WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2023 – 08:13 PM EDT

PDB ID	:	2Q3E
Title	:	Structure of human UDP-glucose dehydrogenase complexed with NADH and UDP-glucose
Authors	:	Kavanagh, K.L.; Guo, K.; Bunkoczi, G.; Savitsky, P.; Pilka, E.; Bhatia, C.; Smee, C.; Berridge, G.; von Delft, F.; Wiegelt, J.; Arrowsmith, C.; Sundstrom, M.; Edwards, A.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2007-05-30
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

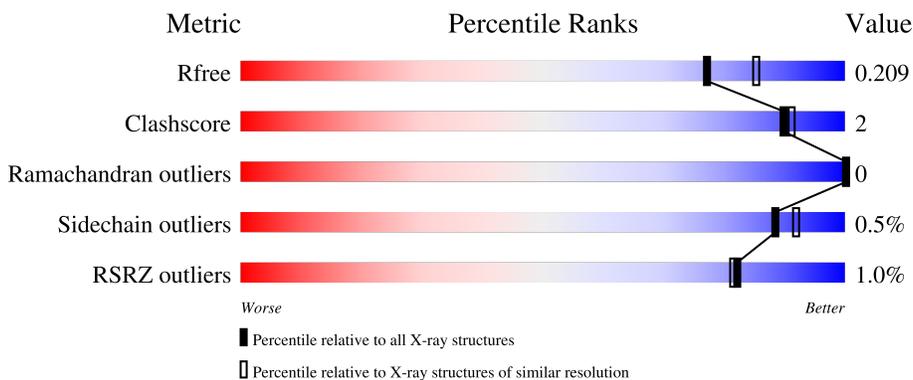|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
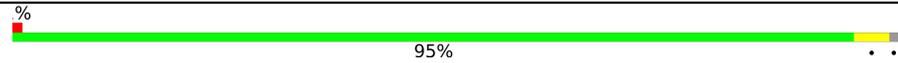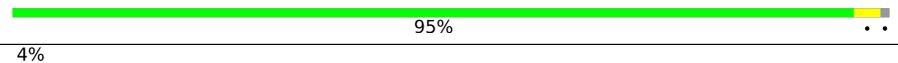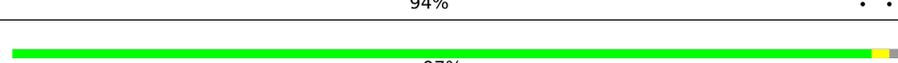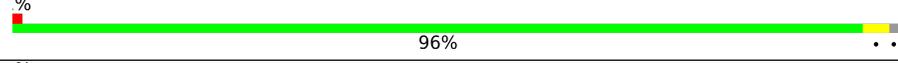
Metric	Percentile Ranks	Value
Rfree		0.209
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		1.0%

Worse   *Better*

█ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	467	95% ··
1	B	467	.% 95% ··
1	C	467	94% ··
1	D	467	95% ··
1	E	467	96% ··

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Mol	Chain	Length	Quality of chain
1	F	467	95%
1	G	467	95%
1	H	467	4% · · 94%
1	I	467	97%
1	J	467	96%
1	K	467	95%
1	L	467	2% 94% 5%
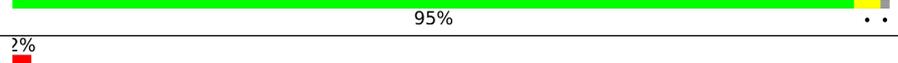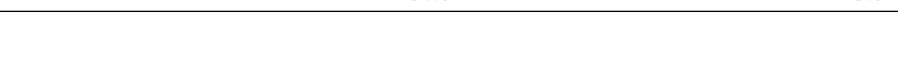
2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 46652 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 UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	7	0
			3629	2299	624	685	21			
1	B	460	Total	C	N	O	S	0	1	0
			3556	2255	609	672	20			
1	C	460	Total	C	N	O	S	0	5	0
			3598	2278	618	682	20			
1	D	458	Total	C	N	O	S	0	3	0
			3569	2264	609	676	20			
1	E	459	Total	C	N	O	S	0	3	0
			3567	2264	612	671	20			
1	F	460	Total	C	N	O	S	0	2	0
			3573	2265	612	676	20			
1	G	460	Total	C	N	O	S	0	2	0
			3579	2268	610	681	20			
1	H	459	Total	C	N	O	S	0	3	0
			3548	2250	604	674	20			
1	I	460	Total	C	N	O	S	0	4	0
			3593	2275	618	679	21			
1	J	460	Total	C	N	O	S	0	3	0
			3575	2266	614	675	20			
1	K	460	Total	C	N	O	S	0	3	0
			3580	2268	615	677	20			
1	L	460	Total	C	N	O	S	0	2	0
			3568	2261	611	676	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP O60701
B	0	SER	-	cloning artifact	UNP O60701
C	0	SER	-	cloning artifact	UNP O60701
D	0	SER	-	cloning artifact	UNP O60701
E	0	SER	-	cloning artifact	UNP O60701

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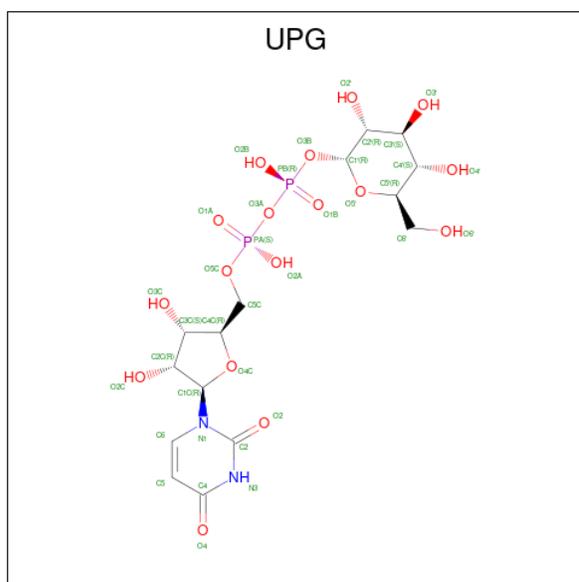
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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	cloning artifact	UNP O60701
G	0	SER	-	cloning artifact	UNP O60701
H	0	SER	-	cloning artifact	UNP O60701
I	0	SER	-	cloning artifact	UNP O60701
J	0	SER	-	cloning artifact	UNP O60701
K	0	SER	-	cloning artifact	UNP O60701
L	0	SER	-	cloning artifact	UNP O60701

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	B	1	Total 1	Cl 1	0	0
2	C	1	Total 1	Cl 1	0	0
2	D	1	Total 1	Cl 1	0	0
2	E	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0
2	G	1	Total 1	Cl 1	0	0
2	H	1	Total 1	Cl 1	0	0
2	I	1	Total 1	Cl 1	0	0
2	J	1	Total 1	Cl 1	0	0
2	K	1	Total 1	Cl 1	0	0
2	L	1	Total 1	Cl 1	0	0

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	B	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	C	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	D	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	E	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	F	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	G	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	H	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	I	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	J	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	K	1	Total 36	C 15	N 2	O 17	P 2	0	0
4	L	1	Total 36	C 15	N 2	O 17	P 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	287	Total 287	O 287	0	0
5	B	175	Total 175	O 175	0	0
5	C	283	Total 283	O 283	0	0
5	D	236	Total 236	O 236	0	0
5	E	268	Total 268	O 268	0	0
5	F	227	Total 227	O 227	0	0
5	G	263	Total 263	O 263	0	0
5	H	130	Total 130	O 130	0	0
5	I	254	Total 254	O 254	0	0
5	J	195	Total 195	O 195	0	0
5	K	234	Total 234	O 234	0	0
5	L	193	Total 193	O 193	0	0

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: UDP-glucose 6-dehydrogenase

Chain A:

- Molecule 1: UDP-glucose 6-dehydrogenase

Chain B:
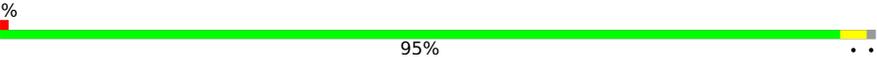
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain C:
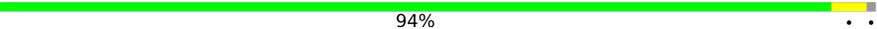
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain D:
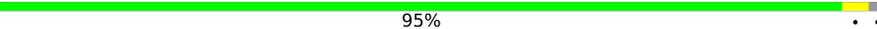
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain E:
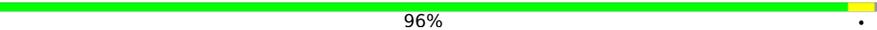
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain F:
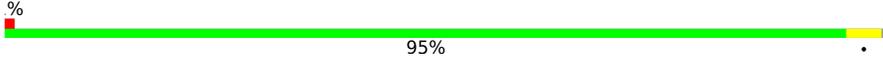
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain G:
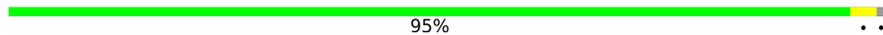
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain H:
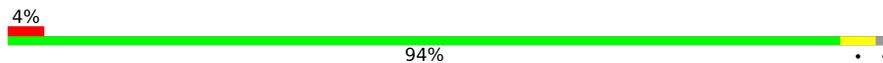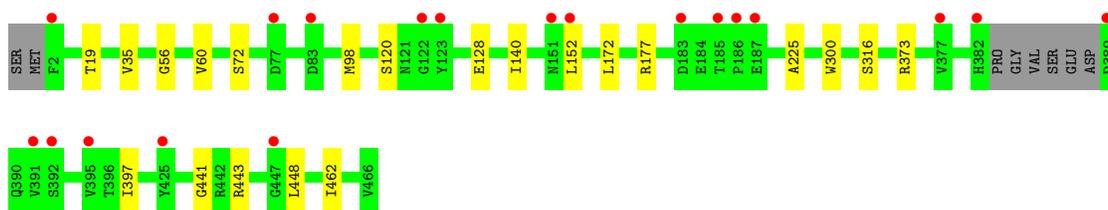
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain I:
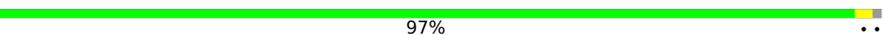
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain J:
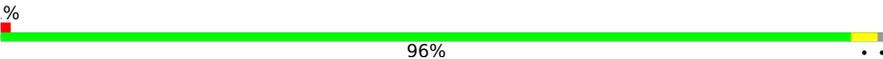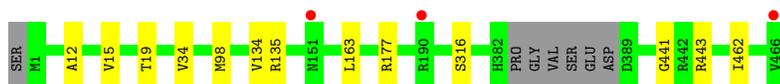
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain K:

- Molecule 1: UDP-glucose 6-dehydrogenase

Chain L:
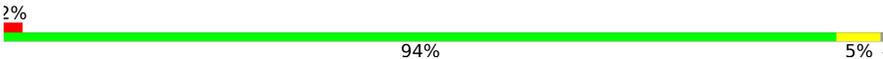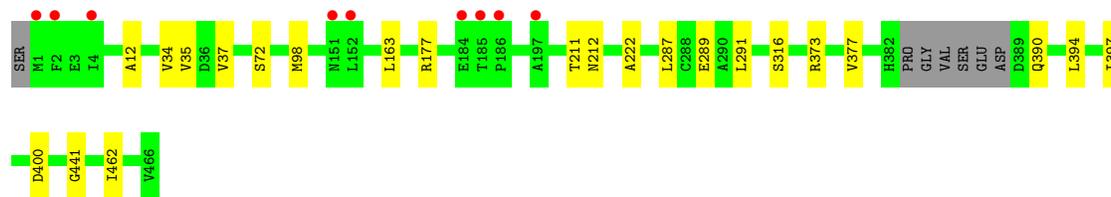
4　Data and refinement statistics　ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.99Å　184.13Å　170.94Å 90.00°　109.23°　90.00°	Depositor
Resolution (Å)	49.09　–　2.00 49.07　–　2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.09-2.00) 99.5 (49.07-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172　,　0.205 0.176　,　0.209	Depositor DCC
R_{free} test set	23473 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.6	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	46652	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4554e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: NAI, UPG, CL

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	0.52	1/3717 (0.0%)	0.61	0/5031
1	B	0.47	0/3624	0.58	0/4911
1	C	0.53	1/3679 (0.0%)	0.62	0/4982
1	D	0.46	1/3642 (0.0%)	0.56	0/4934
1	E	0.49	0/3640	0.59	0/4931
1	F	0.48	0/3644	0.58	0/4937
1	G	0.50	0/3649	0.60	0/4942
1	H	0.45	0/3622	0.55	0/4911
1	I	0.49	0/3669	0.59	0/4970
1	J	0.45	0/3650	0.55	0/4945
1	K	0.48	0/3654	0.58	0/4952
1	L	0.46	0/3638	0.57	0/4931
All	All	0.48	3/43828 (0.0%)	0.58	0/59377

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	CYS	CB-SG	-6.73	1.70	1.82
1	D	288	CYS	CB-SG	-5.44	1.73	1.81
1	A	64	CYS	CB-SG	-5.05	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3629	0	3624	13	0
1	B	3556	0	3526	10	0
1	C	3598	0	3588	16	0
1	D	3569	0	3560	14	0
1	E	3567	0	3560	11	0
1	F	3573	0	3556	15	0
1	G	3579	0	3561	11	0
1	H	3548	0	3506	23	0
1	I	3593	0	3581	6	0
1	J	3575	0	3557	17	0
1	K	3580	0	3562	10	0
1	L	3568	0	3545	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	44	0	27	2	0
3	B	44	0	27	3	0
3	C	44	0	27	2	0
3	D	44	0	27	2	0
3	E	44	0	27	4	0
3	F	44	0	27	2	0
3	G	44	0	27	2	0
3	H	44	0	26	2	0
3	I	44	0	27	2	0
3	J	44	0	27	3	0
3	K	44	0	27	4	0
3	L	44	0	27	3	0
4	A	36	0	22	2	0
4	B	36	0	22	4	0
4	C	36	0	22	2	0
4	D	36	0	22	2	0
4	E	36	0	22	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	36	0	22	4	0
4	G	36	0	22	2	0
4	H	36	0	22	2	0
4	I	36	0	22	2	0
4	J	36	0	22	3	0
4	K	36	0	22	4	0
4	L	36	0	22	2	0
5	A	287	0	0	1	1
5	B	175	0	0	0	0
5	C	283	0	0	0	1
5	D	236	0	0	0	0
5	E	268	0	0	0	0
5	F	227	0	0	1	0
5	G	263	0	0	0	0
5	H	130	0	0	0	0
5	I	254	0	0	0	0
5	J	195	0	0	0	0
5	K	234	0	0	0	0
5	L	193	0	0	0	0
All	All	46652	0	43313	158	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 158 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:J:98[A]:MET:CE	1:L:316[A]:SER:HB2	1.76	1.13
1:H:316[B]:SER:HB3	1:L:98[B]:MET:HE1	1.21	1.11
1:D:98[A]:MET:HE1	1:F:316[A]:SER:HB2	1.34	1.08
1:H:98[B]:MET:HE1	1:J:316[B]:SER:HB3	1.14	1.08
3:E:500:NAI:H4N	4:E:501:UPG:H6'1	1.34	1.05

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3222:HOH:O	5:C:3187:HOH:O[2_444]	2.16	0.04

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	463/467 (99%)	452 (98%)	11 (2%)	0	100	100
1	B	457/467 (98%)	447 (98%)	10 (2%)	0	100	100
1	C	461/467 (99%)	454 (98%)	7 (2%)	0	100	100
1	D	457/467 (98%)	448 (98%)	9 (2%)	0	100	100
1	E	458/467 (98%)	449 (98%)	9 (2%)	0	100	100
1	F	458/467 (98%)	450 (98%)	8 (2%)	0	100	100
1	G	458/467 (98%)	451 (98%)	7 (2%)	0	100	100
1	H	458/467 (98%)	450 (98%)	8 (2%)	0	100	100
1	I	460/467 (98%)	450 (98%)	10 (2%)	0	100	100
1	J	459/467 (98%)	451 (98%)	8 (2%)	0	100	100
1	K	459/467 (98%)	449 (98%)	10 (2%)	0	100	100
1	L	458/467 (98%)	450 (98%)	8 (2%)	0	100	100
All	All	5506/5604 (98%)	5401 (98%)	105 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	395/401 (98%)	393 (100%)	2 (0%)	88	92
1	B	380/401 (95%)	377 (99%)	3 (1%)	81	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	390/401 (97%)	388 (100%)	2 (0%)	88	92
1	D	386/401 (96%)	383 (99%)	3 (1%)	81	86
1	E	384/401 (96%)	383 (100%)	1 (0%)	92	95
1	F	385/401 (96%)	383 (100%)	2 (0%)	88	92
1	G	386/401 (96%)	382 (99%)	4 (1%)	76	81
1	H	380/401 (95%)	379 (100%)	1 (0%)	92	95
1	I	388/401 (97%)	386 (100%)	2 (0%)	88	92
1	J	385/401 (96%)	384 (100%)	1 (0%)	92	95
1	K	386/401 (96%)	384 (100%)	2 (0%)	88	92
1	L	384/401 (96%)	382 (100%)	2 (0%)	88	92
All	All	4629/4812 (96%)	4604 (100%)	25 (0%)	88	92

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	177	ARG
1	H	177	ARG
1	L	400	ASP
1	G	462	ILE
1	I	177	ARG

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

Mol	Chain	Res	Type
1	C	324	ASN
1	D	324	ASN
1	G	302	GLN
1	H	450	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	NAI	B	500	-	42,48,48	1.84	6 (14%)	47,73,73	1.32	4 (8%)
3	NAI	L	500	-	42,48,48	1.82	6 (14%)	47,73,73	1.74	11 (23%)
4	UPG	C	501	-	35,38,38	0.93	0	53,58,58	1.37	6 (11%)
3	NAI	E	500	-	42,48,48	1.81	6 (14%)	47,73,73	1.30	6 (12%)
4	UPG	K	501	-	35,38,38	0.93	0	53,58,58	1.21	5 (9%)
3	NAI	D	500	-	42,48,48	1.81	6 (14%)	47,73,73	1.19	3 (6%)
3	NAI	C	500	-	42,48,48	1.78	6 (14%)	47,73,73	1.44	6 (12%)
4	UPG	B	501	-	35,38,38	0.85	1 (2%)	53,58,58	1.16	6 (11%)
4	UPG	I	501	-	35,38,38	0.91	2 (5%)	53,58,58	1.10	3 (5%)
4	UPG	A	501	-	35,38,38	0.88	0	53,58,58	1.13	6 (11%)
3	NAI	K	500	-	42,48,48	1.80	6 (14%)	47,73,73	1.64	9 (19%)
3	NAI	A	500	-	42,48,48	1.77	6 (14%)	47,73,73	1.33	7 (14%)
4	UPG	E	501	-	35,38,38	1.00	3 (8%)	53,58,58	1.20	4 (7%)
4	UPG	G	501	-	35,38,38	0.84	0	53,58,58	1.16	4 (7%)
3	NAI	H	500	-	42,48,48	1.87	6 (14%)	47,73,73	1.89	8 (17%)
4	UPG	D	501	-	35,38,38	0.84	1 (2%)	53,58,58	1.14	5 (9%)
3	NAI	G	500	-	42,48,48	1.72	5 (11%)	47,73,73	1.35	7 (14%)
3	NAI	I	500	-	42,48,48	1.75	7 (16%)	47,73,73	1.29	5 (10%)
4	UPG	J	501	-	35,38,38	0.93	2 (5%)	53,58,58	1.05	5 (9%)
4	UPG	H	501	-	35,38,38	0.90	1 (2%)	53,58,58	1.31	6 (11%)
4	UPG	L	501	-	35,38,38	1.03	2 (5%)	53,58,58	1.29	8 (15%)
4	UPG	F	501	-	35,38,38	0.94	3 (8%)	53,58,58	1.35	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
3	NAI	J	500	-	42,48,48	1.81	6 (14%)	47,73,73	1.72	11 (23%)
3	NAI	F	500	-	42,48,48	1.85	6 (14%)	47,73,73	1.39	5 (10%)

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	NAI	B	500	-	-	4/25/72/72	0/5/5/5
3	NAI	L	500	-	-	5/25/72/72	0/5/5/5
4	UPG	C	501	-	-	3/23/59/59	0/3/3/3
3	NAI	E	500	-	-	5/25/72/72	0/5/5/5
4	UPG	K	501	-	-	4/23/59/59	0/3/3/3
3	NAI	D	500	-	-	4/25/72/72	0/5/5/5
3	NAI	C	500	-	-	5/25/72/72	0/5/5/5
4	UPG	B	501	-	-	5/23/59/59	0/3/3/3
4	UPG	I	501	-	-	2/23/59/59	0/3/3/3
4	UPG	A	501	-	-	3/23/59/59	0/3/3/3
3	NAI	K	500	-	-	3/25/72/72	0/5/5/5
3	NAI	A	500	-	-	5/25/72/72	0/5/5/5
4	UPG	E	501	-	-	4/23/59/59	0/3/3/3
4	UPG	G	501	-	-	4/23/59/59	0/3/3/3
3	NAI	H	500	-	-	7/25/72/72	0/5/5/5
4	UPG	D	501	-	-	2/23/59/59	0/3/3/3
3	NAI	G	500	-	-	5/25/72/72	0/5/5/5
3	NAI	I	500	-	-	5/25/72/72	0/5/5/5
4	UPG	J	501	-	-	2/23/59/59	0/3/3/3
4	UPG	H	501	-	-	7/23/59/59	0/3/3/3
4	UPG	L	501	-	-	6/23/59/59	0/3/3/3
4	UPG	F	501	-	-	6/23/59/59	0/3/3/3
3	NAI	J	500	-	-	3/25/72/72	0/5/5/5
3	NAI	F	500	-	-	5/25/72/72	0/5/5/5

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	NAI	O7N-C7N	6.92	1.40	1.24
3	H	500	NAI	O7N-C7N	6.81	1.40	1.24
3	J	500	NAI	O7N-C7N	6.71	1.40	1.24
3	K	500	NAI	O7N-C7N	6.68	1.40	1.24
3	L	500	NAI	O7N-C7N	6.65	1.40	1.24

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	500	NAI	N3A-C2A-N1A	-5.96	119.36	128.68
3	K	500	NAI	N3A-C2A-N1A	-5.68	119.80	128.68
3	J	500	NAI	N3A-C2A-N1A	-5.67	119.81	128.68
3	B	500	NAI	N3A-C2A-N1A	-5.60	119.92	128.68
3	C	500	NAI	N3A-C2A-N1A	-5.57	119.97	128.68

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	501	UPG	C4'-C5'-C6'-O6'
4	B	501	UPG	C4'-C5'-C6'-O6'
4	B	501	UPG	O5'-C5'-C6'-O6'
4	F	501	UPG	O5'-C5'-C6'-O6'
3	F	500	NAI	C2D-C1D-N1N-C6N

There are no ring outliers.

24 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	NAI	3	0
3	L	500	NAI	3	0
4	C	501	UPG	2	0
3	E	500	NAI	4	0
4	K	501	UPG	4	0
3	D	500	NAI	2	0
3	C	500	NAI	2	0
4	B	501	UPG	4	0
4	I	501	UPG	2	0
4	A	501	UPG	2	0
3	K	500	NAI	4	0
3	A	500	NAI	2	0
4	E	501	UPG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	501	UPG	2	0
3	H	500	NAI	2	0
4	D	501	UPG	2	0
3	G	500	NAI	2	0
3	I	500	NAI	2	0
4	J	501	UPG	3	0
4	H	501	UPG	2	0
4	L	501	UPG	2	0
4	F	501	UPG	4	0
3	J	500	NAI	3	0
3	F	500	NAI	2	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 NAI B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI L 500

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI E 500

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG K 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI D 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI C 500

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG I 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI K 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG G 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI H 500

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI G 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI I 500

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG J 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG H 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG L 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UPG F 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI J 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI F 500

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	460/467 (98%)	-0.25	1 (0%)	95 | 94	26, 31, 45, 62	0
1	B	460/467 (98%)	-0.19	7 (1%)	73 | 72	25, 31, 45, 62	0
1	C	460/467 (98%)	-0.40	0	100 | 100	25, 31, 44, 59	0
1	D	458/467 (98%)	-0.25	2 (0%)	92 | 92	25, 31, 44, 57	0
1	E	459/467 (98%)	-0.36	1 (0%)	95 | 94	26, 31, 44, 64	0
1	F	460/467 (98%)	-0.30	5 (1%)	80 | 79	25, 31, 44, 60	0
1	G	460/467 (98%)	-0.31	0	100 | 100	26, 31, 44, 60	0
1	H	459/467 (98%)	-0.04	19 (4%)	37 | 36	26, 31, 44, 60	0
1	I	460/467 (98%)	-0.44	2 (0%)	92 | 92	25, 31, 44, 60	0
1	J	460/467 (98%)	-0.24	3 (0%)	87 | 87	25, 31, 44, 59	0
1	K	460/467 (98%)	-0.24	5 (1%)	80 | 79	25, 31, 45, 62	0
1	L	460/467 (98%)	-0.23	9 (1%)	65 | 63	26, 31, 45, 63	0
All	All	5516/5604 (98%)	-0.27	54 (0%)	82 | 81	25, 31, 45, 64	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	183	ASP	4.5
1	H	2	PHE	4.3
1	B	151	ASN	4.1
1	L	186	PRO	4.0
1	H	151	ASN	4.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CL	H	3010	1/1	0.94	0.07	36,36,36,36	0
3	NAI	H	500	44/44	0.96	0.08	23,35,48,50	0
3	NAI	L	500	44/44	0.96	0.08	21,33,45,51	0
3	NAI	B	500	44/44	0.97	0.06	21,31,42,43	0
3	NAI	D	500	44/44	0.97	0.07	20,26,33,34	0
3	NAI	F	500	44/44	0.97	0.07	18,27,38,45	0
2	CL	D	3006	1/1	0.97	0.04	30,30,30,30	0
3	NAI	J	500	44/44	0.97	0.07	17,28,39,40	0
2	CL	K	3008	1/1	0.97	0.04	25,25,25,25	0
4	UPG	E	501	36/36	0.97	0.06	19,23,26,28	0
4	UPG	J	501	36/36	0.97	0.08	20,25,28,30	0
2	CL	L	3007	1/1	0.98	0.04	30,30,30,30	0
3	NAI	G	500	44/44	0.98	0.06	16,22,27,32	0
3	NAI	A	500	44/44	0.98	0.06	13,18,23,26	0
3	NAI	I	500	44/44	0.98	0.06	17,25,30,33	0
2	CL	C	3005	1/1	0.98	0.08	25,25,25,25	0
3	NAI	K	500	44/44	0.98	0.06	19,27,35,37	0
3	NAI	C	500	44/44	0.98	0.06	13,22,25,29	0
4	UPG	B	501	36/36	0.98	0.07	17,22,27,30	0
4	UPG	D	501	36/36	0.98	0.08	18,23,27,36	0
2	CL	B	3009	1/1	0.98	0.07	29,29,29,29	0
4	UPG	F	501	36/36	0.98	0.07	19,25,29,30	0
4	UPG	G	501	36/36	0.98	0.07	16,21,26,26	0
4	UPG	H	501	36/36	0.98	0.06	22,28,34,39	0
4	UPG	I	501	36/36	0.98	0.06	17,24,26,28	0
3	NAI	E	500	44/44	0.98	0.06	19,26,30,31	0
4	UPG	K	501	36/36	0.98	0.06	17,25,29,30	0
4	UPG	L	501	36/36	0.98	0.06	23,28,31,33	0
2	CL	E	3011	1/1	0.99	0.05	29,29,29,29	0
2	CL	I	3003	1/1	0.99	0.07	29,29,29,29	0
4	UPG	A	501	36/36	0.99	0.07	14,20,24,26	0
2	CL	J	3012	1/1	0.99	0.03	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UPG	C	501	36/36	0.99	0.06	18,22,25,29	0
2	CL	F	3004	1/1	0.99	0.06	26,26,26,26	0
2	CL	G	3002	1/1	0.99	0.11	26,26,26,26	0
2	CL	A	3001	1/1	1.00	0.09	21,21,21,21	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.
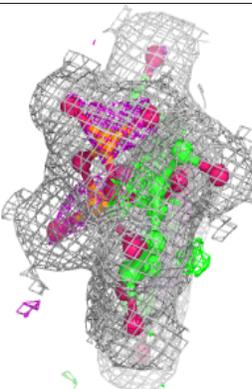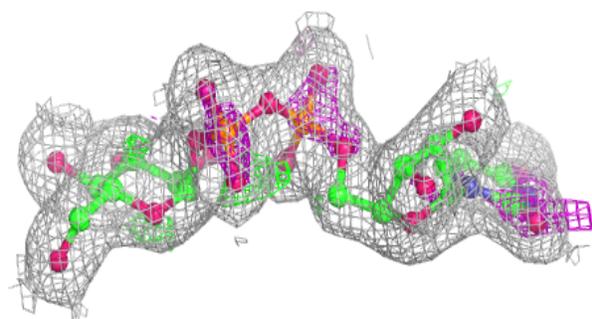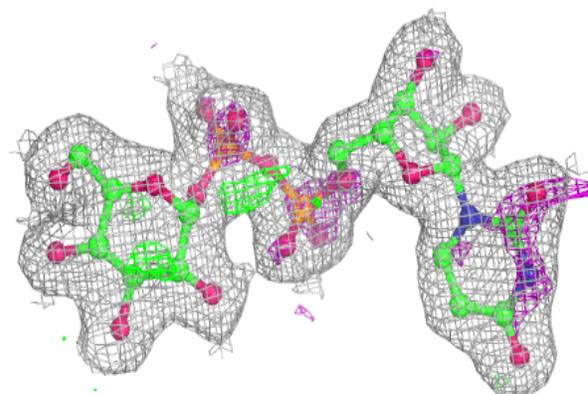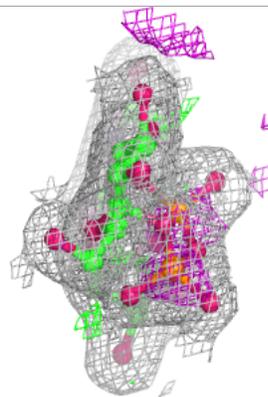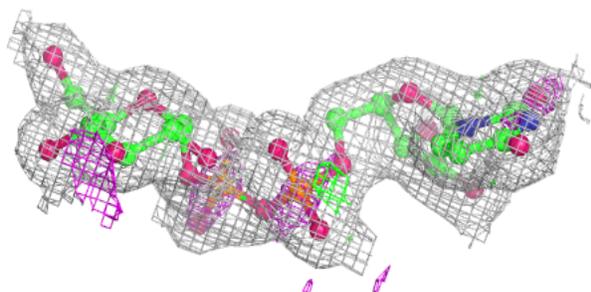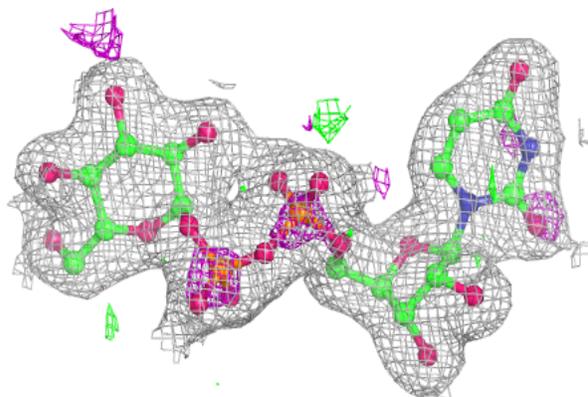

Electron density around NAI H 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
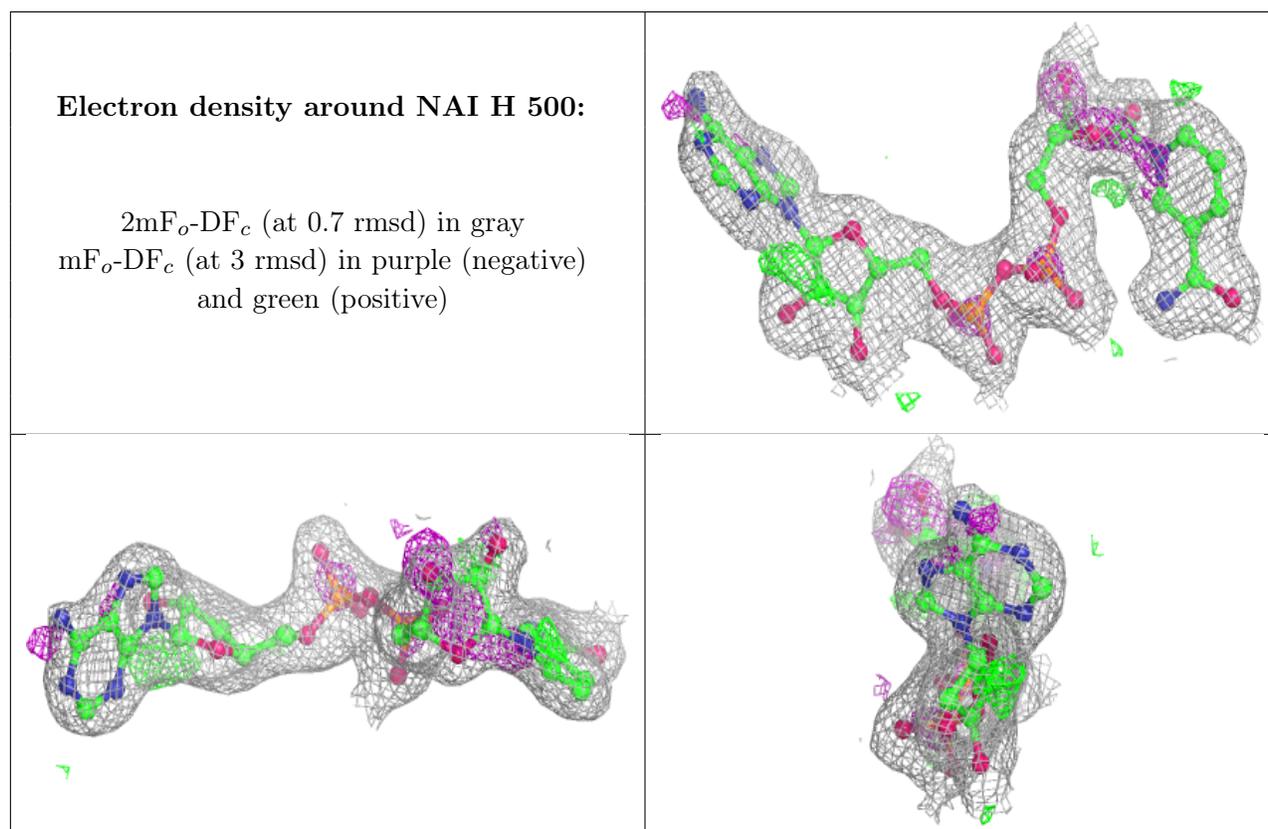
Electron density around NAI L 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
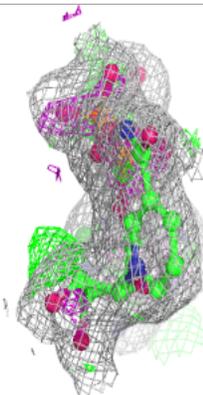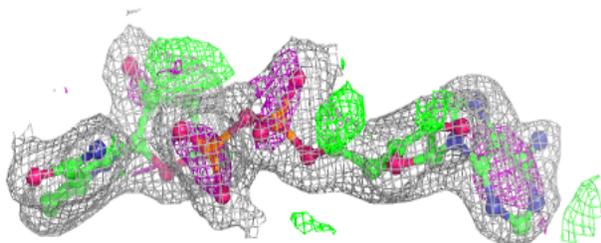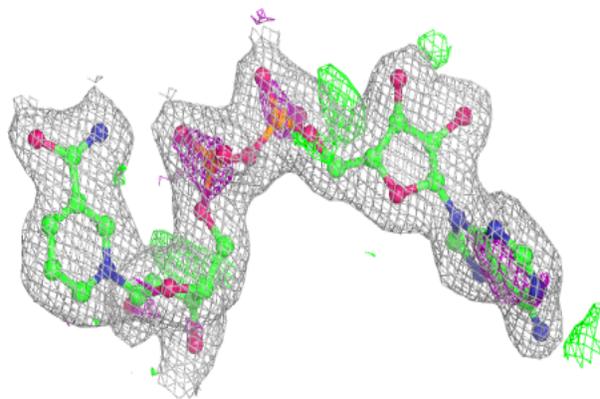
Electron density around NAI B 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
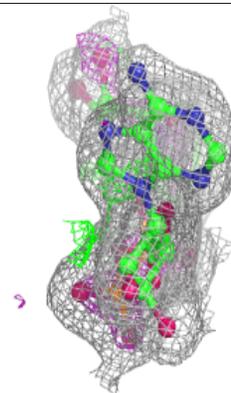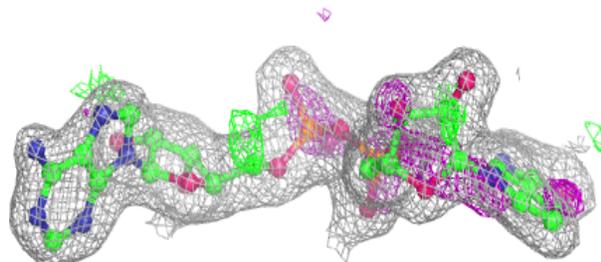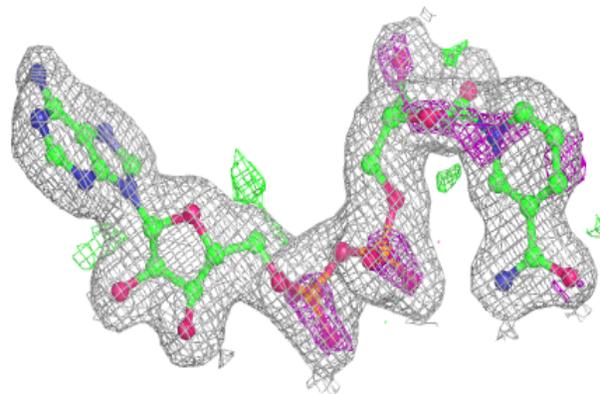
Electron density around NAI D 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
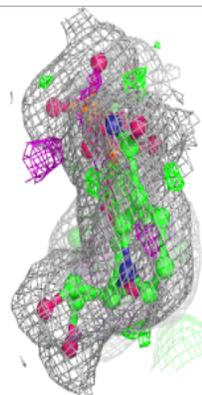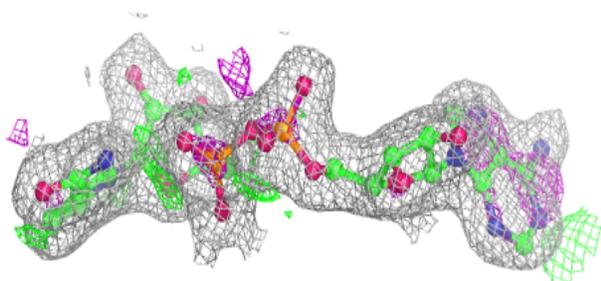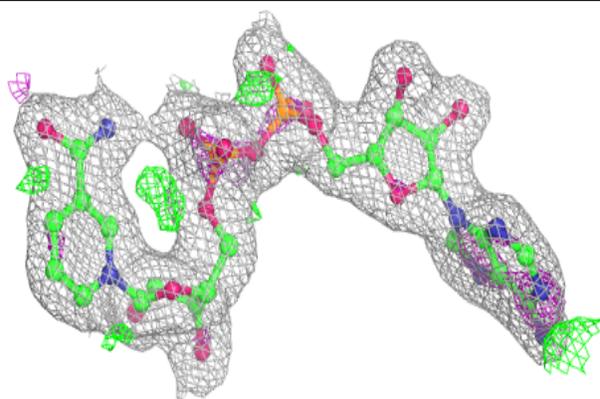
Electron density around NAI F 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
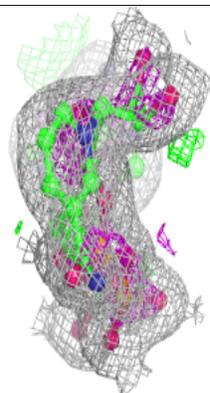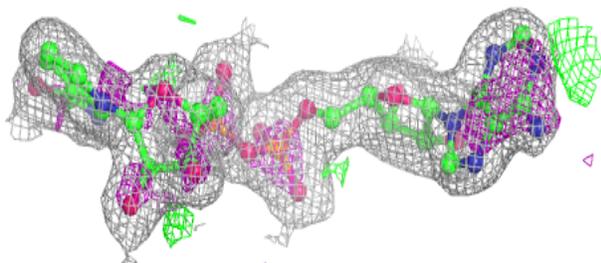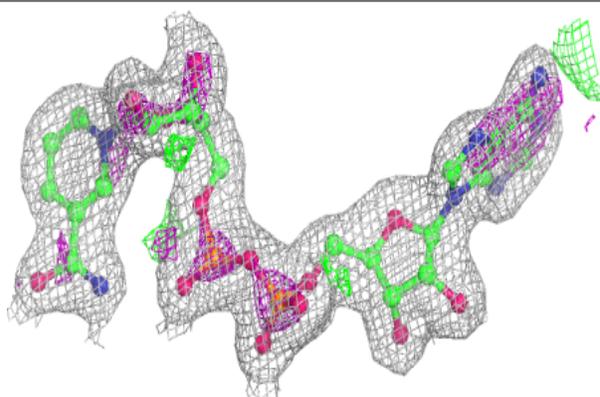
Electron density around NAI J 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
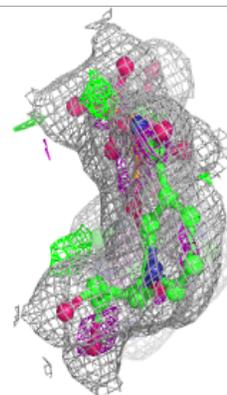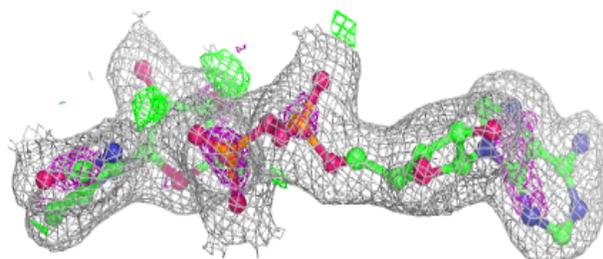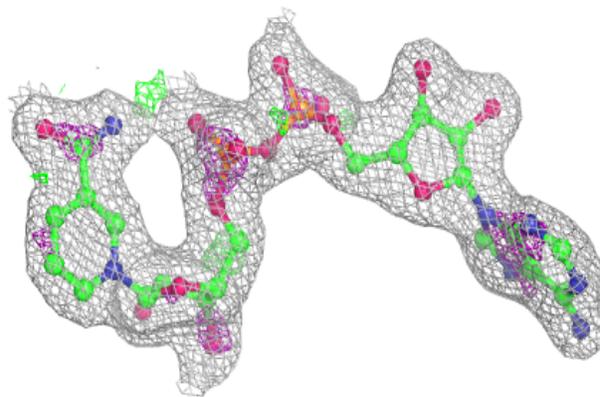
Electron density around UPG E 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
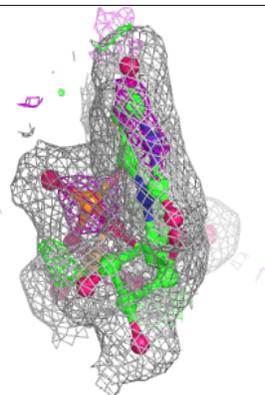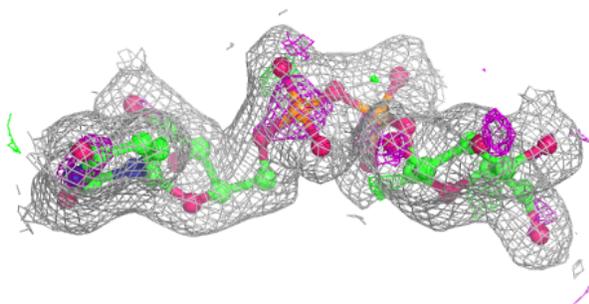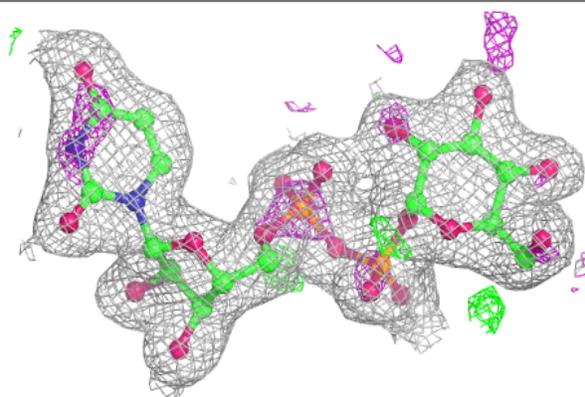$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
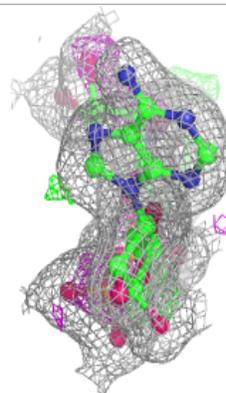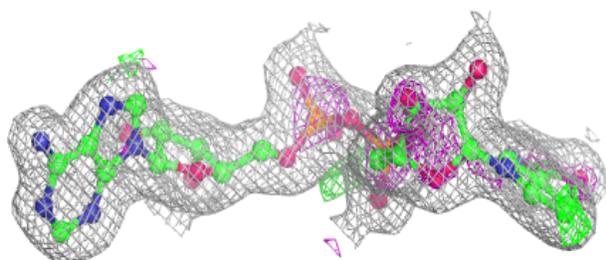and green (positive)
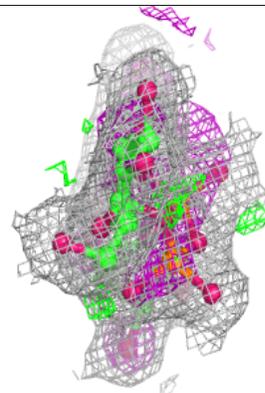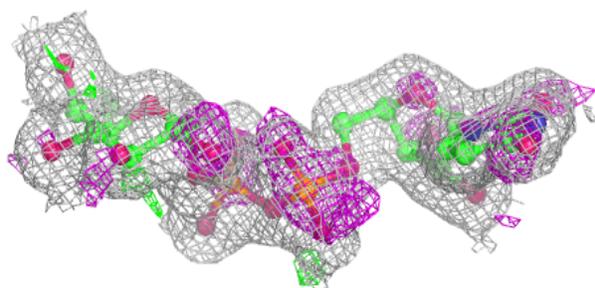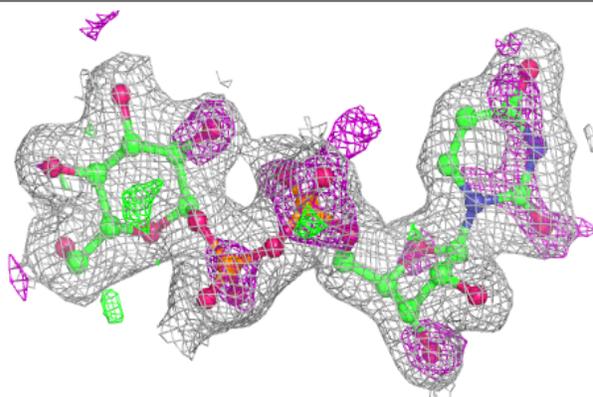
Electron density around UPG J 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
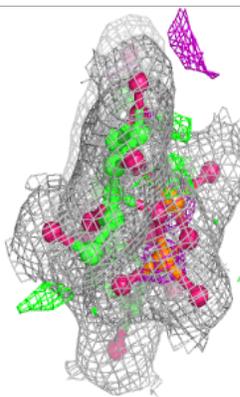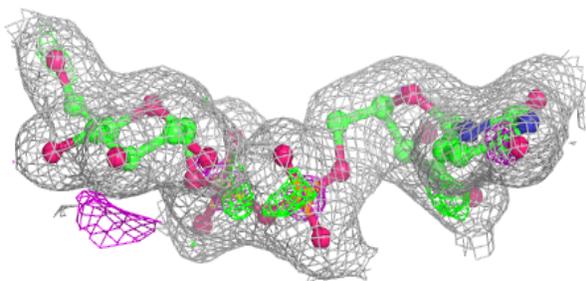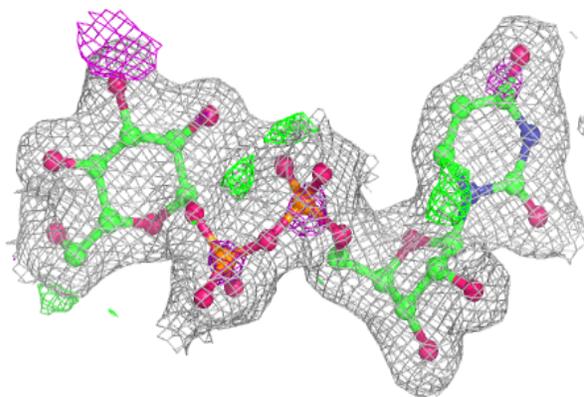
Electron density around NAI G 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
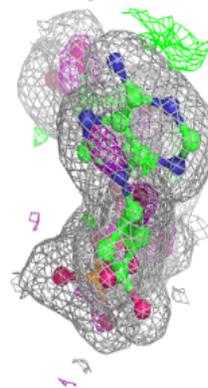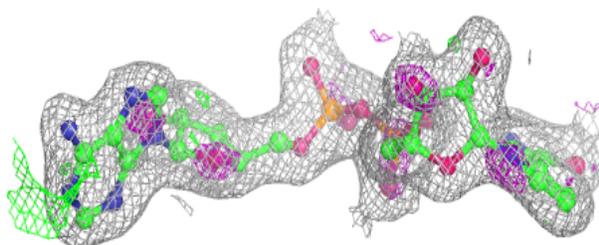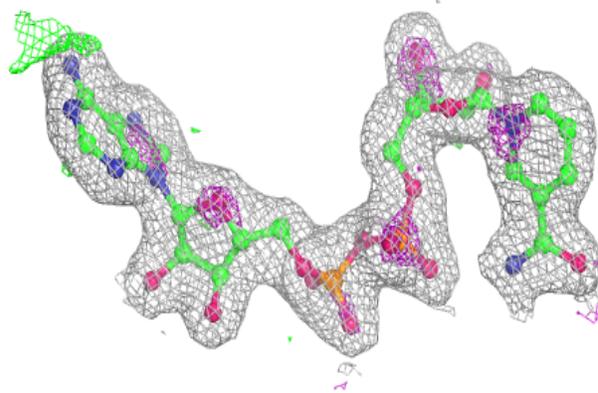
Electron density around NAI A 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
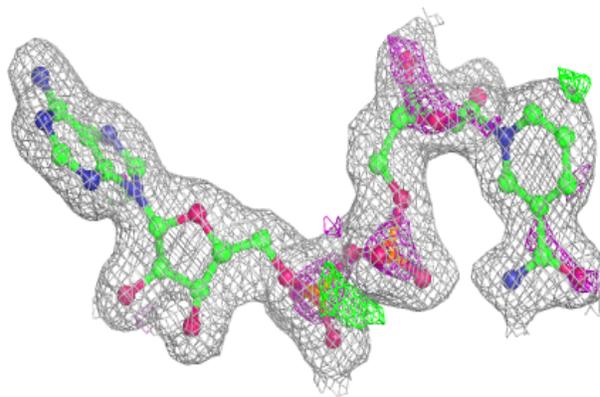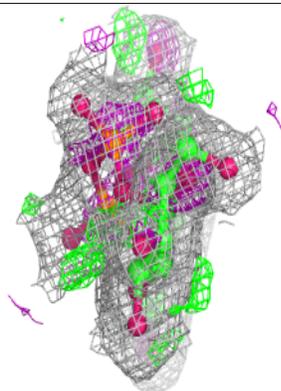and green (positive)
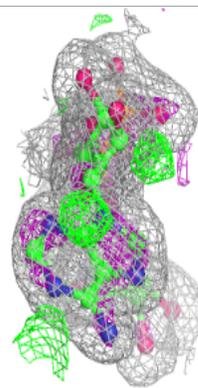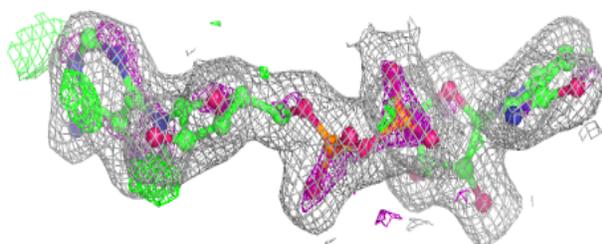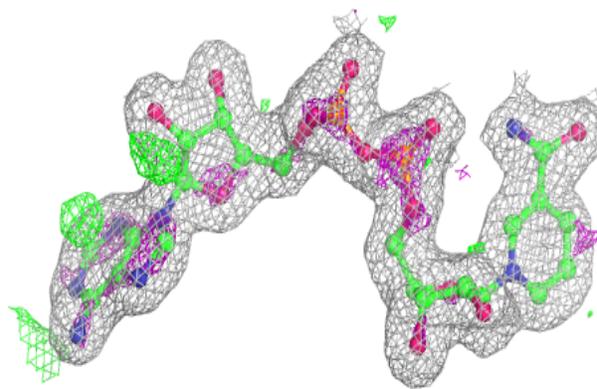
Electron density around NAI I 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
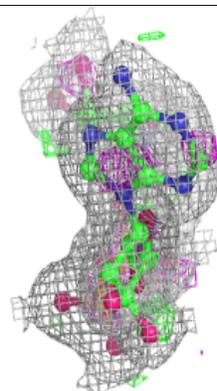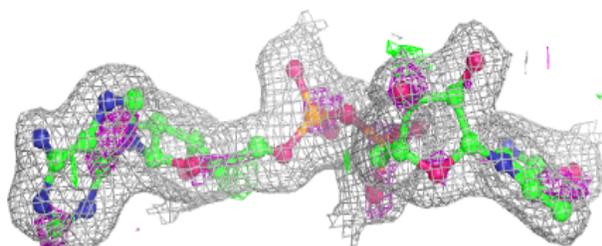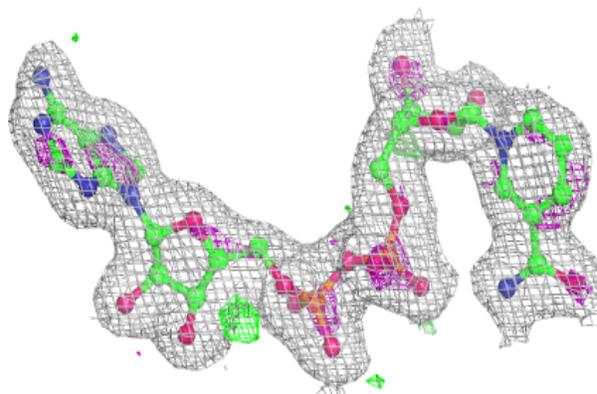
Electron density around NAI K 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
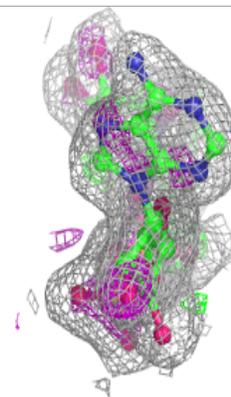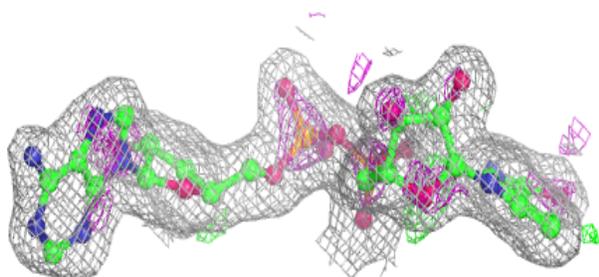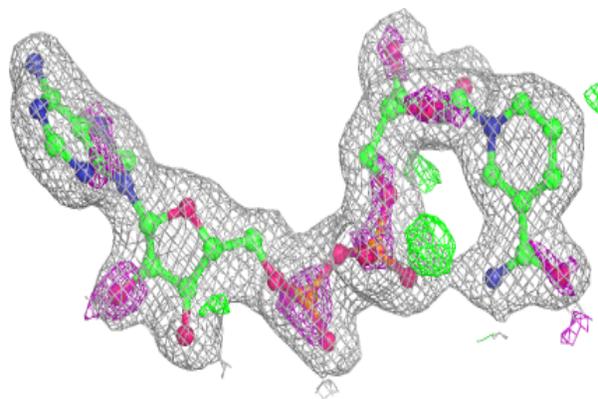
Electron density around NAI C 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
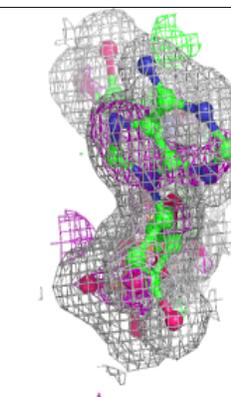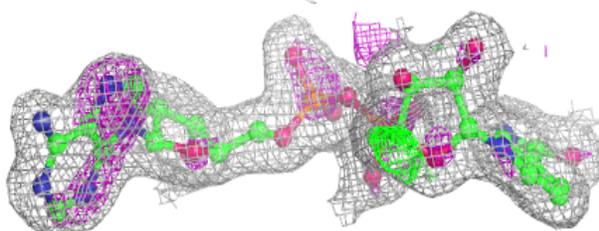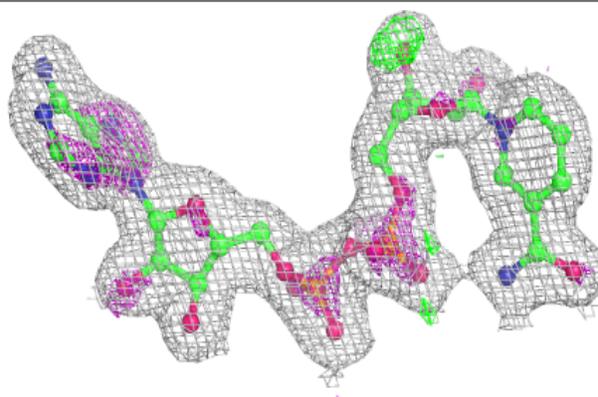
Electron density around UPG B 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
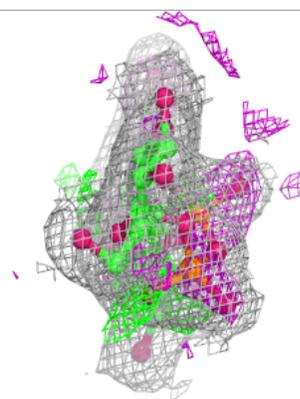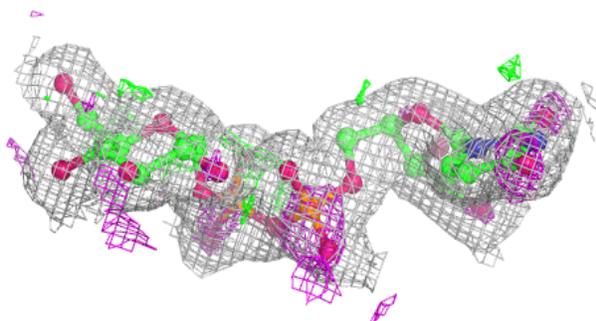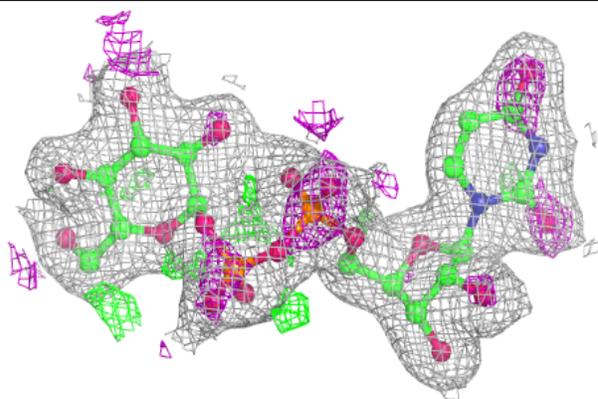
Electron density around UPG D 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
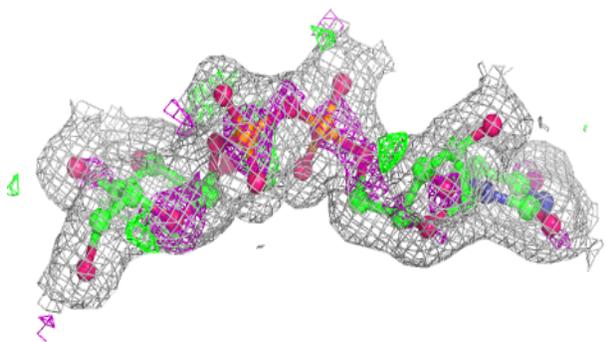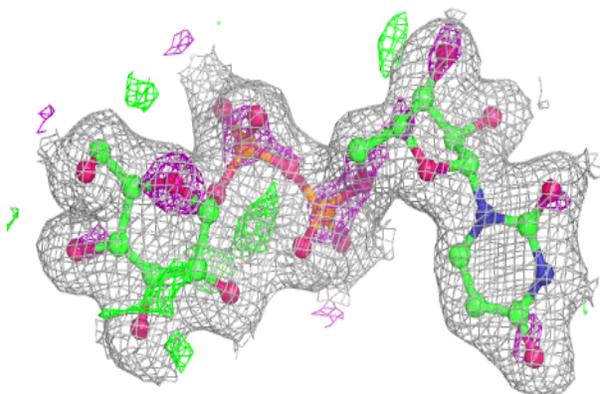mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
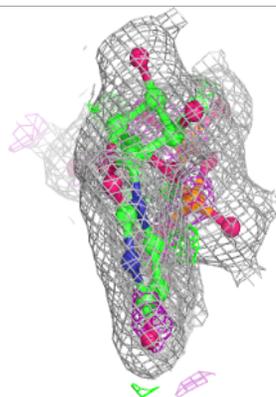and green (positive)
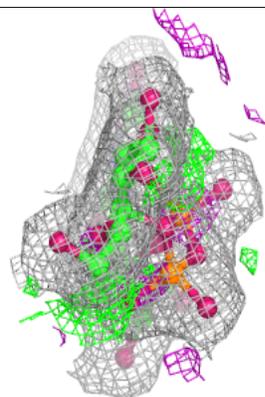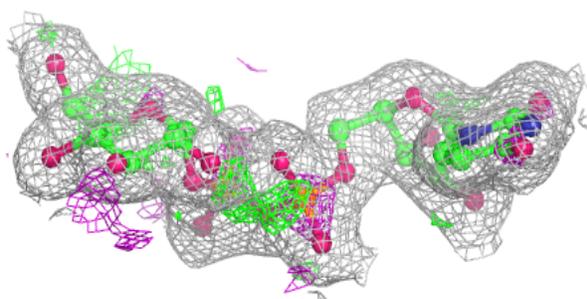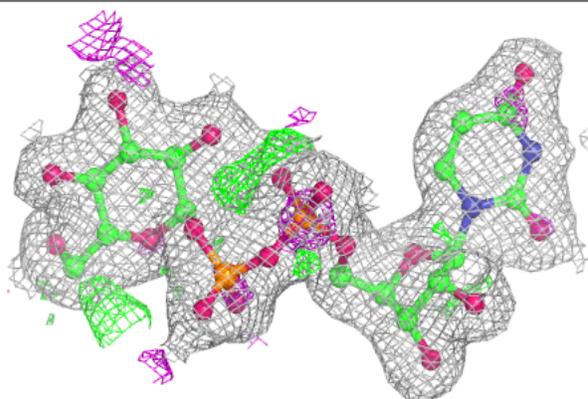
Electron density around UPG F 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
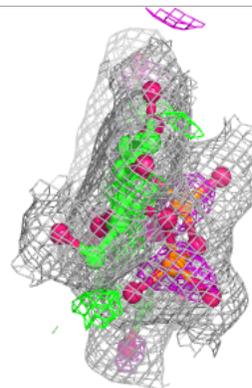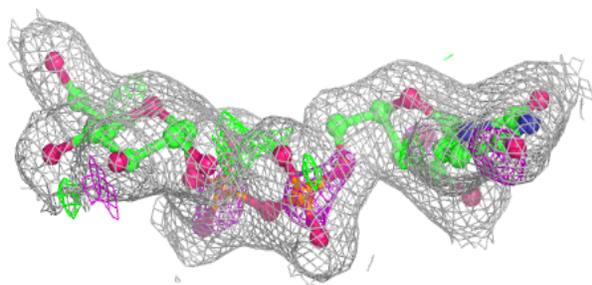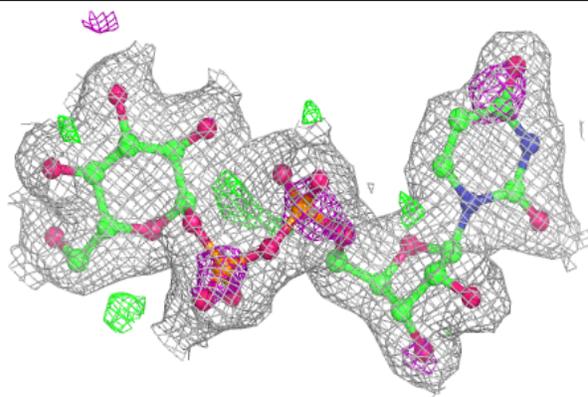
Electron density around UPG G 501:

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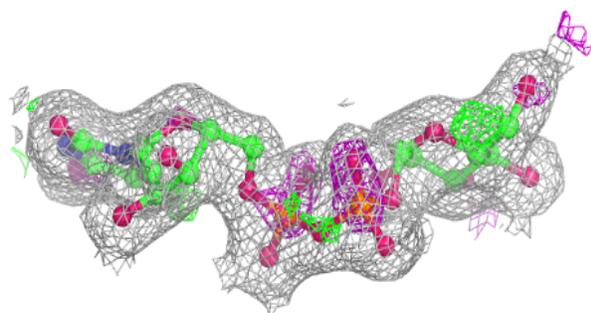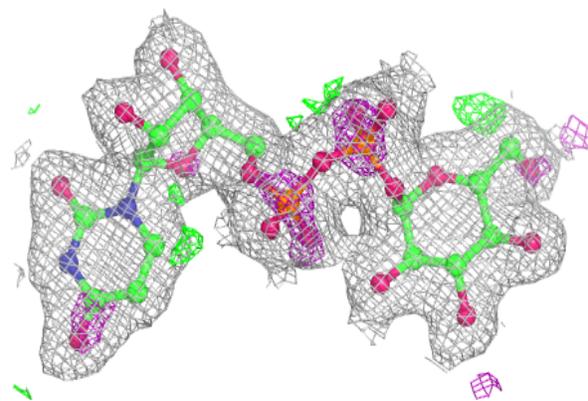mF_o-DF_c (at 3 rmsd) in purple (negative)
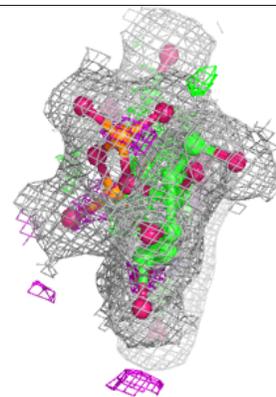and green (positive)

Electron density around UPG H 501:

$2mF_o$-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 I 501:

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

Electron density around NAI E 500:

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

Electron density around UPG K 501:

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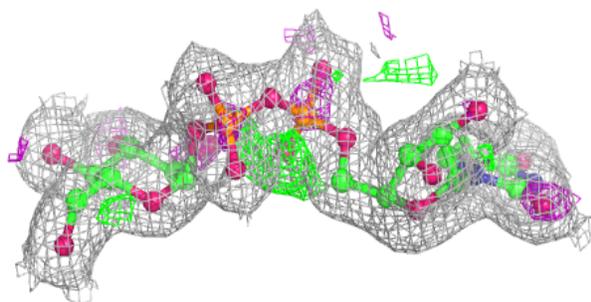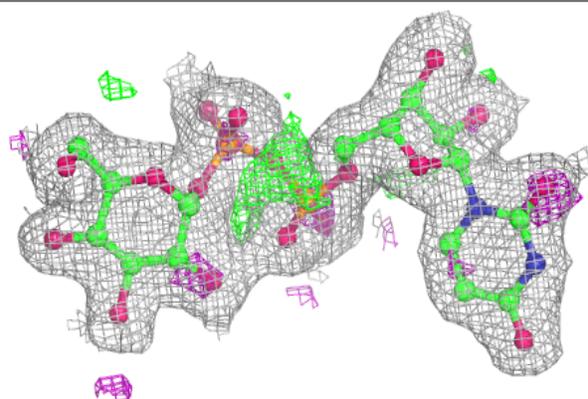$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
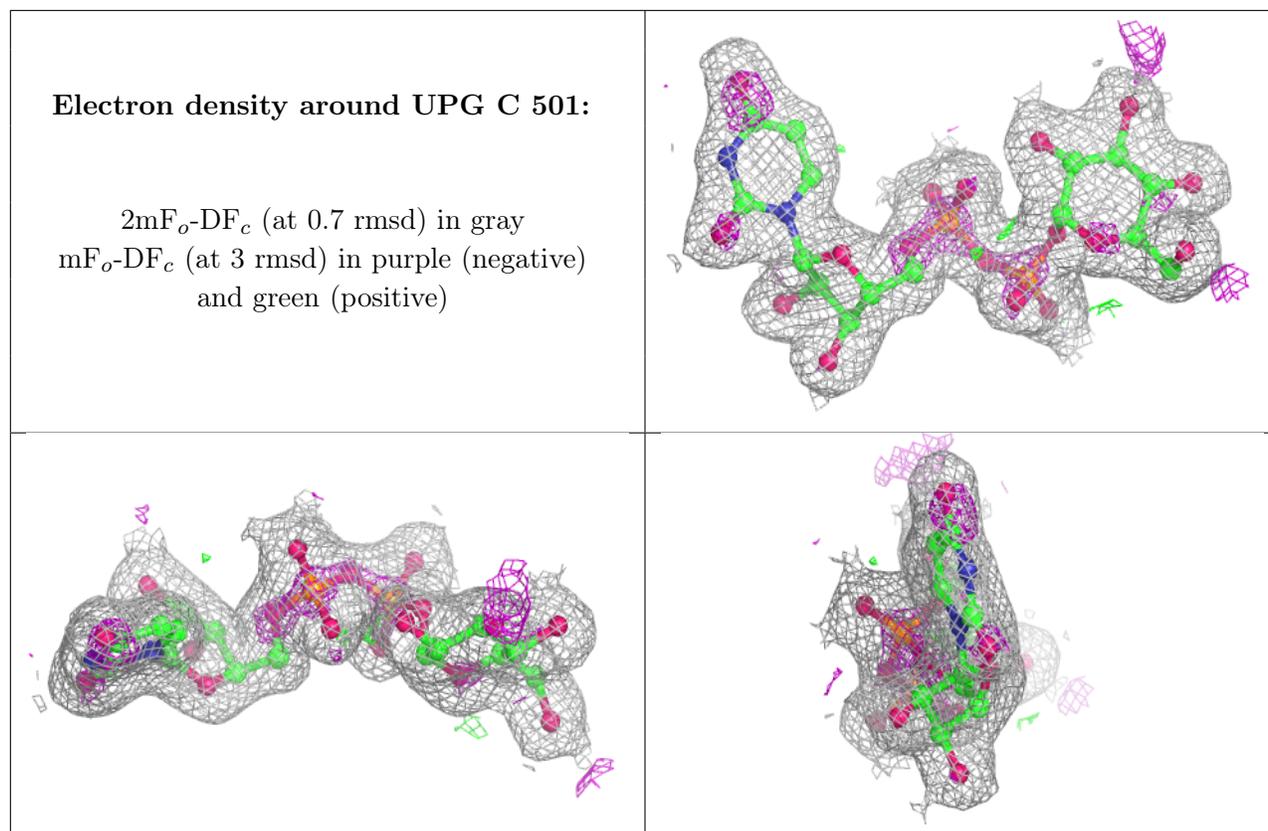and green (positive)

Electron density around UPG L 501:

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 A 501:

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 C 501:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.