



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:38 AM UTC

PDB ID : 5H63 / pdb_00005h63
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

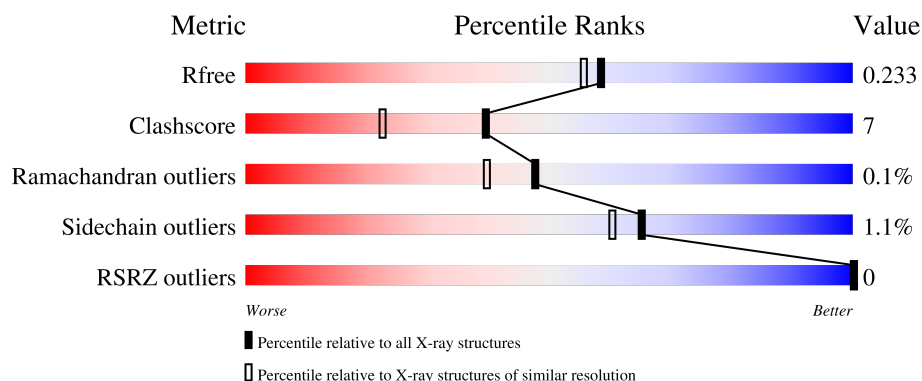
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	348	 79% 9% • 11%
1	B	348	 80% 8% • 11%
1	C	348	 72% 13% • 13%
1	D	348	 76% 10% • 13%

2 Entry composition [i](#)

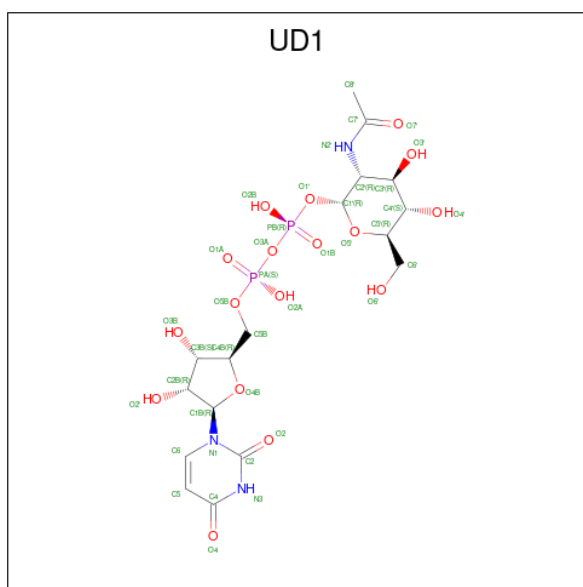
There are 4 unique types of molecules in this entry. The entry contains 10767 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
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-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



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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 (CCD ID: 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.

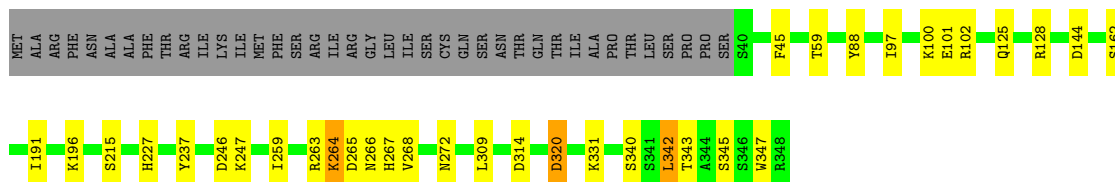
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total	O	0	0
			222	222		
4	B	195	Total	O	0	0
			195	195		
4	C	169	Total	O	0	0
			169	169		
4	D	165	Total	O	0	0
			165	165		

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.

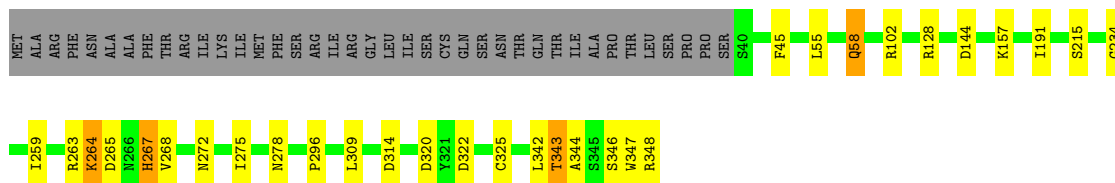
• Molecule 1: Transferase

Chain A: 



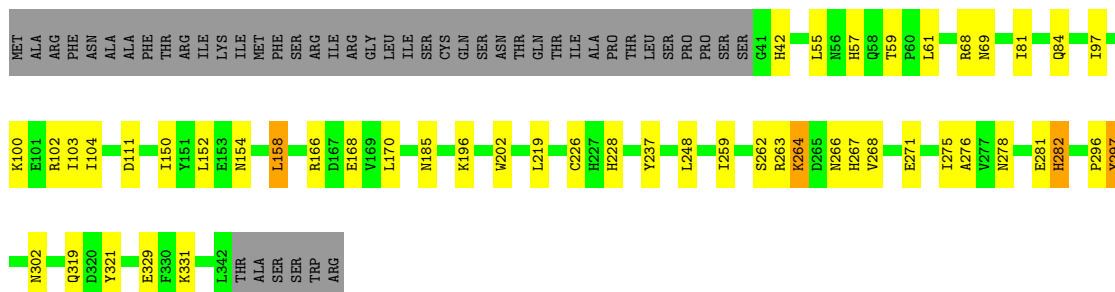
• Molecule 1: Transferase

Chain B: 



• Molecule 1: Transferase

Chain C: 



• Molecule 1: Transferase

Chain D: 

MET	ALA	ARG	PHE	ASN	ALA	ALA	PHE	THR	ARG	ILE	LYS	ILE	MET	PHE	SER	ARG	ILE	ARG	GLY	LEU	ILE	SER	CYS	GLN	SER	ASN	THR	THR	GLN	THR	ILE	ALA	ALA	PRO	THR	LEU	SER	PRO	PRO	SER	SER	G41	H42	Q58	T59	P60	L61	Q84	R102	I103	I150	Y151	L152	T156	L171
M185	K196	W202	H228	L229	Y237	L248	I259	R263	K264	D265	N266	H267	E271	L275	A284	K295	P296	Y297	G298	D299	P300	Y301	L309	R310	Y321	G325	E329	F330	K331	H332	E333	L342	THR	ALA	SER	SER	TRP	ARG																	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.57Å 52.28Å 143.75Å 90.00° 90.00° 108.00°	Depositor
Resolution (Å)	44.80 – 1.92 44.80 – 1.92	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.80-1.92) 94.4 (44.80-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.92Å)	Xtriage
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 (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10767	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	1.22	4/2552 (0.2%)	1.11	2/3453 (0.1%)
1	B	1.24	2/2552 (0.1%)	1.12	10/3453 (0.3%)
1	C	1.24	4/2495 (0.2%)	1.10	3/3375 (0.1%)
1	D	1.19	3/2495 (0.1%)	1.13	6/3375 (0.2%)
All	All	1.22	13/10094 (0.1%)	1.12	21/13656 (0.2%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	325	CYS	N-CA	6.66	1.54	1.46
1	A	246	ASP	C-O	-6.51	1.17	1.24
1	B	102	ARG	C-O	-6.36	1.16	1.23
1	C	282	HIS	CA-C	6.11	1.60	1.53
1	D	271	GLU	CA-C	-5.65	1.45	1.52
1	B	272	ASN	N-CA	-5.49	1.38	1.45
1	A	272	ASN	N-CA	-5.41	1.38	1.45
1	A	340	SER	C-O	-5.39	1.17	1.24
1	D	295	LYS	CA-C	5.20	1.58	1.52
1	C	170	LEU	C-O	-5.14	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	152	LEU	N-CA	5.10	1.52	1.46
1	C	276	ALA	N-CA	-5.09	1.40	1.46
1	A	59	THR	C-O	-5.04	1.17	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	296	PRO	N-CA-C	8.19	124.30	113.57
1	A	246	ASP	O-C-N	-6.69	116.08	123.04
1	B	267	HIS	CA-C-N	-6.36	114.28	123.06
1	B	267	HIS	C-N-CA	-6.36	114.28	123.06
1	B	102	ARG	O-C-N	-5.93	115.69	123.16
1	C	84	GLN	CB-CA-C	-5.87	101.42	110.81
1	D	266	ASN	N-CA-C	5.74	120.78	113.55
1	B	102	ARG	CA-C-N	-5.59	113.14	120.91
1	B	102	ARG	C-N-CA	-5.59	113.14	120.91
1	D	296	PRO	CA-C-N	5.50	131.60	121.70
1	D	296	PRO	C-N-CA	5.50	131.60	121.70
1	A	88	TYR	N-CA-C	5.44	117.29	111.36
1	B	296	PRO	N-CA-C	-5.22	102.39	111.32
1	D	271	GLU	CA-C-O	-5.22	115.69	121.33
1	B	346	SER	N-CA-C	5.18	118.86	112.54
1	B	234	GLY	N-CA-C	5.17	119.65	112.57
1	C	297	TYR	CA-C-N	5.16	125.00	120.10
1	C	297	TYR	C-N-CA	5.16	125.00	120.10
1	B	58	GLN	CB-CA-C	-5.10	102.18	110.85
1	D	84	GLN	CB-CA-C	-5.08	102.91	110.88
1	B	267	HIS	N-CA-C	-5.03	102.74	110.14

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	29	0
1	B	2491	0	2436	26	0
1	C	2436	0	2386	46	0
1	D	2436	0	2386	40	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	5	0
4	B	195	0	0	4	0
4	C	169	0	0	15	0
4	D	165	0	0	9	0
All	All	10767	0	9744	132	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 7.

All (132) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:297:TYR:C	4:D:502:HOH:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ASP:CG	4:C:516:HOH:O	2.48	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: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:144:ASP:CG	1:B:191:ILE:HD12	2.36	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
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:B:342:LEU:C	1:B:343:THR:CG2	2.85	0.49
1:D:171:LEU:C	1:D:171:LEU:HD23	2.38	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:C:237:TYR:CD2	1:C:237:TYR:C	2.91	0.48
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: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:D:237:TYR:CD2	1:D:237:TYR:C	2.92	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:A:237:TYR:CD2	1:A:237:TYR:C	2.92	0.47
1:A:342:LEU:C	1:A:343:THR:CG2	2.88	0.46
1:D:103:ILE:HD12	1:D:229:LEU:CD2	2.46	0.46
1:A:144:ASP:CG	1:A:191:ILE:HD12	2.41	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:HIS:HD2	4:C:507:HOH:O	1.86	0.44
1:A:196:LYS:NZ	4:A:510:HOH:O	2.48	0.44
1:A:342:LEU:C	1:A:343:THR:HG23	2.42	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: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:D:259:ILE:HG13	1:D:309:LEU:HD11	2.00	0.44
1:B:58:GLN:C	4:B:532:HOH:O	2.60	0.43
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:B:267:HIS:ND1	1:B:267:HIS:C	2.77	0.43
1:C:281:GLU:O	1:C:282:HIS:C	2.61	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
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: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: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: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:D:333:GLU:CD	4:D:546:HOH:O	2.63	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: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

5.3.1 Protein backbone

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	100	100
1	B	307/348 (88%)	302 (98%)	4 (1%)	1 (0%)	36	26
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%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	344	ALA

5.3.2 Protein sidechains

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%)	269 (98%)	4 (2%)	57	47
1	B	273/307 (89%)	271 (99%)	2 (1%)	76	73
1	C	267/307 (87%)	263 (98%)	4 (2%)	57	47
1	D	267/307 (87%)	265 (99%)	2 (1%)	76	73
All	All	1080/1228 (88%)	1068 (99%)	12 (1%)	65	60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ARG
1	A	320	ASP
1	A	342	LEU
1	A	345	SER
1	B	157	LYS
1	B	343	THR
1	C	81	ILE
1	C	104	ILE
1	C	158	LEU
1	C	297	TYR
1	D	61	LEU
1	D	310	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	B	42	HIS
1	B	154	ASN
1	B	200	HIS
1	C	42	HIS
1	C	69	ASN
1	C	126	ASN
1	C	228	HIS
1	C	334	ASN
1	D	42	HIS
1	D	317	HIS
1	D	334	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	D	401	3	40,41,41	1.32	4 (10%)	59,62,62	1.70	14 (23%)
2	UD1	B	401	3	40,41,41	1.18	5 (12%)	59,62,62	2.07	16 (27%)
2	UD1	A	401	3	40,41,41	1.32	7 (17%)	59,62,62	1.75	12 (20%)
2	UD1	C	401	3	40,41,41	1.62	6 (15%)	59,62,62	1.31	8 (13%)

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	D	401	3	-	1/26/63/63	0/3/3/3
2	UD1	B	401	3	-	6/26/63/63	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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	UD1	C4-N3	-5.05	1.30	1.38
2	D	401	UD1	C4-N3	-4.11	1.31	1.38
2	C	401	UD1	C2-N3	-3.85	1.31	1.38
2	C	401	UD1	PA-O3A	3.69	1.63	1.59
2	C	401	UD1	PB-O3A	3.69	1.63	1.59
2	D	401	UD1	C2-N3	-3.38	1.32	1.38
2	C	401	UD1	O2-C2	3.29	1.28	1.23
2	B	401	UD1	O2-C2	3.06	1.28	1.23
2	A	401	UD1	O7'-C7'	3.02	1.30	1.23
2	B	401	UD1	C4-N3	-2.90	1.33	1.38
2	A	401	UD1	C2-N3	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	UD1	C8'-C7'	-2.54	1.45	1.50
2	A	401	UD1	C4-N3	-2.35	1.34	1.38
2	D	401	UD1	PB-O3A	2.30	1.62	1.59
2	A	401	UD1	C6-C5	2.27	1.40	1.35
2	D	401	UD1	O7'-C7'	2.23	1.28	1.23
2	B	401	UD1	O6'-C6'	-2.13	1.33	1.42
2	A	401	UD1	C2-N1	2.12	1.41	1.38
2	C	401	UD1	C5-C4	-2.06	1.39	1.43
2	B	401	UD1	C6-C5	2.05	1.39	1.35
2	B	401	UD1	C2-N3	-2.05	1.34	1.38
2	A	401	UD1	PB-O2B	-2.03	1.45	1.55

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	UD1	O2B-PB-O3A	6.86	125.81	107.27
2	B	401	UD1	O5'-C5'-C4'	5.61	119.81	109.70
2	A	401	UD1	C4-N3-C2	-5.09	120.29	126.61
2	A	401	UD1	N3-C2-N1	4.75	121.08	114.89
2	D	401	UD1	N3-C2-N1	4.56	120.82	114.89
2	B	401	UD1	C5-C4-N3	4.46	121.05	114.80
2	B	401	UD1	C6'-C5'-C4'	-4.43	102.15	113.02
2	A	401	UD1	C5-C4-N3	4.31	120.84	114.80
2	C	401	UD1	O2B-PB-O3A	4.16	118.51	107.27
2	D	401	UD1	O2B-PB-O3A	4.02	118.15	107.27
2	B	401	UD1	O1'-C1'-C2'	3.72	115.14	108.40
2	D	401	UD1	O4-C4-C5	-3.56	119.02	125.16
2	B	401	UD1	C4-N3-C2	-3.52	122.25	126.61
2	B	401	UD1	O6'-C6'-C5'	-3.51	99.40	111.33
2	D	401	UD1	C4-N3-C2	-3.48	122.29	126.61
2	A	401	UD1	C4'-C3'-C2'	-3.47	105.35	110.40
2	D	401	UD1	O2-C2-N1	-3.42	118.35	122.80
2	D	401	UD1	O1'-C1'-C2'	3.32	114.40	108.40
2	B	401	UD1	N3-C2-N1	3.14	118.98	114.89
2	A	401	UD1	O4'-C4'-C5'	-3.11	101.66	109.32
2	D	401	UD1	C5-C4-N3	3.08	119.11	114.80
2	A	401	UD1	O3A-PB-O1B	3.07	119.94	110.70
2	C	401	UD1	C5-C4-N3	2.99	118.98	114.80
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	A	401	UD1	O4-C4-C5	-2.87	120.22	125.16
2	B	401	UD1	O4-C4-C5	-2.73	120.46	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	UD1	O3A-PB-O1B	-2.56	103.00	110.70
2	D	401	UD1	C6-N1-C2	-2.55	117.89	121.00
2	D	401	UD1	O5'-C1'-C2'	-2.54	105.78	110.59
2	B	401	UD1	C4'-C3'-C2'	-2.48	106.79	110.40
2	B	401	UD1	O5'-C5'-C6'	-2.47	100.31	106.44
2	C	401	UD1	O5'-C1'-C2'	-2.44	105.99	110.59
2	A	401	UD1	O2-C2-N1	-2.37	119.71	122.80
2	C	401	UD1	N3-C2-N1	2.37	117.98	114.89
2	A	401	UD1	C2'-N2'-C7'	2.36	128.62	123.11
2	B	401	UD1	O5'-C1'-C2'	-2.35	106.15	110.59
2	A	401	UD1	O1'-C1'-C2'	2.34	112.63	108.40
2	A	401	UD1	O5B-PA-O1A	-2.27	99.95	108.94
2	B	401	UD1	O4'-C4'-C5'	-2.26	103.75	109.32
2	C	401	UD1	C3B-C2B-C1B	2.26	105.74	101.46
2	B	401	UD1	O2-C2-N1	-2.25	119.87	122.80
2	C	401	UD1	O3'-C3'-C2'	2.16	113.88	109.58
2	B	401	UD1	C6-C5-C4	-2.16	116.78	119.53
2	D	401	UD1	C8'-C7'-N2'	-2.11	112.62	116.12
2	A	401	UD1	C5-C6-N1	-2.08	118.46	121.84
2	D	401	UD1	O3'-C3'-C2'	2.06	113.68	109.58
2	C	401	UD1	C2B-C3B-C4B	-2.04	98.67	102.61
2	B	401	UD1	C1'-O5'-C5'	2.02	117.67	113.72
2	D	401	UD1	C1B-N1-C2	2.02	121.21	117.59

There are no chirality outliers.

All (15) 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

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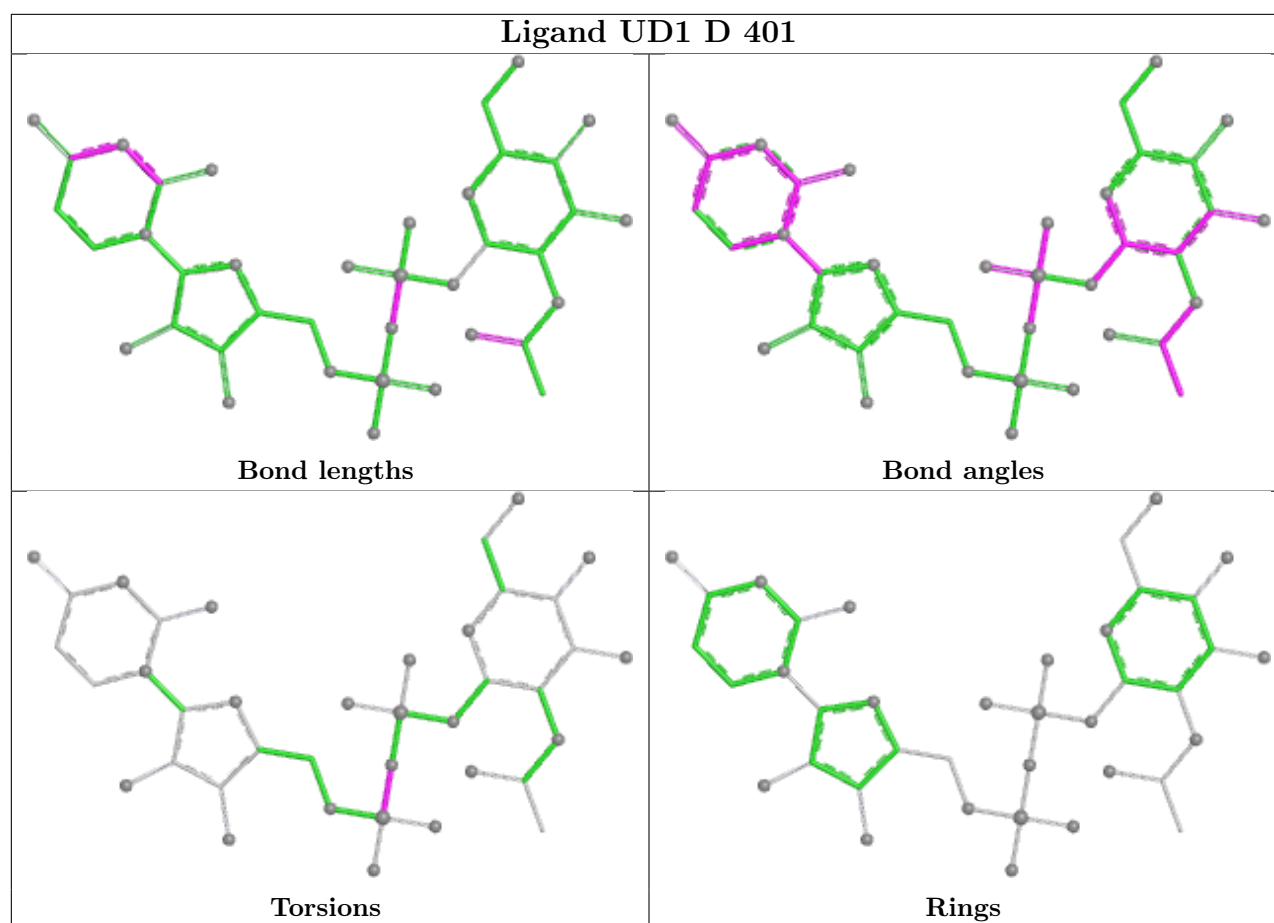
Mol	Chain	Res	Type	Atoms
2	D	401	UD1	PB-O3A-PA-O2A

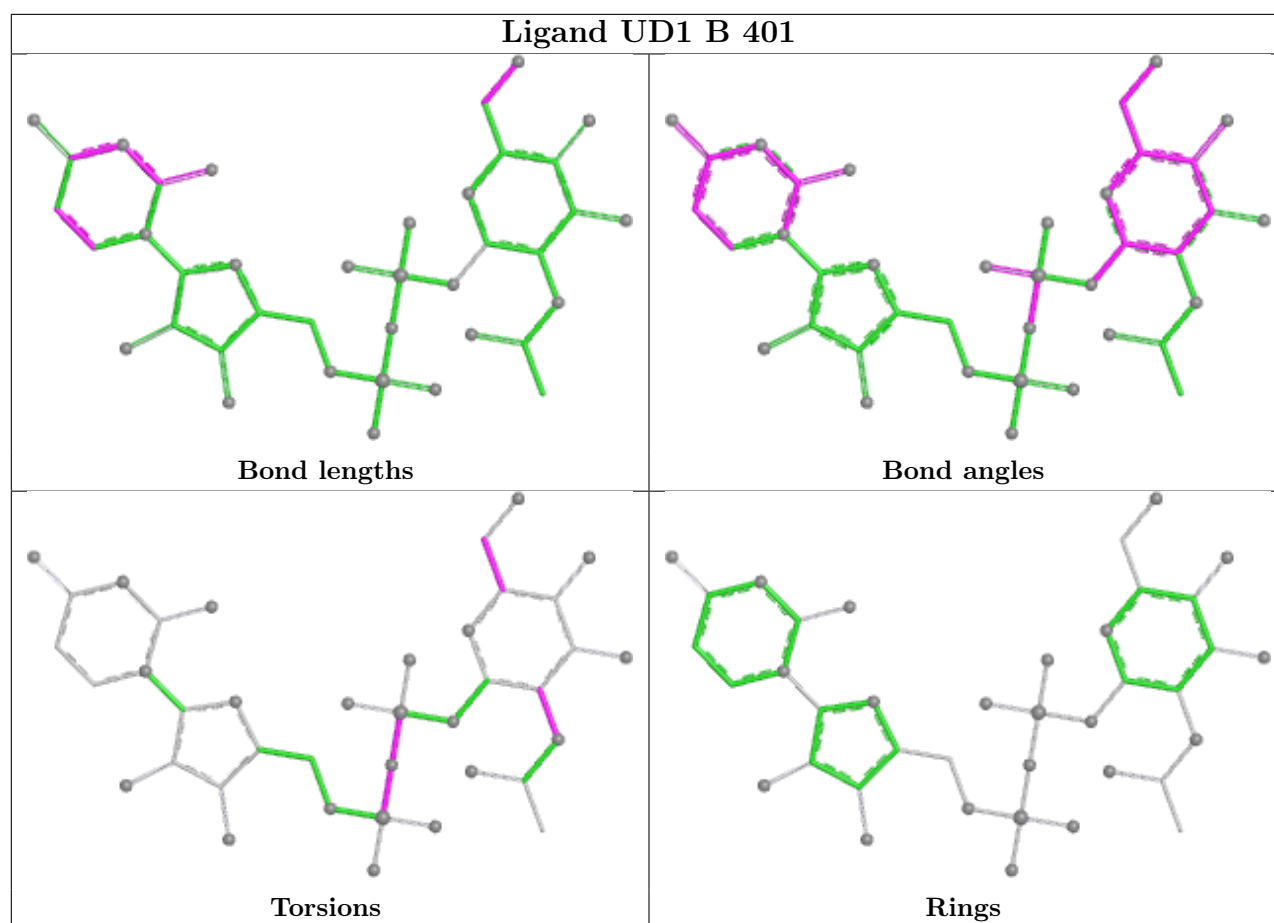
There are no ring outliers.

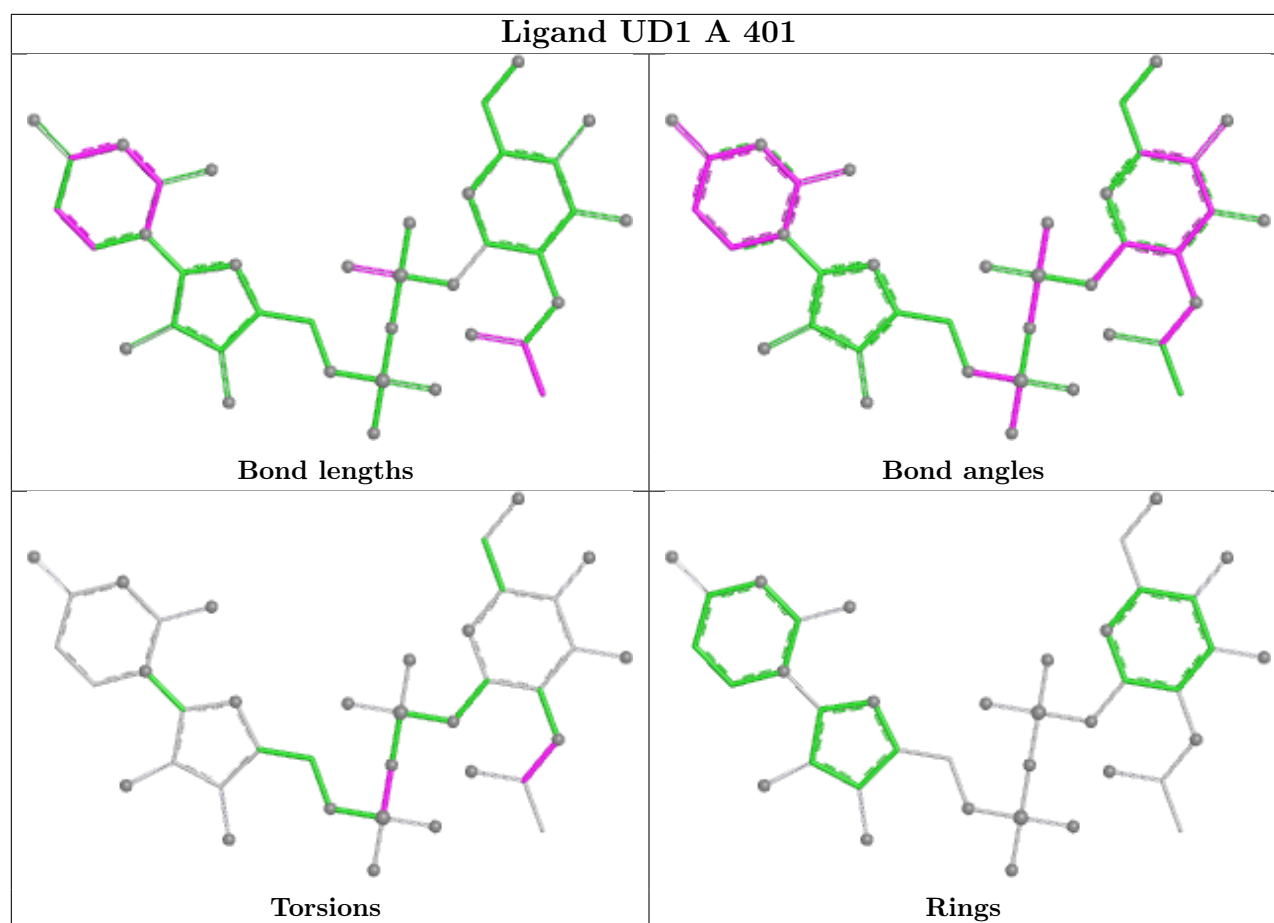
1 monomer is involved in 1 short contact:

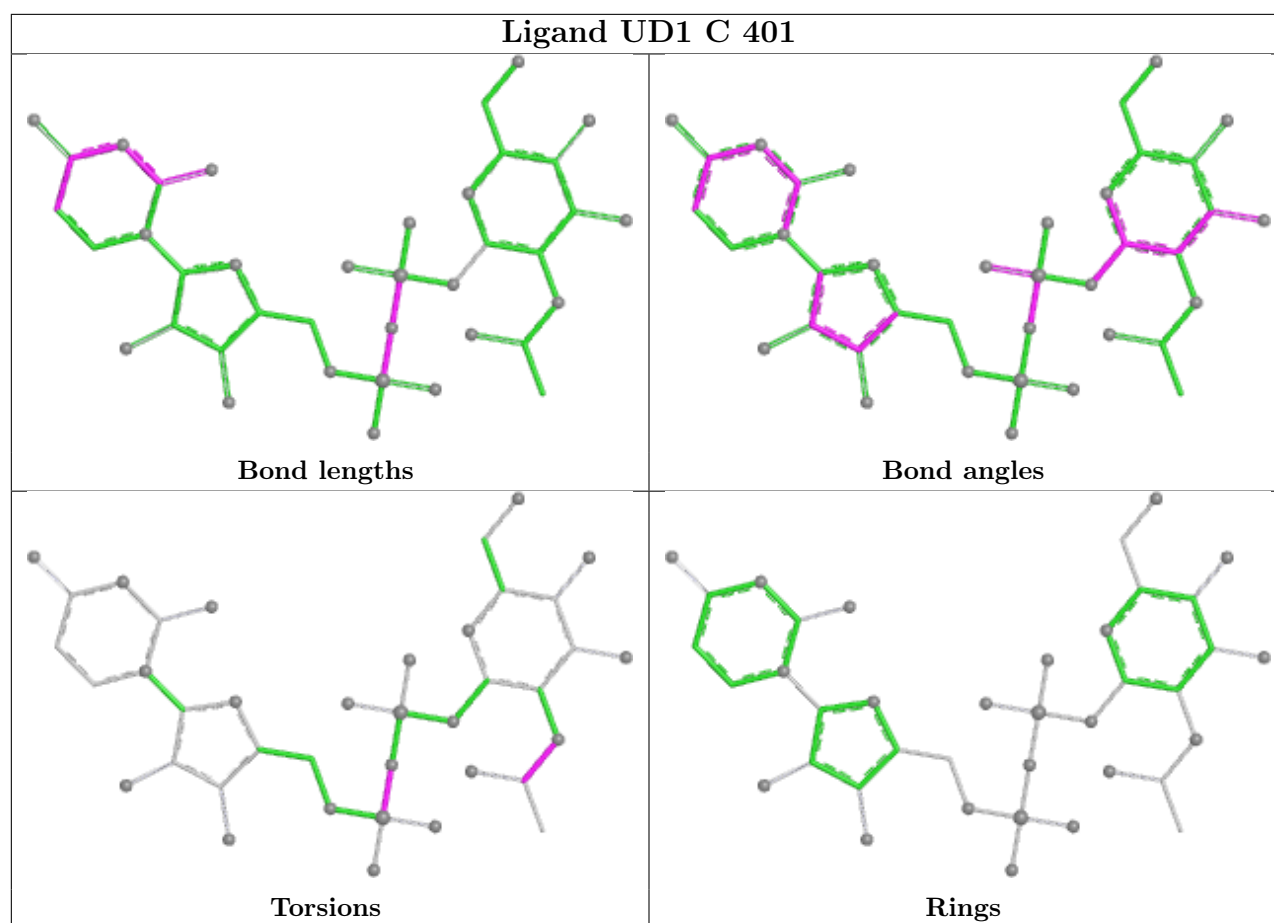
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	UD1	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/348 (88%)	-1.26	0 100 100	13, 23, 48, 84	0
1	B	309/348 (88%)	-1.25	0 100 100	13, 23, 50, 87	0
1	C	302/348 (86%)	-1.17	0 100 100	13, 25, 58, 116	0
1	D	302/348 (86%)	-1.14	0 100 100	13, 25, 56, 116	0
All	All	1222/1392 (87%)	-1.21	0 100 100	13, 24, 52, 116	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

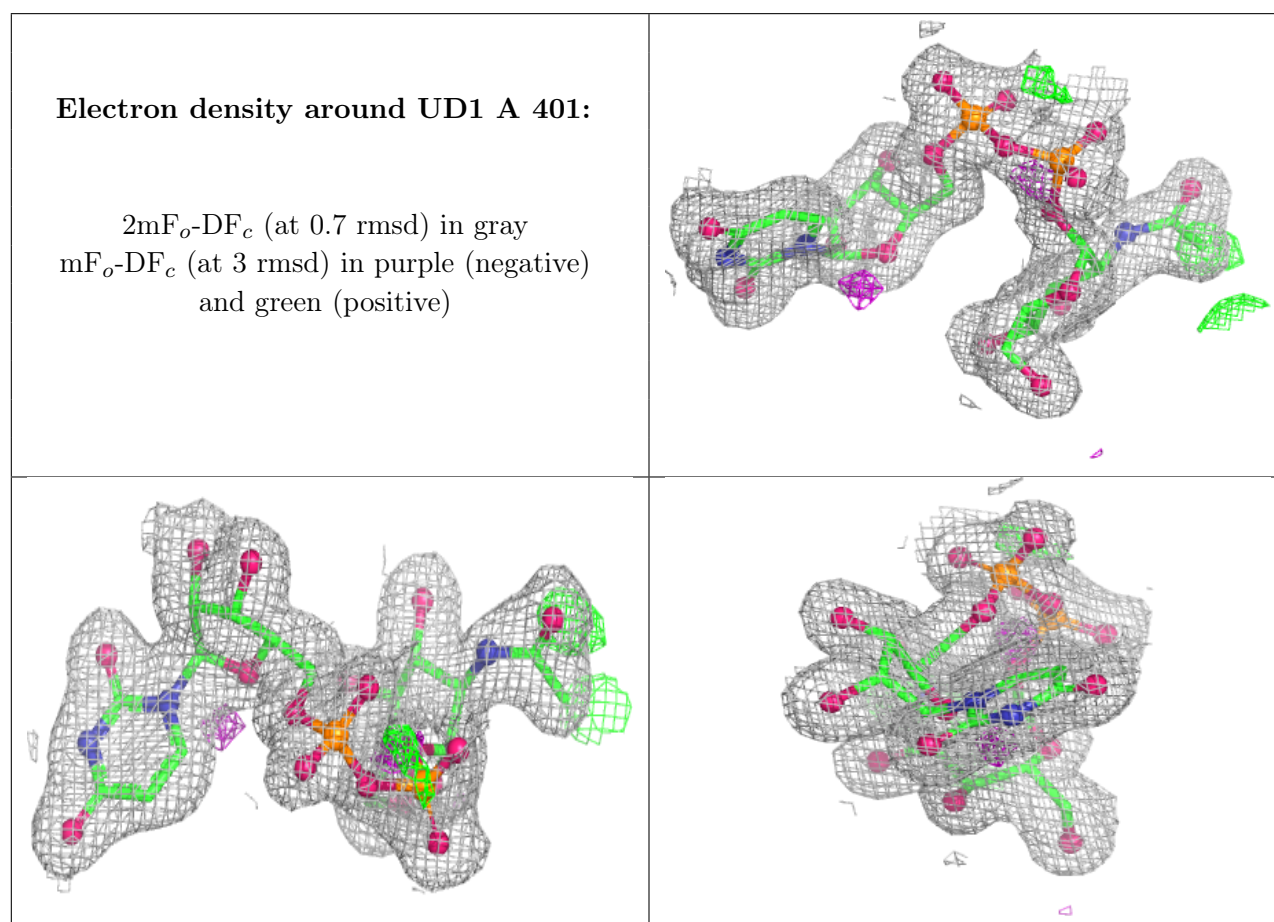
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UD1	A	401	39/39	0.99	0.03	13,17,23,28	0
2	UD1	B	401	39/39	0.99	0.03	13,16,25,28	0
2	UD1	C	401	39/39	0.99	0.03	14,19,30,36	0
2	UD1	D	401	39/39	0.99	0.03	14,20,32,33	0

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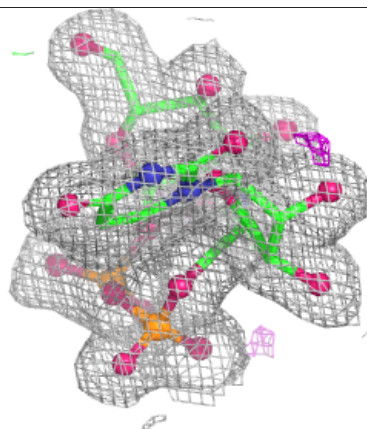
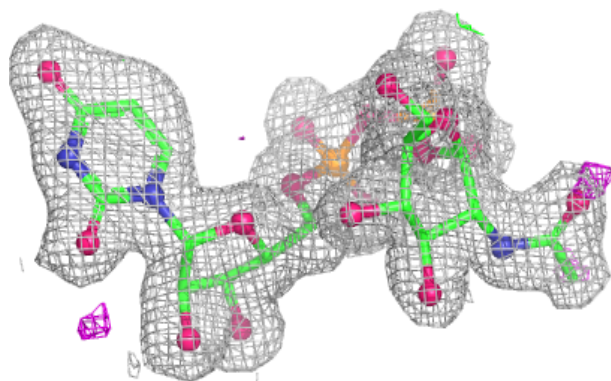
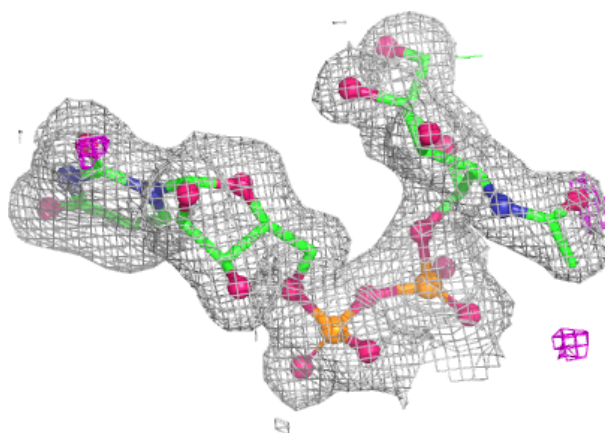
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	B	403	1/1	0.99	0.06	42,42,42,42	0
3	MN	A	403	1/1	1.00	0.05	40,40,40,40	0
3	MN	B	402	1/1	1.00	0.01	19,19,19,19	0
3	MN	A	402	1/1	1.00	0.01	19,19,19,19	0
3	MN	C	402	1/1	1.00	0.01	19,19,19,19	0
3	MN	D	402	1/1	1.00	0.02	19,19,19,19	0

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.



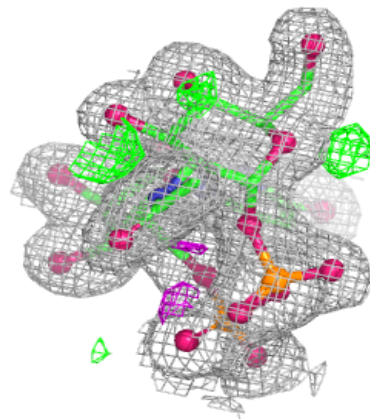
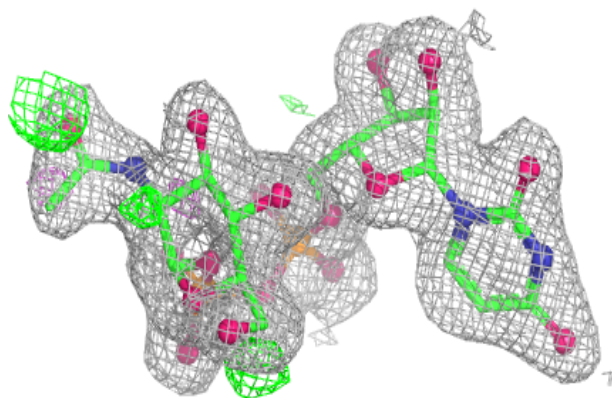
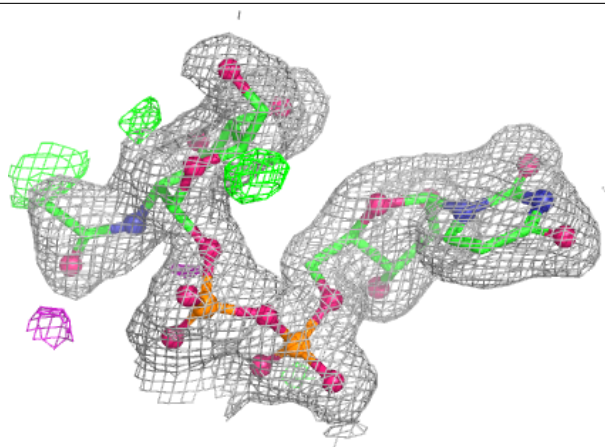
Electron density around UD1 B 401:

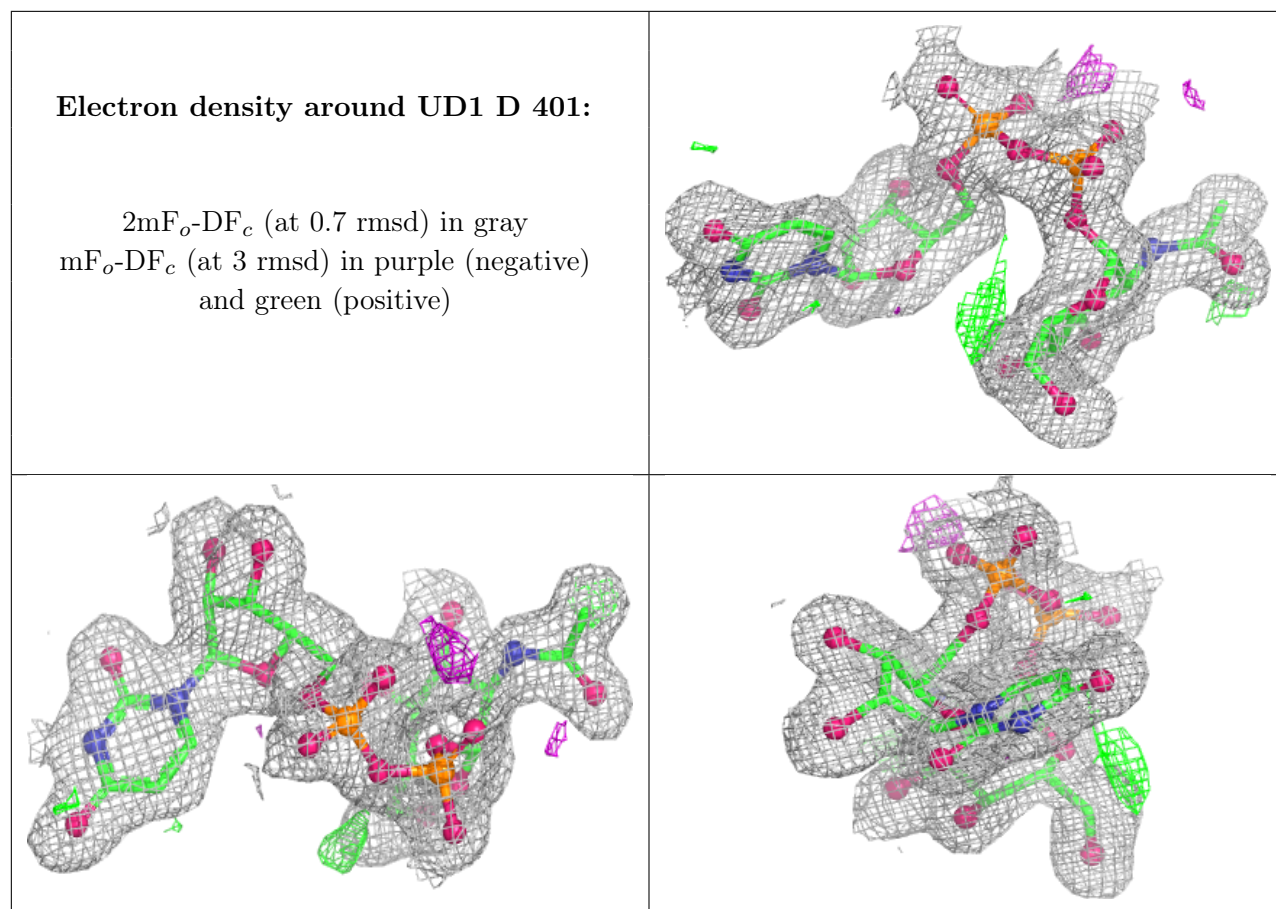
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.