



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:55 PM UTC

PDB ID : 7ZIW / pdb_00007ziw
Title : X-ray structure of the haloalkane dehalogenase HaloTag7 bound to a butyltri fluoromethanesulfonamide tetramethylrhodamine ligand (TMR-T4)
Authors : Tarnawski, M.; Kompa, J.; Johnsson, K.; Hiblot, J.
Deposited on : 2022-04-08
Resolution : 1.99 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

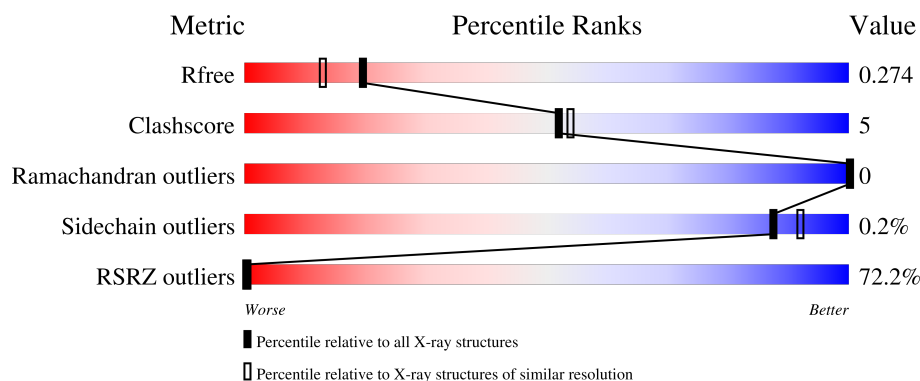
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	293	74% 90% 10%
1	B	293	71% 86% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4996 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 Haloalkane dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2350	1528	395	418	9			
1	B	293	Total	C	N	O	S	0	0	0
			2350	1528	395	418	9			

There are 48 discrepancies between the modelled and reference sequences:

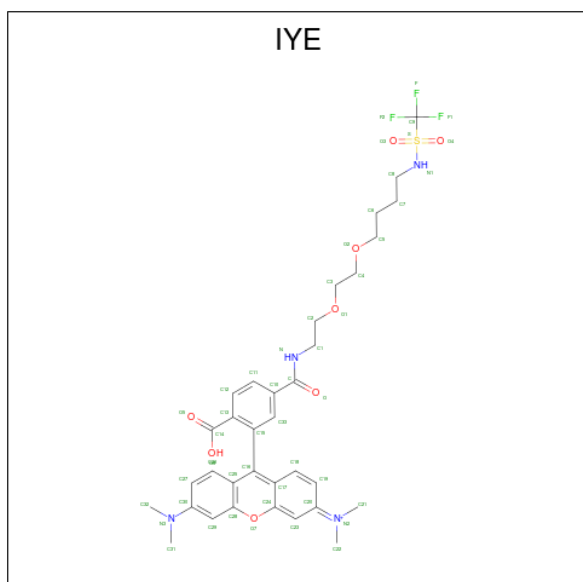
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P0A3G3
A	47	VAL	LEU	engineered mutation	UNP P0A3G3
A	58	THR	SER	engineered mutation	UNP P0A3G3
A	78	GLY	ASP	engineered mutation	UNP P0A3G3
A	87	PHE	TYR	engineered mutation	UNP P0A3G3
A	88	MET	LEU	engineered mutation	UNP P0A3G3
A	128	PHE	CYS	engineered mutation	UNP P0A3G3
A	155	THR	ALA	engineered mutation	UNP P0A3G3
A	160	LYS	GLU	engineered mutation	UNP P0A3G3
A	167	VAL	ALA	engineered mutation	UNP P0A3G3
A	172	THR	ALA	engineered mutation	UNP P0A3G3
A	175	MET	LYS	engineered mutation	UNP P0A3G3
A	176	GLY	CYS	engineered mutation	UNP P0A3G3
A	195	ASN	LYS	engineered mutation	UNP P0A3G3
A	224	GLU	ALA	engineered mutation	UNP P0A3G3
A	227	ASP	ASN	engineered mutation	UNP P0A3G3
A	257	LYS	GLU	engineered mutation	UNP P0A3G3
A	264	ALA	THR	engineered mutation	UNP P0A3G3
A	272	ASN	HIS	engineered mutation	UNP P0A3G3
A	273	LEU	TYR	engineered mutation	UNP P0A3G3
A	291	SER	PRO	engineered mutation	UNP P0A3G3
A	292	THR	ALA	engineered mutation	UNP P0A3G3
A	294	GLU	-	expression tag	UNP P0A3G3
A	295	ILE	-	expression tag	UNP P0A3G3
B	3	GLY	-	expression tag	UNP P0A3G3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	VAL	LEU	engineered mutation	UNP P0A3G3
B	58	THR	SER	engineered mutation	UNP P0A3G3
B	78	GLY	ASP	engineered mutation	UNP P0A3G3
B	87	PHE	TYR	engineered mutation	UNP P0A3G3
B	88	MET	LEU	engineered mutation	UNP P0A3G3
B	128	PHE	CYS	engineered mutation	UNP P0A3G3
B	155	THR	ALA	engineered mutation	UNP P0A3G3
B	160	LYS	GLU	engineered mutation	UNP P0A3G3
B	167	VAL	ALA	engineered mutation	UNP P0A3G3
B	172	THR	ALA	engineered mutation	UNP P0A3G3
B	175	MET	LYS	engineered mutation	UNP P0A3G3
B	176	GLY	CYS	engineered mutation	UNP P0A3G3
B	195	ASN	LYS	engineered mutation	UNP P0A3G3
B	224	GLU	ALA	engineered mutation	UNP P0A3G3
B	227	ASP	ASN	engineered mutation	UNP P0A3G3
B	257	LYS	GLU	engineered mutation	UNP P0A3G3
B	264	ALA	THR	engineered mutation	UNP P0A3G3
B	272	ASN	HIS	engineered mutation	UNP P0A3G3
B	273	LEU	TYR	engineered mutation	UNP P0A3G3
B	291	SER	PRO	engineered mutation	UNP P0A3G3
B	292	THR	ALA	engineered mutation	UNP P0A3G3
B	294	GLU	-	expression tag	UNP P0A3G3
B	295	ILE	-	expression tag	UNP P0A3G3

- Molecule 2 is [9-[2-carboxy-5-[2-[2-[4-(trifluoromethylsulfonylamino)butoxy]ethoxy]ethylcarbamoyl]phenyl]-6-(dimethylamino)xanthen-3-ylidene]-dimethyl-azanium (CCD ID: IYE) (formula: C₃₄H₄₀F₃N₄O₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			50	34	3	4	8	1		
2	B	1	Total	C	F	N	O	S	0	0
			50	34	3	4	8	1		

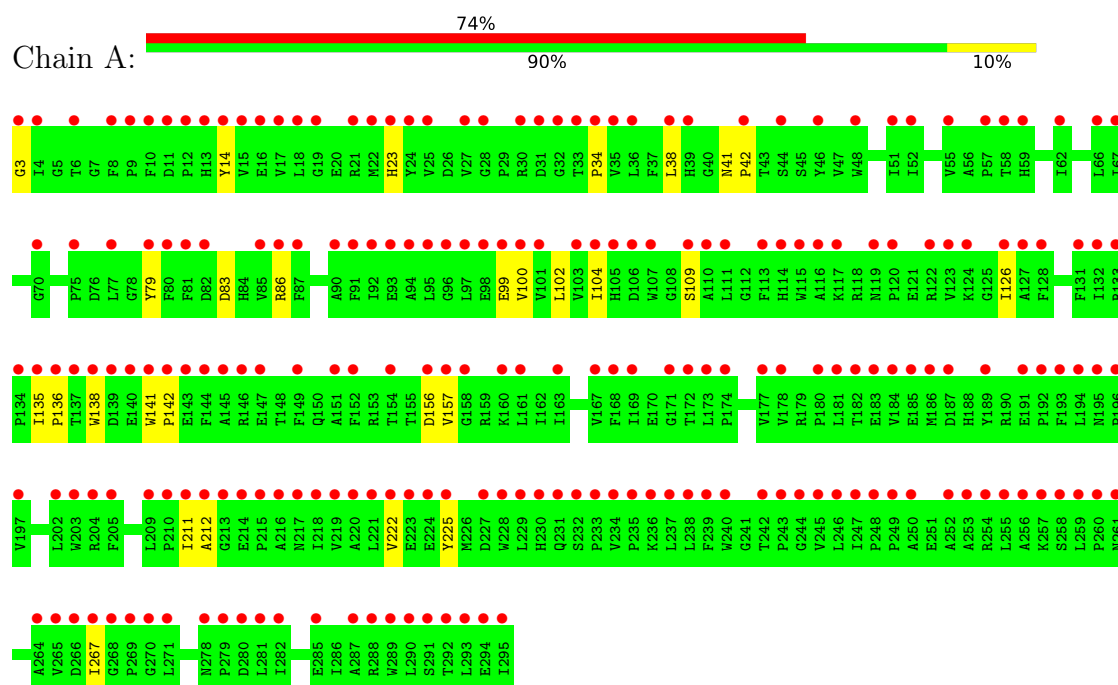
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total	O	0	0
			98	98		
3	B	98	Total	O	0	0
			98	98		

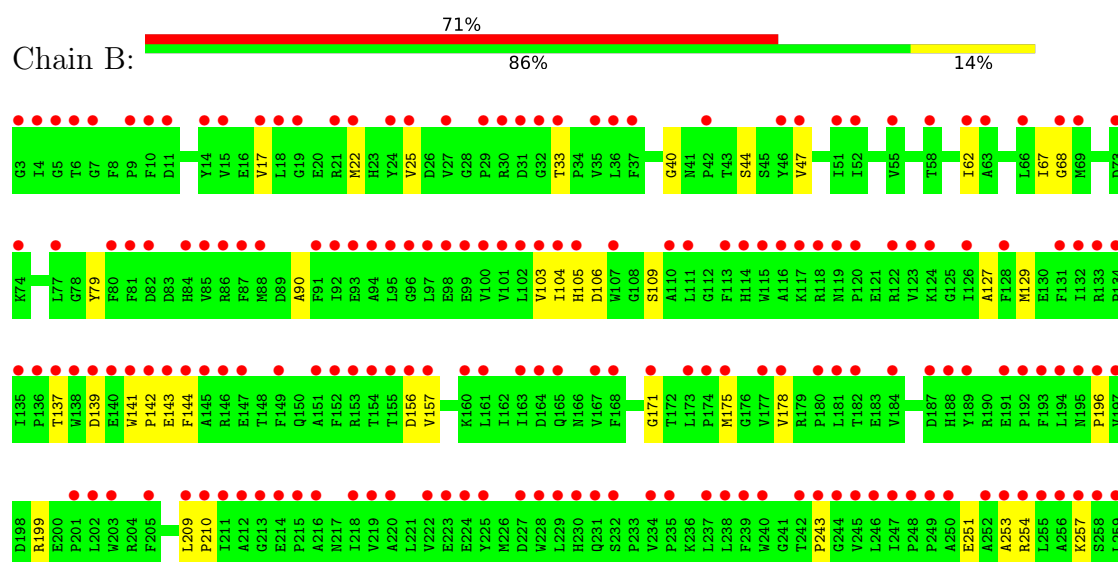
3 Residue-property plots

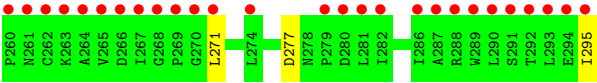
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Haloalkane dehalogenase



• Molecule 1: Haloalkane dehalogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.17Å 49.80Å 78.72Å 71.51° 89.95° 67.99°	Depositor
Resolution (Å)	44.68 – 1.99 44.68 – 1.99	Depositor EDS
% Data completeness (in resolution range)	75.0 (44.68-1.99) 75.1 (44.68-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.248 , 0.274 0.247 , 0.274	Depositor DCC
R_{free} test set	1557 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4996	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.45% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IYE

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	0.17	0/2429	0.38	0/3320
1	B	0.17	0/2429	0.40	0/3320
All	All	0.17	0/4858	0.39	0/6640

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

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	2350	0	2291	18	0
1	B	2350	0	2291	30	0
2	A	50	0	0	0	0
2	B	50	0	0	1	0
3	A	98	0	0	3	0
3	B	98	0	0	1	0
All	All	4996	0	4582	48	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 5.

All (48) 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:137:THR:HG22	1:B:139:ASP:H	1.43	0.83
1:A:135:ILE:HB	1:A:211:ILE:HD12	1.72	0.72
1:A:99:GLU:H	1:A:99:GLU:CD	2.04	0.66
1:B:209:LEU:HD12	1:B:210:PRO:HD2	1.79	0.64
1:B:175:MET:HE3	2:B:301:IYE:C26	2.27	0.63
1:B:143:GLU:HG3	1:B:144:PHE:N	2.17	0.60
1:B:33:THR:HG21	1:B:295:ILE:HB	1.84	0.60
1:B:178:VAL:HB	1:B:277:ASP:OD1	2.10	0.52
1:B:243:PRO:HD2	1:B:271:LEU:HD22	1.93	0.51
1:B:251:GLU:OE1	1:B:254:ARG:NH2	2.45	0.50
1:B:253:ALA:O	1:B:257:LYS:HG3	2.12	0.50
1:A:3:GLY:N	3:A:410:HOH:O	2.45	0.49
1:A:3:GLY:N	3:A:409:HOH:O	2.44	0.49
1:B:171:GLY:O	1:B:175:MET:HG3	2.13	0.49
1:B:104:ILE:HB	1:B:109:SER:HA	1.95	0.49
1:A:104:ILE:HB	1:A:109:SER:HA	1.95	0.48
1:B:33:THR:CG2	1:B:295:ILE:HB	2.42	0.48
1:B:141:TRP:CG	1:B:142:PRO:HD2	2.48	0.48
1:A:156:ASP:OD1	1:A:157:VAL:N	2.42	0.48
1:B:196:PRO:HA	1:B:199:ARG:HD2	1.96	0.48
1:A:83:ASP:OD1	1:A:86:ARG:NH2	2.44	0.47
1:B:156:ASP:OD1	1:B:157:VAL:N	2.45	0.47
1:B:104:ILE:HD12	1:B:109:SER:HA	1.97	0.47
1:B:40:GLY:HA3	1:B:106:ASP:HB3	1.96	0.46
1:B:178:VAL:HG23	1:B:271:LEU:HD23	1.98	0.46
1:B:22:MET:HE2	1:B:22:MET:HB3	1.80	0.46
1:A:104:ILE:HD12	1:A:109:SER:HA	1.99	0.45
1:B:178:VAL:CG2	1:B:271:LEU:HD23	2.46	0.45
1:A:141:TRP:CG	1:A:142:PRO:HD2	2.52	0.44
1:B:103:VAL:HG22	1:B:127:ALA:HB3	2.00	0.44
1:A:79:TYR:HB3	3:A:420:HOH:O	2.18	0.44
1:B:44:SER:O	1:B:47:VAL:HG12	2.17	0.44
1:A:38:LEU:HB2	1:A:104:ILE:HG22	1.99	0.44
1:B:68:GLY:HA3	1:B:79:TYR:CE1	2.53	0.44
1:A:136:PRO:O	1:A:212:ALA:HA	2.18	0.43
1:B:17:VAL:HG13	1:B:90:ALA:HB3	2.00	0.43
1:A:34:PRO:HG2	1:A:100:VAL:HG12	2.00	0.43
1:A:138:TRP:CZ2	1:A:211:ILE:HG21	2.53	0.43
1:B:277:ASP:OD2	3:B:401:HOH:O	2.22	0.42
1:A:14:TYR:CE2	1:A:23:HIS:HB2	2.54	0.42
1:A:102:LEU:HB2	1:A:126:ILE:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:HIS:HD2	1:B:129:MET:O	2.03	0.41
1:B:137:THR:HG22	1:B:139:ASP:N	2.23	0.41
1:A:222:VAL:HG13	1:A:225:TYR:CZ	2.55	0.41
1:B:25:VAL:O	1:B:62:ILE:HA	2.21	0.41
1:B:141:TRP:CD2	1:B:142:PRO:HD2	2.56	0.41
1:A:41:ASN:HA	1:A:42:PRO:HA	1.89	0.40
1:B:67:ILE:HD12	1:B:67:ILE:HA	1.86	0.40

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	291/293 (99%)	278 (96%)	13 (4%)	0	100	100
1	B	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
All	All	582/586 (99%)	558 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	252/252 (100%)	251 (100%)	1 (0%)	84	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	252/252 (100%)	252 (100%)	0	100	100
All	All	504/504 (100%)	503 (100%)	1 (0%)	87	92

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

Mol	Chain	Res	Type
1	A	267	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	B	13	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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
2	IYE	B	301	-	53,53,53	0.55	0	76,76,76	0.58	1 (1%)
2	IYE	A	301	-	53,53,53	0.56	0	76,76,76	0.56	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
2	IYE	B	301	-	-	7/47/49/49	0/4/4/4
2	IYE	A	301	-	-	8/47/49/49	0/4/4/4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	IYE	C9-S-N1	2.01	106.93	105.45

There are no chirality outliers.

All (15) torsion outliers are listed below:

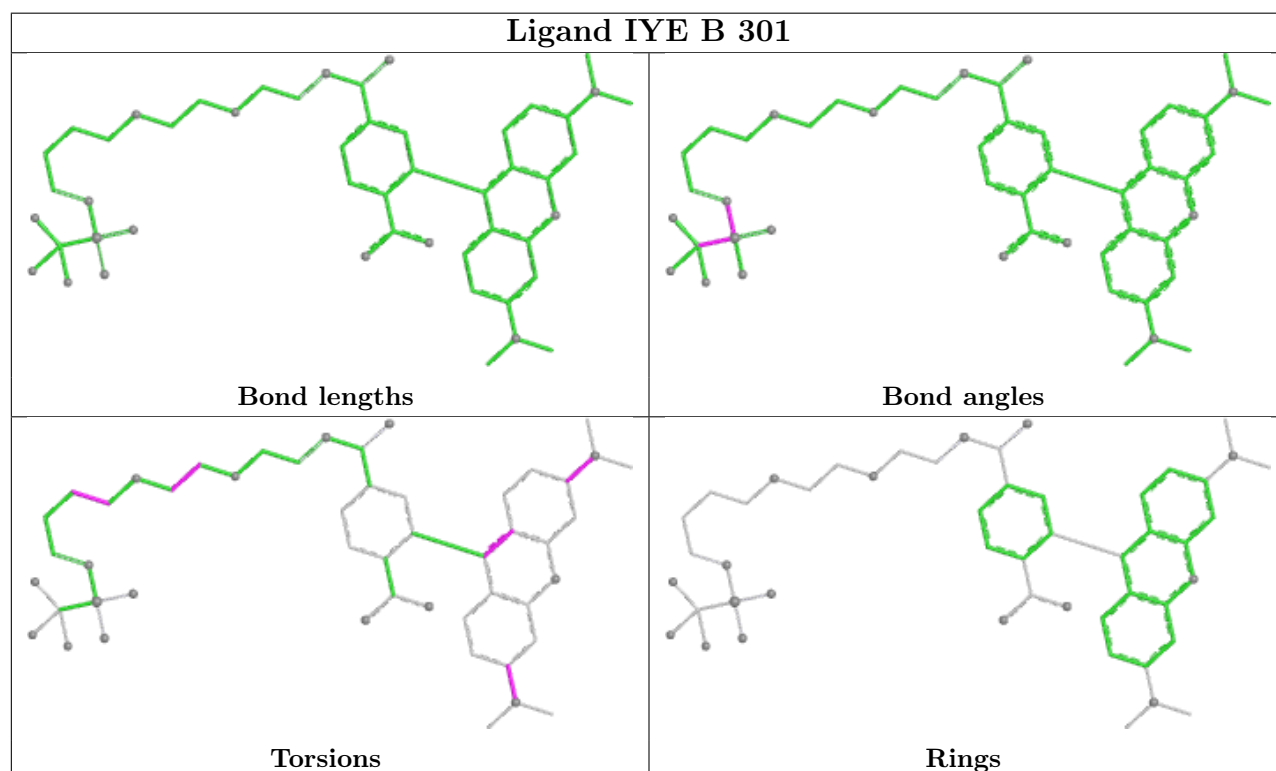
Mol	Chain	Res	Type	Atoms
2	A	301	IYE	C15-C16-C25-C26
2	A	301	IYE	C17-C16-C25-C26
2	B	301	IYE	C15-C16-C25-C26
2	B	301	IYE	C17-C16-C25-C26
2	B	301	IYE	C23-C20-N2-C22
2	B	301	IYE	O1-C3-C4-O2
2	B	301	IYE	C19-C20-N2-C22
2	B	301	IYE	O2-C5-C6-C7
2	A	301	IYE	C23-C20-N2-C22
2	A	301	IYE	C8-N1-S-O3
2	A	301	IYE	C3-C4-O2-C5
2	A	301	IYE	O1-C3-C4-O2
2	A	301	IYE	C19-C20-N2-C22
2	B	301	IYE	C27-C30-N3-C32
2	A	301	IYE	C1-C2-O1-C3

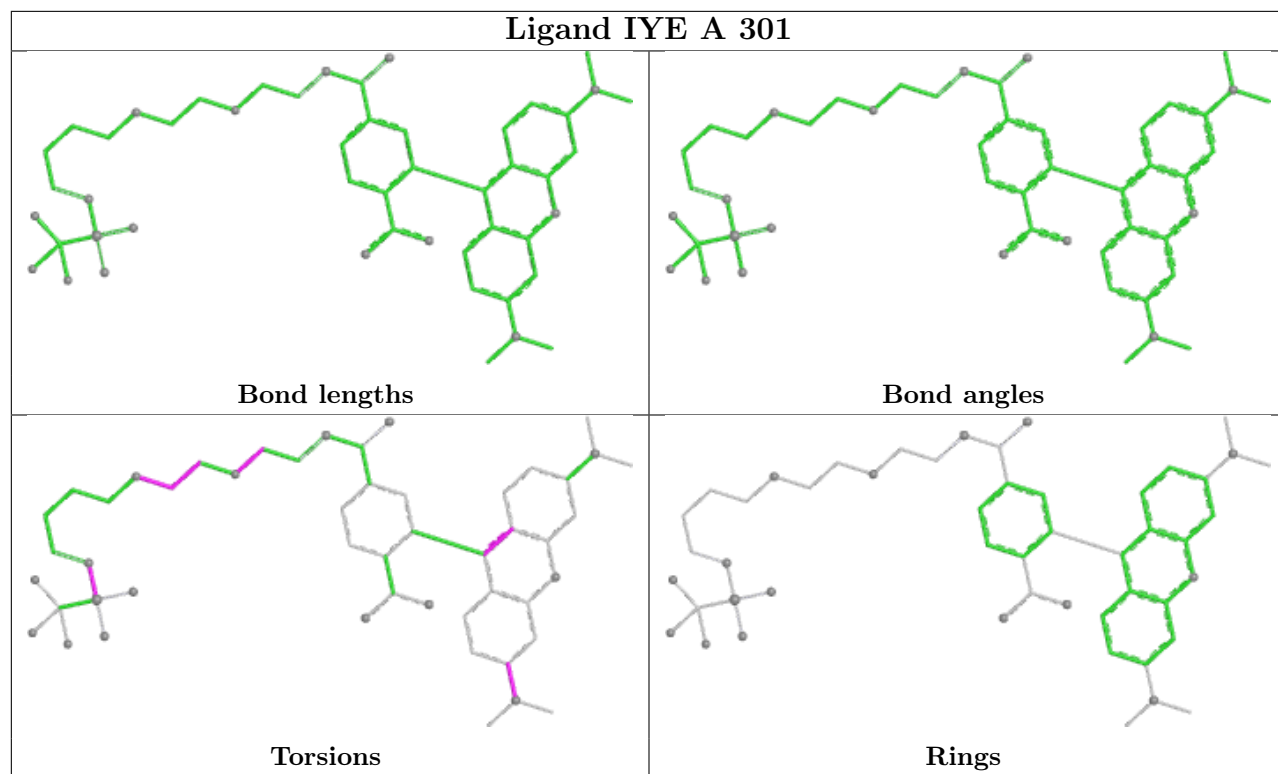
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	IYE	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	293/293 (100%)	2.80	216 (73%) 0 0	28, 39, 53, 76	0
1	B	293/293 (100%)	2.72	207 (70%) 0 0	29, 39, 52, 65	0
All	All	586/586 (100%)	2.76	423 (72%) 0 0	28, 39, 53, 76	0

All (423) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	LEU	8.6
1	B	295	ILE	6.2
1	A	295	ILE	6.1
1	A	291	SER	5.9
1	A	137	THR	5.9
1	A	209	LEU	5.8
1	A	265	VAL	5.8
1	A	167	VAL	5.7
1	B	178	VAL	5.6
1	A	257	LYS	5.6
1	A	256	ALA	5.5
1	A	144	PHE	5.3
1	B	3	GLY	5.3
1	B	31	ASP	5.3
1	B	291	SER	5.2
1	A	99	GLU	5.2
1	B	265	VAL	5.1
1	A	138	TRP	5.1
1	B	30	ARG	5.1
1	A	141	TRP	5.0
1	B	99	GLU	5.0
1	B	140	GLU	4.9
1	B	255	LEU	4.9
1	A	135	ILE	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	142	PRO	4.8
1	A	240	TRP	4.8
1	B	211	ILE	4.8
1	B	141	TRP	4.7
1	A	231	GLN	4.6
1	A	227	ASP	4.6
1	B	254	ARG	4.6
1	A	229	LEU	4.6
1	A	12	PRO	4.6
1	B	294	GLU	4.5
1	A	80	PHE	4.5
1	B	197	VAL	4.5
1	A	254	ARG	4.5
1	A	178	VAL	4.5
1	A	253	ALA	4.4
1	A	228	TRP	4.4
1	B	107	TRP	4.4
1	B	228	TRP	4.4
1	A	246	LEU	4.4
1	A	248	PRO	4.4
1	B	123	VAL	4.3
1	A	282	ILE	4.3
1	A	197	VAL	4.3
1	A	211	ILE	4.3
1	B	4	ILE	4.3
1	B	212	ALA	4.3
1	B	136	PRO	4.3
1	A	182	THR	4.3
1	A	3	GLY	4.2
1	A	31	ASP	4.2
1	B	98	GLU	4.2
1	B	143	GLU	4.2
1	A	259	LEU	4.2
1	A	149	PHE	4.2
1	B	234	VAL	4.2
1	A	252	ALA	4.2
1	B	94	ALA	4.2
1	B	147	GLU	4.2
1	B	149	PHE	4.1
1	B	137	THR	4.1
1	B	167	VAL	4.1
1	B	142	PRO	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	32	GLY	4.1
1	A	194	LEU	4.1
1	B	115	TRP	4.0
1	B	33	THR	4.0
1	A	116	ALA	4.0
1	B	214	GLU	4.0
1	A	62	ILE	4.0
1	B	15	VAL	4.0
1	B	287	ALA	4.0
1	B	263	LYS	3.9
1	A	173	LEU	3.9
1	B	288	ARG	3.9
1	A	210	PRO	3.9
1	A	264	ALA	3.9
1	B	100	VAL	3.9
1	B	135	ILE	3.9
1	B	195	ASN	3.9
1	B	259	LEU	3.9
1	A	225	TYR	3.9
1	A	33	THR	3.9
1	A	131	PHE	3.9
1	A	205	PHE	3.9
1	A	293	LEU	3.8
1	B	229	LEU	3.8
1	A	168	PHE	3.8
1	A	14	TYR	3.8
1	B	209	LEU	3.8
1	A	107	TRP	3.8
1	B	86	ARG	3.8
1	B	95	LEU	3.8
1	A	110	ALA	3.8
1	A	288	ARG	3.8
1	B	213	GLY	3.7
1	A	143	GLU	3.7
1	B	52	ILE	3.7
1	B	126	ILE	3.7
1	A	81	PHE	3.7
1	A	242	THR	3.7
1	B	182	THR	3.7
1	B	113	PHE	3.7
1	B	131	PHE	3.7
1	B	7	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	116	ALA	3.7
1	A	98	GLU	3.7
1	B	224	GLU	3.7
1	B	138	TRP	3.7
1	A	77	LEU	3.6
1	A	103	VAL	3.6
1	B	248	PRO	3.6
1	A	181	LEU	3.6
1	B	252	ALA	3.6
1	B	24	TYR	3.6
1	A	4	ILE	3.6
1	A	258	SER	3.6
1	A	113	PHE	3.6
1	A	21	ARG	3.6
1	A	238	LEU	3.6
1	B	18	LEU	3.6
1	B	97	LEU	3.6
1	A	132	ILE	3.5
1	B	282	ILE	3.5
1	B	157	VAL	3.5
1	B	253	ALA	3.5
1	B	281	LEU	3.5
1	A	280	ASP	3.5
1	B	139	ASP	3.5
1	A	260	PRO	3.5
1	A	163	ILE	3.5
1	A	94	ALA	3.5
1	B	19	GLY	3.5
1	A	139	ASP	3.5
1	A	214	GLU	3.5
1	B	17	VAL	3.5
1	B	36	LEU	3.5
1	B	271	LEU	3.5
1	A	249	PRO	3.4
1	A	151	ALA	3.4
1	B	267	ILE	3.4
1	B	194	LEU	3.4
1	B	210	PRO	3.4
1	B	124	LYS	3.4
1	A	145	ALA	3.4
1	A	220	ALA	3.4
1	B	152	PHE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	117	LYS	3.3
1	B	163	ILE	3.3
1	A	17	VAL	3.3
1	A	136	PRO	3.3
1	A	147	GLU	3.3
1	A	224	GLU	3.3
1	B	258	SER	3.3
1	B	51	ILE	3.3
1	B	91	PHE	3.3
1	B	219	VAL	3.3
1	B	246	LEU	3.3
1	A	120	PRO	3.3
1	A	93	GLU	3.2
1	A	250	ALA	3.2
1	A	38	LEU	3.2
1	B	292	THR	3.2
1	B	261	ASN	3.2
1	B	240	TRP	3.2
1	B	216	ALA	3.2
1	A	290	LEU	3.2
1	A	261	ASN	3.2
1	A	91	PHE	3.2
1	A	268	GLY	3.2
1	B	145	ALA	3.2
1	B	191	GLU	3.2
1	B	223	GLU	3.2
1	A	196	PRO	3.2
1	B	42	PRO	3.2
1	B	269	PRO	3.2
1	A	95	LEU	3.2
1	A	270	GLY	3.2
1	A	294	GLU	3.2
1	B	203	TRP	3.1
1	B	119	ASN	3.1
1	B	160	LYS	3.1
1	A	9	PRO	3.1
1	B	134	PRO	3.1
1	A	25	VAL	3.1
1	B	181	LEU	3.1
1	A	6	THR	3.1
1	B	110	ALA	3.1
1	B	9	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	120	PRO	3.1
1	B	132	ILE	3.1
1	B	247	ILE	3.1
1	A	19	GLY	3.1
1	B	184	VAL	3.1
1	A	134	PRO	3.1
1	A	66	LEU	3.1
1	A	101	VAL	3.1
1	A	123	VAL	3.1
1	A	222	VAL	3.1
1	B	177	VAL	3.1
1	B	231	GLN	3.1
1	B	264	ALA	3.1
1	A	218	ILE	3.0
1	B	227	ASP	3.0
1	B	77	LEU	3.0
1	A	157	VAL	3.0
1	B	14	TYR	3.0
1	A	212	ALA	3.0
1	A	266	ASP	3.0
1	B	220	ALA	3.0
1	B	290	LEU	3.0
1	B	293	LEU	3.0
1	A	177	VAL	3.0
1	A	75	PRO	3.0
1	B	196	PRO	3.0
1	B	280	ASP	3.0
1	B	256	ALA	3.0
1	A	97	LEU	3.0
1	A	223	GLU	3.0
1	B	111	LEU	3.0
1	A	160	LYS	3.0
1	B	80	PHE	3.0
1	B	268	GLY	3.0
1	A	230	HIS	2.9
1	A	133	ARG	2.9
1	A	233	PRO	2.9
1	A	203	TRP	2.9
1	A	247	ILE	2.9
1	B	47	VAL	2.9
1	B	245	VAL	2.9
1	B	96	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	239	PHE	2.9
1	B	10	PHE	2.9
1	A	104	ILE	2.9
1	B	156	ASP	2.9
1	A	111	LEU	2.9
1	B	161	LEU	2.9
1	A	213	GLY	2.9
1	A	245	VAL	2.9
1	A	24	TYR	2.9
1	A	10	PHE	2.9
1	B	122	ARG	2.9
1	A	115	TRP	2.9
1	B	244	GLY	2.9
1	B	35	VAL	2.8
1	A	59	HIS	2.8
1	B	168	PHE	2.8
1	B	250	ALA	2.8
1	A	18	LEU	2.8
1	A	244	GLY	2.8
1	B	55	VAL	2.8
1	B	257	LYS	2.8
1	A	16	GLU	2.8
1	A	106	ASP	2.8
1	A	22	MET	2.8
1	A	92	ILE	2.8
1	B	202	LEU	2.8
1	A	219	VAL	2.8
1	B	225	TYR	2.8
1	B	81	PHE	2.8
1	B	144	PHE	2.8
1	A	191	GLU	2.8
1	A	126	ILE	2.8
1	B	242	THR	2.8
1	B	174	PRO	2.8
1	B	85	VAL	2.8
1	A	127	ALA	2.7
1	A	287	ALA	2.7
1	B	133	ARG	2.7
1	B	188	HIS	2.7
1	A	158	GLY	2.7
1	B	58	THR	2.7
1	A	36	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	11	ASP	2.7
1	A	156	ASP	2.7
1	B	218	ILE	2.7
1	B	249	PRO	2.7
1	B	260	PRO	2.7
1	A	109	SER	2.7
1	B	289	TRP	2.7
1	A	237	LEU	2.7
1	A	67	ILE	2.7
1	A	234	VAL	2.7
1	B	128	PHE	2.7
1	A	267	ILE	2.7
1	A	15	VAL	2.7
1	B	27	VAL	2.7
1	A	171	GLY	2.6
1	A	86	ARG	2.6
1	A	215	PRO	2.6
1	A	271	LEU	2.6
1	B	173	LEU	2.6
1	A	55	VAL	2.6
1	B	6	THR	2.6
1	B	117	LYS	2.6
1	B	205	PHE	2.6
1	B	180	PRO	2.6
1	B	66	LEU	2.6
1	A	140	GLU	2.6
1	B	29	PRO	2.6
1	B	69	MET	2.6
1	B	164	ASP	2.6
1	B	32	GLY	2.6
1	B	68	GLY	2.6
1	B	270	GLY	2.6
1	A	100	VAL	2.6
1	A	184	VAL	2.6
1	A	114	HIS	2.5
1	A	174	PRO	2.5
1	A	243	PRO	2.5
1	B	165	GLN	2.5
1	B	239	PHE	2.5
1	A	183	GLU	2.5
1	A	187	ASP	2.5
1	B	82	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	5	GLY	2.5
1	B	151	ALA	2.5
1	A	146	ARG	2.5
1	B	146	ARG	2.5
1	A	180	PRO	2.5
1	B	266	ASP	2.5
1	A	87	PHE	2.5
1	A	193	PHE	2.5
1	B	74	LYS	2.5
1	B	237	LEU	2.5
1	A	195	ASN	2.5
1	A	30	ARG	2.5
1	B	105	HIS	2.5
1	B	215	PRO	2.5
1	A	46	TYR	2.5
1	A	58	THR	2.5
1	A	27	VAL	2.5
1	B	11	ASP	2.5
1	B	222	VAL	2.5
1	A	57	PRO	2.5
1	B	171	GLY	2.4
1	B	46	TYR	2.4
1	B	87	PHE	2.4
1	B	175	MET	2.4
1	A	51	ILE	2.4
1	B	155	THR	2.4
1	A	122	ARG	2.4
1	B	262	CYS	2.4
1	B	274	LEU	2.4
1	B	37	PHE	2.4
1	B	153	ARG	2.4
1	B	88	MET	2.4
1	A	221	LEU	2.4
1	A	8	PHE	2.4
1	B	73	ASP	2.4
1	B	92	ILE	2.4
1	B	118	ARG	2.4
1	A	35	VAL	2.4
1	A	85	VAL	2.4
1	A	289	TRP	2.4
1	A	202	LEU	2.3
1	B	21	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	128	PHE	2.3
1	A	278	ASN	2.3
1	A	124	LYS	2.3
1	A	281	LEU	2.3
1	A	217	ASN	2.3
1	A	90	ALA	2.3
1	B	104	ILE	2.3
1	B	243	PRO	2.3
1	B	25	VAL	2.3
1	B	154	THR	2.3
1	B	189	TYR	2.3
1	A	52	ILE	2.3
1	A	70	GLY	2.3
1	B	102	LEU	2.3
1	B	238	LEU	2.3
1	B	192	PRO	2.2
1	B	62	ILE	2.2
1	B	103	VAL	2.2
1	A	39	HIS	2.2
1	B	230	HIS	2.2
1	A	236	LYS	2.2
1	B	22	MET	2.2
1	A	292	THR	2.2
1	B	93	GLU	2.2
1	B	187	ASP	2.2
1	B	201	PRO	2.2
1	B	63	ALA	2.2
1	A	79	TYR	2.2
1	A	169	ILE	2.2
1	A	285	GLU	2.2
1	A	82	ASP	2.2
1	A	96	GLY	2.2
1	A	42	PRO	2.2
1	A	192	PRO	2.2
1	A	235	PRO	2.2
1	A	269	PRO	2.2
1	A	216	ALA	2.2
1	A	105	HIS	2.2
1	B	114	HIS	2.2
1	A	172	THR	2.2
1	A	28	GLY	2.2
1	A	34	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	204	ARG	2.2
1	B	84	HIS	2.1
1	A	44	SER	2.1
1	B	232	SER	2.1
1	A	152	PHE	2.1
1	A	48	TRP	2.1
1	B	101	VAL	2.1
1	A	185	GLU	2.1
1	A	161	LEU	2.1
1	A	279	PRO	2.1
1	B	193	PHE	2.1
1	A	189	TYR	2.1
1	B	279	PRO	2.1
1	A	232	SER	2.0
1	A	186	MET	2.0
1	B	235	PRO	2.0
1	A	13	HIS	2.0
1	A	23	HIS	2.0
1	B	286	ILE	2.0
1	A	154	THR	2.0
1	A	119	ASN	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](#)

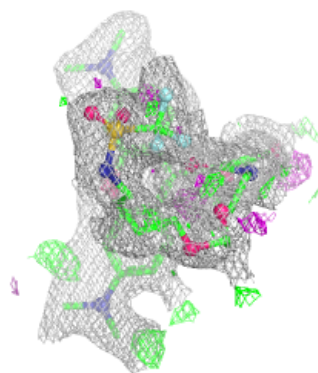
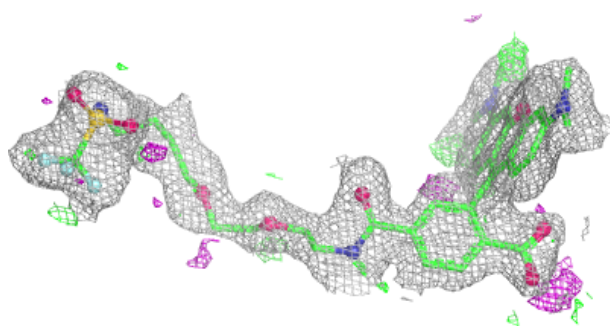
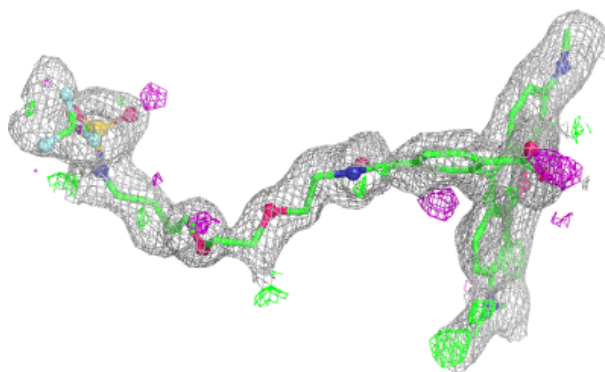
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IYE	A	301	50/50	0.83	0.20	31,38,50,52	0
2	IYE	B	301	50/50	0.85	0.17	29,37,46,53	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.

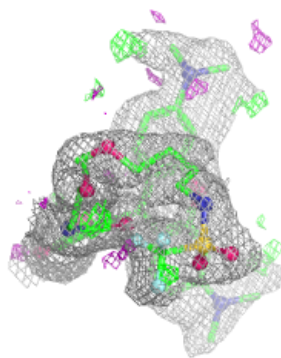
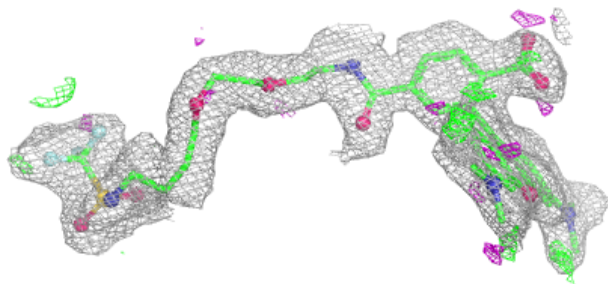
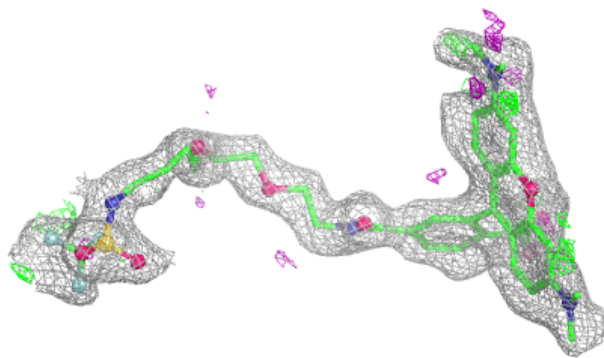
Electron density around IYE A 301:

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



Electron density around IYE B 301:

$2mF_o-DF_c$ (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.