wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2020 – 06:21 AM BST

PDB ID	:	2WVU
Title	:	Crystal structure of a Michaelis complex of alpha-L-fucosidase GH29 from Bacteroides thetaiotaomicron with the synthetic substrate 4- nitrophenyl-alpha-L-fucose
Authors	:	Lammerts van Bueren, A.; Ardevol, A.; Fayers-Kerr, J.; Luo, B.; Zhang, Y.; Sollogoub, M.; Bleriot, Y.; Rovira, C.; Davies, G.J.
Deposited on	:	2009-10-20
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

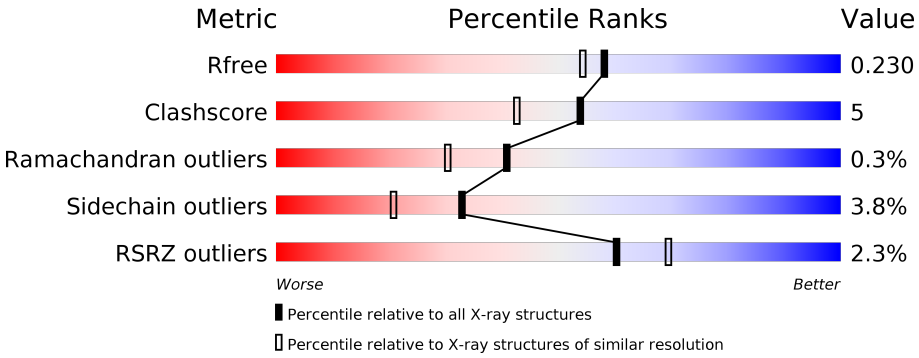
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.95 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 on 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	443	5% 87% 10%
1	B	443	88% 9%
1	C	443	2% 86% 11%
1	D	443	2% 86% 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	1473	-	-	X	-
3	JFZ	A	2001	X	-	-	-
3	JFZ	B	2001	X	-	-	-
3	JFZ	C	2001	X	-	-	-
3	JFZ	D	2001	X	-	-	-

2 Entry composition (i)

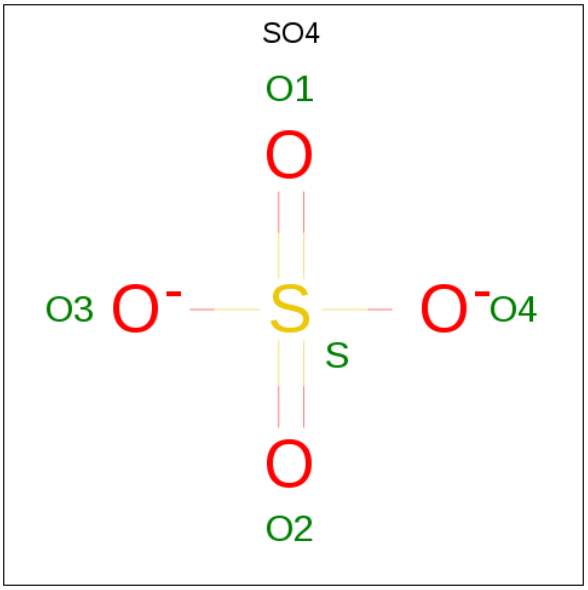
There are 4 unique types of molecules in this entry. The entry contains 15760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-L-FUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3562	2290	601	655	16			
1	B	437	Total	C	N	O	S	0	0	0
			3562	2290	601	655	16			
1	C	437	Total	C	N	O	S	0	1	0
			3565	2292	601	655	17			
1	D	437	Total	C	N	O	S	0	0	0
			3562	2290	601	655	16			

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



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

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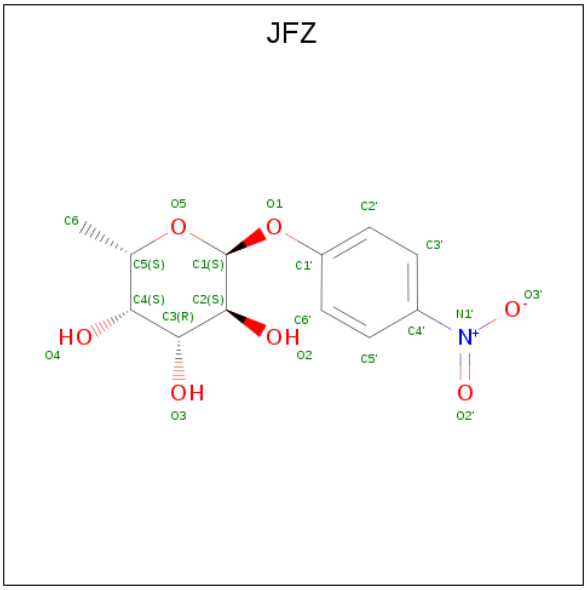
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is 4-nitrophenyl 6-deoxy-alpha-L-galactopyranoside (three-letter code: JFZ) (formula: $C_{12}H_{15}NO_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 20 12 1 7	0	0
3	B	1	Total C N O 20 12 1 7	0	0
3	C	1	Total C N O 20 12 1 7	0	0
3	D	1	Total C N O 20 12 1 7	0	0

- Molecule 4 is water.

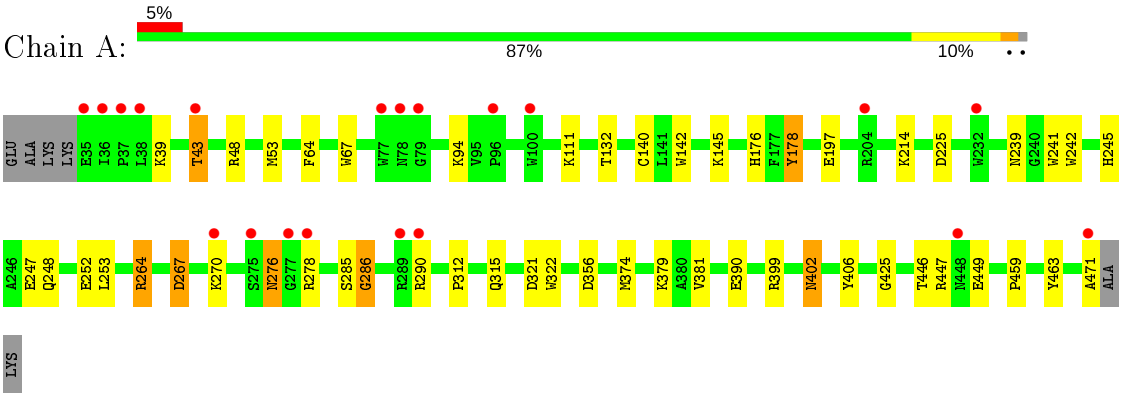
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	306	Total O 306 306	0	0
4	B	342	Total O 342 342	0	0
4	C	390	Total O 390 390	0	0
4	D	356	Total O 356 356	0	0

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.

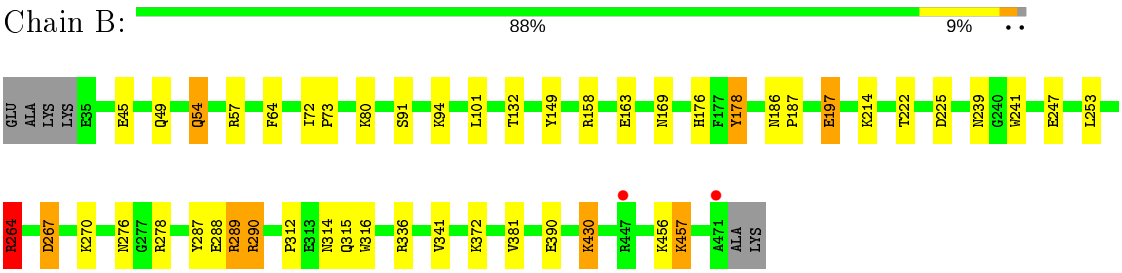
- Molecule 1: ALPHA-L-FUCOSIDASE

Chain A:



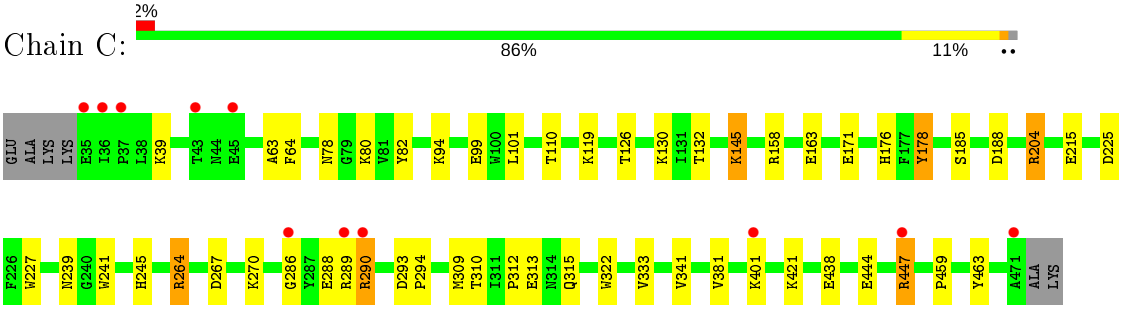
- Molecule 1: ALPHA-L-FUCOSIDASE

Chain B:



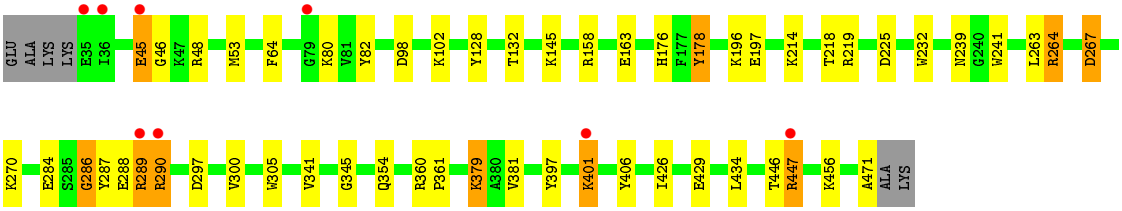
- Molecule 1: ALPHA-L-FUCOSIDASE

Chain C:



- Molecule 1: ALPHA-L-FUCOSIDASE

Chain D:


GLU
ALA
LYS
LYS
E35
I36
E45
G46
K47
R48
M53
F64
G79
K80
V81
Y82
D98
K102
Y128
T132
K145
R158
E163
H176
F177
Y178
K196
E197
K214
T218
R219
D225
W232
N239
G240
W241
L263
R264
D267
K270
E284
S285
G286
Y287
E288
R289
R290
D297
V300
W305
V341
G345
Q354
R360
P361
K379
A380
V381
Y397
K401
Y406
I426
E429
L434
T446
R447
K456
A471
ALA
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.61Å 184.82Å 98.06Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	47.25 – 1.95 47.25 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.25-1.95) 98.3 (47.25-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.179 , 0.229 0.180 , 0.230	Depositor DCC
R_{free} test set	6950 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15760	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: JFZ, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.61	0/3669	0.63	0/4976
1	B	0.68	0/3669	0.68	4/4976 (0.1%)
1	C	0.68	0/3675	0.74	4/4984 (0.1%)
1	D	0.67	0/3669	0.70	2/4976 (0.0%)
All	All	0.66	0/14682	0.69	10/19912 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	204	ARG	NE-CZ-NH2	-12.66	113.97	120.30
1	C	204	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	C	264	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	D	264	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	D	264	ARG	NE-CZ-NH1	8.47	124.54	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	263	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	D	289	ARG	Peptide

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	3562	0	3431	34	0
1	B	3562	0	3431	36	0
1	C	3565	0	3436	35	0
1	D	3562	0	3431	41	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	15	0	0	3	0
3	A	20	0	0	0	0
3	B	20	0	0	1	0
3	C	20	0	0	0	0
3	D	20	0	0	1	0
4	A	306	0	0	8	0
4	B	342	0	0	7	0
4	C	390	0	0	6	0
4	D	356	0	0	15	0
All	All	15760	0	13729	149	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.

The worst 5 of 149 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:D:284:GLU:CD	4:D:2203:HOH:O	1.70	1.24
1:D:289:ARG:HG3	1:D:290:ARG:HB2	1.37	1.04
1:C:145:LYS:HD2	4:D:2182:HOH:O	1.55	1.03
1:C:145:LYS:CD	4:D:2182:HOH:O	2.05	1.01
1:A:239:ASN:HD22	1:A:241:TRP:HE1	1.15	0.95

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	435/443 (98%)	416 (96%)	18 (4%)	1 (0%)	47	38
1	B	435/443 (98%)	424 (98%)	11 (2%)	0	100	100
1	C	436/443 (98%)	423 (97%)	12 (3%)	1 (0%)	47	38
1	D	435/443 (98%)	422 (97%)	10 (2%)	3 (1%)	22	11
All	All	1741/1772 (98%)	1685 (97%)	51 (3%)	5 (0%)	41	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	45	GLU
1	D	290	ARG
1	A	286	GLY
1	C	286	GLY
1	D	286	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	370/377 (98%)	354 (96%)	16 (4%)	29	16
1	B	370/377 (98%)	359 (97%)	11 (3%)	41	30
1	C	371/377 (98%)	356 (96%)	15 (4%)	31	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	370/377 (98%)	356 (96%)	14 (4%)	33 21
All	All	1481/1508 (98%)	1425 (96%)	56 (4%)	33 21

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	430	LYS
1	C	110	THR
1	D	270	LYS
1	B	457	LYS
1	C	64	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	49	GLN
1	C	54	GLN
1	D	54	GLN
1	B	239	ASN
1	D	169	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)

11 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	SO4	C	1473	-	4,4,4	0.16	0	6,6,6	0.42	0
3	JFZ	D	2001	-	20,21,21	3.61	5 (25%)	28,30,30	1.70	6 (21%)
2	SO4	B	1472	-	4,4,4	0.23	0	6,6,6	0.17	0
3	JFZ	B	2001	-	20,21,21	3.47	4 (20%)	28,30,30	1.88	6 (21%)
2	SO4	C	1472	-	4,4,4	0.23	0	6,6,6	0.23	0
2	SO4	D	1472	-	4,4,4	0.22	0	6,6,6	0.26	0
2	SO4	D	1473	-	4,4,4	0.17	0	6,6,6	0.22	0
3	JFZ	A	2001	-	20,21,21	3.58	4 (20%)	28,30,30	1.77	6 (21%)
2	SO4	A	1472	-	4,4,4	0.16	0	6,6,6	0.41	0
3	JFZ	C	2001	-	20,21,21	3.78	5 (25%)	28,30,30	1.84	6 (21%)
2	SO4	D	1474	-	4,4,4	0.13	0	6,6,6	0.16	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
3	JFZ	D	2001	-	1/1/6/6	2/6/28/28	0/2/2/2
3	JFZ	A	2001	-	1/1/6/6	0/6/28/28	0/2/2/2
3	JFZ	C	2001	-	1/1/6/6	0/6/28/28	0/2/2/2
3	JFZ	B	2001	-	1/1/6/6	0/6/28/28	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2001	JFZ	O2'-N1'	12.32	1.43	1.22
3	A	2001	JFZ	O2'-N1'	11.97	1.43	1.22
3	B	2001	JFZ	O2'-N1'	11.62	1.42	1.22
3	D	2001	JFZ	O2'-N1'	11.60	1.42	1.22
3	D	2001	JFZ	O3-C3	-8.39	1.23	1.43

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2001	JFZ	O3-C3-C2	5.07	122.07	110.35
3	A	2001	JFZ	C4-C3-C2	4.91	119.39	110.82
3	C	2001	JFZ	O3-C3-C2	4.90	121.67	110.35
3	A	2001	JFZ	O3-C3-C2	4.83	121.50	110.35
3	D	2001	JFZ	C4-C3-C2	4.31	118.34	110.82

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	2001	JFZ	C3
3	B	2001	JFZ	C3
3	A	2001	JFZ	C3
3	C	2001	JFZ	C3

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2001	JFZ	C3'-C4'-N1'-O2'
3	D	2001	JFZ	C5'-C4'-N1'-O2'

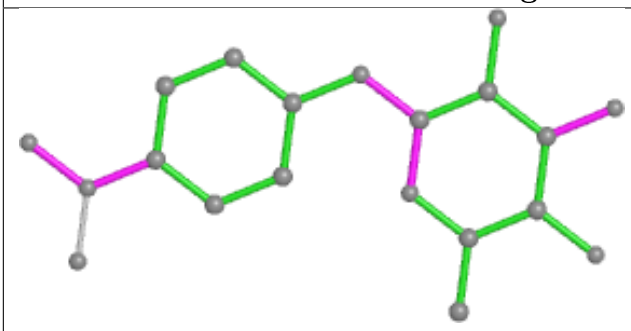
There are no ring outliers.

3 monomers are involved in 5 short contacts:

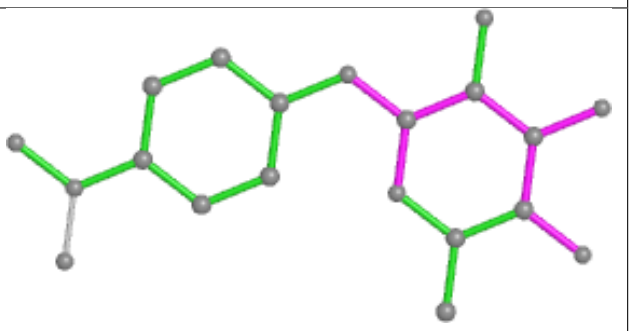
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2001	JFZ	1	0
3	B	2001	JFZ	1	0
2	D	1473	SO4	3	0

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.

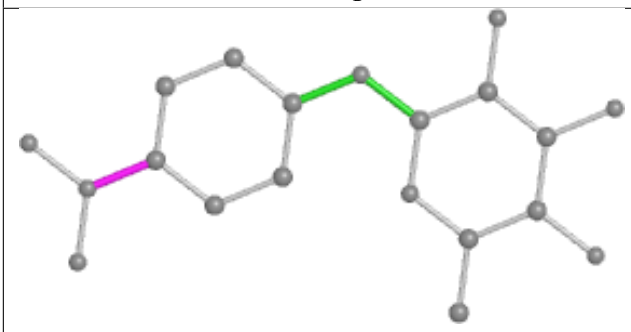
Ligand JFZ D 2001



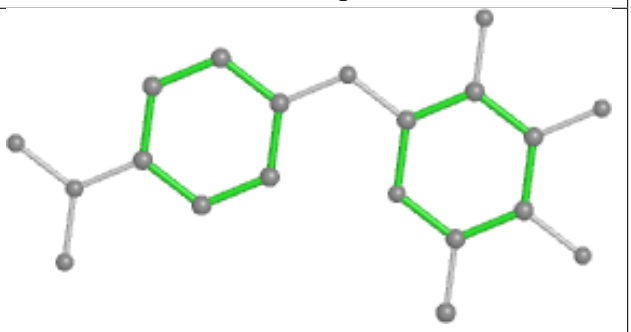
Bond lengths



Bond angles

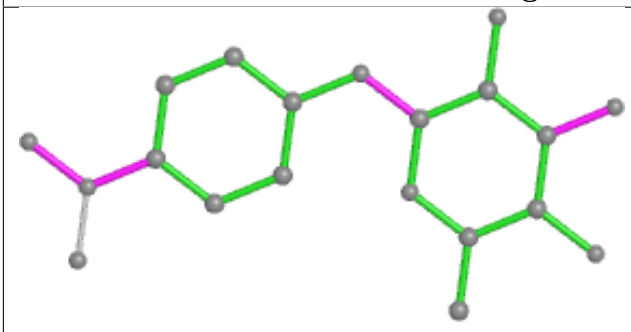


Torsions

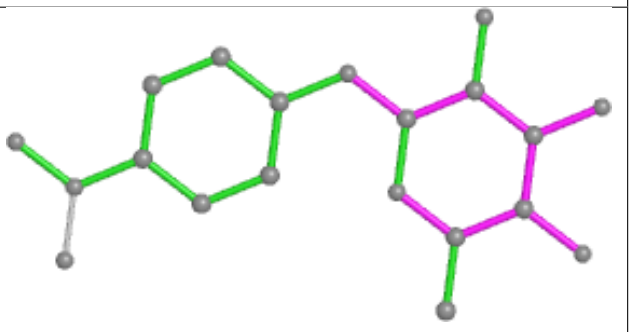


Rings

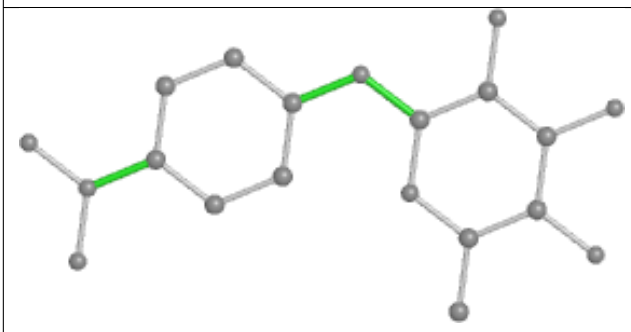
Ligand JFZ B 2001



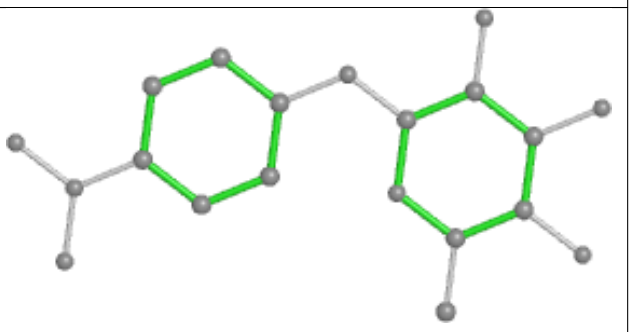
Bond lengths



Bond angles

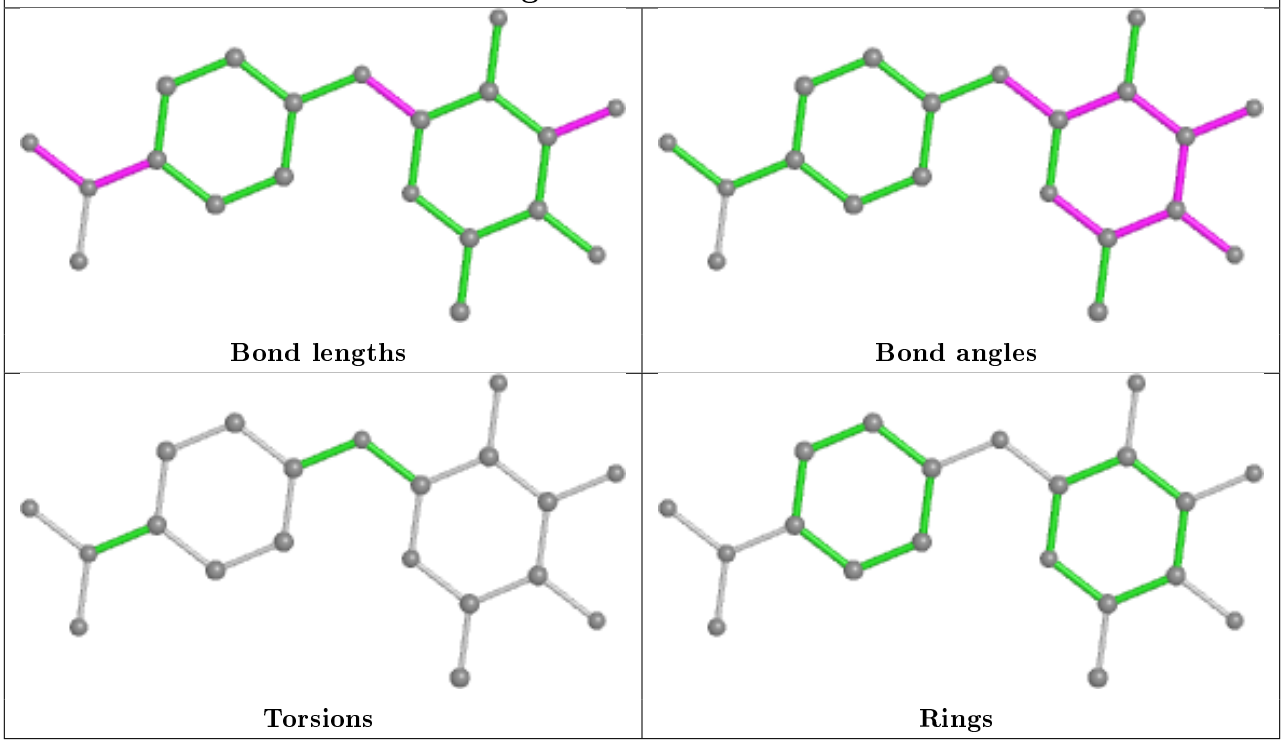


Torsions

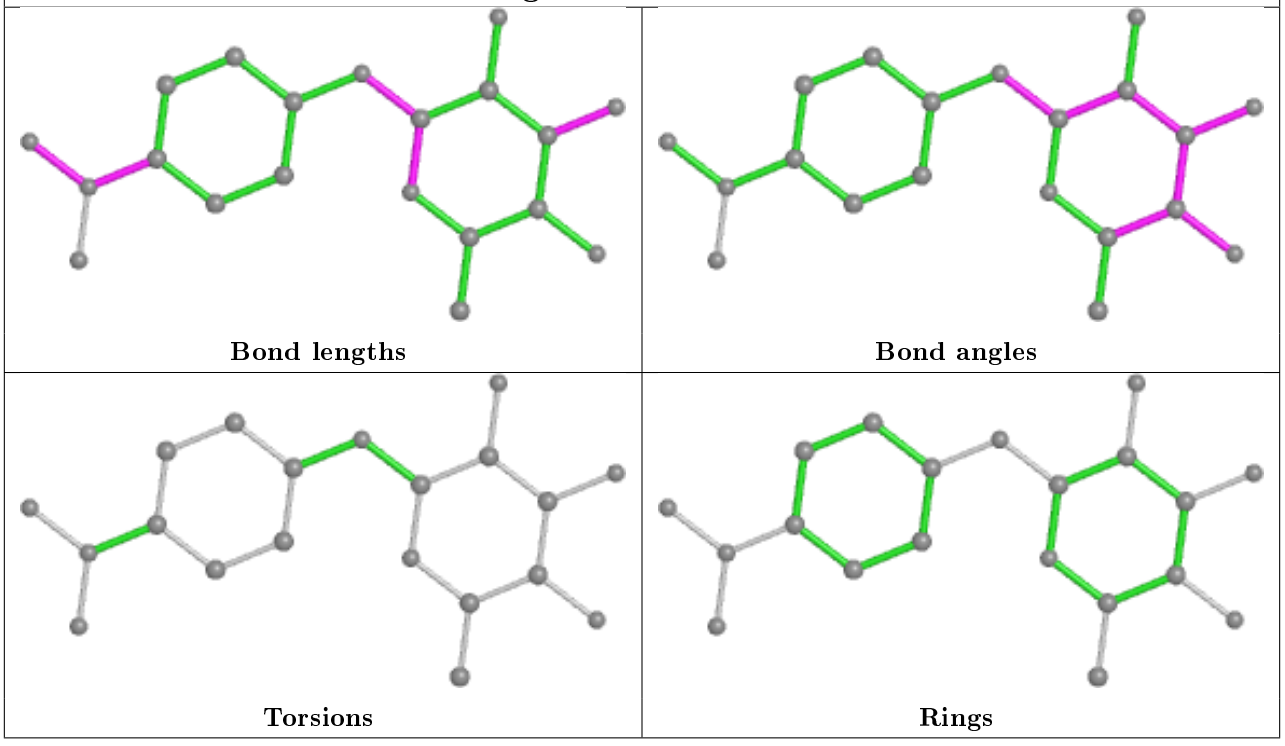


Rings

Ligand JFZ A 2001



Ligand JFZ C 2001



5.7 Other polymers (i)

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	437/443 (98%)	0.23	20 (4%) 32 42	11, 23, 40, 50	1 (0%)
1	B	437/443 (98%)	-0.15	2 (0%) 91 94	9, 18, 30, 41	1 (0%)
1	C	437/443 (98%)	-0.14	11 (2%) 57 66	10, 16, 30, 48	1 (0%)
1	D	437/443 (98%)	-0.10	8 (1%) 68 76	10, 18, 30, 50	1 (0%)
All	All	1748/1772 (98%)	-0.04	41 (2%) 60 69	9, 18, 35, 50	4 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ARG	5.9
1	C	289	ARG	5.1
1	C	290	ARG	5.1
1	A	275	SER	4.1
1	A	471	ALA	3.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

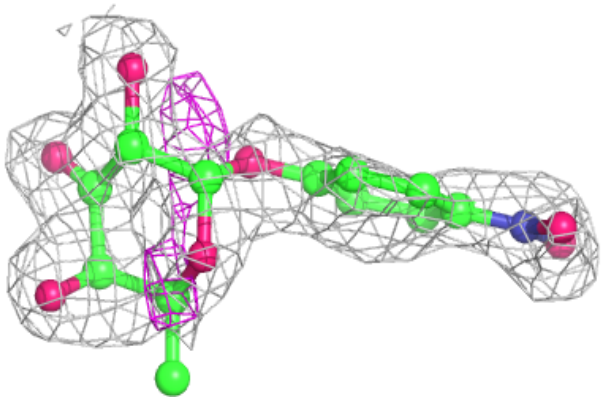
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

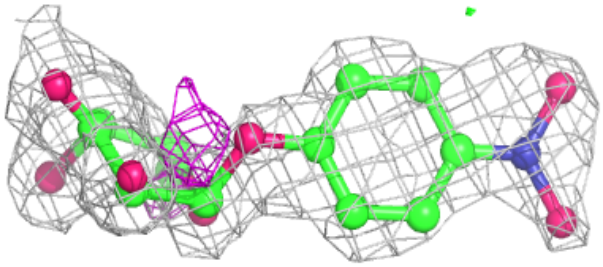
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	JFZ	A	2001	20/20	0.83	0.25	28,37,47,47	0
3	JFZ	C	2001	20/20	0.86	0.17	16,25,40,41	0
3	JFZ	D	2001	20/20	0.89	0.17	18,29,48,49	0
2	SO4	C	1473	5/5	0.90	0.19	58,59,60,61	0
3	JFZ	B	2001	20/20	0.90	0.18	18,29,40,40	0
2	SO4	D	1473	5/5	0.93	0.44	96,96,96,97	0
2	SO4	D	1474	5/5	0.95	0.11	73,73,73,73	0
2	SO4	A	1472	5/5	0.96	0.13	47,47,48,48	0
2	SO4	C	1472	5/5	0.98	0.12	40,41,41,42	0
2	SO4	B	1472	5/5	0.98	0.10	36,37,38,39	0
2	SO4	D	1472	5/5	0.99	0.10	31,32,33,33	0

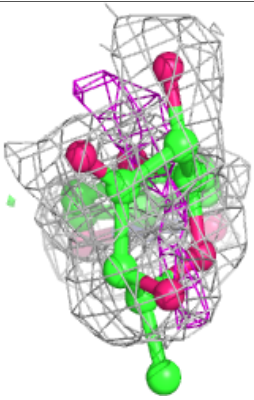
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JFZ A 2001:

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

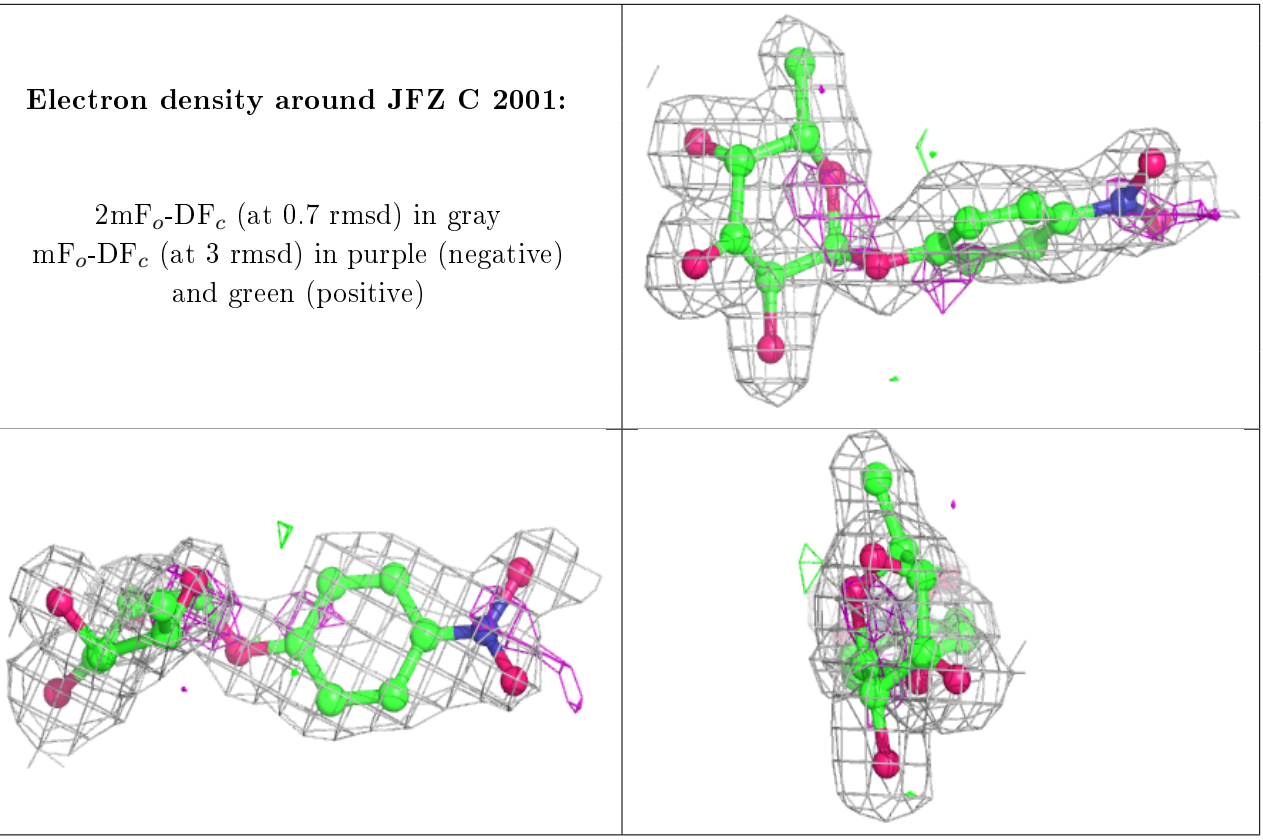






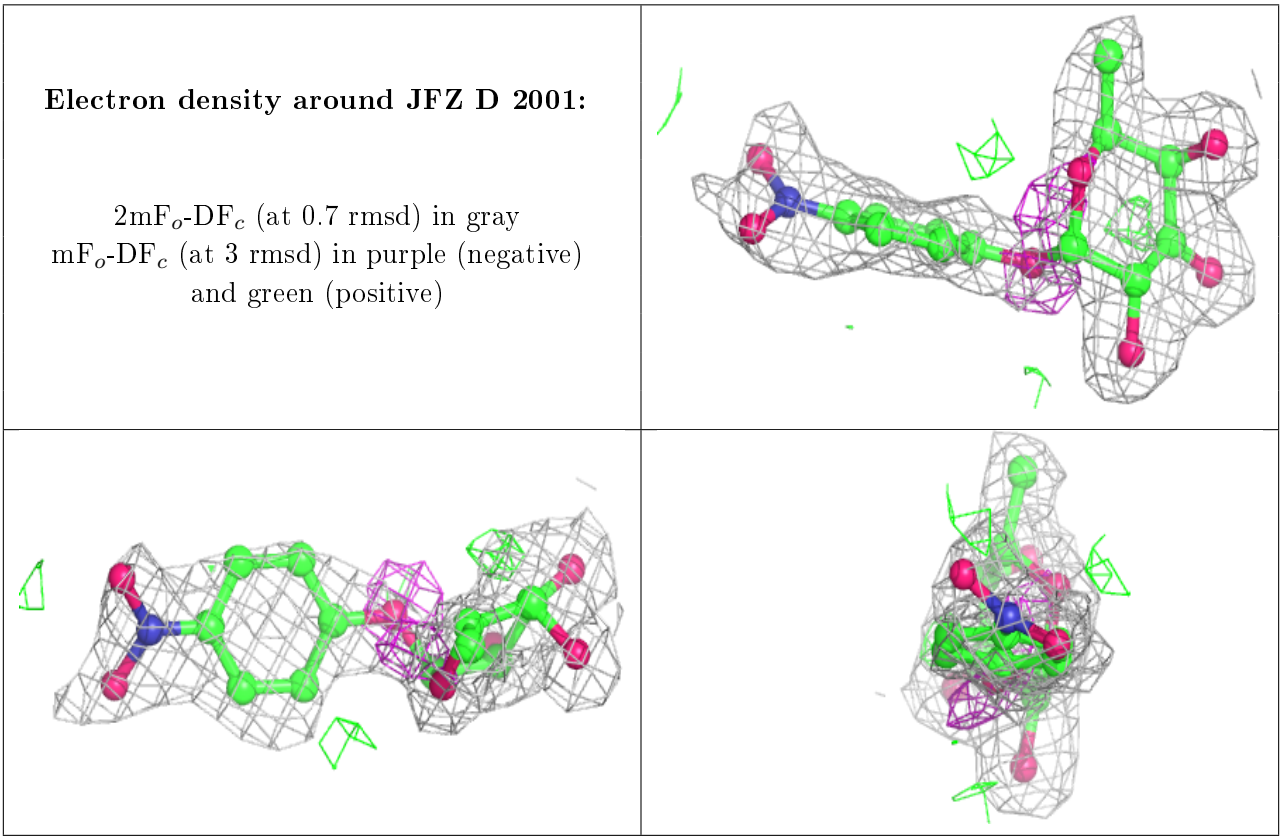
Electron density around JFZ C 2001:

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



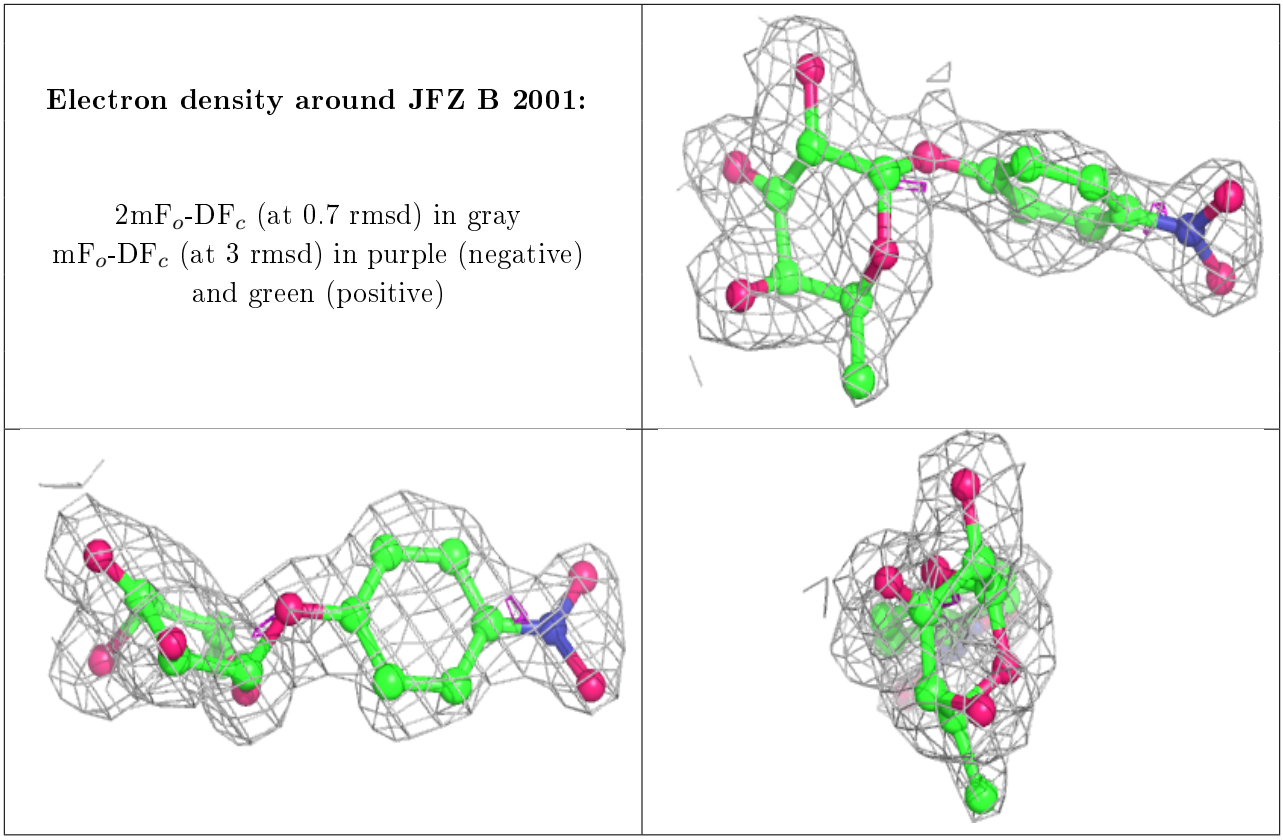
Electron density around JFZ D 2001:

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



Electron density around JFZ B 2001:

$2mF_o$-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.