35	-2.23	116.99	120.75
5	B	1217	O2N	C29-O41-C21	-2.21	102.36	105.32
5	B	1217	O2N	C20-C16-C28	2.20	125.12	120.86
5	A	1219	O2N	C20-C33-N37	-2.20	108.84	112.75
3	A	1217	ACY	O-C-CH3	-2.19	113.55	122.53
5	A	1219	O2N	C7-C12-C23	-2.12	117.31	119.73
5	A	1219	O2N	C2-C1-C3	-2.12	117.62	120.24
5	B	1217	O2N	C11-C6-C17	2.05	123.22	121.18
5	B	1217	O2N	C5-C10-C21	-2.03	116.21	120.06
5	B	1217	O2N	C8-C13-C24	2.03	122.05	119.73
2	A	1211	SO4	O3-S-O2	2.01	120.08	109.56

There are no chirality outliers.

All (14) torsion outliers are listed below:

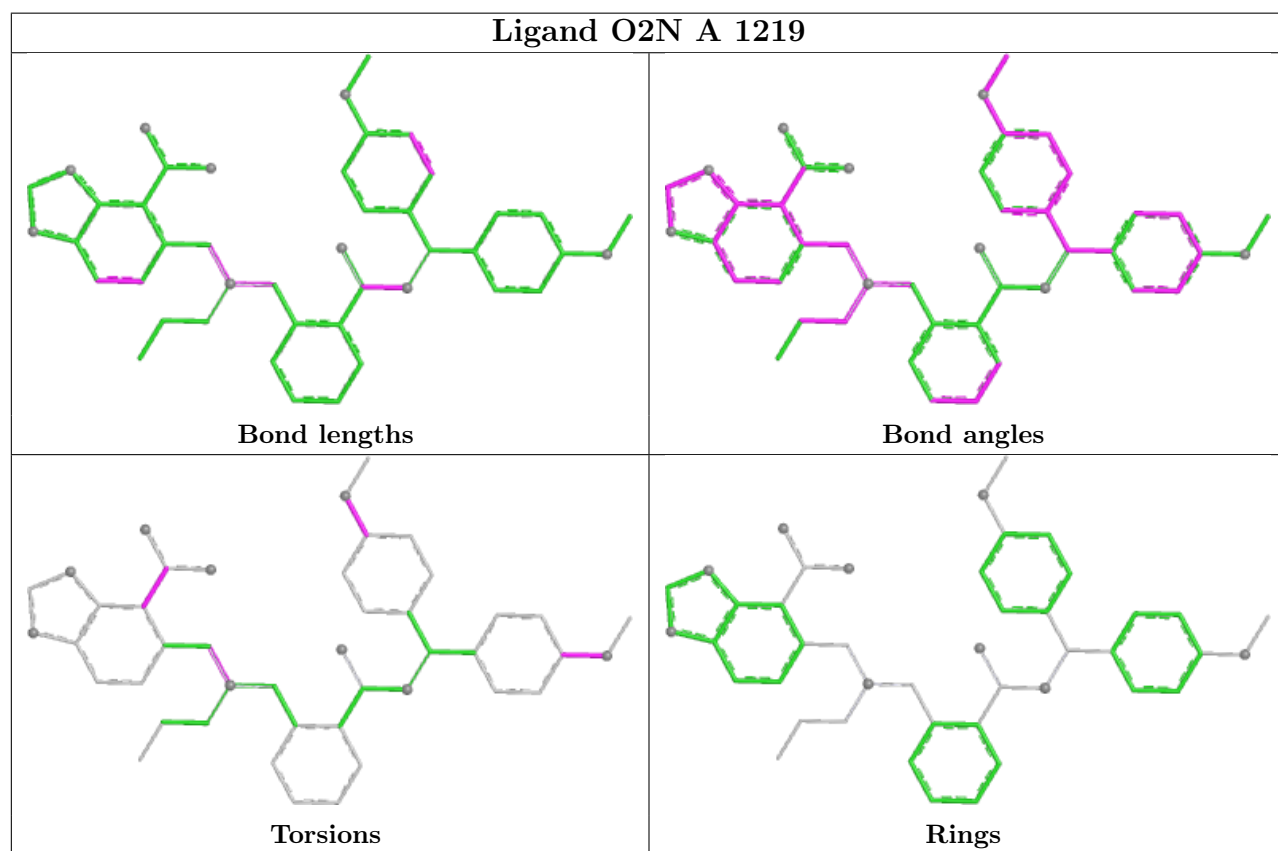
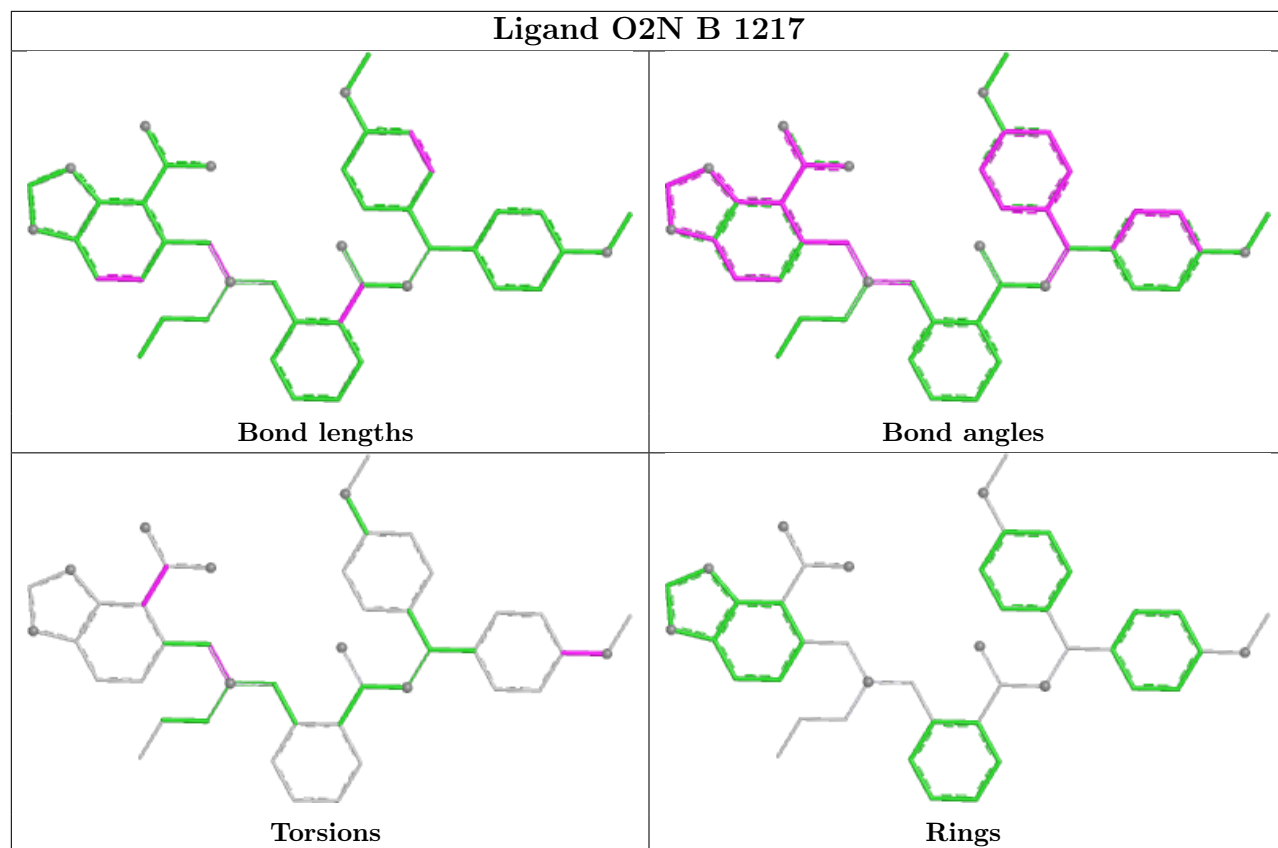
Mol	Chain	Res	Type	Atoms
5	B	1217	O2N	C22-C16-C28-O40
5	A	1219	O2N	C12-C23-O43-C30
5	B	1217	O2N	C12-C23-O43-C30
5	A	1219	O2N	C11-C23-O43-C30
5	B	1217	O2N	C11-C23-O43-C30
5	A	1219	O2N	C22-C16-C28-O40
5	B	1217	O2N	C22-C16-C28-O38
5	A	1219	O2N	C22-C16-C28-O38
5	B	1217	O2N	C20-C16-C28-O38
5	A	1219	O2N	C20-C33-N37-C34
5	B	1217	O2N	C20-C33-N37-C34
5	A	1219	O2N	C14-C24-O44-C31
5	A	1219	O2N	C13-C24-O44-C31
5	A	1219	O2N	C20-C16-C28-O40

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1215	ACY	10	0
5	B	1217	O2N	5	0
3	A	1216	ACY	11	0
3	B	1215	ACY	2	0
2	B	1212	SO4	1	0
2	B	1214	SO4	1	0
2	A	1212	SO4	1	0
3	A	1217	ACY	2	0
5	A	1219	O2N	5	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.



3.6 Other polymers [i](#)

There are no such residues in this entry.

3.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 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	144/167 (86%)	0.05	11 (7%) 20 23	8, 20, 42, 59	36 (25%)
1	B	144/167 (86%)	0.05	10 (6%) 23 26	8, 19, 41, 58	36 (25%)
All	All	288/334 (86%)	0.05	21 (7%) 21 24	8, 19, 42, 59	72 (25%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	GLY	8.6
1	A	193	GLY	8.4
1	A	210	THR	5.3
1	A	143	TYR	4.7
1	B	143	TYR	4.6
1	B	210	THR	4.5
1	A	144[A]	ASN	4.4
1	B	144[A]	ASN	4.3
1	B	145	PRO	3.9
1	A	188	LYS	3.9
1	B	209	GLN	3.8
1	B	146[A]	GLN	3.8
1	A	209	GLN	3.6
1	B	141	ILE	3.2
1	A	145	PRO	3.1
1	B	194	TYR	2.9
1	A	194	TYR	2.8
1	A	146	GLN	2.8
1	A	141[A]	ILE	2.5
1	B	188	LYS	2.3
1	A	142	PRO	2.0

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

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

4.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.4 Ligands [i](#)

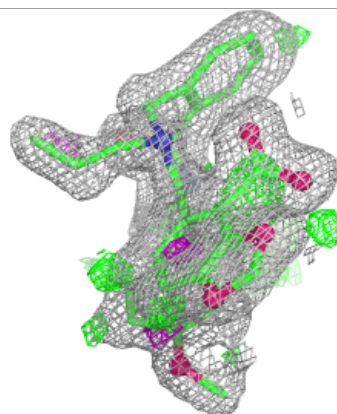
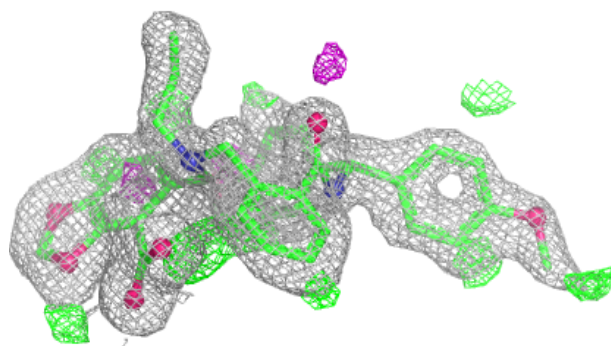
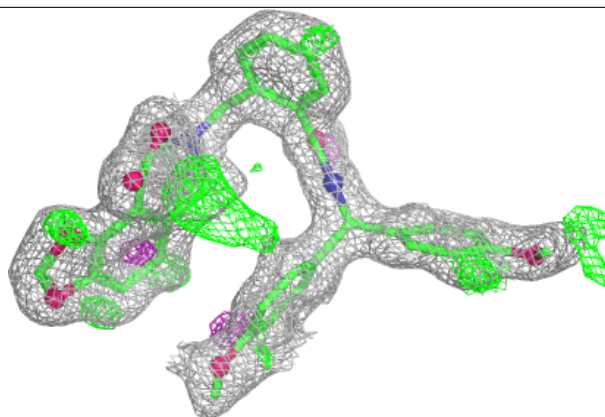
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	1213	5/5	0.76	0.20	35,36,44,48	5
2	SO4	B	1213	5/5	0.80	0.18	33,34,46,48	5
5	O2N	A	1219	44/44	0.87	0.12	18,26,34,37	44
5	O2N	B	1217	44/44	0.87	0.12	19,26,33,36	44
2	SO4	B	1214	5/5	0.88	0.12	27,39,45,46	5
4	NA	A	1218	1/1	0.89	0.09	48,48,48,48	0
2	SO4	A	1214	5/5	0.90	0.12	33,44,47,50	5
4	NA	B	1216	1/1	0.91	0.07	45,45,45,45	0
3	ACY	A	1215	4/4	0.92	0.11	28,29,29,31	0
3	ACY	A	1216	4/4	0.92	0.12	29,30,32,33	0
3	ACY	A	1217	4/4	0.92	0.14	47,48,49,50	0
3	ACY	B	1215	4/4	0.92	0.11	42,43,44,44	0
2	SO4	A	1211	5/5	0.96	0.09	28,28,35,38	5
2	SO4	B	1211	5/5	0.96	0.09	28,31,37,41	5
2	SO4	A	1212	5/5	0.97	0.08	22,26,28,31	5
2	SO4	B	1212	5/5	0.97	0.07	24,29,31,36	5

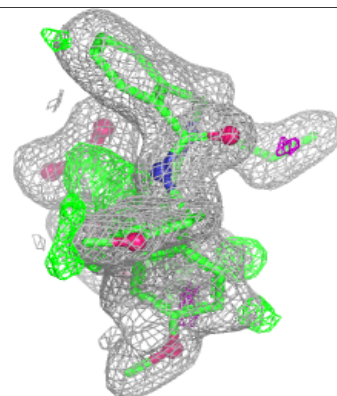
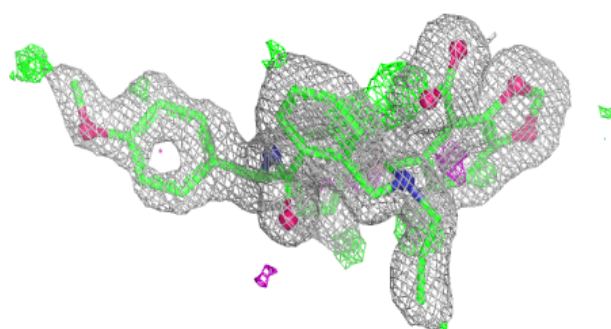
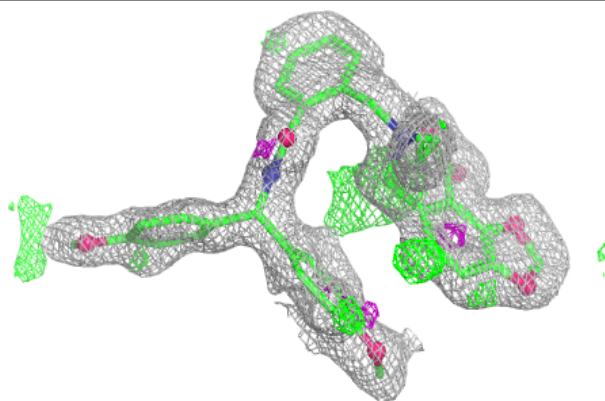
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around O2N A 1219:

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

**Electron density around O2N B 1217:**

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



4.5 Other polymers [i](#)

There are no such residues in this entry.