



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2025 – 01:55 am BST

PDB ID : 9I16 / pdb_00009i16
Title : Structure of RecQL-dsDNA-ADP-AlF₄ complex from *Bos taurus*
Authors : Song, Z.Y.; Liu, N.N.; Ai, X.; Rety, S.; Xi, X.G.
Deposited on : 2025-01-16
Resolution : 2.82 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

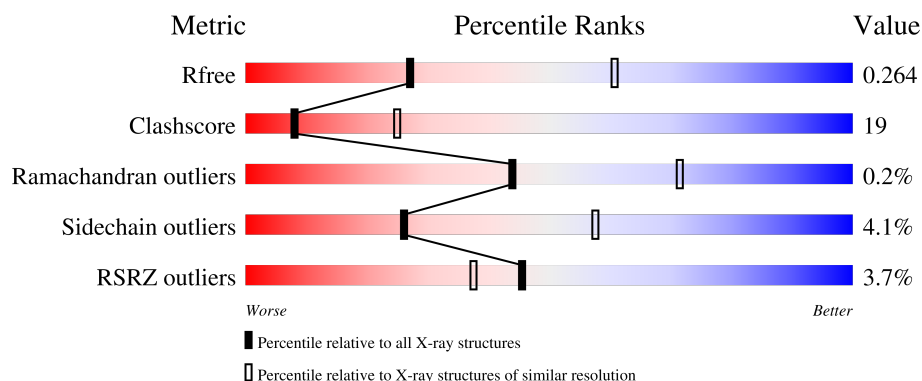
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	164625	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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	531	<div> <div>2%</div> <div>69%</div> <div>30%</div> <div>.</div> </div>
1	B	531	<div> <div>%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>
1	C	531	<div> <div>%</div> <div>76%</div> <div>24%</div> <div>.</div> </div>
1	E	531	<div> <div>8%</div> <div>52%</div> <div>45%</div> <div>.</div> </div>
1	F	531	<div> <div>3%</div> <div>57%</div> <div>39%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	531	
3	G	21	
3	I	21	
3	K	21	
4	H	15	
4	J	15	
4	L	15	

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
8	PO4	F	1003	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 27673 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 ATP-dependent DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			
1	B	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			
1	C	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			
1	E	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			
1	F	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	MET	-	initiating methionine	UNP A0JN36
B	62	MET	-	initiating methionine	UNP A0JN36
C	62	MET	-	initiating methionine	UNP A0JN36
E	62	MET	-	initiating methionine	UNP A0JN36
F	62	MET	-	initiating methionine	UNP A0JN36

- Molecule 2 is a protein called ATP-dependent DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	531	Total	C	N	O	S	0	0	0
			4237	2703	727	772	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	18	Total	C	N	O	P	0	0	0
			362	172	62	110	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	18	Total	C	N	O	P	0	0	0
			362	172	62	110	18			
3	K	18	Total	C	N	O	P	0	0	0
			362	172	62	110	18			

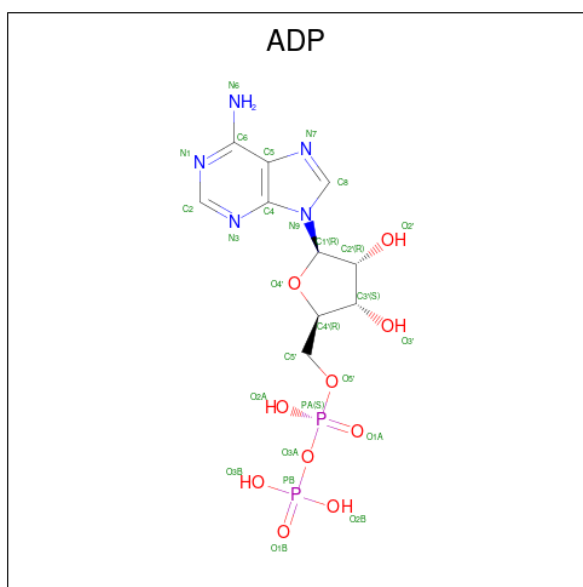
- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*GP*AP*GP*CP*GP*TP*CP*GP*AP*GP*AP*TP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	15	Total	C	N	O	P	0	0	0
			310	146	61	88	15			
4	J	15	Total	C	N	O	P	0	0	0
			310	146	61	88	15			
4	L	15	Total	C	N	O	P	0	0	0
			310	146	61	88	15			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	2	Total	Mg	0	0
			2	2		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	E	1	Total	O	P	0	0
			5	4	1		
8	F	1	Total	O	P	0	0
			5	4	1		
8	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	K	0	0
			2	2		

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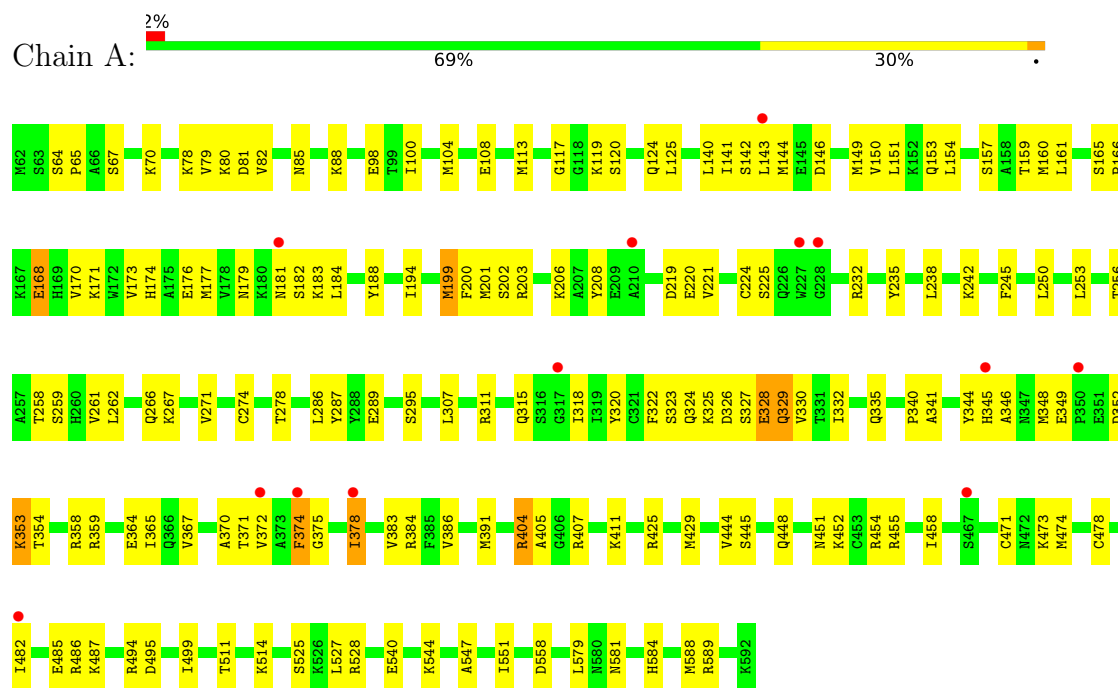
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	4	Total 4	K 4	0	0
9	C	1	Total 1	K 1	0	0
9	G	1	Total 1	K 1	0	0

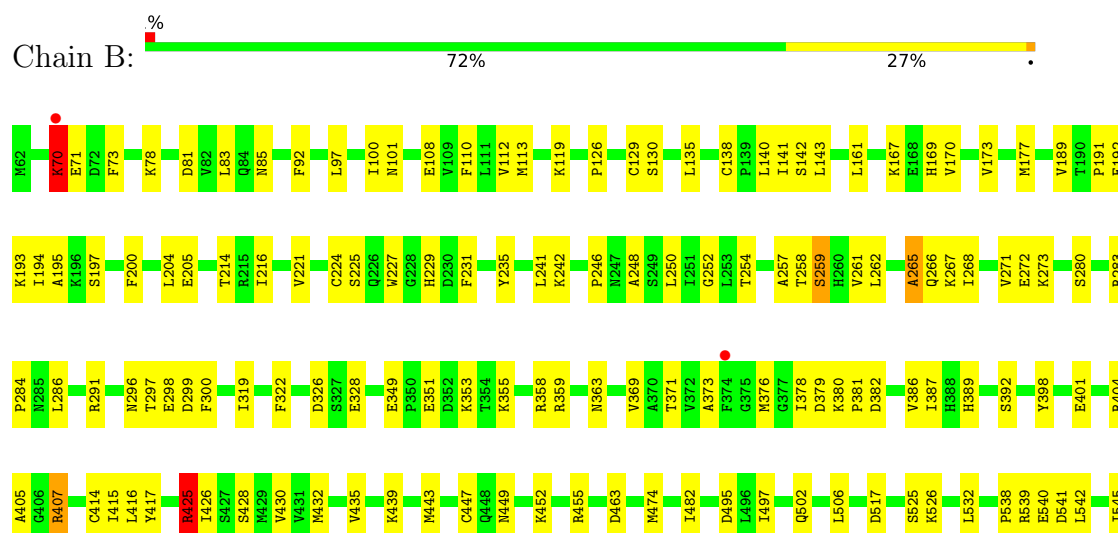
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ATP-dependent DNA helicase

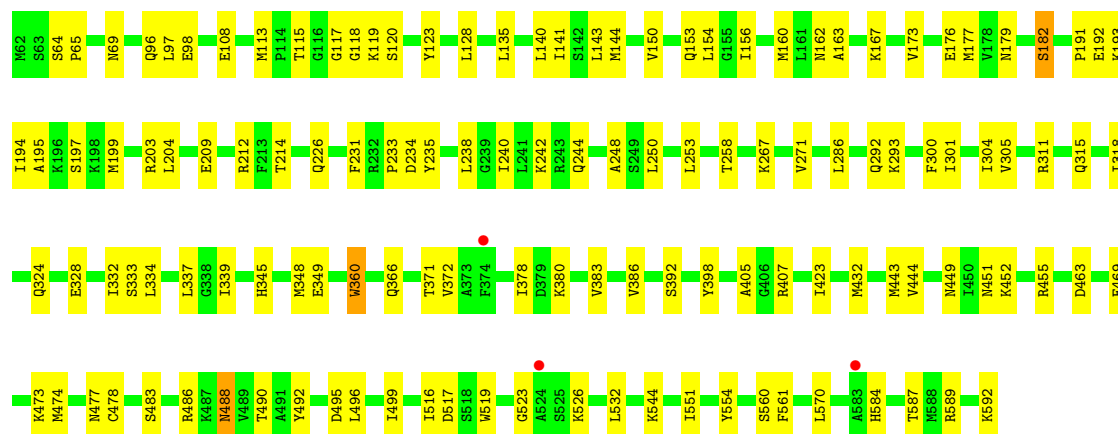
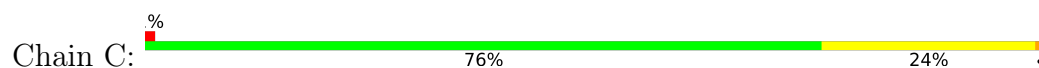


• Molecule 1: ATP-dependent DNA helicase

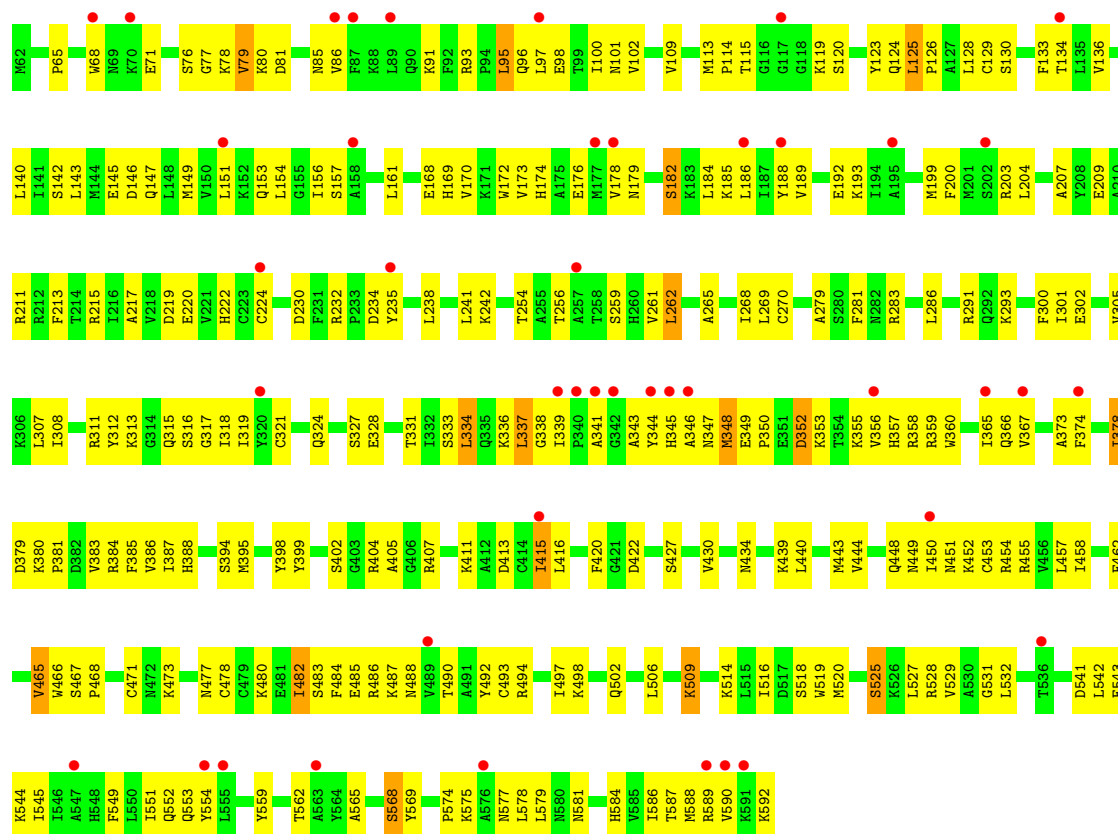




• Molecule 1: ATP-dependent DNA helicase

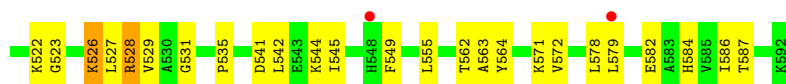


• Molecule 1: ATP-dependent DNA helicase

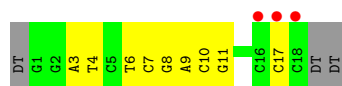
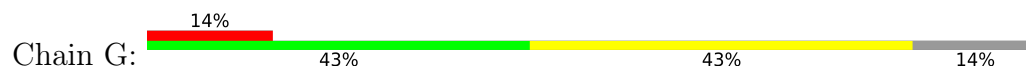


• Molecule 1: ATP-dependent DNA helicase





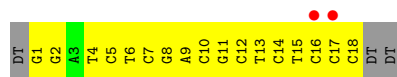
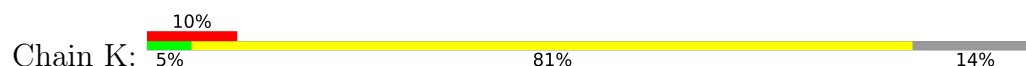
- Molecule 3: DNA (5'-D(P*GP*GP*AP*TP*CP*TP*CP*GP*AP*CP*GP*CP*TP*CP*TP*CP*CP*C)-3')



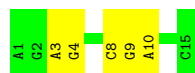
- Molecule 3: DNA (5'-D(P*GP*GP*AP*TP*CP*TP*CP*GP*AP*CP*GP*CP*TP*CP*TP*CP*CP*C)-3')



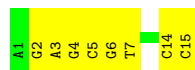
- Molecule 3: DNA (5'-D(P*GP*GP*AP*TP*CP*TP*CP*GP*AP*CP*GP*CP*TP*CP*TP*CP*CP*C)-3')



- Molecule 4: DNA (5'-D(P*AP*GP*AP*GP*CP*GP*TP*CP*GP*AP*GP*AP*TP*CP*CP*C)-3')



- Molecule 4: DNA (5'-D(P*AP*GP*AP*GP*CP*GP*TP*CP*GP*AP*GP*AP*TP*CP*CP*C)-3')



- Molecule 4: DNA (5'-D(P*AP*GP*AP*GP*CP*GP*TP*CP*GP*AP*GP*AP*TP*CP*CP*C)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.56Å 112.08Å 181.79Å 90.00° 92.73° 90.00°	Depositor
Resolution (Å)	29.89 – 2.82 29.89 – 2.82	Depositor EDS
% Data completeness (in resolution range)	69.2 (29.89-2.82) 69.1 (29.89-2.82)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.218 , 0.265 0.218 , 0.264	Depositor DCC
R_{free} test set	3927 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27673	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: PO4, MG, ZN, K, ADP

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	0.28	0/4325	0.61	10/5830 (0.2%)
1	B	0.21	0/4325	0.45	2/5830 (0.0%)
1	C	0.16	0/4325	0.44	3/5830 (0.1%)
1	E	0.24	0/4325	0.57	2/5830 (0.0%)
1	F	0.30	2/4325 (0.0%)	0.58	5/5830 (0.1%)
2	D	0.54	6/4325 (0.1%)	1.00	35/5831 (0.6%)
3	G	0.26	0/403	0.55	0/618
3	I	0.30	0/403	0.66	0/618
3	K	0.33	0/403	0.66	0/618
4	H	0.22	0/348	0.44	0/535
4	J	0.33	0/348	0.50	0/535
4	L	0.35	0/348	0.56	0/535
All	All	0.31	8/28203 (0.0%)	0.63	57/38440 (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	A	0	1
1	B	0	4
1	C	0	1
1	E	0	1
1	F	0	2
2	D	0	4
All	All	0	13

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	132	GLY	C-O	-16.47	1.15	1.24
2	D	401	GLU	CD-OE2	11.49	1.47	1.25
2	D	183	LYS	CD-CE	7.17	1.74	1.52
2	D	404	ARG	CA-CB	5.89	1.63	1.53
1	F	381	PRO	CA-CB	-5.78	1.44	1.53
1	F	381	PRO	N-CA	5.45	1.54	1.47
2	D	401	GLU	CD-OE1	5.40	1.35	1.25
2	D	403	GLY	C-N	-5.36	1.26	1.34

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	192	GLU	CG-CD-OE1	19.04	162.18	118.40
2	D	192	GLU	CB-CG-CD	-18.93	80.42	112.60
2	D	192	GLU	OE1-CD-OE2	-16.01	84.47	122.90
2	D	192	GLU	CG-CD-OE2	-14.47	85.12	118.40
1	A	199	MET	CB-CG-SD	-12.57	74.98	112.70
1	F	381	PRO	N-CA-CB	-11.84	90.56	103.23
2	D	401	GLU	CB-CG-CD	11.68	132.46	112.60
2	D	401	GLU	CA-CB-CG	10.40	134.90	114.10
1	F	381	PRO	N-CD-CG	-10.33	87.71	103.20
2	D	403	GLY	CA-C-N	10.03	135.02	120.38
2	D	403	GLY	C-N-CA	10.03	135.02	120.38
2	D	365	ILE	N-CA-CB	9.94	126.77	110.86
2	D	401	GLU	CG-CD-OE1	-9.80	95.87	118.40
2	D	183	LYS	CG-CD-CE	-9.37	89.76	111.30
1	A	329	GLN	N-CA-CB	-9.15	95.91	109.82
2	D	404	ARG	CG-CD-NE	9.06	131.94	112.00
2	D	365	ILE	CA-CB-CG1	8.70	125.18	110.40
2	D	365	ILE	N-CA-C	-8.43	96.16	108.71
1	A	329	GLN	CB-CA-C	8.32	124.15	110.92
1	F	378	ILE	N-CA-C	8.17	118.17	110.74
1	C	153	GLN	CA-CB-CG	8.09	130.27	114.10
2	D	404	ARG	N-CA-CB	-7.67	98.03	110.14
2	D	203	ARG	CA-CB-CG	-7.65	98.81	114.10
1	F	381	PRO	CA-CB-CG	-7.49	90.27	104.50
2	D	401	GLU	N-CA-CB	-7.39	98.92	110.30
2	D	365	ILE	CB-CA-C	-7.00	101.12	110.98
2	D	142	SER	CA-CB-OG	6.98	125.06	111.10
1	A	353	LYS	CB-CG-CD	-6.97	95.26	111.30
2	D	365	ILE	CG1-CB-CG2	-6.95	89.86	110.70
1	B	70	LYS	CB-CA-C	-6.81	94.36	110.02
2	D	192	GLU	CA-CB-CG	6.77	127.64	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	LYS	CD-CE-NZ	-6.72	90.39	111.90
2	D	142	SER	CB-CA-C	-6.66	97.89	110.67
2	D	79	VAL	CA-CB-CG1	6.65	121.71	110.40
2	D	402	SER	N-CA-C	6.63	121.90	113.55
2	D	401	GLU	CG-CD-OE2	6.59	133.57	118.40
1	C	153	GLN	CB-CA-C	-6.14	100.60	110.79
1	A	329	GLN	CB-CG-CD	6.12	123.01	112.60
1	B	425	ARG	CB-CA-C	-6.12	101.28	110.88
1	A	206	LYS	CG-CD-CE	-6.03	97.44	111.30
2	D	192	GLU	CB-CA-C	5.90	120.71	110.68
2	D	365	ILE	CB-CG1-CD1	5.90	126.18	113.80
2	D	192	GLU	CA-C-N	-5.88	110.90	120.72
2	D	192	GLU	C-N-CA	-5.88	110.90	120.72
1	E	256	THR	CA-C-N	5.87	131.55	121.86
1	E	256	THR	C-N-CA	5.87	131.55	121.86
2	D	209	GLU	CA-CB-CG	5.86	125.82	114.10
2	D	90	GLN	CA-CB-CG	-5.68	102.74	114.10
1	A	161	LEU	CB-CG-CD1	5.60	127.50	110.70
1	C	153	GLN	N-CA-CB	5.57	118.31	110.12
2	D	78	LYS	CA-CB-CG	5.46	125.01	114.10
2	D	398	TYR	N-CA-CB	5.40	118.54	110.22
1	F	381	PRO	CB-CA-C	5.40	121.65	113.06
1	A	328	GLU	CA-C-N	5.15	127.95	120.79
1	A	328	GLU	C-N-CA	5.15	127.95	120.79
2	D	401	GLU	N-CA-C	-5.13	105.76	112.23
2	D	365	ILE	CA-CB-CG2	-5.01	101.98	110.50

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	ARG	Sidechain
1	B	229	HIS	Peptide
1	B	265	ALA	Peptide
1	B	425	ARG	Sidechain
1	B	70	LYS	Peptide
1	C	311	ARG	Sidechain
2	D	192	GLU	Sidechain
2	D	203	ARG	Sidechain
2	D	259	SER	Peptide
2	D	400	GLN	Peptide
1	E	356	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	F	378	ILE	Peptide
1	F	381	PRO	Mainchain

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	4237	0	4295	137	0
1	B	4237	0	4295	119	0
1	C	4237	0	4295	86	0
1	E	4237	0	4294	244	0
1	F	4237	0	4295	175	0
2	D	4237	0	4290	246	0
3	G	362	0	203	14	0
3	I	362	0	203	15	0
3	K	362	0	203	23	0
4	H	310	0	168	4	0
4	J	310	0	168	7	0
4	L	310	0	168	12	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	D	27	0	12	1	0
6	E	27	0	12	3	0
6	F	27	0	12	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
8	A	20	0	0	0	0
8	B	10	0	0	1	0
8	C	10	0	0	1	0
8	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	10	0	0	2	0
9	A	2	0	0	0	0
9	B	4	0	0	0	0
9	C	1	0	0	0	0
9	G	1	0	0	0	0
All	All	27673	0	26949	1045	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 19.

All (1045) 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)
2:D:359:ARG:O	2:D:365:ILE:HD12	1.47	1.16
2:D:398:TYR:CA	2:D:401:GLU:HG3	1.77	1.13
2:D:398:TYR:HA	2:D:401:GLU:CG	1.79	1.13
1:A:140:LEU:HB2	1:A:143:LEU:HD13	1.43	0.98
1:F:565:ALA:HB1	3:K:16:DC:H41	1.33	0.94
1:B:355:LYS:HZ3	1:B:358:ARG:HE	1.12	0.94
4:L:3:DA:H2''	4:L:4:DG:H5''	1.45	0.93
1:A:325:LYS:O	1:A:329:GLN:HB2	1.70	0.91
1:A:429:MET:HE2	3:G:17:DC:H5'	1.54	0.89
1:E:128:LEU:HD21	1:E:156:ILE:HD11	1.55	0.86
1:E:487:LYS:HZ3	1:E:590:VAL:H	1.24	0.86
1:F:429:MET:HE1	3:K:17:DC:H5'	1.57	0.86
1:A:344:TYR:OH	1:A:353:LYS:NZ	2.08	0.86
1:A:143:LEU:HD12	1:A:143:LEU:H	1.42	0.85
1:C:449:ASN:HD21	1:C:452:LYS:HE3	1.39	0.84
2:D:359:ARG:C	2:D:365:ILE:HD12	2.01	0.84
1:F:378:ILE:HD12	1:F:379:ASP:H	1.40	0.83
1:E:174:HIS:HD2	1:E:203:ARG:HG3	1.41	0.82
1:F:378:ILE:HD11	1:F:404:ARG:HD2	1.59	0.82
2:D:134:THR:HG23	2:D:215:ARG:HB2	1.60	0.82
1:B:70:LYS:HE2	1:B:101:ASN:OD1	1.78	0.82
1:E:315:GLN:HB2	1:E:384:ARG:HG3	1.59	0.82
1:C:199:MET:SD	1:C:203:ARG:NH1	2.52	0.81
1:C:301:ILE:HG21	1:C:333:SER:HB3	1.61	0.81
2:D:76:SER:O	2:D:79:VAL:HG12	1.81	0.81
2:D:319:ILE:HG12	2:D:387:ILE:HB	1.61	0.80
1:B:194:ILE:HD12	1:B:241:LEU:HD21	1.63	0.80
2:D:429:MET:HE2	3:I:16:DC:H1'	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:HB3	1:A:182:SER:HB3	1.65	0.79
1:B:326:ASP:OD2	1:B:425:ARG:NH1	2.15	0.79
1:E:529:VAL:HB	1:E:532:LEU:HG	1.66	0.78
2:D:102:VAL:HG11	2:D:109:VAL:HB	1.66	0.78
2:D:293:LYS:HE3	2:D:417:TYR:HB3	1.65	0.77
1:A:140:LEU:CB	1:A:143:LEU:HD13	2.14	0.77
1:A:81:ASP:OD1	1:A:85:ASN:ND2	2.16	0.77
1:E:344:TYR:HE2	1:E:353:LYS:HD3	1.47	0.77
1:E:529:VAL:HG12	1:E:531:GLY:H	1.46	0.77
1:E:115:THR:O	1:E:407:ARG:NH2	2.18	0.77
1:E:230:ASP:O	1:E:232:ARG:NE	2.16	0.77
1:A:199:MET:O	1:A:203:ARG:NH1	2.18	0.77
2:D:67:SER:O	2:D:70:LYS:NZ	2.17	0.76
2:D:316:SER:HA	2:D:366:GLN:OE1	1.85	0.76
1:A:451:ASN:OD1	1:A:452:LYS:N	2.19	0.76
2:D:398:TYR:HA	2:D:401:GLU:HG3	0.86	0.76
1:A:344:TYR:HD2	1:A:374:PHE:CZ	2.04	0.76
1:B:266:GLN:HB3	1:B:272:GLU:HA	1.67	0.75
1:E:480:LYS:HD2	1:E:482:ILE:H	1.51	0.75
1:B:373:ALA:HB3	1:B:376:MET:HE2	1.68	0.75
1:E:315:GLN:HG3	1:E:384:ARG:HB2	1.67	0.74
1:A:344:TYR:CD2	1:A:374:PHE:CZ	2.75	0.74
3:G:6:DT:H2'	3:G:7:DC:C6	2.22	0.74
1:E:102:VAL:HG11	1:E:109:VAL:HB	1.69	0.74
1:F:324:GLN:OE1	1:F:324:GLN:N	2.18	0.74
1:E:68:TRP:O	1:E:101:ASN:ND2	2.21	0.73
1:E:327:SER:HB3	1:E:345:HIS:CE1	2.23	0.73
1:E:549:PHE:HB3	1:E:554:TYR:HB2	1.68	0.73
1:F:301:ILE:HG21	1:F:333:SER:HB3	1.69	0.72
1:E:328:GLU:HA	1:E:331:THR:HG23	1.71	0.72
1:E:259:SER:HA	1:E:262:LEU:HB2	1.71	0.72
1:F:407:ARG:NH1	8:F:1003:PO4:O4	2.22	0.72
2:D:229:HIS:ND1	2:D:230:ASP:OD2	2.22	0.72
1:E:579:LEU:HA	1:E:584:HIS:CD2	2.25	0.72
1:B:110:PHE:HE1	1:B:266:GLN:HG2	1.54	0.72
1:C:177:MET:HE2	1:C:203:ARG:HB2	1.71	0.71
1:E:311:ARG:HG3	1:E:312:TYR:CE1	2.25	0.71
1:F:524:ALA:HB3	1:F:527:LEU:HD12	1.71	0.71
1:A:200:PHE:HA	1:A:203:ARG:HH22	1.55	0.71
1:B:296:ASN:ND2	1:B:299:ASP:H	1.88	0.71
1:F:289:GLU:HB3	1:F:415:ILE:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:6:DT:H2'	3:I:7:DC:C6	2.25	0.71
1:E:193:LYS:HG3	1:E:200:PHE:HD2	1.56	0.71
2:D:453:CYS:SG	2:D:471:CYS:HB2	2.30	0.71
1:B:386:VAL:HG23	1:B:405:ALA:HB2	1.72	0.71
1:A:208:TYR:HE2	1:A:245:PHE:HA	1.55	0.71
1:C:140:LEU:HB2	1:C:143:LEU:HD12	1.72	0.71
1:A:345:HIS:O	1:A:348:MET:HB2	1.91	0.71
1:F:181:ASN:OD1	1:F:181:ASN:N	2.23	0.70
1:E:142:SER:HA	1:E:145:GLU:HG3	1.72	0.70
1:A:78:LYS:O	1:A:82:VAL:HG23	1.90	0.70
1:B:517:ASP:OD1	1:B:539:ARG:NH2	2.25	0.70
1:E:174:HIS:CD2	1:E:203:ARG:HG3	2.24	0.70
1:A:344:TYR:CD2	1:A:374:PHE:HZ	2.09	0.70
2:D:397:ASN:C	2:D:401:GLU:HG2	2.16	0.70
1:A:168:GLU:N	1:A:168:GLU:OE1	2.24	0.70
1:F:565:ALA:HB1	3:K:16:DC:N4	2.07	0.70
1:A:146:ASP:OD1	1:A:353:LYS:HE3	1.92	0.70
2:D:400:GLN:O	2:D:404:ARG:NE	2.25	0.70
3:K:15:DT:H3	4:L:1:DA:H61	1.39	0.70
1:C:179:ASN:O	1:C:212:ARG:NH1	2.25	0.69
2:D:448:GLN:NE2	2:D:544:LYS:O	2.24	0.69
1:E:281:PHE:CD2	1:E:465:VAL:HB	2.28	0.69
4:J:3:DA:H2''	4:J:4:DG:H5'	1.73	0.69
1:B:224:CYS:HB2	1:B:265:ALA:HB2	1.72	0.69
1:F:319:ILE:HD13	1:F:387:ILE:HB	1.75	0.69
1:F:486:ARG:HG3	1:F:486:ARG:O	1.92	0.68
2:D:99:THR:HG1	2:D:122:CYS:HG	1.37	0.68
1:E:487:LYS:HE2	1:E:590:VAL:HG12	1.75	0.68
1:F:301:ILE:O	1:F:305:VAL:HG23	1.94	0.68
1:E:316:SER:HB2	1:E:383:VAL:HA	1.75	0.68
1:E:344:TYR:CE1	1:E:374:PHE:HA	2.29	0.68
1:E:553:GLN:O	1:E:574:PRO:HD2	1.93	0.68
2:D:100:ILE:HD12	2:D:125:LEU:HD22	1.74	0.67
2:D:259:SER:HB3	2:D:262:LEU:HD22	1.76	0.67
1:A:344:TYR:HD2	1:A:374:PHE:HZ	1.41	0.67
1:E:95:LEU:HD23	1:E:279:ALA:HA	1.75	0.67
2:D:109:VAL:HG23	2:D:275:PHE:HB2	1.76	0.67
1:E:349:GLU:OE2	1:E:349:GLU:N	2.28	0.67
1:F:298:GLU:HA	1:F:301:ILE:HD12	1.76	0.67
1:A:194:ILE:HG23	1:A:201:MET:HE1	1.77	0.67
2:D:161:LEU:HD11	2:D:170:VAL:HG12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:545:ILE:O	1:E:549:PHE:HD1	1.78	0.67
1:A:143:LEU:H	1:A:143:LEU:CD1	2.07	0.66
2:D:391:MET:HB2	2:D:443:MET:HE3	1.77	0.66
1:A:235:TYR:HA	1:A:238:LEU:CD2	2.25	0.66
2:D:529:VAL:HG12	2:D:531:GLY:H	1.59	0.66
1:E:224:CYS:SG	1:E:269:LEU:HD11	2.34	0.66
1:F:381:PRO:HA	1:F:407:ARG:HB2	1.77	0.66
3:I:6:DT:H2''	3:I:7:DC:O5'	1.95	0.66
2:D:289:GLU:HB3	2:D:415:ILE:HG22	1.77	0.66
1:E:149:MET:O	1:E:153:GLN:HG2	1.94	0.66
1:E:344:TYR:CE2	1:E:353:LYS:HD3	2.31	0.66
1:E:452:LYS:O	1:E:477:ASN:ND2	2.29	0.66
1:E:316:SER:HA	1:E:366:GLN:HG3	1.78	0.66
1:E:189:VAL:HG11	1:E:200:PHE:CE2	2.31	0.66
1:E:588:MET:HG2	1:E:589:ARG:H	1.61	0.65
1:E:134:THR:HG23	1:E:215:ARG:NH1	2.10	0.65
1:F:486:ARG:HA	1:F:588:MET:O	1.95	0.65
2:D:159:THR:HG21	2:D:172:TRP:CZ3	2.31	0.65
2:D:308:ILE:HA	2:D:312:TYR:HD2	1.61	0.65
1:E:542:LEU:O	1:E:545:ILE:HG13	1.96	0.65
1:F:113:MET:HE3	1:F:119:LYS:HG2	1.77	0.65
1:E:283:ARG:HB3	1:E:286:LEU:HD12	1.79	0.65
1:E:554:TYR:CE2	1:E:575:LYS:HE2	2.32	0.65
2:D:79:VAL:HG22	2:D:125:LEU:HD21	1.79	0.65
2:D:336:LYS:HD2	2:D:336:LYS:O	1.96	0.65
1:F:140:LEU:HB2	1:F:143:LEU:HD22	1.77	0.65
1:E:176:GLU:OE1	1:E:182:SER:OG	2.15	0.64
1:A:494:ARG:HD3	1:A:579:LEU:HD22	1.79	0.64
1:C:144:MET:HE3	1:C:160:MET:HB2	1.78	0.64
1:C:492:TYR:HD2	1:C:519:TRP:HZ2	1.45	0.64
2:D:190:THR:HG23	2:D:193:LYS:H	1.62	0.64
2:D:140:LEU:HD22	2:D:142:SER:HB2	1.80	0.64
1:E:509:LYS:HB2	1:E:569:TYR:CD2	2.33	0.64
1:F:148:LEU:HD11	1:F:160:MET:HB3	1.78	0.64
1:B:143:LEU:HD12	1:B:143:LEU:H	1.63	0.64
1:B:70:LYS:CD	1:B:73:PHE:HD2	2.11	0.64
1:E:509:LYS:HB2	1:E:569:TYR:HD2	1.63	0.64
2:D:258:THR:O	2:D:261:VAL:N	2.30	0.63
2:D:376:MET:HE2	2:D:404:ARG:HD2	1.81	0.63
1:F:431:VAL:HG23	1:F:432:MET:HE1	1.80	0.63
1:F:529:VAL:HG12	1:F:531:GLY:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLU:OE2	1:A:487:LYS:NZ	2.26	0.63
1:E:334:LEU:HD22	1:E:341:ALA:HB2	1.80	0.63
2:D:268:ILE:HG22	2:D:269:LEU:HD23	1.79	0.63
1:F:331:THR:HG21	1:F:343:ALA:HB2	1.81	0.63
1:A:386:VAL:HG23	1:A:405:ALA:HB2	1.81	0.63
1:B:81:ASP:OD1	1:B:85:ASN:ND2	2.31	0.63
1:C:451:ASN:OD1	1:C:589:ARG:NH1	2.32	0.63
2:D:136:VAL:HG22	2:D:217:ALA:HB3	1.81	0.63
1:E:317:GLY:O	1:E:367:VAL:HA	1.99	0.63
1:F:422:ASP:O	1:F:426:ILE:HD12	1.99	0.63
1:E:136:VAL:HG22	1:E:217:ALA:HB3	1.79	0.62
2:D:134:THR:HB	2:D:186:LEU:HD23	1.79	0.62
1:A:141:ILE:H	1:A:141:ILE:HD12	1.63	0.62
2:D:286:LEU:O	2:D:455:ARG:NH2	2.32	0.62
1:F:144:MET:HE2	1:F:188:TYR:HB3	1.81	0.62
1:A:262:LEU:O	1:A:266:GLN:HG3	1.99	0.62
1:E:140:LEU:HB2	1:E:143:LEU:HG	1.81	0.62
1:B:449:ASN:HD21	1:B:452:LYS:HD2	1.64	0.62
1:E:193:LYS:HG3	1:E:200:PHE:CD2	2.34	0.62
1:A:307:LEU:HD11	1:A:311:ARG:HH21	1.63	0.62
1:A:349:GLU:CD	1:A:349:GLU:H	2.06	0.62
2:D:320:TYR:OH	2:D:376:MET:HE3	2.00	0.62
4:L:1:DA:H1'	4:L:2:DG:H5'	1.81	0.62
2:D:395:MET:O	2:D:398:TYR:N	2.33	0.62
2:D:488:ASN:OD1	2:D:490:THR:HG23	1.99	0.62
1:B:432:MET:HE3	1:C:195:ALA:HA	1.82	0.61
1:E:462:PHE:HB3	1:E:465:VAL:HG23	1.82	0.61
1:E:579:LEU:HD23	1:E:584:HIS:CD2	2.35	0.61
1:F:242:LYS:NZ	1:F:248:ALA:O	2.32	0.61
1:F:391:MET:HE2	1:F:443:MET:HG3	1.82	0.61
1:A:345:HIS:HA	1:A:374:PHE:CE1	2.35	0.61
2:D:300:PHE:CE2	2:D:304:ILE:HD11	2.35	0.61
1:F:328:GLU:O	1:F:332:ILE:HD12	2.00	0.61
1:F:354:THR:HA	1:F:358:ARG:HB3	1.81	0.61
1:A:144:MET:SD	1:A:160:MET:HG3	2.40	0.61
1:E:312:TYR:HA	1:E:315:GLN:CD	2.25	0.61
1:F:359:ARG:C	1:F:360:TRP:HE3	2.08	0.61
1:F:96:GLN:O	1:F:100:ILE:HG13	2.00	0.61
1:E:96:GLN:O	1:E:100:ILE:HD12	2.00	0.61
1:E:453:CYS:SG	1:E:471:CYS:HB2	2.41	0.61
1:A:85:ASN:O	1:A:88:LYS:NZ	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:ILE:HD12	2:D:301:ILE:H	1.65	0.61
1:A:340:PRO:HB2	1:A:365:ILE:HA	1.83	0.60
1:C:469:GLU:N	8:C:1005:PO4:O3	2.31	0.60
1:F:289:GLU:HG3	1:F:476:ASP:HB3	1.83	0.60
1:B:371:THR:O	1:B:376:MET:HE3	2.02	0.60
2:D:169:HIS:O	2:D:173:VAL:HG23	2.00	0.60
1:E:520:MET:HE3	1:E:542:LEU:HD22	1.83	0.60
2:D:138:CYS:HB2	2:D:144:MET:SD	2.41	0.60
2:D:381:PRO:HA	2:D:407:ARG:HB2	1.84	0.60
1:E:451:ASN:ND2	1:E:589:ARG:HH21	1.99	0.60
1:F:378:ILE:CD1	1:F:379:ASP:H	2.12	0.60
2:D:157:SER:OG	2:D:183:LYS:O	2.20	0.60
1:B:495:ASP:HB3	1:B:532:LEU:HD21	1.84	0.60
2:D:87:PHE:HB3	2:D:89:LEU:HD13	1.84	0.60
1:A:235:TYR:HA	1:A:238:LEU:HD23	1.83	0.60
1:B:100:ILE:HG23	1:B:126:PRO:HG3	1.82	0.60
1:A:173:VAL:O	1:A:177:MET:HG3	2.01	0.59
2:D:224:CYS:HA	2:D:235:TYR:HB3	1.84	0.59
1:E:574:PRO:O	1:E:577:ASN:ND2	2.34	0.59
1:F:495:ASP:HB3	1:F:532:LEU:HD11	1.84	0.59
2:D:578:LEU:HD21	2:D:584:HIS:CG	2.36	0.59
2:D:235:TYR:HA	2:D:238:LEU:CD2	2.32	0.59
1:B:161:LEU:HD11	1:B:170:VAL:HG22	1.83	0.59
1:C:286:LEU:O	1:C:455:ARG:NH2	2.36	0.59
1:B:463:ASP:OD1	1:B:463:ASP:N	2.35	0.59
1:E:100:ILE:HG23	1:E:126:PRO:HG3	1.84	0.59
2:D:384:ARG:NH2	2:D:408:ASP:OD2	2.35	0.59
2:D:480:LYS:HG3	2:D:482:ILE:HD11	1.84	0.59
1:A:344:TYR:O	1:A:345:HIS:ND1	2.35	0.59
1:B:258:THR:HG23	1:B:261:VAL:HB	1.85	0.58
2:D:324:GLN:O	2:D:328:GLU:HG3	2.03	0.58
1:E:328:GLU:H	1:E:345:HIS:HE1	1.51	0.58
2:D:264:ASP:C	2:D:266:GLN:H	2.10	0.58
1:A:143:LEU:HD12	1:A:143:LEU:N	2.14	0.58
2:D:140:LEU:CD2	2:D:142:SER:H	2.16	0.58
1:B:355:LYS:HZ3	1:B:358:ARG:NE	1.92	0.58
2:D:149:MET:SD	2:D:149:MET:N	2.77	0.58
2:D:453:CYS:O	2:D:457:LEU:HD12	2.04	0.58
1:E:347:ASN:OD1	1:E:348:MET:N	2.32	0.58
1:E:265:ALA:HA	1:E:268:ILE:HG13	1.86	0.58
2:D:113:MET:HG3	2:D:279:ALA:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:397:ASN:C	2:D:401:GLU:CG	2.77	0.58
2:D:498:LYS:HA	2:D:501:LYS:HE3	1.86	0.58
1:E:234:ASP:OD1	1:E:234:ASP:N	2.37	0.58
1:E:518:SER:OG	1:E:527:LEU:O	2.17	0.58
1:A:208:TYR:CE2	1:A:245:PHE:HA	2.38	0.58
1:C:318:ILE:HB	1:C:386:VAL:HG22	1.86	0.57
2:D:163:ALA:CB	2:D:192:GLU:OE1	2.51	0.57
2:D:394:SER:OG	2:D:397:ASN:OD1	2.22	0.57
1:E:308:ILE:HA	1:E:312:TYR:HB2	1.85	0.57
1:A:370:ALA:HB1	1:A:374:PHE:HE2	1.69	0.57
1:B:135:LEU:HD22	1:B:204:LEU:HD21	1.86	0.57
1:B:502:GLN:HE21	1:B:506:LEU:HD11	1.68	0.57
2:D:159:THR:HG21	2:D:172:TRP:HZ3	1.68	0.57
2:D:323:SER:HA	3:I:17:DC:H5''	1.86	0.57
2:D:316:SER:HB2	2:D:382:ASP:O	2.04	0.57
1:E:169:HIS:O	1:E:173:VAL:HG13	2.04	0.57
1:E:324:GLN:HE22	1:E:347:ASN:ND2	2.02	0.57
3:G:6:DT:H2''	3:G:7:DC:O5'	2.02	0.57
2:D:283:ARG:NH2	2:D:405:ALA:O	2.38	0.57
1:E:147:GLN:HG3	1:E:151:LEU:HD11	1.84	0.57
1:F:395:MET:HG3	1:F:461:HIS:CE1	2.39	0.57
2:D:92:PHE:HD2	2:D:97:LEU:HB2	1.69	0.57
1:B:286:LEU:O	1:B:455:ARG:NH2	2.32	0.57
1:B:401:GLU:O	1:B:404:ARG:HG3	2.05	0.57
2:D:75:TRP:O	2:D:78:LYS:HB3	2.04	0.57
1:C:383:VAL:HB	1:C:405:ALA:HA	1.87	0.57
1:E:357:HIS:CE1	1:E:358:ARG:HG3	2.40	0.57
1:E:554:TYR:CE2	1:E:586:ILE:HD12	2.40	0.57
1:F:562:THR:OG1	1:F:565:ALA:O	2.23	0.57
1:F:239:GLY:O	1:F:243:ARG:HG3	2.04	0.57
1:F:431:VAL:HG23	1:F:432:MET:CE	2.35	0.57
1:A:326:ASP:O	1:A:330:VAL:HG23	2.05	0.56
1:A:344:TYR:CZ	1:A:353:LYS:NZ	2.73	0.56
2:D:140:LEU:HD23	2:D:141:ILE:N	2.20	0.56
1:E:360:TRP:CD1	1:E:380:LYS:HZ2	2.23	0.56
2:D:83:LEU:HG	2:D:92:PHE:CE1	2.40	0.56
1:E:374:PHE:HE2	1:E:404:ARG:HD2	1.70	0.56
1:A:429:MET:O	3:G:17:DC:N4	2.37	0.56
2:D:305:VAL:HG21	2:D:337:LEU:HG	1.87	0.56
2:D:519:TRP:CH2	2:D:545:ILE:HD11	2.40	0.56
1:E:113:MET:HG2	1:E:119:LYS:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ALA:HA	1:B:268:ILE:HB	1.85	0.56
1:E:281:PHE:CE2	1:E:465:VAL:HB	2.40	0.56
1:B:296:ASN:HD22	1:B:299:ASP:CG	2.14	0.56
1:E:381:PRO:HA	1:E:407:ARG:HB2	1.86	0.56
3:G:3:DA:H2'	3:G:4:DT:H71	1.87	0.56
1:B:242:LYS:NZ	1:B:248:ALA:O	2.37	0.56
1:F:387:ILE:HD13	1:F:415:ILE:HB	1.86	0.56
1:B:355:LYS:O	1:B:359:ARG:HG3	2.06	0.56
1:C:392:SER:H	1:C:443:MET:HE2	1.71	0.56
1:F:328:GLU:O	1:F:331:THR:OG1	2.17	0.56
1:B:92:PHE:CE2	1:B:97:LEU:HD13	2.40	0.56
2:D:429:MET:HE2	3:I:16:DC:C1'	2.34	0.56
2:D:373:ALA:HA	3:I:18:DC:H4'	1.88	0.56
1:E:301:ILE:H	1:E:301:ILE:HD12	1.70	0.56
2:D:147:GLN:O	2:D:151:LEU:HD12	2.06	0.56
2:D:455:ARG:HG2	2:D:466:TRP:HZ2	1.71	0.56
1:E:219:ASP:OD2	1:E:220:GLU:N	2.39	0.56
1:F:525:SER:HB3	3:K:8:DG:OP1	2.06	0.56
3:I:8:DG:H2''	3:I:9:DA:C8	2.41	0.56
1:B:167:LYS:HD3	1:B:167:LYS:N	2.20	0.55
2:D:227:TRP:HE3	2:D:260:HIS:NE2	2.04	0.55
1:F:292:GLN:OE1	1:F:544:LYS:NZ	2.30	0.55
1:F:292:GLN:HG2	1:F:540:GLU:OE1	2.06	0.55
2:D:348:MET:HE2	2:D:348:MET:HA	1.89	0.55
1:E:97:LEU:O	1:E:101:ASN:ND2	2.38	0.55
1:E:130:SER:O	1:E:185:LYS:NZ	2.38	0.55
1:F:371:THR:HG23	1:F:373:ALA:H	1.72	0.55
1:A:451:ASN:HD22	1:A:589:ARG:NE	2.04	0.55
1:B:173:VAL:HG12	1:B:177:MET:HE2	1.86	0.55
1:B:540:GLU:N	1:B:540:GLU:OE1	2.38	0.55
1:B:541:ASP:O	1:B:545:ILE:HG12	2.07	0.55
1:C:150:VAL:O	1:C:154:LEU:HD13	2.06	0.55
1:E:490:THR:HG22	1:E:586:ILE:H	1.71	0.55
1:F:198:LYS:HD2	1:F:198:LYS:N	2.22	0.55
1:F:547:ALA:O	1:F:551:ILE:HD12	2.07	0.55
4:J:2:DG:H2''	4:J:3:DA:C8	2.42	0.55
1:E:343:ALA:HB1	1:E:345:HIS:NE2	2.22	0.55
3:I:7:DC:H2'	3:I:8:DG:C8	2.42	0.55
2:D:265:ALA:HA	2:D:268:ILE:HB	1.88	0.55
2:D:278:THR:HG21	2:D:465:VAL:HA	1.88	0.55
2:D:490:THR:HG22	2:D:586:ILE:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:MET:HB3	1:E:353:LYS:HG2	1.87	0.55
3:K:17:DC:H1'	3:K:18:DC:H5'	1.88	0.55
1:A:286:LEU:O	1:A:455:ARG:NH2	2.32	0.55
2:D:243:ARG:NH2	1:E:434:ASN:O	2.30	0.55
2:D:541:ASP:O	2:D:545:ILE:HG23	2.06	0.55
1:E:319:ILE:HG12	1:E:387:ILE:HB	1.89	0.55
2:D:304:ILE:O	2:D:308:ILE:HG22	2.07	0.55
1:A:411:LYS:HD2	1:A:474:MET:HE1	1.88	0.55
1:E:395:MET:HE3	1:E:395:MET:O	2.07	0.55
1:F:114:PRO:HG3	1:F:281:PHE:CD2	2.42	0.55
1:C:242:LYS:NZ	1:C:248:ALA:O	2.39	0.54
1:E:98:GLU:OE1	1:E:98:GLU:N	2.37	0.54
1:E:345:HIS:HB2	1:E:348:MET:HE2	1.88	0.54
2:D:234:ASP:OD2	2:D:234:ASP:N	2.38	0.54
2:D:305:VAL:HG11	2:D:337:LEU:HD12	1.89	0.54
2:D:397:ASN:O	2:D:401:GLU:HG2	2.06	0.54
1:B:70:LYS:HE2	1:B:101:ASN:CG	2.31	0.54
1:B:189:VAL:HG11	1:B:200:PHE:CZ	2.42	0.54
1:B:258:THR:O	1:B:261:VAL:N	2.40	0.54
2:D:109:VAL:HG12	2:D:251:ILE:HD12	1.88	0.54
2:D:170:VAL:O	2:D:174:HIS:ND1	2.40	0.54
2:D:227:TRP:HE3	2:D:260:HIS:CE1	2.26	0.54
2:D:244:GLN:O	2:D:246:PRO:HD3	2.07	0.54
1:E:449:ASN:HA	1:E:589:ARG:HH22	1.73	0.54
1:B:113:MET:HE2	1:B:119:LYS:HG3	1.88	0.54
1:E:383:VAL:CG2	1:E:405:ALA:HA	2.38	0.54
2:D:393:LYS:O	2:D:440:LEU:HA	2.08	0.54
1:E:124:GLN:O	1:E:128:LEU:HD23	2.08	0.54
1:B:112:VAL:HG11	1:B:257:ALA:HB2	1.89	0.54
1:B:435:VAL:HG13	1:B:439:LYS:HE2	1.89	0.54
2:D:163:ALA:HB2	2:D:192:GLU:OE1	2.07	0.54
1:E:114:PRO:HG3	1:E:281:PHE:CD1	2.43	0.54
1:E:487:LYS:NZ	1:E:590:VAL:H	2.00	0.54
1:F:225:SER:HB2	1:F:264:ASP:HB3	1.90	0.54
1:A:202:SER:OG	1:A:203:ARG:N	2.40	0.54
1:A:370:ALA:CB	1:A:374:PHE:HE2	2.21	0.54
1:E:380:LYS:HD3	1:E:381:PRO:HD2	1.90	0.54
1:F:355:LYS:O	1:F:359:ARG:HD3	2.06	0.54
1:A:320:TYR:OH	1:A:404:ARG:NH1	2.41	0.53
2:D:301:ILE:HA	2:D:304:ILE:HG13	1.90	0.53
2:D:497:ILE:O	2:D:501:LYS:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:ALA:O	1:E:269:LEU:HD13	2.08	0.53
2:D:82:VAL:HA	2:D:86:VAL:HG23	1.90	0.53
1:E:318:ILE:HG12	1:E:360:TRP:HH2	1.72	0.53
1:B:428:SER:OG	1:B:566:THR:O	2.22	0.53
2:D:75:TRP:O	2:D:79:VAL:N	2.42	0.53
2:D:220:GLU:OE1	2:D:220:GLU:HA	2.09	0.53
1:F:493:CYS:O	1:F:497:ILE:HG13	2.07	0.53
3:I:3:DA:H2'	3:I:4:DT:H71	1.91	0.53
1:B:110:PHE:CE1	1:B:266:GLN:HG2	2.39	0.53
4:J:14:DC:H2''	4:J:15:DC:C6	2.44	0.53
2:D:135:LEU:HD21	2:D:204:LEU:HD11	1.91	0.53
2:D:144:MET:HG3	2:D:160:MET:HG3	1.89	0.53
2:D:359:ARG:HB3	2:D:365:ILE:HG23	1.91	0.53
1:E:86:VAL:O	1:E:154:LEU:HD21	2.09	0.53
1:B:110:PHE:CE2	1:B:252:GLY:HA3	2.43	0.53
1:C:492:TYR:HD2	1:C:519:TRP:CZ2	2.26	0.53
2:D:500:LEU:HD11	2:D:571:LYS:HA	1.91	0.53
1:E:311:ARG:HG2	1:E:311:ARG:HH11	1.73	0.53
1:E:386:VAL:HG23	1:E:405:ALA:HB2	1.91	0.53
3:G:8:DG:H2''	3:G:9:DA:C8	2.44	0.53
1:B:205:GLU:OE1	1:C:561:PHE:N	2.38	0.53
1:B:349:GLU:CD	1:B:349:GLU:H	2.17	0.53
1:B:426:ILE:O	1:B:430:VAL:HG22	2.08	0.53
2:D:98:GLU:OE1	2:D:98:GLU:N	2.28	0.53
2:D:147:GLN:C	2:D:151:LEU:HD12	2.34	0.53
1:B:140:LEU:HB2	1:B:143:LEU:CD1	2.39	0.53
2:D:312:TYR:CE1	2:D:385:PHE:HB3	2.44	0.53
1:F:569:TYR:HE1	4:L:4:DG:OP1	1.91	0.53
1:A:208:TYR:HD2	1:A:245:PHE:HD1	1.55	0.52
1:A:359:ARG:HD2	1:A:364:GLU:OE1	2.09	0.52
1:E:97:LEU:HG	1:E:101:ASN:HD21	1.74	0.52
1:F:476:ASP:OD1	1:F:476:ASP:N	2.41	0.52
3:I:8:DG:H2''	3:I:9:DA:H8	1.73	0.52
1:E:189:VAL:HG11	1:E:200:PHE:CZ	2.45	0.52
1:E:577:ASN:OD1	1:E:578:LEU:N	2.42	0.52
2:D:462:PHE:HB3	2:D:465:VAL:HG23	1.91	0.52
1:E:338:GLY:C	1:E:339:ILE:HD13	2.35	0.52
1:E:386:VAL:HG11	1:E:402:SER:HA	1.91	0.52
1:F:393:LYS:NZ	3:K:17:DC:C2	2.77	0.52
2:D:308:ILE:HG13	2:D:312:TYR:HB2	1.92	0.52
1:C:292:GLN:HE22	1:C:544:LYS:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:PRO:HB2	2:D:234:ASP:HB2	1.92	0.52
2:D:260:HIS:NE2	2:D:261:VAL:HG23	2.23	0.52
2:D:495:ASP:O	2:D:499:ILE:HG13	2.09	0.52
1:E:149:MET:HE2	1:E:153:GLN:HE21	1.74	0.52
1:E:209:GLU:O	1:E:211:ARG:NH1	2.43	0.52
1:E:379:ASP:OD2	6:E:1002:ADP:H4'	2.10	0.52
1:A:250:LEU:HD22	1:A:271:VAL:HG21	1.92	0.52
1:B:224:CYS:HB2	1:B:265:ALA:CB	2.40	0.52
1:C:231:PHE:HE1	1:C:233:PRO:HA	1.75	0.52
1:E:200:PHE:CE1	1:E:204:LEU:HD11	2.45	0.52
1:A:354:THR:HG22	1:A:358:ARG:HD2	1.91	0.52
1:F:579:LEU:HD21	1:F:586:ILE:HD11	1.91	0.52
2:D:272:GLU:HG2	2:D:273:LYS:N	2.25	0.52
2:D:323:SER:OG	2:D:324:GLN:N	2.41	0.52
1:F:161:LEU:HB3	1:F:189:VAL:HG12	1.92	0.52
1:F:428:SER:OG	1:F:568:SER:HB2	2.09	0.52
1:B:380:LYS:HG2	1:B:381:PRO:HD2	1.91	0.52
1:A:391:MET:HE1	1:A:444:VAL:HG22	1.93	0.51
1:E:359:ARG:HB3	1:E:365:ILE:HD12	1.92	0.51
1:F:510:LEU:HD11	1:F:527:LEU:HD22	1.91	0.51
1:A:335:GLN:NE2	1:A:341:ALA:O	2.41	0.51
1:B:112:VAL:HG21	1:B:262:LEU:HD11	1.92	0.51
2:D:99:THR:HG22	2:D:277:PHE:HD2	1.75	0.51
1:F:305:VAL:HG21	1:F:337:LEU:HD12	1.92	0.51
1:E:398:TYR:CD2	1:E:443:MET:HE1	2.45	0.51
1:A:119:LYS:HD2	1:A:253:LEU:HB3	1.91	0.51
2:D:486:ARG:HG3	2:D:486:ARG:HH11	1.74	0.51
1:F:409:ASP:O	1:F:409:ASP:OD2	2.29	0.51
3:I:7:DC:H2'	3:I:8:DG:H8	1.72	0.51
3:K:8:DG:H2''	3:K:9:DA:C8	2.45	0.51
1:B:387:ILE:HG12	1:B:415:ILE:HB	1.92	0.51
1:C:372:VAL:HG23	1:C:372:VAL:O	2.11	0.51
2:D:140:LEU:HD13	2:D:143:LEU:HG	1.92	0.51
1:E:516:ILE:HD11	1:E:542:LEU:HB3	1.93	0.51
1:A:108:GLU:HG3	1:A:250:LEU:HB3	1.90	0.51
2:D:387:ILE:HG12	2:D:415:ILE:HD11	1.93	0.51
1:F:360:TRP:HZ2	1:F:368:VAL:HG22	1.76	0.51
1:A:315:GLN:HB3	1:A:384:ARG:HG3	1.91	0.51
1:A:371:THR:N	1:A:374:PHE:CD2	2.79	0.51
1:C:235:TYR:HA	1:C:238:LEU:HG	1.91	0.51
1:E:134:THR:HG22	1:E:136:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:PHE:HE1	1:E:204:LEU:HD11	1.76	0.51
3:K:13:DT:H1'	3:K:14:DC:H5'	1.91	0.51
1:C:348:MET:HG2	1:C:349:GLU:OE1	2.10	0.51
1:E:281:PHE:HD2	1:E:465:VAL:HB	1.75	0.51
1:F:283:ARG:HB2	1:F:286:LEU:HD12	1.93	0.51
1:F:495:ASP:O	1:F:499:ILE:HD12	2.11	0.51
1:A:371:THR:O	1:A:374:PHE:HD2	1.93	0.51
1:C:452:LYS:O	1:C:477:ASN:ND2	2.43	0.51
2:D:127:ALA:O	2:D:185:LYS:NZ	2.38	0.51
1:E:293:LYS:NZ	1:E:422:ASP:OD2	2.40	0.51
1:F:545:ILE:HA	1:F:588:MET:HE1	1.93	0.51
1:B:173:VAL:O	1:B:177:MET:HG3	2.11	0.51
2:D:296:ASN:OD1	2:D:299:ASP:N	2.32	0.51
1:C:305:VAL:HG12	1:C:339:ILE:HG13	1.93	0.50
1:E:120:SER:HA	1:E:123:TYR:CE2	2.46	0.50
1:E:344:TYR:HE2	1:E:353:LYS:CD	2.18	0.50
1:E:480:LYS:CD	1:E:482:ILE:H	2.23	0.50
1:E:493:CYS:O	1:E:497:ILE:HG13	2.11	0.50
1:B:300:PHE:HE2	1:B:389:HIS:CD2	2.29	0.50
1:B:355:LYS:NZ	1:B:358:ARG:HE	1.97	0.50
1:E:420:PHE:CG	1:E:543:GLU:HB3	2.46	0.50
1:E:486:ARG:HE	1:E:587:THR:HG21	1.76	0.50
2:D:208:TYR:HB2	2:D:213:PHE:HD2	1.75	0.50
1:E:541:ASP:O	1:E:545:ILE:HG23	2.11	0.50
1:F:170:VAL:HG13	1:F:174:HIS:CE1	2.46	0.50
1:F:301:ILE:HA	1:F:304:ILE:HD12	1.93	0.50
1:F:390:SER:HG	1:F:425:ARG:NH2	2.09	0.50
1:C:69:ASN:HD22	1:C:97:LEU:HD23	1.76	0.50
2:D:535:PRO:HG2	2:D:542:LEU:HD21	1.94	0.50
1:E:200:PHE:CE1	1:E:204:LEU:CD1	2.95	0.50
1:E:486:ARG:HG3	1:E:587:THR:HB	1.92	0.50
1:E:549:PHE:HA	1:E:554:TYR:CD1	2.46	0.50
1:E:578:LEU:HD22	1:E:584:HIS:NE2	2.27	0.50
1:F:325:LYS:NZ	3:K:15:DT:OP1	2.44	0.50
1:F:343:ALA:O	1:F:356:VAL:HG21	2.11	0.50
1:B:78:LYS:HG2	1:B:129:CYS:HB3	1.92	0.50
1:B:432:MET:HE1	1:C:240:ILE:HG21	1.94	0.50
2:D:487:LYS:HD3	2:D:488:ASN:H	1.77	0.50
1:F:360:TRP:CH2	1:F:365:ILE:HG12	2.47	0.50
2:D:359:ARG:HA	2:D:359:ARG:NE	2.27	0.50
1:E:444:VAL:HG12	1:E:551:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:SER:OG	1:F:425:ARG:NH2	2.45	0.50
1:C:162:ASN:OD1	1:C:162:ASN:N	2.45	0.50
1:C:324:GLN:HA	1:C:371:THR:HG21	1.94	0.50
1:C:495:ASP:HB3	1:C:532:LEU:HD21	1.93	0.50
2:D:227:TRP:CE3	2:D:260:HIS:NE2	2.80	0.50
1:F:151:LEU:HB3	1:F:156:ILE:HB	1.93	0.50
1:A:159:THR:HB	1:A:184:LEU:HD11	1.93	0.50
2:D:387:ILE:HG23	2:D:415:ILE:HD11	1.94	0.50
1:A:113:MET:HE2	1:A:117:GLY:C	2.37	0.50
1:A:370:ALA:HB1	1:A:374:PHE:CE2	2.45	0.50
1:B:319:ILE:HB	1:B:369:VAL:HG12	1.94	0.50
1:C:242:LYS:HG2	1:C:271:VAL:HG12	1.94	0.50
2:D:294:PRO:HG2	2:D:300:PHE:HB2	1.93	0.50
1:E:242:LYS:HE2	1:E:270:CYS:O	2.12	0.50
1:B:291:ARG:HB2	1:B:417:TYR:CE1	2.47	0.49
1:B:379:ASP:OD1	1:B:404:ARG:NH2	2.42	0.49
2:D:219:ASP:OD1	2:D:220:GLU:N	2.46	0.49
2:D:511:THR:HG22	2:D:514:LYS:HG3	1.94	0.49
1:E:98:GLU:HA	1:E:101:ASN:HD22	1.78	0.49
1:A:168:GLU:H	1:A:168:GLU:CD	2.21	0.49
2:D:229:HIS:CD2	2:D:256:THR:HG21	2.48	0.49
1:E:383:VAL:HG23	1:E:405:ALA:HA	1.92	0.49
1:F:365:ILE:HD13	1:F:367:VAL:O	2.13	0.49
1:E:345:HIS:HD2	1:E:348:MET:HE3	1.77	0.49
1:E:387:ILE:HA	1:E:415:ILE:HD13	1.95	0.49
1:E:549:PHE:O	1:E:554:TYR:HD1	1.96	0.49
1:F:300:PHE:HE1	1:F:417:TYR:CD2	2.31	0.49
1:F:343:ALA:HA	1:F:369:VAL:O	2.12	0.49
1:A:328:GLU:O	1:A:332:ILE:HD12	2.13	0.49
1:B:286:LEU:HD13	1:B:414:CYS:SG	2.52	0.49
1:B:349:GLU:O	1:B:353:LYS:HG3	2.11	0.49
1:C:495:ASP:O	1:C:499:ILE:HG13	2.11	0.49
1:E:450:ILE:HD12	1:E:477:ASN:OD1	2.12	0.49
1:F:347:ASN:OD1	1:F:347:ASN:N	2.44	0.49
1:A:454:ARG:O	1:A:458:ILE:HG13	2.12	0.49
2:D:286:LEU:CD1	2:D:403:GLY:HA2	2.42	0.49
1:E:170:VAL:O	1:E:173:VAL:HG22	2.12	0.49
1:E:327:SER:O	1:E:331:THR:HG23	2.12	0.49
1:A:149:MET:HE1	1:A:353:LYS:HD2	1.95	0.49
1:A:271:VAL:HG12	1:A:274:CYS:HB2	1.94	0.49
2:D:291:ARG:HH22	2:D:307:LEU:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:VAL:HG23	1:F:405:ALA:HB2	1.93	0.49
3:G:7:DC:H2'	3:G:8:DG:C8	2.48	0.49
2:D:67:SER:C	2:D:70:LYS:HZ3	2.14	0.49
1:E:220:GLU:OE1	1:E:222:HIS:NE2	2.46	0.49
1:F:378:ILE:HD12	1:F:379:ASP:N	2.19	0.49
3:K:16:DC:H6	3:K:16:DC:O5'	1.96	0.49
1:A:120:SER:O	1:A:124:GLN:HG3	2.13	0.49
2:D:517:ASP:HB3	2:D:522:LYS:O	2.13	0.49
1:F:76:SER:HA	1:F:79:VAL:HG22	1.95	0.49
1:E:179:ASN:O	1:E:182:SER:HB2	2.13	0.48
1:F:383:VAL:HB	1:F:405:ALA:HA	1.93	0.48
1:F:364:GLU:OE1	1:F:364:GLU:N	2.41	0.48
1:F:497:ILE:O	1:F:501:LYS:HG3	2.12	0.48
1:A:166:PRO:O	1:A:170:VAL:HG23	2.13	0.48
1:A:224:CYS:HA	1:A:235:TYR:HB3	1.94	0.48
2:D:140:LEU:HD23	2:D:142:SER:H	1.78	0.48
1:F:161:LEU:HD22	1:F:173:VAL:HG11	1.95	0.48
1:F:486:ARG:HB2	1:F:589:ARG:HD3	1.95	0.48
4:L:1:DA:C6	4:L:2:DG:C2	3.01	0.48
1:A:144:MET:SD	1:A:188:TYR:HB3	2.53	0.48
1:B:140:LEU:HD12	1:B:143:LEU:HD11	1.95	0.48
1:B:322:PHE:CE1	1:B:426:ILE:HG12	2.48	0.48
2:D:113:MET:HG3	2:D:279:ALA:CB	2.42	0.48
1:E:440:LEU:HD12	1:E:440:LEU:O	2.13	0.48
1:E:529:VAL:CB	1:E:532:LEU:HG	2.41	0.48
1:A:371:THR:HB	1:A:374:PHE:HB3	1.94	0.48
1:F:182:SER:HB3	1:F:212:ARG:NH2	2.29	0.48
2:D:140:LEU:CD2	2:D:142:SER:HB2	2.42	0.48
1:A:149:MET:HE1	1:A:353:LYS:CD	2.44	0.48
2:D:380:LYS:O	2:D:407:ARG:HG3	2.13	0.48
1:E:352:ASP:HA	1:E:355:LYS:HB2	1.96	0.48
1:F:453:CYS:HB3	1:F:456:VAL:HG23	1.94	0.48
1:B:70:LYS:HB2	1:B:71:GLU:HA	1.96	0.48
1:B:161:LEU:HB3	1:B:189:VAL:HG12	1.95	0.48
2:D:216:ILE:HD13	2:D:241:LEU:HB3	1.95	0.48
1:E:451:ASN:OD1	1:E:452:LYS:N	2.47	0.48
3:G:6:DT:H2'	3:G:7:DC:H6	1.74	0.48
1:E:93:ARG:HD2	6:E:1002:ADP:C6	2.49	0.48
1:A:429:MET:HG3	3:G:17:DC:C5	2.49	0.48
1:C:449:ASN:ND2	1:C:452:LYS:HE3	2.19	0.48
2:D:138:CYS:HB2	2:D:144:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:THR:HG23	2:D:193:LYS:N	2.29	0.48
1:E:133:PHE:HZ	1:E:207:ALA:HB1	1.79	0.48
1:E:484:PHE:CD1	1:E:484:PHE:C	2.92	0.48
1:C:135:LEU:HD21	1:C:194:ILE:HD11	1.96	0.47
2:D:223:CYS:HB2	2:D:235:TYR:CD2	2.49	0.47
1:F:345:HIS:O	1:F:348:MET:HG3	2.13	0.47
1:F:373:ALA:HB2	3:K:18:DC:H5''	1.95	0.47
1:B:195:ALA:HA	1:C:432:MET:HE3	1.95	0.47
2:D:496:LEU:HD22	2:D:515:LEU:HD11	1.96	0.47
1:E:451:ASN:HB2	1:E:484:PHE:CE2	2.48	0.47
1:F:340:PRO:HB2	1:F:365:ILE:HA	1.95	0.47
1:F:352:ASP:HA	1:F:355:LYS:HB2	1.95	0.47
1:F:429:MET:SD	3:K:16:DC:H2''	2.54	0.47
1:A:150:VAL:O	1:A:154:LEU:HD12	2.14	0.47
1:F:100:ILE:HG23	1:F:126:PRO:HG3	1.95	0.47
1:B:575:LYS:O	1:B:578:LEU:HB2	2.14	0.47
2:D:500:LEU:HB3	2:D:572:VAL:HG22	1.96	0.47
2:D:508:GLU:OE2	2:D:526:LYS:NZ	2.45	0.47
1:F:119:LYS:HB3	1:F:253:LEU:HD13	1.95	0.47
3:K:5:DC:H2'	3:K:6:DT:H72	1.97	0.47
1:A:429:MET:HG3	3:G:17:DC:C4	2.50	0.47
1:B:92:PHE:CD2	1:B:97:LEU:HD13	2.49	0.47
1:E:399:TYR:HE2	1:E:466:TRP:CZ3	2.32	0.47
1:F:293:LYS:NZ	1:F:422:ASP:OD2	2.40	0.47
1:C:163:ALA:HB2	1:C:192:GLU:OE2	2.14	0.47
2:D:138:CYS:HB2	2:D:144:MET:HE1	1.96	0.47
2:D:485:GLU:OE2	2:D:487:LYS:HB2	2.15	0.47
1:B:78:LYS:NZ	8:B:1005:PO4:O3	2.28	0.47
1:C:193:LYS:O	1:C:197:SER:HB3	2.15	0.47
2:D:511:THR:HG21	4:J:4:DG:P	2.54	0.47
1:E:65:PRO:O	1:E:98:GLU:HG2	2.14	0.47
1:E:427:SER:HA	1:E:430:VAL:HG22	1.97	0.47
1:E:487:LYS:NZ	1:E:589:ARG:HA	2.30	0.47
1:F:407:ARG:HH11	8:F:1003:PO4:P	2.37	0.47
1:F:529:VAL:HB	1:F:532:LEU:HB2	1.96	0.47
1:A:344:TYR:CE2	1:A:378:ILE:HG22	2.50	0.47
2:D:193:LYS:HG3	2:D:200:PHE:CG	2.49	0.47
1:F:318:ILE:HG12	1:F:374:PHE:HE2	1.80	0.47
2:D:221:VAL:HG12	2:D:253:LEU:O	2.15	0.47
2:D:281:PHE:O	2:D:399:TYR:OH	2.20	0.47
2:D:398:TYR:N	2:D:401:GLU:HG3	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:SER:HA	1:E:336:LYS:HG3	1.97	0.47
1:E:490:THR:CG2	1:E:586:ILE:H	2.28	0.47
2:D:259:SER:HA	2:D:262:LEU:HD13	1.96	0.47
1:F:161:LEU:HG	1:F:193:LYS:HE2	1.96	0.47
1:A:495:ASP:O	1:A:499:ILE:HG13	2.15	0.46
1:A:540:GLU:O	1:A:544:LYS:HD2	2.15	0.46
1:F:384:ARG:NH1	1:F:410:MET:O	2.47	0.46
1:F:485:GLU:HB2	1:F:592:LYS:HB2	1.96	0.46
1:F:541:ASP:O	1:F:545:ILE:HG12	2.13	0.46
1:E:199:MET:HE1	1:E:203:ARG:CZ	2.45	0.46
1:E:316:SER:HB3	1:E:360:TRP:HE1	1.80	0.46
1:E:450:ILE:H	1:E:589:ARG:CZ	2.29	0.46
1:F:552:GLN:O	1:F:575:LYS:HE2	2.15	0.46
1:A:100:ILE:HD13	1:A:125:LEU:HD22	1.97	0.46
1:A:149:MET:O	1:A:153:GLN:HB2	2.16	0.46
1:C:332:ILE:HG13	1:C:333:SER:N	2.29	0.46
2:D:193:LYS:HE2	2:D:193:LYS:HA	1.98	0.46
1:E:81:ASP:O	1:E:85:ASN:N	2.47	0.46
1:F:179:ASN:HB3	1:F:182:SER:HB2	1.96	0.46
1:F:509:LYS:HB3	1:F:569:TYR:CD1	2.50	0.46
1:B:214:THR:O	1:B:248:ALA:HA	2.14	0.46
1:B:259:SER:HA	1:B:262:LEU:HB2	1.97	0.46
1:B:392:SER:O	1:B:443:MET:HG2	2.15	0.46
2:D:83:LEU:HG	2:D:92:PHE:HE1	1.80	0.46
2:D:353:LYS:O	2:D:357:HIS:ND1	2.48	0.46
2:D:362:ALA:HB3	2:D:364:GLU:OE2	2.16	0.46
1:E:71:GLU:OE2	1:E:80:LYS:HD3	2.15	0.46
1:E:189:VAL:HG11	1:E:200:PHE:HE2	1.79	0.46
1:E:345:HIS:CD2	1:E:348:MET:HE3	2.51	0.46
1:F:257:ALA:O	1:F:258:THR:OG1	2.30	0.46
1:A:527:LEU:HD23	1:A:527:LEU:HA	1.80	0.46
2:D:519:TRP:CZ3	2:D:545:ILE:HD11	2.51	0.46
1:F:150:VAL:O	1:F:154:LEU:HD22	2.15	0.46
3:G:7:DC:H2'	3:G:8:DG:H8	1.80	0.46
3:K:1:DG:H2''	3:K:2:DG:C8	2.51	0.46
1:C:64:SER:O	1:C:64:SER:OG	2.34	0.46
1:C:96:GLN:NE2	1:C:118:GLY:O	2.48	0.46
1:C:113:MET:HE2	1:C:119:LYS:HG3	1.98	0.46
1:C:231:PHE:CE1	1:C:233:PRO:HA	2.50	0.46
1:E:545:ILE:HA	1:E:588:MET:HE1	1.98	0.46
1:F:141:ILE:HD12	1:F:162:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:500:LEU:HD11	1:F:555:LEU:HD23	1.98	0.46
1:A:208:TYR:HD2	1:A:245:PHE:CD1	2.34	0.46
1:B:177:MET:HE1	1:B:200:PHE:CE2	2.51	0.46
1:E:350:PRO:HA	1:E:353:LYS:HB2	1.98	0.46
1:B:392:SER:OG	1:B:398:TYR:HB2	2.15	0.46
2:D:305:VAL:O	2:D:309:ASN:ND2	2.49	0.46
1:E:76:SER:HA	1:E:79:VAL:HB	1.98	0.46
1:E:488:ASN:HA	1:E:586:ILE:O	2.16	0.46
3:K:6:DT:H2''	3:K:7:DC:O5'	2.16	0.46
1:A:100:ILE:O	1:A:104:MET:HG2	2.16	0.46
1:B:561:PHE:HE2	1:C:244:GLN:HG3	1.81	0.46
1:C:554:TYR:OH	1:C:584:HIS:NE2	2.33	0.46
2:D:205:GLU:HG3	2:D:244:GLN:NE2	2.31	0.46
2:D:286:LEU:HD11	2:D:403:GLY:HA2	1.98	0.46
1:F:489:VAL:O	1:F:489:VAL:HG22	2.16	0.46
1:A:324:GLN:OE1	1:A:345:HIS:NE2	2.49	0.45
2:D:184:LEU:HD23	2:D:184:LEU:HA	1.72	0.45
1:E:378:ILE:HD12	1:E:379:ASP:H	1.81	0.45
1:E:492:TYR:CD1	1:E:519:TRP:HZ2	2.33	0.45
1:E:545:ILE:HG22	1:E:588:MET:SD	2.56	0.45
1:F:224:CYS:SG	1:F:269:LEU:HD21	2.56	0.45
1:F:324:GLN:NE2	3:K:17:DC:OP1	2.48	0.45
1:F:394:SER:O	1:F:443:MET:HE3	2.16	0.45
1:E:312:TYR:CE1	1:E:385:PHE:HB3	2.51	0.45
1:F:113:MET:HB3	1:F:119:LYS:HG2	1.97	0.45
1:A:256:THR:O	1:A:256:THR:OG1	2.32	0.45
1:A:324:GLN:HE22	1:A:345:HIS:CD2	2.34	0.45
1:A:346:ALA:HB2	1:A:374:PHE:O	2.16	0.45
1:B:70:LYS:HD3	1:B:73:PHE:HD2	1.78	0.45
1:B:141:ILE:HD12	1:B:141:ILE:H	1.82	0.45
1:B:495:ASP:CG	1:B:532:LEU:HD11	2.41	0.45
1:B:526:LYS:HB3	1:B:526:LYS:HE2	1.79	0.45
2:D:388:HIS:HB2	2:D:416:LEU:HD12	1.97	0.45
2:D:519:TRP:HH2	2:D:545:ILE:HD11	1.82	0.45
3:G:8:DG:H2''	3:G:9:DA:H8	1.80	0.45
1:A:323:SER:HB2	3:G:17:DC:OP1	2.16	0.45
1:A:486:ARG:HA	1:A:588:MET:O	2.17	0.45
1:C:128:LEU:HD21	1:C:156:ILE:HD13	1.98	0.45
1:C:348:MET:HG2	1:C:349:GLU:H	1.82	0.45
2:D:320:TYR:HB2	2:D:388:HIS:ND1	2.30	0.45
2:D:398:TYR:O	2:D:401:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:LEU:CD1	2:D:571:LYS:HA	2.46	0.45
1:E:554:TYR:HE2	1:E:586:ILE:HD12	1.80	0.45
1:F:189:VAL:HG11	1:F:200:PHE:CZ	2.52	0.45
1:F:564:TYR:HE1	4:L:1:DA:C6	2.33	0.45
4:H:8:DC:H2''	4:H:9:DG:C8	2.52	0.45
1:A:383:VAL:HB	1:A:405:ALA:HA	1.98	0.45
2:D:219:ASP:OD1	2:D:220:GLU:HG2	2.16	0.45
2:D:259:SER:HA	2:D:262:LEU:HB2	1.98	0.45
1:E:78:LYS:HD2	1:E:78:LYS:HA	1.63	0.45
1:E:328:GLU:HB3	1:E:345:HIS:NE2	2.32	0.45
1:E:485:GLU:OE1	1:E:592:LYS:HG3	2.17	0.45
1:F:427:SER:O	1:F:431:VAL:HG13	2.16	0.45
3:G:10:DC:H2''	3:G:11:DG:C8	2.52	0.45
4:L:2:DG:C2	4:L:3:DA:C6	3.05	0.45
1:A:203:ARG:CZ	1:A:203:ARG:HB2	2.43	0.45
1:B:224:CYS:SG	1:B:235:TYR:HD2	2.38	0.45
2:D:159:THR:HG21	2:D:172:TRP:CH2	2.51	0.45
1:E:95:LEU:HD13	1:E:95:LEU:HA	1.78	0.45
1:E:186:LEU:HD22	1:E:188:TYR:CZ	2.52	0.45
1:E:302:GLU:HA	1:E:305:VAL:HG12	1.98	0.45
3:K:12:DC:H2'	3:K:13:DT:H71	1.97	0.45
1:C:328:GLU:O	1:C:332:ILE:HG23	2.17	0.45
1:A:80:LYS:HA	1:A:80:LYS:HD3	1.61	0.45
1:A:344:TYR:HE2	1:A:375:GLY:O	2.00	0.45
1:A:511:THR:OG1	1:A:514:LYS:HG3	2.17	0.45
1:B:373:ALA:HB3	1:B:376:MET:CE	2.43	0.45
1:B:455:ARG:HH21	1:B:474:MET:HB3	1.82	0.45
1:C:69:ASN:ND2	1:C:97:LEU:HD23	2.32	0.45
1:C:305:VAL:HG12	1:C:334:LEU:HD23	1.99	0.45
2:D:216:ILE:HB	2:D:250:LEU:HD12	1.99	0.45
2:D:272:GLU:HG2	2:D:273:LYS:H	1.81	0.45
2:D:427:SER:HA	2:D:430:VAL:HG22	1.99	0.45
2:D:562:THR:HG22	2:D:563:ALA:N	2.32	0.45
1:E:119:LYS:HG3	6:E:1002:ADP:O3B	2.16	0.45
1:E:147:GLN:HG3	1:E:151:LEU:CD1	2.47	0.45
1:E:313:LYS:O	1:E:313:LYS:HG3	2.16	0.45
1:E:448:GLN:NE2	1:E:544:LYS:O	2.46	0.45
1:A:176:GLU:OE1	1:A:182:SER:HB2	2.17	0.45
1:C:570:LEU:HD23	1:C:570:LEU:HA	1.83	0.45
2:D:135:LEU:HD23	2:D:204:LEU:HD21	1.99	0.45
2:D:578:LEU:HD21	2:D:584:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:LYS:HD2	1:E:473:LYS:O	2.17	0.45
1:F:140:LEU:O	1:F:144:MET:HG3	2.17	0.45
1:F:497:ILE:HA	1:F:500:LEU:HD12	1.99	0.45
1:F:502:GLN:O	1:F:506:LEU:HG	2.17	0.45
1:A:547:ALA:O	1:A:551:ILE:HG12	2.17	0.45
1:B:135:LEU:HD21	1:B:194:ILE:HD11	1.98	0.45
1:B:363:ASN:O	1:B:363:ASN:ND2	2.50	0.45
2:D:76:SER:HA	2:D:79:VAL:HG12	1.99	0.45
2:D:102:VAL:HG13	2:D:107:LYS:HB3	1.99	0.45
2:D:180:LYS:HA	2:D:212:ARG:HD2	1.99	0.45
2:D:480:LYS:HD3	2:D:481:GLU:N	2.32	0.45
2:D:502:GLN:O	2:D:506:LEU:HG	2.17	0.45
1:E:312:TYR:HA	1:E:315:GLN:NE2	2.32	0.45
1:F:108:GLU:OE2	1:F:242:LYS:NZ	2.38	0.45
1:C:65:PRO:O	1:C:98:GLU:HG2	2.17	0.44
1:C:191:PRO:HB2	1:C:234:ASP:HB3	1.99	0.44
2:D:260:HIS:CD2	2:D:261:VAL:N	2.85	0.44
1:E:388:HIS:HB2	1:E:416:LEU:HA	1.99	0.44
1:F:168:GLU:O	1:F:171:LYS:N	2.50	0.44
1:F:511:THR:HG21	4:L:5:DC:OP2	2.16	0.44
1:F:578:LEU:HB3	1:F:584:HIS:CD2	2.52	0.44
1:A:143:LEU:CD1	1:A:143:LEU:N	2.78	0.44
1:B:70:LYS:HE3	1:B:97:LEU:HD11	1.97	0.44
1:B:119:LYS:HB2	1:B:119:LYS:HE2	1.73	0.44
1:E:230:ASP:HB2	1:E:232:ARG:HH21	1.81	0.44
1:F:199:MET:HE3	1:F:203:ARG:HG2	1.99	0.44
1:F:216:ILE:HG21	1:F:241:LEU:HD13	1.99	0.44
1:F:402:SER:HB2	1:F:414:CYS:SG	2.58	0.44
1:C:226:GLN:HA	1:C:231:PHE:CD2	2.52	0.44
1:C:407:ARG:HA	1:C:407:ARG:HD3	1.72	0.44
1:E:168:GLU:N	1:E:168:GLU:OE2	2.51	0.44
1:F:519:TRP:CE2	1:F:535:PRO:HG3	2.52	0.44
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.70	0.44
1:A:171:LYS:HD2	1:A:171:LYS:HA	1.71	0.44
1:A:345:HIS:CA	1:A:374:PHE:CE1	3.00	0.44
1:A:407:ARG:HD3	1:A:407:ARG:HA	1.82	0.44
1:B:216:ILE:HD13	1:B:241:LEU:HB3	1.98	0.44
1:C:135:LEU:HD22	1:C:204:LEU:HD11	2.00	0.44
1:C:496:LEU:HD21	1:C:519:TRP:CE3	2.52	0.44
1:E:133:PHE:CZ	1:E:213:PHE:HB2	2.52	0.44
1:F:380:LYS:HA	1:F:381:PRO:HD3	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:THR:HG23	1:F:586:ILE:HG13	2.00	0.44
1:C:226:GLN:HA	1:C:231:PHE:HD2	1.82	0.44
2:D:179:ASN:HB3	2:D:182:SER:HB2	1.99	0.44
2:D:385:PHE:HA	2:D:413:ASP:O	2.17	0.44
1:E:450:ILE:H	1:E:589:ARG:NH2	2.16	0.44
4:L:2:DG:C2	4:L:3:DA:C5	3.06	0.44
1:A:170:VAL:HG12	1:A:174:HIS:NE2	2.32	0.44
1:B:242:LYS:HG2	1:B:271:VAL:HG12	1.99	0.44
1:B:273:LYS:O	1:B:273:LYS:HG2	2.17	0.44
1:C:360:TRP:CZ3	1:C:378:ILE:HG22	2.51	0.44
2:D:395:MET:HG3	2:D:461:HIS:CE1	2.52	0.44
2:D:519:TRP:CZ3	2:D:542:LEU:HG	2.53	0.44
1:E:147:GLN:O	1:E:151:LEU:HD12	2.18	0.44
1:E:259:SER:CA	1:E:262:LEU:HB2	2.45	0.44
1:E:321:CYS:SG	1:E:327:SER:HA	2.57	0.44
1:E:581:ASN:O	1:E:584:HIS:HB2	2.17	0.44
1:A:199:MET:HB3	1:A:199:MET:HE3	1.48	0.44
1:E:454:ARG:O	1:E:458:ILE:HG13	2.18	0.44
1:E:525:SER:HA	1:E:528:ARG:HD3	1.99	0.44
1:F:168:GLU:O	1:F:169:HIS:C	2.61	0.44
1:A:344:TYR:O	1:A:374:PHE:CZ	2.71	0.44
1:B:497:ILE:HG12	1:B:572:VAL:HG13	1.99	0.44
1:C:113:MET:HE3	1:C:117:GLY:HA3	1.99	0.44
2:D:133:PHE:HD2	2:D:187:ILE:HD12	1.82	0.44
2:D:346:ALA:HB3	3:I:18:DC:H5"	2.00	0.44
1:E:161:LEU:HD22	1:E:173:VAL:HG21	1.99	0.44
1:F:326:ASP:O	1:F:330:VAL:HG23	2.18	0.44
4:L:3:DA:C6	4:L:4:DG:C6	3.06	0.44
1:A:208:TYR:CD1	1:A:208:TYR:C	2.96	0.44
1:C:488:ASN:HA	1:C:587:THR:HA	2.00	0.44
2:D:203:ARG:H	2:D:203:ARG:HG2	1.46	0.44
2:D:266:GLN:HA	2:D:266:GLN:OE1	2.17	0.44
1:E:125:LEU:HD23	1:E:129:CYS:SG	2.58	0.44
1:E:450:ILE:HG22	1:E:589:ARG:NH1	2.33	0.44
1:F:444:VAL:CG1	1:F:551:ILE:HD11	2.48	0.44
2:D:371:THR:OG1	2:D:372:VAL:N	2.51	0.43
1:E:283:ARG:O	1:E:455:ARG:NH1	2.49	0.43
1:F:120:SER:HA	1:F:123:TYR:CE2	2.53	0.43
1:A:378:ILE:HD13	1:A:404:ARG:HD3	2.00	0.43
1:B:298:GLU:OE1	1:B:298:GLU:HA	2.18	0.43
1:C:173:VAL:O	1:C:177:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:GLN:O	1:C:366:GLN:NE2	2.51	0.43
1:C:398:TYR:HB2	1:C:443:MET:HE1	2.00	0.43
1:C:444:VAL:HG12	1:C:551:ILE:HD11	1.99	0.43
1:F:289:GLU:HB3	1:F:415:ILE:CD1	2.45	0.43
1:B:221:VAL:HG12	1:B:254:THR:HB	1.99	0.43
2:D:308:ILE:HA	2:D:312:TYR:CD2	2.49	0.43
2:D:398:TYR:HA	2:D:401:GLU:CB	2.47	0.43
1:E:224:CYS:SG	1:E:235:TYR:CD2	3.08	0.43
1:F:162:ASN:HB3	1:F:165:SER:H	1.83	0.43
1:F:494:ARG:HA	1:F:497:ILE:HD12	1.99	0.43
1:A:525:SER:HA	1:A:528:ARG:HG3	2.00	0.43
1:E:200:PHE:HD1	1:E:200:PHE:O	2.01	0.43
1:E:344:TYR:CD1	1:E:374:PHE:HA	2.53	0.43
1:E:473:LYS:HA	1:E:478:CYS:HB2	2.00	0.43
1:F:450:ILE:O	1:F:481:GLU:HG2	2.19	0.43
1:C:324:GLN:HG3	1:C:345:HIS:CE1	2.53	0.43
1:C:380:LYS:O	1:C:383:VAL:HG23	2.19	0.43
2:D:103:THR:O	2:D:215:ARG:NH1	2.51	0.43
2:D:109:VAL:HG23	2:D:275:PHE:CB	2.47	0.43
2:D:203:ARG:HA	2:D:203:ARG:HD2	1.72	0.43
2:D:282:ASN:HA	2:D:466:TRP:CH2	2.52	0.43
1:E:192:GLU:HG2	1:E:234:ASP:OD2	2.19	0.43
1:E:480:LYS:HD3	1:E:482:ILE:HB	2.01	0.43
1:F:183:LYS:HB3	1:F:183:LYS:HE3	1.62	0.43
1:A:451:ASN:HD22	1:A:589:ARG:CZ	2.32	0.43
1:B:407:ARG:HA	1:B:407:ARG:HD3	1.72	0.43
2:D:119:LYS:HG2	6:D:1002:ADP:O3B	2.19	0.43
1:E:224:CYS:HG	1:E:235:TYR:HD2	1.62	0.43
1:E:399:TYR:CD1	1:E:399:TYR:C	2.96	0.43
1:F:113:MET:HG2	1:F:117:GLY:HA3	1.99	0.43
3:K:9:DA:H2"	3:K:10:DC:C6	2.54	0.43
2:D:319:ILE:HG13	2:D:367:VAL:HG21	2.00	0.43
2:D:336:LYS:HE3	2:D:336:LYS:HB3	1.82	0.43
1:E:346:ALA:HA	1:E:373:ALA:CB	2.48	0.43
1:E:552:GLN:HB3	1:E:554:TYR:CE1	2.54	0.43
1:E:554:TYR:HE2	1:E:586:ILE:CD1	2.31	0.43
1:E:588:MET:HG2	1:E:589:ARG:N	2.32	0.43
1:F:208:TYR:HB2	1:F:213:PHE:HD2	1.83	0.43
1:C:554:TYR:HH	1:C:584:HIS:CE1	2.28	0.43
1:E:328:GLU:H	1:E:345:HIS:CE1	2.34	0.43
1:F:109:VAL:O	1:F:251:ILE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:GLU:OE2	1:F:461:HIS:NE2	2.47	0.43
1:A:183:LYS:H	1:A:183:LYS:HG3	1.69	0.43
1:A:224:CYS:SG	1:A:235:TYR:HD2	2.42	0.43
1:C:176:GLU:OE1	1:C:182:SER:OG	2.32	0.43
2:D:259:SER:O	2:D:263:LYS:HE2	2.18	0.43
2:D:293:LYS:HG3	2:D:419:GLY:CA	2.49	0.43
2:D:487:LYS:HD3	2:D:488:ASN:N	2.34	0.43
1:F:144:MET:HB2	1:F:160:MET:HE3	2.01	0.43
4:H:8:DC:H2''	4:H:9:DG:H8	1.84	0.43
1:A:157:SER:OG	1:A:183:LYS:O	2.37	0.42
1:A:232:ARG:HB2	1:A:235:TYR:CD1	2.54	0.42
1:A:318:ILE:HB	1:A:386:VAL:HG22	2.01	0.42
2:D:392:SER:CB	2:D:401:GLU:OE1	2.67	0.42
1:E:378:ILE:O	1:E:379:ASP:OD1	2.37	0.42
1:F:100:ILE:HG21	1:F:125:LEU:HD22	2.01	0.42
1:F:139:PRO:HB2	1:F:232:ARG:NH1	2.34	0.42
1:F:496:LEU:HD13	1:F:515:LEU:HD11	2.01	0.42
2:D:582:GLU:N	2:D:582:GLU:OE1	2.51	0.42
1:E:415:ILE:HG12	1:E:416:LEU:N	2.33	0.42
1:E:575:LYS:HE3	1:E:575:LYS:HB3	1.77	0.42
4:H:3:DA:H1'	4:H:4:DG:H5'	2.01	0.42
4:J:2:DG:H2''	4:J:3:DA:H8	1.81	0.42
1:A:142:SER:OG	1:A:143:LEU:HD12	2.20	0.42
1:A:581:ASN:HB2	1:A:584:HIS:HB2	2.01	0.42
1:C:517:ASP:HB3	1:C:523:GLY:HA3	2.01	0.42
2:D:454:ARG:HG2	2:D:477:ASN:OD1	2.20	0.42
1:F:112:VAL:HG13	1:F:254:THR:HG23	2.01	0.42
1:F:237:ALA:O	1:F:240:ILE:HG22	2.20	0.42
1:C:193:LYS:HD2	1:C:193:LYS:HA	1.67	0.42
2:D:227:TRP:CE3	2:D:260:HIS:CD2	3.08	0.42
2:D:273:LYS:HA	2:D:273:LYS:HD2	1.79	0.42
1:E:411:LYS:HD2	1:E:411:LYS:HA	1.83	0.42
1:F:305:VAL:HG13	1:F:339:ILE:CD1	2.49	0.42
1:A:200:PHE:HA	1:A:203:ARG:NH2	2.30	0.42
1:A:219:ASP:OD1	1:A:220:GLU:HG2	2.20	0.42
1:A:322:PHE:HZ	1:A:429:MET:HG2	1.85	0.42
1:A:511:THR:HG1	1:A:514:LYS:HG3	1.85	0.42
1:B:242:LYS:HE3	1:B:246:PRO:HA	2.02	0.42
2:D:522:LYS:HD2	2:D:523:GLY:N	2.33	0.42
1:E:502:GLN:OE1	1:E:529:VAL:HA	2.19	0.42
1:A:259:SER:HA	1:A:262:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LEU:CD2	1:B:447:CYS:SG	3.08	0.42
2:D:140:LEU:HD23	2:D:141:ILE:H	1.85	0.42
2:D:177:MET:HE1	2:D:200:PHE:CE1	2.55	0.42
2:D:257:ALA:HB2	2:D:465:VAL:HG11	2.02	0.42
2:D:549:PHE:HB3	2:D:555:LEU:CD1	2.49	0.42
1:E:487:LYS:HZ2	1:E:589:ARG:HA	1.85	0.42
1:C:226:GLN:H	1:C:226:GLN:HG2	1.72	0.42
1:C:423:ILE:HG23	1:C:444:VAL:HG21	2.01	0.42
2:D:487:LYS:O	2:D:587:THR:HA	2.20	0.42
1:E:281:PHE:HD2	1:E:465:VAL:O	2.03	0.42
1:E:494:ARG:HA	1:E:497:ILE:HD11	2.00	0.42
1:F:292:GLN:HE21	1:F:292:GLN:HB2	1.65	0.42
1:F:451:ASN:ND2	1:F:452:LYS:HG3	2.35	0.42
1:A:322:PHE:HD2	1:A:425:ARG:NH2	2.17	0.42
1:C:474:MET:HA	1:C:474:MET:HE2	2.00	0.42
1:E:394:SER:HB2	1:E:439:LYS:HD3	2.00	0.42
1:F:462:PHE:HB3	1:F:465:VAL:HG23	2.00	0.42
4:J:5:DC:H2''	4:J:6:DG:H8	1.84	0.42
1:A:346:ALA:H	1:A:374:PHE:HD1	1.68	0.42
1:B:319:ILE:O	1:B:369:VAL:HA	2.20	0.42
1:C:167:LYS:HD3	1:C:167:LYS:N	2.35	0.42
1:E:328:GLU:HA	1:E:331:THR:CG2	2.44	0.42
1:F:391:MET:HA	1:F:416:LEU:HD11	2.02	0.42
3:I:3:DA:H4'	3:I:4:DT:OP1	2.19	0.42
1:B:108:GLU:HA	1:B:250:LEU:O	2.20	0.42
1:C:386:VAL:HG23	1:C:405:ALA:HB2	2.01	0.42
2:D:189:VAL:HG11	2:D:200:PHE:CZ	2.55	0.42
2:D:502:GLN:NE2	2:D:528:ARG:O	2.53	0.42
1:E:77:GLY:O	1:E:81:ASP:HB2	2.20	0.42
1:E:186:LEU:HD22	1:E:188:TYR:CE1	2.55	0.42
1:E:490:THR:HG22	1:E:586:ILE:HG12	2.01	0.42
1:F:314:GLY:H	1:F:366:GLN:NE2	2.18	0.42
3:K:11:DG:C2	4:L:6:DG:N2	2.88	0.42
1:B:83:LEU:HD22	1:B:92:PHE:CZ	2.55	0.41
1:C:108:GLU:HG3	1:C:250:LEU:HB3	2.01	0.41
1:C:120:SER:HA	1:C:123:TYR:CE2	2.55	0.41
1:C:267:LYS:HE2	1:C:267:LYS:HB3	1.49	0.41
2:D:138:CYS:SG	2:D:219:ASP:HB3	2.60	0.41
2:D:444:VAL:O	2:D:448:GLN:HB2	2.20	0.41
1:E:494:ARG:O	1:E:498:LYS:HG3	2.20	0.41
1:F:385:PHE:HA	1:F:413:ASP:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:CYS:O	1:A:474:MET:HB2	2.20	0.41
1:A:558:ASP:OD2	1:A:558:ASP:C	2.64	0.41
1:B:110:PHE:CD2	1:B:252:GLY:HA3	2.55	0.41
1:B:169:HIS:O	1:B:173:VAL:HG23	2.19	0.41
2:D:243:ARG:HH12	1:E:434:ASN:HA	1.84	0.41
2:D:287:TYR:HB3	2:D:413:ASP:HA	2.02	0.41
2:D:510:LEU:HD13	2:D:514:LYS:HB3	2.01	0.41
1:F:569:TYR:CD2	1:F:569:TYR:N	2.88	0.41
4:J:6:DG:H2'	4:J:7:DT:H71	2.02	0.41
1:B:191:PRO:HG3	1:B:235:TYR:CE1	2.55	0.41
1:B:416:LEU:HD21	1:B:447:CYS:SG	2.60	0.41
2:D:108:GLU:HA	2:D:250:LEU:O	2.20	0.41
2:D:199:MET:O	2:D:203:ARG:HG2	2.21	0.41
2:D:454:ARG:O	2:D:458:ILE:HD13	2.20	0.41
1:E:134:THR:HB	1:E:186:LEU:HD23	2.02	0.41
1:E:200:PHE:CD1	1:E:204:LEU:HD13	2.55	0.41
1:A:79:VAL:HG13	1:A:125:LEU:HD21	2.02	0.41
1:B:351:GLU:O	1:B:355:LYS:HG2	2.19	0.41
1:C:214:THR:O	1:C:248:ALA:HA	2.19	0.41
2:D:136:VAL:HG11	2:D:188:TYR:CE1	2.55	0.41
2:D:579:LEU:HD23	2:D:579:LEU:HA	1.89	0.41
1:E:157:SER:OG	1:E:184:LEU:HA	2.20	0.41
1:E:308:ILE:O	1:E:312:TYR:N	2.52	0.41
1:F:224:CYS:SG	1:F:235:TYR:HD2	2.44	0.41
1:A:65:PRO:O	1:A:98:GLU:HG2	2.20	0.41
1:A:287:TYR:CE1	1:A:289:GLU:HB2	2.55	0.41
1:B:70:LYS:CE	1:B:97:LEU:HD11	2.50	0.41
1:B:283:ARG:HG3	1:B:283:ARG:HH11	1.85	0.41
1:B:538:PRO:O	1:B:542:LEU:HG	2.21	0.41
1:C:473:LYS:HA	1:C:478:CYS:HB3	2.02	0.41
2:D:208:TYR:HA	2:D:213:PHE:HB3	2.02	0.41
2:D:293:LYS:HE2	2:D:293:LYS:HA	2.02	0.41
2:D:330:VAL:HG12	2:D:369:VAL:HG21	2.03	0.41
2:D:371:THR:OG1	3:I:17:DC:H4'	2.20	0.41
1:E:305:VAL:HG21	1:E:337:LEU:HD12	2.02	0.41
1:E:562:THR:HG23	1:E:565:ALA:H	1.86	0.41
1:F:462:PHE:N	1:F:462:PHE:CD2	2.88	0.41
1:F:492:TYR:HD1	1:F:519:TRP:HZ2	1.68	0.41
1:A:225:SER:HB3	1:A:261:VAL:HG13	2.02	0.41
2:D:257:ALA:CB	2:D:465:VAL:HG11	2.50	0.41
2:D:336:LYS:NZ	2:D:337:LEU:HD22	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:427:SER:OG	2:D:440:LEU:HD22	2.20	0.41
1:F:111:LEU:HD11	1:F:113:MET:HE2	2.03	0.41
1:F:462:PHE:N	1:F:462:PHE:HD2	2.19	0.41
4:H:9:DG:H2''	4:H:10:DA:H8	1.85	0.41
3:K:6:DT:H2'	3:K:7:DC:C6	2.56	0.41
1:C:293:LYS:HD2	1:C:300:PHE:CE2	2.56	0.41
2:D:348:MET:SD	2:D:349:GLU:N	2.93	0.41
2:D:508:GLU:HG3	2:D:527:LEU:HD21	2.03	0.41
1:E:146:ASP:OD1	1:E:146:ASP:C	2.63	0.41
1:E:293:LYS:HG3	1:E:300:PHE:HE2	1.86	0.41
1:E:307:LEU:HD12	1:E:311:ARG:HB3	2.03	0.41
1:F:494:ARG:NH1	1:F:579:LEU:O	2.54	0.41
1:B:380:LYS:NZ	1:B:382:ASP:OD1	2.37	0.41
1:E:467:SER:HA	1:E:468:PRO:HD3	1.90	0.41
1:F:93:ARG:HG3	6:F:1002:ADP:C6	2.56	0.41
1:F:429:MET:HE3	3:K:17:DC:C6	2.56	0.41
1:A:242:LYS:HD2	1:A:242:LYS:HA	1.84	0.41
1:A:320:TYR:OH	1:A:404:ARG:HD2	2.20	0.41
1:B:193:LYS:O	1:B:197:SER:HB3	2.20	0.41
1:C:486:ARG:HB2	1:C:587:THR:HB	2.02	0.41
2:D:115:THR:HG23	2:D:400:GLN:OE1	2.20	0.41
2:D:148:LEU:HA	2:D:151:LEU:HD13	2.02	0.41
2:D:159:THR:O	2:D:187:ILE:HA	2.21	0.41
2:D:199:MET:O	2:D:202:SER:HB2	2.21	0.41
2:D:334:LEU:HG	2:D:339:ILE:HG21	2.03	0.41
2:D:498:LYS:HG3	2:D:529:VAL:HG21	2.02	0.41
1:E:170:VAL:O	1:E:174:HIS:ND1	2.52	0.41
1:E:241:LEU:HD13	1:E:241:LEU:HA	1.91	0.41
1:E:502:GLN:HE21	1:E:506:LEU:HD11	1.85	0.41
1:F:151:LEU:HD22	1:F:156:ILE:HG21	2.03	0.41
1:F:199:MET:HE1	1:F:203:ARG:NH1	2.36	0.41
1:F:511:THR:HG22	1:F:514:LYS:H	1.85	0.41
3:I:1:DG:H2''	3:I:2:DG:C8	2.55	0.41
1:E:68:TRP:HB3	1:E:101:ASN:HB2	2.02	0.41
1:E:291:ARG:NH2	1:E:307:LEU:HD22	2.36	0.41
1:F:236:LYS:HE3	1:F:236:LYS:HB3	1.81	0.41
1:F:293:LYS:HD2	1:F:419:GLY:HA3	2.03	0.41
1:F:481:GLU:O	1:F:482:ILE:HG22	2.21	0.41
1:F:569:TYR:CE1	4:L:4:DG:OP1	2.72	0.41
1:A:208:TYR:O	1:A:208:TYR:HD1	2.05	0.40
1:B:110:PHE:HE1	1:B:266:GLN:CG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:THR:O	1:B:300:PHE:HB3	2.21	0.40
1:B:532:LEU:HA	1:B:532:LEU:HD12	1.83	0.40
2:D:83:LEU:HA	2:D:87:PHE:HB2	2.03	0.40
2:D:300:PHE:O	2:D:304:ILE:HG13	2.22	0.40
2:D:334:LEU:HD12	2:D:334:LEU:HA	1.92	0.40
1:E:113:MET:HG3	1:E:114:PRO:HD2	2.02	0.40
1:F:133:PHE:CD1	1:F:187:ILE:HD12	2.56	0.40
1:F:535:PRO:HG2	1:F:542:LEU:HD11	2.02	0.40
1:B:227:TRP:CZ2	1:C:226:GLN:HG3	2.56	0.40
2:D:496:LEU:HD13	2:D:555:LEU:HD21	2.02	0.40
1:B:70:LYS:HG3	1:B:101:ASN:ND2	2.36	0.40
2:D:311:ARG:HB3	2:D:312:TYR:CD2	2.56	0.40
1:E:514:LYS:NZ	3:K:4:DT:OP2	2.49	0.40
1:F:199:MET:O	1:F:202:SER:OG	2.37	0.40
1:F:386:VAL:CG2	1:F:405:ALA:HB2	2.51	0.40
1:A:199:MET:SD	1:A:202:SER:HB3	2.61	0.40
1:A:348:MET:HE2	1:A:352:ASP:C	2.47	0.40
1:A:473:LYS:HA	1:A:478:CYS:HB3	2.04	0.40
1:B:224:CYS:HA	1:B:235:TYR:HB3	2.04	0.40
1:B:579:LEU:HD21	1:B:586:ILE:HD11	2.04	0.40
1:C:141:ILE:H	1:C:141:ILE:HD12	1.86	0.40
1:E:242:LYS:HE2	1:E:270:CYS:HB3	2.03	0.40
1:E:301:ILE:HG21	1:E:333:SER:HB2	2.04	0.40
1:E:312:TYR:HB3	1:E:385:PHE:CE1	2.56	0.40
1:E:385:PHE:HA	1:E:413:ASP:O	2.22	0.40
1:E:559:TYR:CE1	1:E:568:SER:HB3	2.56	0.40
1:A:341:ALA:HA	1:A:367:VAL:O	2.21	0.40
1:B:225:SER:O	1:B:231:PHE:HB2	2.22	0.40
1:B:284:PRO:O	1:B:474:MET:HG2	2.22	0.40
1:C:483:SER:O	1:C:592:LYS:HG2	2.22	0.40
2:D:292:GLN:OE1	2:D:544:LYS:NZ	2.42	0.40
1:E:381:PRO:HA	1:E:407:ARG:CB	2.50	0.40
1:F:300:PHE:CE1	1:F:417:TYR:CD2	3.08	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	529/531 (100%)	528 (100%)	1 (0%)	0	100	100
1	B	529/531 (100%)	524 (99%)	5 (1%)	0	100	100
1	C	529/531 (100%)	528 (100%)	1 (0%)	0	100	100
1	E	529/531 (100%)	523 (99%)	5 (1%)	1 (0%)	44	71
1	F	529/531 (100%)	520 (98%)	4 (1%)	5 (1%)	14	39
2	D	529/531 (100%)	522 (99%)	6 (1%)	1 (0%)	44	71
All	All	3174/3186 (100%)	3145 (99%)	22 (1%)	7 (0%)	44	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	335	GLN
1	F	482	ILE
1	E	348	MET
1	F	346	ALA
1	F	348	MET
1	F	376	MET
1	F	258	THR

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	469/469 (100%)	451 (96%)	18 (4%)	28	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	469/469 (100%)	456 (97%)	13 (3%)	38	71
1	C	469/469 (100%)	455 (97%)	14 (3%)	36	69
1	E	469/469 (100%)	446 (95%)	23 (5%)	21	50
1	F	469/469 (100%)	447 (95%)	22 (5%)	22	52
2	D	469/469 (100%)	445 (95%)	24 (5%)	20	49
All	All	2814/2814 (100%)	2700 (96%)	114 (4%)	26	57

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	67	SER
1	A	70	LYS
1	A	165	SER
1	A	168	GLU
1	A	181	ASN
1	A	221	VAL
1	A	258	THR
1	A	267	LYS
1	A	278	THR
1	A	295	SER
1	A	327	SER
1	A	372	VAL
1	A	374	PHE
1	A	378	ILE
1	A	445	SER
1	A	448	GLN
1	A	482	ILE
1	B	70	LYS
1	B	130	SER
1	B	138	CYS
1	B	142	SER
1	B	192	GLU
1	B	259	SER
1	B	267	LYS
1	B	280	SER
1	B	328	GLU
1	B	378	ILE
1	B	407	ARG
1	B	482	ILE

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Mol	Chain	Res	Type
1	B	525	SER
1	C	115	THR
1	C	182	SER
1	C	209	GLU
1	C	253	LEU
1	C	258	THR
1	C	304	ILE
1	C	337	LEU
1	C	360	TRP
1	C	463	ASP
1	C	488	ASN
1	C	490	THR
1	C	516	ILE
1	C	526	LYS
1	C	560	SER
2	D	79	VAL
2	D	108	GLU
2	D	115	THR
2	D	129	CYS
2	D	214	THR
2	D	234	ASP
2	D	271	VAL
2	D	274	CYS
2	D	328	GLU
2	D	334	LEU
2	D	337	LEU
2	D	339	ILE
2	D	365	ILE
2	D	368	VAL
2	D	371	THR
2	D	378	ILE
2	D	383	VAL
2	D	392	SER
2	D	393	LYS
2	D	469	GLU
2	D	479	CYS
2	D	526	LYS
2	D	528	ARG
2	D	564	TYR
1	E	79	VAL
1	E	91	LYS
1	E	95	LEU

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Mol	Chain	Res	Type
1	E	125	LEU
1	E	172	TRP
1	E	178	VAL
1	E	182	SER
1	E	238	LEU
1	E	254	THR
1	E	261	VAL
1	E	262	LEU
1	E	334	LEU
1	E	337	LEU
1	E	352	ASP
1	E	378	ILE
1	E	415	ILE
1	E	457	LEU
1	E	465	VAL
1	E	482	ILE
1	E	483	SER
1	E	509	LYS
1	E	525	SER
1	E	568	SER
1	F	64	SER
1	F	67	SER
1	F	76	SER
1	F	115	THR
1	F	138	CYS
1	F	170	VAL
1	F	181	ASN
1	F	198	LYS
1	F	234	ASP
1	F	301	ILE
1	F	334	LEU
1	F	347	ASN
1	F	367	VAL
1	F	368	VAL
1	F	380	LYS
1	F	381	PRO
1	F	426	ILE
1	F	450	ILE
1	F	478	CYS
1	F	485	GLU
1	F	486	ARG
1	F	510	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	A	324	GLN
1	A	577	ASN
1	B	226	GLN
1	B	244	GLN
1	B	296	ASN
1	B	397	ASN
1	B	438	GLN
1	B	507	ASN
1	C	69	ASN
1	C	174	HIS
1	C	226	GLN
1	C	292	GLN
1	C	345	HIS
1	C	477	ASN
1	C	552	GLN
1	C	580	ASN
2	D	169	HIS
2	D	244	GLN
1	E	101	ASN
1	E	124	GLN
1	E	147	GLN
1	E	324	GLN
1	E	400	GLN
1	E	548	HIS
1	F	174	HIS
1	F	247	ASN
1	F	266	GLN
1	F	366	GLN
1	F	438	GLN
1	F	472	ASN
1	F	548	HIS
1	F	577	ASN
1	F	581	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 18 are monoatomic - leaving 17 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$
6	ADP	E	1002	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)
8	PO4	B	1004	-	4,4,4	0.92	0	6,6,6	0.40	0
8	PO4	A	1007	-	4,4,4	0.92	0	6,6,6	0.48	0
8	PO4	A	1004	-	4,4,4	0.88	0	6,6,6	0.44	0
8	PO4	E	1003	-	4,4,4	0.92	0	6,6,6	0.43	0
6	ADP	D	1002	-	24,29,29	0.97	1 (4%)	29,45,45	1.35	4 (13%)
6	ADP	A	1002	-	24,29,29	0.97	1 (4%)	29,45,45	1.42	4 (13%)
6	ADP	F	1002	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
8	PO4	A	1005	-	4,4,4	0.93	0	6,6,6	0.41	0
8	PO4	C	1004	-	4,4,4	0.91	0	6,6,6	0.44	0
8	PO4	F	1004	-	4,4,4	0.91	0	6,6,6	0.43	0
8	PO4	A	1006	-	4,4,4	0.89	0	6,6,6	0.45	0
8	PO4	F	1003	-	4,4,4	0.93	0	6,6,6	0.41	0
6	ADP	C	1002	-	24,29,29	0.93	1 (4%)	29,45,45	1.38	4 (13%)
6	ADP	B	1002	-	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)
8	PO4	C	1005	-	4,4,4	1.02	0	6,6,6	0.54	0
8	PO4	B	1005	-	4,4,4	0.99	0	6,6,6	0.48	0

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
6	ADP	E	1002	-	-	0/12/32/32	0/3/3/3
6	ADP	D	1002	-	-	4/12/32/32	0/3/3/3
6	ADP	A	1002	-	-	3/12/32/32	0/3/3/3
6	ADP	F	1002	-	-	3/12/32/32	0/3/3/3
6	ADP	C	1002	-	-	3/12/32/32	0/3/3/3
6	ADP	B	1002	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1002	ADP	C5-C4	2.51	1.47	1.40
6	A	1002	ADP	C5-C4	2.51	1.47	1.40
6	F	1002	ADP	C5-C4	2.47	1.47	1.40
6	C	1002	ADP	C5-C4	2.46	1.47	1.40
6	B	1002	ADP	C5-C4	2.46	1.47	1.40
6	E	1002	ADP	C5-C4	2.40	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1002	ADP	N3-C2-N1	-3.35	123.45	128.68
6	B	1002	ADP	PA-O3A-PB	-3.34	121.38	132.83
6	A	1002	ADP	PA-O3A-PB	-3.32	121.43	132.83
6	F	1002	ADP	PA-O3A-PB	-3.32	121.45	132.83
6	F	1002	ADP	C3'-C2'-C1'	3.27	105.91	100.98
6	F	1002	ADP	N3-C2-N1	-3.26	123.59	128.68
6	C	1002	ADP	N3-C2-N1	-3.25	123.61	128.68
6	B	1002	ADP	N3-C2-N1	-3.21	123.66	128.68
6	A	1002	ADP	N3-C2-N1	-3.17	123.73	128.68
6	D	1002	ADP	N3-C2-N1	-3.15	123.75	128.68
6	E	1002	ADP	PA-O3A-PB	-3.10	122.18	132.83
6	C	1002	ADP	PA-O3A-PB	-3.06	122.32	132.83
6	F	1002	ADP	C4-C5-N7	-2.82	106.46	109.40
6	D	1002	ADP	C4-C5-N7	-2.81	106.47	109.40
6	A	1002	ADP	C3'-C2'-C1'	2.76	105.14	100.98
6	B	1002	ADP	C4-C5-N7	-2.68	106.61	109.40
6	A	1002	ADP	C4-C5-N7	-2.67	106.61	109.40
6	C	1002	ADP	C4-C5-N7	-2.61	106.68	109.40
6	D	1002	ADP	C3'-C2'-C1'	2.56	104.83	100.98
6	E	1002	ADP	C4-C5-N7	-2.52	106.77	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1002	ADP	C3'-C2'-C1'	2.51	104.75	100.98
6	D	1002	ADP	PA-O3A-PB	-2.51	124.23	132.83
6	B	1002	ADP	C3'-C2'-C1'	2.48	104.71	100.98
6	C	1002	ADP	C3'-C2'-C1'	2.37	104.55	100.98

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	ADP	C5'-O5'-PA-O1A
6	A	1002	ADP	C5'-O5'-PA-O2A
6	B	1002	ADP	C5'-O5'-PA-O1A
6	B	1002	ADP	C5'-O5'-PA-O2A
6	C	1002	ADP	C5'-O5'-PA-O1A
6	C	1002	ADP	C5'-O5'-PA-O2A
6	D	1002	ADP	C5'-O5'-PA-O2A
6	F	1002	ADP	C5'-O5'-PA-O1A
6	F	1002	ADP	C5'-O5'-PA-O2A
6	D	1002	ADP	C5'-O5'-PA-O3A
6	F	1002	ADP	C5'-O5'-PA-O3A
6	D	1002	ADP	C5'-O5'-PA-O1A
6	D	1002	ADP	PA-O3A-PB-O1B
6	A	1002	ADP	C5'-O5'-PA-O3A
6	B	1002	ADP	C5'-O5'-PA-O3A
6	C	1002	ADP	C5'-O5'-PA-O3A

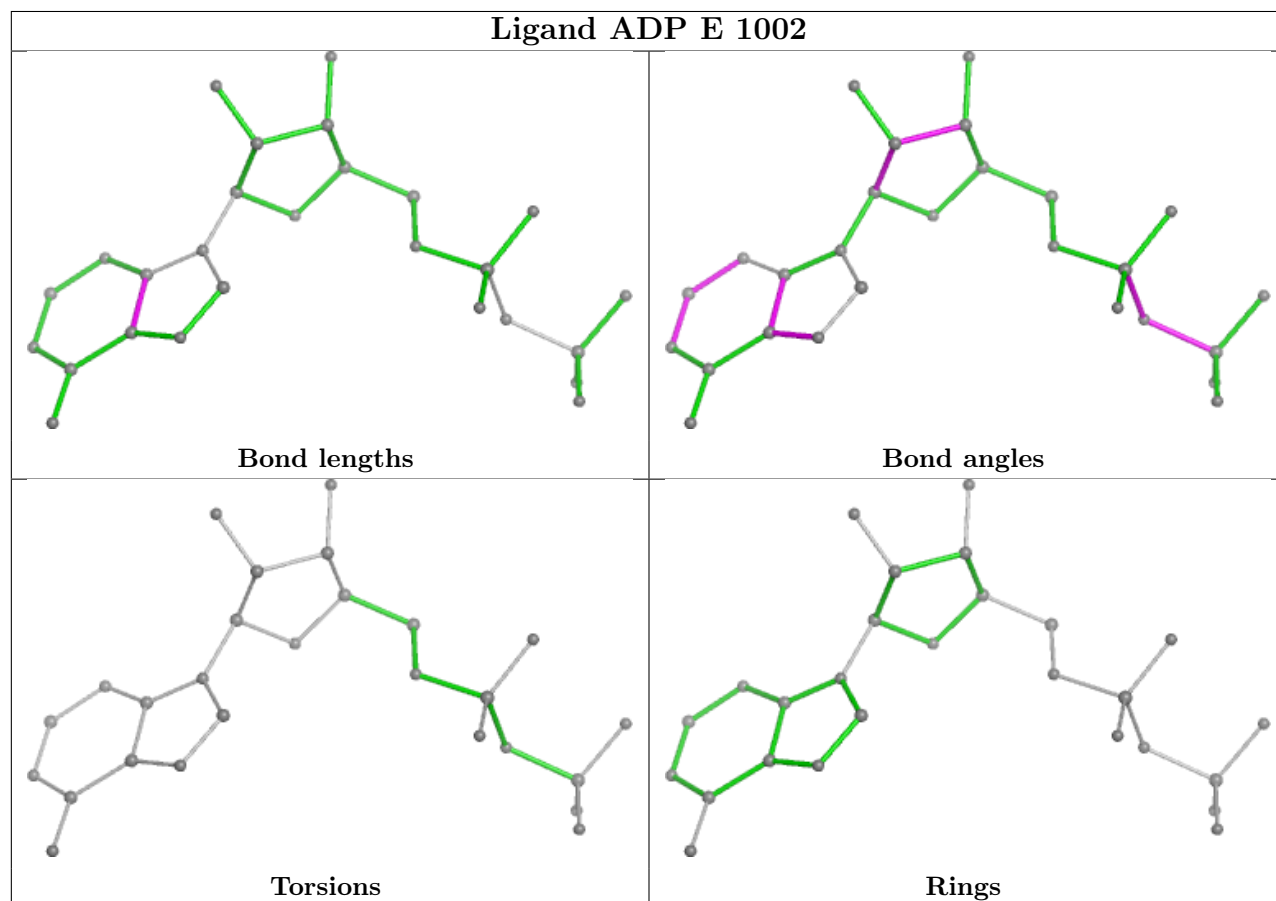
There are no ring outliers.

6 monomers are involved in 9 short contacts:

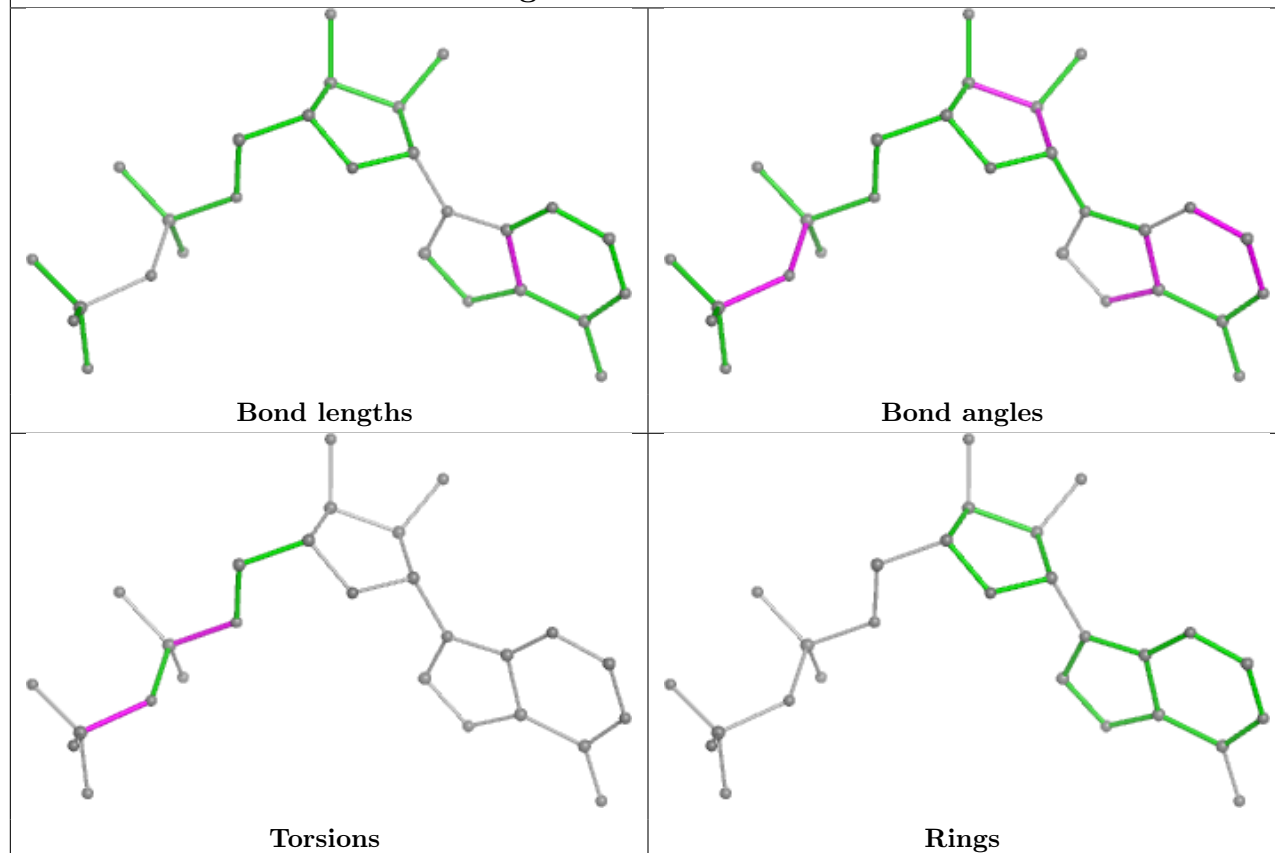
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1002	ADP	3	0
6	D	1002	ADP	1	0
6	F	1002	ADP	1	0
8	F	1003	PO4	2	0
8	C	1005	PO4	1	0
8	B	1005	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

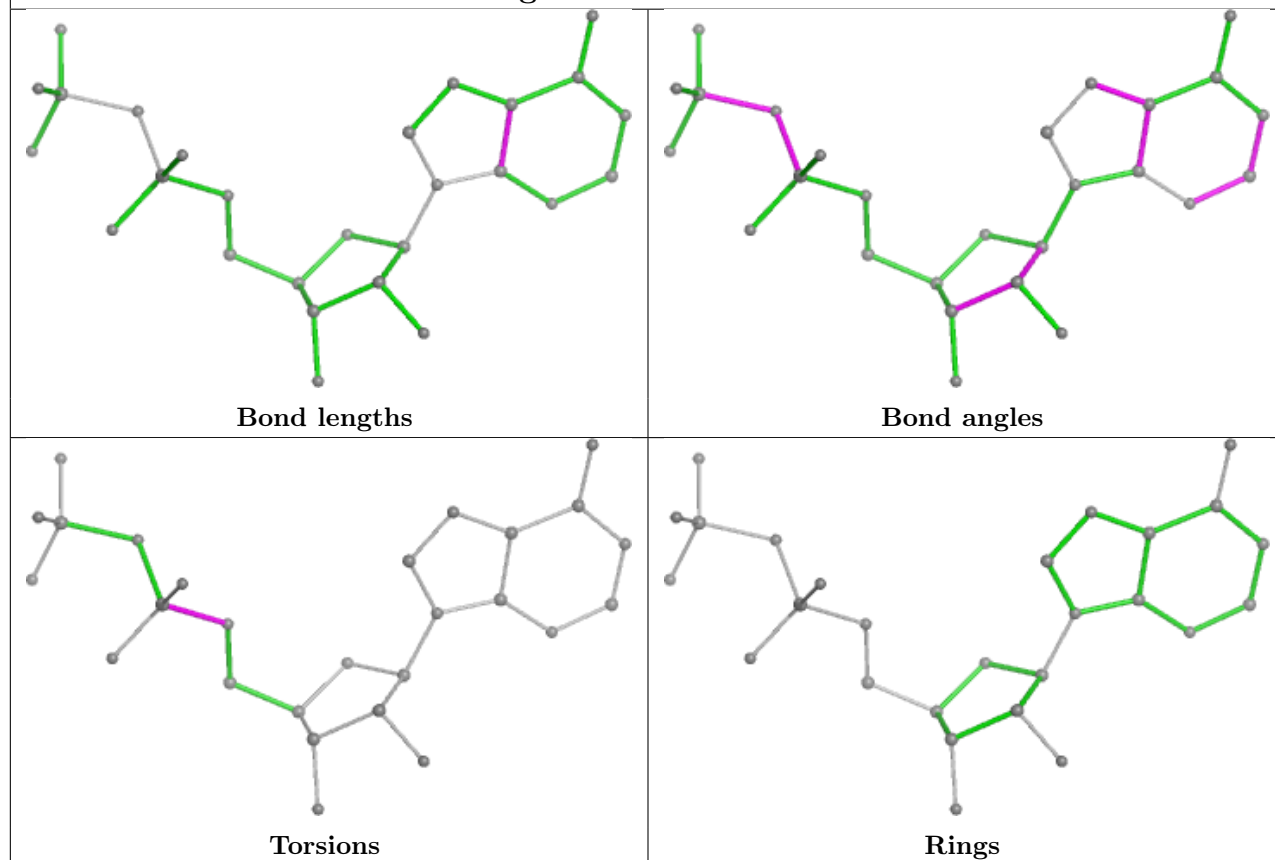
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



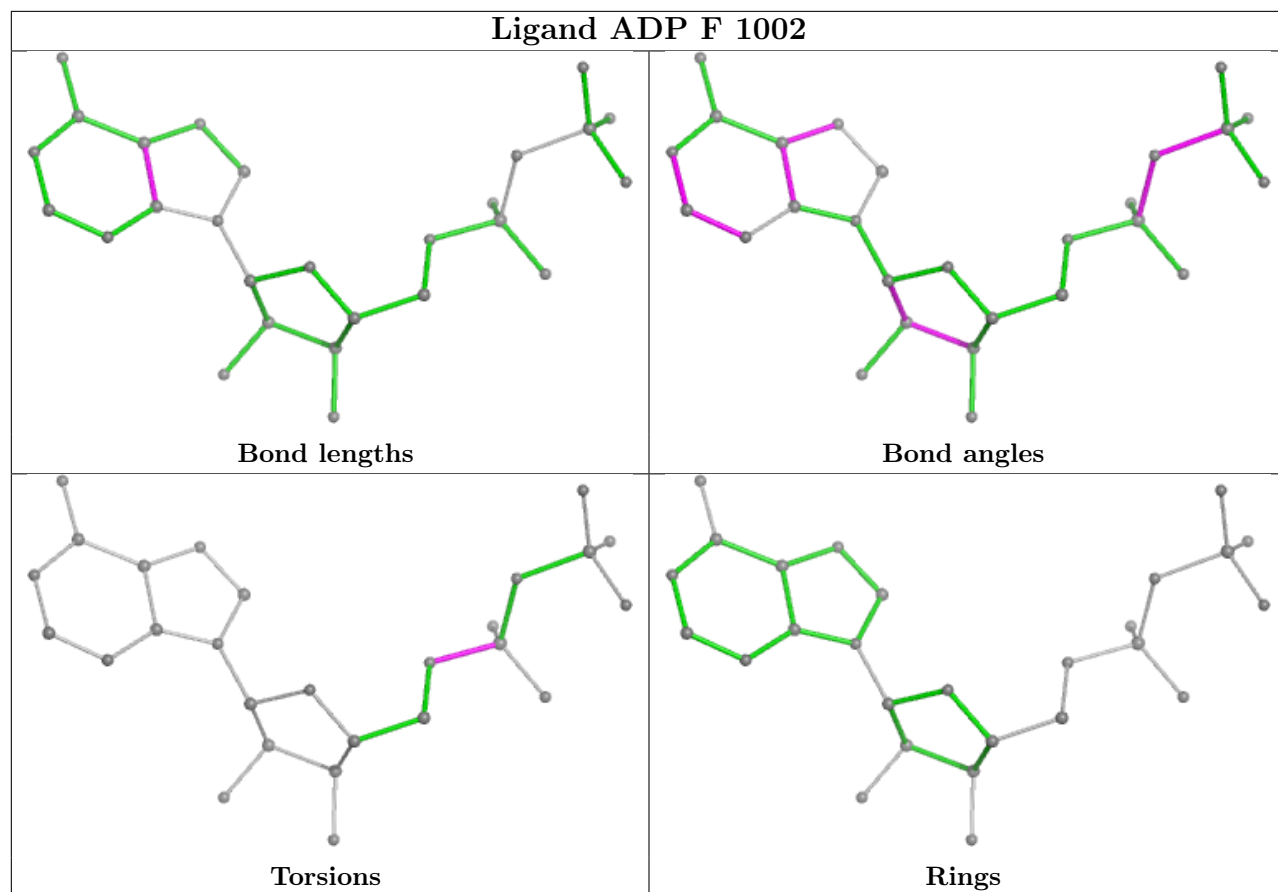
Ligand ADP D 1002



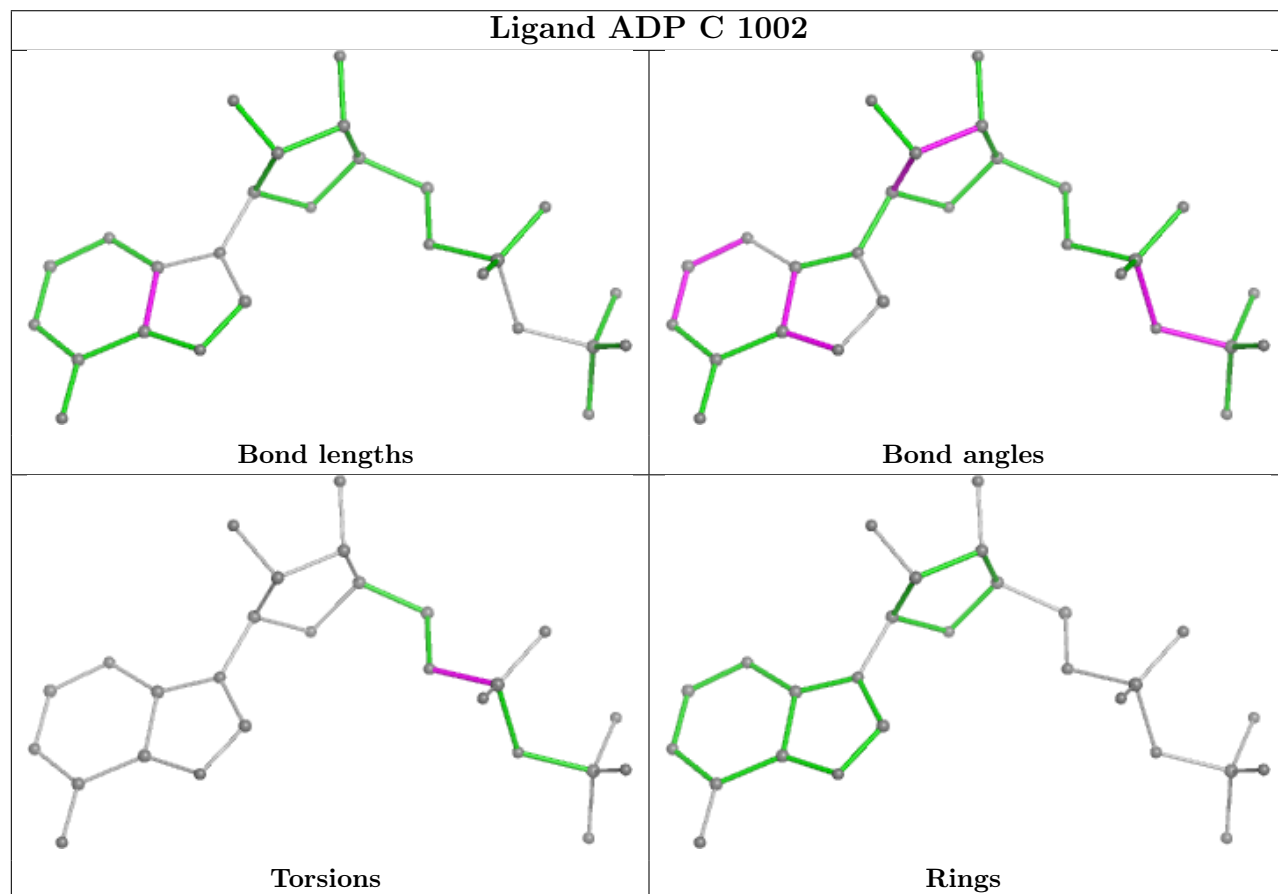
Ligand ADP A 1002

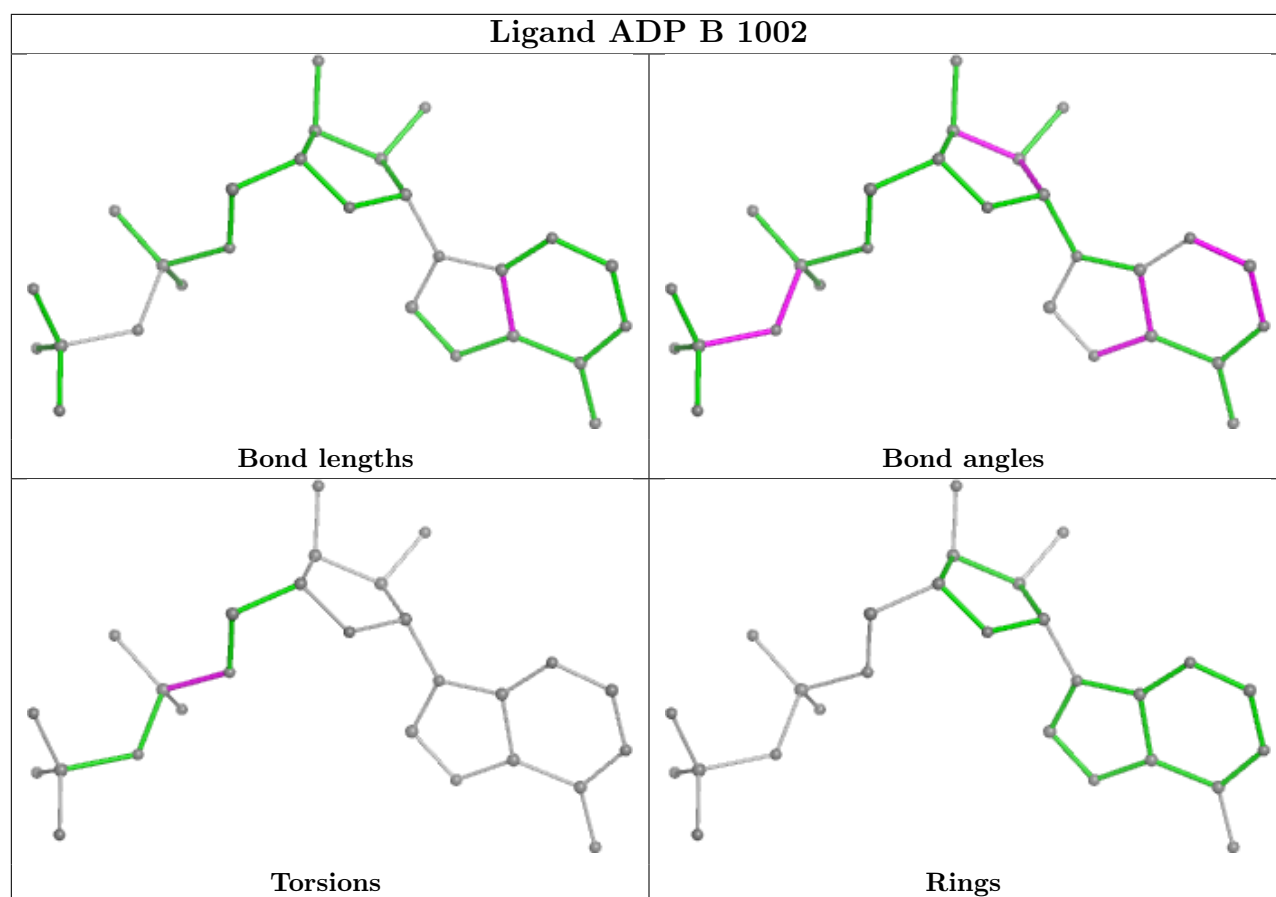


Ligand ADP F 1002



Ligand ADP C 1002





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	531/531 (100%)	-0.10	13 (2%) 59 52	29, 59, 107, 157	0
1	B	531/531 (100%)	-0.21	3 (0%) 85 81	37, 62, 91, 129	0
1	C	531/531 (100%)	-0.41	3 (0%) 85 81	26, 57, 100, 168	0
1	E	531/531 (100%)	0.63	43 (8%) 19 15	86, 127, 172, 227	0
1	F	531/531 (100%)	0.05	16 (3%) 52 44	38, 86, 135, 221	0
2	D	531/531 (100%)	0.62	34 (6%) 27 20	83, 131, 178, 270	0
3	G	18/21 (85%)	0.43	3 (16%) 5 5	78, 104, 230, 249	0
3	I	18/21 (85%)	0.57	1 (5%) 31 24	83, 142, 206, 298	0
3	K	18/21 (85%)	0.67	2 (11%) 12 9	123, 172, 245, 293	0
4	H	15/15 (100%)	0.06	0 100 100	72, 102, 133, 141	0
4	J	15/15 (100%)	0.32	0 100 100	100, 134, 157, 174	0
4	L	15/15 (100%)	0.98	2 (13%) 8 7	130, 167, 194, 235	0
All	All	3285/3294 (99%)	0.11	120 (3%) 45 37	26, 84, 161, 298	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	392	SER	5.1
1	F	356	VAL	5.1
1	E	177	MET	4.3
1	C	374	PHE	4.2
2	D	403	GLY	4.1
1	F	257	ALA	4.1
3	K	16	DC	4.1
1	E	547	ALA	4.0
1	E	320	TYR	3.9
1	E	591	LYS	3.8
1	F	362	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	345	HIS	3.7
2	D	465	VAL	3.6
1	E	345	HIS	3.6
2	D	374	PHE	3.6
1	E	590	VAL	3.5
3	G	16	DC	3.5
1	F	360	TRP	3.3
1	B	374	PHE	3.3
1	E	554	TYR	3.3
1	E	341	ALA	3.2
1	E	374	PHE	3.2
2	D	213	PHE	3.2
2	D	320	TYR	3.1
1	A	374	PHE	3.1
1	E	415	ILE	3.0
2	D	258	THR	3.0
1	B	70	LYS	3.0
1	E	68	TRP	3.0
2	D	350	PRO	2.9
1	E	89	LEU	2.9
4	L	1	DA	2.9
3	I	16	DC	2.9
2	D	373	ALA	2.9
1	A	467	SER	2.8
3	G	18	DC	2.8
2	D	224	CYS	2.8
1	E	158	ALA	2.8
1	E	257	ALA	2.8
2	D	115	THR	2.8
1	F	567	ILE	2.8
1	A	350	PRO	2.7
1	F	450	ILE	2.7
2	D	391	MET	2.7
1	A	210	ALA	2.7
1	E	86	VAL	2.7
1	E	346	ALA	2.6
1	E	339	ILE	2.6
1	E	340	PRO	2.6
1	A	372	VAL	2.6
1	E	356	VAL	2.6
1	E	224	CYS	2.6
2	D	300	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	379	ASP	2.6
1	C	583	ALA	2.5
1	F	481	GLU	2.5
1	A	378	ILE	2.5
2	D	332	ILE	2.5
1	A	482	ILE	2.5
2	D	198	LYS	2.5
2	D	400	GLN	2.5
1	E	87	PHE	2.4
3	K	17	DC	2.4
2	D	548	HIS	2.4
1	E	70	LYS	2.4
1	E	365	ILE	2.3
2	D	354	THR	2.3
1	E	186	LEU	2.3
1	E	188	TYR	2.3
1	E	235	TYR	2.3
1	E	576	ALA	2.3
2	D	405	ALA	2.3
2	D	368	VAL	2.3
1	C	524	ALA	2.3
1	F	563	ALA	2.3
1	F	434	ASN	2.3
1	E	589	ARG	2.3
2	D	257	ALA	2.3
2	D	262	LEU	2.3
1	E	178	VAL	2.2
2	D	383	VAL	2.2
1	F	361	ALA	2.2
2	D	395	MET	2.2
1	E	151	LEU	2.2
2	D	416	LEU	2.2
2	D	288	TYR	2.2
2	D	346	ALA	2.2
1	E	536	THR	2.2
1	A	228	GLY	2.2
1	F	343	ALA	2.2
1	E	555	LEU	2.2
3	G	17	DC	2.2
1	E	450	ILE	2.2
1	A	317	GLY	2.1
1	E	117	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	163	ALA	2.1
4	L	2	DG	2.1
1	E	202	SER	2.1
1	E	134	THR	2.1
1	F	365	ILE	2.1
2	D	304	ILE	2.1
2	D	415	ILE	2.1
1	E	489	VAL	2.1
2	D	178	VAL	2.1
2	D	116	GLY	2.1
1	F	484	PHE	2.1
1	E	195	ALA	2.1
1	E	563	ALA	2.1
1	B	580	ASN	2.1
1	A	227	TRP	2.1
1	E	342	GLY	2.1
2	D	263	LYS	2.1
1	E	97	LEU	2.1
1	F	368	VAL	2.1
2	D	579	LEU	2.0
1	E	344	TYR	2.0
1	A	181	ASN	2.0
1	E	367	VAL	2.0
1	A	143	LEU	2.0
2	D	386	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

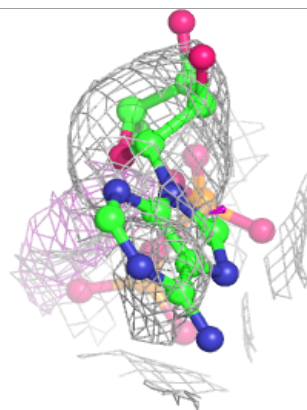
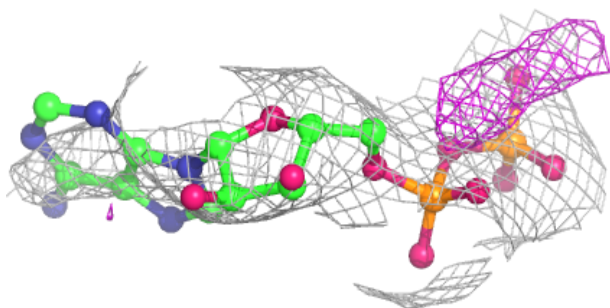
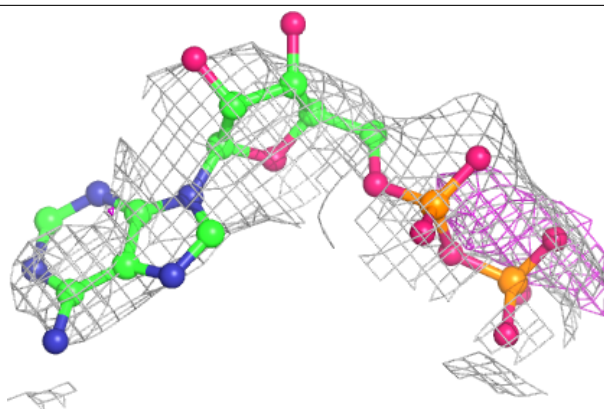
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PO4	E	1003	5/5	0.62	0.13	102,113,121,126	0
8	PO4	C	1004	5/5	0.77	0.08	108,146,166,182	0
6	ADP	D	1002	27/27	0.80	0.11	116,135,157,167	0
8	PO4	A	1005	5/5	0.82	0.16	95,106,138,139	0
8	PO4	A	1006	5/5	0.82	0.25	97,106,107,130	0
8	PO4	F	1003	5/5	0.82	0.27	88,119,124,136	0
8	PO4	F	1004	5/5	0.82	0.19	93,97,121,125	0
8	PO4	C	1005	5/5	0.83	0.28	89,112,117,120	0
6	ADP	E	1002	27/27	0.83	0.12	111,149,164,168	0
8	PO4	B	1004	5/5	0.84	0.17	71,85,119,124	0
9	K	B	1008	1/1	0.86	0.10	84,84,84,84	0
8	PO4	B	1005	5/5	0.87	0.28	107,116,130,163	0
8	PO4	A	1004	5/5	0.88	0.13	56,66,97,118	0
7	MG	C	1007	1/1	0.89	0.10	52,52,52,52	0
9	K	B	1006	1/1	0.89	0.07	70,70,70,70	0
8	PO4	A	1007	5/5	0.89	0.26	87,102,128,136	0
9	K	B	1009	1/1	0.89	0.10	68,68,68,68	0
9	K	C	1006	1/1	0.89	0.07	58,58,58,58	0
9	K	A	1008	1/1	0.90	0.08	65,65,65,65	0
9	K	G	101	1/1	0.91	0.09	91,91,91,91	0
9	K	B	1007	1/1	0.93	0.07	62,62,62,62	0
7	MG	C	1003	1/1	0.94	0.06	57,57,57,57	0
5	ZN	D	1001	1/1	0.94	0.07	149,149,149,149	0
6	ADP	B	1002	27/27	0.95	0.07	41,57,70,81	0
7	MG	B	1003	1/1	0.96	0.06	53,53,53,53	0
6	ADP	A	1002	27/27	0.96	0.06	37,52,67,72	0
6	ADP	C	1002	27/27	0.96	0.07	34,48,61,69	0
6	ADP	F	1002	27/27	0.96	0.06	53,67,78,89	0
7	MG	A	1003	1/1	0.96	0.12	79,79,79,79	0
9	K	A	1009	1/1	0.96	0.09	60,60,60,60	0
5	ZN	E	1001	1/1	0.97	0.05	122,122,122,122	0
5	ZN	F	1001	1/1	0.99	0.03	80,80,80,80	0
5	ZN	B	1001	1/1	0.99	0.07	66,66,66,66	0
5	ZN	C	1001	1/1	0.99	0.09	60,60,60,60	0
5	ZN	A	1001	1/1	1.00	0.12	53,53,53,53	0

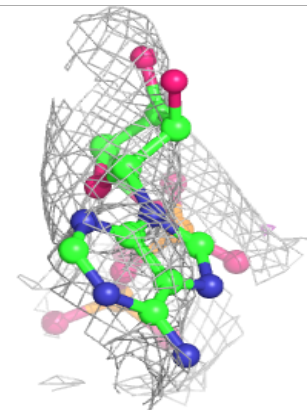
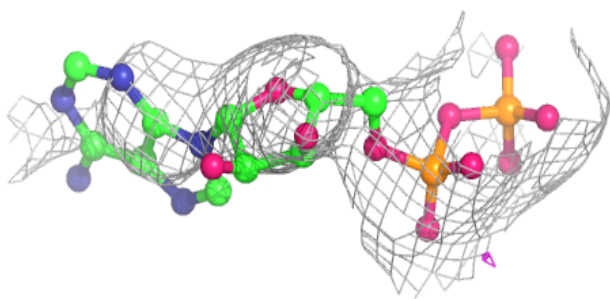
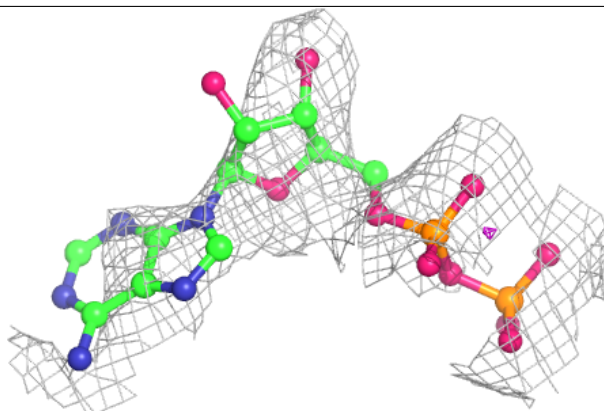
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP D 1002:

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

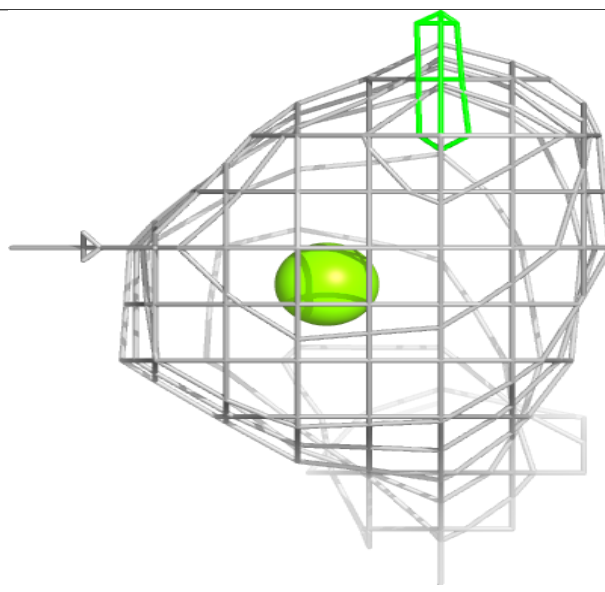
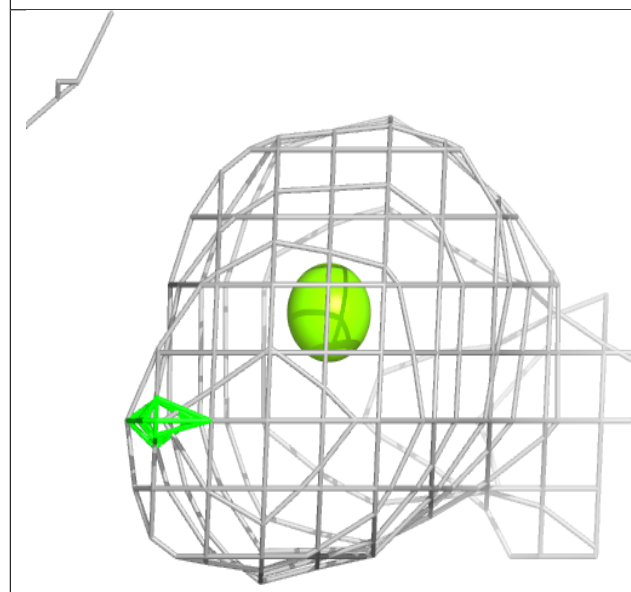
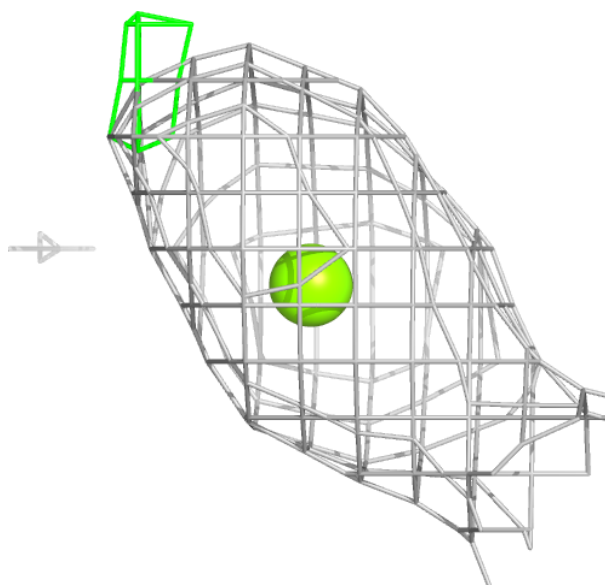
**Electron density around ADP E 1002:**

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



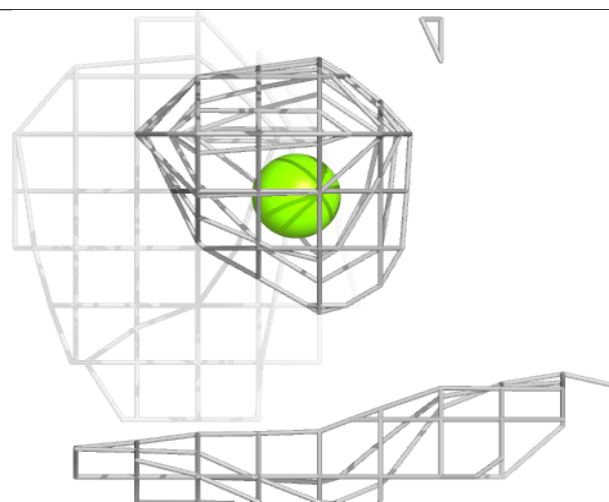
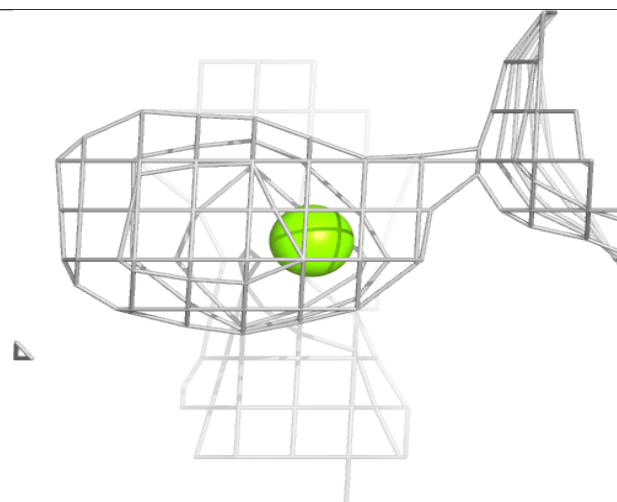
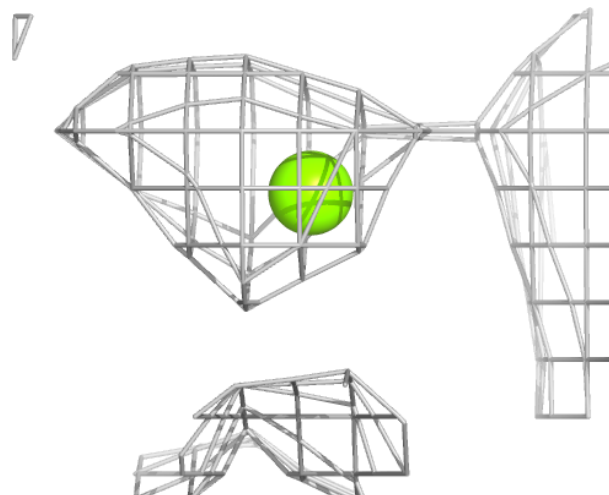
Electron density around MG C 1007:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



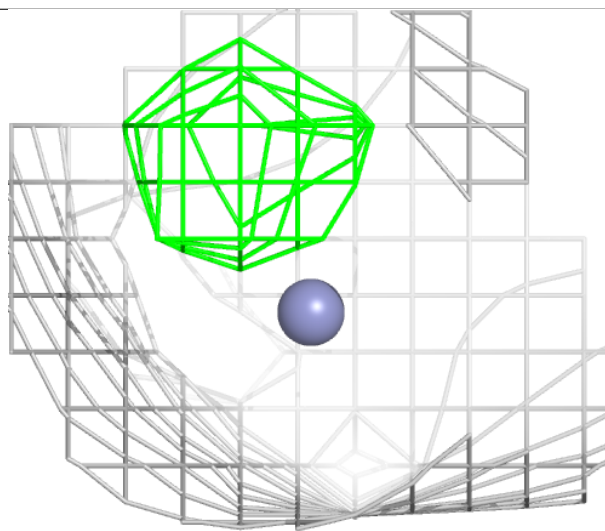
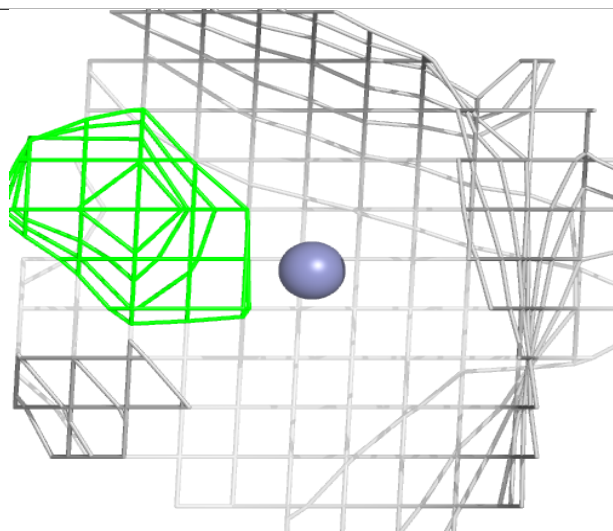
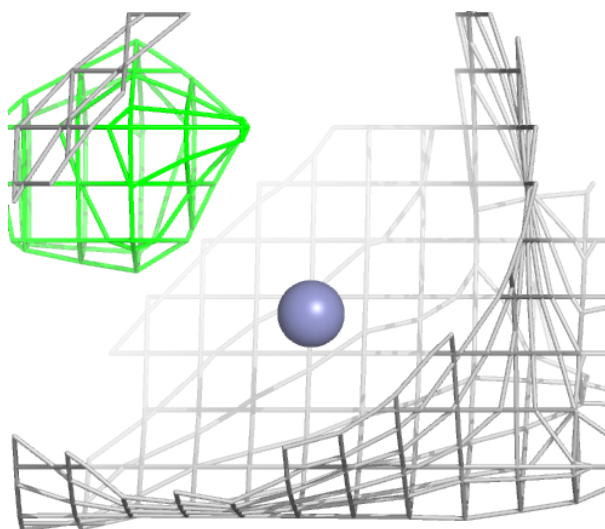
Electron density around MG C 1003:

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



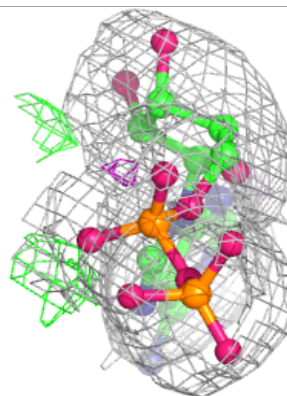
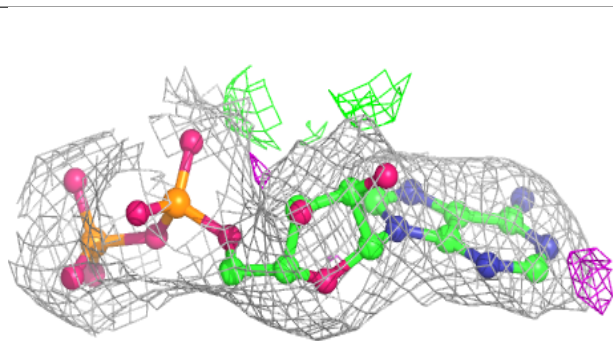
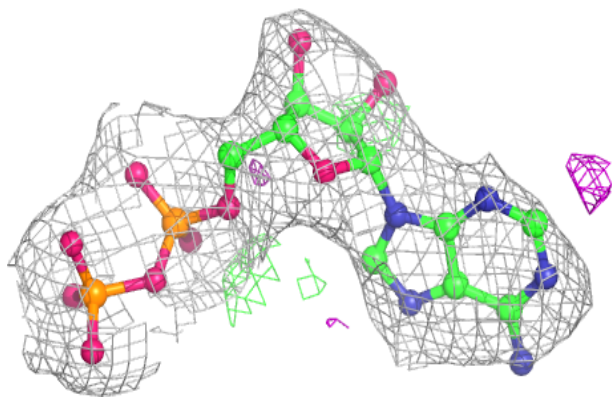
Electron density around ZN D 1001:

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



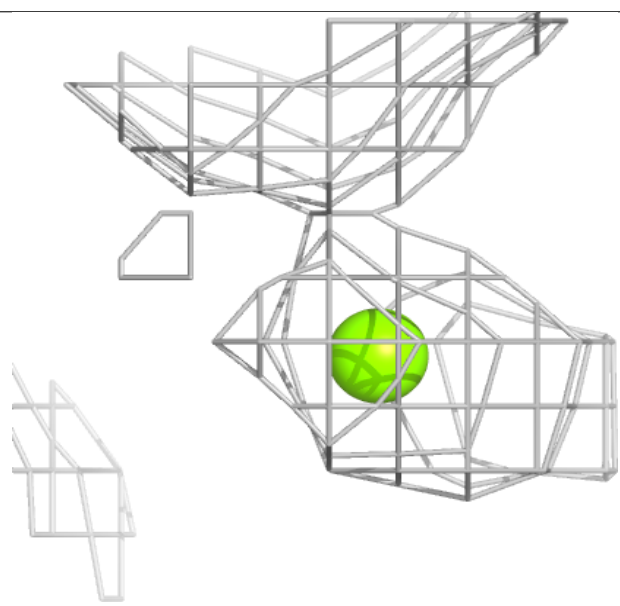
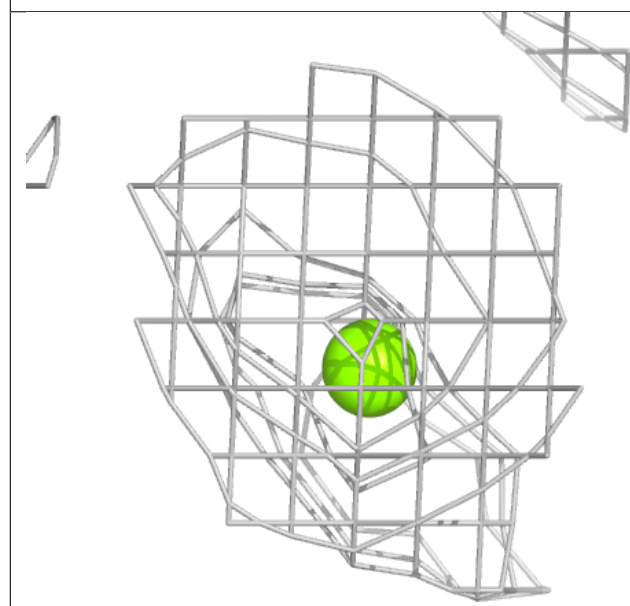
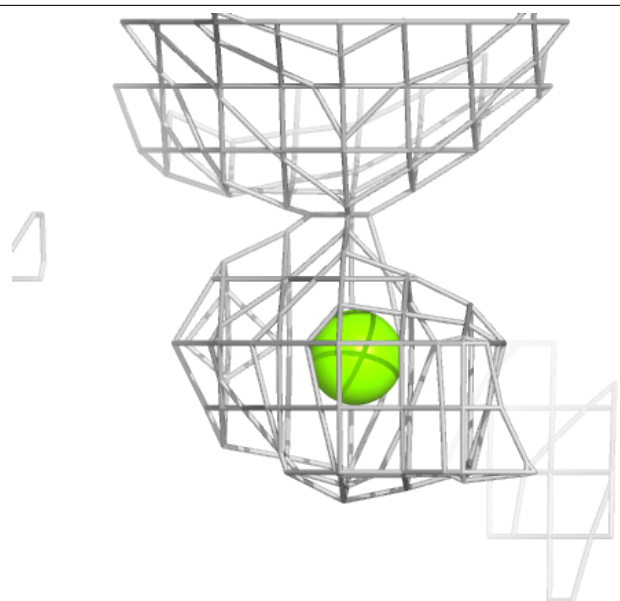
Electron density around ADP B 1002:

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



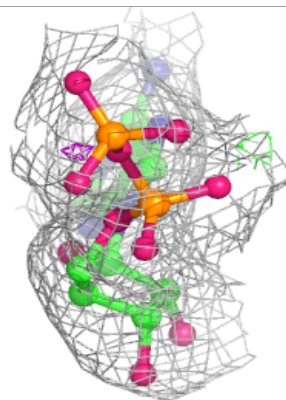
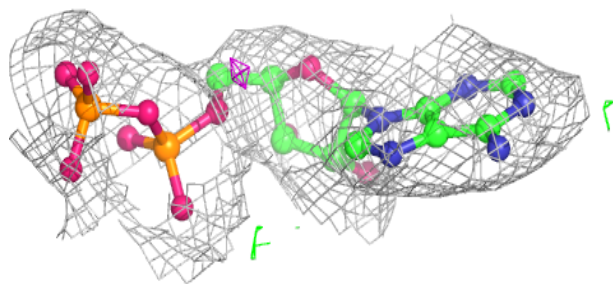
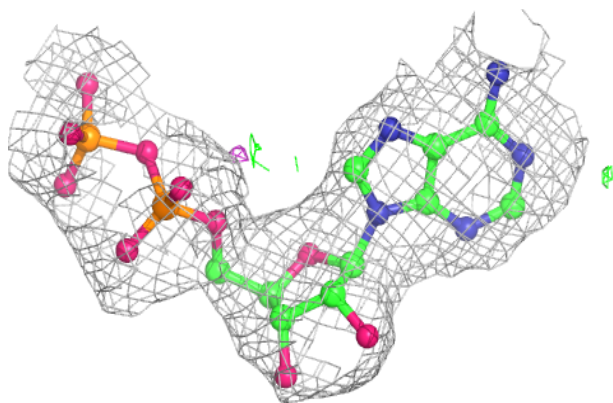
Electron density around MG B 1003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

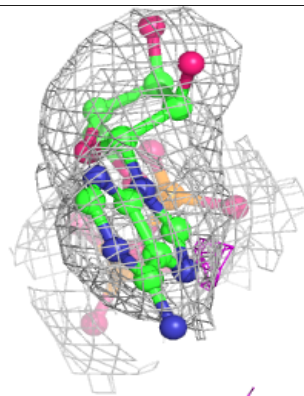
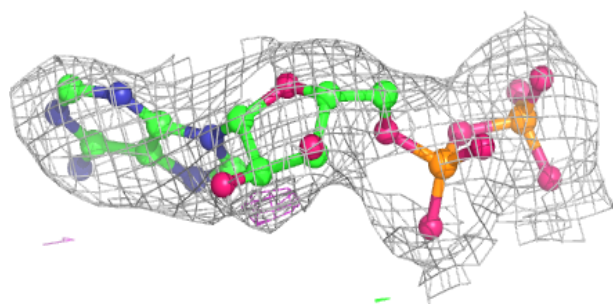
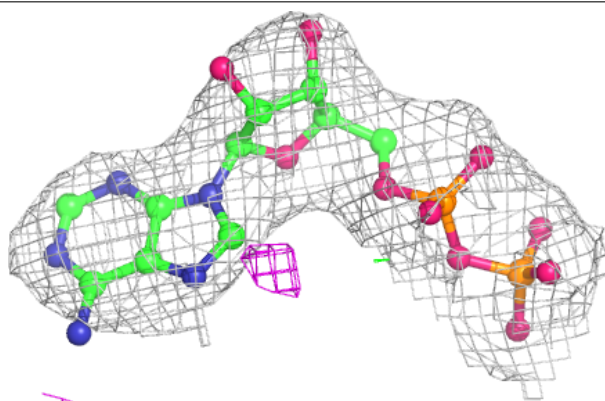


Electron density around ADP A 1002:

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

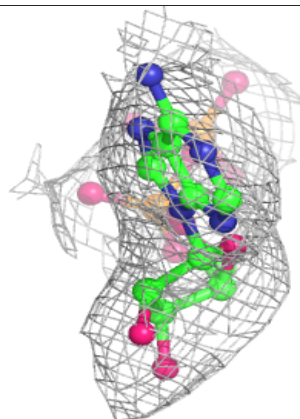
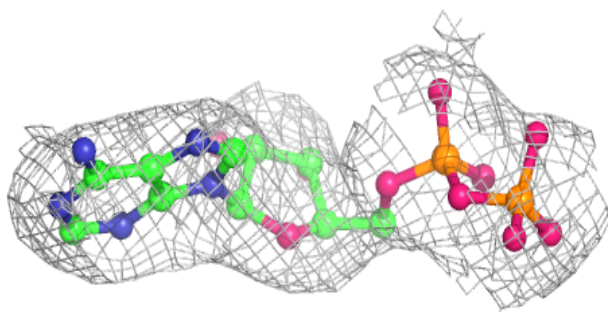
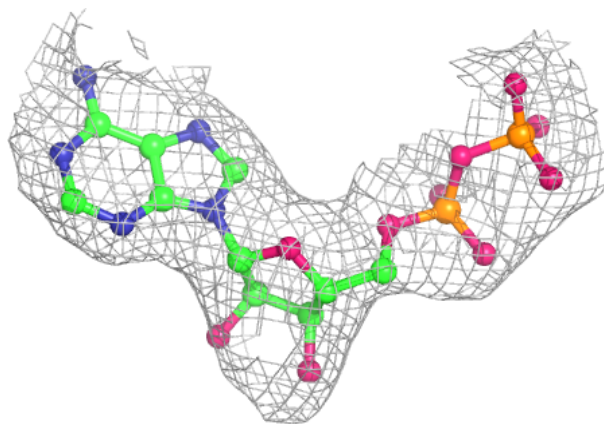
**Electron density around ADP C 1002:**

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



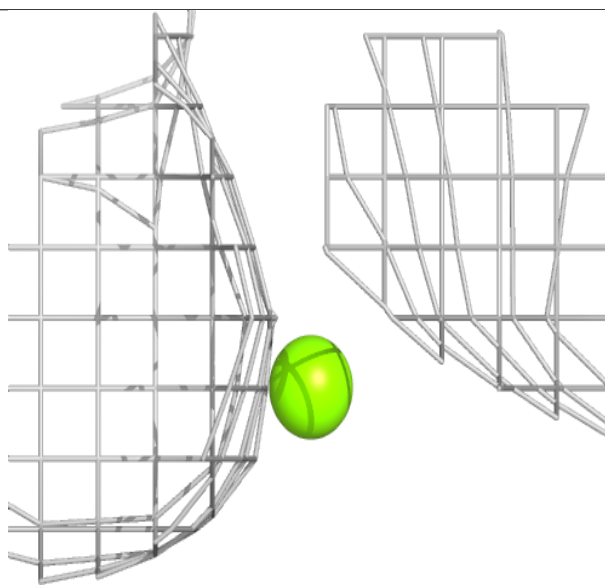
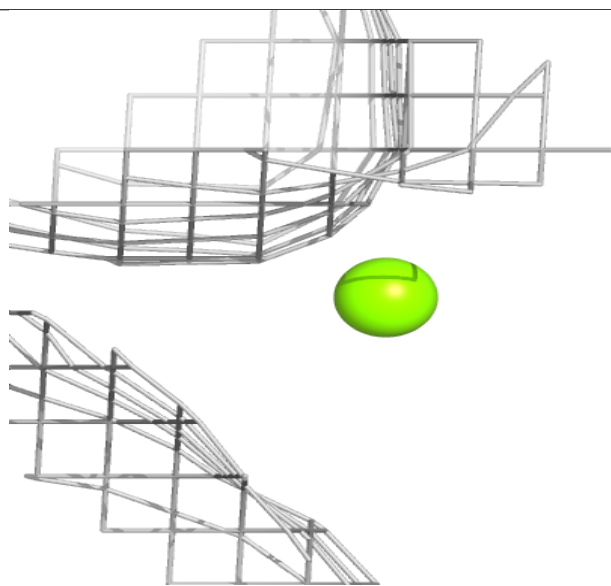
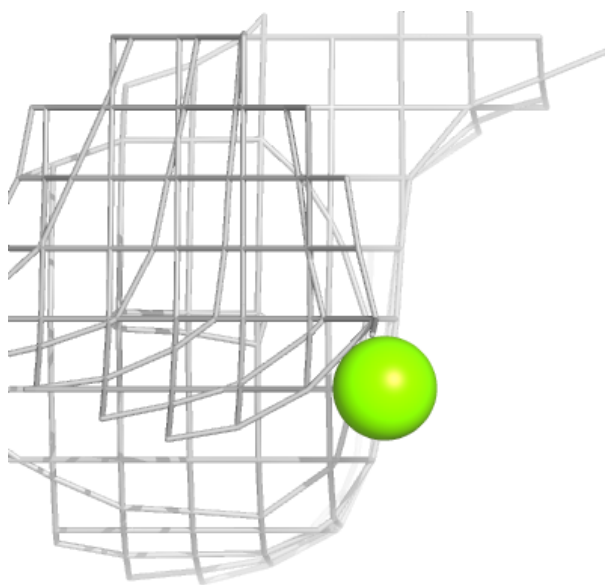
Electron density around ADP F 1002:

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



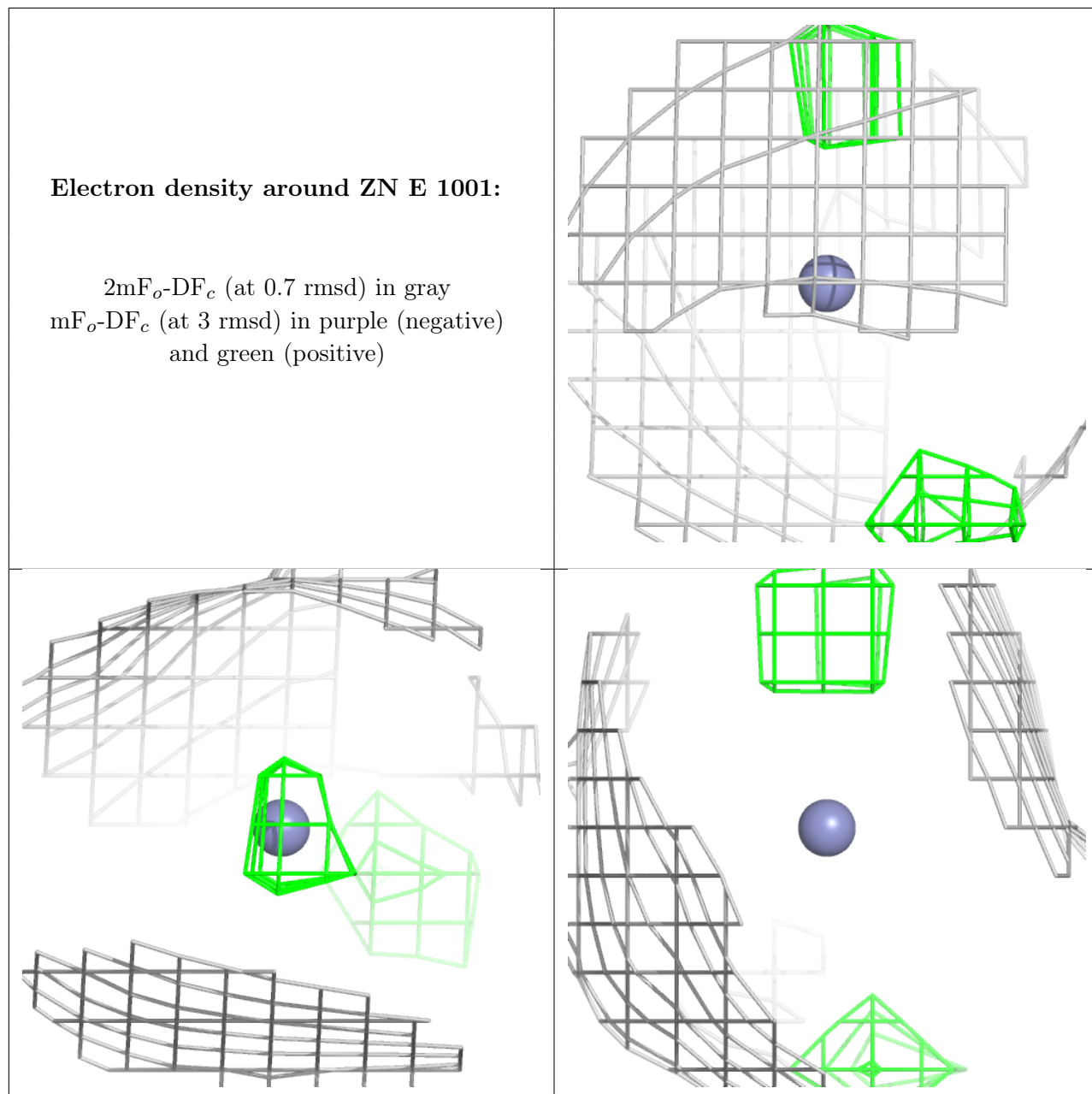
Electron density around MG A 1003:

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



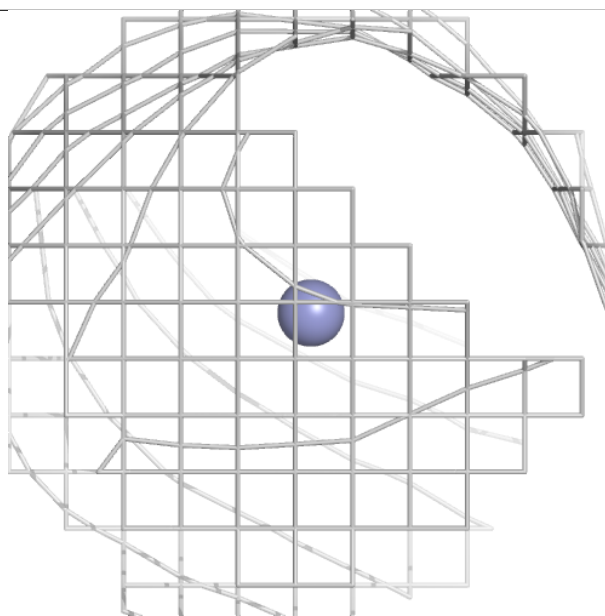
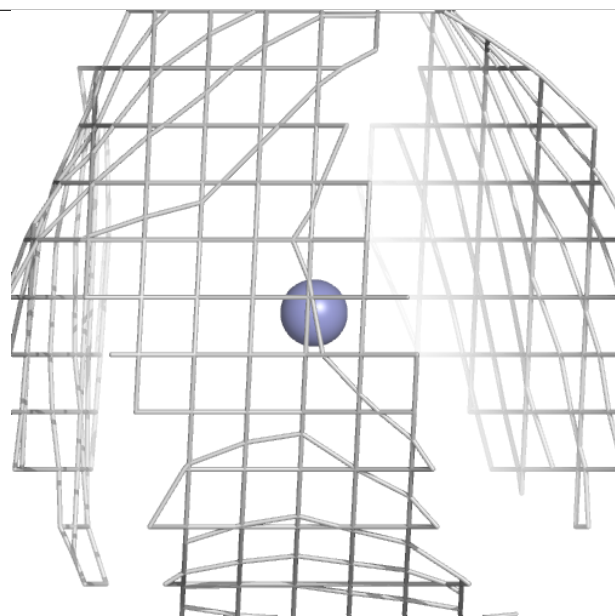
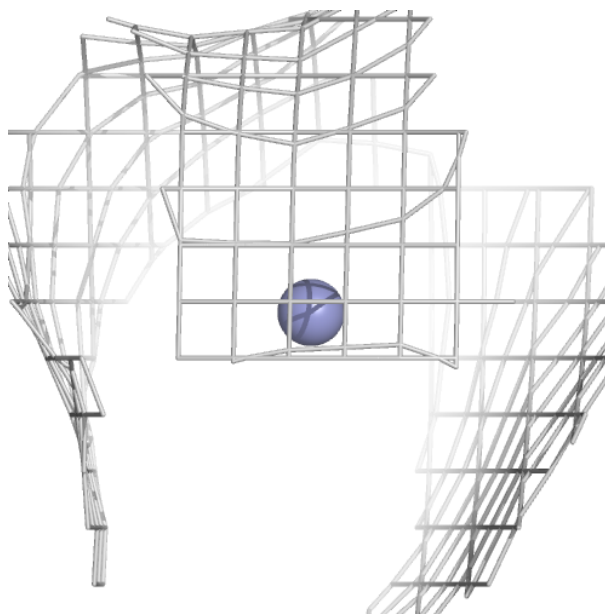
Electron density around ZN E 1001:

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



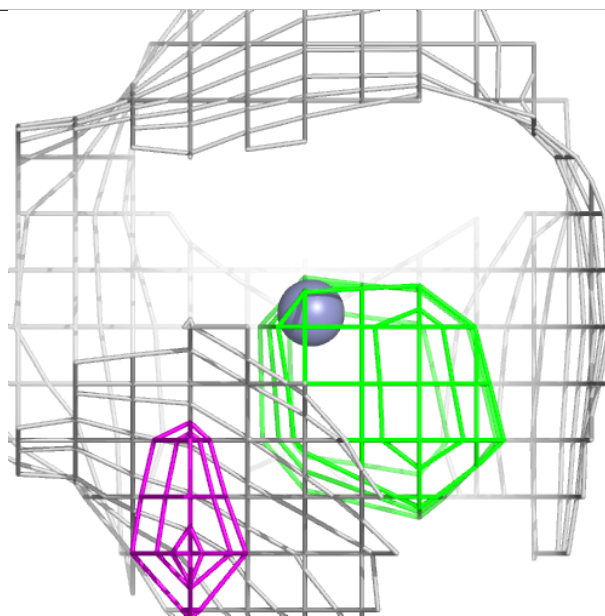
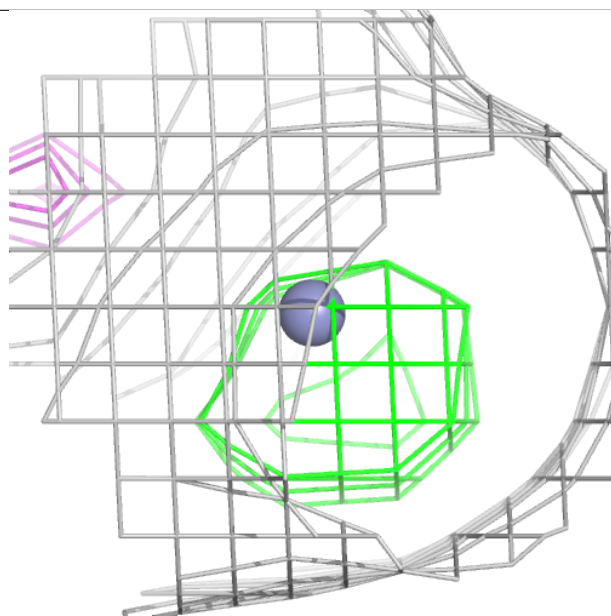
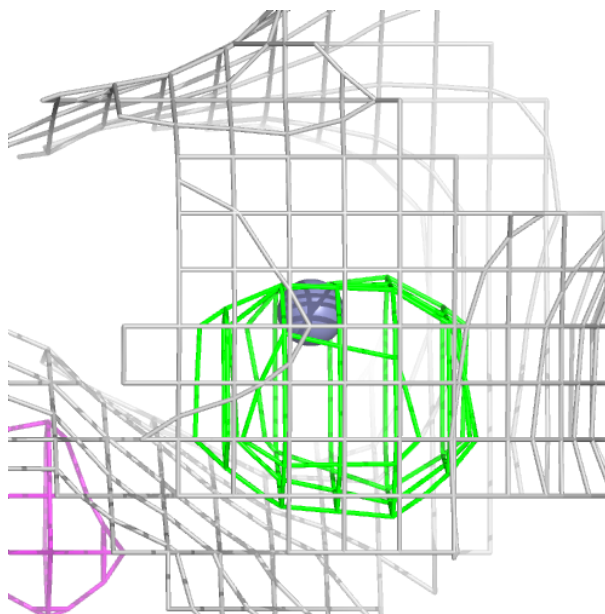
Electron density around ZN F 1001:

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



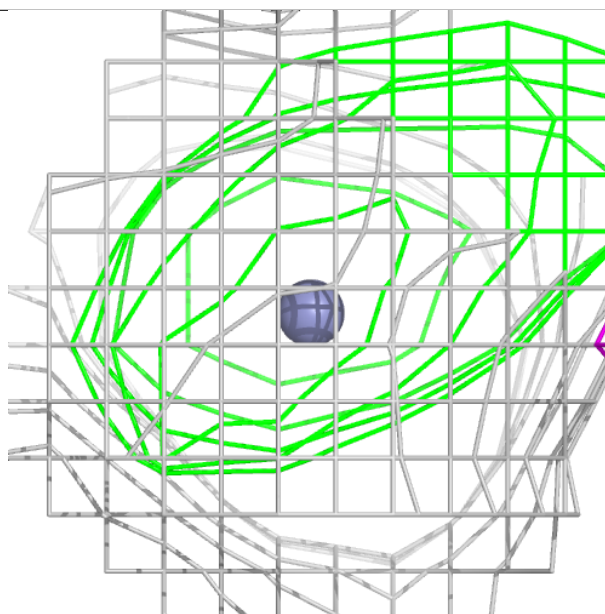
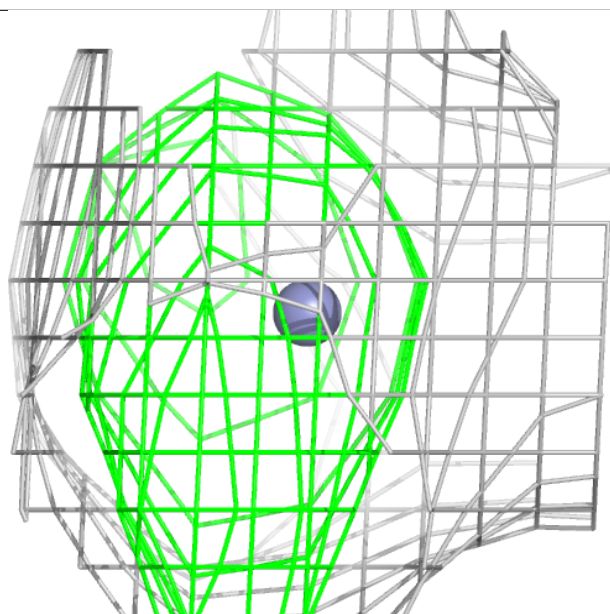
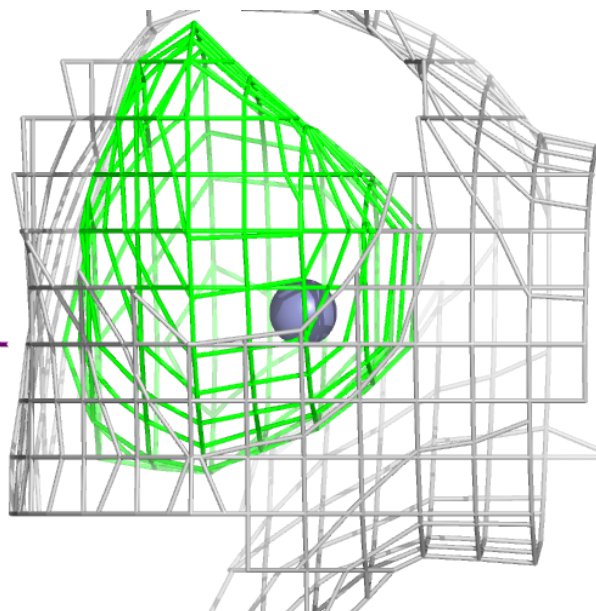
Electron density around ZN B 1001:

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



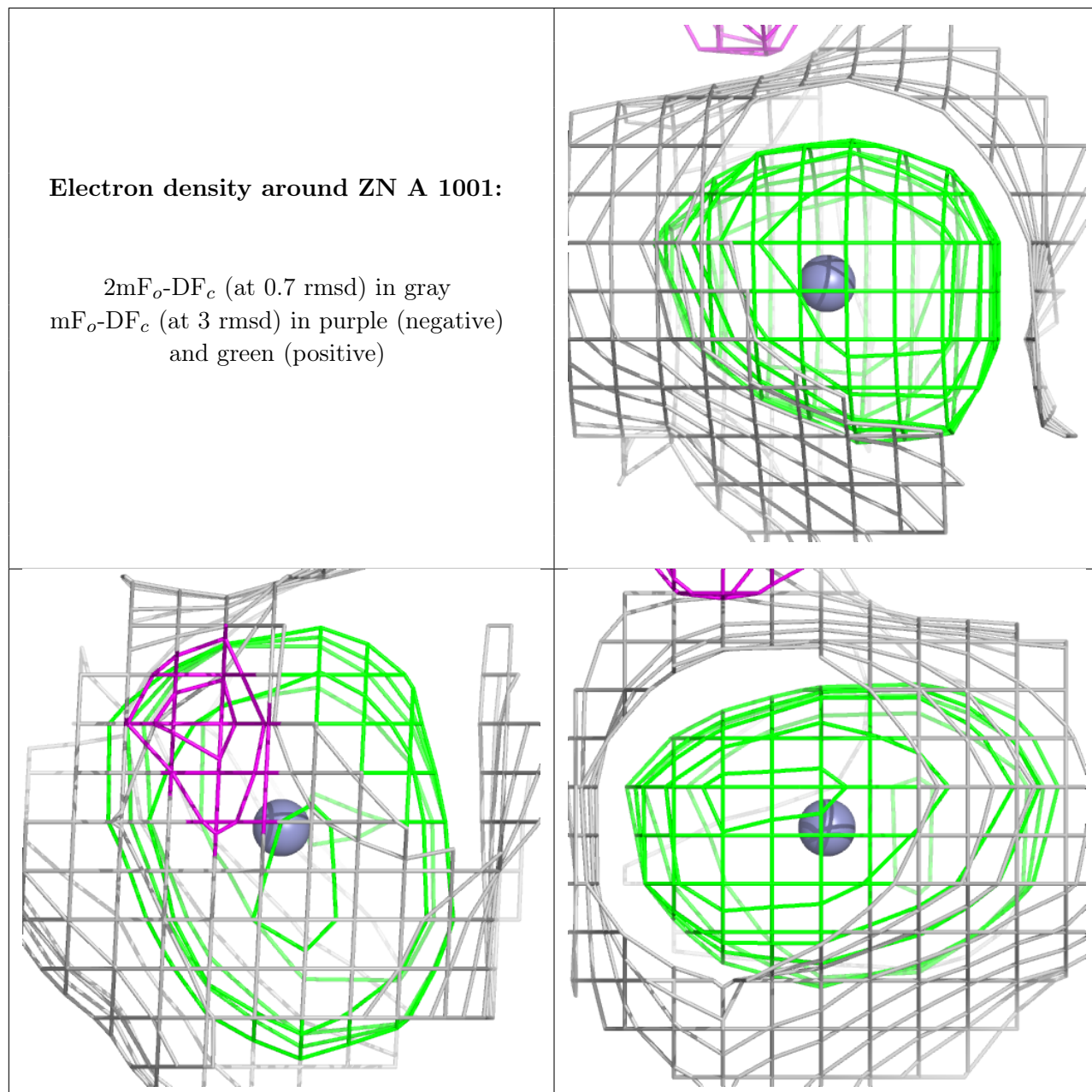
Electron density around ZN C 1001:

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



Electron density around ZN A 1001:

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

**6.5 Other polymers** ⓘ

There are no such residues in this entry.