



wwPDB X-ray Structure Validation Summary Report

Oct 10, 2023 – 12:13 AM EDT

PDB ID : 7RQ0
Title : HIV Integrase CORE domain in complex with 2-{2-[2-(3-{[4-(2-{{(3-{2-[3-(carboxymethyl)-5-methyl-1-benzofuran-2-yl]ethynyl}phenyl)methyl]amino}ethyl)piperazin-1-yl]methyl}phenyl)ethynyl]-5-methyl-1-benzofuran-3-yl}acetic acid
Authors : Gorman, M.A.; Parker, M.W.
Deposited on : 2021-08-05
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : ?? (??), CSD ??CSD?? (????)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

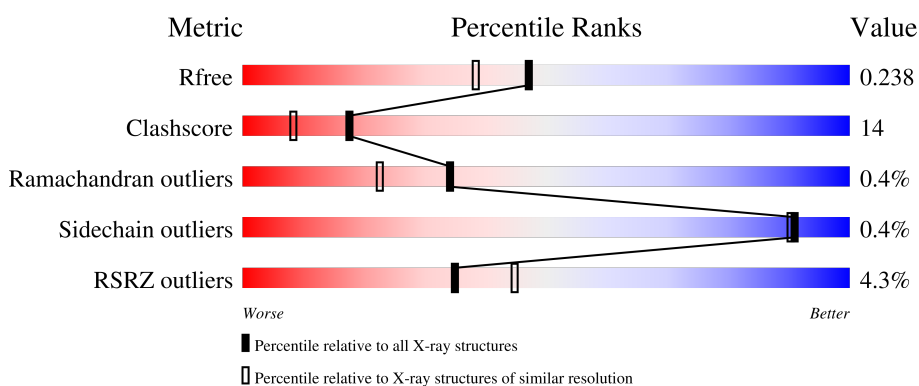
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 $\leq 5\%$. 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	163	 4% 57% 27% 16%
1	B	163	 4% 68% 16% •• 15%

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	A	303	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4413 atoms, of which 2133 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.

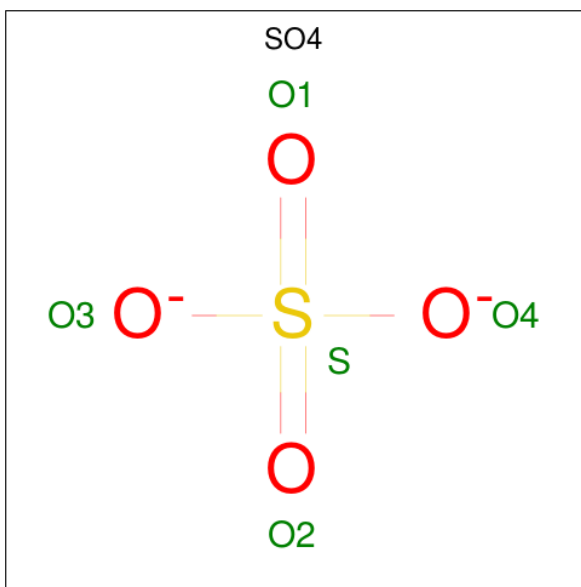
- Molecule 1 is a protein called Integrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	137	2109	674	1053	183	195	4	0	0	0
1	B	139	2155	687	1080	186	198	4	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	GLU	GLN	conflict	UNP Q76353
A	56	SER	CYS	conflict	UNP Q76353
A	131	GLU	TRP	conflict	UNP Q76353
A	185	LYS	PHE	conflict	UNP Q76353
A	209	GLU	GLN	conflict	UNP Q76353
B	53	GLU	GLN	conflict	UNP Q76353
B	56	SER	CYS	conflict	UNP Q76353
B	131	GLU	TRP	conflict	UNP Q76353
B	185	LYS	PHE	conflict	UNP Q76353
B	209	GLU	GLN	conflict	UNP Q76353

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

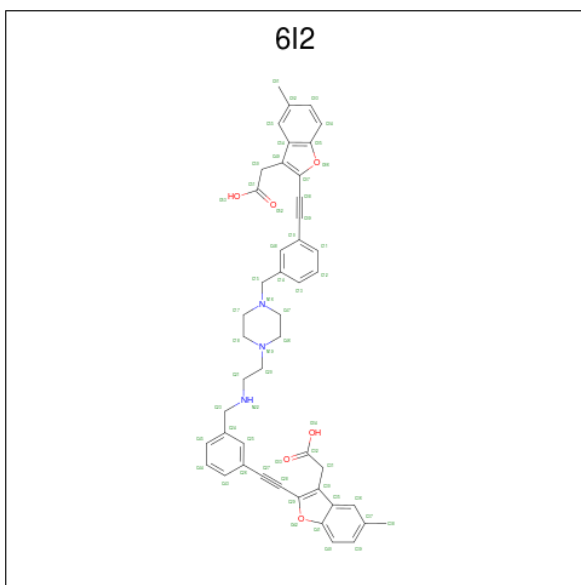


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total I 3 3	0	0
3	B	2	Total I 2 2	0	0

- Molecule 4 is {2-[(3-{[4-(2-{[(3-{[3-(carboxymethyl)-5-methyl-1-benzofuran-2-yl]ethynyl}phenyl)methyl]amino}ethyl)piperazin-1-yl]methyl}phenyl)ethynyl]-5-methyl-1-benzofuran-3-yl}acetic acid (three-letter code: 6I2) (formula: C₄₆H₄₃N₃O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	55	46	3	6	0	0

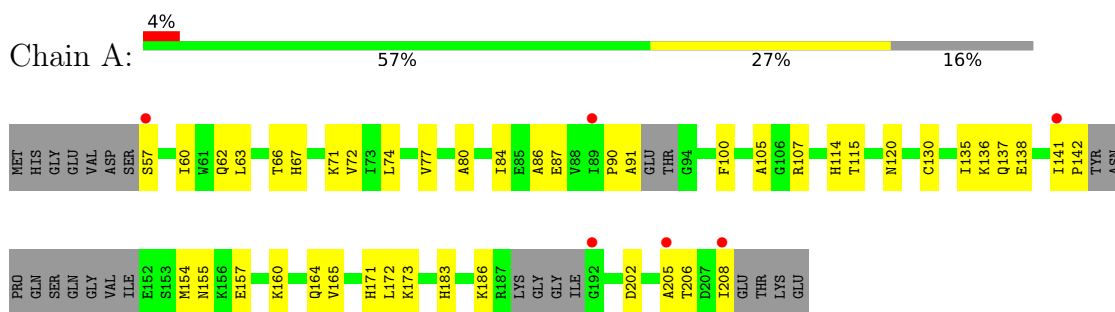
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	33	33	33	0	0
5	B	26	26	26	0	0

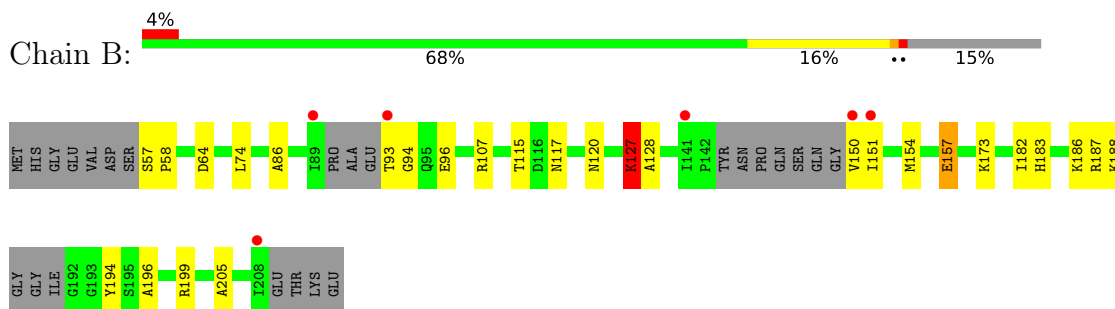
3 Residue-property plots [i](#)

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



- Molecule 1: Integrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	46.42Å 46.42Å 138.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.54 – 1.95 46.42 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.54-1.95) 92.8 (46.42-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 1.95Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.230 , 0.270 0.239 , 0.238	Depositor DCC
R_{free} test set	1994 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.007	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4413	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.01% 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: 6I2, 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	A	0.53	1/1074 (0.1%)	0.78	2/1449 (0.1%)
1	B	0.65	3/1092 (0.3%)	1.43	6/1472 (0.4%)
All	All	0.60	4/2166 (0.2%)	1.16	8/2921 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	GLU	CB-CG	9.92	1.71	1.52
1	B	157	GLU	CD-OE1	9.51	1.36	1.25
1	B	157	GLU	CD-OE2	7.20	1.33	1.25
1	A	136	LYS	CE-NZ	6.64	1.65	1.49

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	GLU	OE1-CD-OE2	-35.80	80.34	123.30
1	B	157	GLU	CG-CD-OE2	-21.49	75.31	118.30
1	B	157	GLU	CG-CD-OE1	16.93	152.16	118.30
1	B	127	LYS	CD-CE-NZ	-13.13	81.50	111.70
1	B	127	LYS	CB-CG-CD	-10.00	85.60	111.60

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	1056	1053	1065	38	0
1	B	1075	1080	1093	25	0
2	A	10	0	0	0	0
2	B	20	0	0	0	0
3	A	3	0	0	9	0
3	B	2	0	0	1	0
4	B	55	0	0	0	0
5	A	33	0	0	0	0
5	B	26	0	0	2	0
All	All	2280	2133	2158	60	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 14.

The worst 5 of 60 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:B:127:LYS:HD2	1:B:127:LYS:C	1.82	1.00
1:B:117:ASN:ND2	5:B:401:HOH:O	2.06	0.88
1:A:173:LYS:HE3	3:A:303:IOD:I	2.48	0.83
1:A:173:LYS:NZ	3:A:303:IOD:I	2.86	0.78
1:B:173:LYS:HG3	3:B:307:IOD:I	2.56	0.75

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	129/163 (79%)	127 (98%)	2 (2%)	0	100 100
1	B	131/163 (80%)	128 (98%)	2 (2%)	1 (1%)	19 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	260/326 (80%)	255 (98%)	4 (2%)	1 (0%)	34 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	GLY

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	111/133 (84%)	111 (100%)	0	100 100
1	B	114/133 (86%)	113 (99%)	1 (1%)	78 77
All	All	225/266 (85%)	224 (100%)	1 (0%)	91 90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

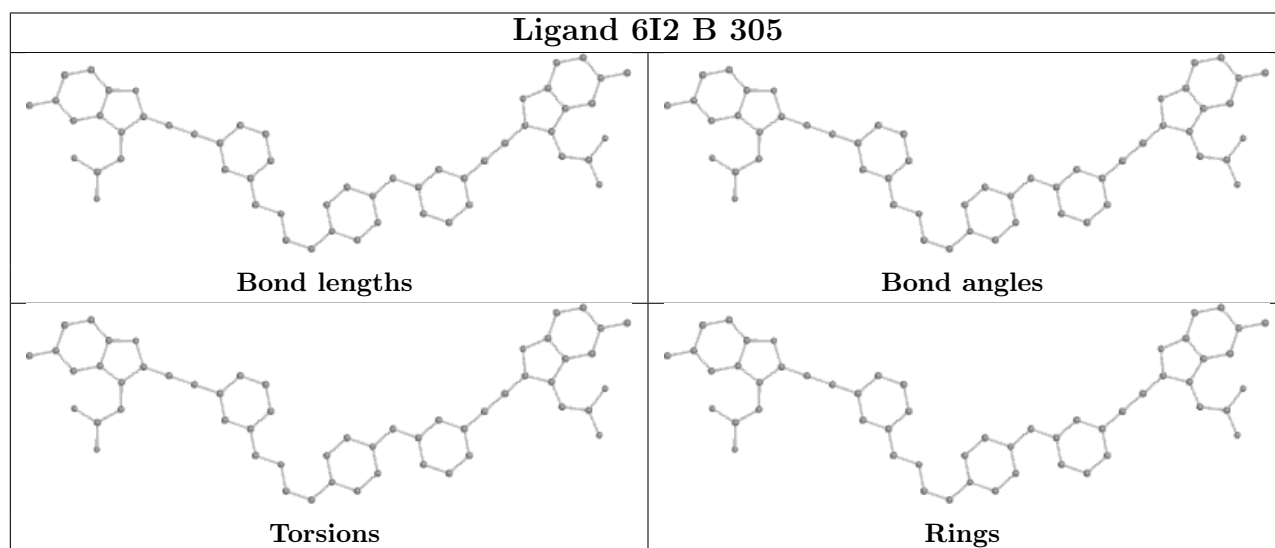
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	137/163 (84%)	0.34	6 (4%) 34 44	21, 36, 66, 100	0
1	B	139/163 (85%)	0.39	6 (4%) 35 45	22, 36, 69, 127	0
All	All	276/326 (84%)	0.37	12 (4%) 35 45	21, 36, 67, 127	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	ILE	8.2
1	B	150	VAL	4.4
1	A	57	SER	4.4
1	B	89	ILE	3.3
1	A	208	ILE	3.3

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](#)

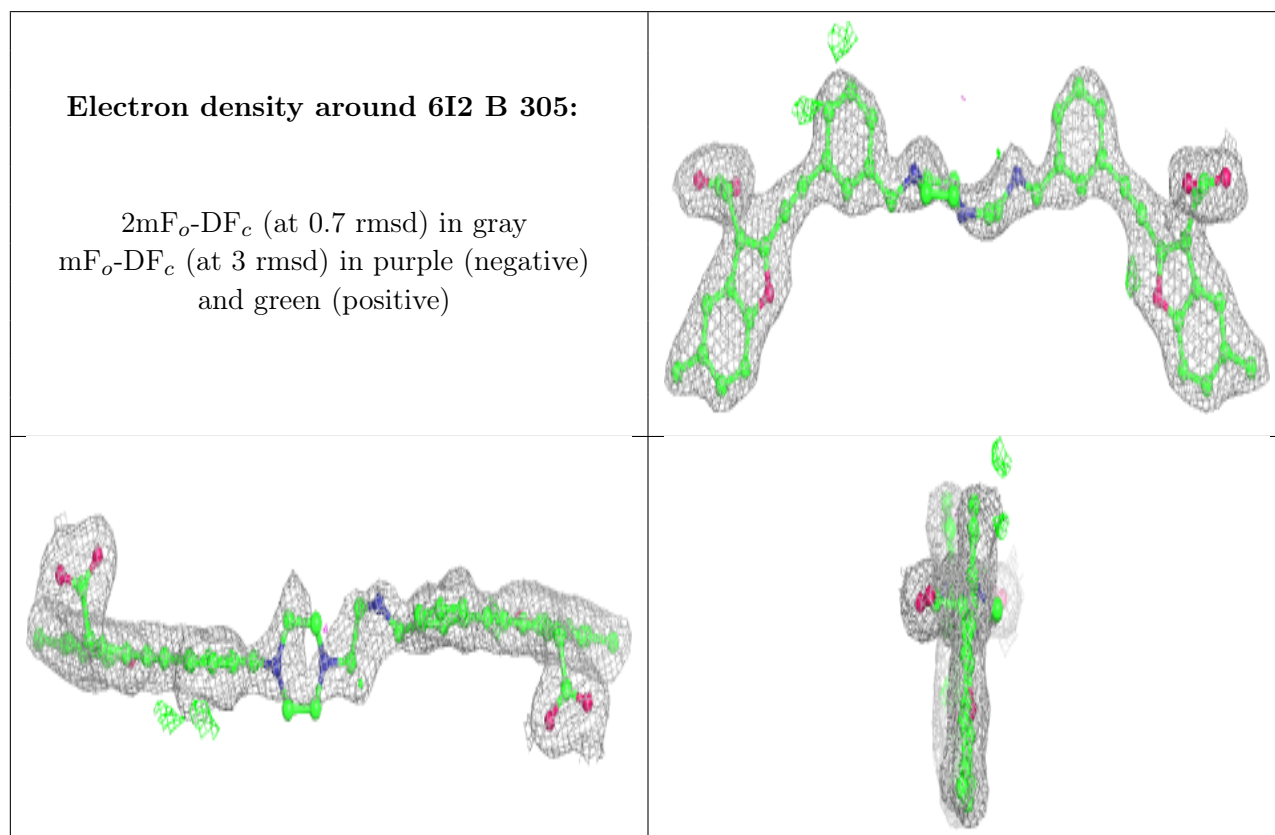
There are no monosaccharides in this entry.

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, 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	SO4	B	303	5/5	0.85	0.21	65,67,79,90	0
3	IOD	A	303	1/1	0.89	0.13	78,78,78,78	0
2	SO4	B	302	5/5	0.91	0.16	64,71,77,85	0
4	6I2	B	305	55/55	0.92	0.16	30,40,66,73	0
3	IOD	B	307	1/1	0.94	0.06	62,62,62,62	0
2	SO4	A	301	5/5	0.94	0.10	57,66,78,90	0
2	SO4	B	304	5/5	0.95	0.10	61,68,75,75	0
2	SO4	B	301	5/5	0.96	0.10	59,67,72,75	0
2	SO4	A	302	5/5	0.97	0.11	58,61,70,84	0
3	IOD	B	306	1/1	0.98	0.05	45,45,45,45	0
3	IOD	A	304	1/1	0.98	0.05	47,47,47,47	0
3	IOD	A	305	1/1	0.98	0.04	66,66,66,66	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.