Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2023 – 02:06 PM EDT

PDB ID	:	8FUR
Title	:	Crystal structure of human IDO1 with compound 11
Authors	:	Critton, D.A.; Lewis, H.A.
Deposited on	:	2023-01-18
Resolution	:	2.29 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:

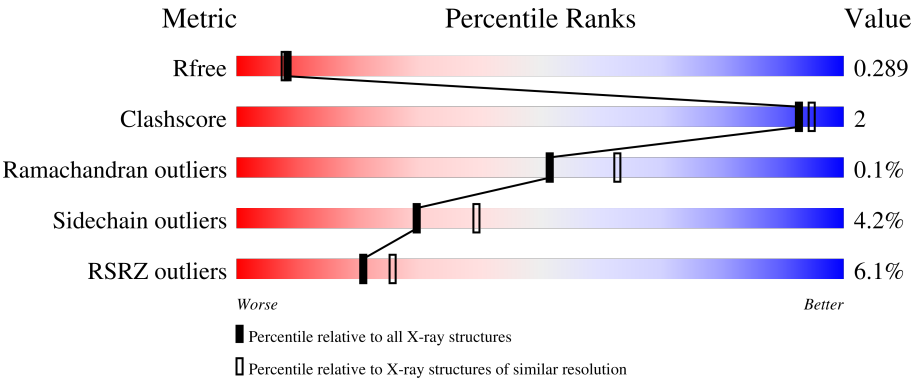
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.29 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	A	406	% 84% 5% 11%
1	B	406	2% 83% 7% 11%
1	C	406	7% 81% 6% 13%
1	D	406	11% 82% 5% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22495 atoms, of which 10914 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.

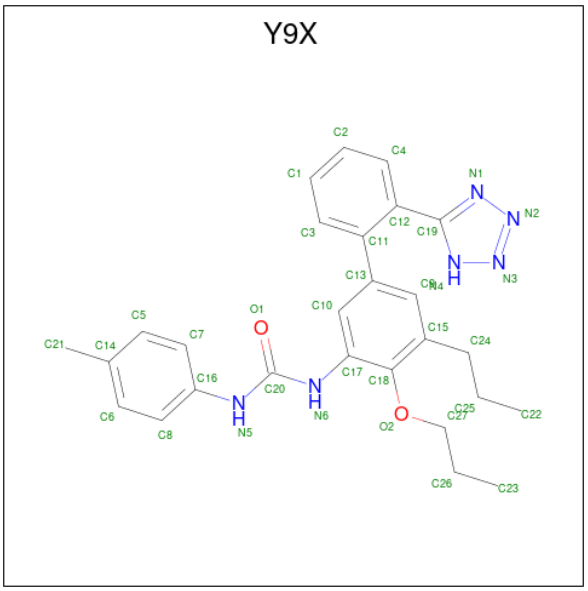
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	H	N	O	S	2723	0	0
			5526	1811	2723	470	505	17			
1	B	363	Total	C	H	N	O	S	2747	0	0
			5566	1823	2747	473	506	17			
1	C	353	Total	C	H	N	O	S	2669	0	0
			5411	1776	2669	458	491	17			
1	D	358	Total	C	H	N	O	S	2655	0	0
			5415	1786	2655	459	498	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P14902
A	-1	SER	-	expression tag	UNP P14902
A	0	HIS	-	expression tag	UNP P14902
B	-2	GLY	-	expression tag	UNP P14902
B	-1	SER	-	expression tag	UNP P14902
B	0	HIS	-	expression tag	UNP P14902
C	-2	GLY	-	expression tag	UNP P14902
C	-1	SER	-	expression tag	UNP P14902
C	0	HIS	-	expression tag	UNP P14902
D	-2	GLY	-	expression tag	UNP P14902
D	-1	SER	-	expression tag	UNP P14902
D	0	HIS	-	expression tag	UNP P14902

- Molecule 2 is N-(4-methylphenyl)-N'-[(1P,2'P)-4-propoxy-5-propyl-2'-(1H-tetrazol-5-yl)[1,1' -biphenyl]-3-yl]urea (three-letter code: Y9X) (formula: $C_{27}H_{30}N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	30	0
			65	27	30	6	2		
2	B	1	Total	C	H	N	O	30	0
			65	27	30	6	2		
2	C	1	Total	C	H	N	O	30	0
			65	27	30	6	2		
2	D	1	Total	C	H	N	O	30	0
			65	27	30	6	2		

- Molecule 3 is water.

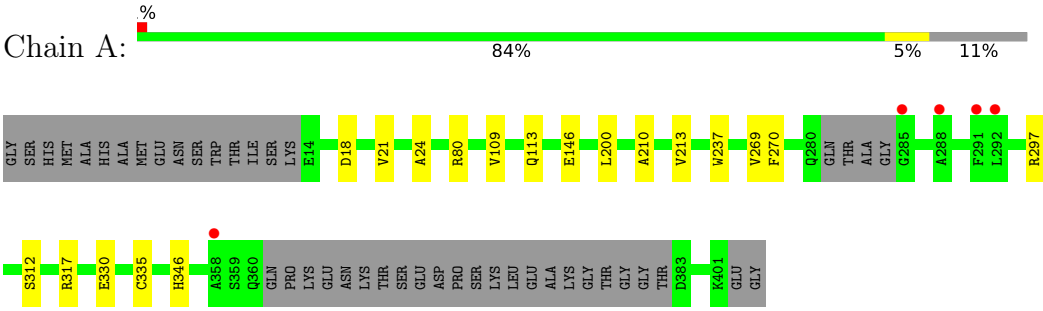
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	86	Total	O	0	0
			86	86		
3	C	75	Total	O	0	0
			75	75		
3	D	75	Total	O	0	0
			75	75		

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.

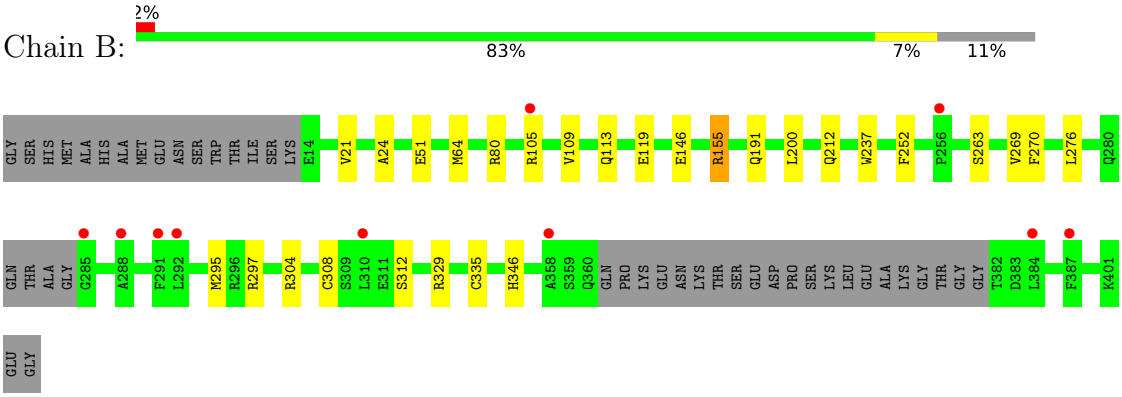
• Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain A:



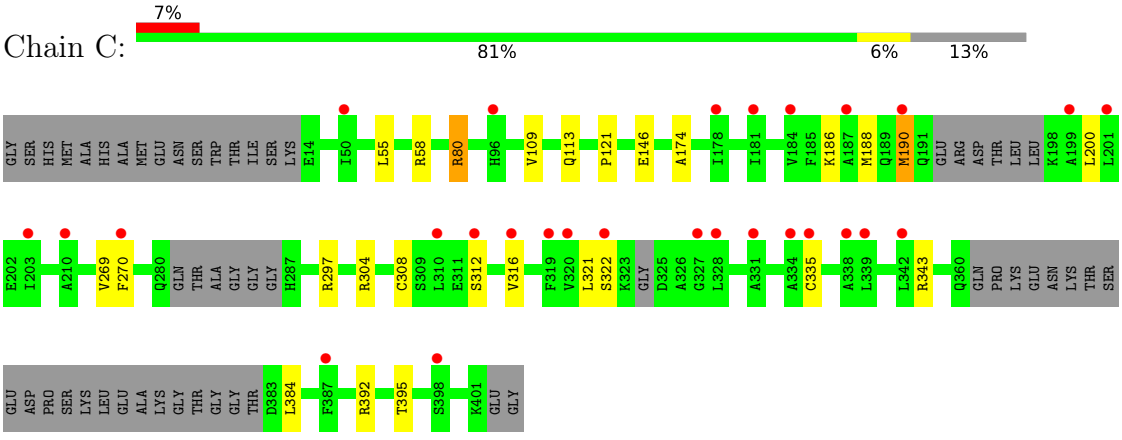
• Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain B:



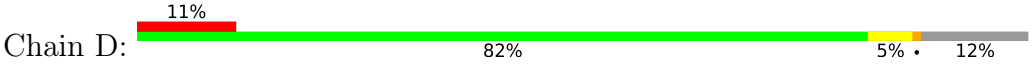
• Molecule 1: Indoleamine 2,3-dioxygenase 1

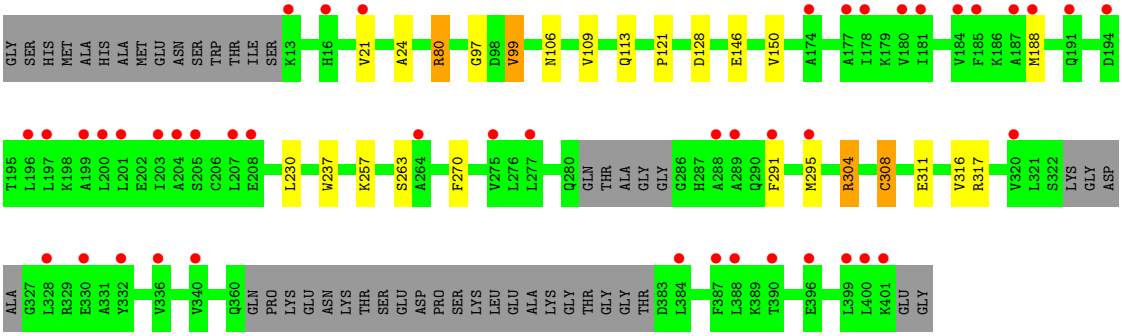
Chain C:



• Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.88Å 120.29Å 100.82Å 90.00° 119.38° 90.00°	Depositor
Resolution (Å)	19.76 – 2.29 19.76 – 2.29	Depositor EDS
% Data completeness (in resolution range)	56.6 (19.76-2.29) 56.7 (19.76-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.28Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.279 , 0.300 0.269 , 0.289	Depositor DCC
R_{free} test set	2839 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 21.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.428 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22495	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: Y9X

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	0.38	0/2869	0.51	0/3897
1	B	0.36	0/2886	0.51	0/3920
1	C	0.38	0/2806	0.53	0/3810
1	D	0.37	0/2825	0.52	0/3842
All	All	0.37	0/11386	0.52	0/15469

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	2803	2723	2724	8	0
1	B	2819	2747	2747	10	0
1	C	2742	2669	2669	10	0
1	D	2760	2655	2655	11	0
2	A	35	30	0	1	0
2	B	35	30	0	1	0
2	C	35	30	0	0	0
2	D	35	30	0	0	0
3	A	81	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	86	0	0	0	0
3	C	75	0	0	0	0
3	D	75	0	0	1	0
All	All	11581	10914	10795	34	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 (34) 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:C:80:ARG:NH1	1:C:121:PRO:O	2.14	0.81
1:D:21:VAL:HG12	1:D:24:ALA:HB3	1.67	0.77
1:B:21:VAL:HG12	1:B:24:ALA:HB3	1.68	0.73
1:D:21:VAL:CG1	1:D:24:ALA:HB3	2.24	0.68
1:B:21:VAL:CG1	1:B:24:ALA:HB3	2.25	0.67
1:D:80:ARG:NH1	1:D:121:PRO:O	2.28	0.67
1:A:21:VAL:HG22	1:A:24:ALA:HB3	1.76	0.67
1:C:297:ARG:NH2	1:D:311:GLU:O	2.31	0.64
1:A:297:ARG:HG2	1:B:312:SER:O	2.02	0.59
1:D:188:MET:HE1	1:D:316:VAL:HG22	1.84	0.58
1:A:312:SER:O	1:B:297:ARG:HG2	2.03	0.57
1:D:291:PHE:O	1:D:295:MET:HG2	2.05	0.56
1:B:109:VAL:O	1:B:113:GLN:HG3	2.09	0.52
1:C:312:SER:O	1:D:304:ARG:HD2	2.09	0.52
1:A:210:ALA:O	1:A:213:VAL:HG12	2.11	0.51
1:D:97:GLY:O	1:D:99:VAL:HG12	2.10	0.50
1:B:346:HIS:NE2	2:B:501:Y9X:N1	2.59	0.50
1:C:343:ARG:NH2	1:C:395:THR:OG1	2.41	0.49
1:D:109:VAL:O	1:D:113:GLN:HG3	2.14	0.48
1:C:109:VAL:O	1:C:113:GLN:HG3	2.14	0.47
1:D:106:ASN:HB2	3:D:630:HOH:O	2.13	0.47
1:A:109:VAL:O	1:A:113:GLN:HG3	2.14	0.46
1:C:174:ALA:HB1	1:C:269:VAL:HG21	1.98	0.45
1:B:109:VAL:HG23	1:B:252:PHE:HD1	1.80	0.45
1:B:51:GLU:OE1	1:B:155:ARG:NH2	2.50	0.44
1:C:308:CYS:O	1:D:308:CYS:SG	2.75	0.44
1:A:18:ASP:HB3	1:A:21:VAL:HG12	2.00	0.42
1:A:200:LEU:O	1:A:335:CYS:SG	2.78	0.41
1:B:200:LEU:O	1:B:335:CYS:SG	2.79	0.41
1:A:346:HIS:NE2	2:A:501:Y9X:N1	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LEU:O	1:C:335:CYS:SG	2.78	0.41
1:B:119:GLU:O	1:B:304:ARG:NH2	2.53	0.41
1:C:186:LYS:O	1:C:190:MET:SD	2.79	0.41
1:C:316:VAL:HG12	1:C:316:VAL:O	2.21	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	356/406 (88%)	346 (97%)	10 (3%)	0	100	100
1	B	357/406 (88%)	345 (97%)	12 (3%)	0	100	100
1	C	343/406 (84%)	333 (97%)	9 (3%)	1 (0%)	41	49
1	D	350/406 (86%)	340 (97%)	10 (3%)	0	100	100
All	All	1406/1624 (87%)	1364 (97%)	41 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	322	SER

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	291/350 (83%)	282 (97%)	9 (3%)	40	53
1	B	294/350 (84%)	279 (95%)	15 (5%)	24	31
1	C	287/350 (82%)	276 (96%)	11 (4%)	33	44
1	D	284/350 (81%)	271 (95%)	13 (5%)	27	35
All	All	1156/1400 (83%)	1108 (96%)	48 (4%)	30	39

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	146	GLU
1	A	237	TRP
1	A	269	VAL
1	A	270	PHE
1	A	304	ARG
1	A	308	CYS
1	A	317	ARG
1	A	330	GLU
1	B	64	MET
1	B	80	ARG
1	B	105	ARG
1	B	146	GLU
1	B	155	ARG
1	B	191	GLN
1	B	212	GLN
1	B	237	TRP
1	B	263	SER
1	B	269	VAL
1	B	270	PHE
1	B	276	LEU
1	B	295	MET
1	B	308	CYS
1	B	329	ARG
1	C	55	LEU
1	C	58	ARG
1	C	80	ARG
1	C	146	GLU
1	C	188	MET
1	C	190	MET
1	C	270	PHE
1	C	304	ARG
1	C	321	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	384	LEU
1	C	392	ARG
1	D	80	ARG
1	D	99	VAL
1	D	128	ASP
1	D	146	GLU
1	D	150	VAL
1	D	230	LEU
1	D	237	TRP
1	D	257	LYS
1	D	263	SER
1	D	270	PHE
1	D	304	ARG
1	D	308	CYS
1	D	317	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	B	313	ASN
1	C	113	GLN
1	C	305	ASN
1	C	313	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)

4 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	Y9X	C	501	-	38,38,38	0.32	0	49,51,51	1.26	3 (6%)
2	Y9X	D	501	-	38,38,38	0.31	0	49,51,51	1.26	3 (6%)
2	Y9X	B	501	-	38,38,38	0.33	0	49,51,51	1.24	4 (8%)
2	Y9X	A	501	-	38,38,38	0.32	0	49,51,51	1.33	4 (8%)

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	Y9X	C	501	-	-	5/23/23/23	0/4/4/4
2	Y9X	D	501	-	-	5/23/23/23	0/4/4/4
2	Y9X	B	501	-	-	3/23/23/23	0/4/4/4
2	Y9X	A	501	-	-	5/23/23/23	0/4/4/4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	Y9X	N4-N3-N2	-5.17	106.16	109.53
2	C	501	Y9X	N4-N3-N2	-5.13	106.18	109.53
2	B	501	Y9X	N4-N3-N2	-5.04	106.24	109.53
2	D	501	Y9X	N4-N3-N2	-4.96	106.29	109.53
2	A	501	Y9X	C19-N4-N3	4.73	109.08	104.87
2	C	501	Y9X	C19-N4-N3	4.69	109.04	104.87
2	D	501	Y9X	C19-N4-N3	4.63	108.99	104.87
2	B	501	Y9X	C19-N4-N3	4.57	108.94	104.87
2	A	501	Y9X	C27-O2-C18	3.26	124.08	114.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	Y9X	N4-C19-N1	-3.21	107.80	111.39
2	D	501	Y9X	N4-C19-N1	-3.17	107.86	111.39
2	C	501	Y9X	N4-C19-N1	-3.15	107.87	111.39
2	B	501	Y9X	N4-C19-N1	-3.11	107.92	111.39
2	B	501	Y9X	C27-O2-C18	2.07	120.48	114.23

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	Y9X	C23-C26-C27-O2
2	D	501	Y9X	C4-C12-C19-N4
2	A	501	Y9X	C26-C27-O2-C18
2	D	501	Y9X	C4-C12-C19-N1
2	D	501	Y9X	C8-C16-N5-C20
2	D	501	Y9X	C7-C16-N5-C20
2	A	501	Y9X	C15-C18-O2-C27
2	C	501	Y9X	C8-C16-N5-C20
2	C	501	Y9X	C7-C16-N5-C20
2	B	501	Y9X	C8-C16-N5-C20
2	A	501	Y9X	C4-C12-C19-N4
2	C	501	Y9X	C4-C12-C19-N4
2	B	501	Y9X	C7-C16-N5-C20
2	C	501	Y9X	C23-C26-C27-O2
2	A	501	Y9X	C4-C12-C19-N1
2	C	501	Y9X	C4-C12-C19-N1
2	D	501	Y9X	C26-C27-O2-C18
2	B	501	Y9X	C26-C27-O2-C18

There are no ring outliers.

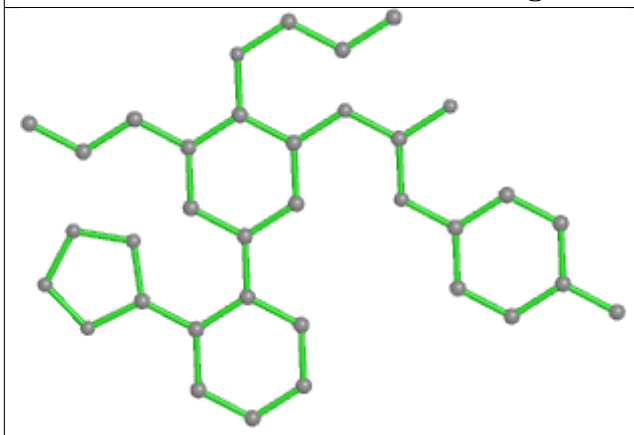
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	Y9X	1	0
2	A	501	Y9X	1	0

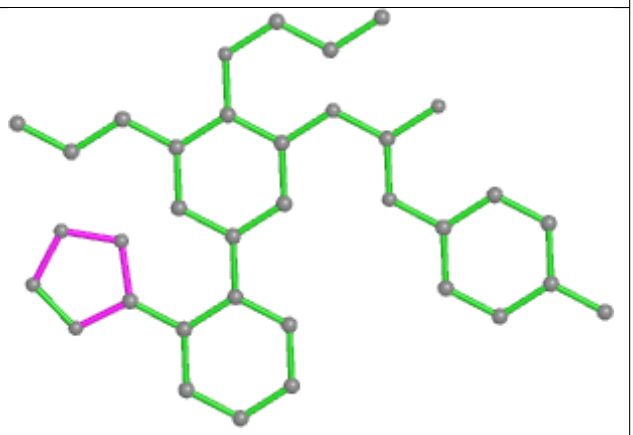
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

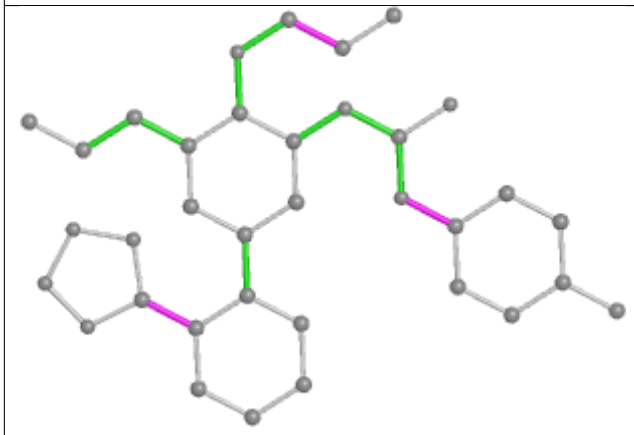
Ligand Y9X C 501



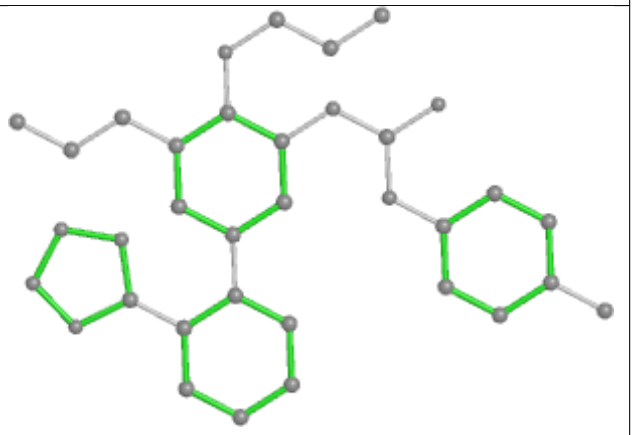
Bond lengths



Bond angles

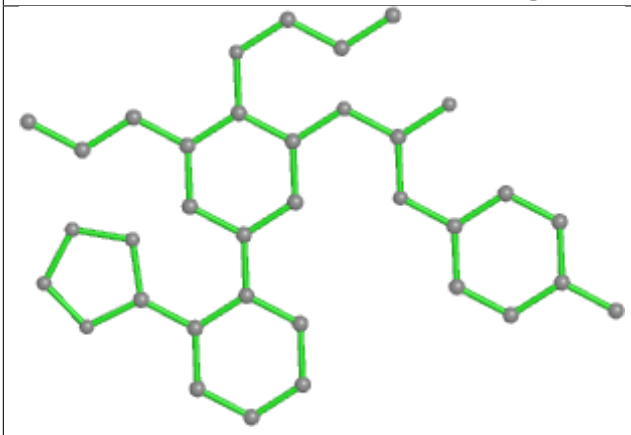


Torsions

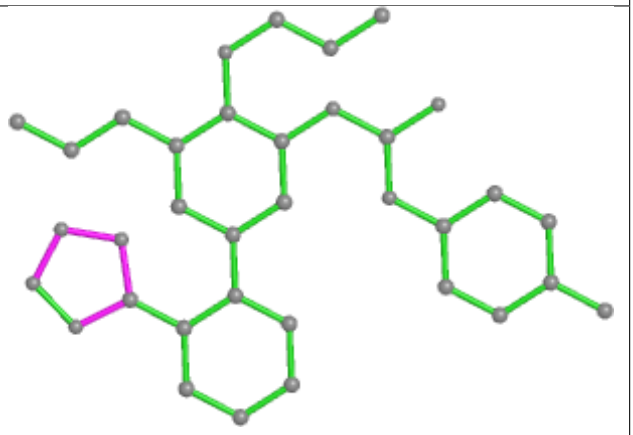


Rings

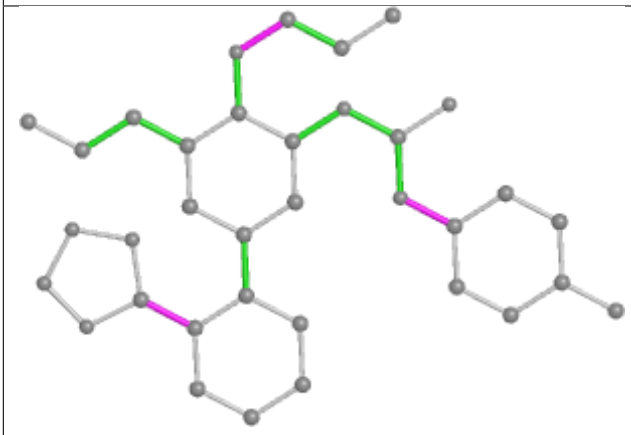
Ligand Y9X D 501



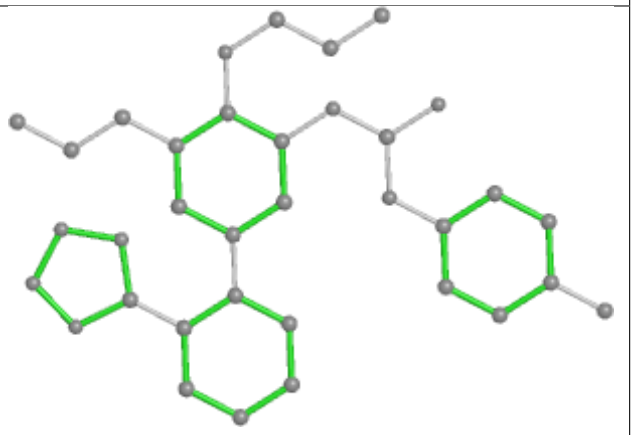
Bond lengths



Bond angles

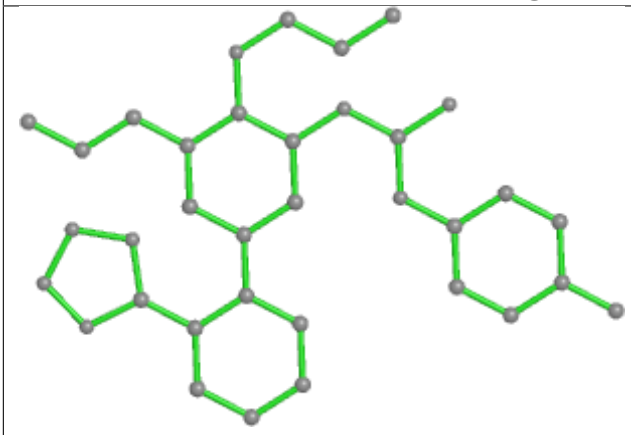


Torsions

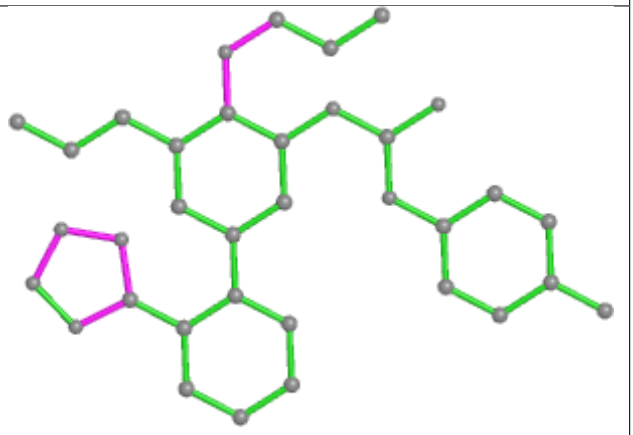


Rings

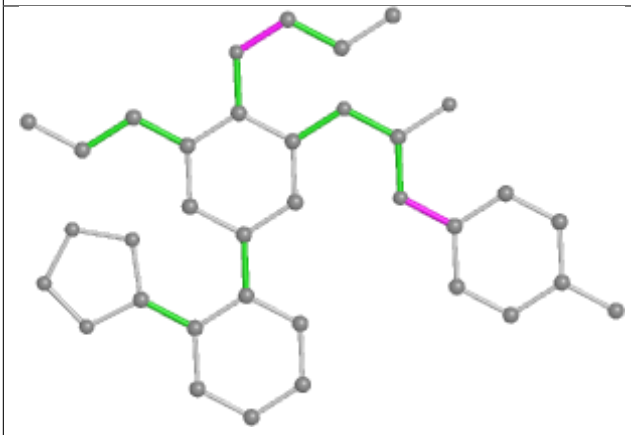
Ligand Y9X B 501



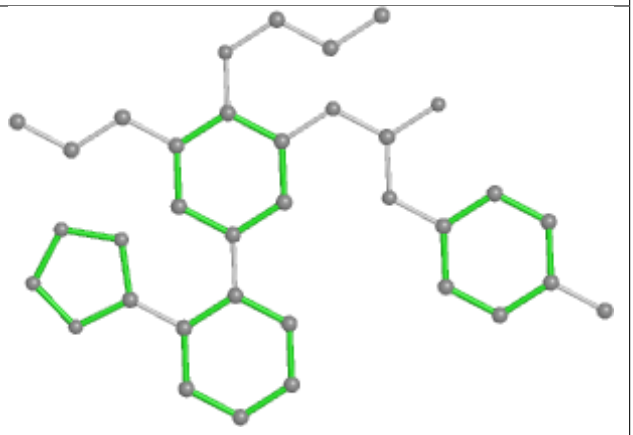
Bond lengths



Bond angles

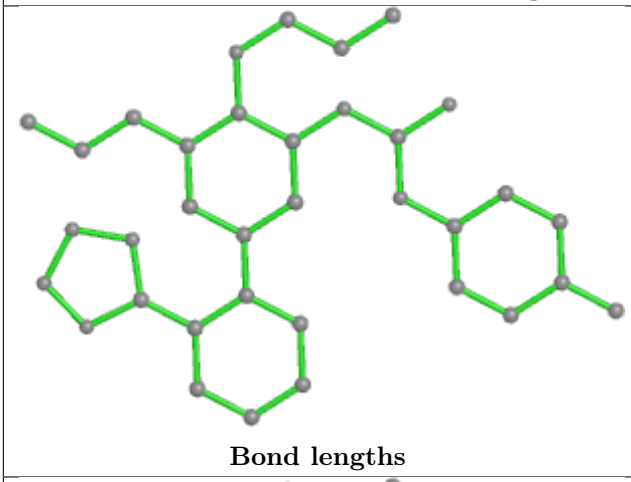


Torsions

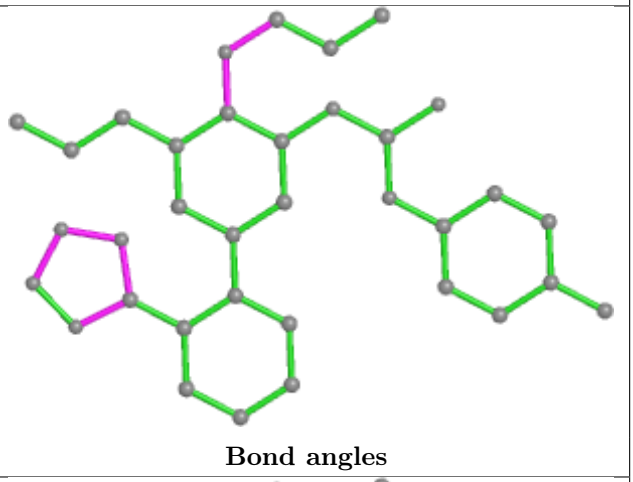


Rings

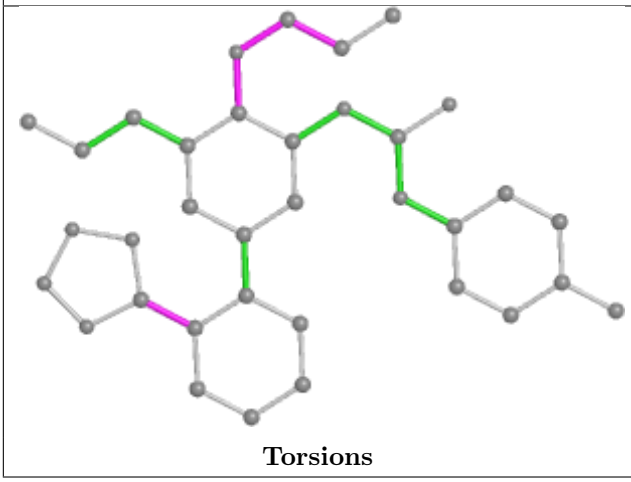
Ligand Y9X A 501



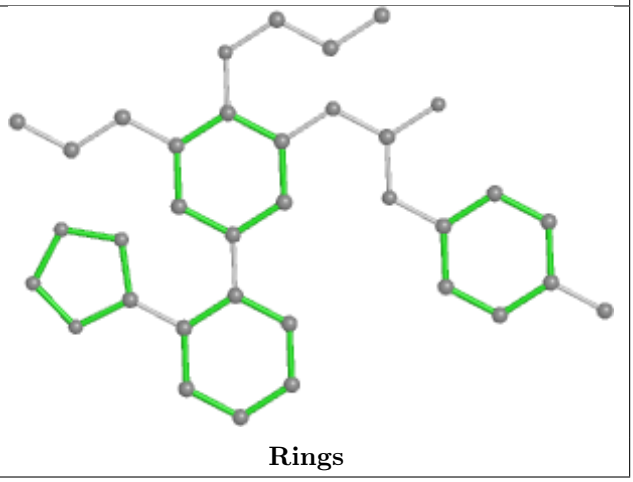
Bond lengths



Bond angles



Torsions



Rings

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, 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	A	362/406 (89%)	0.13	5 (1%) 75 79	31, 52, 68, 82	0
1	B	363/406 (89%)	0.19	10 (2%) 53 59	28, 50, 66, 85	0
1	C	353/406 (86%)	0.57	28 (7%) 12 16	32, 61, 123, 139	0
1	D	358/406 (88%)	0.63	45 (12%) 3 4	35, 63, 128, 138	0
All	All	1436/1624 (88%)	0.38	88 (6%) 21 26	28, 55, 115, 139	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	GLY	11.9
1	C	328	LEU	10.8
1	D	400	LEU	6.1
1	D	201	LEU	5.6
1	D	197	LEU	5.3
1	D	181	ILE	4.6
1	D	178	ILE	4.5
1	D	187	ALA	4.4
1	D	203	ILE	4.3
1	C	320	VAL	4.3
1	C	190	MET	4.1
1	C	334	ALA	4.1
1	D	328	LEU	4.0
1	C	387	PHE	3.8
1	D	277	LEU	3.7
1	A	285	GLY	3.7
1	D	13	LYS	3.6
1	C	331	ALA	3.6
1	D	399	LEU	3.5
1	D	401	LYS	3.5
1	C	339	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	327	GLY	3.4
1	B	288	ALA	3.3
1	C	322	SER	3.3
1	C	319	PHE	3.2
1	D	340	VAL	3.2
1	C	96	HIS	3.1
1	C	398	SER	3.1
1	D	185	PHE	3.0
1	D	174	ALA	3.0
1	D	336	VAL	3.0
1	B	292	LEU	3.0
1	D	332	TYR	2.9
1	D	396	GLU	2.9
1	C	203	ILE	2.8
1	D	205	SER	2.8
1	B	387	PHE	2.8
1	D	184	VAL	2.8
1	C	201	LEU	2.8
1	D	200	LEU	2.7
1	C	50	ILE	2.7
1	A	292	LEU	2.7
1	C	335	CYS	2.7
1	C	342	LEU	2.7
1	C	316	VAL	2.6
1	D	384	LEU	2.6
1	C	210	ALA	2.6
1	B	291	PHE	2.6
1	C	310	LEU	2.6
1	B	384	LEU	2.5
1	A	291	PHE	2.5
1	D	194	ASP	2.5
1	B	105	ARG	2.5
1	D	387	PHE	2.5
1	D	275	VAL	2.5
1	C	181	ILE	2.5
1	D	177	ALA	2.5
1	D	191	GLN	2.5
1	C	338	ALA	2.4
1	D	264	ALA	2.4
1	D	289	ALA	2.4
1	D	291	PHE	2.4
1	C	270	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	208	GLU	2.3
1	D	188	MET	2.3
1	C	178	ILE	2.3
1	D	288	ALA	2.3
1	C	312	SER	2.3
1	A	358	ALA	2.3
1	D	207	LEU	2.3
1	B	256	PRO	2.2
1	D	16	HIS	2.2
1	D	388	LEU	2.2
1	B	358	ALA	2.2
1	C	187	ALA	2.2
1	C	184	VAL	2.1
1	D	199	ALA	2.1
1	B	310	LEU	2.1
1	D	295	MET	2.1
1	A	288	ALA	2.1
1	D	180	VAL	2.1
1	D	390	THR	2.1
1	C	199	ALA	2.1
1	D	204	ALA	2.1
1	D	21	VAL	2.1
1	D	196	LEU	2.0
1	D	320	VAL	2.0
1	D	330	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

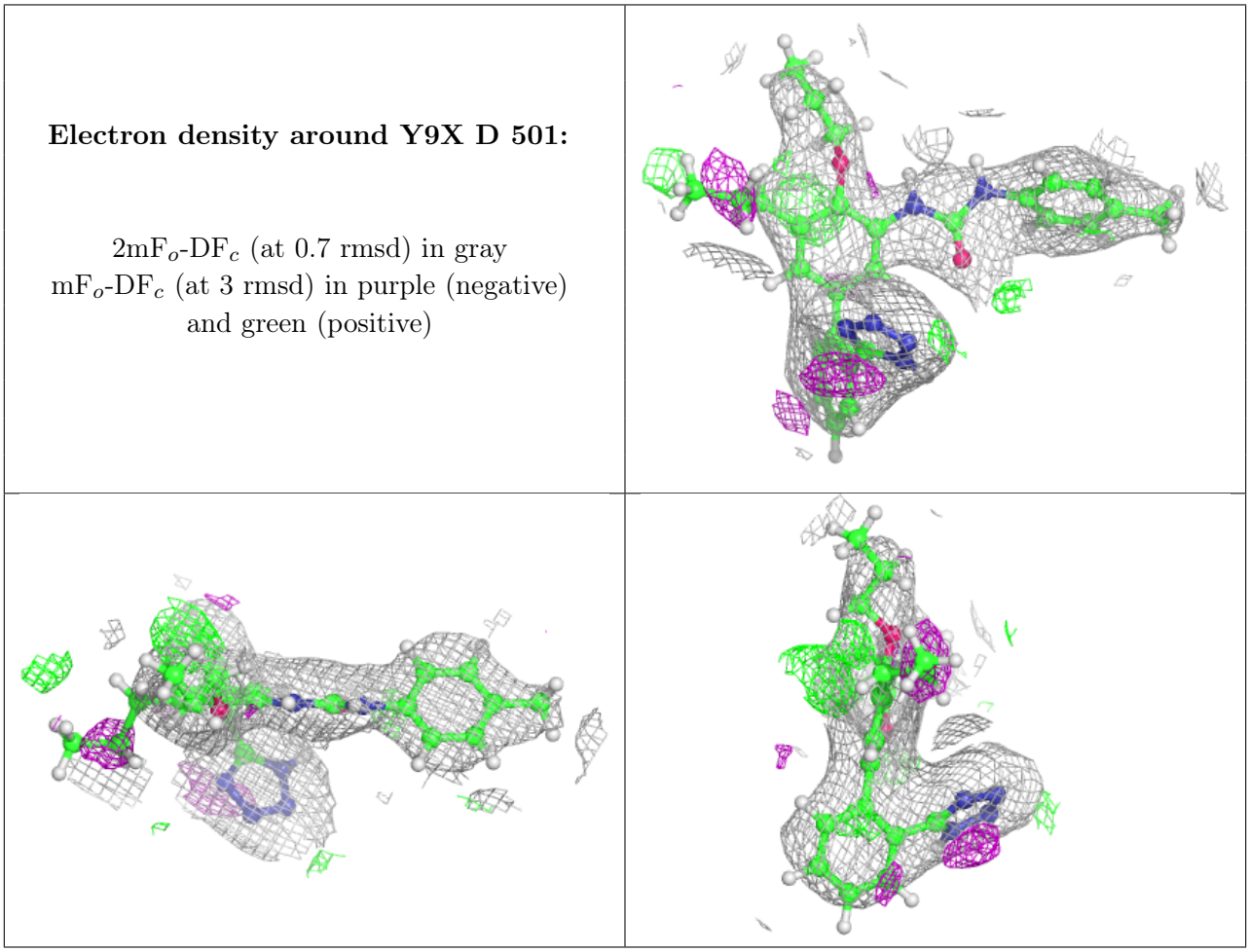
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	Y9X	D	501	35/35	0.80	0.21	64,65,67,67	30
2	Y9X	A	501	35/35	0.86	0.18	45,47,48,48	30
2	Y9X	C	501	35/35	0.87	0.17	60,62,62,62	30
2	Y9X	B	501	35/35	0.91	0.15	43,44,44,44	30

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.

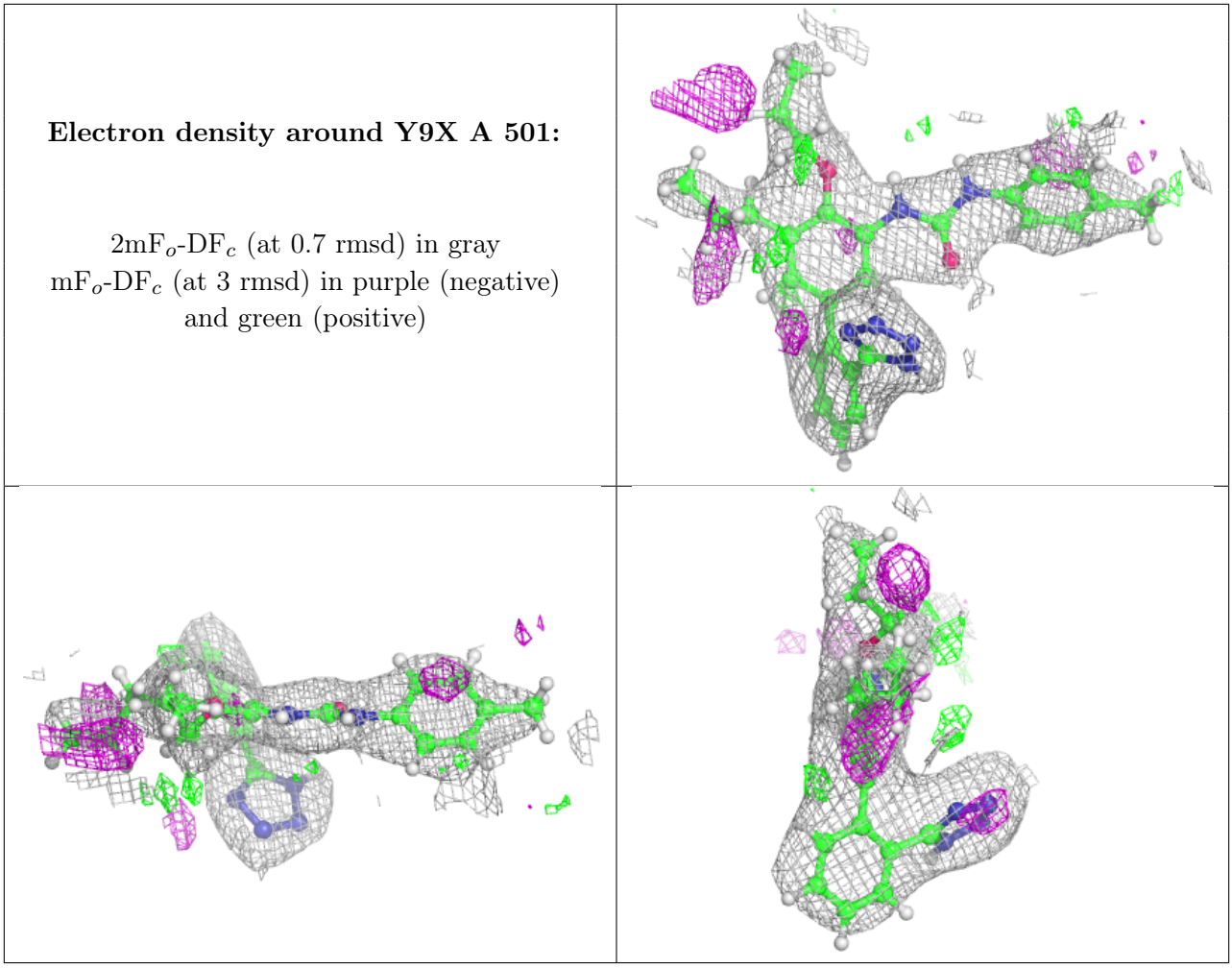
Electron density around Y9X D 501:

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



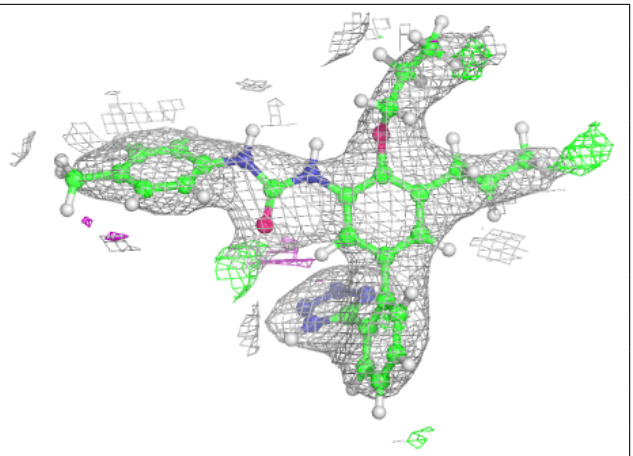
Electron density around Y9X A 501:

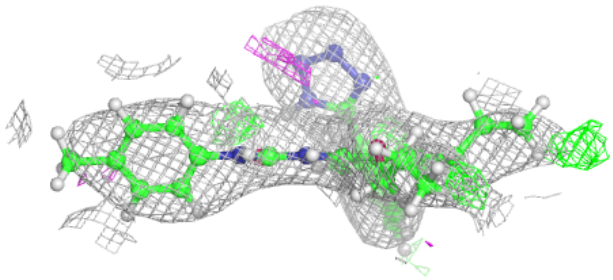
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

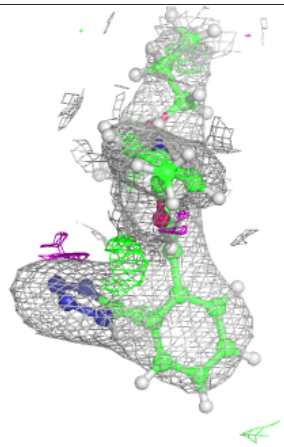


Electron density around Y9X C 501:

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

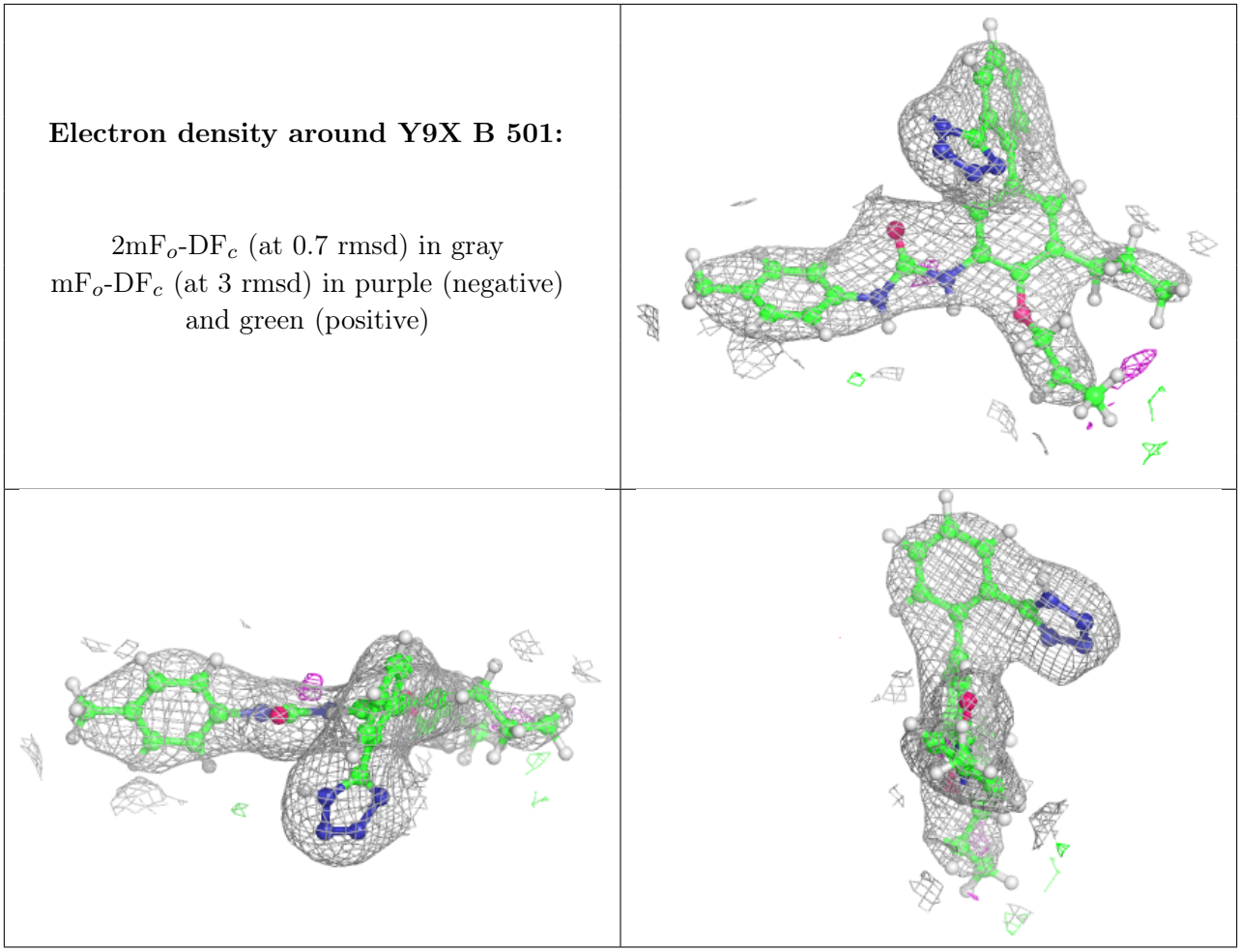






Electron density around Y9X B 501:

$2mF_o$-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.