W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2023 – 09:54 PM EDT

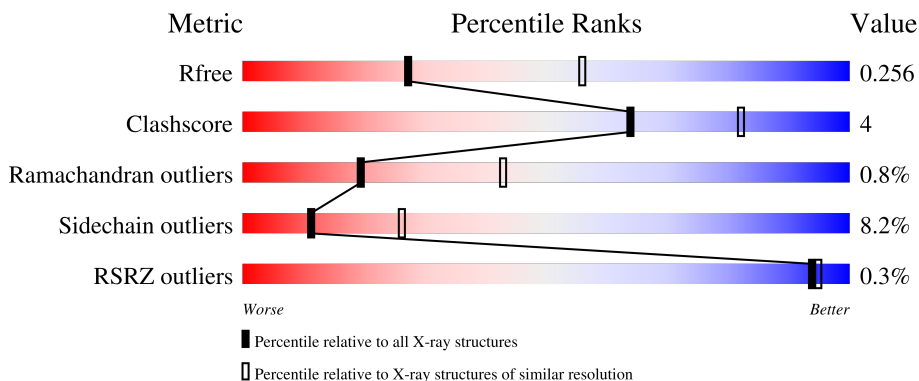|		
PDB ID	:	6BWC
Title	:	X-ray structure of Pen from Bacillus thuringiensis
Authors	:	Delvaux, N.A.; Thoden, J.B.; Holden, H.M.
Deposited on	:	2017-12-14
Resolution	:	2.70 Å(reported)

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 2.70 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.
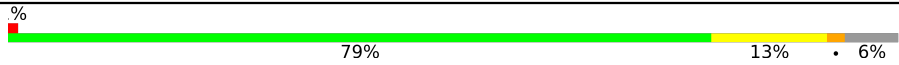
Metric	Percentile Ranks	Value
Rfree		0.256
Clashscore		4
Ramachandran outliers		0.8%
Sidechain outliers		8.2%
RSRZ outliers		0.3%

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	343	78% / 15% · 6%
1	B	343	80% / 10% · 8%
1	C	343	78% / 14% · 5%
1	D	343	74% / 18% · 6%
1	E	343	80% / 13% · 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	343	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 16002 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 Polysaccharide biosynthesis protein CapD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2559	1631	427	486	15			
1	B	316	Total	C	N	O	S	0	0	0
			2504	1595	420	474	15			
1	C	327	Total	C	N	O	S	0	0	0
			2590	1650	436	489	15			
1	D	324	Total	C	N	O	S	0	0	0
			2566	1636	431	484	15			
1	E	322	Total	C	N	O	S	0	0	0
			2553	1625	429	484	15			
1	F	323	Total	C	N	O	S	0	0	0
			2549	1624	425	485	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP J3UJH9
A	0	HIS	-	expression tag	UNP J3UJH9
A	128	ASN	ASP	engineered mutation	UNP J3UJH9
A	129	ALA	LYS	engineered mutation	UNP J3UJH9
B	-1	GLY	-	expression tag	UNP J3UJH9
B	0	HIS	-	expression tag	UNP J3UJH9
B	128	ASN	ASP	engineered mutation	UNP J3UJH9
B	129	ALA	LYS	engineered mutation	UNP J3UJH9
C	-1	GLY	-	expression tag	UNP J3UJH9
C	0	HIS	-	expression tag	UNP J3UJH9
C	128	ASN	ASP	engineered mutation	UNP J3UJH9
C	129	ALA	LYS	engineered mutation	UNP J3UJH9
D	-1	GLY	-	expression tag	UNP J3UJH9
D	0	HIS	-	expression tag	UNP J3UJH9
D	128	ASN	ASP	engineered mutation	UNP J3UJH9
D	129	ALA	LYS	engineered mutation	UNP J3UJH9
E	-1	GLY	-	expression tag	UNP J3UJH9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP J3UJH9
E	128	ASN	ASP	engineered mutation	UNP J3UJH9
E	129	ALA	LYS	engineered mutation	UNP J3UJH9
F	-1	GLY	-	expression tag	UNP J3UJH9
F	0	HIS	-	expression tag	UNP J3UJH9
F	128	ASN	ASP	engineered mutation	UNP J3UJH9
F	129	ALA	LYS	engineered mutation	UNP J3UJH9

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP
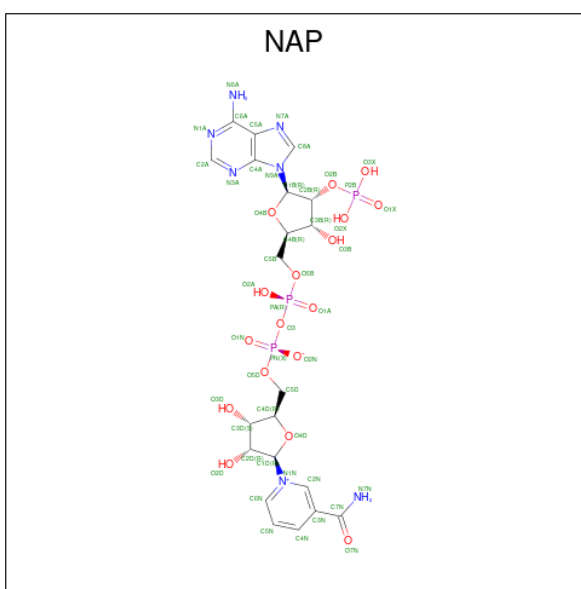
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).

UD1
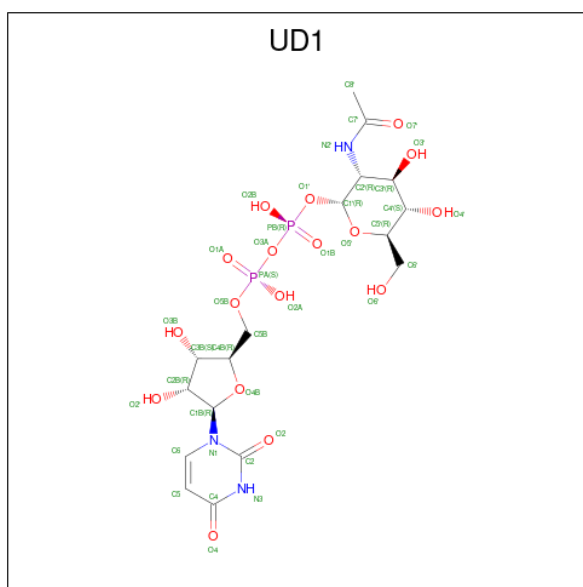
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	E	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	F	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total O S 5 4 1			0	0
4	A	1	Total O S 5 4 1			0	0
4	B	1	Total O S 5 4 1			0	0
4	F	1	Total O S 5 4 1			0	0
4	F	1	Total O S 5 4 1			0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total O 34 34		0	0
5	B	21	Total O 21 21		0	0
5	C	25	Total O 25 25		0	0
5	D	21	Total O 21 21		0	0
5	E	18	Total O 18 18		0	0
5	F	15	Total O 15 15		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.
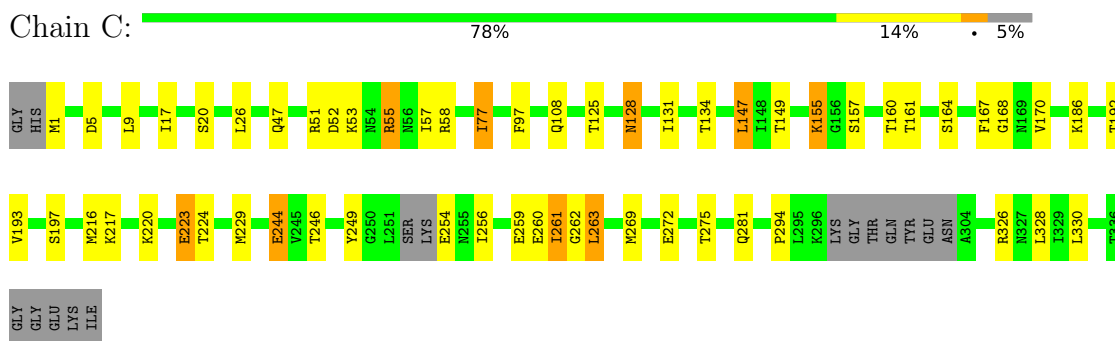
• Molecule 1: Polysaccharide biosynthesis protein CapD
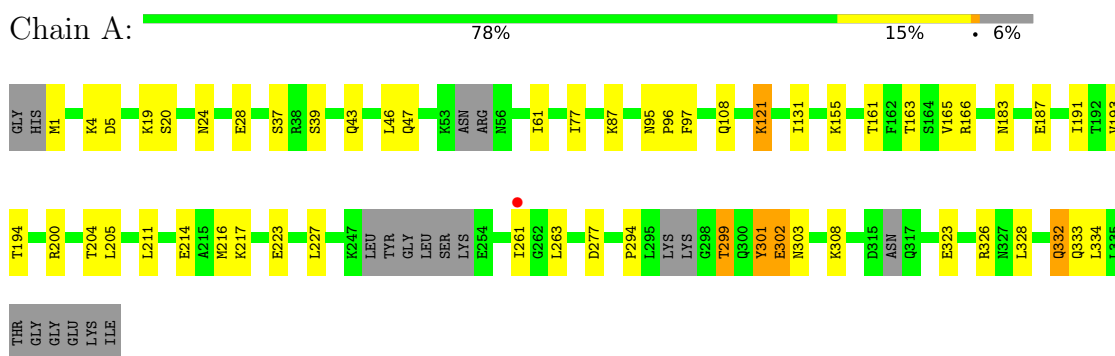
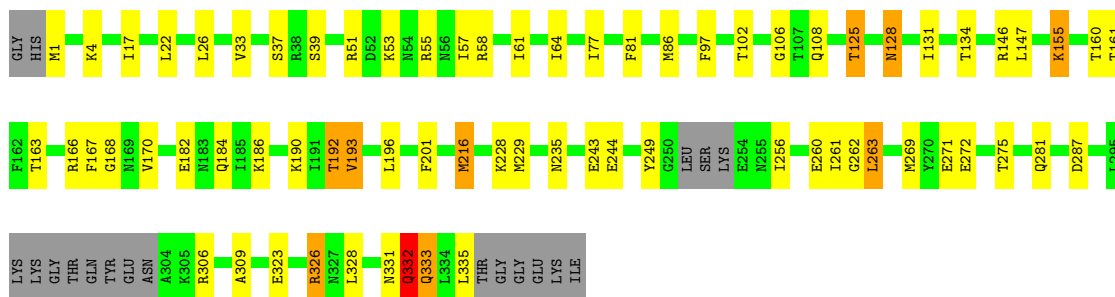• Molecule 1: Polysaccharide biosynthesis protein CapD
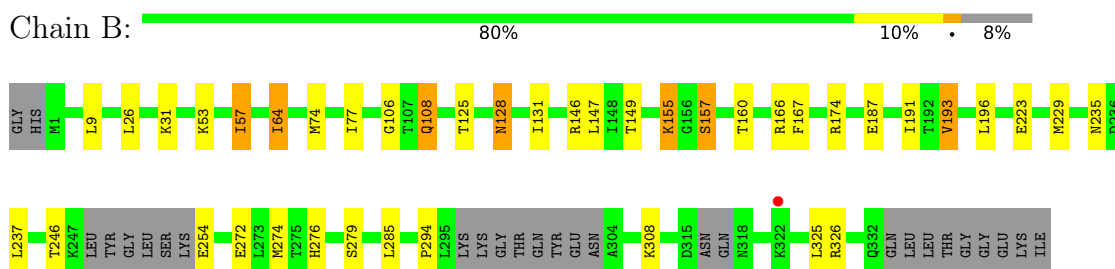
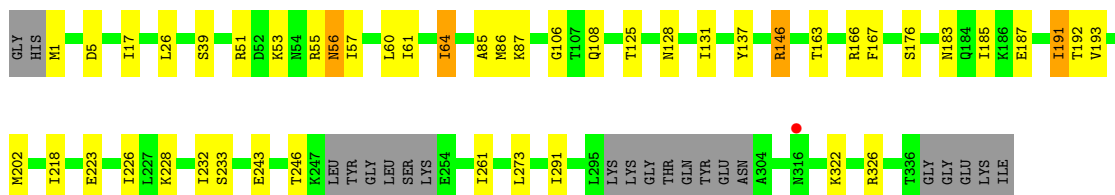• Molecule 1: Polysaccharide biosynthesis protein CapD

• Molecule 1: Polysaccharide biosynthesis protein CapD

Chain D:

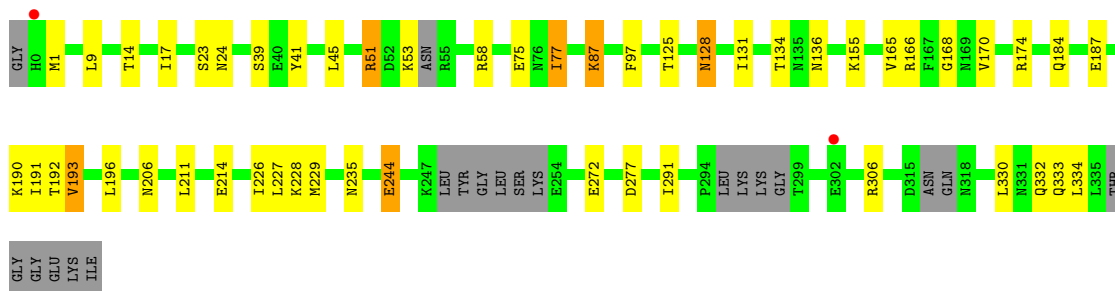74%　　　18%　　•　6%

GLY HIS M1 K4 I17 L22 L26 V33 S37 R38 S39 R51 D52 K53 N54 R55 N56 I57 R58 I61 I64 I77 F81 M86 F97 T102 G106 T107 Q108 T125 N128 I131 T134 R146 L147 K155 T160 T161

F162 T163 R166 F167 G168 N169 V170 E182 N183 Q184 I185 K186 K190 I191 T192 V193 L196 F201 M216 K228 M229 N235 E243 E244 Y249 G250 LEU SER LYS E254 N255 I256 E260 I261 G262 L263 M269 Y270 E271 E272 T275 Q281 D287 L295

LYS LYS GLY THR GLN TYR GLU ASN A304 K305 R306 A309 E323 R326 N327 L328 N331 Q332 Q333 L334 L335 THR GLY GLU LYS ILE

• Molecule 1: Polysaccharide biosynthesis protein CapD

Chain E:

80%　　　13%　　•　6%

GLY HIS M1 D5 I17 L26 S39 R51 D52 K53 N54 R55 N56 I57 L60 I61 I64 A85 M86 K87 G106 T107 Q108 T125 N128 I131 Y137 R146 T163 R166 F167 S176 N183 Q184 I185 K186 E187 I191 T192 V193

M202 I218 E223 I226 L227 K228 I232 S233 E243 T246 K247 LEU TYR GLY LEU SER LYS E254 I261 L273 I291 L295 LYS LYS GLY THR GLN TYR GLU ASN A304 N316 K322 R326 T336 GLY GLY GLU LYS ILE

• Molecule 1: Polysaccharide biosynthesis protein CapD

Chain F:

%

79%　　　13%　　•　6%

GLY H0 M1 L9 T14 I17 S23 N24 S39 E40 Y41 L45 R51 D52 K53 ASN R55 R58 E75 N76 I77 K87 F97 T125 N128 I131 T134 N135 N136 K155 V165 R166 F167 G168 N169 V170 R174 Q184 E187

K190 I191 T192 V193 L196 N206 L211 E214 I226 L227 K228 M229 N235 E244 K247 LEU TYR GLY LEU SER LYS E254 E272 D277 I291 P294 LEU LYS LYS GLY T299 E302 R306 D315 ASN GLN N318 L330 N331 Q332 Q333 L334 L335 THR

GLY GLY GLU LYS ILE

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.52Å 141.88Å 93.24Å 90.00° 111.66° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.7 (30.00-2.70) 88.7 (29.82-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.201 , 0.251 0.206 , 0.256	Depositor DCC
R_{free} test set	2898 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , -2.6	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.399 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16002	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: NAP, SO4, UD1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.64	1/2595 (0.0%)	0.82	1/3486 (0.0%)
1	B	0.57	0/2540	0.75	0/3412
1	C	0.59	0/2628	0.80	1/3533 (0.0%)
1	D	0.61	0/2604	0.83	4/3501 (0.1%)
1	E	0.59	0/2590	0.78	0/3482
1	F	0.59	0/2585	0.79	1/3475 (0.0%)
All	All	0.60	1/15542 (0.0%)	0.80	7/20889 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	TYR	CE2-CZ	-5.25	1.31	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	333	GLN	N-CA-C	5.87	126.86	111.00
1	D	58	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	326	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	174	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	200	ARG	NE-CZ-NH1	5.23	122.91	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2559	0	2598	20	0
1	B	2504	0	2552	18	0
1	C	2590	0	2642	28	0
1	D	2566	0	2616	38	0
1	E	2553	0	2604	20	0
1	F	2549	0	2576	21	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
2	E	48	0	25	0	0
2	F	48	0	25	2	0
3	A	39	0	25	1	0
3	B	39	0	25	0	0
3	C	39	0	25	0	0
3	D	39	0	25	0	0
3	E	39	0	25	0	0
3	F	39	0	25	1	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	F	10	0	0	1	0
5	A	34	0	0	0	0
5	B	21	0	0	1	0
5	C	25	0	0	0	0
5	D	21	0	0	0	0
5	E	18	0	0	0	0
5	F	15	0	0	0	0
All	All	16002	0	15888	133	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 4.

The worst 5 of 133 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:D:182:GLU:OE1	1:D:335:LEU:HD12	1.82	0.79
1:D:17:ILE:HD11	1:D:170:VAL:HG21	1.72	0.72
1:F:17:ILE:HD11	1:F:170:VAL:HG21	1.72	0.71
1:B:31:LYS:NZ	5:B:501:HOH:O	2.18	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ILE:HD13	1:B:106:GLY:HA3	1.74	0.70

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	314/343 (92%)	294 (94%)	17 (5%)	3 (1%)	15	37
1	B	308/343 (90%)	297 (96%)	10 (3%)	1 (0%)	41	66
1	C	321/343 (94%)	300 (94%)	19 (6%)	2 (1%)	25	50
1	D	318/343 (93%)	300 (94%)	15 (5%)	3 (1%)	17	40
1	E	316/343 (92%)	296 (94%)	16 (5%)	4 (1%)	12	30
1	F	313/343 (91%)	292 (93%)	19 (6%)	2 (1%)	25	50
All	All	1890/2058 (92%)	1779 (94%)	96 (5%)	15 (1%)	19	43

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	155	LYS
1	E	322	LYS
1	F	51	ARG
1	F	155	LYS
1	A	155	LYS

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	284/302 (94%)	259 (91%)	25 (9%)	10	23
1	B	279/302 (92%)	261 (94%)	18 (6%)	17	38
1	C	288/302 (95%)	262 (91%)	26 (9%)	9	22
1	D	285/302 (94%)	256 (90%)	29 (10%)	7	17
1	E	285/302 (94%)	265 (93%)	20 (7%)	15	35
1	F	282/302 (93%)	260 (92%)	22 (8%)	12	29
All	All	1703/1812 (94%)	1563 (92%)	140 (8%)	11	26

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	228	LYS
1	F	23	SER
1	F	187	GLU
1	C	52	ASP
1	C	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	56	ASN
1	F	47	GLN
1	F	235	ASN
1	F	183	ASN
1	B	184	GLN

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 ⓘ

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	UD1	D	401	-	38,41,41	0.86	1 (2%)	57,62,62	1.54	9 (15%)
2	NAP	E	400	-	45,52,52	1.52	5 (11%)	56,80,80	1.69	9 (16%)
2	NAP	B	401	-	45,52,52	1.45	3 (6%)	56,80,80	1.91	12 (21%)
3	UD1	A	402	-	38,41,41	0.96	3 (7%)	57,62,62	1.37	6 (10%)
4	SO4	F	403	-	4,4,4	0.34	0	6,6,6	0.25	0
4	SO4	F	404	-	4,4,4	0.33	0	6,6,6	0.60	0
4	SO4	A	404	-	4,4,4	0.44	0	6,6,6	0.41	0
2	NAP	D	400	-	45,52,52	1.56	5 (11%)	56,80,80	1.56	8 (14%)
3	UD1	E	401	-	38,41,41	1.05	2 (5%)	57,62,62	1.43	7 (12%)
4	SO4	B	403	-	4,4,4	0.38	0	6,6,6	0.65	0
2	NAP	F	401	-	45,52,52	1.47	4 (8%)	56,80,80	1.65	9 (16%)
3	UD1	B	402	-	38,41,41	1.05	2 (5%)	57,62,62	1.49	10 (17%)
3	UD1	C	401	-	38,41,41	0.95	2 (5%)	57,62,62	1.47	8 (14%)
4	SO4	A	403	-	4,4,4	0.36	0	6,6,6	0.39	0
2	NAP	A	401	-	45,52,52	1.62	4 (8%)	56,80,80	1.48	6 (10%)
3	UD1	F	402	-	38,41,41	1.01	2 (5%)	57,62,62	1.70	12 (21%)
2	NAP	C	400	-	45,52,52	1.38	3 (6%)	56,80,80	1.59	10 (17%)

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	UD1	D	401	-	-	4/26/63/63	0/3/3/3
2	NAP	E	400	-	-	10/31/67/67	0/5/5/5
2	NAP	B	401	-	-	4/31/67/67	0/5/5/5
3	UD1	A	402	-	-	2/26/63/63	0/3/3/3
2	NAP	D	400	-	-	4/31/67/67	0/5/5/5
3	UD1	E	401	-	-	5/26/63/63	0/3/3/3
2	NAP	F	401	-	-	9/31/67/67	0/5/5/5
3	UD1	B	402	-	-	1/26/63/63	0/3/3/3
3	UD1	C	401	-	-	5/26/63/63	0/3/3/3
2	NAP	A	401	-	-	9/31/67/67	0/5/5/5
3	UD1	F	402	-	-	7/26/63/63	0/3/3/3
2	NAP	C	400	-	-	5/31/67/67	0/5/5/5

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	C4N-C3N	7.51	1.52	1.39
2	E	400	NAP	C4N-C3N	7.44	1.52	1.39
2	A	401	NAP	C4N-C3N	7.37	1.51	1.39
2	F	401	NAP	C4N-C3N	6.83	1.51	1.39
2	D	400	NAP	C4N-C3N	6.21	1.49	1.39

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAP	C5N-C4N-C3N	-7.21	111.81	120.34
2	D	400	NAP	C5N-C4N-C3N	-6.70	112.41	120.34
2	B	401	NAP	C5N-C4N-C3N	-6.67	112.45	120.34
2	E	400	NAP	C5N-C4N-C3N	-6.21	112.99	120.34
2	C	400	NAP	C5N-C4N-C3N	-5.91	113.35	120.34

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	C5B-O5B-PA-O2A
2	A	401	NAP	C2B-O2B-P2B-O1X
2	A	401	NAP	C5D-O5D-PN-O1N
2	C	400	NAP	C5B-O5B-PA-O2A

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	UD1	1	0
4	F	404	SO4	1	0
2	D	400	NAP	2	0
2	F	401	NAP	2	0
2	A	401	NAP	1	0
3	F	402	UD1	1	0
2	C	400	NAP	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 UD1 D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP E 400

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 400

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 F 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 400

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(Å²)	Q<0.9
1	A	324/343 (94%)	-0.42	1 (0%)	94	95	10, 23, 45, 61	0
1	B	316/343 (92%)	-0.34	1 (0%)	94	95	9, 26, 53, 74	0
1	C	327/343 (95%)	-0.43	0	100	100	10, 22, 40, 68	0
1	D	324/343 (94%)	-0.43	0	100	100	9, 21, 43, 60	0
1	E	322/343 (93%)	-0.31	1 (0%)	94	95	10, 28, 57, 75	0
1	F	323/343 (94%)	-0.39	2 (0%)	89	91	10, 24, 49, 77	0
All	All	1936/2058 (94%)	-0.39	5 (0%)	94	95	9, 24, 49, 77	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	316	ASN	2.8
1	A	261	ILE	2.7
1	F	0	HIS	2.3
1	B	322	LYS	2.3
1	F	302	GLU	2.2

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
4	SO4	F	404	5/5	0.89	0.21	66,68,72,73	0
4	SO4	A	403	5/5	0.93	0.16	60,62,64,65	0
4	SO4	F	403	5/5	0.95	0.10	57,58,62,66	0
4	SO4	B	403	5/5	0.96	0.14	49,50,52,53	0
2	NAP	F	401	48/48	0.97	0.11	13,14,24,26	0
3	UD1	A	402	39/39	0.97	0.12	17,20,25,25	0
3	UD1	B	402	39/39	0.97	0.14	19,20,31,32	0
3	UD1	C	401	39/39	0.97	0.13	12,15,19,20	0
3	UD1	D	401	39/39	0.97	0.12	13,16,18,18	0
3	UD1	E	401	39/39	0.97	0.13	23,25,30,31	0
3	UD1	F	402	39/39	0.97	0.13	16,19,26,27	0
2	NAP	A	401	48/48	0.97	0.12	10,12,23,25	0
4	SO4	A	404	5/5	0.97	0.13	57,58,61,63	0
2	NAP	B	401	48/48	0.97	0.12	14,19,30,34	0
2	NAP	D	400	48/48	0.97	0.12	11,14,24,27	0
2	NAP	E	400	48/48	0.97	0.12	14,17,27,29	0
2	NAP	C	400	48/48	0.98	0.10	11,14,19,20	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 NAP F 401:

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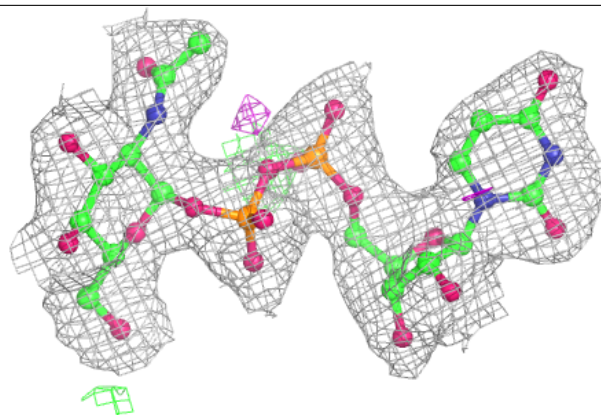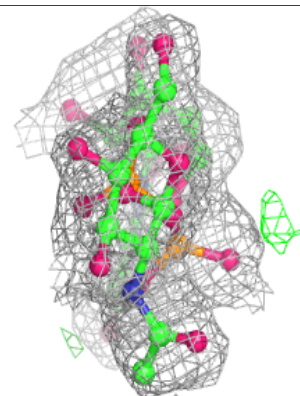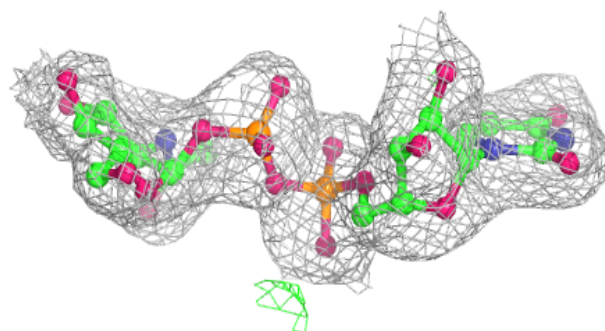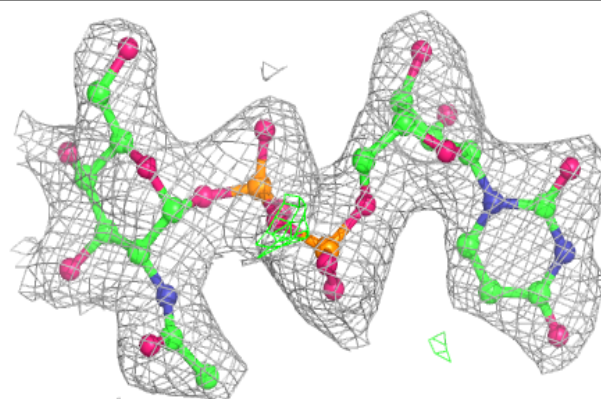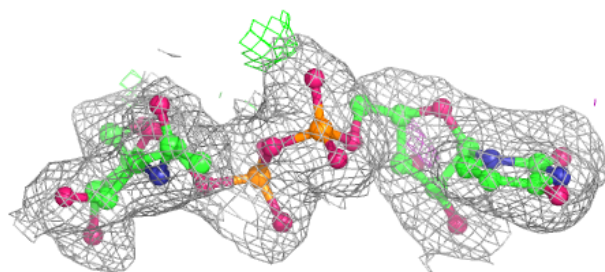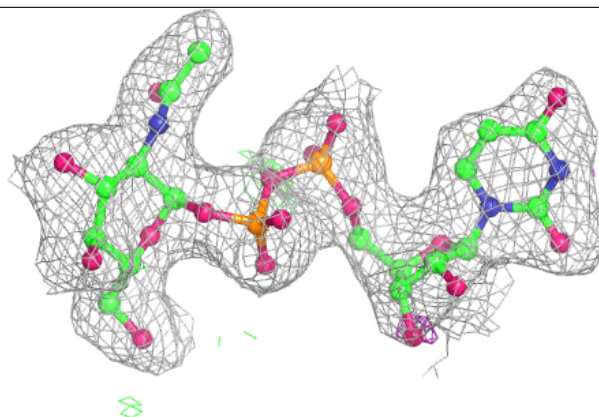mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around UD1 A 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
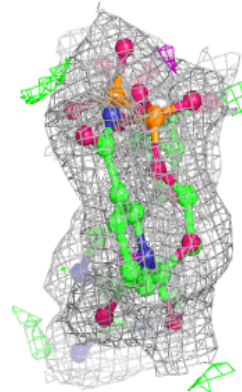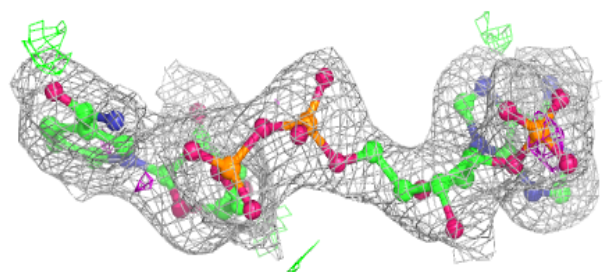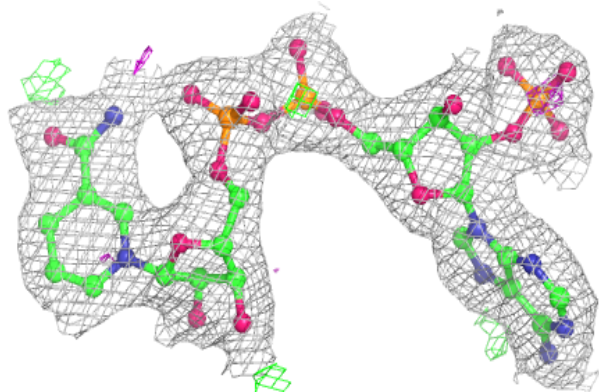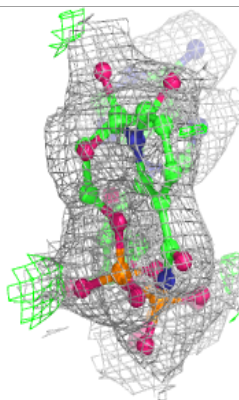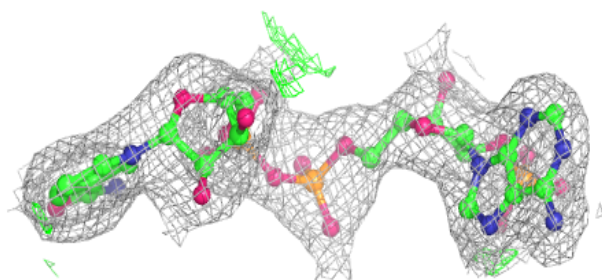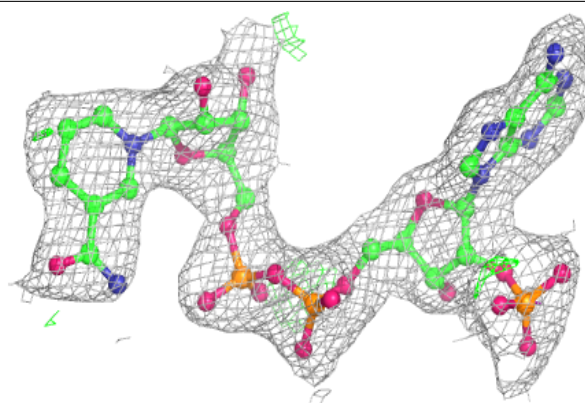mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
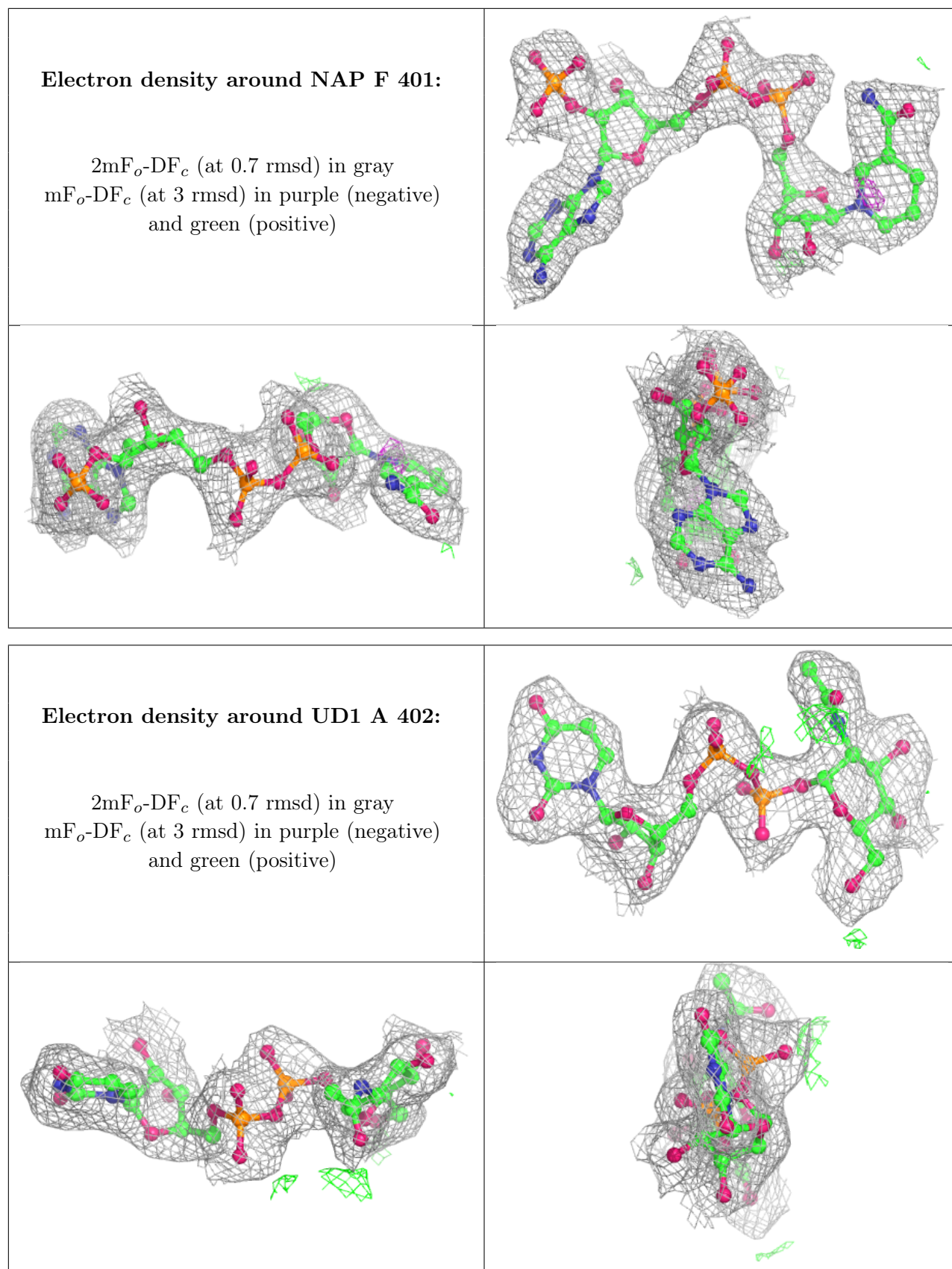
Electron density around UD1 B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
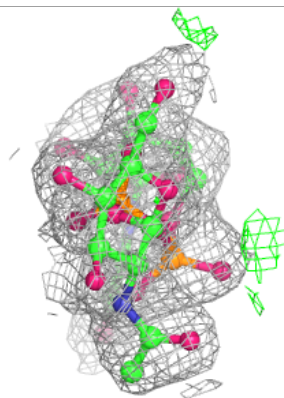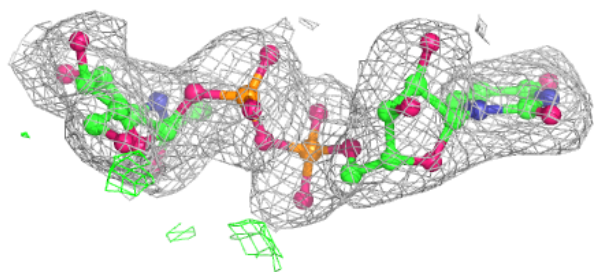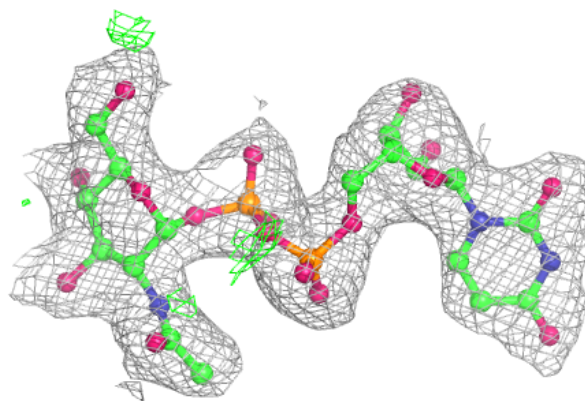
Electron density around UD1 C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
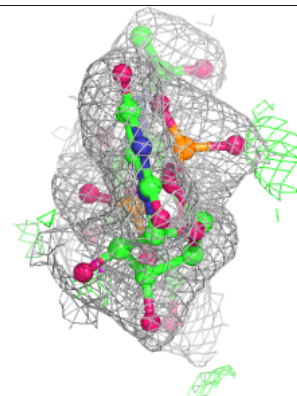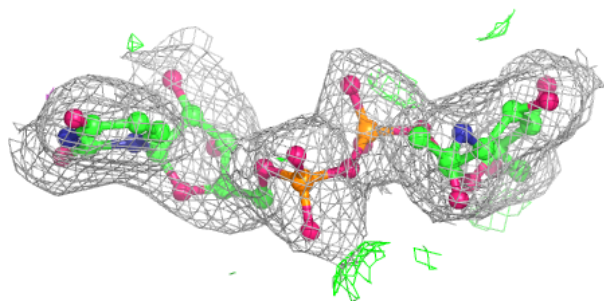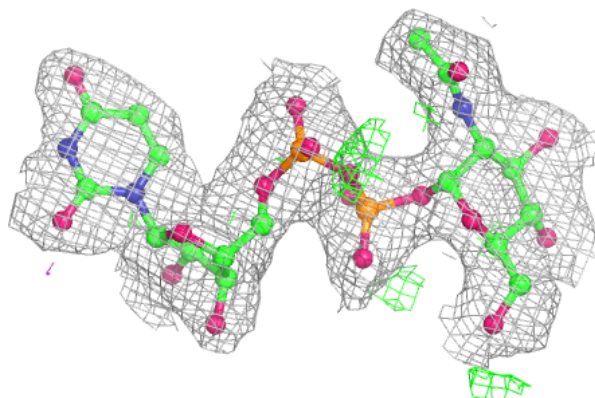
Electron density around UD1 D 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
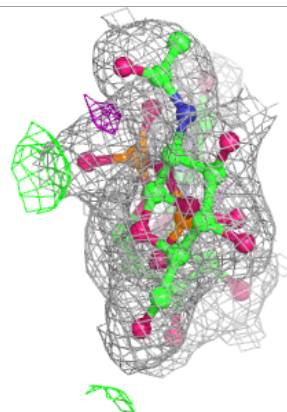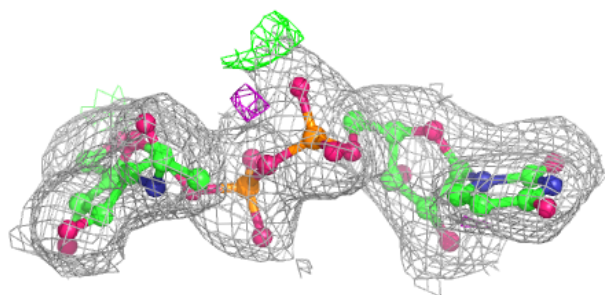
Electron density around UD1 E 401:

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 F 402:

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

Electron density around NAP A 401:

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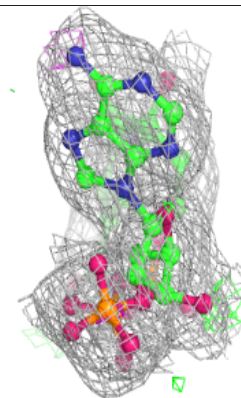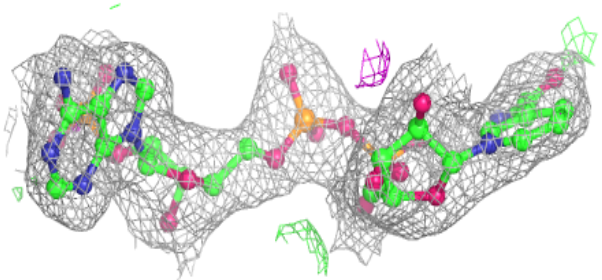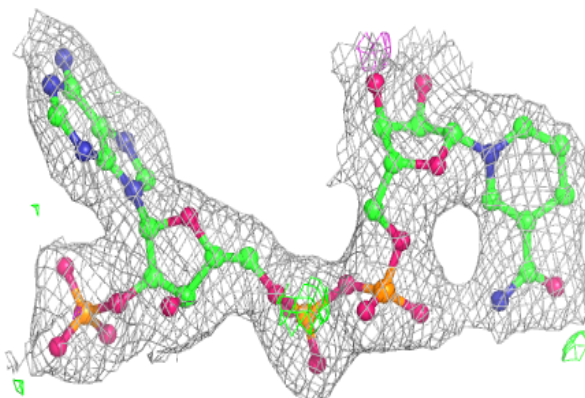and green (positive)

Electron density around NAP B 401:

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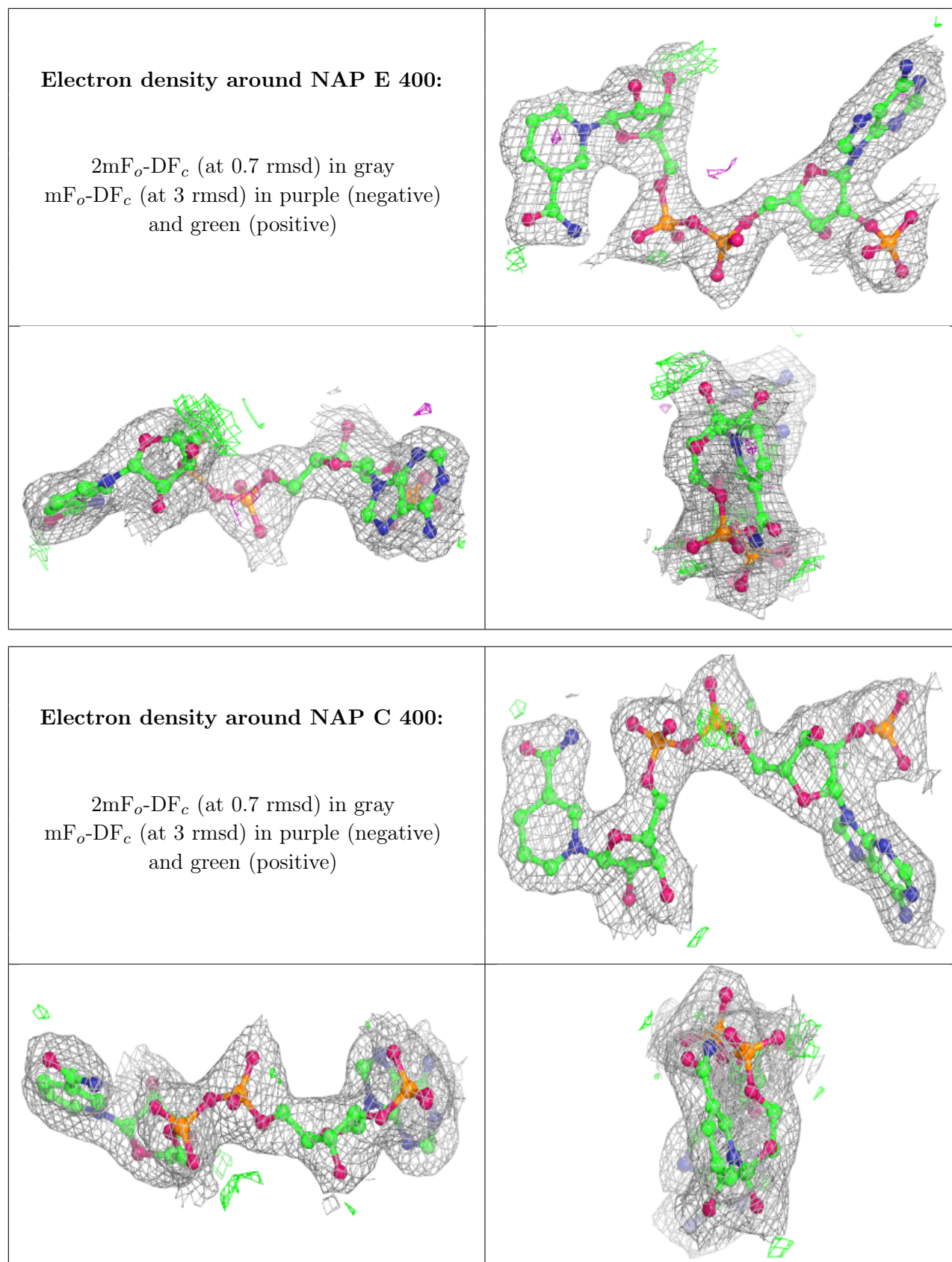mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAP D 400:

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

Electron density around NAP E 400:

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

Electron density around NAP C 400:

$2mF_o$-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.