



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 03:18 PM EST

PDB ID : 3PW7  
Title : Ternary complex of Aflatoxin B1 Adduct modified DNA (AFB1-N7-Gua) with DNA Polymerase IV and incoming dCTP  
Authors : Banerjee, S.  
Deposited on : 2010-12-07  
Resolution : 2.90 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

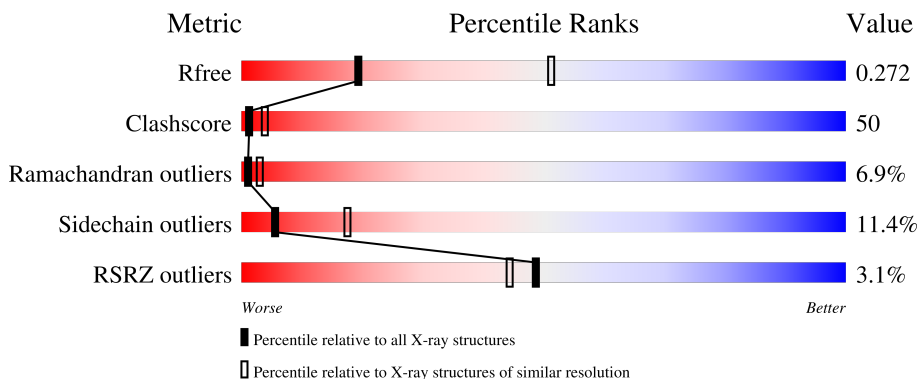
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



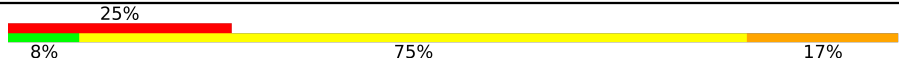
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	347	 2% 31% 56% 11%
1	E	347	 0% 33% 53% 12%
2	B	16	 25% 31% 56% 12%
2	F	16	 12% 6% 88% 6%
3	C	12	 25% 25% 75%

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Mol	Chain	Length	Quality of chain
3	G	12	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DCP	A	400	-	-	X	-
6	AFN	B	387	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 6857 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 DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2764	1772	478	507	7	0	0	0
1	E	343	2764	1772	478	507	7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	expression tag	UNP Q97W02
A	-1	HIS	-	expression tag	UNP Q97W02
A	0	HIS	-	expression tag	UNP Q97W02
A	1	HIS	-	expression tag	UNP Q97W02
A	2	HIS	-	expression tag	UNP Q97W02
A	3	HIS	-	expression tag	UNP Q97W02
E	-2	HIS	-	expression tag	UNP Q97W02
E	-1	HIS	-	expression tag	UNP Q97W02
E	0	HIS	-	expression tag	UNP Q97W02
E	1	HIS	-	expression tag	UNP Q97W02
E	2	HIS	-	expression tag	UNP Q97W02
E	3	HIS	-	expression tag	UNP Q97W02

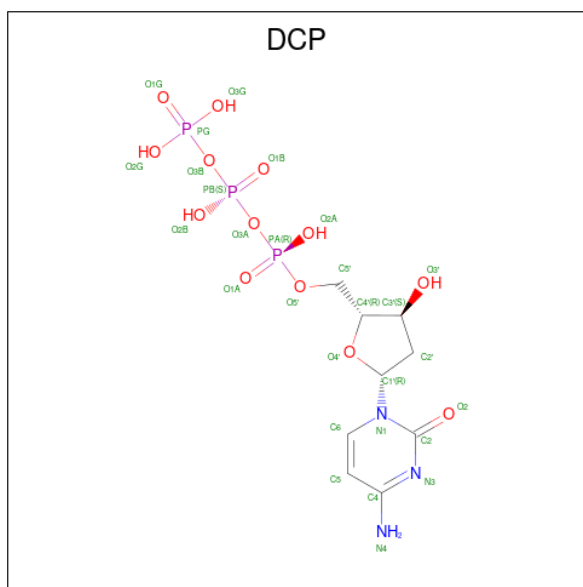
- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*TP\*TP\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	16	315	153	51	96	15	0	0	0
2	F	16	315	153	51	96	15	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	12	Total 254	C 120	N 54	O 69	P 11	0	0	0
3	G	12	Total 254	C 120	N 54	O 69	P 11	0	0	0

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula:  $C_9H_{16}N_3O_{13}P_3$ ).

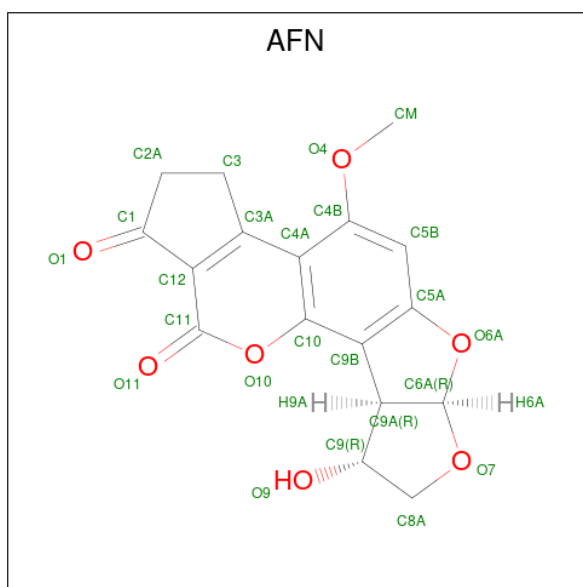


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
4	E	1	Total 28	C 9	N 3	O 13	P 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	Total 1	Ca 1	0	0
5	E	1	Total 1	Ca 1	0	0

- Molecule 6 is 8,9-DIHYDRO-9-HYDROXY-AFLATOXIN B1 (three-letter code: AFN) (formula:  $C_{17}H_{14}O_7$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	B	1	Total	C	O	0	0
			24	17	7		
6	F	1	Total	C	O	0	0
			24	17	7		

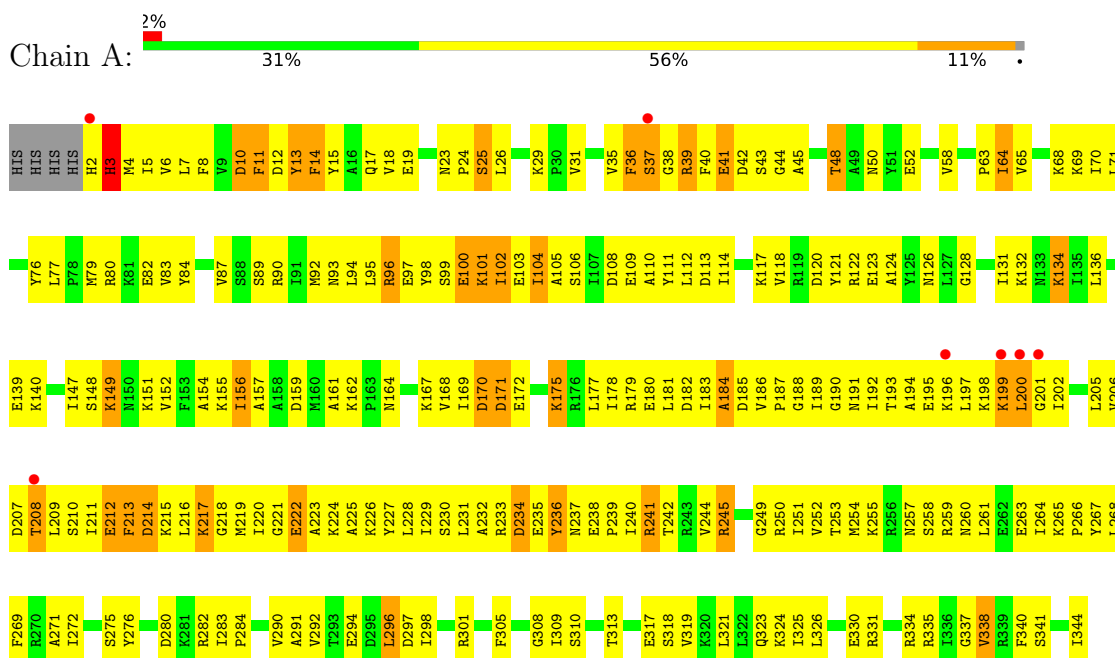
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	B	3	Total	O	0	0
			3	3		
7	C	3	Total	O	0	0
			3	3		
7	E	34	Total	O	0	0
			34	34		
7	F	3	Total	O	0	0
			3	3		
7	G	1	Total	O	0	0
			1	1		

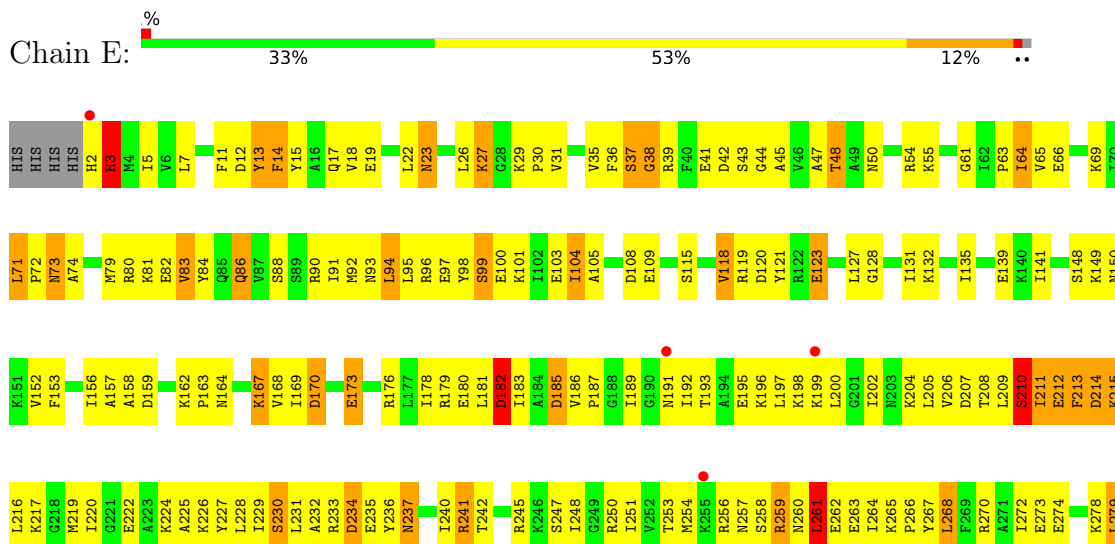
### 3 Residue-property plots i

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: DNA polymerase IV

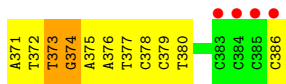


#### • Molecule 1: DNA polymerase IV

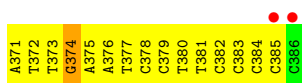




- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3')



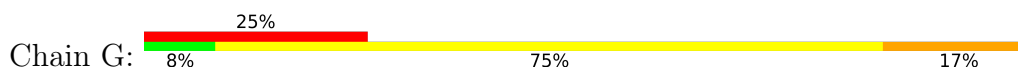
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3')



- Molecule 3: DNA (5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP\*T)-3')



- Molecule 3: DNA (5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP\*T)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.15Å 99.79Å 52.12Å 75.02° 70.95° 80.91°	Depositor
Resolution (Å)	29.52 – 2.90 29.52 – 2.88	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.52-2.90) 87.5 (29.52-2.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.90Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.284 0.225 , 0.272	Depositor DCC
$R_{free}$ test set	880 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtrriage
Anisotropy	0.180	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6857	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DCP, AFN, CA

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	0.44	0/2805	0.68	0/3766
1	E	0.42	0/2805	0.68	0/3766
2	B	1.15	3/350 (0.9%)	1.44	6/536 (1.1%)
2	F	1.16	3/350 (0.9%)	1.34	4/536 (0.7%)
3	C	0.72	0/287	0.90	0/444
3	G	0.75	0/287	0.95	2/444 (0.5%)
All	All	0.58	6/6884 (0.1%)	0.81	12/9492 (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
2	B	1	0
2	F	1	0
All	All	2	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	374	DG	C5-C6	9.68	1.52	1.42
2	F	374	DG	C8-N7	9.08	1.36	1.30
2	B	374	DG	C5-C6	8.12	1.50	1.42
2	B	374	DG	C8-N7	6.17	1.34	1.30
2	B	374	DG	C2-N3	5.85	1.37	1.32
2	F	374	DG	N1-C2	5.49	1.42	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	374	DG	O4'-C1'-N9	12.43	116.70	108.00
2	B	373	DT	OP1-P-O3'	-12.20	78.35	105.20
2	B	373	DT	OP2-P-O3'	-11.89	79.04	105.20
2	B	374	DG	OP1-P-OP2	10.91	135.96	119.60
2	B	374	DG	O4'-C1'-N9	7.71	113.40	108.00
2	F	374	DG	N9-C4-C5	7.28	108.31	105.40
2	F	374	DG	C2-N3-C4	6.90	115.35	111.90
2	B	373	DT	O3'-P-O5'	-6.48	91.69	104.00
2	B	374	DG	C2-N3-C4	6.04	114.92	111.90
3	G	350	DG	O4'-C4'-C3'	-5.96	102.11	104.50
3	G	357	DT	C4'-C3'-C2'	5.87	108.38	103.10
2	F	374	DG	C6-C5-N7	5.26	133.55	130.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	374	DG	C4'
2	F	374	DG	C4'

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2764	0	2900	300	0
1	E	2764	0	2900	257	0
2	B	315	0	183	42	0
2	F	315	0	183	56	0
3	C	254	0	136	18	0
3	G	254	0	136	28	0
4	A	28	0	11	13	0
4	E	28	0	11	5	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	B	24	0	13	10	0
6	F	24	0	13	2	0
7	A	41	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	3	0	0	3	0
7	C	3	0	0	3	0
7	E	34	0	0	5	0
7	F	3	0	0	4	0
7	G	1	0	0	0	0
All	All	6857	0	6486	657	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 50.

All (657) 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:E:335:ARG:NH1	2:F:373:DT:H2''	1.62	1.15
2:B:372:DT:H2''	2:B:373:DT:H5''	1.32	1.10
1:E:297:ASP:HB3	1:E:331:ARG:HH12	1.08	1.08
1:A:260:ASN:HD22	1:A:263:GLU:HB2	1.18	1.08
3:G:347:DG:H2''	3:G:348:DG:O5'	1.55	1.06
2:B:371:DA:H4'	2:B:372:DT:H5''	1.37	1.05
2:B:371:DA:H4'	2:B:372:DT:C5'	1.88	1.04
1:E:202:ILE:HG23	1:E:207:ASP:HB2	1.40	0.99
2:F:379:DC:H42	3:G:354:DG:H1	1.09	0.95
1:A:202:ILE:HD13	1:A:208:THR:HG22	1.48	0.93
1:A:39:ARG:HH12	1:A:334:ARG:HH21	1.06	0.92
1:E:335:ARG:HH11	2:F:373:DT:H2''	1.34	0.91
3:G:349:DG:H2''	3:G:350:DG:H5''	1.53	0.89
2:F:383:DC:H42	3:G:350:DG:H1	1.21	0.89
2:F:371:DA:H4'	2:F:372:DT:H5''	1.56	0.88
1:A:14:PHE:O	1:A:18:VAL:HG23	1.73	0.87
1:E:259:ARG:NH2	1:E:330:GLU:HA	1.89	0.86
1:E:297:ASP:HB3	1:E:331:ARG:NH1	1.89	0.86
1:A:39:ARG:HH12	1:A:334:ARG:NH2	1.74	0.86
2:F:373:DT:H4'	2:F:374:DG:OP1	1.74	0.85
4:A:400:DCP:H2'2	6:B:387:AFN:H2A2	1.58	0.85
1:A:260:ASN:HD22	1:A:263:GLU:CB	1.89	0.85
1:E:176:ARG:HG2	1:E:180:GLU:OE2	1.76	0.85
1:A:292:VAL:HB	1:A:335:ARG:HB3	1.59	0.85
2:B:371:DA:C4'	2:B:372:DT:H5''	2.06	0.84
1:E:42:ASP:HB3	1:E:64:ILE:HD11	1.59	0.84
1:E:118:VAL:HG22	1:E:123:GLU:HB2	1.60	0.84
1:E:293:THR:HG21	1:E:331:ARG:HD2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:379:DC:N4	3:G:354:DG:H1	1.75	0.83
1:A:190:GLY:HA3	3:C:357:DT:H5'	1.60	0.83
1:A:39:ARG:NH1	1:A:334:ARG:HH21	1.76	0.83
1:E:193:THR:HG21	1:E:224:LYS:NZ	1.93	0.83
1:A:121:TYR:HE2	1:A:170:ASP:HA	1.44	0.83
2:B:373:DT:H1'	7:B:501:HOH:O	1.77	0.82
2:F:371:DA:H4'	2:F:372:DT:C5'	2.09	0.82
1:A:37:SER:HB3	2:B:373:DT:O5'	1.78	0.82
1:A:178:ILE:HG23	1:A:232:ALA:HA	1.61	0.82
1:A:250:ARG:HG3	1:A:250:ARG:HH11	1.43	0.81
1:E:257:ASN:HD21	1:E:334:ARG:HD2	1.44	0.80
1:E:267:TYR:HD1	1:E:270:ARG:HH12	1.25	0.80
1:A:15:TYR:HB2	1:A:48:THR:HG21	1.64	0.80
1:E:335:ARG:CZ	2:F:373:DT:H2''	2.12	0.78
1:A:120:ASP:HB3	7:A:533:HOH:O	1.83	0.78
1:E:294:GLU:C	1:E:296:LEU:H	1.86	0.77
1:E:27:LYS:HB2	1:E:27:LYS:NZ	1.99	0.77
1:A:106:SER:HB2	7:A:528:HOH:O	1.85	0.77
1:A:202:ILE:HA	1:A:207:ASP:HB3	1.67	0.77
2:F:379:DC:H4'	7:F:500:HOH:O	1.85	0.76
1:E:31:VAL:HB	1:E:50:ASN:ND2	2.00	0.76
1:A:24:PRO:C	1:A:26:LEU:H	1.87	0.76
1:A:202:ILE:HA	1:A:207:ASP:CB	2.16	0.76
1:E:63:PRO:HB3	2:F:371:DA:H5'	1.68	0.76
1:E:157:ALA:HB1	1:E:167:LYS:HG2	1.69	0.75
2:B:371:DA:H4'	2:B:372:DT:H5'	1.66	0.75
1:E:237:ASN:C	1:E:237:ASN:HD22	1.91	0.74
2:B:372:DT:C2'	2:B:373:DT:H5''	2.14	0.74
1:A:79:MET:SD	6:B:387:AFN:HM2	2.27	0.74
1:A:260:ASN:ND2	1:A:263:GLU:HB2	1.99	0.73
1:A:272:ILE:HG13	1:A:338:VAL:HG11	1.71	0.73
4:A:400:DCP:H6	7:C:500:HOH:O	1.88	0.73
1:E:88:SER:O	1:E:92:MET:HB2	1.88	0.73
1:E:193:THR:HG21	1:E:224:LYS:HZ3	1.51	0.73
1:A:200:LEU:O	1:A:200:LEU:HD23	1.89	0.73
1:E:292:VAL:HG22	1:E:298:ILE:HG12	1.71	0.73
3:G:349:DG:C2'	3:G:350:DG:H5''	2.18	0.73
1:A:226:LYS:O	1:A:230:SER:HB3	1.88	0.72
2:F:376:DA:H2''	2:F:377:DT:H5''	1.72	0.72
2:F:373:DT:C4'	2:F:374:DG:OP1	2.38	0.72
1:A:202:ILE:HD11	1:A:208:THR:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:O	1:A:275:SER:HB2	1.90	0.72
1:A:280:ASP:CB	1:A:282:ARG:HH21	2.03	0.71
1:A:94:LEU:O	1:A:97:GLU:HG2	1.90	0.71
1:A:216:LEU:C	1:A:218:GLY:H	1.93	0.71
1:A:236:TYR:CE2	1:A:238:GLU:HB2	2.26	0.71
1:A:98:TYR:CE2	1:A:131:ILE:HG13	2.26	0.71
2:F:378:DC:H2''	2:F:379:DC:OP2	1.91	0.70
1:A:265:LYS:NZ	1:A:265:LYS:HB2	2.06	0.70
1:A:231:LEU:HD23	1:A:236:TYR:HB3	1.73	0.70
1:E:192:ILE:HG22	1:E:196:LYS:NZ	2.06	0.70
1:A:292:VAL:HB	1:A:335:ARG:CB	2.22	0.70
3:C:357:DT:H2'	3:C:358:DT:H71	1.74	0.69
1:E:156:ILE:HD11	1:E:187:PRO:HD3	1.74	0.69
1:A:310:SER:O	1:A:313:THR:HG22	1.91	0.69
1:E:253:THR:OG1	2:F:373:DT:H3'	1.93	0.69
1:E:192:ILE:O	1:E:196:LYS:HG3	1.93	0.69
1:E:293:THR:CG2	1:E:331:ARG:HD2	2.22	0.69
1:E:329:ASP:OD1	1:E:331:ARG:HG3	1.93	0.69
1:A:8:PHE:CD2	1:A:155:LYS:HA	2.27	0.69
1:A:253:THR:OG1	2:B:373:DT:H5'	1.92	0.69
1:A:241:ARG:HD3	7:A:516:HOH:O	1.92	0.68
1:E:291:ALA:HA	1:E:335:ARG:O	1.93	0.68
1:E:291:ALA:HB2	1:E:336:ILE:HD12	1.74	0.68
1:A:126:ASN:HB3	7:A:534:HOH:O	1.93	0.68
2:B:374:DG:H2'	2:B:375:DA:C8	2.29	0.68
1:E:301:ARG:NE	1:E:328:GLU:OE2	2.21	0.68
1:E:121:TYR:HB3	1:E:168:VAL:HG11	1.76	0.68
1:E:80:ARG:O	1:E:83:VAL:HG23	1.94	0.68
1:E:211:ILE:HD12	1:E:212:GLU:H	1.58	0.68
1:A:167:LYS:HG3	1:A:168:VAL:N	2.09	0.68
1:A:292:VAL:HA	7:A:520:HOH:O	1.93	0.68
1:E:36:PHE:O	1:E:37:SER:HB3	1.91	0.68
2:B:376:DA:H2	3:C:357:DT:H3	1.42	0.67
1:A:31:VAL:H	1:A:50:ASN:HD21	1.41	0.67
1:E:63:PRO:HG2	1:E:66:GLU:CG	2.23	0.67
1:E:335:ARG:NH1	2:F:373:DT:C2'	2.51	0.67
3:G:349:DG:H2''	3:G:350:DG:C5'	2.24	0.67
1:A:305:PHE:HZ	1:A:317:GLU:HG2	1.61	0.66
1:A:252:VAL:O	1:A:335:ARG:HG3	1.95	0.66
1:E:335:ARG:HD2	2:F:373:DT:H2'	1.77	0.66
1:A:45:ALA:HB3	6:B:387:AFN:H6A	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ILE:HG22	1:A:308:GLY:HA3	1.75	0.66
1:E:247:SER:O	1:E:339:ARG:NH2	2.29	0.66
1:A:268:LEU:HD21	1:A:318:SER:HB3	1.78	0.66
1:E:195:GLU:OE2	1:E:198:LYS:HD3	1.96	0.66
1:A:45:ALA:HB3	2:B:373:DT:O2	1.95	0.66
1:E:192:ILE:HG22	1:E:196:LYS:HZ2	1.60	0.66
1:A:11:PHE:N	1:A:11:PHE:CD1	2.62	0.66
1:E:65:VAL:O	1:E:69:LYS:HG3	1.96	0.66
1:A:15:TYR:HB2	1:A:48:THR:CG2	2.25	0.66
1:A:220:ILE:HD11	1:A:225:ALA:HA	1.78	0.66
4:A:400:DCP:C2'	6:B:387:AFN:H2A2	2.27	0.65
1:E:101:LYS:NZ	1:E:101:LYS:HB3	2.10	0.65
1:E:208:THR:O	1:E:229:ILE:HG12	1.96	0.65
1:E:176:ARG:HG2	1:E:176:ARG:HH11	1.61	0.65
1:A:79:MET:HG3	1:A:84:TYR:HE2	1.61	0.65
1:A:19:GLU:HA	1:A:19:GLU:OE2	1.96	0.65
1:A:31:VAL:H	1:A:50:ASN:ND2	1.94	0.65
1:E:183:ILE:HD13	1:E:197:LEU:HD13	1.79	0.65
1:E:224:LYS:O	1:E:227:TYR:HB3	1.97	0.65
1:E:272:ILE:HG12	1:E:338:VAL:HG11	1.78	0.65
1:A:178:ILE:CG2	1:A:232:ALA:HA	2.26	0.65
1:A:191:ASN:HA	1:A:194:ALA:HB3	1.78	0.64
1:A:236:TYR:HD2	1:A:237:ASN:N	1.96	0.64
1:A:245:ARG:HH12	2:B:376:DA:H4'	1.63	0.64
1:E:109:GLU:HG3	7:E:524:HOH:O	1.97	0.64
1:A:233:ARG:HG2	1:A:235:GLU:HB2	1.80	0.64
1:A:123:GLU:HA	1:A:126:ASN:OD1	1.97	0.63
1:A:161:ALA:HB2	1:A:167:LYS:HB2	1.79	0.63
1:E:233:ARG:O	1:E:235:GLU:HG3	1.98	0.63
1:A:38:GLY:O	1:A:255:LYS:HE3	1.99	0.63
1:A:118:VAL:HG11	1:A:124:ALA:HB2	1.79	0.63
1:E:225:ALA:C	1:E:227:TYR:H	2.01	0.63
1:E:251:ILE:HD11	1:E:290:VAL:HG21	1.79	0.63
1:A:207:ASP:C	1:A:209:LEU:H	2.01	0.63
1:E:335:ARG:HD2	2:F:373:DT:C2'	2.28	0.63
2:F:376:DA:H2	3:G:357:DT:H3	1.46	0.63
1:A:19:GLU:HG3	1:A:77:LEU:HD12	1.81	0.62
1:A:250:ARG:HG3	1:A:250:ARG:NH1	2.13	0.62
1:A:280:ASP:HB2	1:A:282:ARG:HH21	1.62	0.62
1:A:236:TYR:HD2	1:A:236:TYR:C	2.03	0.62
1:A:240:ILE:O	1:A:240:ILE:HG22	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:MET:HG3	1:E:84:TYR:HE2	1.64	0.62
1:A:98:TYR:OH	1:A:134:LYS:HD2	1.99	0.62
1:E:178:ILE:HG23	1:E:232:ALA:HA	1.81	0.62
1:E:211:ILE:HD12	1:E:212:GLU:N	2.14	0.62
1:E:259:ARG:HA	1:E:264:ILE:HD11	1.82	0.62
1:A:23:ASN:OD1	1:A:25:SER:HB3	2.00	0.61
1:A:196:LYS:HD3	1:A:219:MET:HG3	1.82	0.61
1:A:259:ARG:HH21	1:A:330:GLU:C	2.04	0.61
1:A:310:SER:OG	1:A:313:THR:HG22	2.01	0.61
3:G:350:DG:H2''	3:G:351:DG:O5'	1.99	0.61
1:E:64:ILE:C	1:E:64:ILE:HD12	2.20	0.61
1:A:309:ILE:HG23	1:A:313:THR:HG23	1.83	0.61
1:E:293:THR:CB	1:E:331:ARG:HD2	2.30	0.61
1:E:294:GLU:O	1:E:296:LEU:N	2.34	0.61
1:A:220:ILE:HD11	1:A:225:ALA:CA	2.30	0.61
1:E:219:MET:HA	1:E:219:MET:CE	2.30	0.61
1:E:305:PHE:HZ	1:E:317:GLU:HG2	1.65	0.61
2:F:371:DA:H4'	2:F:372:DT:O5'	1.99	0.61
4:A:400:DCP:H6	3:C:358:DT:H2''	1.82	0.61
1:E:240:ILE:HG22	1:E:240:ILE:O	1.99	0.61
3:C:349:DG:H2''	3:C:350:DG:O5'	2.01	0.61
1:E:245:ARG:NH2	1:E:248:ILE:HG12	2.16	0.60
1:A:101:LYS:HB3	1:A:113:ASP:HB3	1.83	0.60
1:A:268:LEU:HD21	1:A:318:SER:CB	2.32	0.60
1:E:27:LYS:HB2	1:E:27:LYS:HZ2	1.66	0.60
1:A:108:ASP:OD2	4:A:400:DCP:O3'	2.20	0.60
2:B:376:DA:H2''	2:B:377:DT:H5'	1.83	0.60
1:E:103:GLU:O	1:E:104:ILE:HB	2.02	0.60
1:E:294:GLU:C	1:E:296:LEU:N	2.55	0.60
1:A:102:ILE:HG12	1:A:112:LEU:HG	1.82	0.60
4:A:400:DCP:C6	3:C:358:DT:H2''	2.32	0.60
1:A:191:ASN:O	1:A:195:GLU:HG2	2.00	0.60
2:B:378:DC:H2''	2:B:379:DC:OP2	2.02	0.60
1:E:260:ASN:HB3	1:E:263:GLU:HB3	1.81	0.60
3:G:356:DA:C8	3:G:357:DT:H72	2.36	0.60
1:A:231:LEU:HD23	1:A:236:TYR:CB	2.32	0.60
4:A:400:DCP:H5'2	7:C:500:HOH:O	2.02	0.60
1:E:19:GLU:O	1:E:26:LEU:HD12	2.01	0.60
1:A:151:LYS:HD3	1:A:240:ILE:HG13	1.84	0.59
1:E:120:ASP:HB3	1:E:123:GLU:OE2	2.02	0.59
1:A:236:TYR:C	1:A:236:TYR:CD2	2.74	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:LYS:O	1:E:280:ASP:N	2.35	0.59
1:E:317:GLU:OE2	1:E:320:LYS:HD2	2.02	0.59
2:B:376:DA:H2''	2:B:377:DT:C5'	2.32	0.59
1:A:233:ARG:HG2	1:A:233:ARG:O	2.03	0.59
1:E:43:SER:O	2:F:373:DT:OP1	2.20	0.59
1:A:280:ASP:HB3	1:A:282:ARG:HH21	1.68	0.59
1:A:211:ILE:HD12	1:A:212:GLU:H	1.67	0.59
1:A:231:LEU:O	1:A:234:ASP:N	2.35	0.59
2:B:371:DA:O4'	2:B:372:DT:H72	2.02	0.59
1:A:13:TYR:CE1	1:A:17:GLN:HB2	2.38	0.59
1:A:201:GLY:O	1:A:207:ASP:HB3	2.03	0.59
1:A:283:ILE:HB	1:A:344:ILE:HD12	1.84	0.58
2:B:379:DC:H42	3:C:354:DG:H1	1.49	0.58
1:E:291:ALA:HB1	1:E:333:ILE:HD12	1.84	0.58
1:E:297:ASP:CB	1:E:331:ARG:HH12	2.00	0.58
1:A:4:MET:HG3	1:A:149:LYS:O	2.03	0.58
1:A:245:ARG:NH1	2:B:376:DA:H4'	2.19	0.58
1:E:268:LEU:HD12	1:E:268:LEU:O	2.04	0.58
4:E:400:DCP:H6	4:E:400:DCP:H5'2	1.86	0.58
1:A:233:ARG:O	1:A:234:ASP:C	2.42	0.58
1:E:44:GLY:HA2	2:F:372:DT:O3'	2.03	0.58
1:A:272:ILE:HD11	1:A:318:SER:OG	2.04	0.58
1:E:251:ILE:CD1	1:E:290:VAL:HG21	2.33	0.58
1:A:272:ILE:CG1	1:A:338:VAL:HG11	2.33	0.58
1:A:100:GLU:CD	1:A:100:GLU:H	2.08	0.58
1:E:35:VAL:O	1:E:35:VAL:HG13	2.03	0.57
1:A:68:LYS:HD3	1:A:76:TYR:CZ	2.39	0.57
1:E:82:GLU:O	1:E:86:GLN:HG2	2.03	0.57
1:E:245:ARG:NH2	2:F:376:DA:OP1	2.37	0.57
1:A:179:ARG:HA	1:A:206:VAL:HB	1.86	0.57
1:A:224:LYS:O	1:A:227:TYR:HB3	2.04	0.57
1:A:233:ARG:O	1:A:233:ARG:CG	2.51	0.57
1:A:103:GLU:O	1:A:104:ILE:CB	2.53	0.57
1:A:103:GLU:O	1:A:104:ILE:HB	2.04	0.57
1:E:322:LEU:HD12	1:E:322:LEU:O	2.04	0.57
1:A:298:ILE:HD13	7:A:520:HOH:O	2.03	0.57
2:B:376:DA:N1	3:C:357:DT:O4	2.37	0.57
1:E:169:ILE:HG23	1:E:173:GLU:HB3	1.86	0.57
1:E:214:ASP:O	1:E:215:LYS:HB2	2.05	0.57
3:G:349:DG:C1'	3:G:350:DG:H5''	2.34	0.57
1:A:36:PHE:CD1	1:A:36:PHE:N	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HD2	1:A:199:LYS:O	2.05	0.57
1:A:265:LYS:HG2	1:A:269:PHE:CE2	2.40	0.56
1:E:14:PHE:O	1:E:15:TYR:C	2.43	0.56
1:A:12:ASP:O	1:A:14:PHE:N	2.39	0.56
2:B:372:DT:H1'	2:B:373:DT:C6	2.40	0.56
1:E:205:LEU:HG	1:E:232:ALA:HB2	1.87	0.56
1:E:233:ARG:NH1	1:E:235:GLU:OE1	2.38	0.56
1:A:292:VAL:CB	1:A:335:ARG:HB3	2.32	0.56
1:E:231:LEU:HD23	1:E:236:TYR:HB3	1.87	0.56
1:A:171:ASP:O	1:A:175:LYS:HD3	2.06	0.56
1:A:79:MET:SD	6:B:387:AFN:CM	2.94	0.55
1:E:90:ARG:HA	1:E:93:ASN:HD22	1.70	0.55
1:A:102:ILE:HD13	1:A:111:TYR:O	2.06	0.55
1:A:213:PHE:HD2	1:A:213:PHE:N	2.04	0.55
1:A:236:TYR:CD2	1:A:237:ASN:N	2.73	0.55
1:E:109:GLU:CG	7:E:524:HOH:O	2.53	0.55
1:A:167:LYS:HG3	1:A:168:VAL:H	1.72	0.55
1:E:273:GLU:OE2	1:E:273:GLU:HA	2.05	0.55
1:A:271:ALA:O	1:A:275:SER:CB	2.53	0.55
1:E:196:LYS:HD3	1:E:219:MET:CE	2.36	0.55
1:A:40:PHE:O	1:A:41:GLU:CB	2.54	0.55
1:A:152:VAL:HG13	1:A:187:PRO:HG2	1.89	0.55
1:A:152:VAL:HG11	1:A:231:LEU:HD11	1.87	0.55
1:A:213:PHE:O	1:A:217:LYS:N	2.30	0.55
2:B:375:DA:H2''	2:B:376:DA:C5'	2.37	0.55
1:E:18:VAL:O	1:E:22:LEU:HG	2.07	0.55
6:B:387:AFN:H8A2	7:B:500:HOH:O	2.06	0.55
1:A:24:PRO:C	1:A:26:LEU:N	2.56	0.55
1:A:98:TYR:CD2	1:A:131:ILE:HG13	2.41	0.55
1:E:219:MET:HA	1:E:219:MET:HE2	1.88	0.55
1:E:265:LYS:N	1:E:266:PRO:HD2	2.22	0.55
1:A:2:HIS:O	1:A:3:HIS:HB3	2.06	0.54
1:A:261:LEU:HD22	1:A:323:GLN:HG2	1.88	0.54
1:E:335:ARG:HH11	2:F:373:DT:C2'	2.13	0.54
1:A:265:LYS:HB2	1:A:265:LYS:HZ3	1.70	0.54
1:A:90:ARG:NH1	1:A:139:GLU:OE2	2.41	0.54
3:G:347:DG:C2'	3:G:348:DG:O5'	2.39	0.54
1:A:255:LYS:HG2	7:A:517:HOH:O	2.05	0.54
1:A:283:ILE:CG2	1:A:308:GLY:HA3	2.37	0.54
1:E:90:ARG:O	1:E:94:LEU:HG	2.08	0.54
3:G:349:DG:H1'	3:G:350:DG:H5''	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:VAL:CG2	1:E:123:GLU:HB2	2.36	0.54
1:E:258:SER:OG	1:E:259:ARG:N	2.41	0.54
1:E:265:LYS:HE2	1:E:319:VAL:HG21	1.90	0.54
1:E:209:LEU:HD21	1:E:233:ARG:HB3	1.89	0.54
1:E:236:TYR:C	1:E:236:TYR:CD2	2.81	0.54
1:A:36:PHE:HB3	1:A:43:SER:O	2.08	0.54
1:A:206:VAL:O	1:A:209:LEU:HB2	2.09	0.53
1:E:98:TYR:O	1:E:99:SER:HB2	2.06	0.53
1:A:199:LYS:O	1:A:200:LEU:HB2	2.08	0.53
1:E:11:PHE:CD1	1:E:11:PHE:N	2.75	0.53
2:B:377:DT:H5'	2:B:377:DT:H6	1.74	0.53
1:E:90:ARG:HD2	1:E:139:GLU:OE2	2.08	0.53
2:F:376:DA:C2'	2:F:377:DT:H5''	2.36	0.53
1:A:48:THR:HG21	7:A:505:HOH:O	2.08	0.53
1:A:64:ILE:HD12	1:A:64:ILE:O	2.09	0.53
1:A:103:GLU:O	1:A:104:ILE:HG13	2.09	0.53
1:E:296:LEU:C	1:E:296:LEU:HD13	2.29	0.53
1:A:196:LYS:HD3	1:A:219:MET:O	2.07	0.53
1:A:254:MET:HA	1:A:267:TYR:CZ	2.44	0.53
1:E:237:ASN:C	1:E:237:ASN:ND2	2.58	0.53
1:A:190:GLY:CA	3:C:357:DT:H5'	2.35	0.53
1:E:191:ASN:OD1	1:E:192:ILE:HG13	2.09	0.53
1:A:183:ILE:C	1:A:185:ASP:H	2.11	0.53
1:A:183:ILE:O	1:A:186:VAL:HG23	2.08	0.53
1:A:213:PHE:C	1:A:215:LYS:H	2.13	0.53
1:E:120:ASP:OD1	1:E:121:TYR:N	2.42	0.53
1:E:170:ASP:O	1:E:173:GLU:N	2.41	0.53
1:E:193:THR:HG21	1:E:224:LYS:HZ1	1.73	0.53
1:A:108:ASP:OD1	4:A:400:DCP:O1B	2.27	0.52
1:E:291:ALA:HB1	1:E:333:ILE:HG23	1.91	0.52
2:B:373:DT:H2''	2:B:374:DG:H5''	1.91	0.52
1:E:296:LEU:HD23	2:F:372:DT:O4	2.09	0.52
1:A:217:LYS:O	1:A:217:LYS:HG2	2.08	0.52
1:E:103:GLU:O	1:E:104:ILE:CB	2.57	0.52
1:E:341:SER:O	1:E:342:LYS:HB2	2.08	0.52
2:F:374:DG:H2''	2:F:375:DA:C8	2.44	0.52
3:G:357:DT:C2'	3:G:358:DT:O5'	2.57	0.52
1:A:213:PHE:N	1:A:213:PHE:CD2	2.75	0.52
1:E:30:PRO:HG2	1:E:74:ALA:HA	1.91	0.52
1:A:260:ASN:ND2	1:A:263:GLU:N	2.57	0.52
3:G:357:DT:H2''	3:G:358:DT:O5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PHE:O	1:A:41:GLU:HB2	2.10	0.52
1:E:43:SER:C	2:F:373:DT:OP1	2.48	0.52
1:A:103:GLU:OE2	7:A:516:HOH:O	2.19	0.52
4:E:400:DCP:C5	3:G:358:DT:H1'	2.40	0.52
1:A:45:ALA:CB	6:B:387:AFN:H6A	2.40	0.52
1:A:52:GLU:N	1:A:52:GLU:OE1	2.43	0.52
3:C:349:DG:H1'	3:C:350:DG:H5'	1.91	0.51
3:C:357:DT:H2''	3:C:358:DT:O5'	2.10	0.51
1:A:123:GLU:HA	1:A:126:ASN:CG	2.31	0.51
1:A:151:LYS:CG	1:A:240:ILE:HD11	2.41	0.51
1:A:211:ILE:HD11	1:A:215:LYS:CB	2.41	0.51
1:A:7:LEU:HB2	1:A:114:ILE:HD13	1.92	0.51
1:A:291:ALA:HA	1:A:335:ARG:O	2.11	0.51
1:E:183:ILE:CD1	1:E:197:LEU:HD13	2.40	0.51
1:E:321:LEU:O	1:E:325:ILE:HG13	2.10	0.51
1:A:39:ARG:HG3	1:A:40:PHE:CD1	2.45	0.51
7:F:501:HOH:O	3:G:348:DG:N1	2.43	0.51
1:A:44:GLY:HA2	2:B:372:DT:H4'	1.92	0.51
1:A:195:GLU:O	1:A:199:LYS:HE2	2.09	0.51
1:A:253:THR:CB	2:B:373:DT:H5'	2.41	0.51
1:E:41:GLU:HA	1:E:41:GLU:OE1	2.10	0.51
1:E:54:ARG:O	1:E:55:LYS:C	2.49	0.51
1:E:241:ARG:HB2	1:E:241:ARG:NH1	2.25	0.51
1:E:260:ASN:HD22	1:E:263:GLU:CB	2.24	0.51
1:A:236:TYR:HE2	1:A:238:GLU:HB2	1.75	0.50
1:E:148:SER:OG	1:E:149:LYS:N	2.44	0.50
1:E:293:THR:HA	1:E:332:LYS:O	2.11	0.50
1:A:251:ILE:HG12	1:A:337:GLY:HA3	1.92	0.50
1:A:258:SER:HB2	1:A:263:GLU:OE1	2.11	0.50
1:E:256:ARG:HG2	1:E:257:ASN:O	2.11	0.50
1:A:102:ILE:CD1	1:A:110:ALA:HB1	2.42	0.50
1:A:136:LEU:HD12	1:A:136:LEU:O	2.10	0.50
1:A:124:ALA:HB1	1:A:147:ILE:HD13	1.92	0.50
1:A:297:ASP:HB3	1:A:331:ARG:HH12	1.77	0.50
1:E:42:ASP:O	1:E:65:VAL:HG13	2.11	0.50
1:E:189:ILE:HG23	1:E:193:THR:HG22	1.94	0.50
1:E:260:ASN:O	1:E:262:GLU:N	2.45	0.50
1:A:12:ASP:C	1:A:14:PHE:N	2.65	0.50
1:A:149:LYS:CB	1:A:149:LYS:NZ	2.75	0.50
1:A:90:ARG:O	1:A:94:LEU:HG	2.12	0.50
1:A:216:LEU:C	1:A:218:GLY:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:ALA:O	1:E:318:SER:HB3	2.12	0.50
1:A:35:VAL:HG21	7:B:501:HOH:O	2.11	0.49
1:A:39:ARG:HH12	1:A:334:ARG:CZ	2.24	0.49
2:B:375:DA:H2''	2:B:376:DA:H5'	1.93	0.49
1:E:95:LEU:HD21	1:E:135:ILE:HD11	1.93	0.49
1:E:296:LEU:O	1:E:297:ASP:C	2.50	0.49
1:A:82:GLU:H	1:A:82:GLU:CD	2.15	0.49
1:E:196:LYS:HD3	1:E:219:MET:HE2	1.93	0.49
1:A:131:ILE:HG22	1:A:132:LYS:N	2.26	0.49
1:A:284:PRO:O	1:A:309:ILE:HG13	2.13	0.49
1:E:282:ARG:C	1:E:283:ILE:HD13	2.33	0.49
1:E:310:SER:H	1:E:313:THR:HG23	1.77	0.49
1:A:232:ALA:C	1:A:234:ASP:H	2.15	0.49
1:E:259:ARG:HB2	1:E:326:LEU:CD2	2.42	0.49
1:A:207:ASP:C	1:A:209:LEU:N	2.66	0.49
1:E:63:PRO:HG2	1:E:66:GLU:HG2	1.94	0.49
1:A:18:VAL:CG1	1:A:87:VAL:HG21	2.42	0.49
1:A:292:VAL:HG13	7:A:520:HOH:O	2.12	0.49
1:E:231:LEU:HD23	1:E:236:TYR:CB	2.42	0.49
1:E:108:ASP:OD2	4:E:400:DCP:O1G	2.31	0.49
1:A:117:LYS:N	1:A:117:LYS:HD2	2.28	0.49
1:E:272:ILE:CG1	1:E:338:VAL:HG11	2.42	0.49
2:B:373:DT:N3	6:B:387:AFN:O7	2.46	0.48
1:E:80:ARG:HB3	1:E:83:VAL:CG2	2.43	0.48
1:E:225:ALA:C	1:E:227:TYR:N	2.66	0.48
1:E:250:ARG:HG3	1:E:251:ILE:N	2.28	0.48
1:A:6:VAL:HG11	1:A:151:LYS:HA	1.96	0.48
1:A:123:GLU:O	1:A:126:ASN:HB2	2.13	0.48
1:A:284:PRO:HG3	1:A:340:PHE:CD1	2.48	0.48
3:C:347:DG:H2''	3:C:348:DG:O5'	2.13	0.48
1:A:44:GLY:HA2	2:B:372:DT:O3'	2.12	0.48
1:A:93:ASN:O	1:A:96:ARG:HB2	2.13	0.48
1:A:233:ARG:O	1:A:235:GLU:N	2.46	0.48
3:C:358:DT:H2''	7:C:500:HOH:O	2.13	0.48
1:E:291:ALA:CB	1:E:333:ILE:HD12	2.43	0.48
1:E:260:ASN:O	1:E:260:ASN:ND2	2.46	0.48
1:E:303:ARG:NH1	1:E:317:GLU:OE2	2.46	0.48
2:F:374:DG:O6	6:F:387:AFN:H9	2.13	0.48
2:F:377:DT:H2''	2:F:378:DC:H5'	1.95	0.48
3:G:351:DG:H1'	3:G:352:DA:H5''	1.95	0.48
1:A:24:PRO:O	1:A:26:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:DA:H2	3:C:358:DT:H3	1.61	0.48
1:E:226:LYS:O	1:E:226:LYS:HG2	2.14	0.48
2:F:375:DA:OP1	7:F:502:HOH:O	2.19	0.48
1:A:102:ILE:HD11	1:A:110:ALA:HB1	1.96	0.48
1:A:170:ASP:O	1:A:172:GLU:N	2.46	0.48
1:A:197:LEU:O	1:A:202:ILE:HB	2.14	0.48
1:E:210:SER:OG	1:E:211:ILE:N	2.46	0.48
1:E:248:ILE:HD12	1:E:279:LEU:HD23	1.95	0.48
1:E:251:ILE:HA	1:E:337:GLY:HA3	1.96	0.48
1:A:102:ILE:HG23	1:A:103:GLU:N	2.29	0.48
1:A:182:ASP:OD2	1:A:183:ILE:N	2.45	0.48
1:A:183:ILE:HG23	1:A:184:ALA:N	2.28	0.48
1:E:39:ARG:HH22	1:E:334:ARG:HE	1.60	0.48
1:E:61:GLY:HA2	6:F:387:AFN:H9A	1.96	0.48
1:E:80:ARG:HB3	1:E:83:VAL:HG23	1.94	0.48
1:E:231:LEU:O	1:E:234:ASP:N	2.47	0.48
1:E:250:ARG:HD2	2:F:375:DA:OP1	2.14	0.48
1:A:8:PHE:CE2	1:A:155:LYS:HG3	2.49	0.48
1:A:31:VAL:HB	1:A:50:ASN:ND2	2.28	0.48
2:B:377:DT:H2''	2:B:378:DC:C6	2.48	0.48
1:E:179:ARG:HG3	1:E:180:GLU:N	2.29	0.48
1:A:122:ARG:O	1:A:126:ASN:ND2	2.47	0.47
1:E:305:PHE:CZ	1:E:317:GLU:HG2	2.47	0.47
1:E:35:VAL:HG12	1:E:45:ALA:O	2.14	0.47
1:E:253:THR:HB	2:F:373:DT:H5'	1.95	0.47
2:F:377:DT:H6	2:F:377:DT:H5'	1.79	0.47
1:A:259:ARG:NH2	1:A:330:GLU:C	2.66	0.47
1:E:183:ILE:C	1:E:185:ASP:H	2.16	0.47
1:E:196:LYS:HD2	1:E:219:MET:O	2.15	0.47
4:E:400:DCP:H5	3:G:358:DT:H2''	1.96	0.47
1:A:208:THR:O	1:A:229:ILE:HG12	2.14	0.47
1:A:284:PRO:CB	1:A:340:PHE:HB3	2.44	0.47
1:A:292:VAL:HG22	1:A:298:ILE:HD12	1.97	0.47
4:A:400:DCP:H3'	7:A:502:HOH:O	2.15	0.47
1:E:157:ALA:HA	1:E:167:LYS:HD3	1.95	0.47
1:A:4:MET:O	1:A:149:LYS:HA	2.14	0.47
1:A:101:LYS:CB	1:A:113:ASP:HB3	2.44	0.47
1:A:111:TYR:OH	1:A:155:LYS:HD2	2.14	0.47
1:A:148:SER:OG	1:A:149:LYS:N	2.48	0.47
2:B:386:DC:O2	2:B:386:DC:O4'	2.31	0.47
1:E:176:ARG:NH1	1:E:180:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:381:DT:H2''	2:F:382:DC:O5'	2.15	0.47
1:E:22:LEU:O	1:E:23:ASN:HB2	2.14	0.47
1:E:217:LYS:HE3	1:E:222:GLU:HG3	1.97	0.47
1:A:238:GLU:OE2	1:A:239:PRO:HD2	2.14	0.47
1:A:10:ASP:OD2	4:A:400:DCP:O2A	2.33	0.47
1:A:58:VAL:HG12	1:A:58:VAL:O	2.14	0.47
1:E:29:LYS:HG3	1:E:30:PRO:HD2	1.96	0.47
1:E:260:ASN:HD22	1:E:263:GLU:HB2	1.79	0.47
1:E:301:ARG:HD2	1:E:324:LYS:HD3	1.96	0.47
1:A:191:ASN:OD1	1:A:192:ILE:N	2.48	0.46
1:A:305:PHE:N	1:A:305:PHE:CD1	2.83	0.46
1:A:310:SER:O	1:A:313:THR:CG2	2.60	0.46
2:B:371:DA:C4'	2:B:372:DT:C5'	2.74	0.46
1:E:63:PRO:HB3	2:F:371:DA:H3'	1.96	0.46
1:A:44:GLY:CA	2:B:372:DT:H4'	2.45	0.46
1:A:335:ARG:NH2	2:B:373:DT:H72	2.29	0.46
1:E:162:LYS:HA	1:E:163:PRO:HA	1.73	0.46
2:F:377:DT:H6	2:F:377:DT:C5'	2.28	0.46
1:A:250:ARG:NH1	1:A:250:ARG:CG	2.78	0.46
2:B:377:DT:H2'	2:B:378:DC:C5	2.50	0.46
1:E:120:ASP:CB	1:E:123:GLU:OE2	2.63	0.46
1:E:189:ILE:HD11	1:E:228:LEU:HD21	1.96	0.46
1:A:211:ILE:HD12	1:A:212:GLU:N	2.30	0.46
1:A:284:PRO:HB3	1:A:340:PHE:HB3	1.98	0.46
2:F:383:DC:N4	3:G:350:DG:H1	2.01	0.46
2:B:371:DA:O5'	2:B:372:DT:H5''	2.16	0.46
1:E:7:LEU:HD11	1:E:128:GLY:HA2	1.97	0.46
1:E:179:ARG:HA	1:E:206:VAL:HB	1.96	0.46
1:E:296:LEU:HD13	1:E:296:LEU:O	2.15	0.46
1:A:18:VAL:HG11	1:A:87:VAL:HG21	1.97	0.46
1:A:39:ARG:NH1	1:A:334:ARG:HE	2.14	0.46
1:A:152:VAL:HG13	1:A:187:PRO:CG	2.46	0.46
1:E:279:LEU:HD13	1:E:284:PRO:HD3	1.97	0.46
1:A:250:ARG:CG	1:A:251:ILE:N	2.79	0.46
1:A:261:LEU:HD12	1:A:261:LEU:O	2.16	0.46
1:E:193:THR:HG22	1:E:193:THR:O	2.15	0.46
1:A:213:PHE:O	1:A:215:LYS:N	2.48	0.46
1:E:63:PRO:CB	2:F:371:DA:H5'	2.44	0.46
1:E:310:SER:OG	1:E:313:THR:CG2	2.63	0.46
1:A:179:ARG:HG3	1:A:180:GLU:HG3	1.98	0.46
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ASN:HD21	1:E:153:PHE:HD1	1.64	0.46
1:E:158:ALA:O	1:E:162:LYS:HG3	2.16	0.45
2:F:377:DT:H2''	2:F:378:DC:O4'	2.16	0.45
4:A:400:DCP:H2'1	6:B:387:AFN:O1	2.16	0.45
1:E:39:ARG:NH2	1:E:257:ASN:OD1	2.49	0.45
1:E:47:ALA:O	1:E:48:THR:HG22	2.15	0.45
1:E:181:LEU:HD12	1:E:182:ASP:H	1.80	0.45
1:E:254:MET:HE1	1:E:333:ILE:CG2	2.46	0.45
2:F:374:DG:H2''	2:F:375:DA:H8	1.80	0.45
1:A:178:ILE:HG21	1:A:232:ALA:O	2.15	0.45
1:E:22:LEU:O	1:E:23:ASN:CB	2.64	0.45
1:E:91:ILE:HA	1:E:94:LEU:CD1	2.46	0.45
1:E:186:VAL:HG21	1:E:205:LEU:HD13	1.97	0.45
1:E:193:THR:N	3:G:357:DT:OP1	2.48	0.45
1:E:325:ILE:C	1:E:327:GLU:N	2.70	0.45
2:F:374:DG:C2	2:F:375:DA:C4	3.04	0.45
1:A:186:VAL:O	1:A:189:ILE:HG12	2.17	0.45
1:A:192:ILE:HD12	3:C:356:DA:H3'	1.97	0.45
1:E:260:ASN:O	1:E:261:LEU:C	2.54	0.45
1:E:303:ARG:HG3	1:E:305:PHE:CE1	2.52	0.45
1:A:121:TYR:CE2	1:A:170:ASP:HA	2.36	0.45
1:E:12:ASP:C	1:E:13:TYR:CD2	2.90	0.45
1:E:37:SER:O	1:E:39:ARG:N	2.49	0.45
1:E:335:ARG:HD2	2:F:373:DT:H2''	1.98	0.45
1:A:95:LEU:HD13	1:A:112:LEU:HD11	1.98	0.45
1:A:301:ARG:HD2	1:A:324:LYS:HD2	1.99	0.45
1:E:39:ARG:HD2	1:E:39:ARG:HA	1.70	0.45
1:E:119:ARG:N	1:E:123:GLU:OE1	2.45	0.45
1:E:325:ILE:C	1:E:327:GLU:H	2.20	0.45
2:F:376:DA:H2''	2:F:377:DT:C5'	2.45	0.45
1:A:335:ARG:NH2	2:B:373:DT:C7	2.80	0.45
2:B:377:DT:C2'	2:B:378:DC:C6	3.00	0.45
1:E:3:HIS:HA	7:E:512:HOH:O	2.16	0.45
1:A:37:SER:CB	2:B:373:DT:O5'	2.57	0.45
1:E:22:LEU:CD1	1:E:80:ARG:NH2	2.79	0.45
1:E:334:ARG:NH1	2:F:372:DT:N3	2.64	0.45
1:A:37:SER:OG	1:A:39:ARG:HB2	2.17	0.44
1:E:335:ARG:CD	2:F:373:DT:H2''	2.47	0.44
1:A:169:ILE:HD13	1:A:177:LEU:CD1	2.47	0.44
1:E:301:ARG:NH2	1:E:328:GLU:OE2	2.49	0.44
1:A:7:LEU:HD12	1:A:114:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:348:DG:N2	3:C:349:DG:O6	2.50	0.44
1:E:5:ILE:N	1:E:115:SER:OG	2.45	0.44
1:E:12:ASP:C	1:E:14:PHE:N	2.70	0.44
1:E:38:GLY:O	1:E:39:ARG:C	2.55	0.44
1:A:7:LEU:C	1:A:7:LEU:HD23	2.38	0.44
1:A:43:SER:O	2:B:373:DT:OP1	2.36	0.44
1:A:188:GLY:C	1:A:189:ILE:HD13	2.38	0.44
1:E:253:THR:CB	2:F:373:DT:H3'	2.47	0.44
1:A:93:ASN:OD1	1:A:96:ARG:NH1	2.51	0.44
1:E:195:GLU:OE2	1:E:195:GLU:HA	2.17	0.44
4:E:400:DCP:N4	3:G:358:DT:C6	2.86	0.44
2:F:372:DT:C6	2:F:373:DT:C4	3.06	0.44
3:G:349:DG:O6	3:G:350:DG:N2	2.50	0.44
1:A:236:TYR:CZ	1:A:238:GLU:HB2	2.53	0.44
3:C:348:DG:N3	3:C:349:DG:N7	2.66	0.44
1:E:250:ARG:HG3	1:E:251:ILE:H	1.82	0.44
1:E:292:VAL:HB	1:E:335:ARG:HB2	1.99	0.44
1:A:70:ILE:HG23	7:A:511:HOH:O	2.17	0.44
1:A:149:LYS:HZ3	1:A:149:LYS:HB3	1.83	0.44
1:E:14:PHE:O	1:E:17:GLN:N	2.49	0.44
1:E:152:VAL:O	1:E:156:ILE:HG12	2.18	0.44
1:E:204:LYS:HG3	7:E:500:HOH:O	2.18	0.44
1:A:168:VAL:HG12	1:A:169:ILE:N	2.32	0.43
1:A:211:ILE:HD11	1:A:215:LYS:HB2	1.99	0.43
1:A:39:ARG:HH12	1:A:334:ARG:HE	1.64	0.43
1:A:105:ALA:HB3	1:A:109:GLU:HB2	2.00	0.43
3:C:350:DG:H2''	3:C:351:DG:C8	2.53	0.43
1:E:233:ARG:HG3	1:E:235:GLU:OE1	2.18	0.43
1:E:264:ILE:O	1:E:264:ILE:HG22	2.17	0.43
1:A:39:ARG:HH12	1:A:334:ARG:NE	2.16	0.43
1:A:319:VAL:N	7:A:521:HOH:O	2.51	0.43
1:E:17:GLN:NE2	1:E:141:ILE:HG23	2.33	0.43
1:E:37:SER:HB3	2:F:373:DT:O5'	2.17	0.43
3:G:351:DG:H2''	3:G:352:DA:OP2	2.18	0.43
1:A:206:VAL:HG23	1:A:209:LEU:HD12	1.99	0.43
1:A:216:LEU:O	1:A:219:MET:N	2.50	0.43
1:A:197:LEU:O	1:A:202:ILE:O	2.36	0.43
1:E:176:ARG:HG2	1:E:176:ARG:NH1	2.31	0.43
1:E:288:HIS:CD2	1:E:302:GLY:HA3	2.53	0.43
2:F:378:DC:C2'	2:F:379:DC:OP2	2.65	0.43
1:A:36:PHE:HB2	1:A:37:SER:H	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD12	1:A:140:LYS:HA	2.01	0.43
1:A:292:VAL:HG22	1:A:298:ILE:CD1	2.49	0.43
1:E:176:ARG:O	1:E:180:GLU:HG3	2.18	0.43
1:E:229:ILE:O	1:E:231:LEU:N	2.52	0.43
1:E:237:ASN:ND2	1:E:237:ASN:O	2.52	0.43
2:F:376:DA:N1	3:G:357:DT:O4	2.51	0.43
1:A:259:ARG:HG3	1:A:326:LEU:CD2	2.49	0.43
1:A:265:LYS:N	1:A:266:PRO:HD2	2.34	0.43
1:A:321:LEU:O	1:A:325:ILE:HG13	2.18	0.43
1:A:168:VAL:CG1	1:A:169:ILE:N	2.82	0.43
1:A:231:LEU:O	1:A:232:ALA:C	2.55	0.43
1:A:264:ILE:C	1:A:266:PRO:HD2	2.39	0.43
1:E:196:LYS:HD3	1:E:219:MET:HE1	2.01	0.43
1:E:196:LYS:HB3	1:E:219:MET:HG3	2.00	0.43
1:A:263:GLU:O	1:A:266:PRO:HD2	2.19	0.42
1:E:131:ILE:O	1:E:132:LYS:C	2.58	0.42
1:A:151:LYS:HG2	1:A:240:ILE:HD11	2.01	0.42
1:A:245:ARG:NH2	1:A:245:ARG:HG3	2.34	0.42
1:A:80:ARG:HB3	1:A:83:VAL:HG23	2.01	0.42
1:A:117:LYS:O	1:A:118:VAL:HG23	2.19	0.42
1:A:259:ARG:NH2	1:A:331:ARG:O	2.51	0.42
1:E:197:LEU:HB3	1:E:202:ILE:HB	2.00	0.42
1:A:128:GLY:O	1:A:132:LYS:HG3	2.19	0.42
1:A:196:LYS:CD	1:A:219:MET:O	2.66	0.42
1:A:264:ILE:O	1:A:267:TYR:HB2	2.18	0.42
1:E:101:LYS:HB3	1:E:101:LYS:HZ2	1.82	0.42
1:E:189:ILE:HG23	1:E:193:THR:CG2	2.50	0.42
1:E:250:ARG:O	1:E:251:ILE:HG13	2.19	0.42
1:A:221:GLY:O	1:A:222:GLU:C	2.57	0.42
1:E:65:VAL:HG22	2:F:372:DT:OP1	2.19	0.42
1:E:72:PRO:O	1:E:73:ASN:O	2.38	0.42
2:F:380:DT:H2''	2:F:381:DT:OP2	2.18	0.42
1:A:323:GLN:O	1:A:324:LYS:C	2.58	0.42
1:E:63:PRO:HG2	1:E:66:GLU:HG3	1.98	0.42
1:E:128:GLY:O	1:E:132:LYS:HG3	2.20	0.42
1:E:229:ILE:HG22	1:E:230:SER:N	2.34	0.42
3:G:357:DT:C5	3:G:358:DT:C4	3.08	0.42
1:A:10:ASP:OD1	1:A:10:ASP:O	2.38	0.41
1:A:70:ILE:HG22	1:A:71:LEU:HG	2.02	0.41
1:A:159:ASP:HA	1:A:162:LYS:HD2	2.01	0.41
1:A:272:ILE:O	1:A:276:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:DC:H1'	2:B:380:DT:H5'	2.02	0.41
1:E:71:LEU:N	1:E:72:PRO:HD3	2.35	0.41
1:E:101:LYS:HB3	1:E:101:LYS:HZ3	1.82	0.41
1:E:295:ASP:N	1:E:295:ASP:OD2	2.52	0.41
3:G:355:DG:C2	3:G:356:DA:C2	3.08	0.41
1:A:213:PHE:C	1:A:215:LYS:N	2.73	0.41
1:A:260:ASN:ND2	1:A:263:GLU:H	2.18	0.41
1:A:309:ILE:HG22	1:A:310:SER:O	2.19	0.41
1:E:274:GLU:OE1	1:E:274:GLU:HA	2.21	0.41
1:A:79:MET:HG3	1:A:84:TYR:CE2	2.50	0.41
1:A:156:ILE:HD13	1:A:181:LEU:HD22	2.03	0.41
1:A:207:ASP:O	1:A:209:LEU:N	2.53	0.41
1:A:249:GLY:HA2	1:A:275:SER:OG	2.20	0.41
1:A:257:ASN:HD22	1:A:294:GLU:HB2	1.84	0.41
1:E:96:ARG:O	1:E:97:GLU:C	2.58	0.41
7:F:501:HOH:O	3:G:348:DG:N2	2.53	0.41
1:A:102:ILE:HD13	1:A:103:GLU:H	1.85	0.41
1:A:193:THR:HG21	1:A:224:LYS:NZ	2.35	0.41
1:A:109:GLU:OE1	4:A:400:DCP:O2A	2.38	0.41
1:E:5:ILE:H	1:E:115:SER:HG	1.64	0.41
2:F:378:DC:H6	2:F:378:DC:H2'	1.72	0.41
2:F:384:DC:H1'	2:F:385:DC:H5'	2.02	0.41
1:A:89:SER:O	1:A:93:ASN:ND2	2.53	0.41
1:A:233:ARG:O	1:A:235:GLU:HB2	2.21	0.41
1:A:251:ILE:CG2	1:A:335:ARG:HG2	2.51	0.41
1:E:170:ASP:N	1:E:173:GLU:HB2	2.36	0.41
1:E:245:ARG:NH2	1:E:245:ARG:HG2	2.36	0.41
1:A:29:LYS:NZ	1:E:265:LYS:NZ	2.69	0.41
1:A:213:PHE:HD2	1:A:213:PHE:H	1.69	0.41
1:A:228:LEU:O	1:A:229:ILE:C	2.58	0.41
1:E:96:ARG:O	1:E:99:SER:N	2.42	0.41
1:E:104:ILE:O	1:E:104:ILE:HG22	2.21	0.41
1:E:179:ARG:HG3	1:E:180:GLU:HG3	2.01	0.41
1:E:189:ILE:CD1	1:E:228:LEU:HD21	2.51	0.41
1:E:305:PHE:CD1	1:E:305:PHE:N	2.89	0.41
1:A:5:ILE:HG23	1:A:121:TYR:HE1	1.86	0.41
1:A:35:VAL:HG12	1:A:79:MET:HE2	2.03	0.41
1:A:104:ILE:HA	1:A:110:ALA:HA	2.03	0.41
1:A:319:VAL:O	1:A:323:GLN:HG3	2.21	0.41
1:A:6:VAL:HG21	1:A:151:LYS:N	2.36	0.40
1:A:41:GLU:O	1:A:42:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:MET:HE2	1:A:79:MET:HB3	1.97	0.40
1:A:154:ALA:O	1:A:157:ALA:HB3	2.21	0.40
1:E:95:LEU:O	1:E:96:ARG:C	2.58	0.40
1:E:181:LEU:HD12	1:E:182:ASP:N	2.36	0.40
1:E:204:LYS:HE3	7:E:500:HOH:O	2.22	0.40
1:E:229:ILE:C	1:E:231:LEU:N	2.73	0.40
1:E:2:HIS:O	1:E:3:HIS:HB3	2.21	0.40
1:E:261:LEU:HD21	1:E:323:GLN:HG2	2.03	0.40
1:A:63:PRO:C	1:A:65:VAL:N	2.74	0.40
1:A:95:LEU:O	1:A:97:GLU:N	2.54	0.40
1:A:202:ILE:CD1	1:A:208:THR:HA	2.45	0.40
1:E:344:ILE:OXT	1:E:344:ILE:CG2	2.69	0.40
4:A:400:DCP:H2'1	6:B:387:AFN:C1	2.51	0.40
1:E:63:PRO:CB	2:F:371:DA:H3'	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	341/347 (98%)	265 (78%)	54 (16%)	22 (6%)	<b>1</b> <b>3</b>
1	E	341/347 (98%)	265 (78%)	51 (15%)	25 (7%)	<b>1</b> <b>3</b>
All	All	682/694 (98%)	530 (78%)	105 (15%)	47 (7%)	<b>1</b> <b>3</b>

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	13	TYR
1	A	41	GLU
1	A	104	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	198	LYS
1	A	200	LEU
1	A	222	GLU
1	E	14	PHE
1	E	23	ASN
1	E	37	SER
1	E	73	ASN
1	E	104	ILE
1	E	210	SER
1	E	215	LYS
1	E	261	LEU
1	E	279	LEU
1	E	295	ASP
1	E	331	ARG
1	A	37	SER
1	A	39	ARG
1	A	171	ASP
1	A	205	LEU
1	A	214	ASP
1	A	234	ASP
1	E	38	GLY
1	E	81	LYS
1	E	182	ASP
1	E	213	PHE
1	E	234	ASP
1	E	293	THR
1	E	343	PHE
1	A	14	PHE
1	A	25	SER
1	A	184	ALA
1	A	223	ALA
1	E	3	HIS
1	E	99	SER
1	E	105	ALA
1	E	214	ASP
1	A	96	ARG
1	A	99	SER
1	A	208	THR
1	E	13	TYR
1	E	230	SER
1	A	217	LYS
1	A	296	LEU

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Mol	Chain	Res	Type
1	E	220	ILE

### 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	302/306 (99%)	271 (90%)	31 (10%)	7	22
1	E	302/306 (99%)	264 (87%)	38 (13%)	4	13
All	All	604/612 (99%)	535 (89%)	69 (11%)	5	17

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	10	ASP
1	A	11	PHE
1	A	36	PHE
1	A	48	THR
1	A	64	ILE
1	A	69	LYS
1	A	92	MET
1	A	100	GLU
1	A	101	LYS
1	A	102	ILE
1	A	134	LYS
1	A	149	LYS
1	A	156	ILE
1	A	164	ASN
1	A	170	ASP
1	A	175	LYS
1	A	199	LYS
1	A	210	SER
1	A	212	GLU
1	A	213	PHE
1	A	214	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	236	TYR
1	A	241	ARG
1	A	242	THR
1	A	244	VAL
1	A	245	ARG
1	A	290	VAL
1	A	296	LEU
1	A	338	VAL
1	A	341	SER
1	E	3	HIS
1	E	27	LYS
1	E	48	THR
1	E	64	ILE
1	E	71	LEU
1	E	83	VAL
1	E	86	GLN
1	E	94	LEU
1	E	100	GLU
1	E	118	VAL
1	E	123	GLU
1	E	127	LEU
1	E	159	ASP
1	E	164	ASN
1	E	167	LYS
1	E	170	ASP
1	E	173	GLU
1	E	182	ASP
1	E	185	ASP
1	E	199	LYS
1	E	200	LEU
1	E	210	SER
1	E	211	ILE
1	E	212	GLU
1	E	213	PHE
1	E	216	LEU
1	E	237	ASN
1	E	241	ARG
1	E	242	THR
1	E	259	ARG
1	E	261	LEU
1	E	268	LEU
1	E	299	VAL

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Mol	Chain	Res	Type
1	E	313	THR
1	E	318	SER
1	E	324	LYS
1	E	332	LYS
1	E	335	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	3	HIS
1	A	50	ASN
1	A	85	GLN
1	A	86	GLN
1	A	164	ASN
1	A	260	ASN
1	E	3	HIS
1	E	93	ASN
1	E	164	ASN
1	E	237	ASN
1	E	260	ASN
1	E	288	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DCP	E	400	-	25,29,29	2.71	4 (16%)	37,45,45	2.22	11 (29%)
6	AFN	B	387	2	24,28,28	1.90	6 (25%)	32,44,44	2.35	12 (37%)
4	DCP	A	400	5	25,29,29	2.66	6 (24%)	37,45,45	2.24	10 (27%)
6	AFN	F	387	2	24,28,28	1.67	7 (29%)	32,44,44	2.27	10 (31%)

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	DCP	E	400	-	-	12/22/34/34	0/2/2/2
6	AFN	B	387	2	-	0/2/32/32	0/5/5/5
4	DCP	A	400	5	-	11/22/34/34	0/2/2/2
6	AFN	F	387	2	-	0/2/32/32	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	DCP	O3'-C3'	-9.82	1.22	1.43
4	E	400	DCP	O3'-C3'	-9.50	1.23	1.43
4	E	400	DCP	O5'-C5'	-6.50	1.19	1.44
6	B	387	AFN	C8A-C9	5.97	1.61	1.51
4	A	400	DCP	O5'-C5'	-5.26	1.24	1.44
4	E	400	DCP	C1'-N1	4.07	1.58	1.48
6	F	387	AFN	C8A-C9	3.93	1.58	1.51
4	A	400	DCP	C1'-N1	3.40	1.56	1.48
4	A	400	DCP	O4'-C4'	2.93	1.51	1.45
6	F	387	AFN	O10-C10	2.91	1.41	1.36
4	A	400	DCP	PG-O1G	2.90	1.59	1.50
6	F	387	AFN	C4B-C4A	2.81	1.48	1.42
6	B	387	AFN	C5B-C4B	2.75	1.46	1.37
6	B	387	AFN	C3-C2A	-2.67	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	387	AFN	C2A-C1	2.53	1.54	1.51
4	E	400	DCP	PG-O1G	2.49	1.58	1.50
6	F	387	AFN	C4A-C10	2.45	1.44	1.41
6	F	387	AFN	O7-C6A	2.33	1.46	1.41
4	A	400	DCP	C2'-C3'	-2.30	1.46	1.52
6	B	387	AFN	C4B-C4A	2.29	1.47	1.42
6	F	387	AFN	C5A-C9B	2.29	1.38	1.36
6	B	387	AFN	C5B-C5A	2.23	1.42	1.38
6	F	387	AFN	C5B-C4B	2.16	1.44	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	DCP	O4'-C1'-N1	8.01	122.19	107.86
6	B	387	AFN	CM-O4-C4B	6.68	127.09	117.75
6	F	387	AFN	CM-O4-C4B	6.17	126.38	117.75
4	E	400	DCP	O4'-C1'-N1	5.97	118.53	107.86
4	E	400	DCP	O5'-C5'-C4'	5.80	128.97	108.99
4	E	400	DCP	O4'-C4'-C5'	-5.42	91.54	109.37
6	B	387	AFN	O7-C8A-C9	-5.25	95.84	105.99
4	A	400	DCP	C2'-C1'-N1	-4.92	102.44	113.77
6	B	387	AFN	O1-C1-C12	4.84	132.12	127.19
4	E	400	DCP	C2'-C1'-N1	-4.71	102.92	113.77
6	F	387	AFN	O1-C1-C12	4.68	131.96	127.19
6	F	387	AFN	O7-C8A-C9	-4.63	97.03	105.99
6	F	387	AFN	O1-C1-C2A	-4.53	121.58	125.72
6	B	387	AFN	O1-C1-C2A	-3.96	122.10	125.72
4	A	400	DCP	O5'-C5'-C4'	3.64	121.51	108.99
4	A	400	DCP	C4'-O4'-C1'	-3.56	100.84	109.45
6	F	387	AFN	O10-C10-C9B	3.55	120.38	116.17
4	A	400	DCP	O5'-PA-O1A	3.35	122.17	109.07
4	A	400	DCP	C1'-N1-C2	3.18	123.31	117.74
4	E	400	DCP	O2A-PA-O5'	3.15	122.36	107.75
6	B	387	AFN	C5B-C5A-C9B	-3.03	120.39	124.07
4	E	400	DCP	C1'-N1-C2	3.01	123.02	117.74
6	B	387	AFN	C2A-C1-C12	-2.93	105.77	107.39
4	A	400	DCP	O4'-C4'-C5'	-2.93	99.74	109.37
4	A	400	DCP	C1'-N1-C6	-2.88	115.86	121.55
4	A	400	DCP	O4'-C4'-C3'	2.71	111.99	105.67
6	B	387	AFN	C10-O10-C11	2.69	124.29	119.19
4	E	400	DCP	O4'-C4'-C3'	2.69	111.95	105.67
6	B	387	AFN	C5A-C9B-C10	2.65	122.78	120.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	387	AFN	C3-C3A-C12	-2.63	109.11	111.38
6	F	387	AFN	C10-O10-C11	2.51	123.93	119.19
6	F	387	AFN	C5B-C5A-C9B	-2.45	121.09	124.07
6	B	387	AFN	C3-C2A-C1	2.45	107.56	106.38
6	B	387	AFN	O6A-C5A-C5B	2.30	126.57	123.36
6	F	387	AFN	O4-C4B-C4A	2.28	119.25	115.89
4	A	400	DCP	O4'-C1'-C2'	2.25	110.50	106.25
6	B	387	AFN	O10-C10-C9B	2.22	118.81	116.17
4	E	400	DCP	C1'-N1-C6	-2.15	117.30	121.55
6	F	387	AFN	C8A-O7-C6A	2.13	109.71	106.86
4	E	400	DCP	O2G-PG-O3B	2.10	111.68	104.64
4	E	400	DCP	O4'-C1'-C2'	2.09	110.20	106.25
6	B	387	AFN	C3-C3A-C12	-2.07	109.59	111.38
4	E	400	DCP	PB-O3A-PA	-2.00	125.95	132.83

There are no chirality outliers.

All (23) torsion outliers are listed below:

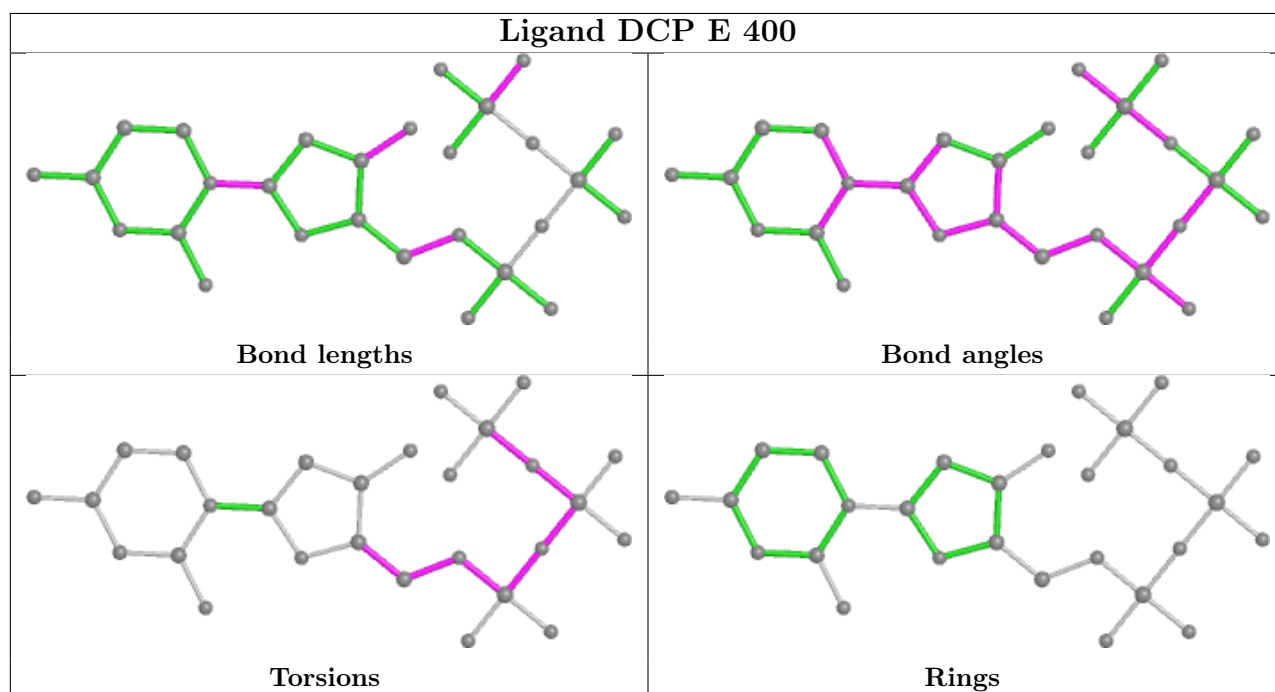
Mol	Chain	Res	Type	Atoms
4	A	400	DCP	C5'-O5'-PA-O1A
4	A	400	DCP	PB-O3A-PA-O5'
4	A	400	DCP	PB-O3B-PG-O2G
4	E	400	DCP	C5'-O5'-PA-O1A
4	E	400	DCP	C5'-O5'-PA-O2A
4	E	400	DCP	PB-O3A-PA-O5'
4	E	400	DCP	PB-O3B-PG-O2G
4	A	400	DCP	PA-O3A-PB-O1B
4	A	400	DCP	PG-O3B-PB-O2B
4	E	400	DCP	PA-O3A-PB-O1B
4	E	400	DCP	PG-O3B-PB-O2B
4	A	400	DCP	C5'-O5'-PA-O2A
4	E	400	DCP	C4'-C5'-O5'-PA
4	A	400	DCP	O4'-C4'-C5'-O5'
4	E	400	DCP	O4'-C4'-C5'-O5'
4	A	400	DCP	PB-O3B-PG-O3G
4	E	400	DCP	PB-O3B-PG-O3G
4	A	400	DCP	C5'-O5'-PA-O3A
4	E	400	DCP	C5'-O5'-PA-O3A
4	A	400	DCP	PA-O3A-PB-O2B
4	A	400	DCP	PG-O3B-PB-O1B
4	E	400	DCP	PA-O3A-PB-O2B
4	E	400	DCP	PG-O3B-PB-O1B

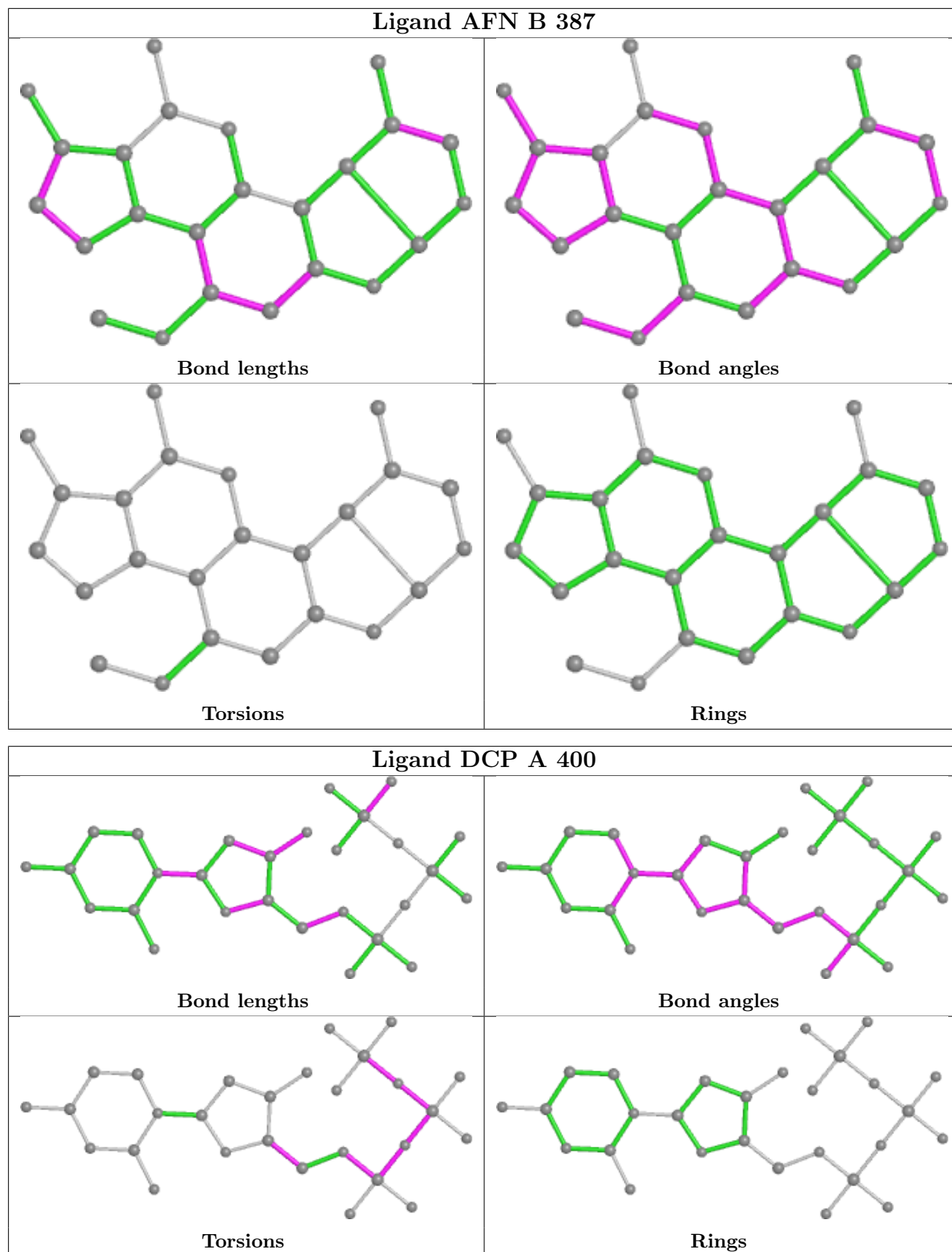
There are no ring outliers.

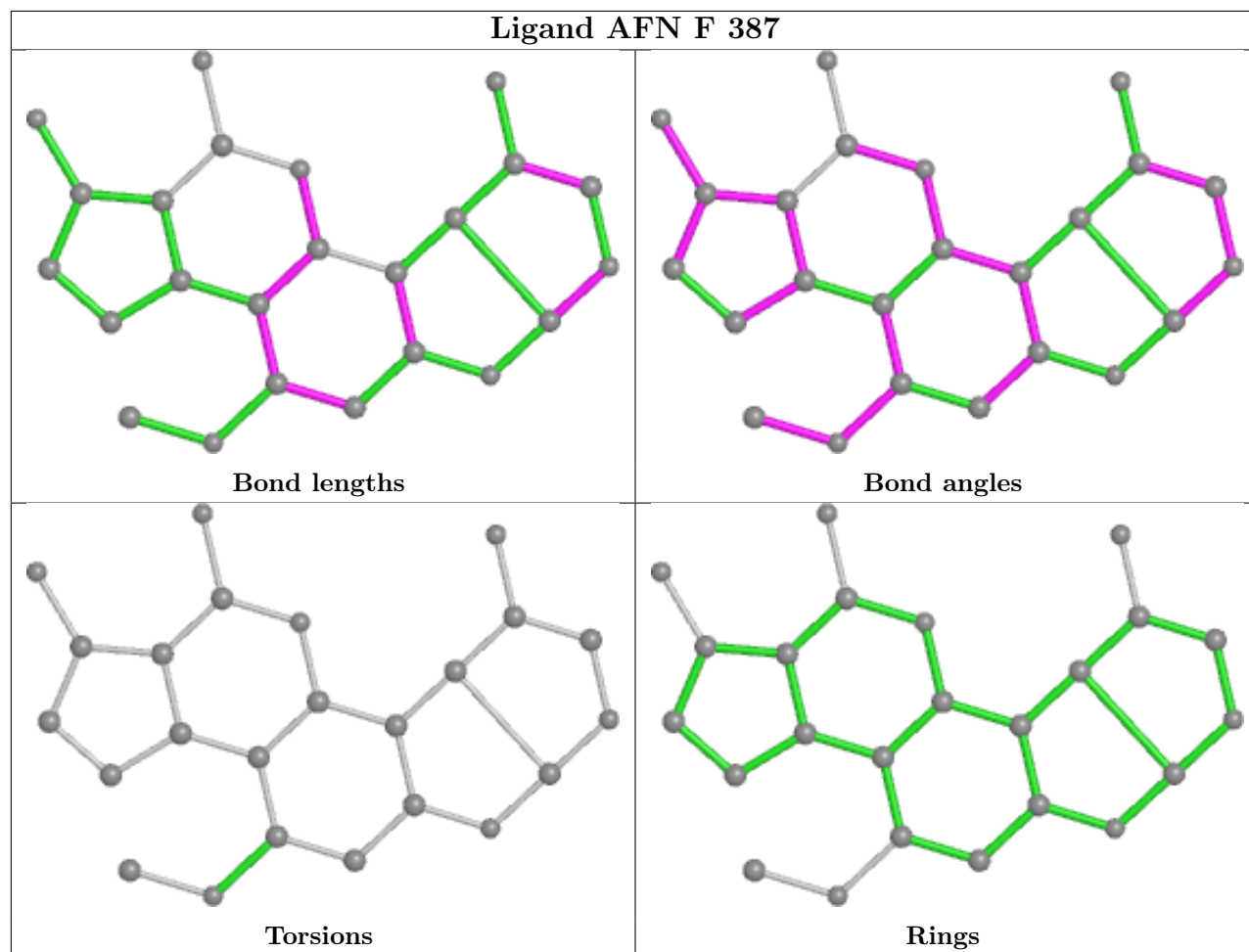
4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	400	DCP	5	0
6	B	387	AFN	10	0
4	A	400	DCP	13	0
6	F	387	AFN	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	343/347 (98%)	-0.15	7 (2%) 65 63	23, 52, 85, 106	0
1	E	343/347 (98%)	-0.21	4 (1%) 79 79	23, 49, 84, 103	0
2	B	16/16 (100%)	1.40	4 (25%) 0 0	42, 93, 158, 160	0
2	F	16/16 (100%)	1.52	2 (12%) 3 3	49, 104, 164, 167	0
3	C	12/12 (100%)	0.92	3 (25%) 0 0	73, 80, 162, 167	0
3	G	12/12 (100%)	0.91	3 (25%) 0 0	75, 88, 162, 167	0
All	All	742/750 (98%)	-0.07	23 (3%) 49 44	23, 52, 98, 167	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	386	DC	7.6
2	F	385	DC	6.7
2	F	386	DC	6.2
3	C	348	DG	5.1
3	C	347	DG	5.0
1	A	201	GLY	4.7
3	G	347	DG	4.0
2	B	385	DC	3.9
1	A	2	HIS	3.5
1	E	2	HIS	3.1
1	E	191	ASN	3.1
1	A	200	LEU	3.0
1	A	37	SER	2.9
2	B	383	DC	2.8
2	B	384	DC	2.7
3	G	349	DG	2.7
3	G	348	DG	2.6
1	A	199	LYS	2.5
1	E	199	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	208	THR	2.3
1	E	255	LYS	2.3
3	C	349	DG	2.1
1	A	196	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

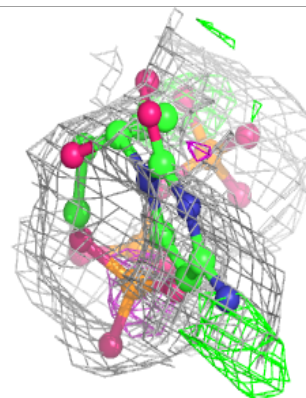
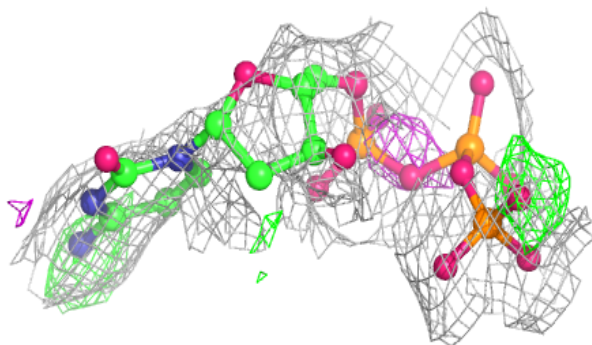
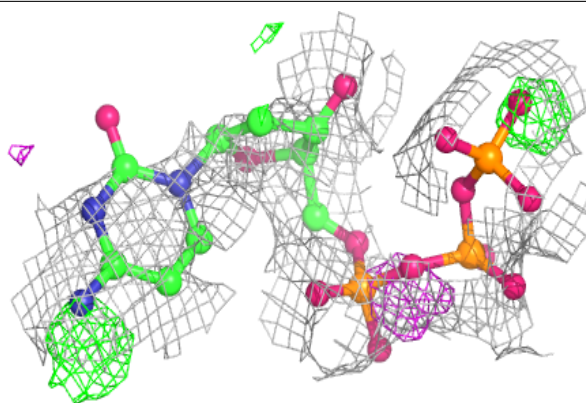
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	DCP	E	400	28/28	0.75	0.28	76,89,100,100	0
5	CA	E	345	1/1	0.80	0.24	84,84,84,84	0
5	CA	A	345	1/1	0.84	0.12	78,78,78,78	0
6	AFN	B	387	24/24	0.85	0.23	60,64,68,70	0
6	AFN	F	387	24/24	0.85	0.27	43,58,68,72	0
4	DCP	A	400	28/28	0.88	0.19	74,88,94,95	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.

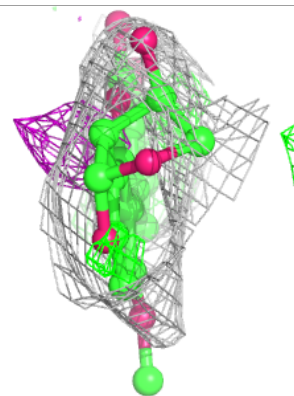
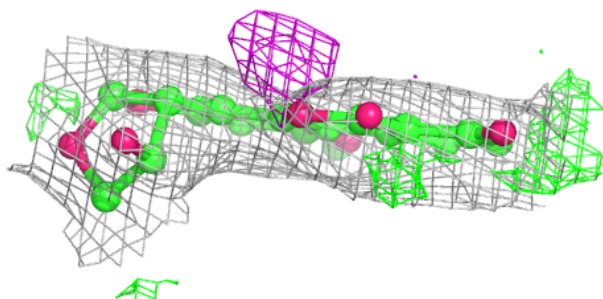
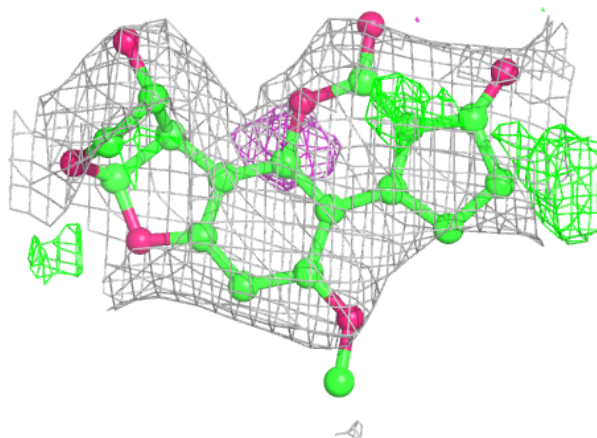


**Electron density around DCP E 400:**

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

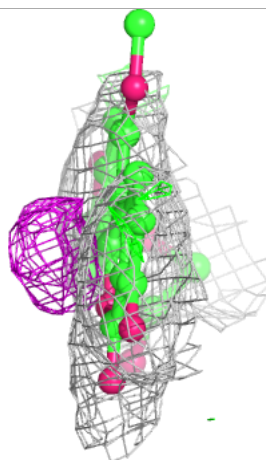
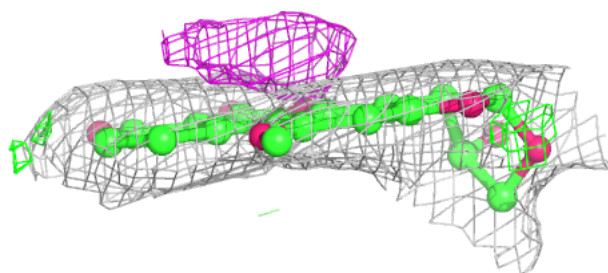
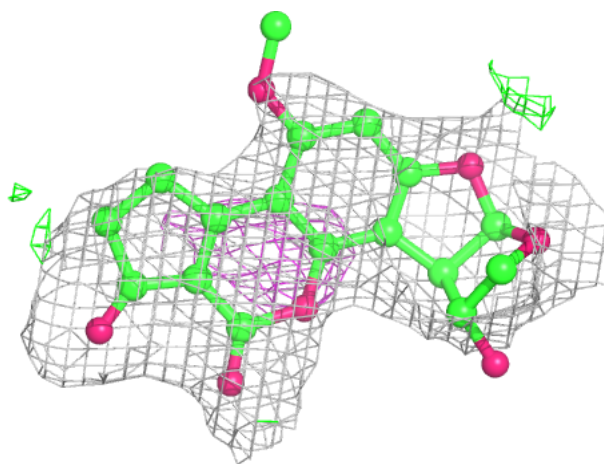
**Electron density around AFN B 387:**

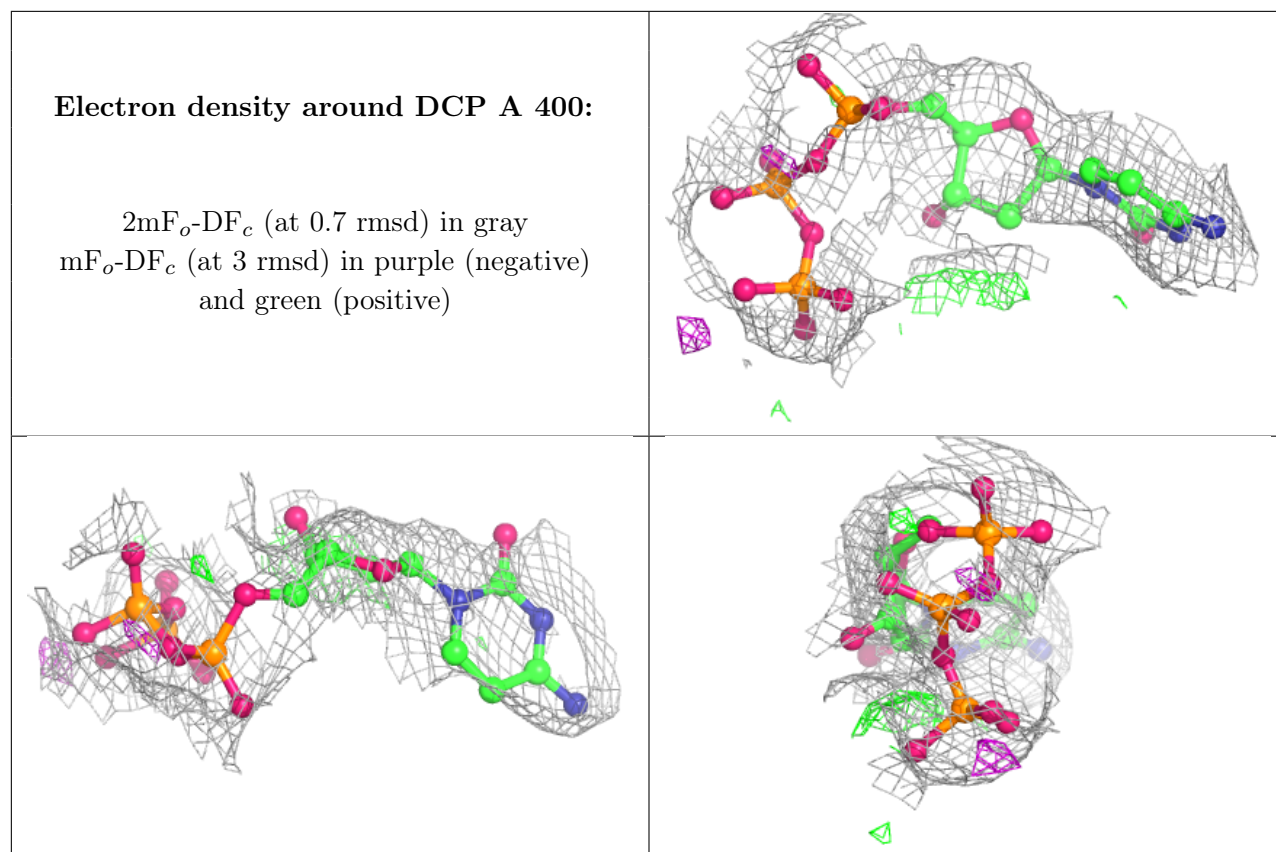
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AFN F 387:**

$2mF_o-DF_c$  (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.