Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2021 – 01:27 PM EST

PDB ID	:	7L2Y
Title	:	HIV Integrase core domain in complex with inhibitor 2-(5-(3-fluorophenyl)-2-(2-(thiophen-2-yl)ethynyl)-1- benzofuran-3-yl)ethanoic acid
Authors	:	Gorman, M.A.; Parker, M.W.
Deposited on	:	2020-12-17
Resolution	:	1.98 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:

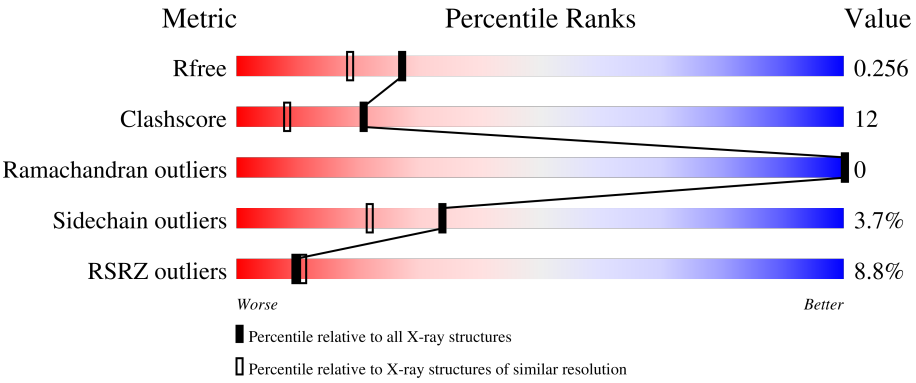
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	AAA	162	7% 66% 19% 14%

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	IOD	AAA	306	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	AAA	307	-	-	X	-
3	IOD	AAA	308	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1170 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.

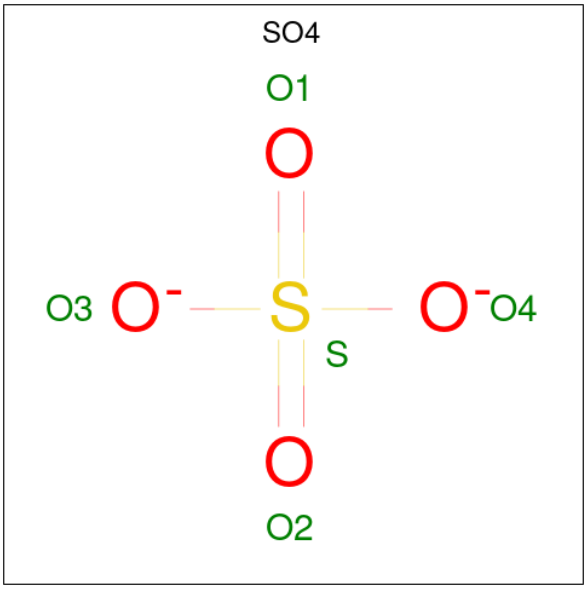
- Molecule 1 is a protein called Integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	139	1078	684	187	204	3	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	53	GLU	GLN	conflict	UNP F2WR52
AAA	56	SER	CYS	conflict	UNP F2WR52
AAA	131	GLU	TRP	conflict	UNP F2WR52
AAA	?	-	MET	deletion	UNP F2WR52
AAA	185	LYS	PHE	conflict	UNP F2WR52
AAA	209	GLU	GLN	conflict	UNP F2WR52

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

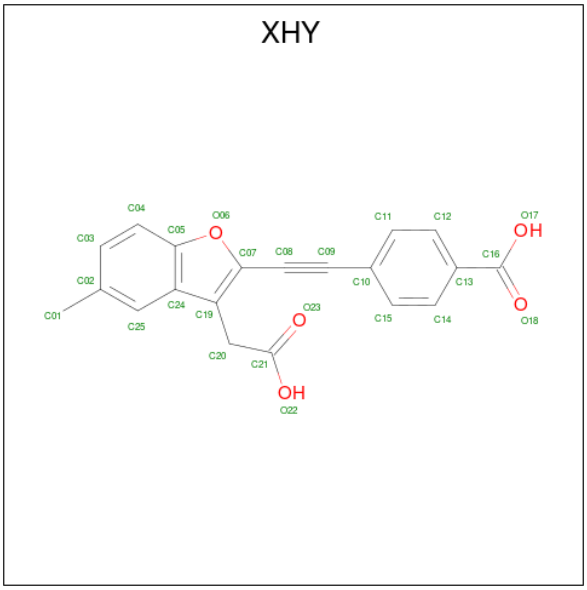


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total O S 5 4 1	0	0
2	AAA	1	Total O S 5 4 1	0	0
2	AAA	1	Total O S 5 4 1	0	0
2	AAA	1	Total O S 5 4 1	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	5	Total I 5 5	0	0

- Molecule 4 is 4-{[3-(carboxymethyl)-5-methyl-1-benzofuran-2-yl]ethynyl}benzoic acid (three-letter code: XHY) (formula: $C_{20}H_{14}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 25 20 5	0	0

- Molecule 5 is water.

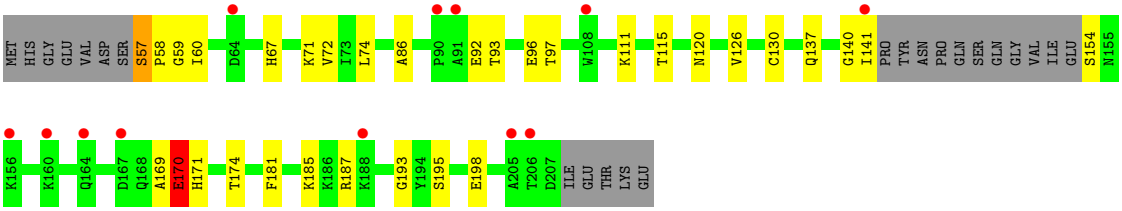
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	42	Total O 42 42	0	0

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: Integrase

Chain AAA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	45.98Å 45.98Å 138.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.62 – 1.98 32.62 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.62-1.98) 99.7 (32.62-1.98)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.249 0.217 , 0.256	Depositor DCC
R_{free} test set	835 reflections (7.59%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	1170	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OCS, XHY, SO4, IOD

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	AAA	0.74	0/1085	0.85	1/1463 (0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	170	GLU	CB-CA-C	5.34	121.08	110.40

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	AAA	1078	0	1087	27	0
2	AAA	20	0	0	1	0
3	AAA	5	0	0	7	0
4	AAA	25	0	0	0	0
5	AAA	42	0	0	1	1
All	All	1170	0	1087	27	1

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 12.

All (27) 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:AAA:137:GLN:NE2	3:AAA:306:IOD:I	2.42	1.23
1:AAA:187:ARG:CZ	1:AAA:193:GLY:O	2.43	0.67
1:AAA:93:THR:HG23	1:AAA:96:GLU:H	1.63	0.64
1:AAA:120[A]:ASN:HB3	1:AAA:137:GLN:HE22	1.61	0.64
1:AAA:126:VAL:O	1:AAA:130:OCS:OD3	2.17	0.63
1:AAA:67:HIS:CD2	1:AAA:72:VAL:HG22	2.35	0.62
1:AAA:57:SER:N	3:AAA:308:IOD:I	3.02	0.62
1:AAA:71:LYS:HE2	3:AAA:307:IOD:I	2.73	0.58
1:AAA:71:LYS:CE	3:AAA:307:IOD:I	3.22	0.57
1:AAA:195:SER:OG	1:AAA:198:GLU:HG3	2.06	0.56
1:AAA:115[A]:THR:HG21	5:AAA:419:HOH:O	2.06	0.54
1:AAA:57:SER:N	1:AAA:58:PRO:HD2	2.24	0.54
1:AAA:170:GLU:HG2	1:AAA:171:HIS:CD2	2.45	0.52
1:AAA:137:GLN:CD	3:AAA:306:IOD:I	3.18	0.52
1:AAA:120[B]:ASN:HB3	1:AAA:137:GLN:HE22	1.75	0.50
1:AAA:71:LYS:HE3	3:AAA:307:IOD:I	2.83	0.48
1:AAA:72:VAL:HG11	1:AAA:92:GLU:HG3	1.95	0.48
1:AAA:181:PHE:O	1:AAA:185:LYS:HG2	2.15	0.46
1:AAA:111:LYS:HD2	3:AAA:308:IOD:I	2.86	0.46
1:AAA:57:SER:HA	1:AAA:60:ILE:HG12	1.98	0.45
1:AAA:74:LEU:O	1:AAA:86:ALA:HA	2.16	0.45
1:AAA:140:GLY:HA3	2:AAA:310:SO4:O2	2.17	0.44
1:AAA:187:ARG:NH2	1:AAA:193:GLY:O	2.51	0.43
1:AAA:59:GLY:HA3	1:AAA:111:LYS:HD2	2.02	0.42
1:AAA:169:ALA:HB1	1:AAA:174:THR:HB	2.02	0.42
1:AAA:97:THR:HG21	1:AAA:120[B]:ASN:ND2	2.35	0.41
1:AAA:67:HIS:NE2	1:AAA:72:VAL:HG22	2.36	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AAA:434:HOH:O	5:AAA:436:HOH:O[7_545]	1.74	0.46

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	AAA	135/162 (83%)	132 (98%)	3 (2%)	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	AAA	111/130 (85%)	107 (96%)	4 (4%)	35 23

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	57	SER
1	AAA	141	ILE
1	AAA	154	SER
1	AAA	170	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OCS	AAA	65	1	2,7,9	0.85	0	2,8,13	1.27	0
1	OCS	AAA	130	1	2,7,9	0.83	0	2,8,13	0.58	0

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	OCS	AAA	65	1	-	0/3/6/9	-
1	OCS	AAA	130	1	-	1/3/6/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	130	OCS	CA-CB-SG-OD3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	130	OCS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	AAA	303	-	4,4,4	0.35	0	6,6,6	0.18	0
2	SO4	AAA	301	-	4,4,4	0.42	0	6,6,6	0.14	0
2	SO4	AAA	310	-	4,4,4	0.39	0	6,6,6	0.18	0
4	XHY	AAA	309	-	17,27,27	1.40	2 (11%)	21,38,38	1.85	4 (19%)
2	SO4	AAA	302	-	4,4,4	0.35	0	6,6,6	0.14	0

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
4	XHY	AAA	309	-	-	0/4/13/13	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	309	XHY	C13-C16	4.42	1.51	1.47
4	AAA	309	XHY	C10-C09	2.05	1.49	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AAA	309	XHY	C19-C20-C21	-4.63	106.94	115.96
4	AAA	309	XHY	C07-C19-C24	-4.16	104.35	109.56
4	AAA	309	XHY	C03-C02-C25	2.69	121.72	118.40
4	AAA	309	XHY	C02-C25-C24	-2.56	118.74	121.64

There are no chirality outliers.

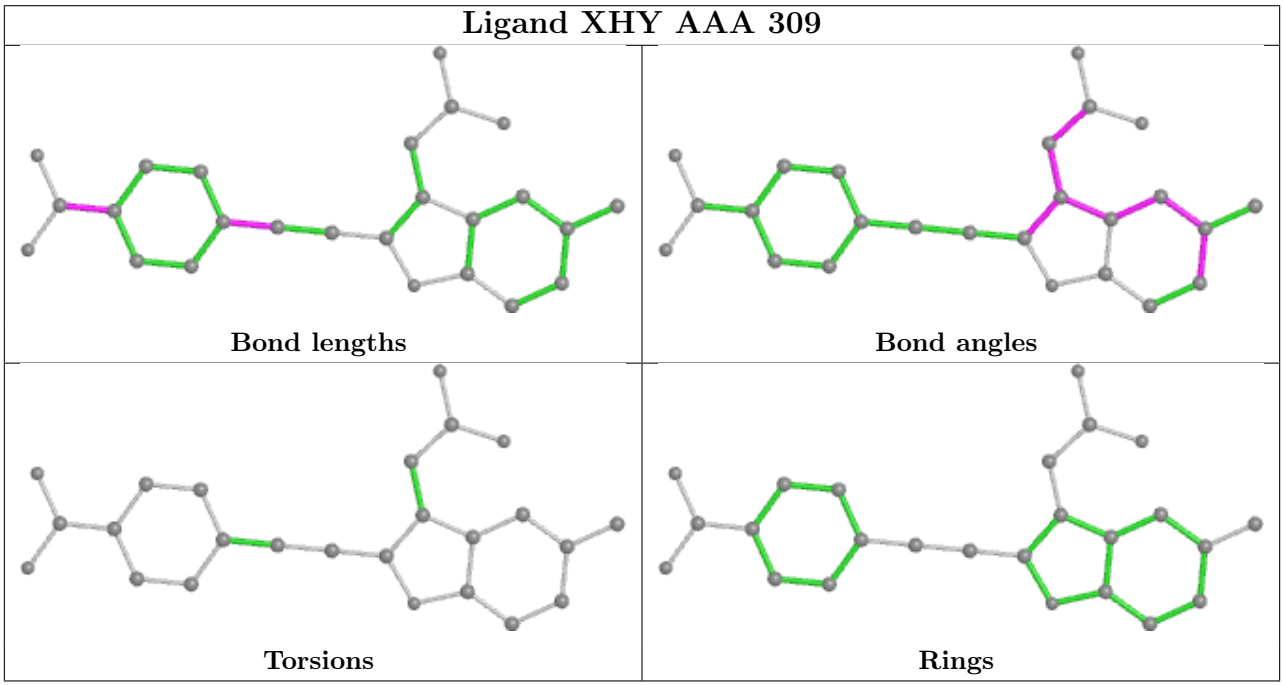
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	310	SO4	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 then 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^{th} 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	AAA	137/162 (84%)	0.71	12 (8%)	10	11	17, 31, 55, 68	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	141	ILE	5.9
1	AAA	167	ASP	4.2
1	AAA	156	LYS	3.4
1	AAA	160	LYS	3.3
1	AAA	90	PRO	3.3
1	AAA	91	ALA	3.2
1	AAA	64	ASP	2.6
1	AAA	164	GLN	2.6
1	AAA	188	LYS	2.3
1	AAA	108	TRP	2.3
1	AAA	205	ALA	2.3
1	AAA	206	THR	2.2

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^{th} 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^2)	Q<0.9
1	OCS	AAA	65	8/10	0.78	0.16	35,42,70,78	0
1	OCS	AAA	130	8/10	0.96	0.12	22,24,30,50	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

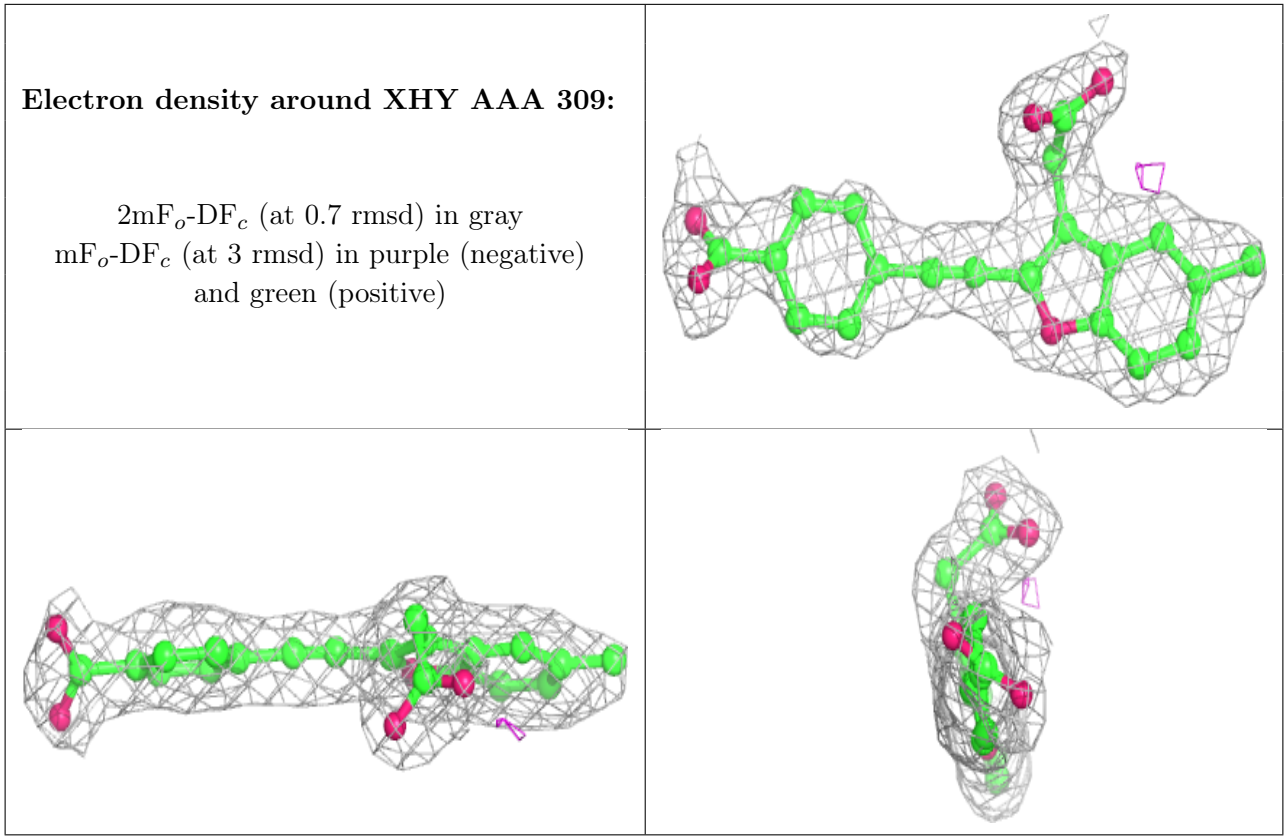
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	AAA	302	5/5	0.88	0.27	67,73,74,77	0
4	XHY	AAA	309	25/25	0.90	0.15	23,30,60,64	0
2	SO4	AAA	303	5/5	0.92	0.46	48,49,65,73	0
2	SO4	AAA	310	5/5	0.94	0.37	43,47,62,70	0
3	IOD	AAA	308	1/1	0.95	0.10	68,68,68,68	1
3	IOD	AAA	305	1/1	0.96	0.11	26,26,26,26	1
2	SO4	AAA	301	5/5	0.97	0.07	59,59,62,63	0
3	IOD	AAA	307	1/1	0.98	0.05	36,36,36,36	1
3	IOD	AAA	304	1/1	0.99	0.04	33,33,33,33	1
3	IOD	AAA	306	1/1	1.00	0.12	17,17,17,17	1

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 XHY AAA 309:

$2mF_o$-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.