Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2021 – 10:15 PM JST

PDB ID	:	7CK2
Title	:	Crystal structure of Arabidopsis CESA3 catalytic domain with UDP-Glucose
Authors	:	Qiao, Z.; Gao, Y.G.
Deposited on	:	2020-07-15
Resolution	:	2.05 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 following versions of software and data (see references ⓘ) were used in the production of this report:

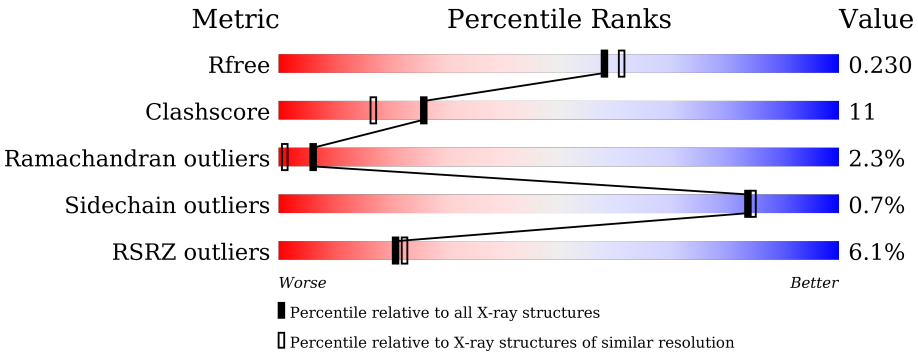
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	410	6% 72% 11% • • 14%
1	B	410	4% 69% 12% • • 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5851 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 Cellulose synthase A catalytic subunit 3 [UDP-forming],Cellulose synthase A catalytic subunit 3 [UDP-forming].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total 2775	C 1773	N 471	O 512	S 19	0	0	0
1	B	351	Total 2764	C 1767	N 469	O 509	S 19	0	0	0

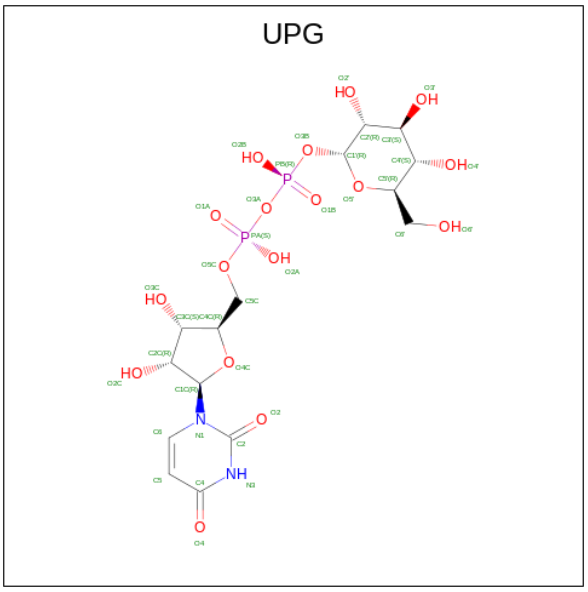
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	GLY	-	linker	UNP Q941L0
A	698	SER	-	linker	UNP Q941L0
A	699	GLY	-	linker	UNP Q941L0
A	700	SER	-	linker	UNP Q941L0
A	701	GLY	-	linker	UNP Q941L0
B	697	GLY	-	linker	UNP Q941L0
B	698	SER	-	linker	UNP Q941L0
B	699	GLY	-	linker	UNP Q941L0
B	700	SER	-	linker	UNP Q941L0
B	701	GLY	-	linker	UNP Q941L0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

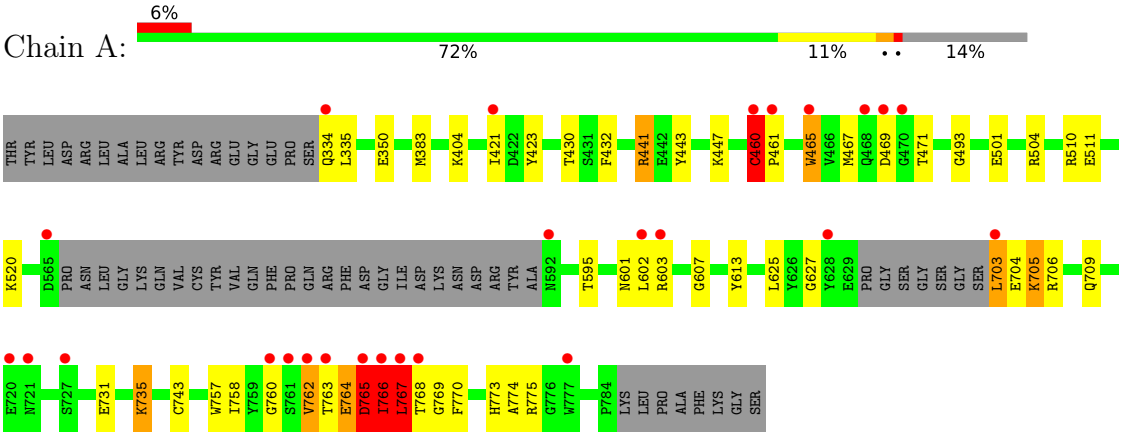
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	113	Total	O	0	0
			113	113		

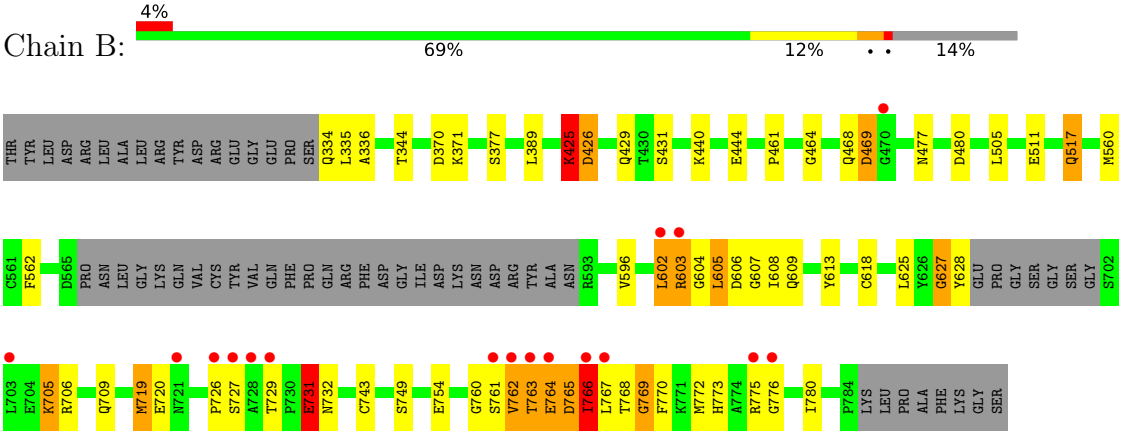
3 Residue-property plots (i)

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: Cellulose synthase A catalytic subunit 3 [UDP-forming],Cellulose synthase A catalytic subunit 3 [UDP-forming]



• Molecule 1: Cellulose synthase A catalytic subunit 3 [UDP-forming],Cellulose synthase A catalytic subunit 3 [UDP-forming]



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.36Å 148.53Å 94.09Å 90.00° 103.15° 90.00°	Depositor
Resolution (Å)	43.78 – 2.05 49.86 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.78-2.05) 99.0 (49.86-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.214 , 0.231 0.214 , 0.230	Depositor DCC
R_{free} test set	4500 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5851	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: UPG, MN

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	0.58	6/2842 (0.2%)	0.96	24/3849 (0.6%)
1	B	0.54	3/2831 (0.1%)	1.06	15/3834 (0.4%)
All	All	0.56	9/5673 (0.2%)	1.01	39/7683 (0.5%)

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	5
1	B	0	5
All	All	0	10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	TRP	CE3-CZ3	-8.95	1.23	1.38
1	A	767	LEU	CG-CD2	-7.46	1.24	1.51
1	B	425	LYS	CD-CE	6.22	1.66	1.51
1	A	735	LYS	CD-CE	5.96	1.66	1.51
1	B	764	GLU	CG-CD	-5.95	1.43	1.51
1	A	764	GLU	CD-OE2	5.67	1.31	1.25
1	B	603	ARG	CZ-NH2	-5.26	1.26	1.33
1	A	465	TRP	CE2-CZ2	-5.22	1.30	1.39
1	A	465	TRP	CZ3-CH2	-5.10	1.31	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	731	GLU	OE1-CD-OE2	-30.03	87.26	123.30
1	B	731	GLU	CG-CD-OE1	17.39	153.08	118.30
1	B	731	GLU	CG-CD-OE2	-15.28	87.74	118.30
1	B	603	ARG	NE-CZ-NH2	-13.27	113.66	120.30
1	A	767	LEU	CB-CG-CD2	12.87	132.87	111.00
1	B	425	LYS	CB-CA-C	-12.83	84.74	110.40
1	B	603	ARG	NE-CZ-NH1	12.44	126.52	120.30
1	A	465	TRP	CB-CG-CD2	-12.11	110.86	126.60
1	A	441	ARG	CB-CG-CD	-11.97	80.48	111.60
1	A	767	LEU	CA-CB-CG	11.34	141.39	115.30
1	A	441	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	B	764	GLU	CA-CB-CG	-10.38	90.55	113.40
1	A	764	GLU	CA-CB-CG	10.28	136.01	113.40
1	A	465	TRP	CD1-CG-CD2	-9.12	99.00	106.30
1	A	767	LEU	CB-CA-C	8.78	126.87	110.20
1	B	603	ARG	CD-NE-CZ	8.59	135.62	123.60
1	A	735	LYS	CB-CA-C	-8.03	94.34	110.40
1	B	763	THR	C-N-CA	-7.86	102.06	121.70
1	A	766	ILE	CG1-CB-CG2	7.79	128.54	111.40
1	B	766	ILE	CG1-CB-CG2	7.58	128.07	111.40
1	B	425	LYS	CD-CE-NZ	-7.03	95.54	111.70
1	B	517	GLN	N-CA-CB	-6.93	98.13	110.60
1	A	465	TRP	N-CA-CB	6.92	123.06	110.60
1	A	735	LYS	CG-CD-CE	-6.72	91.75	111.90
1	A	441	ARG	CD-NE-CZ	6.56	132.78	123.60
1	A	735	LYS	N-CA-CB	6.47	122.24	110.60
1	A	764	GLU	N-CA-CB	-6.06	99.69	110.60
1	B	705	LYS	CA-CB-CG	-6.00	100.19	113.40
1	A	735	LYS	CD-CE-NZ	5.99	125.48	111.70
1	A	602	LEU	N-CA-CB	5.98	122.36	110.40
1	A	441	ARG	CA-CB-CG	5.76	126.07	113.40
1	A	460	CYS	CA-CB-SG	5.74	124.33	114.00
1	B	425	LYS	N-CA-CB	5.73	120.91	110.60
1	A	703	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	764	GLU	CB-CA-C	5.54	121.48	110.40
1	A	602	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	765	ASP	CB-CA-C	-5.25	99.89	110.40
1	B	705	LYS	CB-CG-CD	5.22	125.18	111.60
1	A	465	TRP	CD1-NE1-CE2	-5.22	104.30	109.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	441	ARG	Sidechain
1	A	460	CYS	Peptide
1	A	603	ARG	Peptide
1	A	705	LYS	Peptide
1	A	767	LEU	Peptide
1	B	425	LYS	Peptide
1	B	719	MET	Peptide
1	B	731	GLU	Sidechain
1	B	760	GLY	Peptide
1	B	762	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2775	0	2726	66	0
1	B	2764	0	2719	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	36	0	22	1	0
3	B	36	0	22	0	0
4	A	123	0	0	6	0
4	B	113	0	0	1	0
All	All	5851	0	5489	117	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 11.

All (117) 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:460:CYS:HA	1:A:465:TRP:HH2	1.19	1.08
1:A:460:CYS:HA	1:A:465:TRP:CH2	2.03	0.93
1:A:758:ILE:O	1:A:767:LEU:HB3	1.70	0.90
1:A:430:THR:HG22	1:A:432:PHE:H	1.41	0.86
1:B:336:ALA:H	1:B:560:MET:HE2	1.37	0.85
1:B:613:TYR:CG	1:B:766:ILE:HG21	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:TYR:CD2	1:B:766:ILE:HG21	2.14	0.82
1:B:705:LYS:HE2	1:B:709:GLN:HE22	1.42	0.82
1:A:757:TRP:NE1	1:A:767:LEU:HA	1.94	0.81
1:A:460:CYS:CA	1:A:465:TRP:HH2	1.93	0.79
1:A:757:TRP:CD1	1:A:767:LEU:HA	2.17	0.78
1:A:465:TRP:HA	1:A:465:TRP:CE3	2.20	0.77
1:B:729:THR:HG23	1:B:732:ASN:H	1.54	0.72
1:B:768:THR:HG22	1:B:769:GLY:H	1.53	0.72
1:B:517:GLN:HG3	4:B:996:HOH:O	1.89	0.72
1:A:758:ILE:HB	1:A:766:ILE:CG2	2.20	0.71
1:A:762:VAL:HG22	1:A:763:THR:HG23	1.74	0.69
1:A:601:ASN:ND2	1:A:774:ALA:HB1	2.09	0.68
1:A:758:ILE:HB	1:A:766:ILE:HG21	1.75	0.67
1:B:731:GLU:OE2	1:B:731:GLU:N	2.22	0.67
1:A:404:LYS:NZ	4:A:904:HOH:O	2.25	0.67
1:B:761:SER:O	1:B:763:THR:N	2.26	0.65
1:A:601:ASN:HD22	1:A:774:ALA:HB1	1.61	0.64
1:A:766:ILE:HG13	1:A:767:LEU:N	2.13	0.63
1:B:336:ALA:H	1:B:560:MET:CE	2.10	0.63
1:B:425:LYS:HB2	1:B:426:ASP:CB	2.29	0.63
1:A:762:VAL:HG13	1:A:763:THR:H	1.63	0.62
1:A:504:ARG:NH1	4:A:905:HOH:O	2.29	0.61
1:A:520:LYS:NZ	3:A:803:UPG:O1B	2.32	0.61
1:B:705:LYS:HE2	1:B:709:GLN:NE2	2.16	0.58
1:B:511:GLU:HG2	1:B:743:CYS:HB3	1.85	0.58
1:A:430:THR:HG22	1:A:432:PHE:N	2.14	0.58
1:B:389:LEU:HG	1:B:505:LEU:HD21	1.85	0.58
1:B:628:TYR:CZ	1:B:754:GLU:HG3	2.38	0.58
1:B:625:LEU:HD21	1:B:770:PHE:HB3	1.86	0.57
1:B:425:LYS:HB2	1:B:426:ASP:HB2	1.86	0.57
1:B:425:LYS:O	1:B:426:ASP:O	2.22	0.57
1:B:344:THR:HG22	1:B:377:SER:O	2.05	0.56
1:A:465:TRP:HA	1:A:465:TRP:HE3	1.65	0.56
1:B:469:ASP:N	1:B:469:ASP:OD1	2.38	0.56
1:B:763:THR:C	1:B:764:GLU:HG2	2.23	0.56
1:A:766:ILE:HG13	1:A:767:LEU:H	1.72	0.55
1:B:764:GLU:O	1:B:765:ASP:HB2	2.06	0.55
1:B:767:LEU:HD12	1:B:767:LEU:H	1.71	0.55
1:B:768:THR:HG22	1:B:769:GLY:N	2.18	0.55
1:A:757:TRP:HE1	1:A:767:LEU:HA	1.66	0.55
1:A:504:ARG:HG3	1:A:504:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLY:O	4:A:901:HOH:O	2.19	0.54
1:A:766:ILE:C	1:A:768:THR:H	2.12	0.53
1:A:460:CYS:HB3	1:A:461:PRO:O	2.08	0.53
1:B:602:LEU:O	1:B:603:ARG:HD3	2.08	0.52
1:A:625:LEU:HD21	1:A:770:PHE:HB3	1.91	0.52
1:A:768:THR:HG23	1:B:605:LEU:CD2	2.40	0.52
1:A:465:TRP:CE3	1:A:465:TRP:CA	2.90	0.52
1:A:764:GLU:O	1:A:766:ILE:N	2.43	0.52
1:A:350:GLU:OE2	4:A:902:HOH:O	2.19	0.50
1:A:768:THR:HG23	1:B:605:LEU:HD22	1.93	0.50
1:A:383:MET:CE	1:A:467:MET:HG2	2.41	0.50
1:A:510:ARG:HD2	4:A:917:HOH:O	2.11	0.50
1:B:468:GLN:HG2	1:B:469:ASP:H	1.76	0.50
1:A:703:LEU:O	1:A:706:ARG:NH1	2.37	0.50
1:B:335:LEU:O	1:B:371:LYS:NZ	2.34	0.50
1:A:760:GLY:N	1:A:767:LEU:HD23	2.27	0.49
1:B:562:PHE:CZ	1:B:596:VAL:HG13	2.47	0.49
1:A:383:MET:HE2	1:A:467:MET:HG2	1.94	0.49
1:A:758:ILE:O	1:A:767:LEU:CB	2.54	0.49
1:B:429:GLN:O	1:B:431:SER:N	2.45	0.49
1:A:705:LYS:HG3	1:A:709:GLN:OE1	2.12	0.49
1:B:602:LEU:C	1:B:603:ARG:HD3	2.33	0.49
1:B:705:LYS:O	1:B:749:SER:HA	2.13	0.49
1:B:606:ASP:O	1:B:609:GLN:NE2	2.47	0.48
1:B:468:GLN:HG2	1:B:469:ASP:N	2.28	0.48
1:B:613:TYR:CD2	1:B:766:ILE:CG2	2.93	0.48
1:A:760:GLY:H	1:A:767:LEU:HD23	1.79	0.47
1:A:421:ILE:HG23	1:A:423:TYR:CE2	2.49	0.47
1:A:443:TYR:CE2	1:A:447:LYS:HD2	2.49	0.47
1:B:370:ASP:OD1	1:B:370:ASP:N	2.48	0.47
1:B:334:GLN:CD	1:B:335:LEU:H	2.18	0.47
1:A:511:GLU:HG2	1:A:743:CYS:HB3	1.97	0.47
1:A:461:PRO:HD2	1:A:465:TRP:CZ3	2.50	0.47
1:A:613:TYR:CD2	1:A:766:ILE:HD13	2.50	0.47
1:A:627:GLY:HA3	1:A:773:HIS:HB2	1.97	0.47
1:A:766:ILE:C	1:A:768:THR:N	2.69	0.47
1:A:501:GLU:OE1	4:A:903:HOH:O	2.21	0.45
1:A:766:ILE:HD11	1:A:769:GLY:N	2.32	0.45
1:B:726:PRO:O	1:B:727:SER:OG	2.30	0.45
1:B:772:MET:HE3	1:B:780:ILE:HD11	1.99	0.45
1:A:461:PRO:CG	1:A:465:TRP:HZ3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:PRO:HG2	1:B:464:GLY:O	2.17	0.45
1:A:595:THR:HG21	1:B:608:ILE:HG12	1.98	0.44
1:B:768:THR:CG2	1:B:769:GLY:H	2.25	0.44
1:B:729:THR:OG1	1:B:731:GLU:OE2	2.30	0.44
1:B:764:GLU:O	1:B:765:ASP:CB	2.64	0.44
1:B:627:GLY:CA	1:B:775:ARG:HD2	2.48	0.44
1:A:768:THR:O	1:B:609:GLN:HG3	2.16	0.44
1:A:766:ILE:CG1	1:A:767:LEU:N	2.78	0.44
1:A:758:ILE:HB	1:A:766:ILE:HG23	1.96	0.44
1:A:461:PRO:CD	1:A:465:TRP:CZ3	3.01	0.43
1:B:765:ASP:OD1	1:B:766:ILE:N	2.52	0.43
1:A:469:ASP:HB2	1:A:471:THR:H	1.84	0.43
1:B:440:LYS:O	1:B:444:GLU:HG2	2.19	0.43
1:B:719:MET:HA	1:B:720:GLU:OE1	2.18	0.43
1:B:754:GLU:O	1:B:773:HIS:NE2	2.52	0.43
1:A:607:GLY:HA2	1:B:618:CYS:SG	2.59	0.43
1:A:766:ILE:HD12	1:A:766:ILE:HA	1.80	0.43
1:A:762:VAL:HG13	1:A:763:THR:N	2.33	0.43
1:B:628:TYR:HD1	1:B:706:ARG:HH21	1.66	0.42
1:A:504:ARG:NH1	1:A:504:ARG:HG3	2.34	0.42
1:A:705:LYS:HE2	1:A:709:GLN:HA	2.01	0.42
1:A:758:ILE:CB	1:A:766:ILE:HG21	2.47	0.41
1:B:606:ASP:OD1	1:B:607:GLY:N	2.53	0.41
1:A:334:GLN:HG2	1:A:335:LEU:H	1.86	0.41
1:B:628:TYR:HB3	1:B:706:ARG:HH22	1.85	0.41
1:A:703:LEU:HB3	1:A:704:GLU:H	1.41	0.41
1:A:731:GLU:H	1:A:731:GLU:HG3	1.40	0.40
1:A:768:THR:HG21	1:B:609:GLN:OE1	2.21	0.40
1:B:477:ASN:ND2	1:B:480:ASP:HB3	2.36	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	346/410 (84%)	328 (95%)	13 (4%)	5 (1%)	11 3
1	B	345/410 (84%)	318 (92%)	16 (5%)	11 (3%)	4 0
All	All	691/820 (84%)	646 (94%)	29 (4%)	16 (2%)	6 1

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	ASP
1	A	767	LEU
1	B	426	ASP
1	B	469	ASP
1	B	762	VAL
1	B	765	ASP
1	B	769	GLY
1	A	762	VAL
1	A	766	ILE
1	A	775	ARG
1	B	605	LEU
1	B	766	ILE
1	B	776	GLY
1	B	602	LEU
1	B	627	GLY
1	B	604	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	298/346 (86%)	295 (99%)	3 (1%)	76 75
1	B	297/346 (86%)	296 (100%)	1 (0%)	92 93
All	All	595/692 (86%)	591 (99%)	4 (1%)	84 84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	735	LYS
1	A	765	ASP
1	A	767	LEU
1	B	425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	491	GLN
1	A	548	HIS
1	A	601	ASN
1	B	709	GLN

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	UPG	B	803	-	31,38,38	3.77	11 (35%)	41,58,58	1.13	4 (9%)
3	UPG	A	803	-	31,38,38	3.78	11 (35%)	41,58,58	1.29	5 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UPG	B	803	-	-	6/21/59/59	0/3/3/3
3	UPG	A	803	-	-	7/21/59/59	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	UPG	O4C-C1C	11.90	1.57	1.41
3	A	803	UPG	O4C-C1C	11.54	1.57	1.41
3	A	803	UPG	C4-N3	7.43	1.46	1.33
3	B	803	UPG	C4-N3	7.28	1.45	1.33
3	B	803	UPG	C3C-C2C	-7.03	1.34	1.53
3	A	803	UPG	C3C-C2C	-7.01	1.34	1.53
3	A	803	UPG	C6-N1	6.88	1.44	1.35
3	B	803	UPG	C6-N1	6.68	1.44	1.35
3	A	803	UPG	O4C-C4C	-6.15	1.31	1.45
3	B	803	UPG	O4C-C4C	-6.08	1.31	1.45
3	A	803	UPG	C2-N3	5.87	1.49	1.38
3	B	803	UPG	C2-N3	5.47	1.49	1.38
3	A	803	UPG	C6-C5	5.27	1.49	1.38
3	B	803	UPG	C6-C5	4.99	1.49	1.38
3	B	803	UPG	C3C-C4C	4.52	1.64	1.53
3	A	803	UPG	C3C-C4C	4.18	1.63	1.53
3	B	803	UPG	O5'-C1'	3.84	1.51	1.41
3	A	803	UPG	O5'-C1'	3.81	1.51	1.41
3	A	803	UPG	PA-O5C	2.97	1.71	1.59
3	B	803	UPG	PA-O5C	2.76	1.70	1.59
3	B	803	UPG	O2C-C2C	2.17	1.48	1.43
3	A	803	UPG	O2C-C2C	2.04	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	UPG	O3A-PB-O3B	3.82	110.18	102.48
3	B	803	UPG	O3A-PB-O3B	2.91	108.36	102.48
3	A	803	UPG	O3B-C1'-C2'	2.72	113.37	108.38
3	B	803	UPG	PB-O3A-PA	-2.42	124.52	132.83
3	A	803	UPG	O4C-C1C-C2C	-2.36	103.47	106.93
3	B	803	UPG	O4C-C1C-C2C	-2.33	103.52	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	UPG	C3C-C2C-C1C	2.29	104.42	100.98
3	B	803	UPG	C4'-C3'-C2'	2.19	114.65	110.82
3	A	803	UPG	O5'-C5'-C4'	2.17	113.63	109.69

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	UPG	O4C-C1C-N1-C6
3	A	803	UPG	C1'-O3B-PB-O2B
3	B	803	UPG	C1'-O3B-PB-O3A
3	B	803	UPG	O5'-C1'-O3B-PB
3	B	803	UPG	O5'-C5'-C6'-O6'
3	B	803	UPG	C4'-C5'-C6'-O6'
3	A	803	UPG	C3C-C4C-C5C-O5C
3	A	803	UPG	O4C-C4C-C5C-O5C
3	A	803	UPG	C1'-O3B-PB-O3A
3	A	803	UPG	C2'-C1'-O3B-PB
3	A	803	UPG	PA-O3A-PB-O3B
3	B	803	UPG	PB-O3A-PA-O1A
3	B	803	UPG	C1'-O3B-PB-O1B

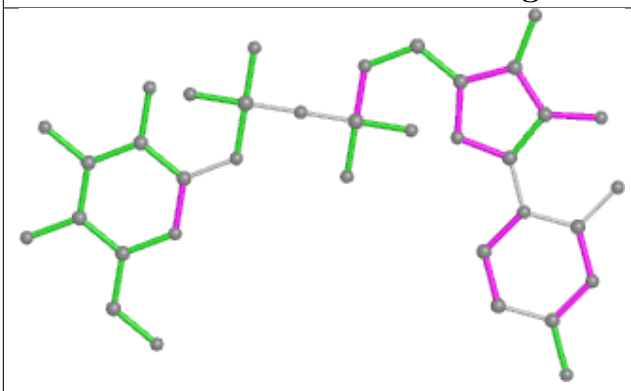
There are no ring outliers.

1 monomer is involved in 1 short contact:

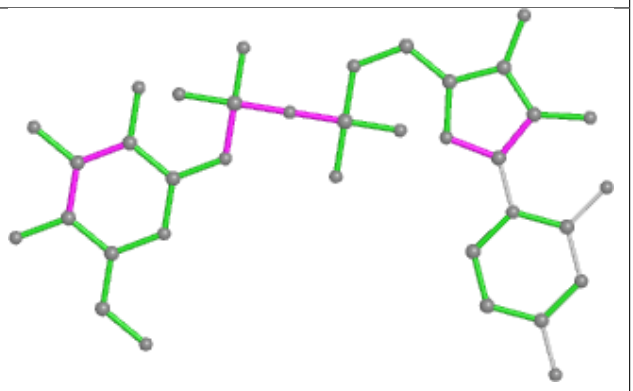
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	UPG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

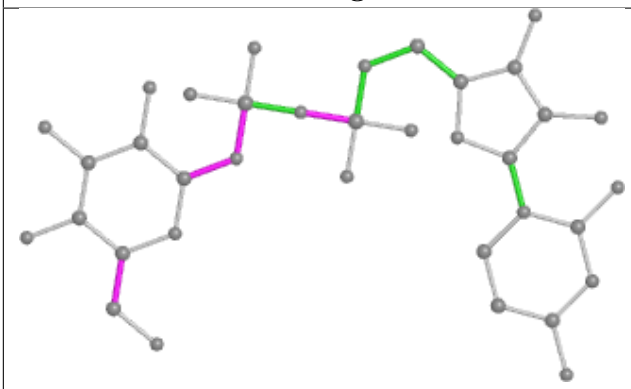
Ligand UPG B 803



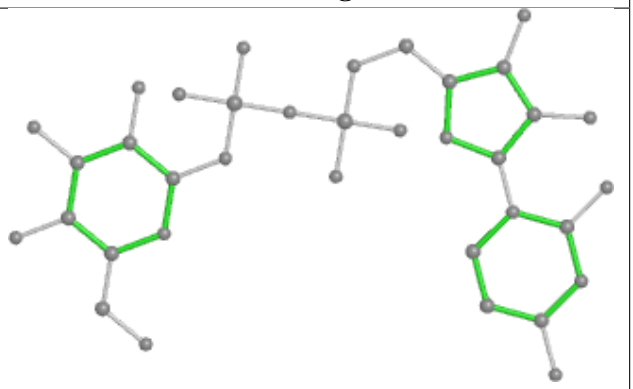
Bond lengths



Bond angles

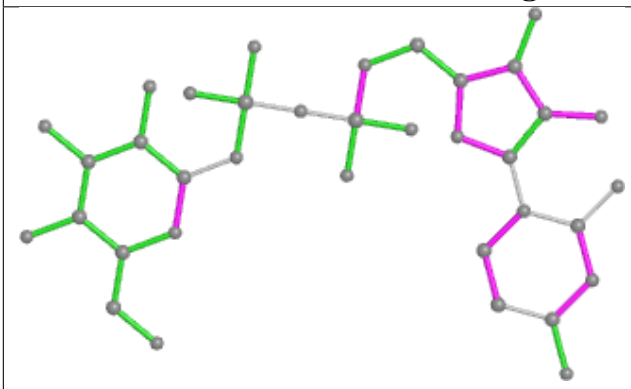


Torsions

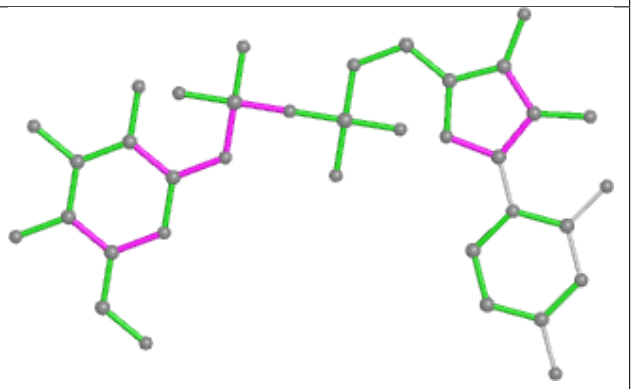


Rings

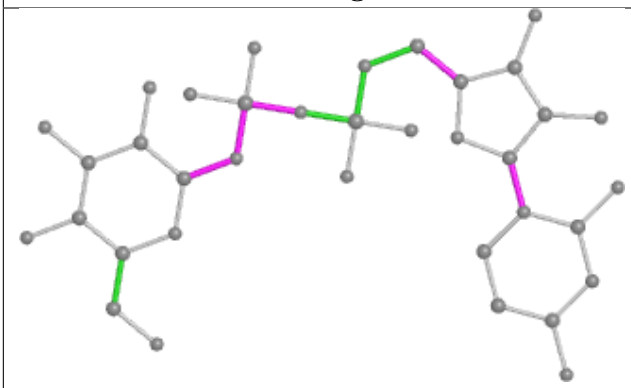
Ligand UPG A 803



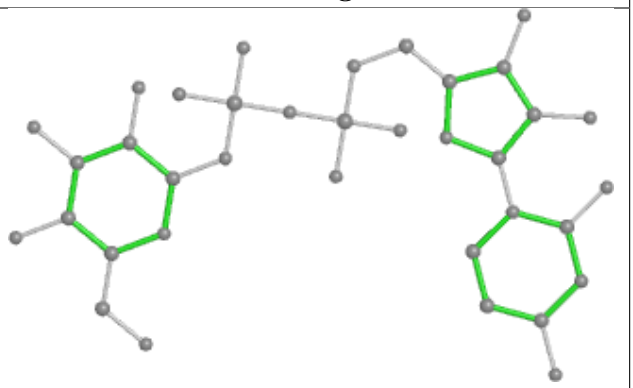
Bond lengths



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	352/410 (85%)	0.34	26 (7%)	14	16	46, 59, 95, 121	0
1	B	351/410 (85%)	0.36	17 (4%)	30	33	46, 58, 91, 134	0
All	All	703/820 (85%)	0.35	43 (6%)	21	22	46, 59, 93, 134	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	LEU	8.9
1	B	763	THR	8.2
1	A	628	TYR	7.4
1	B	762	VAL	6.8
1	B	603	ARG	4.5
1	A	703	LEU	4.4
1	A	470	GLY	4.4
1	A	720	GLU	4.4
1	A	727	SER	4.4
1	B	728	ALA	4.4
1	B	761	SER	4.2
1	A	762	VAL	4.1
1	A	761	SER	4.0
1	A	465	TRP	3.8
1	B	727	SER	3.7
1	A	765	ASP	3.7
1	A	603	ARG	3.6
1	A	602	LEU	3.5
1	A	469	ASP	3.5
1	B	470	GLY	3.3
1	A	763	THR	3.3
1	A	468	GLN	3.1
1	A	766	ILE	3.0
1	B	726	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	775	ARG	2.8
1	A	592	ASN	2.7
1	A	460	CYS	2.7
1	A	461	PRO	2.7
1	A	768	THR	2.6
1	B	729	THR	2.6
1	A	421	ILE	2.6
1	B	602	LEU	2.5
1	A	565	ASP	2.4
1	A	334	GLN	2.3
1	B	767	LEU	2.3
1	B	776	GLY	2.3
1	A	777	TRP	2.2
1	A	721	ASN	2.2
1	B	764	GLU	2.1
1	A	760	GLY	2.1
1	B	766	ILE	2.1
1	B	721	ASN	2.0
1	B	703	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UPG	A	803	36/36	0.79	0.19	54,82,101,102	36
3	UPG	B	803	36/36	0.79	0.21	54,83,98,98	36
2	MN	A	801	1/1	0.90	0.10	58,58,58,58	1
2	MN	B	802	1/1	0.90	0.18	77,77,77,77	1

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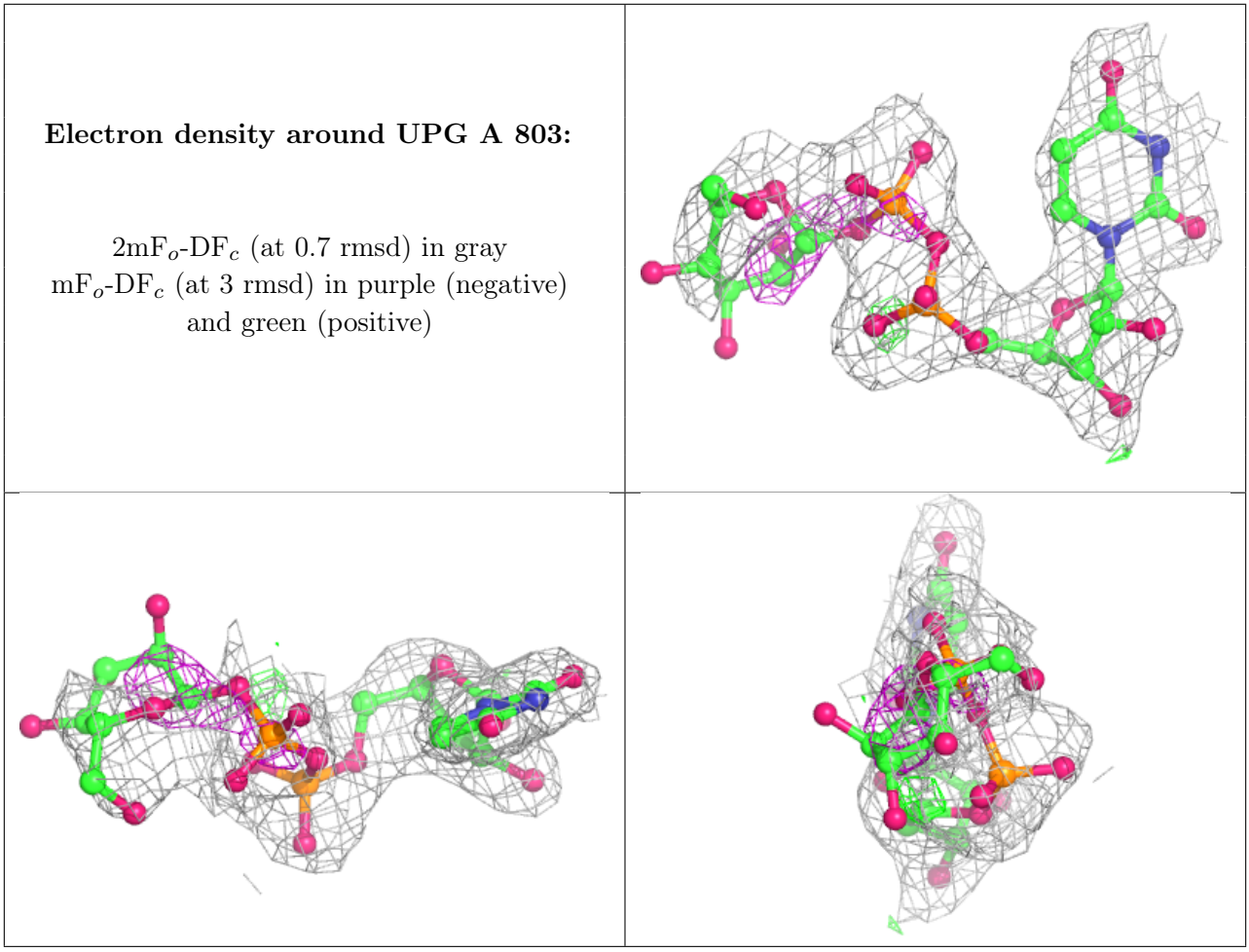
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	B	801	1/1	0.93	0.15	57,57,57,57	1
2	MN	A	802	1/1	0.93	0.11	59,59,59,59	1

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.

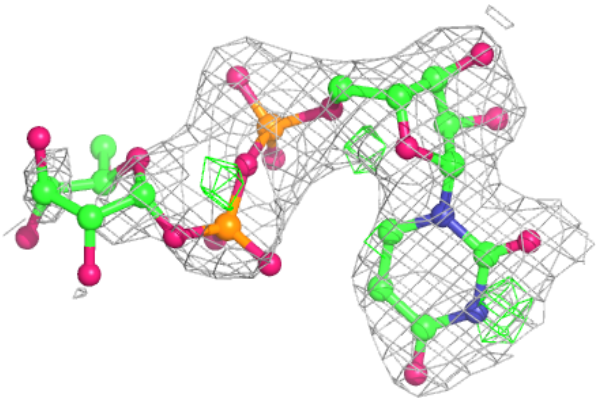
Electron density around UPG A 803:

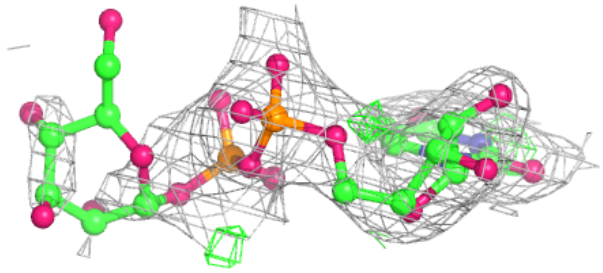
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

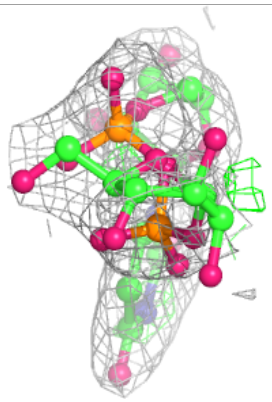


Electron density around UPG B 803:

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

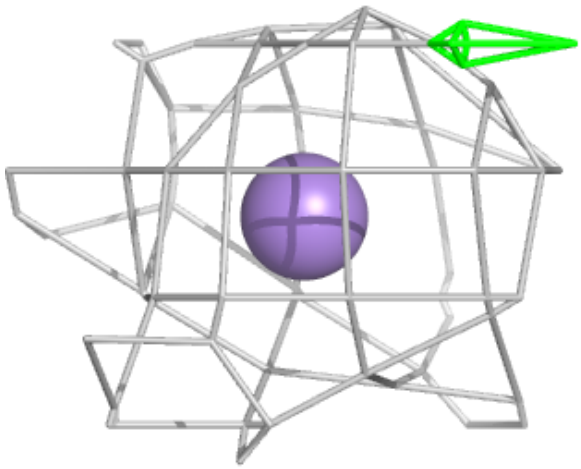


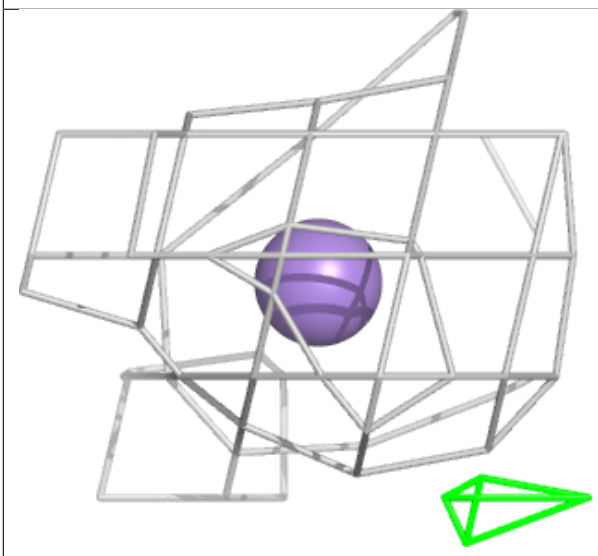


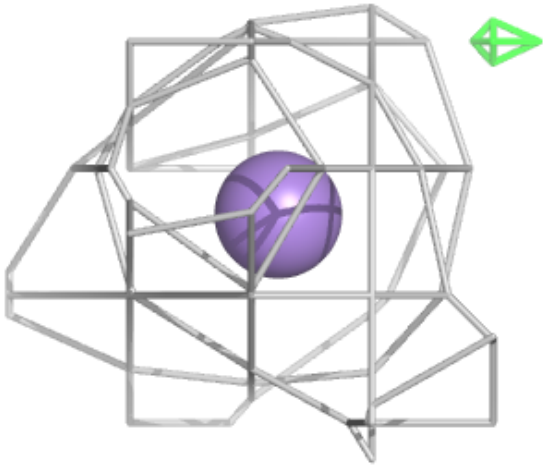


Electron density around MN A 801:

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

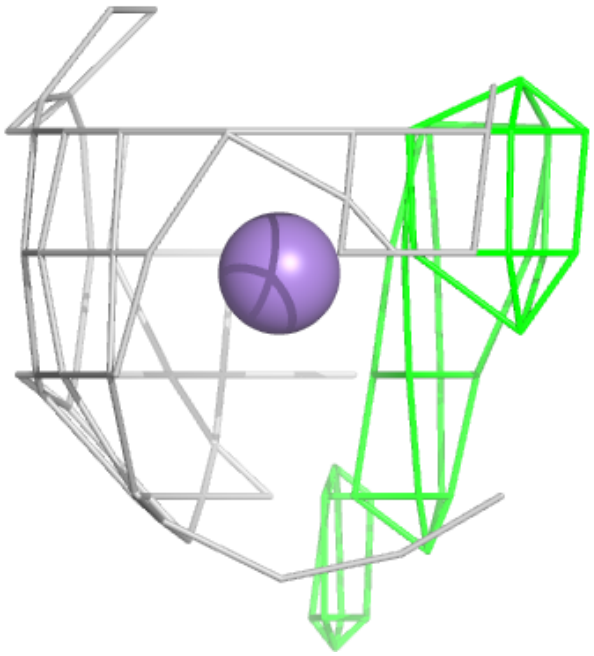


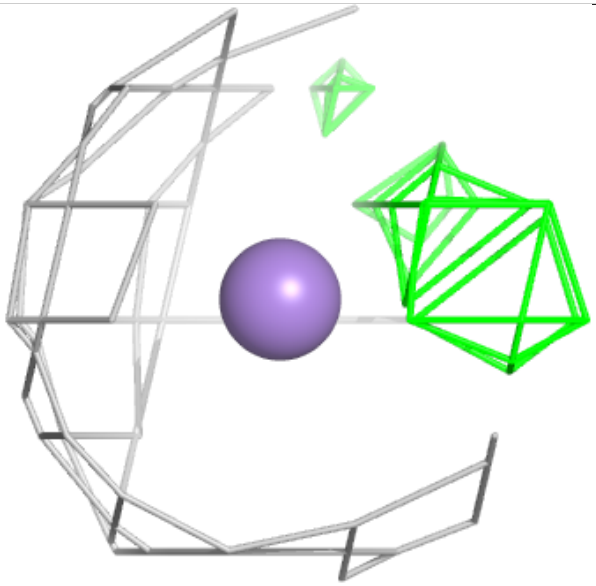


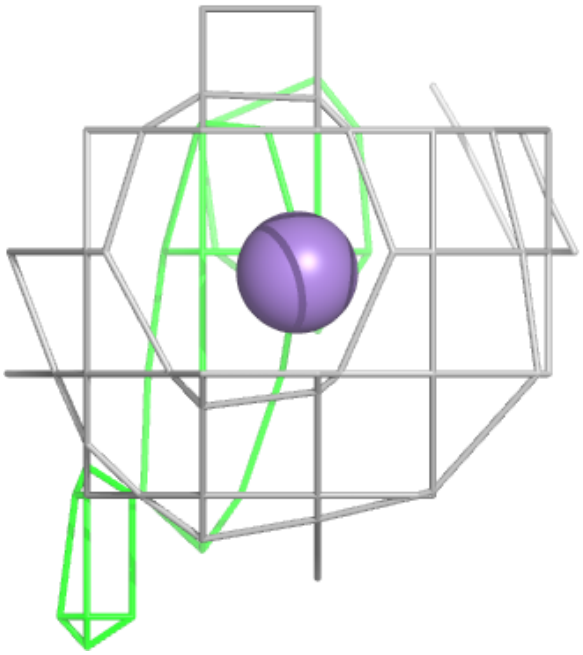


Electron density around MN B 802:

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

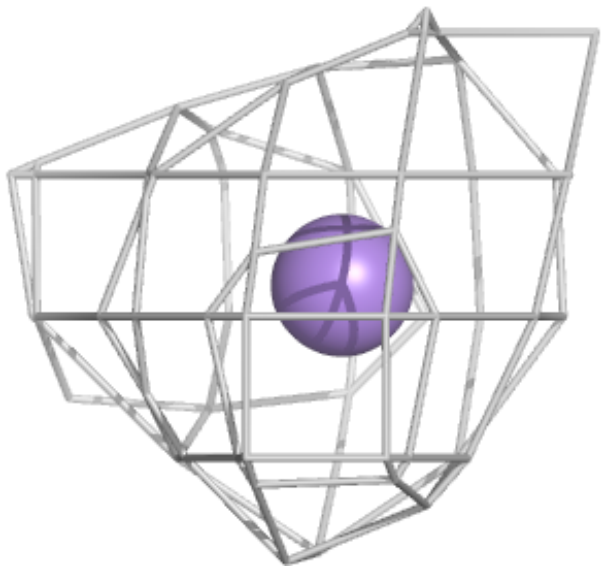


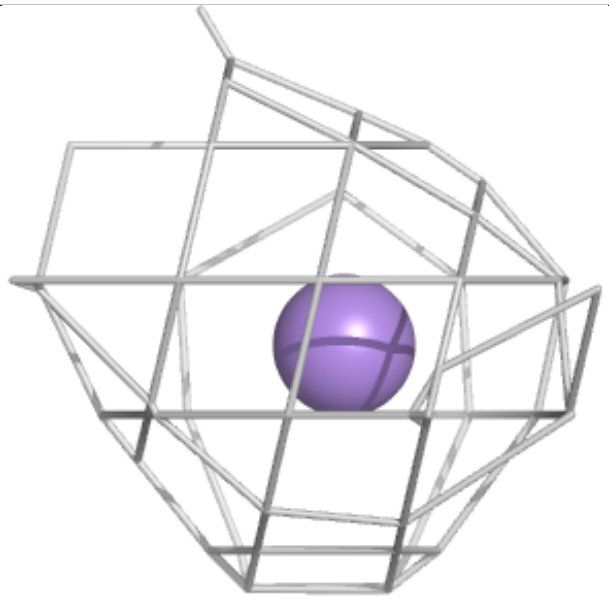


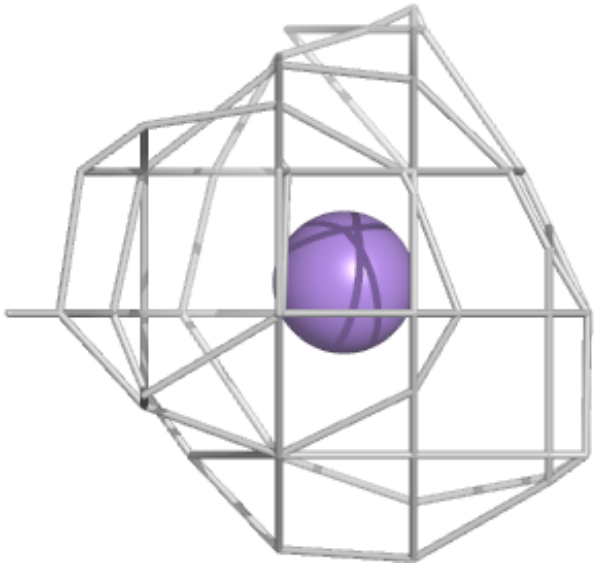


Electron density around MN B 801:

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

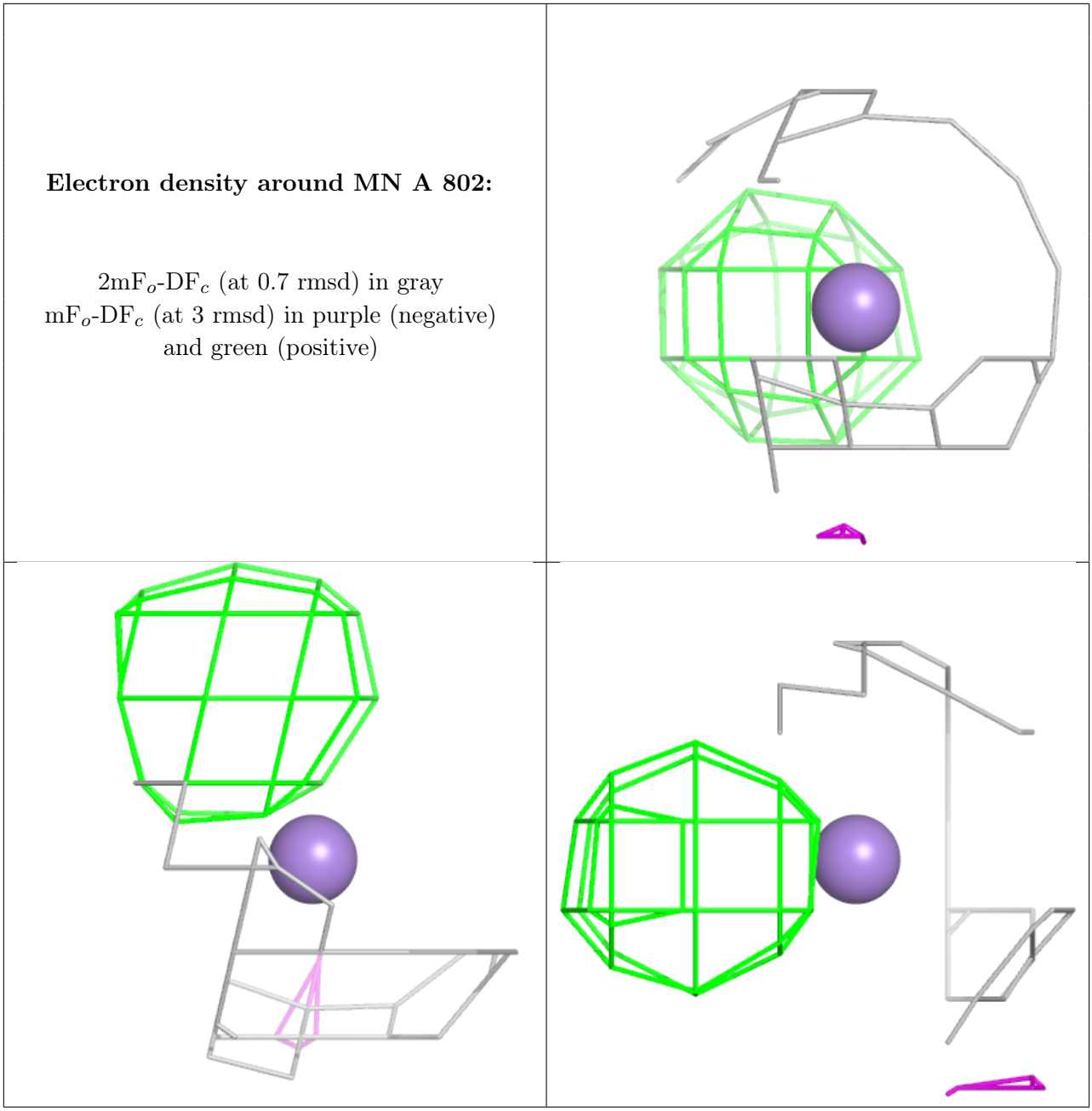






Electron density around MN A 802:

$2mF_o$-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.