



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:08 AM UTC

PDB ID : 8JFH / pdb_00008jfh
Title : Crystal structure of 3-oxoacyl-ACP reductase FabG in complex with NADP+ and 3-keto-octanoyl-ACP from Helicobacter pylori in an inactive form that priors the acyl substrate delivery
Authors : Zhou, J.S.; Zhang, L.
Deposited on : 2023-05-18
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

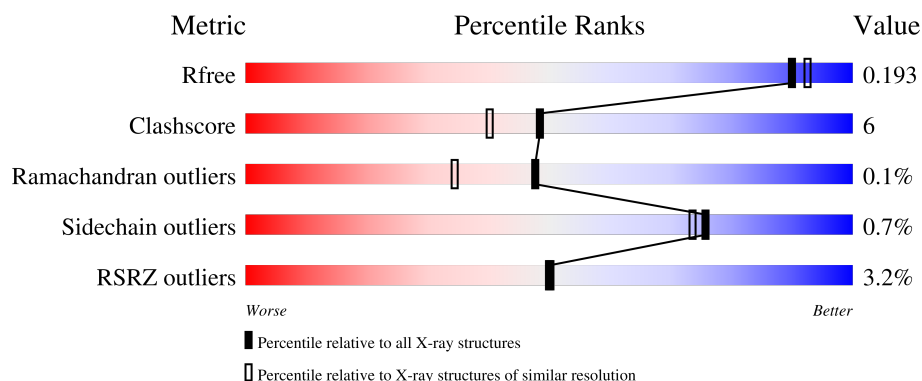
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	248	2% 87% 8% .
1	B	248	3% 81% 13% 6%
1	C	248	3% 84% 11% .
1	D	248	2% 85% 10% .

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Mol	Chain	Length	Quality of chain
2	E	84	4% 79% 13% .. 6%
2	F	84	10% 81% 13% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9733 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 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	4	0
			1808	1141	310	348	9			
1	B	234	Total	C	N	O	S	0	6	0
			1796	1138	306	343	9			
1	C	238	Total	C	N	O	S	0	3	0
			1805	1138	310	348	9			
1	D	238	Total	C	N	O	S	0	3	0
			1806	1140	310	347	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP G2M827
B	0	SER	-	expression tag	UNP G2M827
C	0	SER	-	expression tag	UNP G2M827
D	0	SER	-	expression tag	UNP G2M827

- Molecule 2 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	79	Total	C	N	O	S	0	0	0
			608	388	91	127	2			
2	F	81	Total	C	N	O	S	0	0	0
			622	395	92	132	3			

There are 12 discrepancies between the modelled and reference sequences:

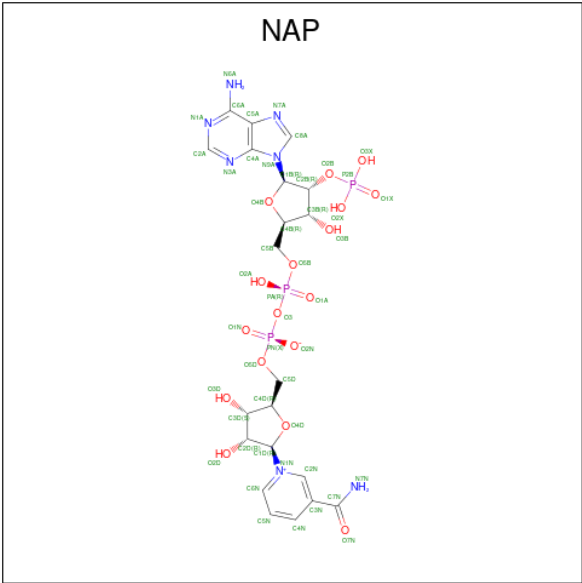
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	SER	-	expression tag	UNP Q5EDC8
E	-4	SER	-	expression tag	UNP Q5EDC8
E	-3	MET	-	expression tag	UNP Q5EDC8
E	-2	GLY	-	expression tag	UNP Q5EDC8

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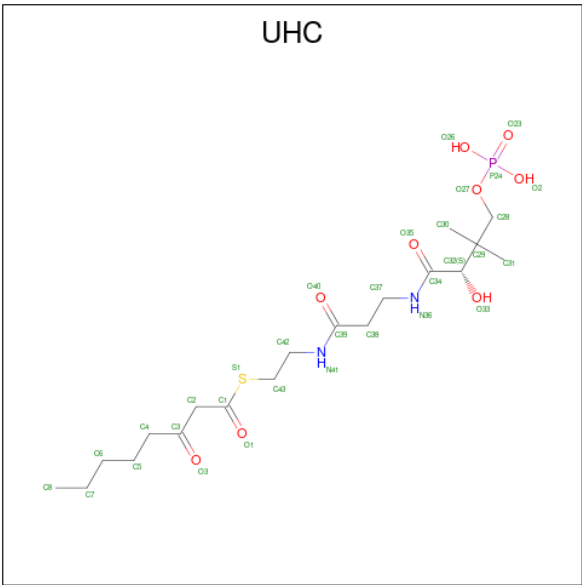
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	TYR	-	expression tag	UNP Q5EDC8
E	0	LEU	-	expression tag	UNP Q5EDC8
F	-5	SER	-	expression tag	UNP Q5EDC8
F	-4	SER	-	expression tag	UNP Q5EDC8
F	-3	MET	-	expression tag	UNP Q5EDC8
F	-2	GLY	-	expression tag	UNP Q5EDC8
F	-1	TYR	-	expression tag	UNP Q5EDC8
F	0	LEU	-	expression tag	UNP Q5EDC8

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



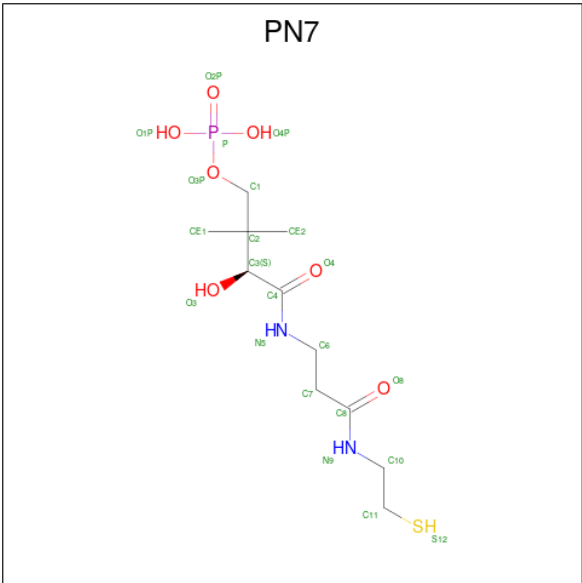
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 23	10	5	7	1	0	0
3	B	1	Total 27	10	5	10	2	0	0
3	D	1	Total 23	10	5	7	1	0	0

- Molecule 4 is {S}-[2-[3-[(2 {S})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl] amino]propanoylamino]ethyl] 3-oxidanylideneoctanethioate (CCD ID: UHC) (formula: C₁₉H₃₅N₂O₉PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	E	1	Total	C	N	O	P	S	0	0
			31	19	2	8	1	1		

- Molecule 5 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfanylet hyl)-beta-alaninamide (CCD ID: PN7) (formula: C₁₁H₂₃N₂O₇PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	F	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

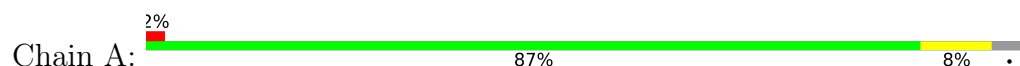
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	275	Total 275	O 275	0	0
6	B	257	Total 257	O 257	0	0
6	C	255	Total 255	O 255	0	0
6	D	236	Total 236	O 236	0	0
6	E	67	Total 67	O 67	0	0
6	F	73	Total 73	O 73	0	0

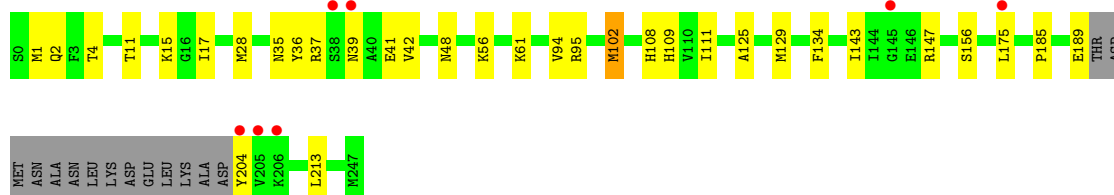
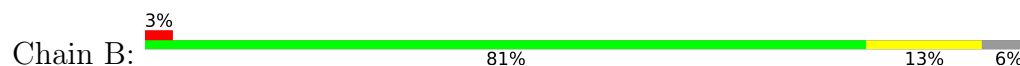
3 Residue-property plots [i](#)

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.

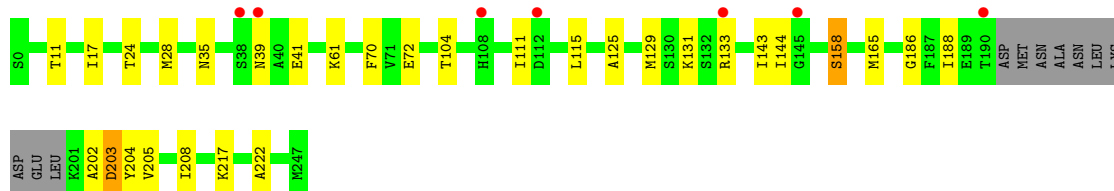
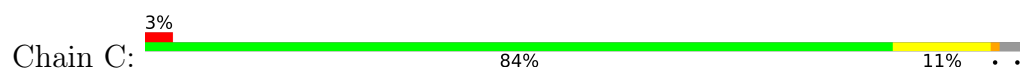
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



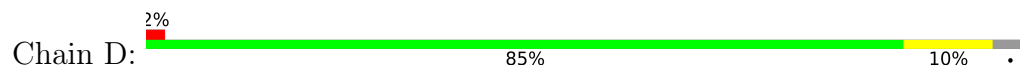
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

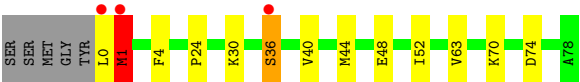
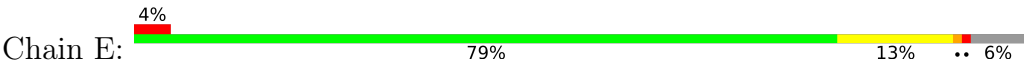


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

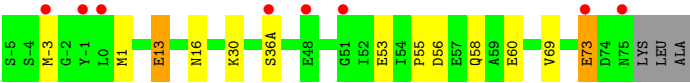
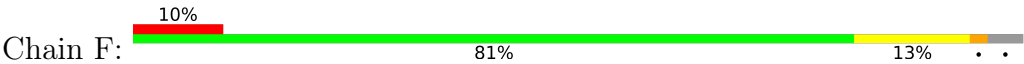




● Molecule 2: Acyl carrier protein



● Molecule 2: Acyl carrier protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.94Å 117.26Å 142.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.24 – 1.80 45.24 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.24-1.80) 99.6 (45.24-1.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.164 , 0.190 0.166 , 0.193	Depositor DCC
R_{free} test set	5274 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9733	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UHC, PN7, NAP

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	0.49	2/1837 (0.1%)	0.68	1/2470 (0.0%)
1	B	0.49	2/1834 (0.1%)	0.71	6/2465 (0.2%)
1	C	0.59	4/1837 (0.2%)	0.82	5/2468 (0.2%)
1	D	0.63	6/1838 (0.3%)	0.72	1/2470 (0.0%)
2	E	0.54	1/613 (0.2%)	0.70	1/831 (0.1%)
2	F	0.50	0/628	0.82	1/851 (0.1%)
All	All	0.55	15/8587 (0.2%)	0.74	15/11555 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	MET	C-O	-7.72	1.15	1.24
1	D	70	PHE	C-O	-6.63	1.16	1.24
1	B	111[A]	ILE	C-O	6.53	1.31	1.24
1	B	111[B]	ILE	C-O	6.53	1.31	1.24
1	D	183[A]	VAL	C-O	6.19	1.30	1.24
1	D	183[B]	VAL	C-O	6.19	1.30	1.24
1	A	187	PHE	C-O	-6.04	1.16	1.24
1	C	202	ALA	C-O	-5.85	1.17	1.24
1	D	162	MET	C-O	-5.80	1.17	1.24
1	C	204	TYR	C-O	-5.70	1.17	1.24
1	A	70	PHE	C-O	-5.62	1.17	1.24
1	D	38[A]	SER	C-O	5.50	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	38[B]	SER	C-O	5.50	1.30	1.24
1	C	158[A]	SER	C-O	5.22	1.30	1.24
1	C	158[B]	SER	C-O	5.22	1.30	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158[A]	SER	CA-C-O	9.47	130.77	120.82
1	C	158[B]	SER	CA-C-O	9.47	130.77	120.82
1	C	72	GLU	CB-CG-CD	7.45	125.26	112.60
1	B	111[A]	ILE	N-CA-C	6.38	117.13	110.62
1	B	111[B]	ILE	N-CA-C	6.38	117.13	110.62
2	F	13	GLU	CA-CB-CG	-6.12	101.87	114.10
1	B	111[A]	ILE	CA-C-O	6.02	127.21	120.95
1	B	111[B]	ILE	CA-C-O	6.02	127.21	120.95
1	C	203	ASP	CB-CA-C	5.83	121.41	110.63
1	A	189	GLU	CB-CA-C	5.72	120.29	110.79
2	E	36	SER	CA-CB-OG	-5.66	99.78	111.10
1	B	102	MET	CB-CA-C	-5.29	101.62	110.29
1	B	15	LYS	CB-CG-CD	-5.27	99.17	111.30
1	C	70	PHE	CA-CB-CG	5.26	119.06	113.80
1	D	103	LYS	CB-CG-CD	5.03	122.86	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	37	ARG	Sidechain

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	1808	0	1833	15	0
1	B	1796	0	1835	24	0
1	C	1805	0	1833	18	0
1	D	1806	0	1837	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	608	0	608	12	0
2	F	622	0	610	8	0
3	A	23	0	11	1	0
3	B	27	0	11	0	0
3	D	23	0	11	0	0
4	E	31	0	0	0	0
5	F	21	0	21	3	0
6	A	275	0	0	7	0
6	B	257	0	0	7	0
6	C	255	0	0	5	0
6	D	236	0	0	13	0
6	E	67	0	0	5	0
6	F	73	0	0	3	0
All	All	9733	0	8610	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (95) 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:B:37:ARG:HD2	6:B:542:HOH:O	1.58	1.02
2:E:1:MET:HA	2:E:1:MET:HE2	1.46	0.98
1:A:131:LYS:HG2	6:A:481:HOH:O	1.87	0.74
1:C:17:ILE:HD11	1:C:188:ILE:HG21	1.75	0.67
1:D:108:HIS:HD2	6:D:520:HOH:O	1.79	0.65
1:B:147:ARG:HG2	1:B:204:TYR:CD1	2.32	0.65
1:B:39:ASN:HA	6:B:415:HOH:O	1.96	0.64
2:E:30:LYS:HG3	6:E:215:HOH:O	1.98	0.64
1:A:12:GLY:H	1:A:35:ASN:HD22	1.46	0.64
1:B:17:ILE:HD11	1:B:143[A]:ILE:HD11	1.79	0.63
1:C:217:LYS:HE3	6:C:438:HOH:O	1.97	0.62
1:B:94:VAL:O	1:B:95:ARG:HD3	2.00	0.61
2:E:63:VAL:HG11	6:E:264:HOH:O	2.00	0.60
1:A:131:LYS:HG3	6:A:643:HOH:O	1.99	0.60
1:C:222:ALA:HB2	6:C:333:HOH:O	2.01	0.60
2:E:1:MET:HA	2:E:1:MET:CE	2.25	0.60
1:A:157:ALA:HB2	1:C:165:MET:HB2	1.84	0.59
1:B:2:GLN:NE2	6:B:403:HOH:O	2.35	0.59
1:B:17:ILE:CD1	1:B:143[A]:ILE:HD11	2.33	0.58
1:C:131:LYS:HG3	6:C:306:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:ND2	1:B:41:GLU:OE1	2.38	0.57
2:F:55:PRO:HD2	2:F:58:GLN:HG3	1.87	0.57
1:B:1:MET:HB2	1:B:28:MET:SD	2.45	0.56
1:B:108:HIS:HE1	6:D:560:HOH:O	1.88	0.56
2:F:53:GLU:HG3	6:F:252:HOH:O	2.04	0.56
1:A:102:MET:HG2	1:A:106:ASP:HB2	1.88	0.55
1:C:144:ILE:HD12	1:C:186:GLY:HA2	1.89	0.55
2:F:56:ASP:O	2:F:60:GLU:HG3	2.07	0.55
1:D:131:LYS:HG2	6:D:479:HOH:O	2.08	0.54
1:A:144[B]:ILE:HD13	6:A:420:HOH:O	2.07	0.54
2:E:52:ILE:HB	6:E:250:HOH:O	2.07	0.53
1:D:151:GLY:HA3	5:F:101:PN7:H19	1.90	0.53
2:E:1:MET:CE	2:E:1:MET:CA	2.84	0.53
1:D:39:ASN:HB3	6:D:453:HOH:O	2.09	0.53
1:D:108:HIS:CD2	6:D:520:HOH:O	2.59	0.53
2:E:1:MET:HE2	2:E:1:MET:CA	2.25	0.52
1:D:98:LEU:HD11	5:F:101:PN7:H5	1.91	0.52
2:F:-3:MET:O	2:F:1:MET:HG2	2.10	0.52
2:E:4:PHE:CZ	2:E:24:PRO:HD3	2.46	0.52
1:B:143[A]:ILE:HD13	1:B:185:PRO:HB2	1.92	0.51
1:B:125:ALA:O	1:B:129:MET:HB2	2.11	0.50
1:D:37:ARG:HG2	6:D:487:HOH:O	2.11	0.50
1:D:56:LYS:NZ	6:D:411:HOH:O	2.40	0.50
1:C:24:THR:O	1:C:28:MET:HG3	2.11	0.50
1:C:111:ILE:HG23	1:C:115:LEU:HD12	1.94	0.50
1:A:95:ARG:HG3	6:A:550:HOH:O	2.12	0.49
1:C:11:THR:HA	1:C:35:ASN:HB3	1.93	0.49
2:F:30:LYS:HG3	6:F:216:HOH:O	2.13	0.49
5:F:101:PN7:O4	5:F:101:PN7:H8	2.11	0.49
1:A:131:LYS:CG	6:A:481:HOH:O	2.53	0.48
1:A:39:ASN:CG	6:A:403:HOH:O	2.56	0.48
1:D:39:ASN:N	6:D:413:HOH:O	2.46	0.47
1:B:109:HIS:HD2	6:B:587:HOH:O	1.97	0.47
1:D:11:THR:HA	1:D:35:ASN:HB3	1.95	0.47
1:C:133:ARG:O	1:C:133:ARG:HG3	2.14	0.47
1:D:189:GLU:HB2	6:D:586:HOH:O	2.13	0.47
1:A:67:GLU:OE1	1:C:104:THR:HG23	2.15	0.47
1:D:24:THR:O	1:D:28:MET:HG3	2.16	0.46
1:B:147:ARG:HG2	1:B:204:TYR:HD1	1.78	0.46
1:C:61:LYS:HE3	6:C:477:HOH:O	2.16	0.46
1:C:125:ALA:O	1:C:129:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:16:ASN:ND2	6:F:202:HOH:O	2.35	0.46
1:B:39:ASN:OD1	1:B:42:VAL:HG23	2.16	0.45
1:C:111:ILE:HD13	1:C:158[A]:SER:OG	2.17	0.45
1:D:75:GLN:NE2	6:D:402:HOH:O	2.49	0.45
1:D:101:LYS:NZ	6:D:401:HOH:O	2.21	0.45
1:D:203:ASP:HA	1:D:206:LYS:HG3	1.97	0.45
1:A:222:ALA:HB2	6:A:422:HOH:O	2.16	0.45
2:E:48:GLU:HG3	6:E:244:HOH:O	2.17	0.44
1:B:189:GLU:HB3	1:B:213:LEU:HD13	2.00	0.44
2:E:40:VAL:O	2:E:44:MET:HG3	2.17	0.44
1:B:48:ASN:ND2	6:B:402:HOH:O	2.34	0.43
1:C:205:VAL:HA	1:C:208:ILE:HD12	1.99	0.43
1:A:217:LYS:O	1:A:221:GLU:HG3	2.19	0.43
1:B:56:LYS:NZ	6:B:410:HOH:O	2.52	0.43
1:D:75:GLN:CD	6:D:402:HOH:O	2.62	0.42
2:F:13:GLU:O	2:F:13:GLU:HG3	2.17	0.42
1:B:175:LEU:C	6:B:435:HOH:O	2.62	0.42
1:A:37:ARG:HG3	3:A:301:NAP:C2A	2.49	0.42
1:B:36:TYR:CZ	1:B:61:LYS:HB2	2.54	0.42
1:B:102:MET:HB3	1:D:119:PHE:HZ	1.84	0.42
1:C:144:ILE:CD1	1:C:186:GLY:HA2	2.50	0.42
1:A:183[A]:VAL:HG12	1:A:185:PRO:HD3	2.01	0.41
1:C:39:ASN:OD1	1:C:41:GLU:HG3	2.20	0.41
1:D:190:THR:C	6:D:419:HOH:O	2.63	0.41
1:B:11:THR:HA	1:B:35:ASN:HB3	2.03	0.41
1:C:143:ILE:CG2	6:C:461:HOH:O	2.69	0.41
1:D:11:THR:O	1:D:90:ASN:HB3	2.20	0.41
1:B:156[B]:SER:OG	1:D:165:MET:HA	2.19	0.41
1:B:4:THR:HB	1:B:134:PHE:CZ	2.55	0.41
2:E:48:GLU:HG2	6:E:247:HOH:O	2.21	0.41
2:E:70:LYS:HE2	2:E:74:ASP:OD1	2.20	0.40
1:A:11:THR:O	1:A:90:ASN:HB3	2.22	0.40
2:F:69:VAL:O	2:F:73:GLU:HB3	2.22	0.40
1:D:202:ALA:O	1:D:206:LYS:HG3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/248 (96%)	231 (98%)	6 (2%)	0	100	100
1	B	236/248 (95%)	232 (98%)	4 (2%)	0	100	100
1	C	237/248 (96%)	232 (98%)	5 (2%)	0	100	100
1	D	237/248 (96%)	230 (97%)	7 (3%)	0	100	100
2	E	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
2	F	79/84 (94%)	74 (94%)	4 (5%)	1 (1%)	9	3
All	All	1103/1160 (95%)	1073 (97%)	29 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	73	GLU

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	191/197 (97%)	191 (100%)	0	100	100
1	B	191/197 (97%)	191 (100%)	0	100	100
1	C	191/197 (97%)	190 (100%)	1 (0%)	81	80
1	D	191/197 (97%)	190 (100%)	1 (0%)	81	80
2	E	66/70 (94%)	63 (96%)	3 (4%)	24	12
2	F	68/70 (97%)	67 (98%)	1 (2%)	57	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	898/928 (97%)	892 (99%)	6 (1%)	76	73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	203	ASP
1	D	105	GLU
2	E	0	LEU
2	E	1	MET
2	E	36	SER
2	F	36(A)	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	89	ASN
1	A	109	HIS
1	B	108	HIS
1	B	152	GLN
1	C	75	GLN
1	C	108	HIS
1	D	89	ASN
1	D	108	HIS
2	E	58	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 oligosaccharides in this entry.

5.6 Ligand geometry

5 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
4	UHC	E	101	2	24,30,31	0.79	1 (4%)	30,38,41	4.28	13 (43%)
3	NAP	D	301	-	25,25,52	0.43	0	38,38,80	0.81	1 (2%)
3	NAP	B	301	-	29,29,52	0.54	0	44,45,80	0.90	1 (2%)
3	NAP	A	301	-	25,25,52	0.43	0	38,38,80	0.88	1 (2%)
5	PN7	F	101	-	14,20,21	1.63	3 (21%)	18,26,29	2.45	7 (38%)

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
4	UHC	E	101	2	-	20/36/38/39	-
3	NAP	D	301	-	-	1/11/27/67	0/3/3/5
3	NAP	B	301	-	-	2/15/31/67	0/3/3/5
3	NAP	A	301	-	-	0/11/27/67	0/3/3/5
5	PN7	F	101	-	-	14/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	PN7	O4-C4	-3.69	1.16	1.23
5	F	101	PN7	O8-C8	-2.97	1.17	1.23
4	E	101	UHC	O27-C28	-2.62	1.36	1.44
5	F	101	PN7	CE1-C2	-2.31	1.49	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	101	UHC	C32-C34-N36	16.62	148.02	116.48
4	E	101	UHC	O35-C34-C32	-10.62	91.25	120.89
4	E	101	UHC	C43-C42-N41	-5.66	100.60	112.41
4	E	101	UHC	C37-N36-C34	4.97	131.48	122.55
4	E	101	UHC	C3-C2-C1	-4.75	103.33	112.45
3	B	301	NAP	P2B-O2B-C2B	-4.52	111.37	123.43
3	A	301	NAP	P2B-O2B-C2B	-4.41	111.65	123.43
5	F	101	PN7	C7-C8-N9	4.36	124.29	116.34
5	F	101	PN7	C7-C6-N5	-4.35	102.74	112.00
4	E	101	UHC	O33-C32-C34	-4.29	91.46	109.38
5	F	101	PN7	C6-N5-C4	3.56	128.94	122.55
5	F	101	PN7	CE1-C2-C3	-3.54	102.73	108.77
4	E	101	UHC	C37-C38-C39	-3.26	106.97	112.39
5	F	101	PN7	O8-C8-N9	-3.22	116.71	123.03
5	F	101	PN7	CE2-C2-C3	3.18	114.19	108.77
4	E	101	UHC	C5-C4-C3	-3.11	106.70	114.59
3	D	301	NAP	P2B-O2B-C2B	-3.09	115.17	123.43
4	E	101	UHC	C38-C37-N36	-2.77	106.11	112.00
5	F	101	PN7	O3-C3-C2	2.56	116.10	110.18
4	E	101	UHC	O33-C32-C29	2.51	116.00	110.18
4	E	101	UHC	O35-C34-N36	-2.46	117.77	122.98
4	E	101	UHC	O1-C1-S1	2.15	125.42	122.68
4	E	101	UHC	C43-S1-C1	-2.00	95.93	101.84

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	NAP	C5B-O5B-PA-O1A
4	E	101	UHC	C1-C2-C3-O3
4	E	101	UHC	O27-C28-C29-C32
4	E	101	UHC	C28-C29-C32-O33
4	E	101	UHC	C28-C29-C32-C34
4	E	101	UHC	C30-C29-C32-O33
4	E	101	UHC	C30-C29-C32-C34
4	E	101	UHC	C31-C29-C32-C34
4	E	101	UHC	C32-C34-N36-C37
4	E	101	UHC	N41-C42-C43-S1
5	F	101	PN7	C1-C2-C3-O3
5	F	101	PN7	CE1-C2-C3-O3
5	F	101	PN7	CE2-C2-C3-O3
5	F	101	PN7	CE2-C2-C3-C4
5	F	101	PN7	O3-C3-C4-O4

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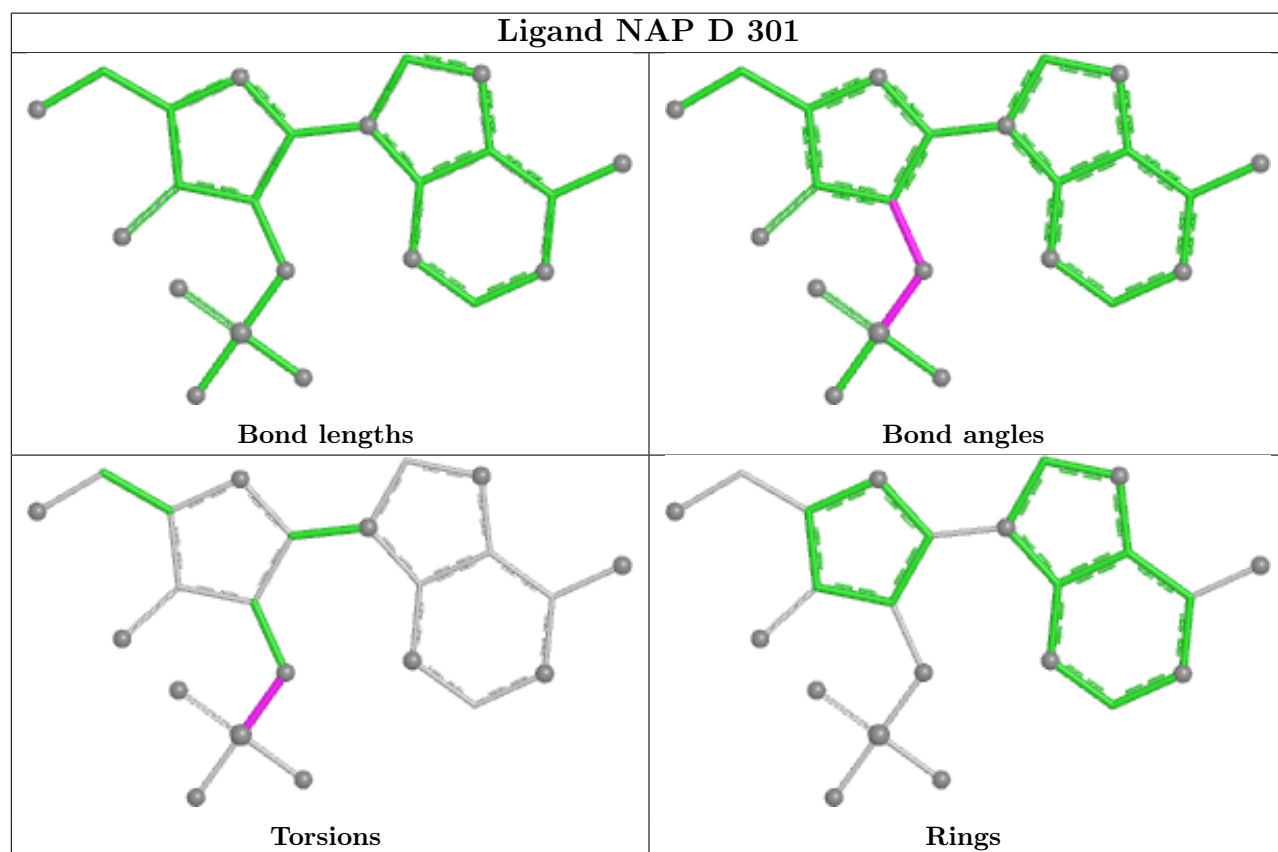
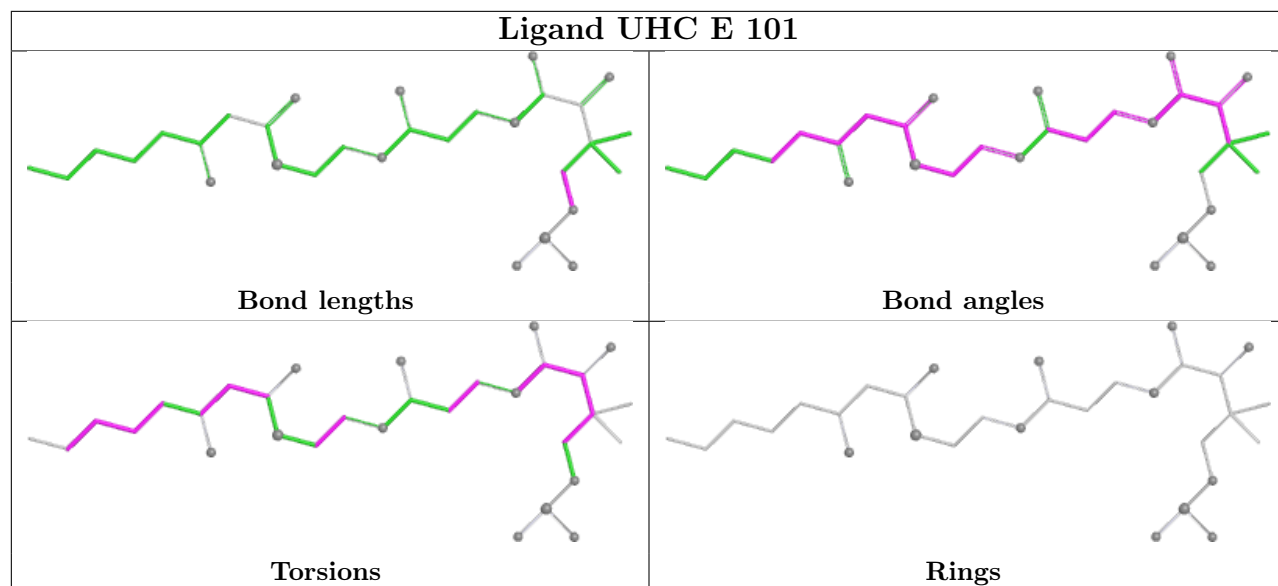
Mol	Chain	Res	Type	Atoms
5	F	101	PN7	O3-C3-C4-N5
5	F	101	PN7	N5-C6-C7-C8
5	F	101	PN7	N9-C10-C11-S12
4	E	101	UHC	O35-C34-N36-C37
4	E	101	UHC	C3-C4-C5-C6
4	E	101	UHC	N36-C37-C38-C39
4	E	101	UHC	C5-C6-C7-C8
4	E	101	UHC	C31-C29-C32-O33
4	E	101	UHC	C29-C32-C34-N36
4	E	101	UHC	C4-C5-C6-C7
4	E	101	UHC	O1-C1-C2-C3
5	F	101	PN7	CE1-C2-C3-C4
4	E	101	UHC	O27-C28-C29-C30
4	E	101	UHC	O27-C28-C29-C31
3	D	301	NAP	C2B-O2B-P2B-O1X
5	F	101	PN7	C6-C7-C8-N9
5	F	101	PN7	C2-C3-C4-O4
3	B	301	NAP	C2B-O2B-P2B-O3X
5	F	101	PN7	C2-C3-C4-N5
4	E	101	UHC	C1-C2-C3-C4
5	F	101	PN7	C6-C7-C8-O8
5	F	101	PN7	C11-C10-N9-C8

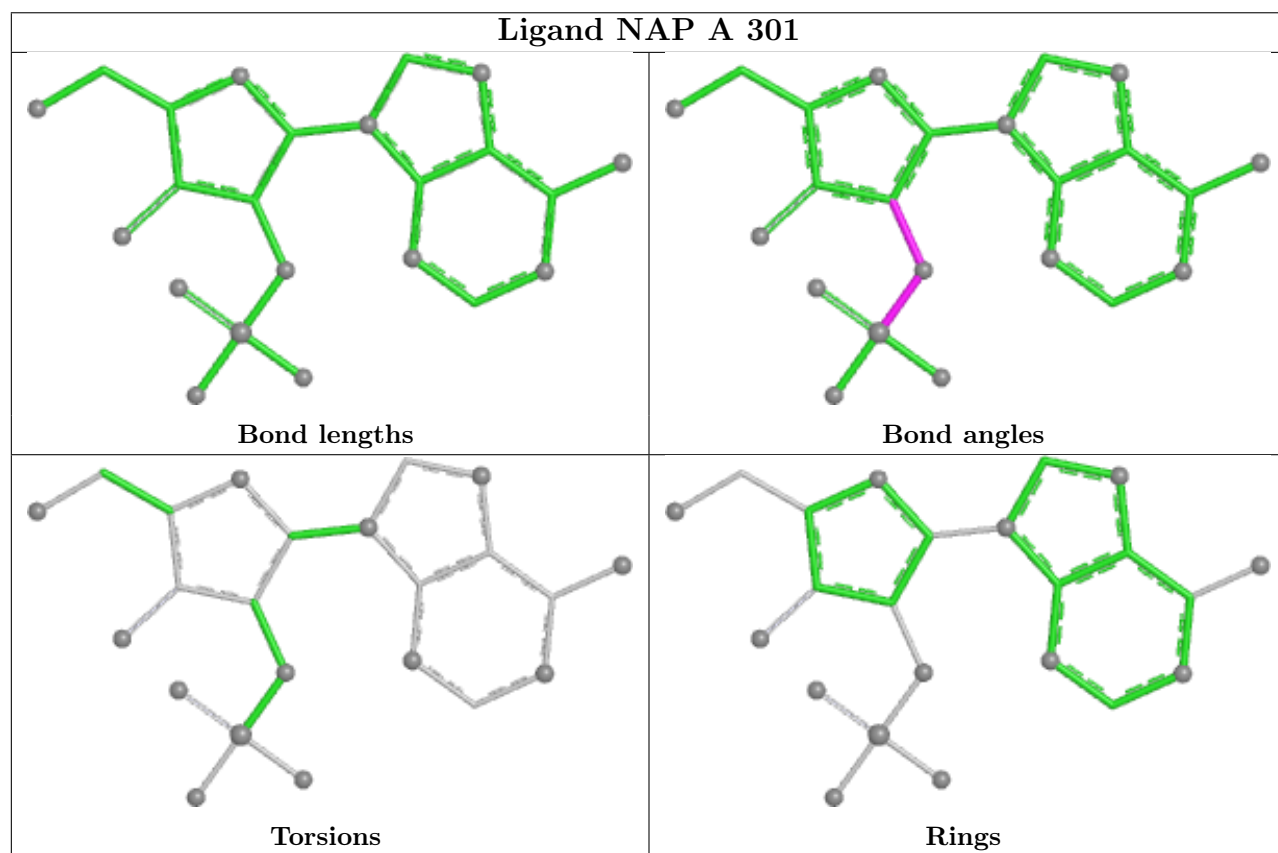
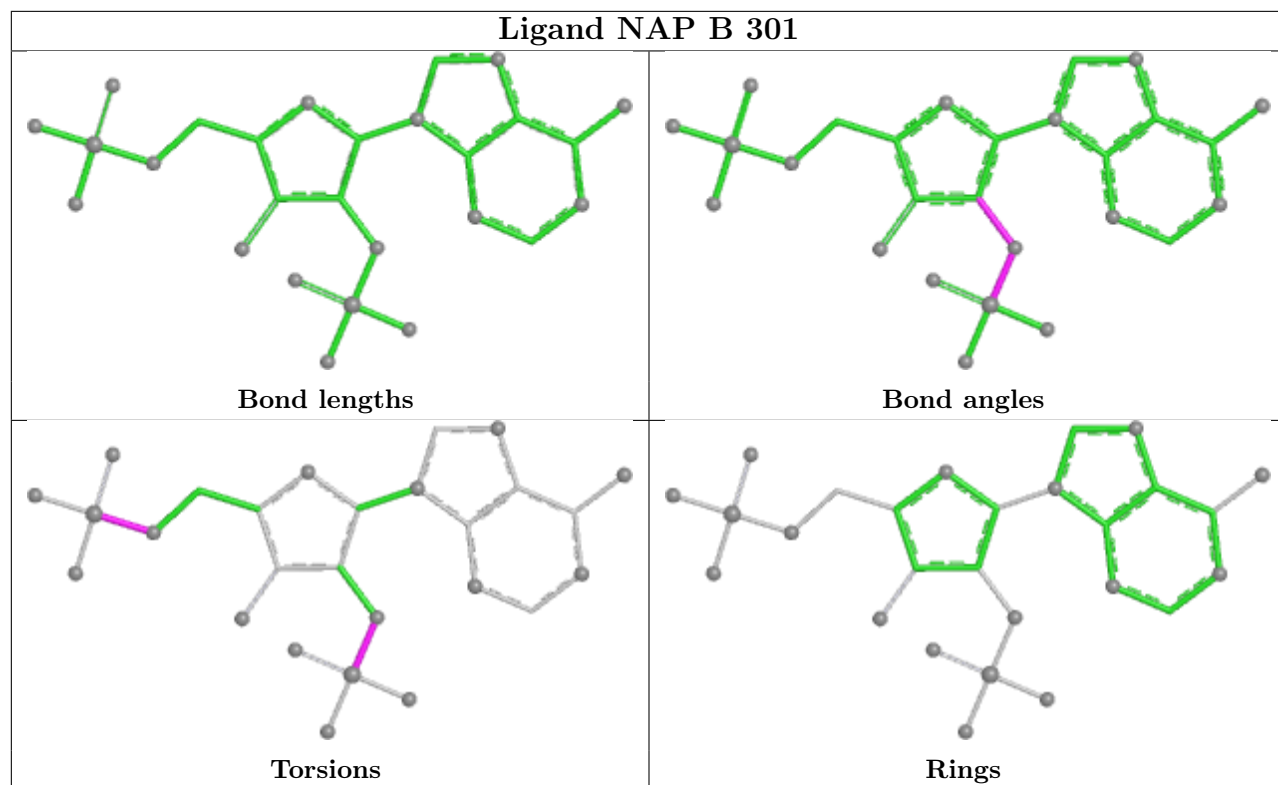
There are no ring outliers.

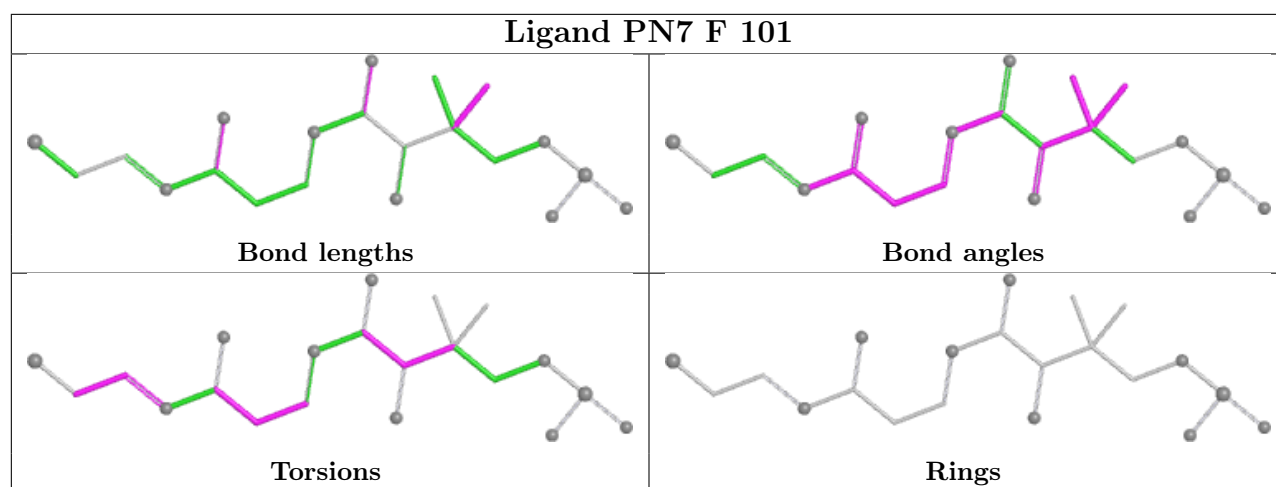
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAP	1	0
5	F	101	PN7	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	237/248 (95%)	-0.44	5 (2%)	63	64	8, 15, 35, 63	4 (1%)
1	B	234/248 (94%)	-0.34	7 (2%)	52	52	7, 16, 35, 55	6 (2%)
1	C	238/248 (95%)	-0.24	7 (2%)	53	53	9, 17, 40, 53	3 (1%)
1	D	238/248 (95%)	-0.35	5 (2%)	63	64	8, 17, 35, 59	3 (1%)
2	E	79/84 (94%)	0.58	3 (3%)	44	44	19, 30, 51, 65	0
2	F	81/84 (96%)	0.71	8 (9%)	13	11	20, 32, 55, 60	0
All	All	1107/1160 (95%)	-0.20	35 (3%)	50	50	7, 17, 43, 65	16 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	TYR	4.6
1	C	38	SER	3.9
1	D	190	THR	3.9
1	C	145	GLY	3.8
1	D	38[A]	SER	3.7
1	C	190	THR	3.7
1	D	39	ASN	3.5
2	F	-3	MET	3.5
2	E	0	LEU	3.5
1	D	204	TYR	3.5
2	F	75	ASN	3.5
1	A	39	ASN	3.4
2	E	36	SER	3.3
1	A	204	TYR	3.1
1	B	205	VAL	3.0
1	C	39	ASN	3.0
1	D	206	LYS	3.0
1	A	190	THR	2.8
1	A	202	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	145	GLY	2.6
1	B	206	LYS	2.6
1	B	38	SER	2.6
2	F	36(A)	SER	2.6
1	C	112	ASP	2.5
2	F	48	GLU	2.3
1	B	39	ASN	2.3
1	B	175	LEU	2.3
2	F	-1	TYR	2.2
2	E	1	MET	2.2
2	F	0	LEU	2.2
2	F	51	GLY	2.1
1	C	133	ARG	2.1
1	C	108	HIS	2.1
1	A	37	ARG	2.1
2	F	73	GLU	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 oligosaccharides in this entry.

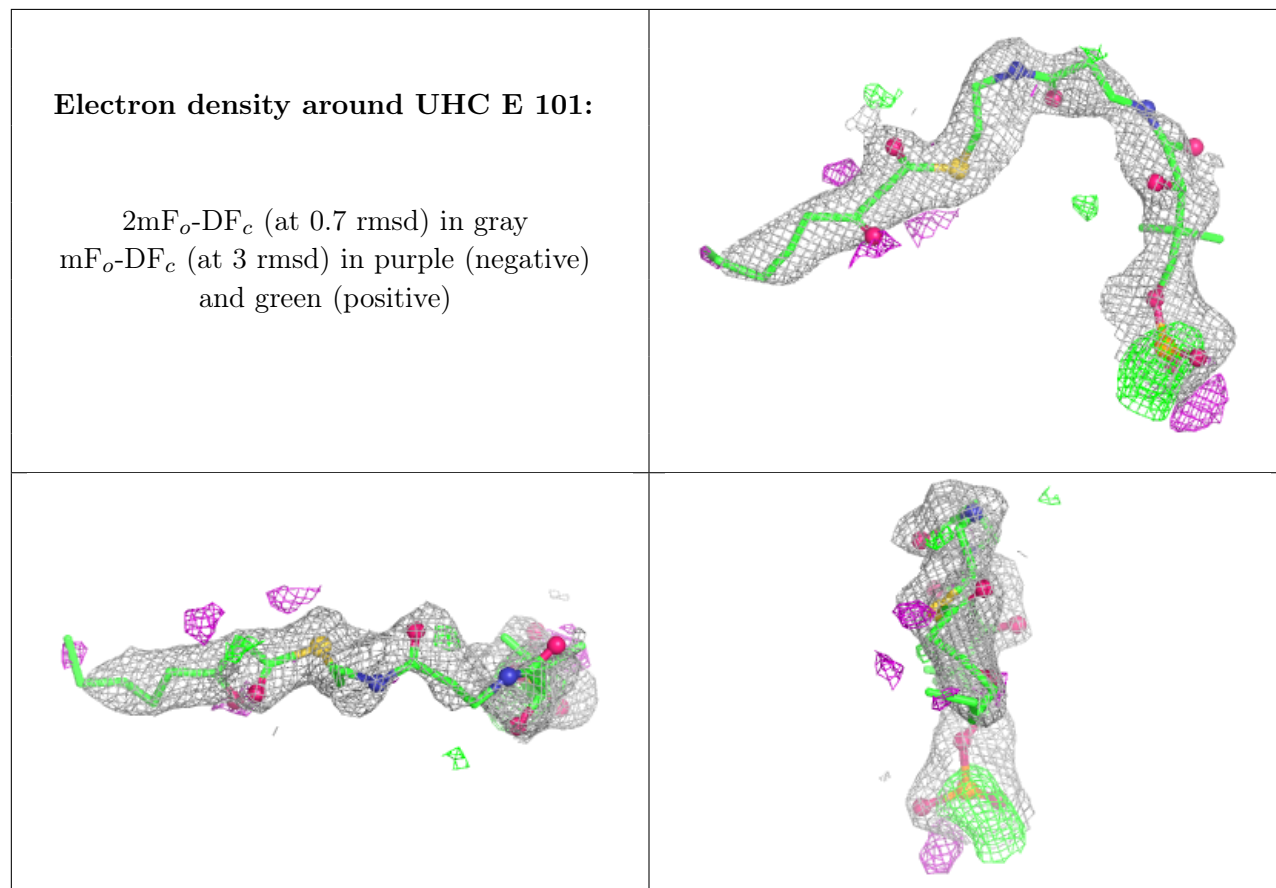
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	UHC	E	101	31/32	0.73	0.20	38,67,84,91	0
5	PN7	F	101	21/22	0.77	0.24	37,61,82,85	0
3	NAP	D	301	23/48	0.80	0.13	31,42,59,69	0
3	NAP	A	301	23/48	0.80	0.12	23,32,51,61	0
3	NAP	B	301	27/48	0.80	0.12	21,39,58,65	0

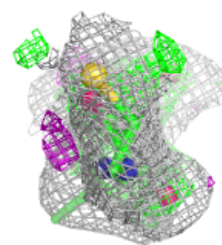
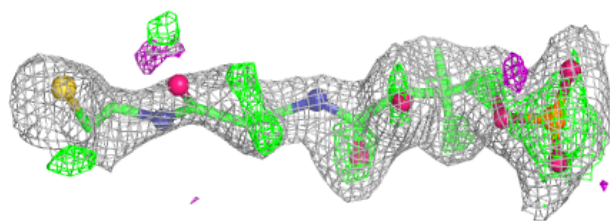
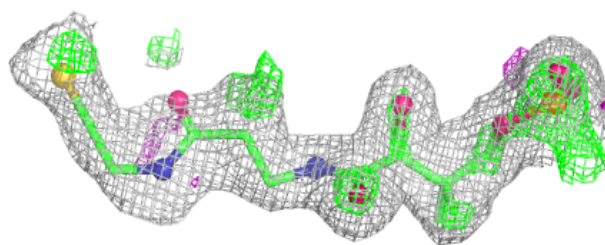
The following is a graphical depiction of the model fit to experimental electron density of all

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.



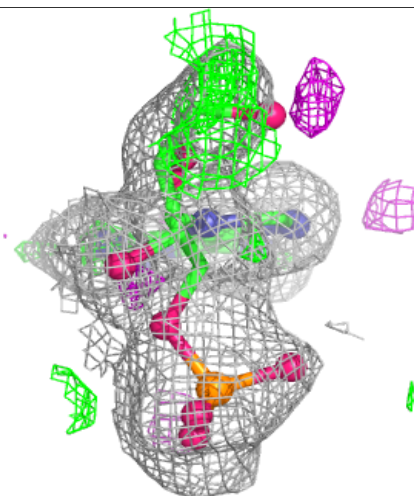
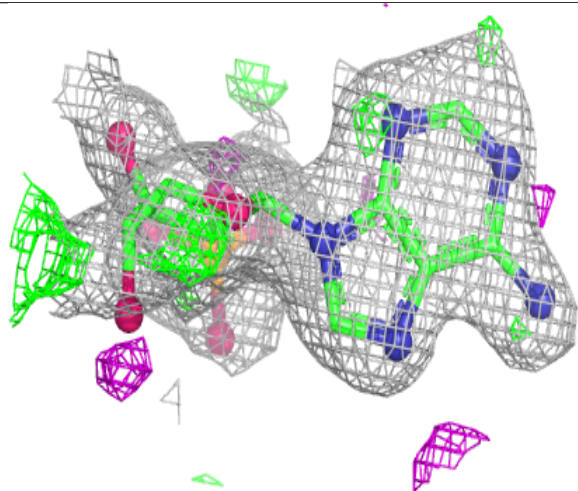
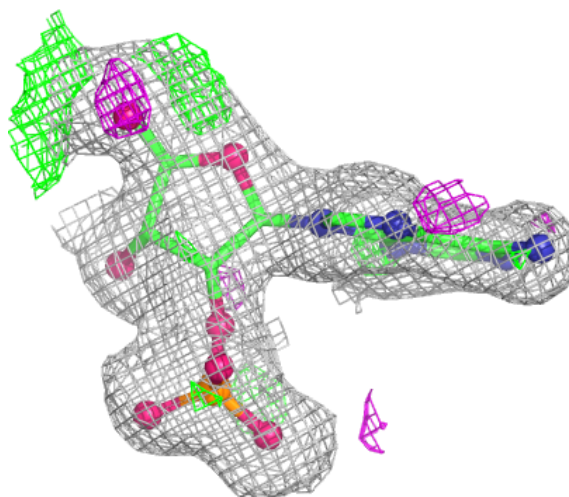
Electron density around PN7 F 101:

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



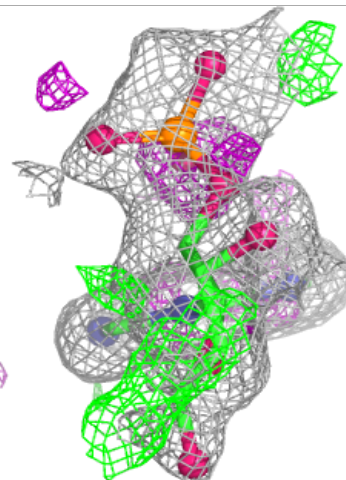
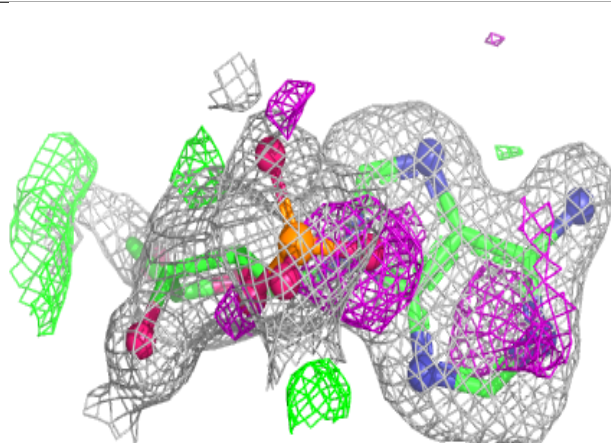
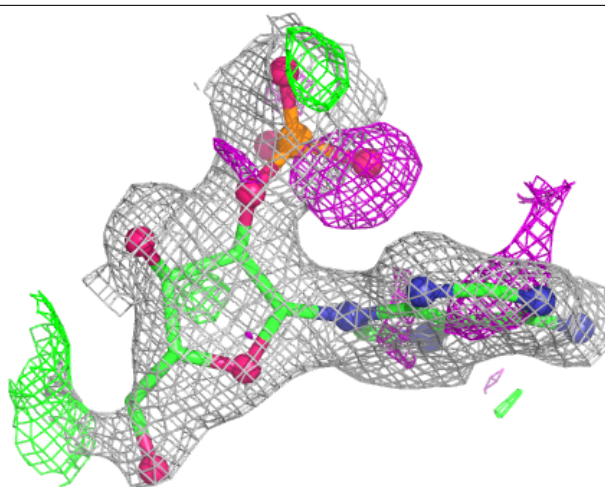
Electron density around NAP D 301:

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



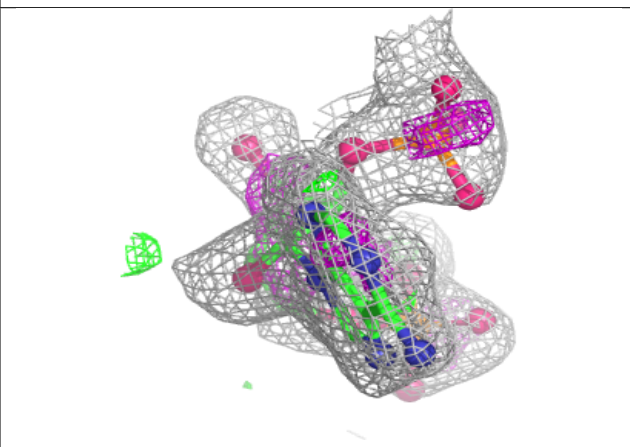
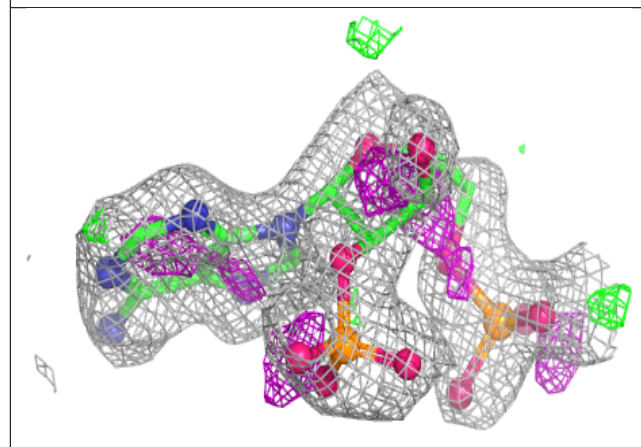
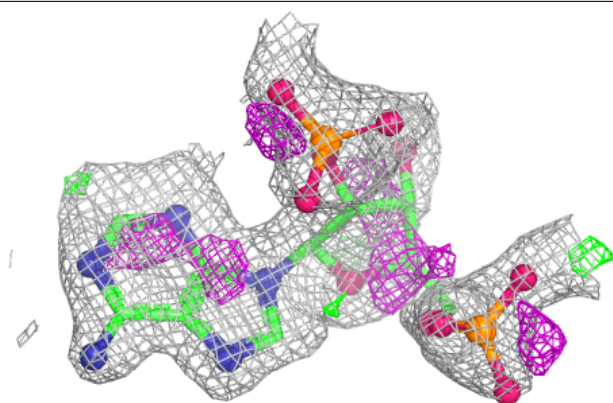
Electron density around NAP A 301:

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



Electron density around NAP B 301:

$2mF_o-DF_c$ (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.