Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 08:40 AM EDT

PDB ID	:	4Q18
Title	:	Human dCK C4S-S74E mutant in complex with UDP and the inhibitor 4 [1-[5-(4-{[(2,6-diaminopyrimidin-4-yl)sulfanyl]methyl}-5-propyl-1,3-thiazol-2-yl)-2-methoxyphenoxy]-2-methylpropan-2-ol]
Authors	:	Nomme, J.; Lavie, A.
Deposited on	:	2014-04-03
Resolution	:	2.00 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:

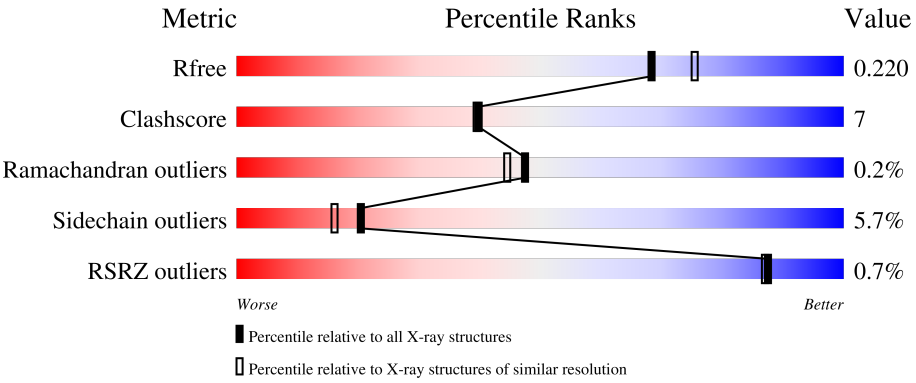
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	280	66% 15% · 18%
1	B	280	% 68% 14% · 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4089 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	3	0
			1921	1236	315	362	8			
1	B	231	Total	C	N	O	S	0	3	0
			1902	1224	314	356	8			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P27707
A	-18	GLY	-	expression tag	UNP P27707
A	-17	SER	-	expression tag	UNP P27707
A	-16	SER	-	expression tag	UNP P27707
A	-15	HIS	-	expression tag	UNP P27707
A	-14	HIS	-	expression tag	UNP P27707
A	-13	HIS	-	expression tag	UNP P27707
A	-12	HIS	-	expression tag	UNP P27707
A	-11	HIS	-	expression tag	UNP P27707
A	-10	HIS	-	expression tag	UNP P27707
A	-9	SER	-	expression tag	UNP P27707
A	-8	SER	-	expression tag	UNP P27707
A	-7	GLY	-	expression tag	UNP P27707
A	-6	LEU	-	expression tag	UNP P27707
A	-5	VAL	-	expression tag	UNP P27707
A	-4	PRO	-	expression tag	UNP P27707
A	-3	ARG	-	expression tag	UNP P27707
A	-2	GLY	-	expression tag	UNP P27707
A	-1	SER	-	expression tag	UNP P27707
A	0	HIS	-	expression tag	UNP P27707
A	9	SER	CYS	engineered mutation	UNP P27707
A	45	SER	CYS	engineered mutation	UNP P27707
A	59	SER	CYS	engineered mutation	UNP P27707
A	74	GLU	SER	engineered mutation	UNP P27707
A	146	SER	CYS	engineered mutation	UNP P27707

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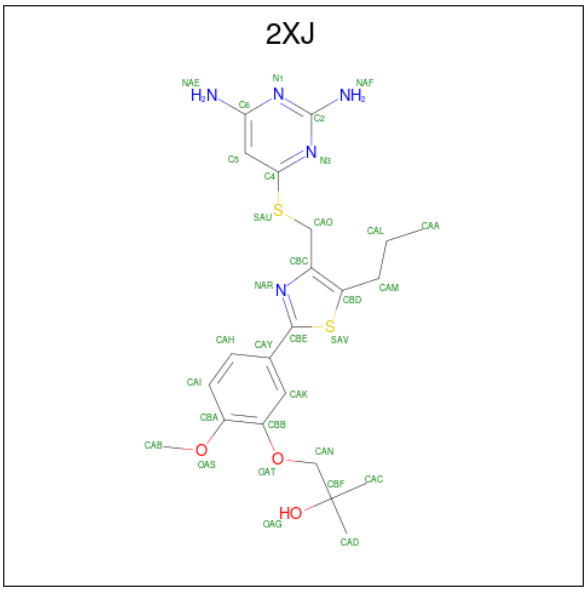
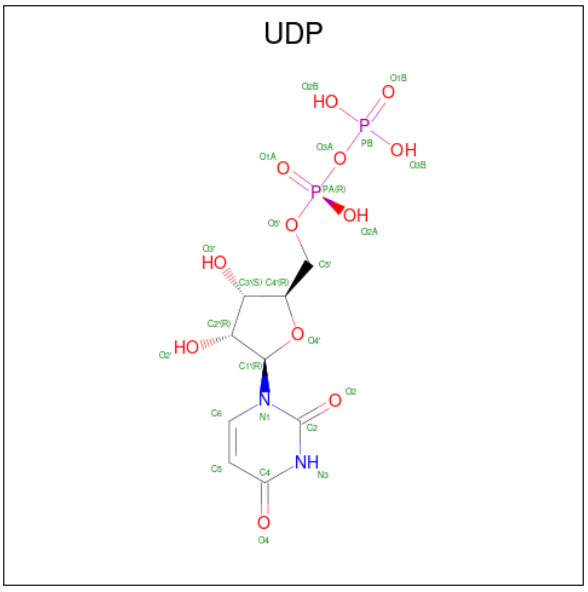
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP P27707
B	-18	GLY	-	expression tag	UNP P27707
B	-17	SER	-	expression tag	UNP P27707
B	-16	SER	-	expression tag	UNP P27707
B	-15	HIS	-	expression tag	UNP P27707
B	-14	HIS	-	expression tag	UNP P27707
B	-13	HIS	-	expression tag	UNP P27707
B	-12	HIS	-	expression tag	UNP P27707
B	-11	HIS	-	expression tag	UNP P27707
B	-10	HIS	-	expression tag	UNP P27707
B	-9	SER	-	expression tag	UNP P27707
B	-8	SER	-	expression tag	UNP P27707
B	-7	GLY	-	expression tag	UNP P27707
B	-6	LEU	-	expression tag	UNP P27707
B	-5	VAL	-	expression tag	UNP P27707
B	-4	PRO	-	expression tag	UNP P27707
B	-3	ARG	-	expression tag	UNP P27707
B	-2	GLY	-	expression tag	UNP P27707
B	-1	SER	-	expression tag	UNP P27707
B	0	HIS	-	expression tag	UNP P27707
B	9	SER	CYS	engineered mutation	UNP P27707
B	45	SER	CYS	engineered mutation	UNP P27707
B	59	SER	CYS	engineered mutation	UNP P27707
B	74	GLU	SER	engineered mutation	UNP P27707
B	146	SER	CYS	engineered mutation	UNP P27707

- Molecule 2 is 1-(5-(4-(((2,6-diaminopyrimidin-4-yl)thio)methyl)-5-propylthiazol-2-yl)-2-methoxyphenoxy)-2-methylpropan-2-ol (three-letter code: 2XJ) (formula: $C_{22}H_{29}N_5O_3S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	22	5	3	2		
2	A	1	Total	C	N	O	S	0	0
			32	22	5	3	2		
2	B	1	Total	C	N	O	S	0	0
			32	22	5	3	2		
2	B	1	Total	C	N	O	S	0	0
			32	22	5	3	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is water.

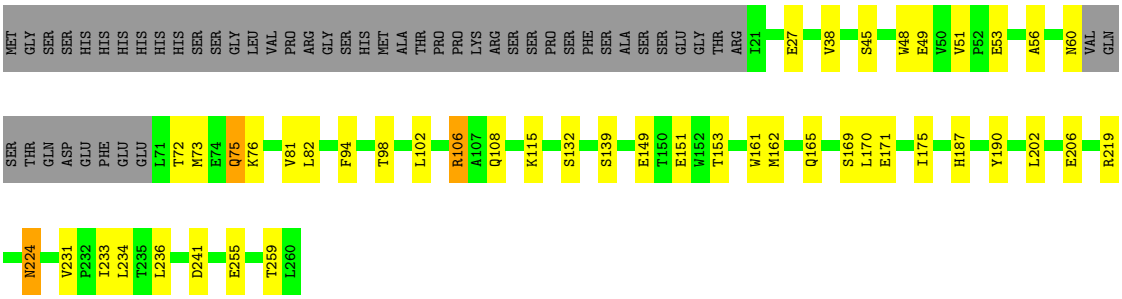
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	44	Total	O	0	0
			44	44		

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.

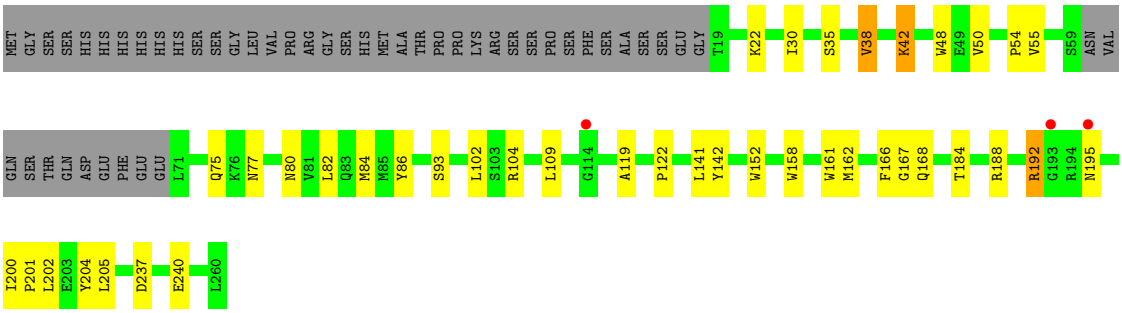
• Molecule 1: Deoxycytidine kinase

Chain A:



• Molecule 1: Deoxycytidine kinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	68.75Å 68.75Å 122.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.97 – 2.00 27.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (27.97-2.00) 99.4 (27.97-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.183 , 0.216 0.190 , 0.220	Depositor DCC
R_{free} test set	1911 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.504 for H, K, L 0.496 for -H, K, -L	Depositor
Outliers	1 of 38119 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4089	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: 2XJ, UDP

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	0/1977	0.74	1/2675 (0.0%)
1	B	0.53	0/1957	0.72	0/2652
All	All	0.53	0/3934	0.73	1/5327 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	ARG	NE-CZ-NH1	6.31	123.45	120.30

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	1921	0	1854	25	0
1	B	1902	0	1823	32	0
2	A	64	0	56	2	0
2	B	64	0	57	14	0
3	A	25	0	11	0	0
3	B	25	0	11	0	0
4	A	44	0	0	2	1
4	B	44	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4089	0	3812	57	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (57) 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)
2:B:403:2XJ:CAO	2:B:403:2XJ:CAL	2.32	1.04
2:B:403:2XJ:CAO	2:B:403:2XJ:H18	1.94	0.96
2:A:301:2XJ:H19	2:A:302:2XJ:H22	1.49	0.90
1:B:86[B]:TYR:CE2	2:B:403:2XJ:N3	2.29	0.90
2:B:403:2XJ:CAO	2:B:403:2XJ:H19	2.10	0.79
1:B:42:LYS:O	4:B:534:HOH:O	2.06	0.72
1:B:166:PHE:HA	4:B:536:HOH:O	1.91	0.70
1:A:82:LEU:HD11	2:A:301:2XJ:H22	1.72	0.70
1:A:49:GLU:HG3	4:A:433:HOH:O	1.93	0.69
1:B:86[B]:TYR:HE1	2:B:403:2XJ:NAR	1.90	0.68
1:A:72:THR:N	1:A:75:GLN:OE1	2.27	0.67
1:B:48:TRP:O	4:B:534:HOH:O	2.13	0.66
1:A:151:GLU:OE2	4:A:404:HOH:O	2.14	0.66
1:B:86[B]:TYR:OH	2:B:403:2XJ:H19	2.02	0.60
1:A:219:ARG:CZ	1:A:233:ILE:HD12	2.32	0.60
1:B:166:PHE:CA	4:B:536:HOH:O	2.49	0.59
1:B:38:VAL:HG13	1:B:50:VAL:HG11	1.87	0.56
1:B:192:ARG:HB3	4:B:533:HOH:O	2.06	0.55
1:A:161:TRP:CZ2	1:A:165:GLN:HG3	2.43	0.53
2:B:403:2XJ:H18	2:B:403:2XJ:H24	1.86	0.52
1:B:204:TYR:HE1	2:B:402:2XJ:H3	1.75	0.51
1:A:161:TRP:CE2	1:A:165:GLN:HG3	2.47	0.50
1:A:187:HIS:O	1:A:190:TYR:HB3	2.12	0.50
1:B:80:ASN:O	1:B:84[B]:MET:HG3	2.13	0.48
1:B:201:PRO:HD3	2:B:403:2XJ:CBB	2.44	0.47
1:B:158:TRP:O	1:B:162:MET:HB3	2.14	0.47
1:A:202:LEU:O	1:A:206:GLU:N	2.41	0.46
1:B:167:GLY:O	1:B:168:GLN:HB2	2.15	0.46
1:B:200:ILE:HG12	2:B:403:2XJ:CBE	2.45	0.46
1:B:119:ALA:HB3	1:B:122:PRO:HB3	1.97	0.46
1:B:184:THR:O	1:B:188:ARG:N	2.40	0.46
1:B:142:TYR:CD2	1:B:152:TRP:CD1	3.04	0.46
1:B:54:PRO:HG2	1:B:104:ARG:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HD11	1:B:166:PHE:CE1	2.51	0.45
1:B:86[B]:TYR:OH	2:B:403:2XJ:CAL	2.64	0.44
1:B:86[B]:TYR:HE2	2:B:403:2XJ:N3	2.02	0.44
1:B:237:ASP:OD1	1:B:237:ASP:C	2.56	0.44
1:A:234:LEU:HD21	1:A:236:LEU:HD21	1.99	0.44
1:A:153:THR:HG22	1:B:77:ASN:HD21	1.83	0.44
1:A:53:GLU:O	1:A:56:ALA:HB3	2.18	0.43
1:B:141:LEU:HD23	2:B:402:2XJ:H1	2.00	0.43
1:A:162:MET:SD	1:B:162:MET:CE	3.06	0.43
1:A:161:TRP:CE3	1:B:102:LEU:CD1	3.02	0.42
1:A:170:LEU:O	1:A:171:GLU:C	2.57	0.42
1:A:94:PHE:O	1:A:98:THR:HG23	2.20	0.42
1:A:106:ARG:HH21	1:B:161:TRP:CB	2.33	0.41
1:A:27:GLU:OE2	1:A:132:SER:OG	2.35	0.41
1:B:38:VAL:CG1	1:B:50:VAL:HG11	2.50	0.41
1:A:175:ILE:HB	1:A:233:ILE:HG12	2.02	0.41
1:A:72:THR:O	1:A:75:GLN:HG2	2.21	0.41
1:A:102:LEU:HD11	1:B:158:TRP:CD1	2.55	0.41
1:A:51:VAL:HG11	1:A:108:GLN:HG2	2.02	0.41
1:A:224:ASN:HD22	1:A:224:ASN:HA	1.69	0.41
1:B:30:ILE:HD13	2:B:403:2XJ:H17	2.02	0.40
1:A:45:SER:HB3	1:A:48:TRP:CG	2.56	0.40
1:A:255:GLU:O	1:A:259:THR:HG23	2.22	0.40
1:B:202:LEU:HA	1:B:205:LEU:HD12	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:444:HOH:O	4:B:541:HOH:O[3_455]	1.61	0.59

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	229/280 (82%)	215 (94%)	13 (6%)	1 (0%)	34 30
1	B	230/280 (82%)	222 (96%)	8 (4%)	0	100 100
All	All	459/560 (82%)	437 (95%)	21 (5%)	1 (0%)	47 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	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	209/256 (82%)	197 (94%)	12 (6%)	20 16
1	B	203/256 (79%)	192 (95%)	11 (5%)	22 18
All	All	412/512 (80%)	389 (94%)	23 (6%)	20 17

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	60	ASN
1	A	73	MET
1	A	75	GLN
1	A	76	LYS
1	A	81	VAL
1	A	115	LYS
1	A	139	SER
1	A	149	GLU
1	A	224	ASN
1	A	231	VAL
1	A	241	ASP
1	B	22	LYS

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Mol	Chain	Res	Type
1	B	35	SER
1	B	38	VAL
1	B	42	LYS
1	B	55	VAL
1	B	75	GLN
1	B	82	LEU
1	B	93	SER
1	B	192	ARG
1	B	195	ASN
1	B	240	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	168	GLN
1	A	224	ASN
1	A	229	GLN
1	B	75	GLN
1	B	163	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)

6 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	2XJ	B	402	-	32,34,34	2.88	6 (18%)	30,48,48	3.16	10 (33%)
2	2XJ	A	302	-	32,34,34	1.79	3 (9%)	30,48,48	2.52	9 (30%)
2	2XJ	A	301	-	32,34,34	1.99	6 (18%)	30,48,48	2.92	6 (20%)
3	UDP	A	303	-	24,26,26	1.11	3 (12%)	37,40,40	1.61	8 (21%)
3	UDP	B	401	-	24,26,26	1.21	3 (12%)	37,40,40	1.62	6 (16%)
2	2XJ	B	403	-	32,34,34	2.68	5 (15%)	30,48,48	2.73	9 (30%)

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	2XJ	B	402	-	-	10/17/20/20	0/3/3/3
2	2XJ	A	302	-	-	4/17/20/20	0/3/3/3
2	2XJ	A	301	-	-	7/17/20/20	0/3/3/3
3	UDP	A	303	-	-	1/16/32/32	0/2/2/2
3	UDP	B	401	-	-	1/16/32/32	0/2/2/2
2	2XJ	B	403	-	-	6/17/20/20	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	2XJ	CBD-SAV	-12.50	1.50	1.74
2	B	402	2XJ	CBE-SAV	-11.94	1.57	1.73
2	B	402	2XJ	CBD-SAV	-7.69	1.59	1.74
2	A	302	2XJ	CBE-SAV	-7.35	1.63	1.73
2	A	301	2XJ	CBD-SAV	-6.26	1.62	1.74
2	B	403	2XJ	CBE-SAV	-5.29	1.66	1.73
2	B	402	2XJ	CBC-CBD	-4.90	1.33	1.42
2	A	301	2XJ	CBE-SAV	-4.86	1.67	1.73
2	B	403	2XJ	CBC-CBD	-4.55	1.33	1.42
2	A	302	2XJ	CBC-CBD	-4.30	1.34	1.42
2	A	301	2XJ	CBC-CBD	-4.29	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	2XJ	CBD-SAV	-4.11	1.66	1.74
2	A	301	2XJ	C4-SAU	3.94	1.83	1.76
2	A	301	2XJ	CAM-CBD	3.73	1.52	1.50
2	B	402	2XJ	CBE-NAR	2.86	1.35	1.31
3	B	401	UDP	C4-N3	-2.73	1.33	1.38
2	B	402	2XJ	C4-SAU	2.70	1.81	1.76
3	B	401	UDP	C2-N3	-2.44	1.33	1.38
3	A	303	UDP	C2-N1	2.39	1.42	1.38
2	A	301	2XJ	CAO-CBC	-2.38	1.48	1.50
2	B	403	2XJ	C4-SAU	2.38	1.80	1.76
3	B	401	UDP	C2-N1	2.31	1.42	1.38
3	A	303	UDP	C4-N3	-2.12	1.34	1.38
2	B	402	2XJ	C4-N3	2.08	1.35	1.33
2	B	403	2XJ	CAM-CBD	-2.05	1.50	1.50
3	A	303	UDP	C6-C5	2.00	1.39	1.35

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	2XJ	C2-N3-C4	10.50	123.23	115.50
2	B	402	2XJ	C2-N3-C4	10.38	123.15	115.50
2	A	301	2XJ	C5-C4-N3	-9.46	116.94	123.55
2	B	402	2XJ	C5-C4-N3	-9.46	116.94	123.55
2	B	403	2XJ	C2-N3-C4	7.17	120.78	115.50
2	A	302	2XJ	C2-N3-C4	6.89	120.57	115.50
2	B	403	2XJ	C5-C4-N3	-6.88	118.74	123.55
2	B	403	2XJ	CAB-OAS-CBA	-6.71	107.40	117.53
2	A	302	2XJ	C5-C4-N3	-5.94	119.40	123.55
2	B	403	2XJ	CAO-SAU-C4	-5.58	95.34	102.65
2	B	402	2XJ	CAO-SAU-C4	5.38	109.69	102.65
2	B	402	2XJ	CAM-CBD-CBC	-4.68	123.65	127.47
2	A	302	2XJ	CAB-OAS-CBA	-4.52	110.71	117.53
2	A	302	2XJ	CAO-SAU-C4	4.49	108.53	102.65
3	A	303	UDP	N3-C2-N1	4.30	120.59	114.89
3	B	401	UDP	C4-N3-C2	-4.27	120.94	126.58
3	A	303	UDP	C4-N3-C2	-4.14	121.12	126.58
3	B	401	UDP	N3-C2-N1	3.90	120.06	114.89
3	B	401	UDP	C5-C4-N3	3.88	120.65	114.84
2	A	302	2XJ	CAN-OAT-CBB	-3.77	108.47	117.67
2	A	302	2XJ	CAL-CAM-CBD	-3.44	102.65	115.27
3	A	303	UDP	C5-C4-N3	3.28	119.75	114.84
2	A	301	2XJ	N1-C2-N3	-3.27	120.29	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	2XJ	CBC-CAO-SAU	-3.14	102.98	109.96
3	A	303	UDP	O4-C4-C5	-2.93	120.01	125.16
2	A	301	2XJ	NAE-C6-N1	2.88	121.04	116.49
2	A	302	2XJ	CBC-CAO-SAU	-2.86	103.61	109.96
2	B	402	2XJ	N1-C2-N3	-2.80	121.02	125.42
2	A	302	2XJ	N1-C2-N3	-2.78	121.05	125.42
3	B	401	UDP	O4'-C1'-N1	2.61	114.33	108.36
2	B	403	2XJ	CAA-CAL-CAM	-2.56	100.61	112.87
3	B	401	UDP	PA-O3A-PB	-2.54	124.11	132.83
3	A	303	UDP	C2'-C1'-N1	2.53	120.39	113.22
2	B	403	2XJ	NAE-C6-N1	2.49	120.42	116.49
2	B	402	2XJ	CAN-OAT-CBB	-2.47	111.64	117.67
2	B	403	2XJ	N1-C2-N3	-2.45	121.58	125.42
2	B	403	2XJ	SAU-C4-N3	2.37	122.86	118.78
2	B	402	2XJ	CAK-CBB-CBA	2.36	122.98	119.84
3	B	401	UDP	O4-C4-C5	-2.32	121.08	125.16
2	A	301	2XJ	CAO-SAU-C4	2.29	105.65	102.65
3	A	303	UDP	O2-C2-N1	-2.27	119.77	122.79
2	B	402	2XJ	CAL-CAM-CBD	-2.27	106.94	115.27
2	B	403	2XJ	CAL-CAM-CBD	-2.25	106.99	115.27
2	A	302	2XJ	NAE-C6-N1	2.21	119.98	116.49
3	A	303	UDP	O3B-PB-O1B	2.17	119.18	110.68
2	B	402	2XJ	OAS-CBA-CBB	2.15	118.40	115.41
3	A	303	UDP	O4'-C1'-N1	-2.09	103.59	108.36
2	B	402	2XJ	NAF-C2-N3	2.08	120.48	117.25

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	2XJ	OAT-CAN-CBF-CAC
2	A	301	2XJ	OAT-CAN-CBF-CAD
2	A	301	2XJ	OAT-CAN-CBF-OAG
2	A	301	2XJ	CBC-CAO-SAU-C4
2	A	302	2XJ	C5-C4-SAU-CAO
2	A	302	2XJ	N3-C4-SAU-CAO
2	B	402	2XJ	OAT-CAN-CBF-CAC
2	B	402	2XJ	OAT-CAN-CBF-CAD
2	B	402	2XJ	OAT-CAN-CBF-OAG
2	B	403	2XJ	OAT-CAN-CBF-CAC
2	B	403	2XJ	CAL-CAM-CBD-CBC
3	A	303	UDP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
2	A	301	2XJ	CAA-CAL-CAM-CBD
2	B	402	2XJ	CAA-CAL-CAM-CBD
2	B	402	2XJ	N3-C4-SAU-CAO
2	B	402	2XJ	CBA-CBB-OAT-CAN
2	B	402	2XJ	C5-C4-SAU-CAO
2	B	403	2XJ	OAT-CAN-CBF-CAD
2	B	403	2XJ	CAK-CBB-OAT-CAN
2	B	402	2XJ	CAK-CBB-OAT-CAN
3	B	401	UDP	PA-O3A-PB-O3B
2	B	403	2XJ	CBA-CBB-OAT-CAN
2	B	403	2XJ	OAT-CAN-CBF-OAG
2	B	402	2XJ	CAL-CAM-CBD-CBC
2	A	301	2XJ	C5-C4-SAU-CAO
2	A	301	2XJ	N3-C4-SAU-CAO
2	A	302	2XJ	CAL-CAM-CBD-CBC
2	A	302	2XJ	CBC-CAO-SAU-C4
2	B	402	2XJ	CBC-CAO-SAU-C4

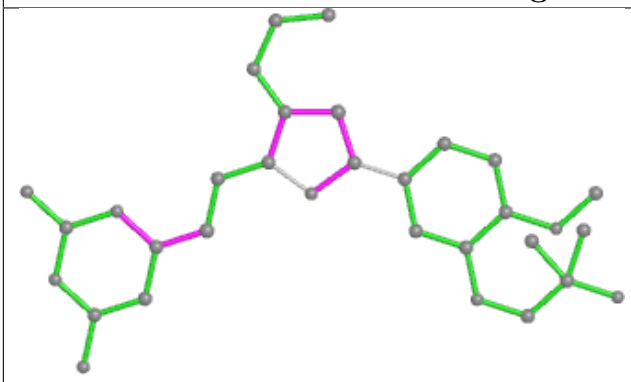
There are no ring outliers.

4 monomers are involved in 16 short contacts:

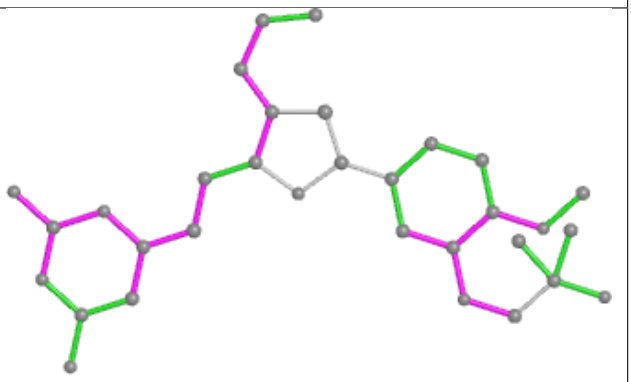
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	2XJ	2	0
2	A	302	2XJ	1	0
2	A	301	2XJ	2	0
2	B	403	2XJ	12	0

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.

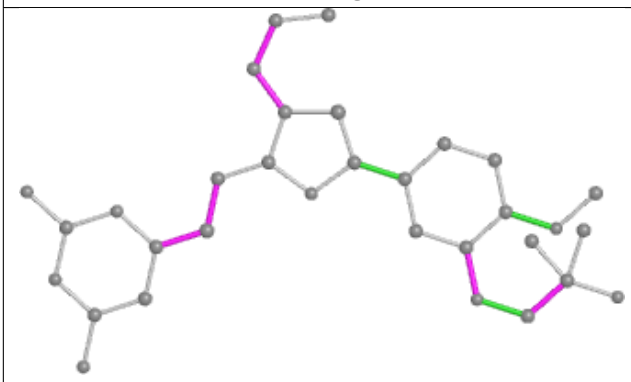
Ligand 2XJ B 402



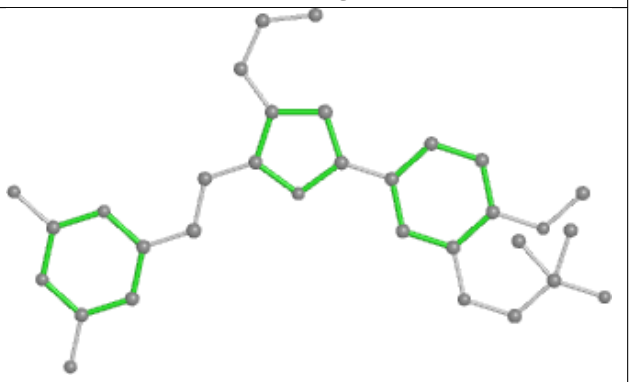
Bond lengths



Bond angles

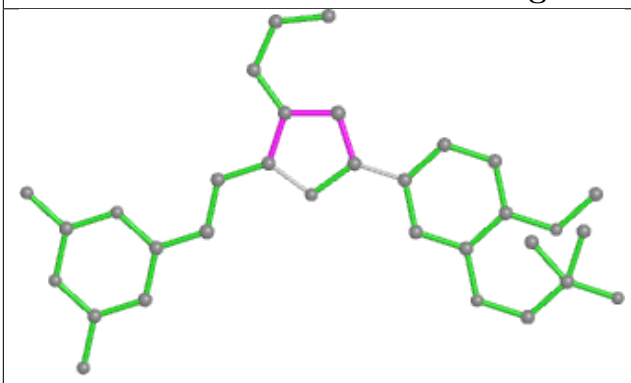


Torsions

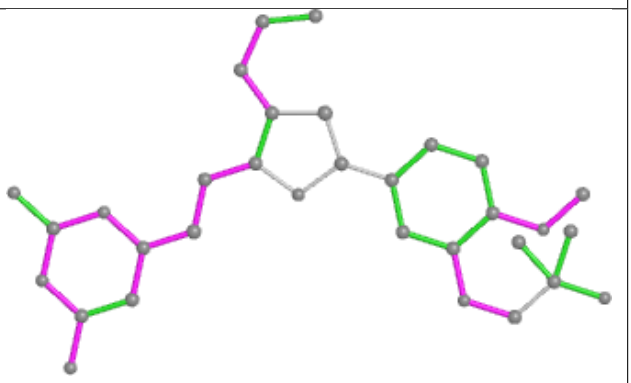


Rings

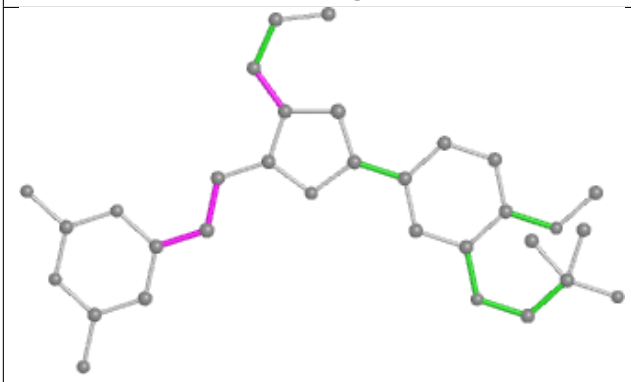
Ligand 2XJ A 302



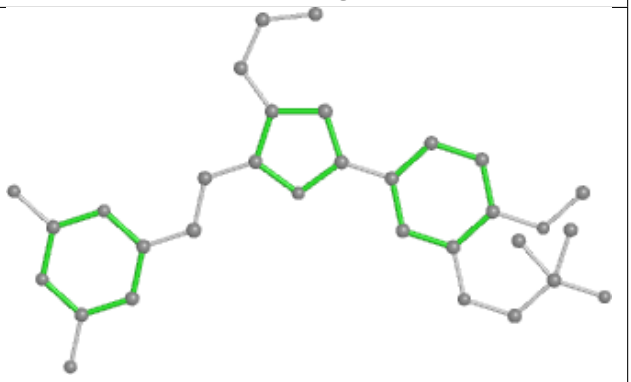
Bond lengths



Bond angles

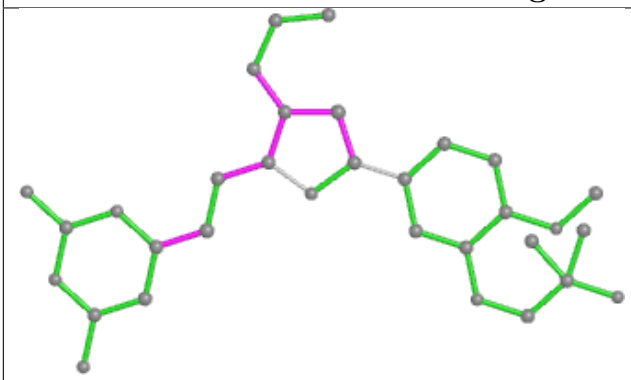


Torsions

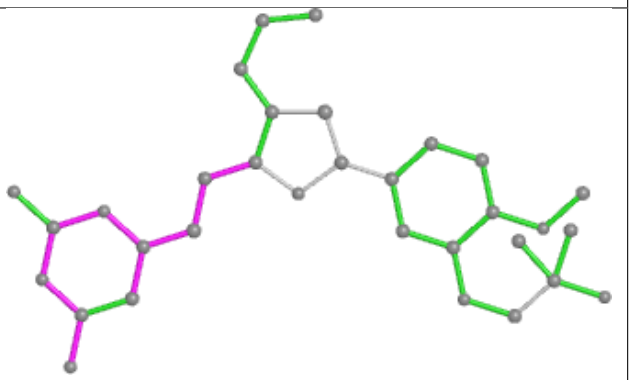


Rings

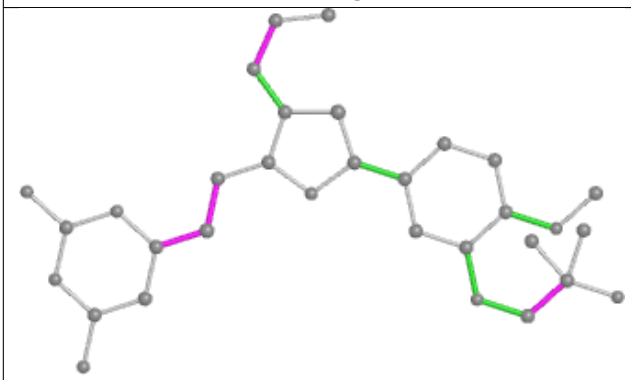
Ligand 2XJ A 301



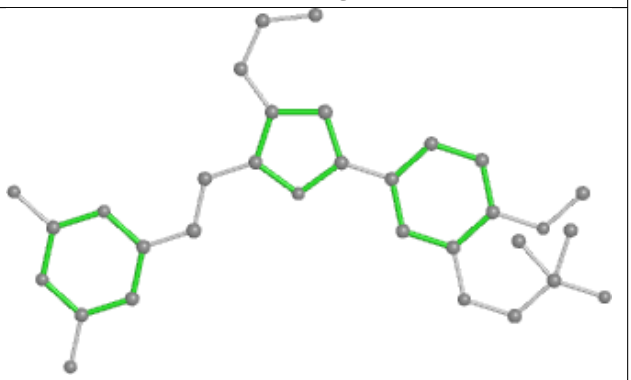
Bond lengths



Bond angles

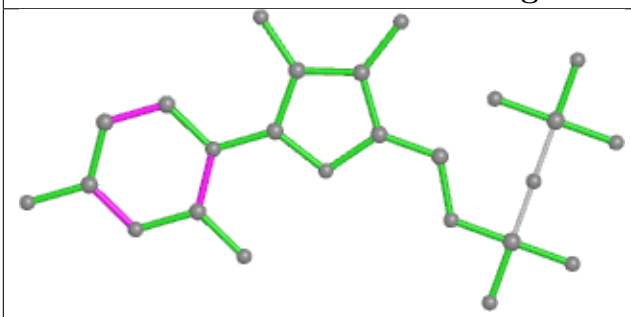


Torsions

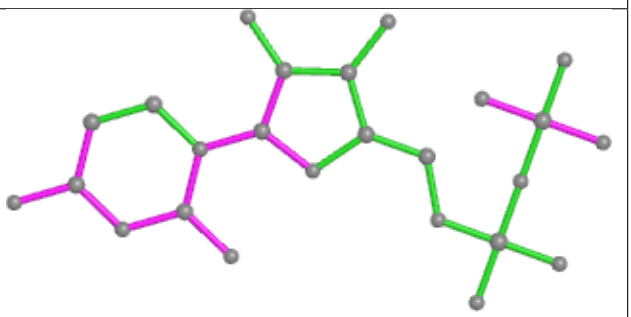


Rings

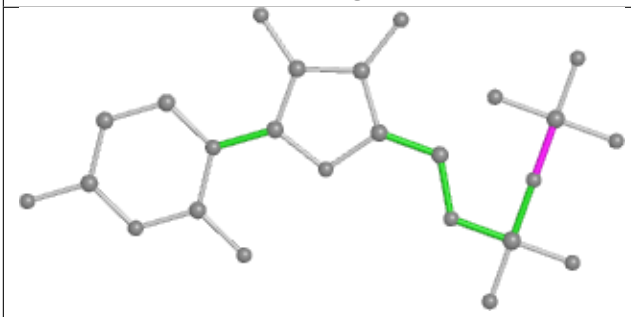
Ligand UDP A 303



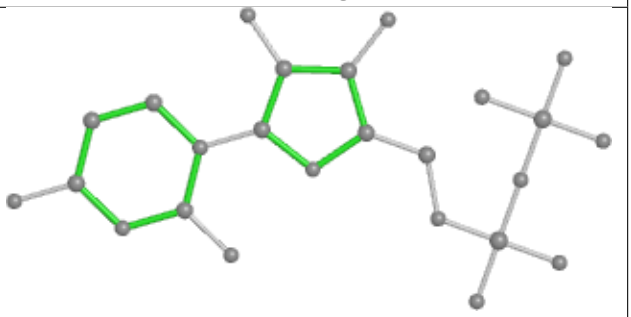
Bond lengths



Bond angles

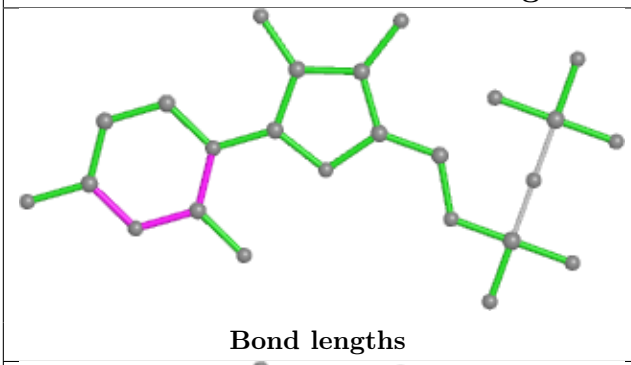


Torsions

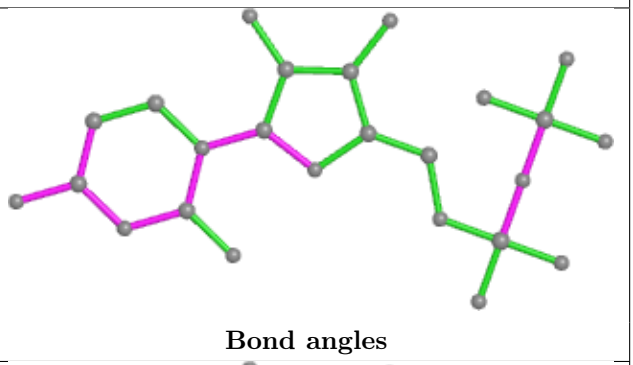


Rings

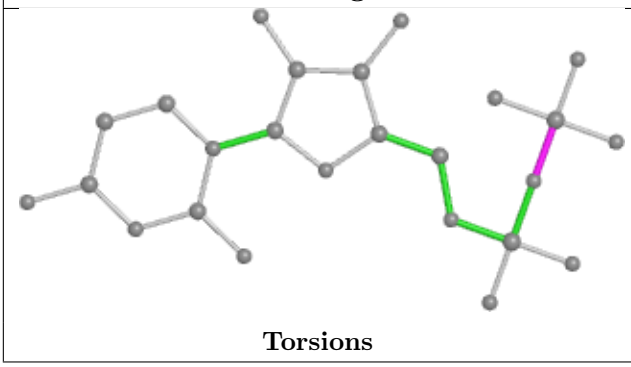
Ligand UDP B 401



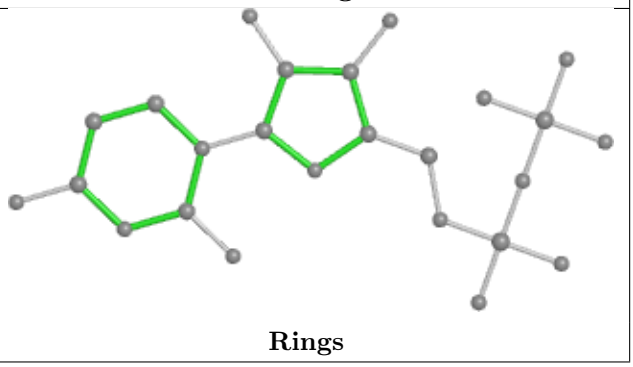
Bond lengths



Bond angles

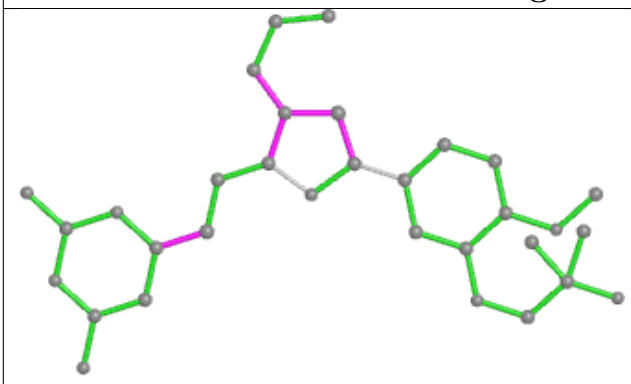


Torsions

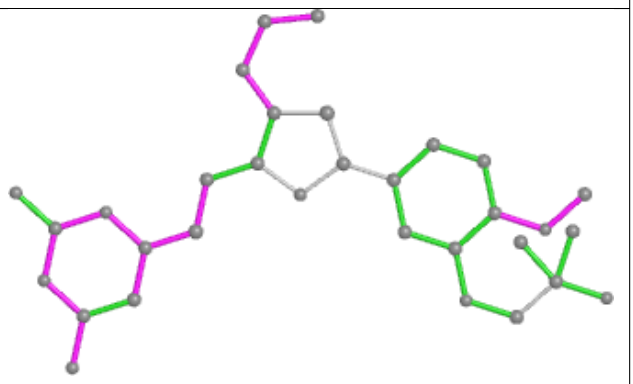


Rings

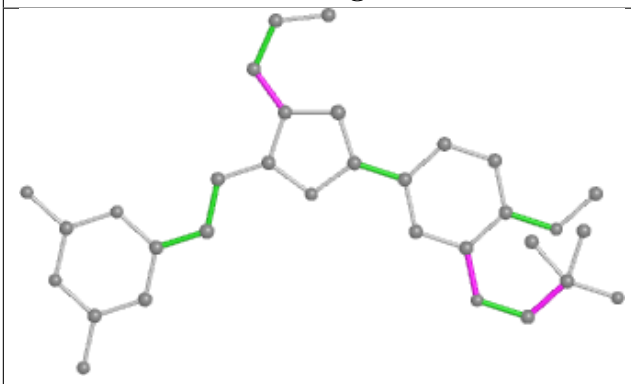
Ligand 2XJ B 403



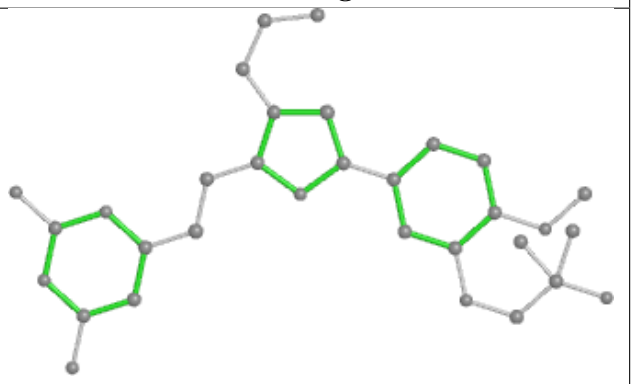
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	230/280 (82%)	-0.25	0 100 100	31, 45, 64, 71	0
1	B	231/280 (82%)	-0.21	3 (1%) 77 76	33, 45, 63, 84	0
All	All	461/560 (82%)	-0.23	3 (0%) 87 87	31, 45, 64, 84	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	GLY	3.7
1	B	193	GLY	2.8
1	B	195	ASN	2.4

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
2	2XJ	A	302	32/32	0.89	0.21	38,43,54,59	32
2	2XJ	B	403	32/32	0.91	0.23	36,40,45,45	32

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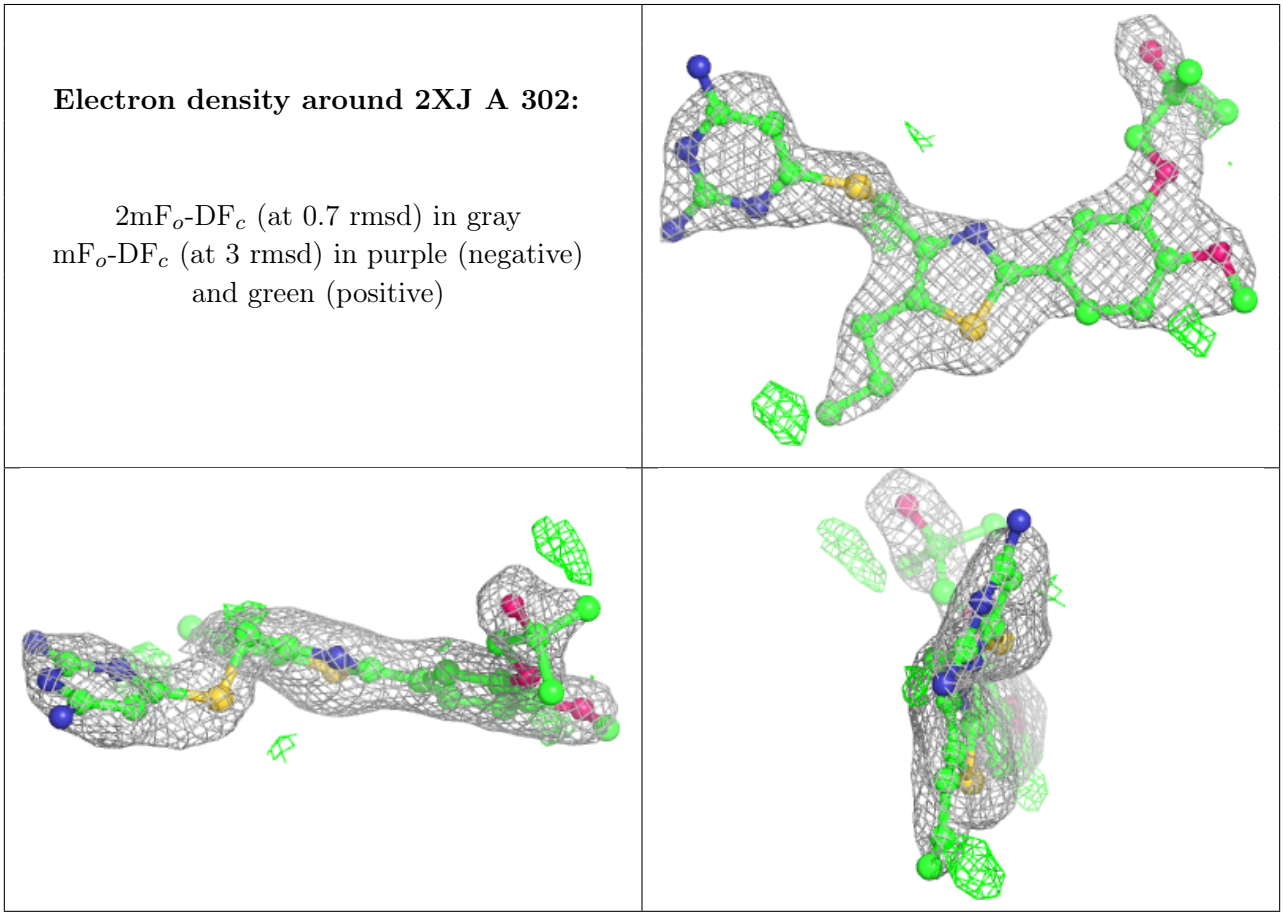
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	2XJ	B	402	32/32	0.96	0.13	36,52,67,71	0
2	2XJ	A	301	32/32	0.96	0.13	34,47,57,63	0
3	UDP	A	303	25/25	0.98	0.09	42,49,59,61	0
3	UDP	B	401	25/25	0.98	0.09	37,50,54,57	0

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.

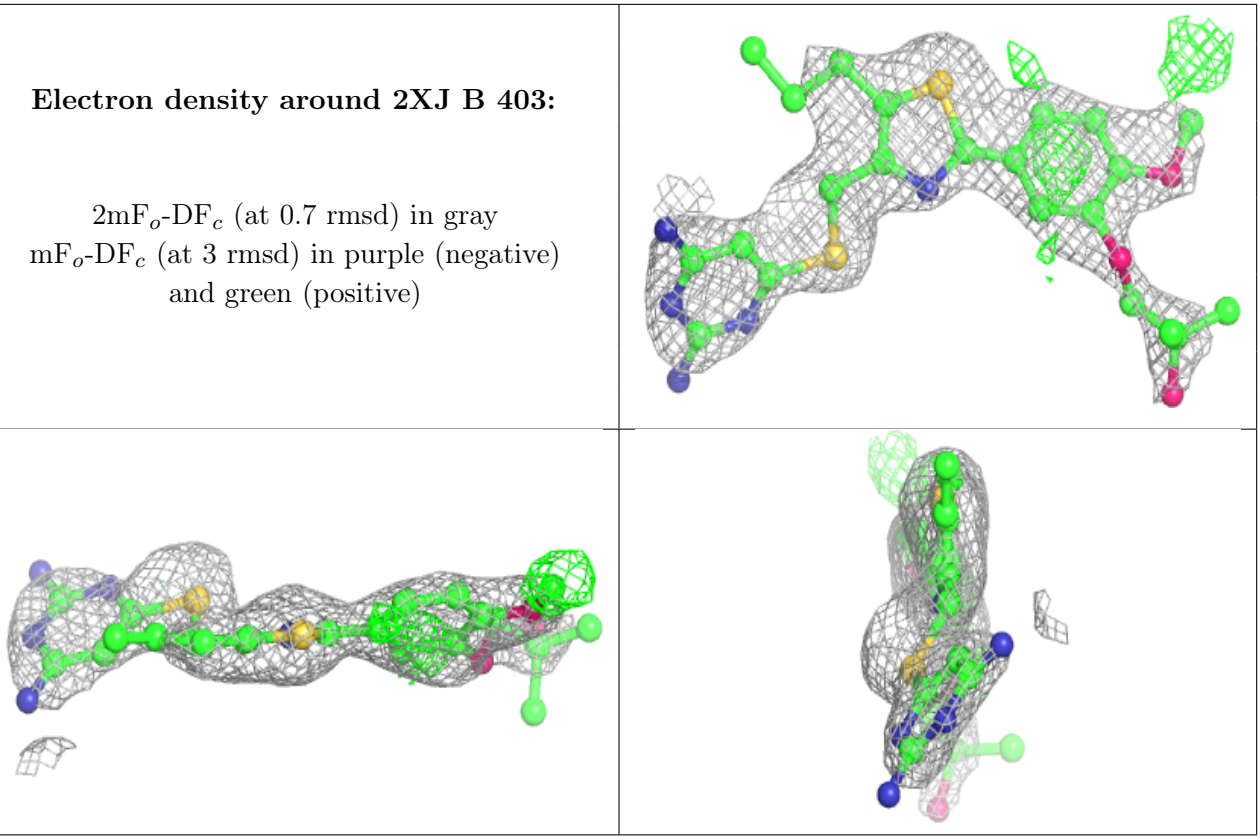
Electron density around 2XJ A 302:

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



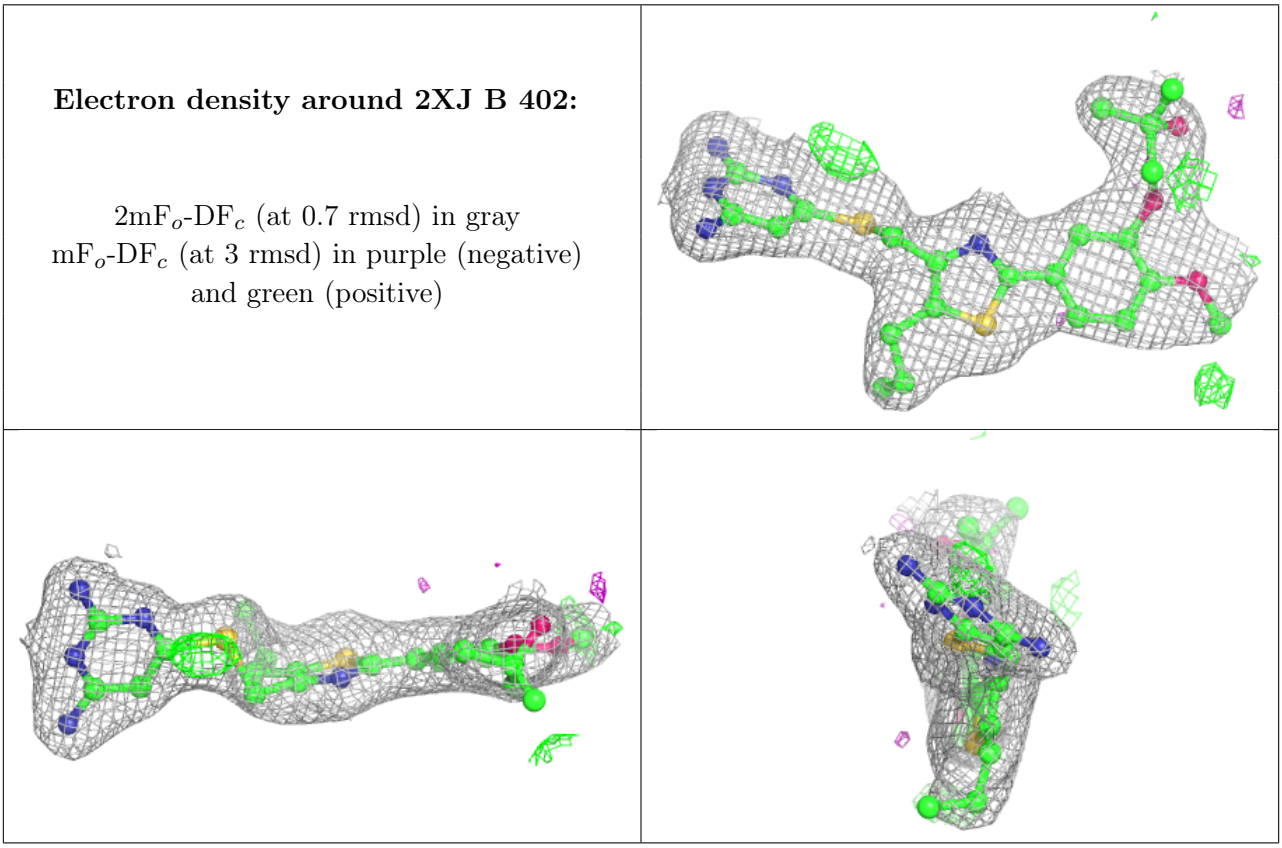
Electron density around 2XJ B 403:

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



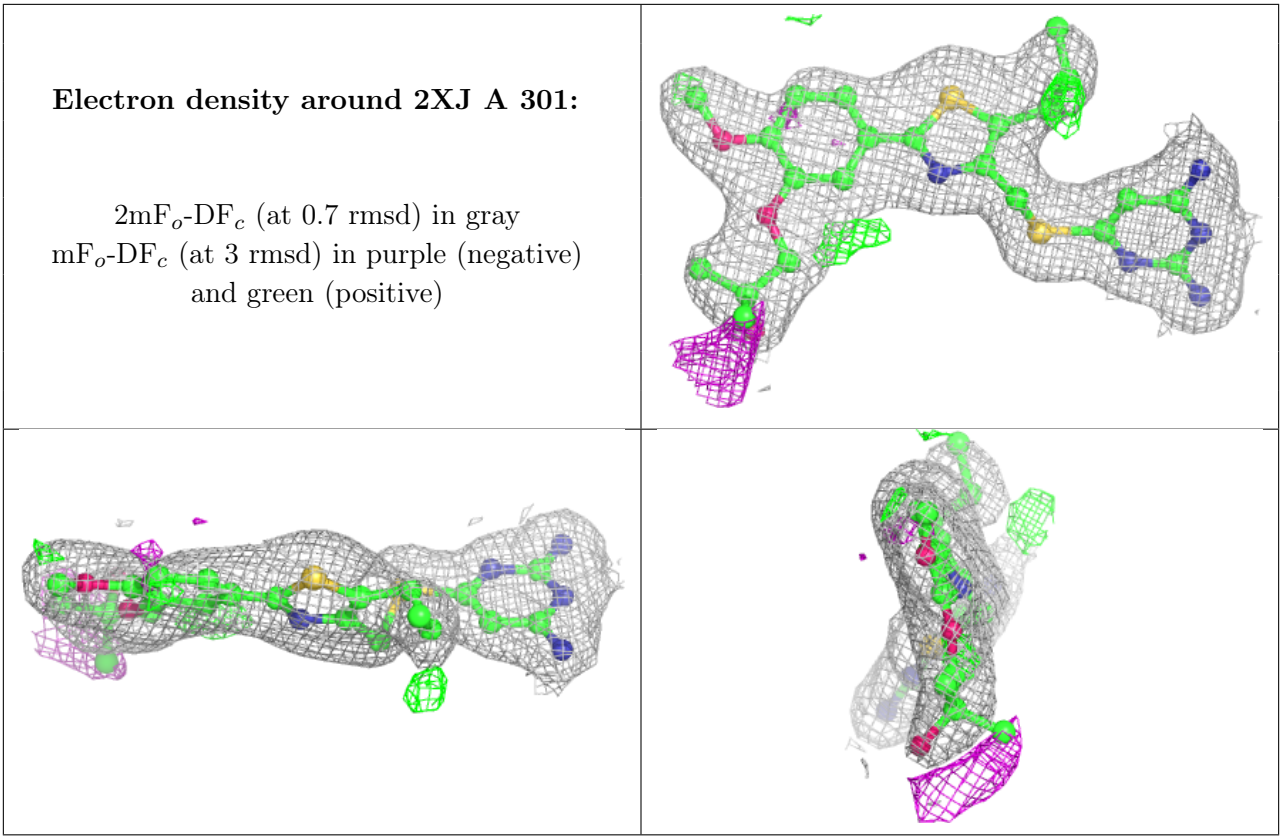
Electron density around 2XJ B 402:

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



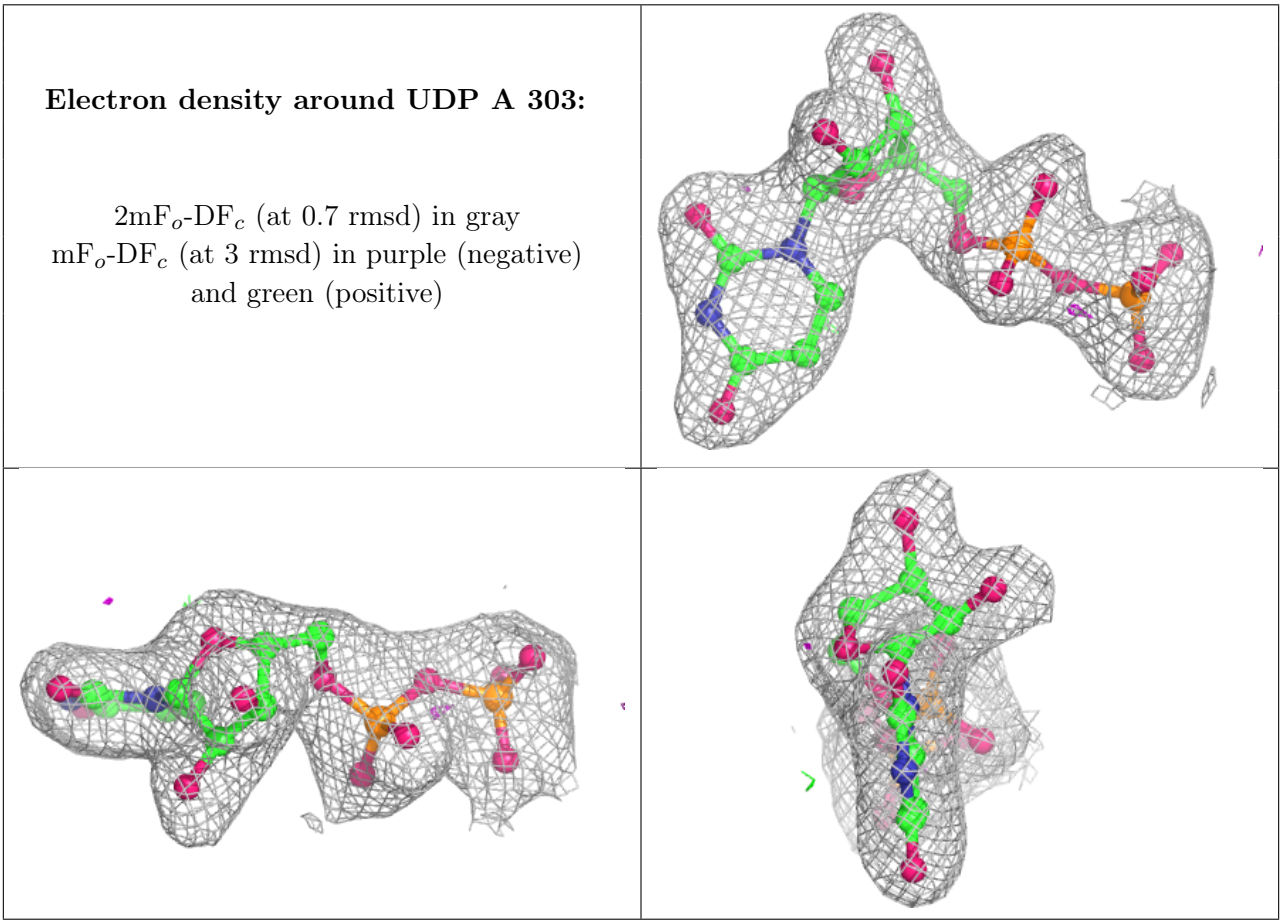
Electron density around 2XJ A 301:

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



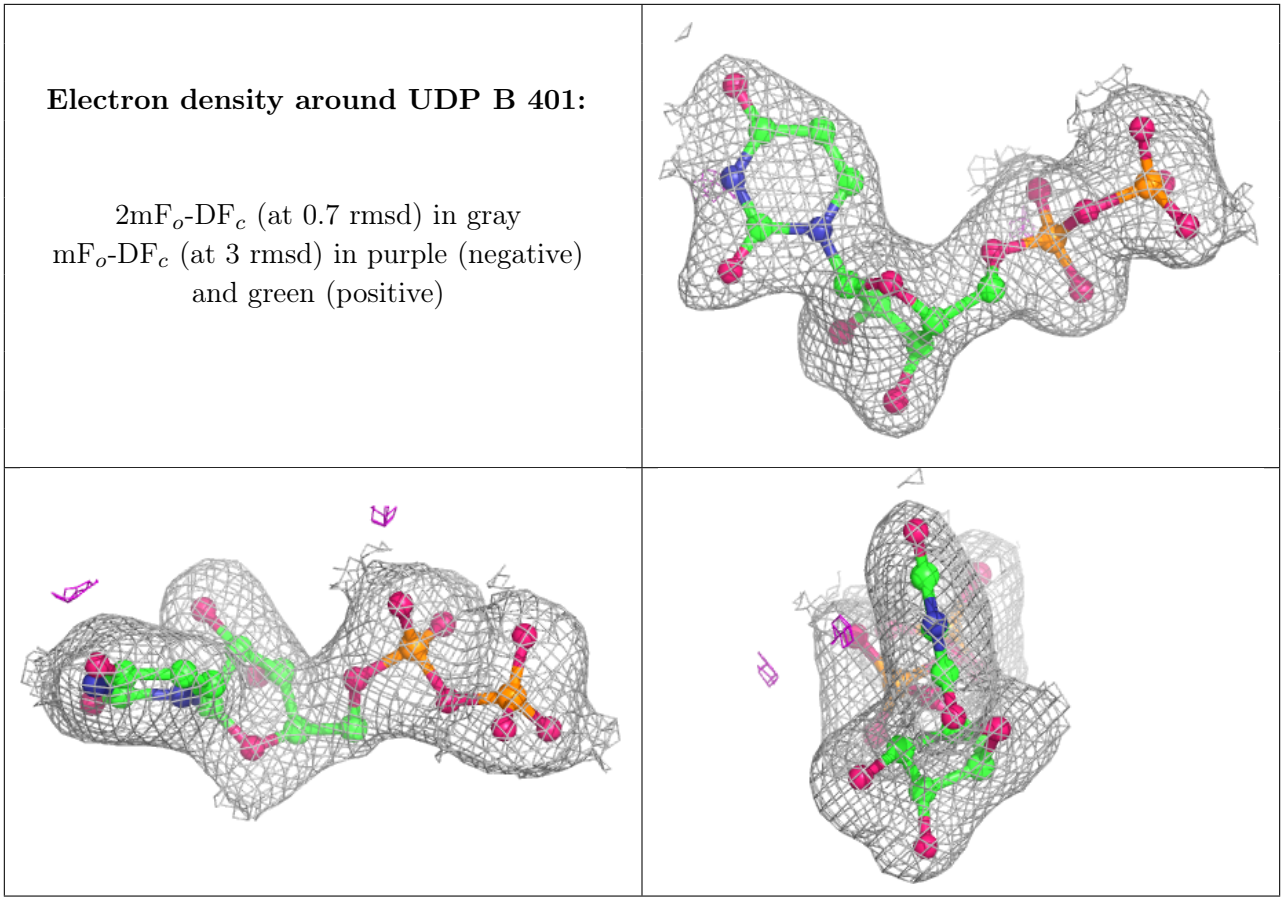
Electron density around UDP A 303:

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



Electron density around UDP B 401:

$2mF_o$-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.