



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 06:36 PM JST

PDB ID : 5H63  
Title : Structure of Transferase mutant-C23S,C199S  
Authors : Park, J.B.; Yoo, Y.; Kim, J.  
Deposited on : 2016-11-10  
Resolution : 1.92 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](mailto: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>.

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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 : 2.36  
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) : 2.36

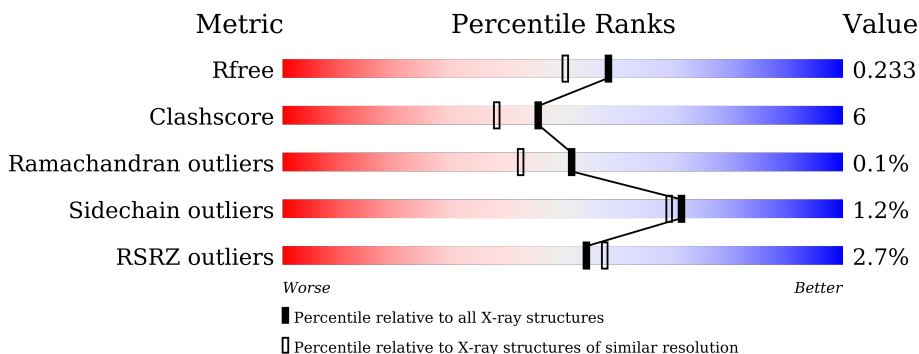
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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  $\geq 3$ , 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	348	2% 78% 9% • 11%
1	B	348	% 80% 8% • 11%
1	C	348	3% 74% 12% • 13%
1	D	348	3% 75% 11% • 13%

## 2 Entry composition [i](#)

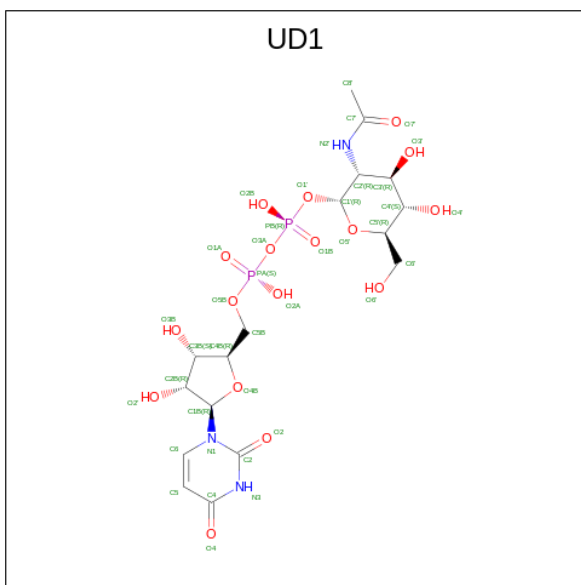
There are 4 unique types of molecules in this entry. The entry contains 10767 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	Total	C	N	O	S	0	0	0
			2491	1590	427	467	7			
1	B	309	Total	C	N	O	S	0	0	0
			2491	1590	427	467	7			
1	C	302	Total	C	N	O	S	0	0	0
			2436	1557	416	456	7			
1	D	302	Total	C	N	O	S	0	0	0
			2436	1557	416	456	7			

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGUCOSAMINE (three-letter code: UD1) (formula:  $C_{17}H_{27}N_3O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

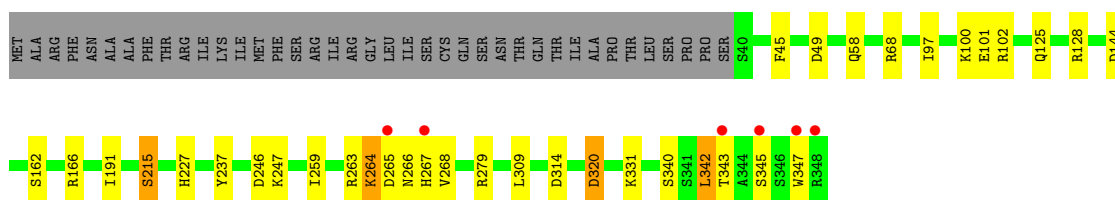
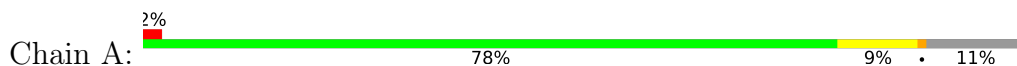
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total	O	0	0
			222	222		
4	B	195	Total	O	0	0
			195	195		
4	C	169	Total	O	0	0
			169	169		
4	D	165	Total	O	0	0
			165	165		

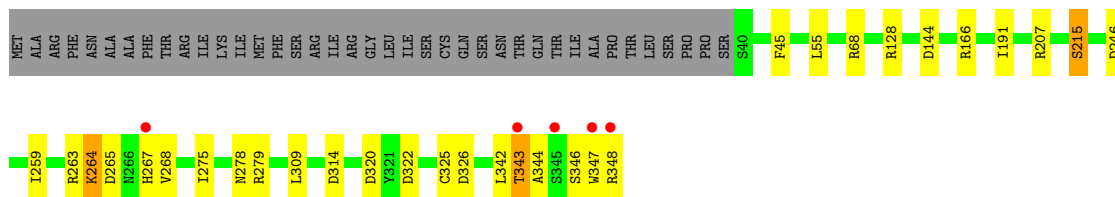
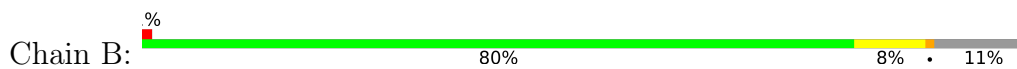
### 3 Residue-property plots

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.

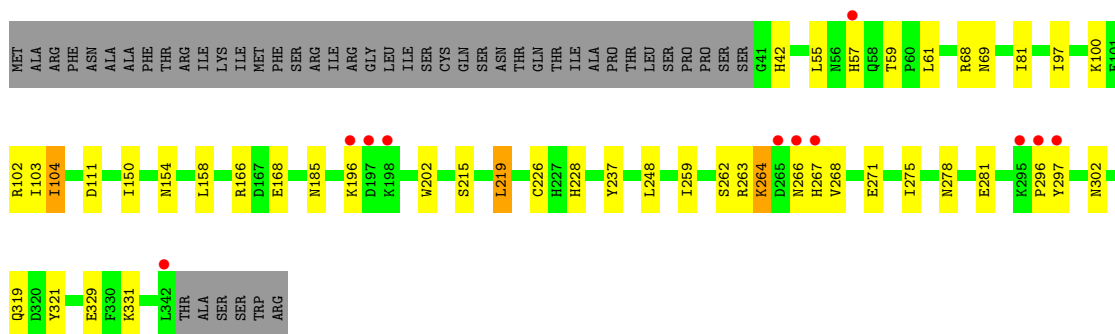
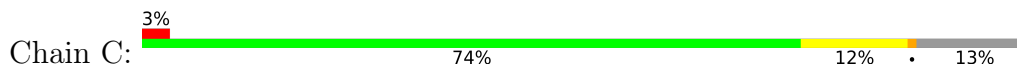
- Molecule 1: Transferase



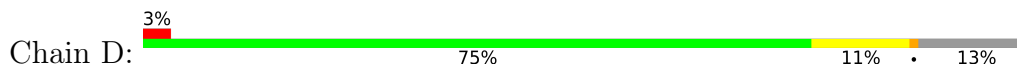
- Molecule 1: Transferase

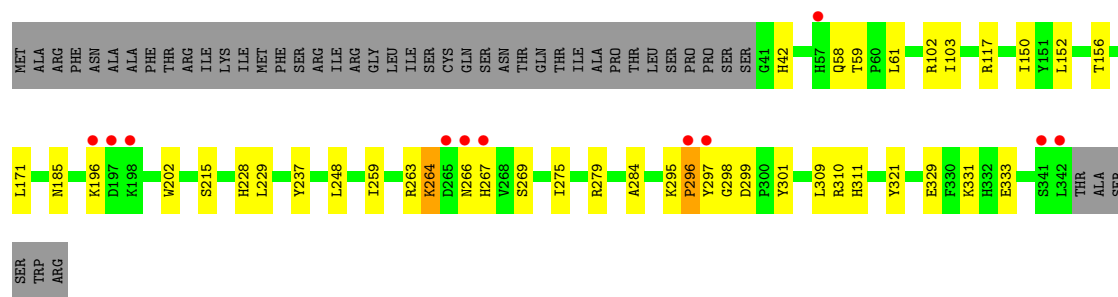


- Molecule 1: Transferase



- Molecule 1: Transferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.57Å 52.28Å 143.75Å 90.00° 90.00° 108.00°	Depositor
Resolution (Å)	44.80 – 1.92 41.14 – 1.92	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.80-1.92) 94.4 (41.14-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 1.92Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.184 , 0.228 0.192 , 0.233	Depositor DCC
$R_{free}$ test set	4960 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 28.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.457 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10767	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, UD1

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	0.93	2/2552 (0.1%)	0.96	7/3453 (0.2%)
1	B	0.93	2/2552 (0.1%)	0.97	7/3453 (0.2%)
1	C	0.93	1/2495 (0.0%)	0.93	2/3375 (0.1%)
1	D	0.89	1/2495 (0.0%)	0.95	3/3375 (0.1%)
All	All	0.92	6/10094 (0.1%)	0.95	19/13656 (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	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	SER	CB-OG	-7.38	1.32	1.42
1	B	215	SER	CB-OG	-6.99	1.33	1.42
1	C	215	SER	CB-OG	-6.11	1.34	1.42
1	D	215	SER	CB-OG	-5.43	1.35	1.42
1	A	340	SER	CB-OG	-5.43	1.35	1.42
1	B	346	SER	CB-OG	-5.27	1.35	1.42

All (19) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	166	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	68	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	279	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	B	68	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	246	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	246	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	166	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	326	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	166	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	279	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	104	ILE	CG1-CB-CG2	-5.86	98.51	111.40
1	A	279	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	279	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	68	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	117	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	219	LEU	CA-CB-CG	-5.41	102.86	115.30
1	B	207	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	58	GLN	CB-CA-C	-5.07	100.25	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	LYS	Peptide
1	A	266	ASN	Peptide
1	B	264	LYS	Peptide
1	C	264	LYS	Peptide
1	D	264	LYS	Peptide
1	D	296	PRO	Peptide

## 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	2491	0	2437	27	0
1	B	2491	0	2436	24	0
1	C	2436	0	2386	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2436	0	2386	39	0
2	A	39	0	25	1	0
2	B	39	0	24	0	0
2	C	39	0	25	0	0
2	D	39	0	25	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	222	0	0	4	0
4	B	195	0	0	3	0
4	C	169	0	0	15	0
4	D	165	0	0	8	0
All	All	10767	0	9744	126	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 6.

All (126) 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:A:128:ARG:HD3	4:C:566:HOH:O	1.50	1.11
1:C:111:ASP:HB2	4:C:516:HOH:O	1.62	0.98
1:B:264:LYS:O	1:B:267:HIS:CD2	2.25	0.89
1:D:296:PRO:CD	1:D:297:TYR:HB2	2.04	0.87
1:C:57:HIS:CD2	4:C:507:HOH:O	2.27	0.86
1:C:266:ASN:OD1	1:C:267:HIS:ND1	2.08	0.85
1:C:196:LYS:HB2	4:C:549:HOH:O	1.78	0.81
1:D:296:PRO:N	1:D:297:TYR:HB2	1.95	0.81
1:A:264:LYS:HA	1:A:265:ASP:HB2	1.63	0.80
1:B:265:ASP:HB3	4:B:544:HOH:O	1.83	0.77
1:D:333:GLU:HG3	4:D:546:HOH:O	1.85	0.76
1:C:68:ARG:HG3	4:C:549:HOH:O	1.84	0.75
1:B:320:ASP:HB3	1:C:321:TYR:CZ	2.22	0.75
1:A:227:HIS:ND1	1:C:219:LEU:HD13	2.04	0.72
1:D:264:LYS:O	1:D:264:LYS:HG3	1.93	0.69
1:C:42:HIS:HE1	4:C:642:HOH:O	1.76	0.67
1:D:296:PRO:HG2	1:D:297:TYR:HD1	1.60	0.67
1:C:319:GLN:HG3	4:C:532:HOH:O	1.94	0.66
1:C:111:ASP:CB	4:C:516:HOH:O	2.30	0.65
1:A:128:ARG:CD	4:C:566:HOH:O	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LEU:O	1:D:156:THR:HG23	1.97	0.65
1:D:42:HIS:HE1	4:D:635:HOH:O	1.80	0.64
1:C:266:ASN:O	1:C:268:VAL:HG23	1.97	0.64
1:C:266:ASN:OD1	1:C:267:HIS:N	2.30	0.64
1:A:331:LYS:HE3	4:A:694:HOH:O	1.99	0.63
1:B:320:ASP:HB3	1:C:321:TYR:CE1	2.32	0.63
1:D:103:ILE:HD12	1:D:229:LEU:HD21	1.81	0.62
1:D:42:HIS:CE1	4:D:635:HOH:O	2.53	0.62
1:C:154:ASN:O	1:C:158:LEU:HD22	1.99	0.61
1:C:264:LYS:O	1:C:267:HIS:HB2	2.00	0.61
1:D:331:LYS:HE2	4:D:644:HOH:O	1.99	0.61
1:A:101:GLU:OE2	1:A:247:LYS:NZ	2.34	0.61
1:C:154:ASN:O	1:C:158:LEU:CD2	2.49	0.61
1:D:103:ILE:HD11	1:D:228:HIS:NE2	2.17	0.60
1:B:215:SER:HB3	4:B:539:HOH:O	2.01	0.59
1:A:97:ILE:O	1:A:100:LYS:HG3	2.03	0.58
1:A:125:GLN:HG2	1:C:281:GLU:OE2	2.03	0.58
1:C:69:ASN:HB3	4:C:652:HOH:O	2.02	0.58
1:C:42:HIS:CE1	4:C:642:HOH:O	2.54	0.57
1:A:215:SER:HB3	4:A:604:HOH:O	2.05	0.56
1:B:347:TRP:CH2	1:B:348:ARG:NH1	2.73	0.56
1:B:128:ARG:HG3	1:B:128:ARG:NH1	2.20	0.56
1:B:343:THR:O	1:B:343:THR:OG1	2.19	0.56
1:B:320:ASP:CB	1:C:321:TYR:CZ	2.88	0.56
1:D:296:PRO:HG2	1:D:297:TYR:CD1	2.41	0.56
1:C:103:ILE:HD13	1:C:226:CYS:SG	2.46	0.56
1:D:266:ASN:OD1	1:D:267:HIS:N	2.39	0.56
1:D:296:PRO:HD2	1:D:297:TYR:HB2	1.85	0.55
1:D:259:ILE:HD11	1:D:275:ILE:HG23	1.90	0.54
1:A:264:LYS:HA	1:A:265:ASP:CB	2.36	0.54
1:B:259:ILE:HG13	1:B:309:LEU:CD1	2.38	0.53
1:C:196:LYS:HA	1:C:202:TRP:CD2	2.43	0.53
1:C:97:ILE:O	1:C:100:LYS:HG2	2.08	0.53
1:A:347:TRP:CZ2	2:A:401:UD1:H6'2	2.44	0.52
1:C:263:ARG:HG2	1:C:268:VAL:HG22	1.91	0.52
1:D:297:TYR:C	4:D:502:HOH:O	2.48	0.52
1:D:296:PRO:CG	1:D:297:TYR:HB2	2.39	0.51
1:C:69:ASN:CB	4:C:652:HOH:O	2.59	0.51
1:B:128:ARG:HG3	1:B:128:ARG:HH11	1.74	0.51
1:B:347:TRP:CZ2	1:B:348:ARG:CZ	2.93	0.50
1:D:298:GLY:N	4:D:502:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:GLU:CG	4:D:546:HOH:O	2.50	0.50
1:D:61:LEU:HD11	1:D:248:LEU:HD12	1.93	0.50
1:D:263:ARG:HH11	1:D:263:ARG:HG2	1.77	0.50
1:D:329:GLU:HG2	1:D:331:LYS:HG3	1.94	0.50
1:A:320:ASP:HB3	1:D:321:TYR:CZ	2.46	0.49
1:C:259:ILE:CD1	1:C:275:ILE:HG23	2.42	0.49
1:C:262:SER:OG	1:C:271:GLU:OE1	2.29	0.49
1:C:59:THR:O	1:C:102:ARG:HD3	2.12	0.49
1:A:263:ARG:HG2	1:A:268:VAL:HG22	1.94	0.48
1:A:128:ARG:HG3	1:A:128:ARG:NH1	2.28	0.48
1:D:259:ILE:CD1	1:D:275:ILE:HG23	2.44	0.48
1:D:196:LYS:HA	1:D:202:TRP:CD2	2.49	0.48
1:C:111:ASP:CG	4:C:516:HOH:O	2.48	0.48
1:D:59:THR:O	1:D:102:ARG:HD3	2.14	0.47
1:A:227:HIS:CE1	1:C:219:LEU:HD13	2.48	0.47
1:B:259:ILE:CD1	1:B:275:ILE:HG23	2.44	0.47
1:B:268:VAL:HG12	1:B:325:CYS:SG	2.55	0.47
1:B:347:TRP:CZ2	1:B:348:ARG:NH1	2.83	0.47
1:D:295:LYS:HG2	1:D:297:TYR:O	2.15	0.47
1:A:128:ARG:HG3	1:A:128:ARG:HH11	1.80	0.47
1:B:144:ASP:CG	1:B:191:ILE:HD12	2.36	0.46
1:D:103:ILE:HD12	1:D:229:LEU:CD2	2.46	0.46
1:A:227:HIS:CE1	1:C:219:LEU:CD1	2.99	0.45
1:A:259:ILE:HG13	1:A:309:LEU:CD1	2.47	0.44
1:B:342:LEU:O	1:B:343:THR:HG22	2.16	0.44
1:C:57:HIS:HD2	4:C:507:HOH:O	1.86	0.44
1:B:342:LEU:C	1:B:343:THR:CG2	2.85	0.44
1:C:329:GLU:HG2	1:C:331:LYS:HG3	1.99	0.44
1:C:166:ARG:HD2	1:C:168:GLU:OE2	2.16	0.44
1:D:150:ILE:HG21	1:D:296:PRO:HD3	2.00	0.44
1:D:171:LEU:C	1:D:171:LEU:HD23	2.38	0.44
1:B:322:ASP:OD1	1:C:302:ASN:ND2	2.27	0.44
1:C:228:HIS:CD2	1:C:228:HIS:H	2.35	0.44
1:C:237:TYR:CD2	1:C:237:TYR:C	2.91	0.44
1:D:259:ILE:HG13	1:D:309:LEU:HD11	2.00	0.44
1:A:45:PHE:HE2	1:A:314:ASP:HB2	1.83	0.43
1:A:263:ARG:HA	1:A:267:HIS:O	2.19	0.43
1:C:228:HIS:HD2	4:C:647:HOH:O	2.01	0.43
1:C:55:LEU:HD11	1:C:278:ASN:HB3	2.01	0.43
1:D:185:ASN:OD1	1:D:185:ASN:N	2.52	0.43
1:D:58:GLN:HB3	4:D:610:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASP:CA	4:B:544:HOH:O	2.67	0.42
1:A:331:LYS:NZ	4:A:514:HOH:O	2.51	0.42
1:B:263:ARG:HG2	1:B:268:VAL:HG22	2.01	0.42
1:C:61:LEU:HD11	1:C:248:LEU:HD12	2.01	0.42
1:D:237:TYR:CD2	1:D:237:TYR:C	2.92	0.42
1:D:264:LYS:O	1:D:264:LYS:CG	2.66	0.42
1:C:154:ASN:O	1:C:158:LEU:HD23	2.19	0.42
1:B:144:ASP:HB2	1:B:191:ILE:HD12	2.01	0.42
1:C:185:ASN:N	1:C:185:ASN:OD1	2.52	0.42
1:A:237:TYR:CD2	1:A:237:TYR:C	2.92	0.42
1:B:45:PHE:HE2	1:B:314:ASP:HB2	1.85	0.42
1:C:150:ILE:HG21	1:C:296:PRO:HD3	2.01	0.42
1:A:162:SER:HA	4:A:631:HOH:O	2.20	0.42
1:A:342:LEU:C	1:A:343:THR:CG2	2.88	0.42
1:D:259:ILE:HD13	1:D:275:ILE:HA	2.02	0.42
1:B:55:LEU:HD11	1:B:278:ASN:HB3	2.02	0.41
1:A:342:LEU:O	1:A:343:THR:HG22	2.20	0.41
1:D:263:ARG:HG2	1:D:263:ARG:NH1	2.35	0.41
1:C:259:ILE:HD11	1:C:275:ILE:HG23	2.02	0.41
1:A:144:ASP:HB2	1:A:191:ILE:HD12	2.02	0.41
1:D:299:ASP:OD2	1:D:301:TYR:HB3	2.20	0.41
1:A:144:ASP:CG	1:A:191:ILE:HD12	2.41	0.41
1:D:284:ALA:HB1	1:D:309:LEU:HD23	2.03	0.40
1:C:61:LEU:HD13	1:C:102:ARG:HD2	2.03	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	307/348 (88%)	295 (96%)	12 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	307/348 (88%)	302 (98%)	4 (1%)	1 (0%)	41	31
1	C	300/348 (86%)	294 (98%)	6 (2%)	0	100	100
1	D	300/348 (86%)	295 (98%)	5 (2%)	0	100	100
All	All	1214/1392 (87%)	1186 (98%)	27 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	344	ALA

### 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	273/307 (89%)	268 (98%)	5 (2%)	59	53
1	B	273/307 (89%)	271 (99%)	2 (1%)	84	83
1	C	267/307 (87%)	264 (99%)	3 (1%)	73	72
1	D	267/307 (87%)	264 (99%)	3 (1%)	73	72
All	All	1080/1228 (88%)	1067 (99%)	13 (1%)	71	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	102	ARG
1	A	320	ASP
1	A	342	LEU
1	A	345	SER
1	B	246	ASP
1	B	343	THR
1	C	81	ILE
1	C	104	ILE
1	C	297	TYR

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Mol	Chain	Res	Type
1	D	269	SER
1	D	310	ARG
1	D	311	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	HIS
1	B	200	HIS
1	C	42	HIS
1	C	228	HIS
1	C	334	ASN
1	D	42	HIS
1	D	228	HIS
1	D	317	HIS
1	D	334	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	UD1	B	401	3	38,41,41	1.17	5 (13%)	57,62,62	1.99	16 (28%)
2	UD1	D	401	3	38,41,41	1.27	3 (7%)	57,62,62	1.63	14 (24%)
2	UD1	A	401	3	38,41,41	1.31	6 (15%)	57,62,62	1.79	12 (21%)
2	UD1	C	401	3	38,41,41	1.39	3 (7%)	57,62,62	1.32	9 (15%)

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	UD1	B	401	3	-	6/26/63/63	0/3/3/3
2	UD1	D	401	3	-	0/26/63/63	0/3/3/3
2	UD1	A	401	3	-	4/26/63/63	0/3/3/3
2	UD1	C	401	3	-	4/26/63/63	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	UD1	C4-N3	-4.80	1.30	1.38
2	D	401	UD1	C4-N3	-3.90	1.31	1.38
2	C	401	UD1	C2-N3	-3.77	1.31	1.38
2	D	401	UD1	C2-N3	-3.31	1.32	1.38
2	C	401	UD1	O2-C2	3.20	1.28	1.23
2	A	401	UD1	O7'-C7'	2.99	1.30	1.23
2	B	401	UD1	O2-C2	2.97	1.28	1.23
2	B	401	UD1	C4-N3	-2.74	1.33	1.38
2	A	401	UD1	C2-N3	-2.72	1.33	1.38
2	A	401	UD1	C8'-C7'	-2.53	1.45	1.50
2	A	401	UD1	C6-C5	2.29	1.40	1.35
2	A	401	UD1	C4-N3	-2.21	1.34	1.38
2	D	401	UD1	O7'-C7'	2.21	1.28	1.23
2	B	401	UD1	O6'-C6'	-2.12	1.33	1.42
2	B	401	UD1	C6-C5	2.08	1.39	1.35
2	A	401	UD1	C2-N1	2.07	1.41	1.38
2	B	401	UD1	C2-N3	-2.00	1.34	1.38

All (51) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	UD1	O5'-C5'-C4'	5.57	119.81	109.69
2	A	401	UD1	O3A-PB-O1'	-5.34	91.72	102.48
2	B	401	UD1	O3A-PB-O1'	-5.03	92.35	102.48
2	A	401	UD1	C4-N3-C2	-4.77	120.29	126.58
2	A	401	UD1	N3-C2-N1	4.66	121.08	114.89
2	B	401	UD1	C6'-C5'-C4'	-4.63	102.15	113.00
2	D	401	UD1	N3-C2-N1	4.47	120.82	114.89
2	B	401	UD1	C5-C4-N3	4.15	121.05	114.84
2	A	401	UD1	C5-C4-N3	4.01	120.84	114.84
2	C	401	UD1	O3A-PB-O1'	-3.91	94.60	102.48
2	B	401	UD1	O1'-C1'-C2'	3.72	115.14	108.40
2	D	401	UD1	O4-C4-C5	-3.49	119.02	125.16
2	B	401	UD1	O6'-C6'-C5'	-3.47	99.40	111.29
2	A	401	UD1	C4'-C3'-C2'	-3.41	105.35	110.34
2	D	401	UD1	O2-C2-N1	-3.34	118.35	122.79
2	D	401	UD1	O1'-C1'-C2'	3.32	114.40	108.40
2	B	401	UD1	C4-N3-C2	-3.29	122.25	126.58
2	D	401	UD1	C4-N3-C2	-3.25	122.29	126.58
2	B	401	UD1	N3-C2-N1	3.08	118.98	114.89
2	A	401	UD1	O4'-C4'-C5'	-3.08	101.66	109.30
2	D	401	UD1	O5'-C1'-O1'	-2.98	107.47	111.36
2	C	401	UD1	O1'-C1'-C2'	2.98	113.79	108.40
2	C	401	UD1	PB-O3A-PA	-2.87	122.98	132.83
2	D	401	UD1	C5-C4-N3	2.86	119.11	114.84
2	A	401	UD1	O4-C4-C5	-2.81	120.22	125.16
2	C	401	UD1	C5-C4-N3	2.77	118.98	114.84
2	B	401	UD1	O4-C4-C5	-2.67	120.46	125.16
2	B	401	UD1	O5'-C5'-C6'	-2.46	100.31	106.44
2	D	401	UD1	O5'-C1'-C2'	-2.45	105.78	110.58
2	D	401	UD1	O3A-PB-O1'	-2.45	97.54	102.48
2	D	401	UD1	C6-N1-C2	-2.43	117.89	120.99
2	B	401	UD1	C4'-C3'-C2'	-2.43	106.79	110.34
2	C	401	UD1	O5'-C1'-C2'	-2.35	105.99	110.58
2	A	401	UD1	O1'-C1'-C2'	2.34	112.63	108.40
2	A	401	UD1	O5B-PA-O1A	-2.33	99.95	109.07
2	C	401	UD1	N3-C2-N1	2.33	117.98	114.89
2	A	401	UD1	O2-C2-N1	-2.31	119.71	122.79
2	D	401	UD1	PB-O3A-PA	-2.29	124.98	132.83
2	C	401	UD1	C3B-C2B-C1B	2.27	105.74	101.43
2	B	401	UD1	O5'-C1'-C2'	-2.27	106.15	110.58
2	A	401	UD1	C2'-N2'-C7'	2.24	128.62	123.18
2	B	401	UD1	O4'-C4'-C5'	-2.23	103.75	109.30
2	B	401	UD1	O2-C2-N1	-2.19	119.87	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	UD1	O3'-C3'-C2'	2.09	113.88	109.66
2	D	401	UD1	PB-O1'-C1'	2.06	127.71	119.74
2	D	401	UD1	C8'-C7'-N2'	-2.06	112.62	116.10
2	C	401	UD1	C2B-C3B-C4B	-2.04	98.67	102.64
2	B	401	UD1	C1'-O5'-C5'	2.03	117.67	113.69
2	D	401	UD1	C1B-N1-C2	2.01	121.21	117.57
2	B	401	UD1	C6-C5-C4	-2.01	116.78	119.52
2	A	401	UD1	C5-C6-N1	-2.00	118.46	121.81

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	UD1	O5'-C5'-C6'-O6'
2	B	401	UD1	C4'-C5'-C6'-O6'
2	A	401	UD1	C8'-C7'-N2'-C2'
2	A	401	UD1	O7'-C7'-N2'-C2'
2	C	401	UD1	C8'-C7'-N2'-C2'
2	C	401	UD1	O7'-C7'-N2'-C2'
2	A	401	UD1	PB-O3A-PA-O2A
2	B	401	UD1	PB-O3A-PA-O1A
2	C	401	UD1	PB-O3A-PA-O1A
2	C	401	UD1	PB-O3A-PA-O2A
2	A	401	UD1	PB-O3A-PA-O1A
2	B	401	UD1	C3'-C2'-N2'-C7'
2	B	401	UD1	PB-O3A-PA-O2A
2	B	401	UD1	PA-O3A-PB-O2B

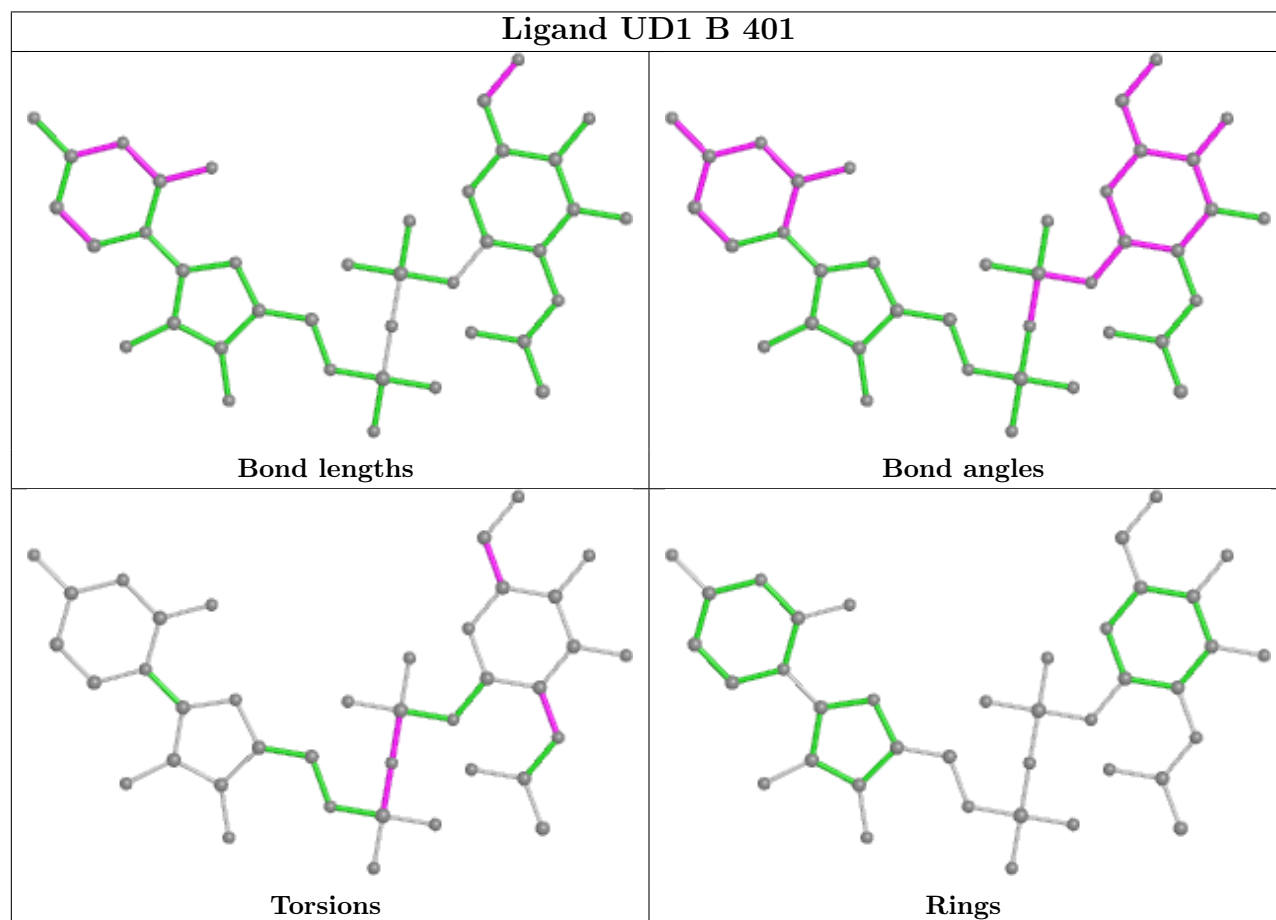
There are no ring outliers.

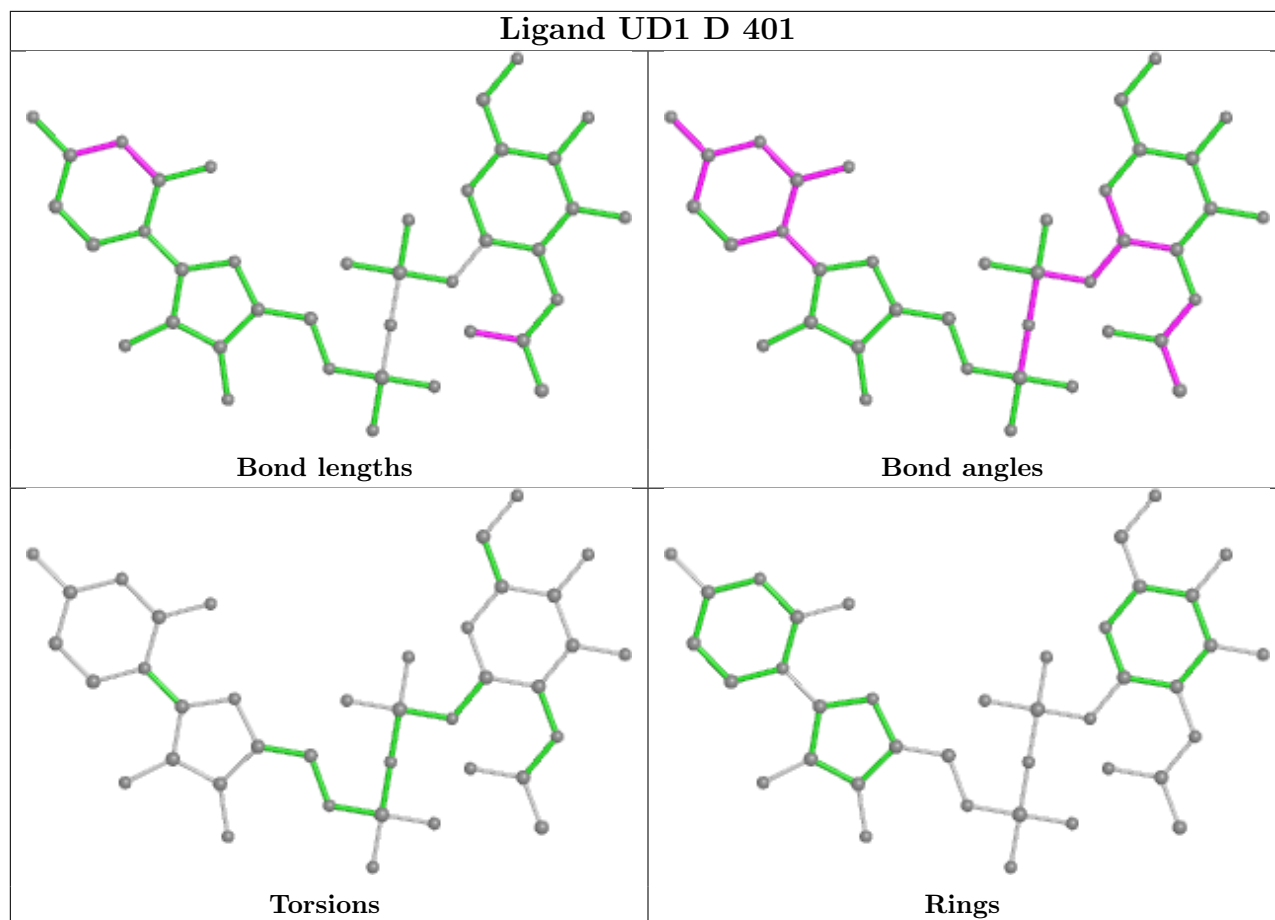
1 monomer is involved in 1 short contact:

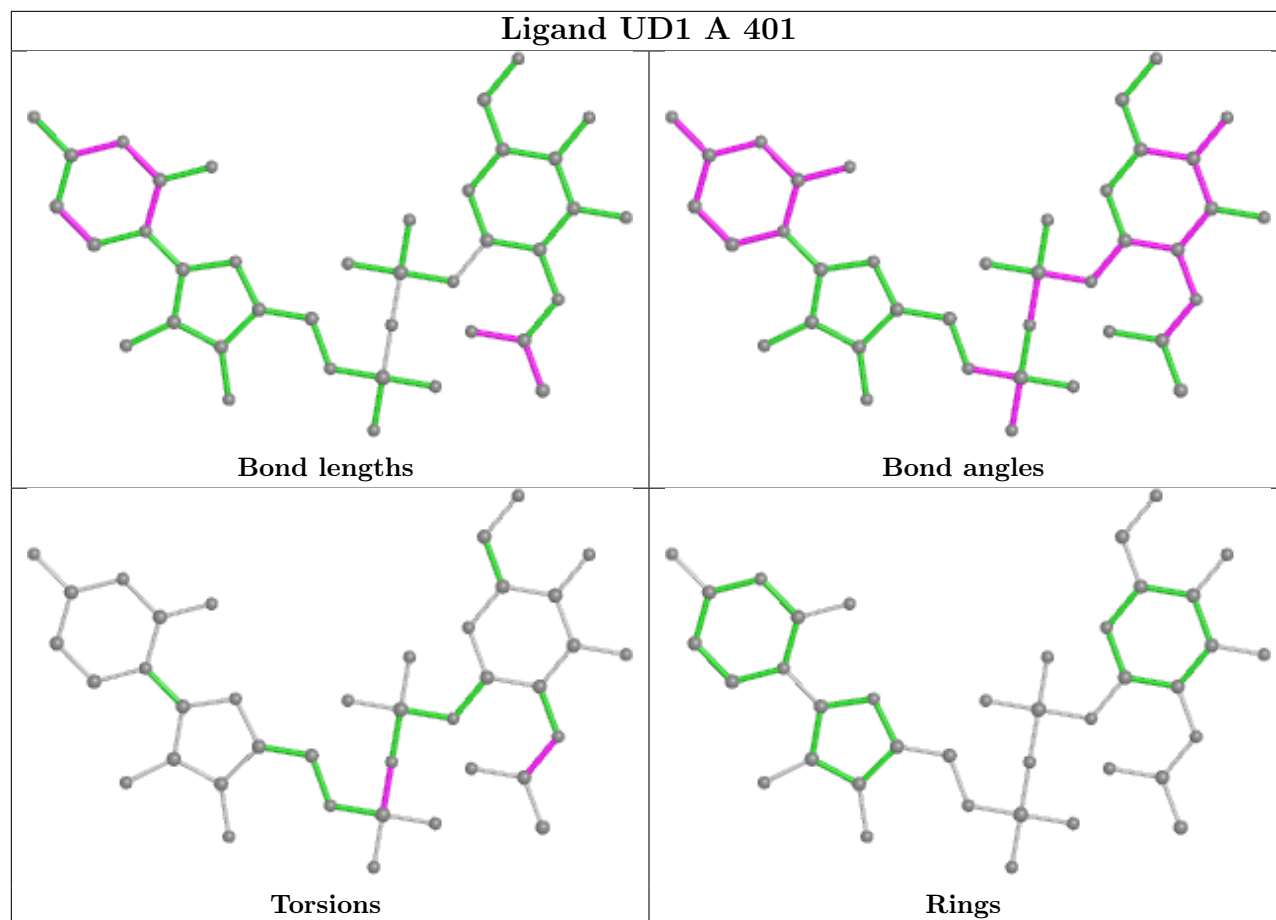
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	UD1	1	0

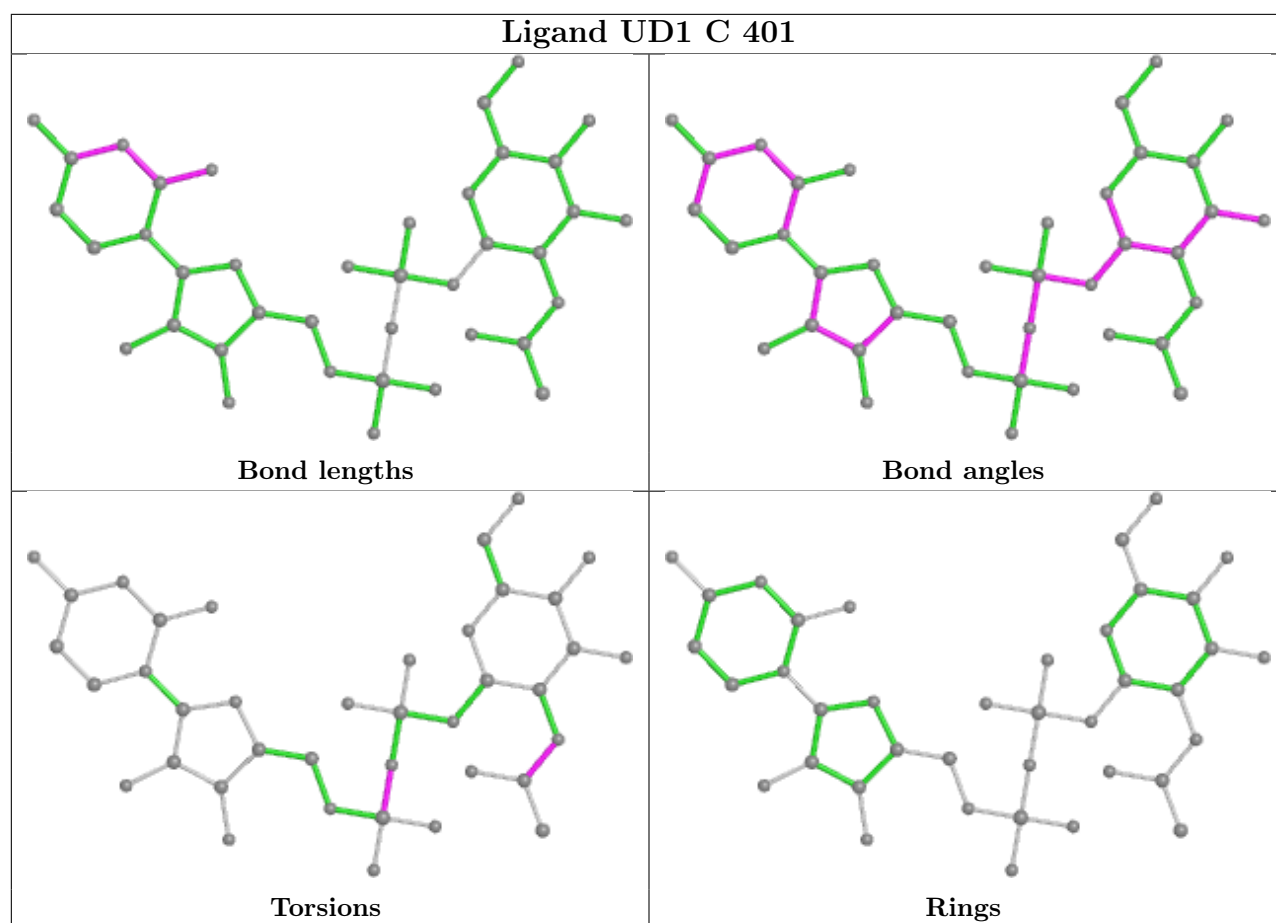
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	309/348 (88%)	-0.45	6 (1%) 66 69	13, 23, 48, 84	0
1	B	309/348 (88%)	-0.42	5 (1%) 72 74	13, 23, 50, 87	0
1	C	302/348 (86%)	-0.20	11 (3%) 42 46	13, 25, 58, 116	0
1	D	302/348 (86%)	-0.20	11 (3%) 42 46	13, 25, 56, 116	0
All	All	1222/1392 (87%)	-0.31	33 (2%) 54 57	13, 24, 52, 116	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	ASP	9.4
1	C	197	ASP	8.1
1	D	297	TYR	6.6
1	C	265	ASP	6.3
1	C	198	LYS	5.8
1	D	198	LYS	4.9
1	C	267	HIS	4.5
1	B	348	ARG	4.1
1	C	295	LYS	3.8
1	C	297	TYR	3.6
1	A	348	ARG	3.6
1	D	265	ASP	3.5
1	A	347	TRP	3.5
1	D	266	ASN	3.4
1	D	342	LEU	3.4
1	A	267	HIS	3.3
1	C	196	LYS	3.3
1	D	296	PRO	3.2
1	B	343	THR	3.2
1	D	196	LYS	3.0
1	D	57	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	347	TRP	2.9
1	C	296	PRO	2.9
1	D	267	HIS	2.9
1	B	267	HIS	2.8
1	C	342	LEU	2.7
1	B	345	SER	2.7
1	A	343	THR	2.6
1	A	345	SER	2.6
1	C	266	ASN	2.2
1	A	265	ASP	2.2
1	C	57	HIS	2.2
1	D	341	SER	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.

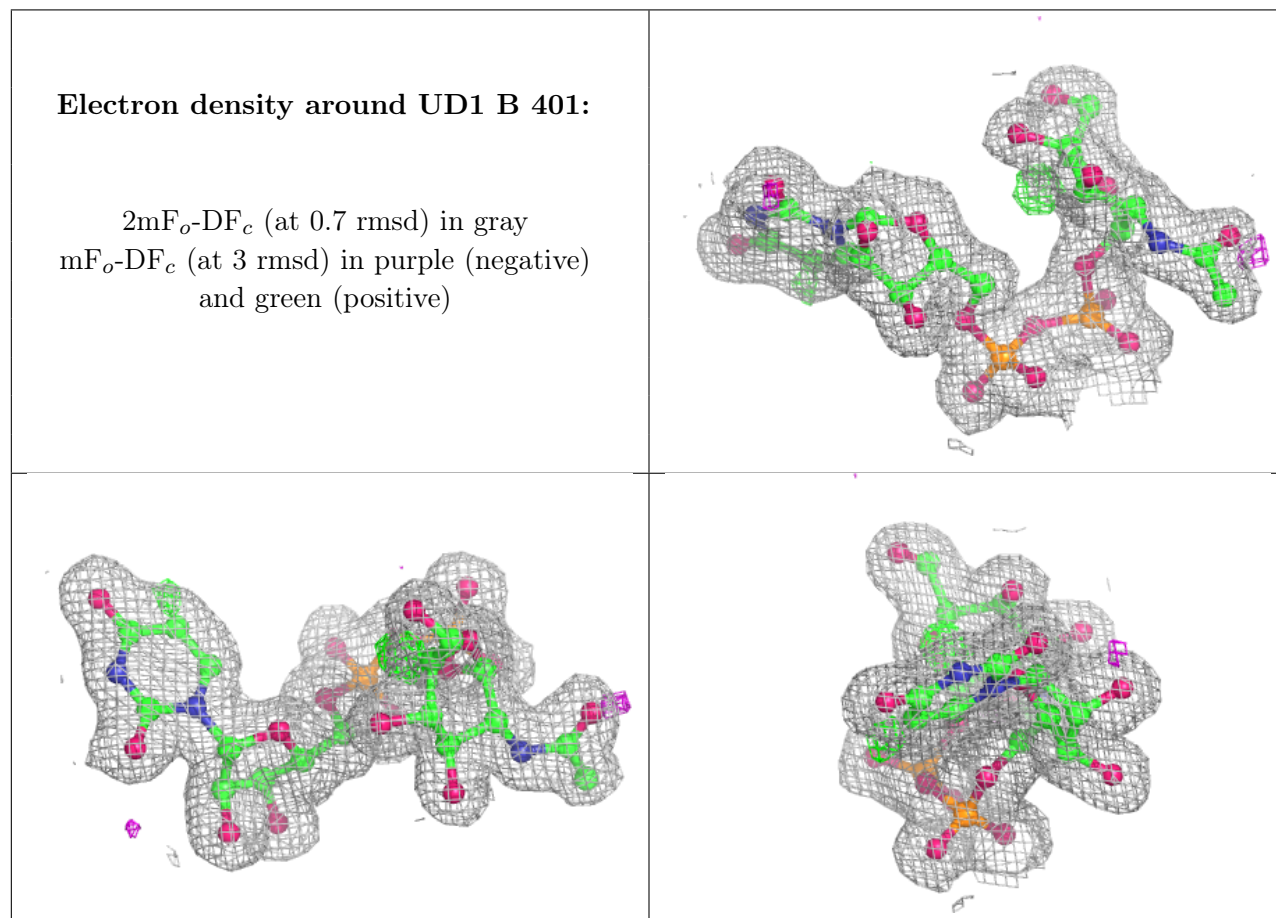
## 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	UD1	B	401	39/39	0.97	0.07	13,16,25,28	0
2	UD1	C	401	39/39	0.97	0.07	14,19,30,36	0
2	UD1	D	401	39/39	0.97	0.07	14,20,32,33	0
3	MN	B	403	1/1	0.97	0.07	42,42,42,42	0
3	MN	A	403	1/1	0.98	0.06	40,40,40,40	0
2	UD1	A	401	39/39	0.98	0.08	13,17,23,28	0
3	MN	A	402	1/1	0.99	0.11	19,19,19,19	0
3	MN	B	402	1/1	1.00	0.08	19,19,19,19	0
3	MN	C	402	1/1	1.00	0.08	19,19,19,19	0
3	MN	D	402	1/1	1.00	0.06	19,19,19,19	0

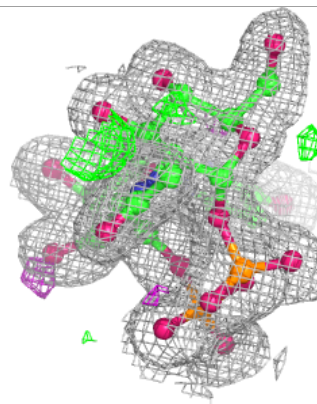
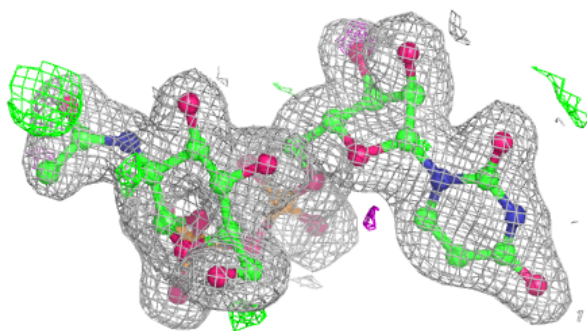
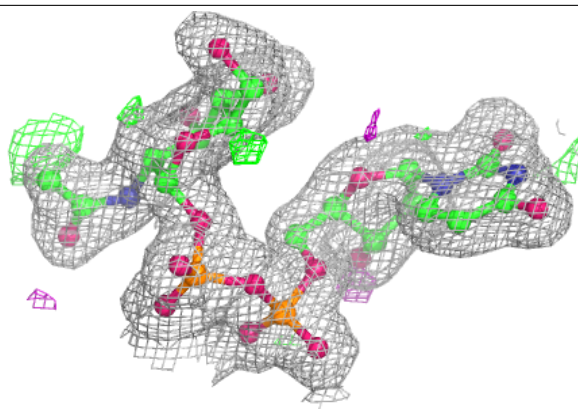


The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

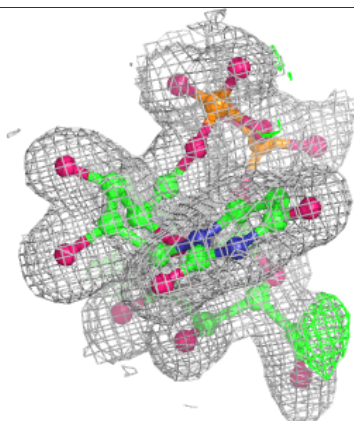
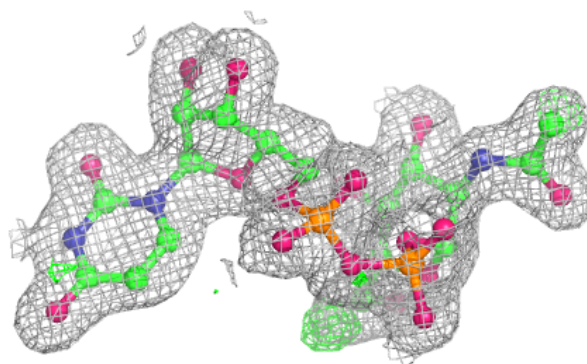
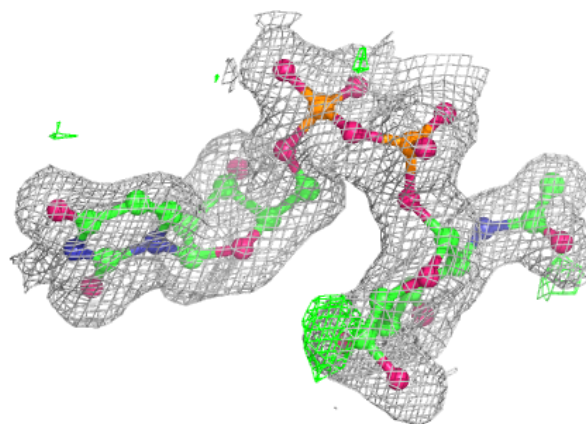


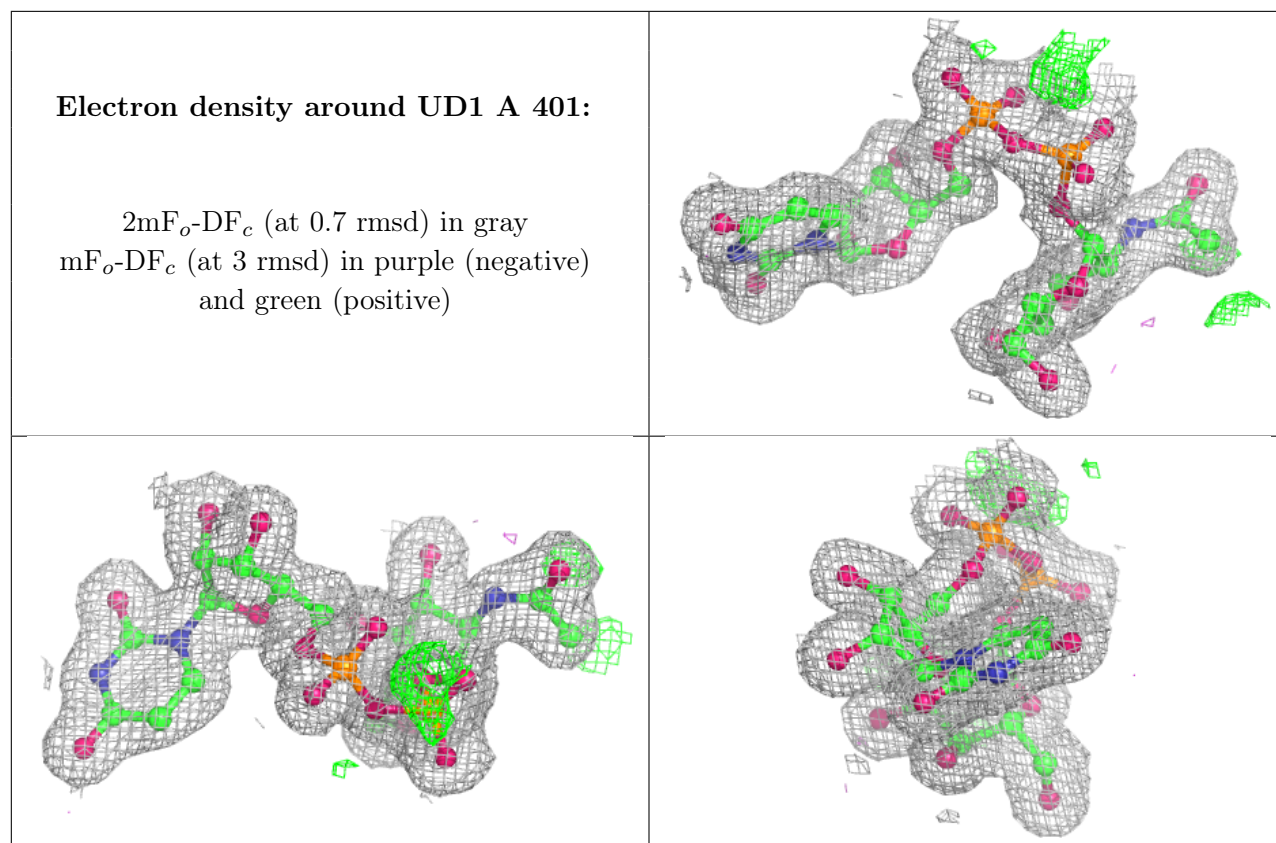
**Electron density around UD1 C 401:**

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

**Electron density around UD1 D 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.