Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 10:10 PM EST

PDB ID	:	8UK9
Title	:	Structure of T4 Bacteriophage clamp loader mutant D110C bound to the T4 clamp, primer-template DNA, and ATP analog
Authors	:	Marcus, K.; Ghaffari-Kashani, S.; Gee, C.L.
Deposited on	:	2023-10-12
Resolution	:	3.10 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:

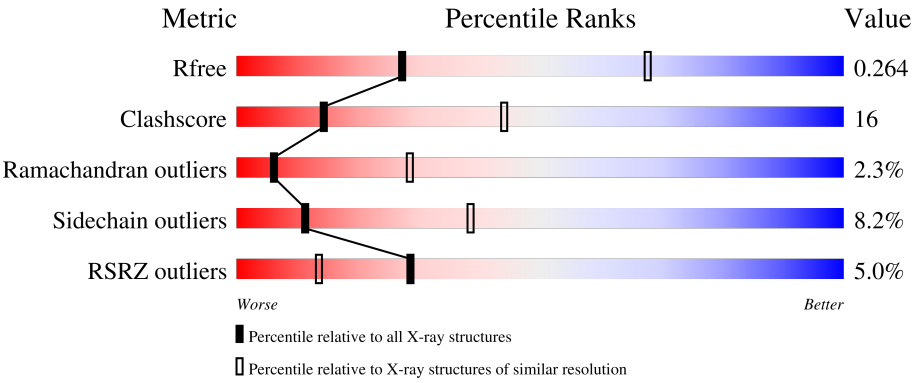
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	187	7% 52% 36% 8%
1	Q	187	18% 51% 37% 10%
2	B	320	67% 30%
2	C	320	69% 28%
2	D	320	60% 36%

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Mol	Chain	Length	Quality of chain
2	E	320	2% 53% 40% 6%
2	K	320	4% 65% 31%
2	L	320	3% 65% 32%
2	M	320	3% 59% 37%
2	N	320	8% 53% 35% 7% 5%
3	F	228	12% 54% 39% 7%
3	G	228	2% 75% 22%
3	H	228	4% 73% 26%
3	R	228	8% 68% 31%
3	S	228	10% 62% 36%
3	T	228	10% 66% 29%
4	I	24	4% 33% 67%
4	O	24	29% 71%
5	J	20	40% 60%
5	P	20	15% 55% 45%

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
6	AF3	B	901	-	-	X	-
6	AF3	K	402	-	-	X	-
6	AF3	L	402	-	-	X	-
6	AF3	M	402	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 35422 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 Sliding-clamp-loader small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	1	0
			1474	951	242	275	6			
1	Q	183	Total	C	N	O	S	0	0	0
			1469	947	244	272	6			

- Molecule 2 is a protein called Sliding-clamp-loader large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2507	1586	431	472	18			
2	C	320	Total	C	N	O	S	0	0	0
			2513	1589	432	474	18			
2	D	318	Total	C	N	O	S	0	0	0
			2499	1581	430	471	17			
2	E	318	Total	C	N	O	S	0	0	0
			2499	1581	430	471	17			
2	K	319	Total	C	N	O	S	0	0	0
			2507	1586	431	472	18			
2	L	320	Total	C	N	O	S	0	0	0
			2513	1589	432	474	18			
2	M	317	Total	C	N	O	S	0	0	0
			2492	1578	426	470	18			
2	N	305	Total	C	N	O	S	0	0	0
			2407	1526	413	451	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P04526
B	110	CYS	ASP	engineered mutation	UNP P04526
C	0	SER	-	expression tag	UNP P04526
C	110	CYS	ASP	engineered mutation	UNP P04526
D	0	SER	-	expression tag	UNP P04526

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Chain	Residue	Modelled	Actual	Comment	Reference
D	110	CYS	ASP	engineered mutation	UNP P04526
E	0	SER	-	expression tag	UNP P04526
E	110	CYS	ASP	engineered mutation	UNP P04526
K	0	SER	-	expression tag	UNP P04526
K	110	CYS	ASP	engineered mutation	UNP P04526
L	0	SER	-	expression tag	UNP P04526
L	110	CYS	ASP	engineered mutation	UNP P04526
M	0	SER	-	expression tag	UNP P04526
M	110	CYS	ASP	engineered mutation	UNP P04526
N	0	SER	-	expression tag	UNP P04526
N	110	CYS	ASP	engineered mutation	UNP P04526

- Molecule 3 is a protein called Sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	G	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	H	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	R	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	S	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	T	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			

- Molecule 4 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			
4	O	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			

- Molecule 5 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	20	Total	C	N	O	P	0	0	0
			408	195	81	113	19			

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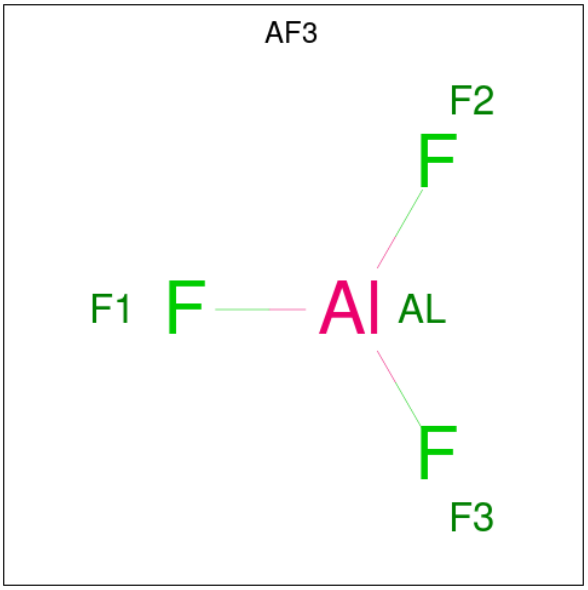
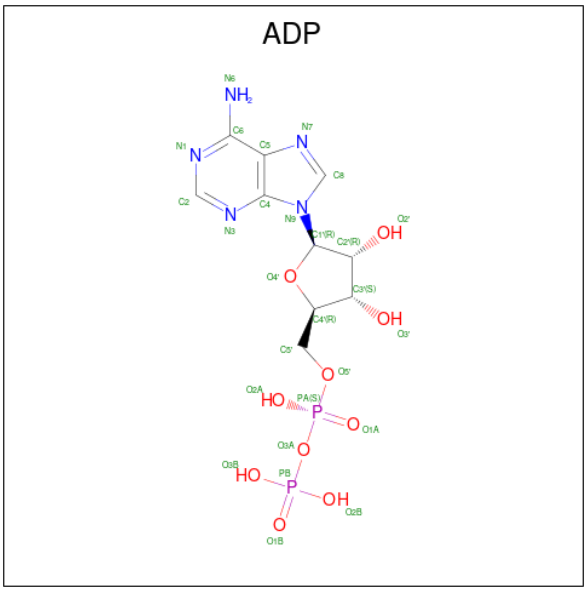
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	20	Total	C	N	O	P	0	0	0
			408	195	81	113	19			

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Al	F	0	0
			4	1	3		
6	C	1	Total	Al	F	0	0
			4	1	3		
6	D	1	Total	Al	F	0	0
			4	1	3		
6	K	1	Total	Al	F	0	0
			4	1	3		
6	L	1	Total	Al	F	0	0
			4	1	3		
6	M	1	Total	Al	F	0	0
			4	1	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	E	1	Total	Mg	0	0
			1	1		

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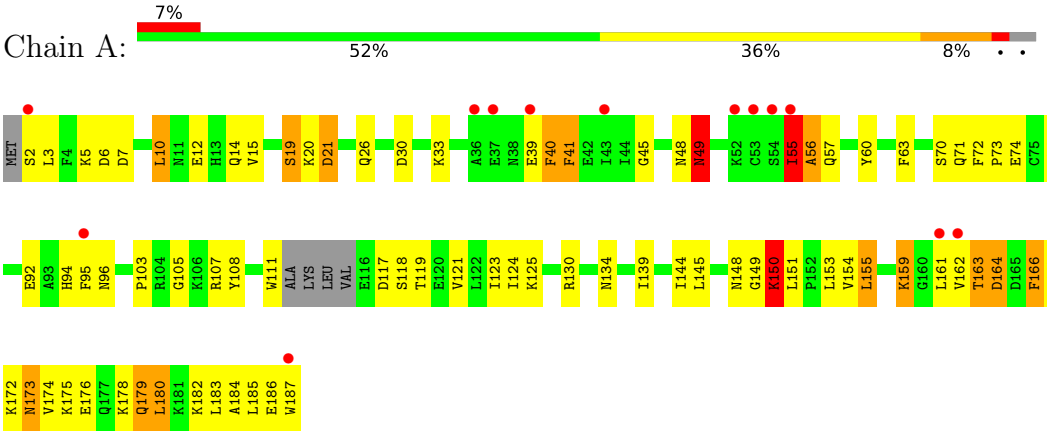
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	1	Total Mg 1 1	0	0
8	L	1	Total Mg 1 1	0	0
8	M	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

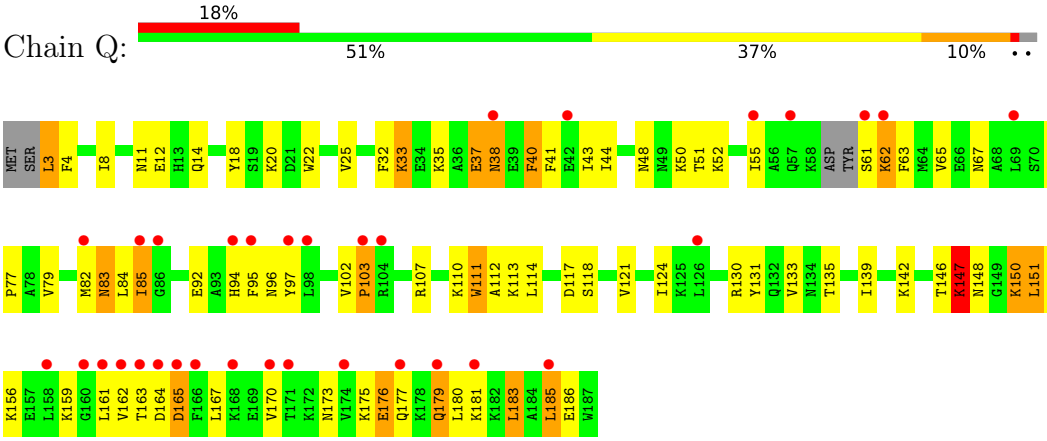
• Molecule 1: Sliding-clamp-loader small subunit

Chain A:



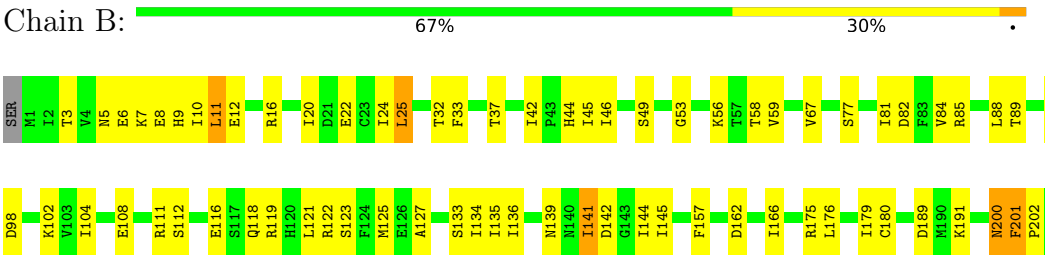
• Molecule 1: Sliding-clamp-loader small subunit

Chain Q:



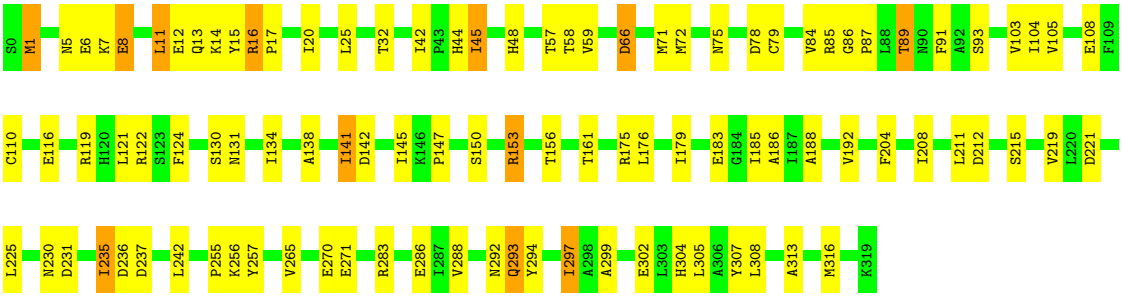
• Molecule 2: Sliding-clamp-loader large subunit

Chain B:



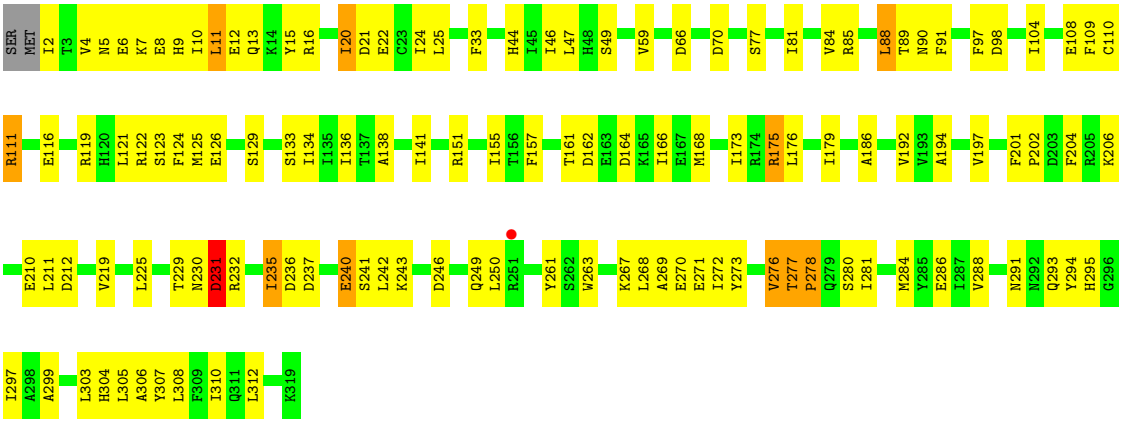
• Molecule 2: Sliding-clamp-loader large subunit

Chain C:



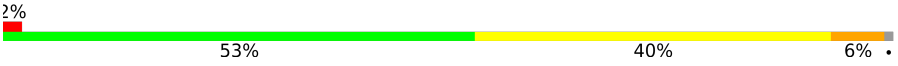
• Molecule 2: Sliding-clamp-loader large subunit

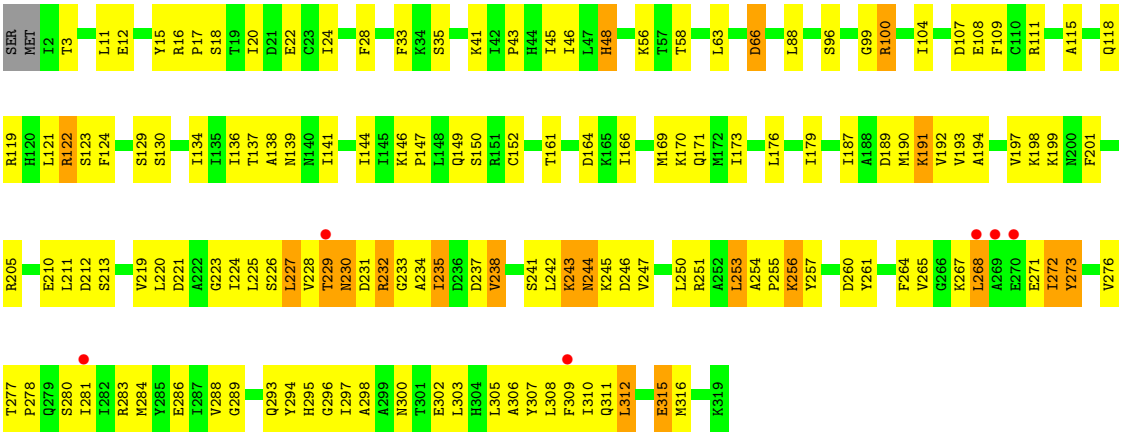
Chain D:



• Molecule 2: Sliding-clamp-loader large subunit

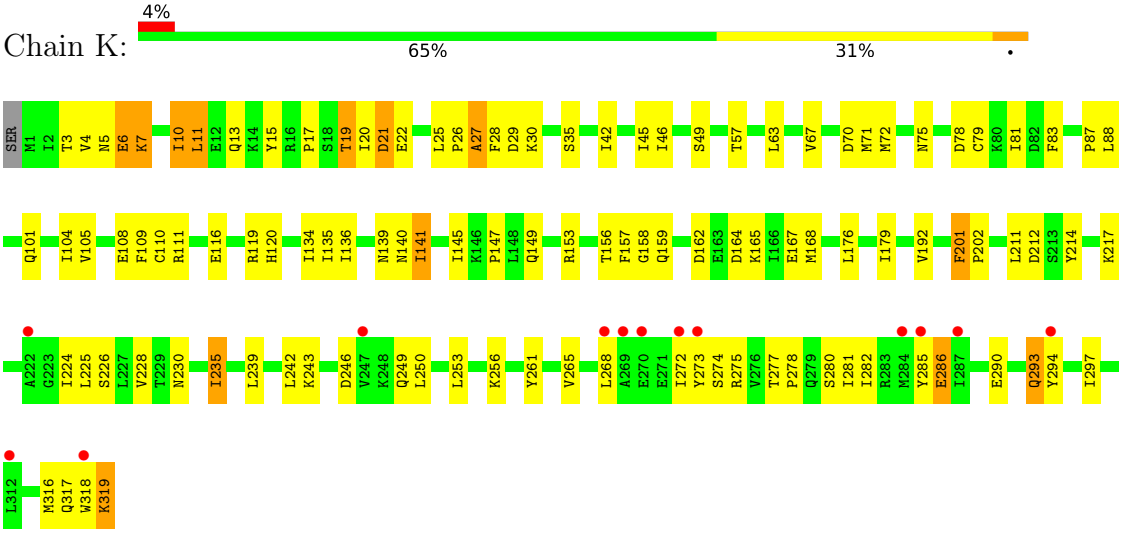
Chain E:





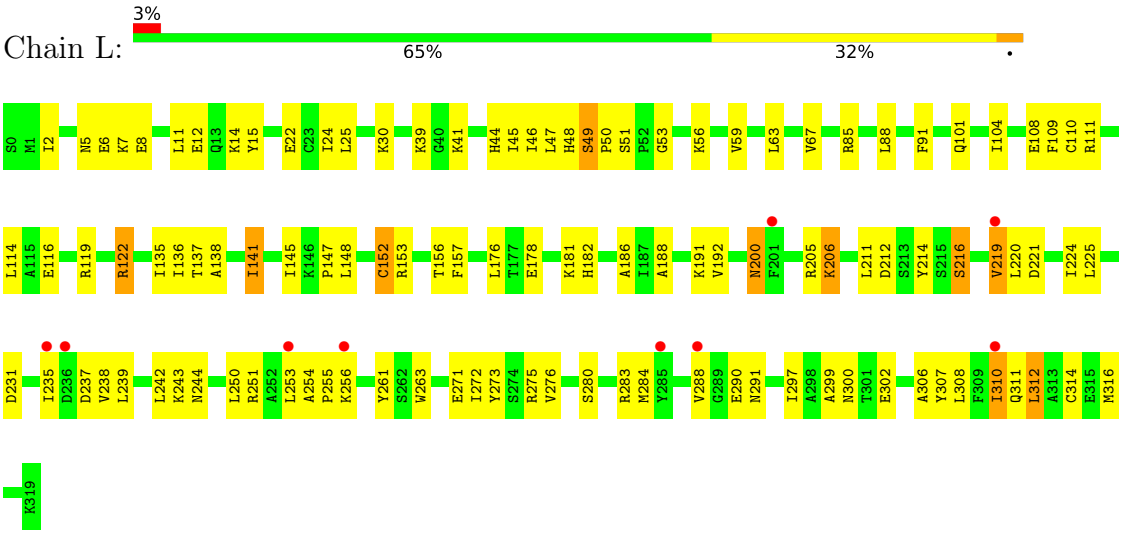
• Molecule 2: Sliding-clamp-loader large subunit

Chain K:



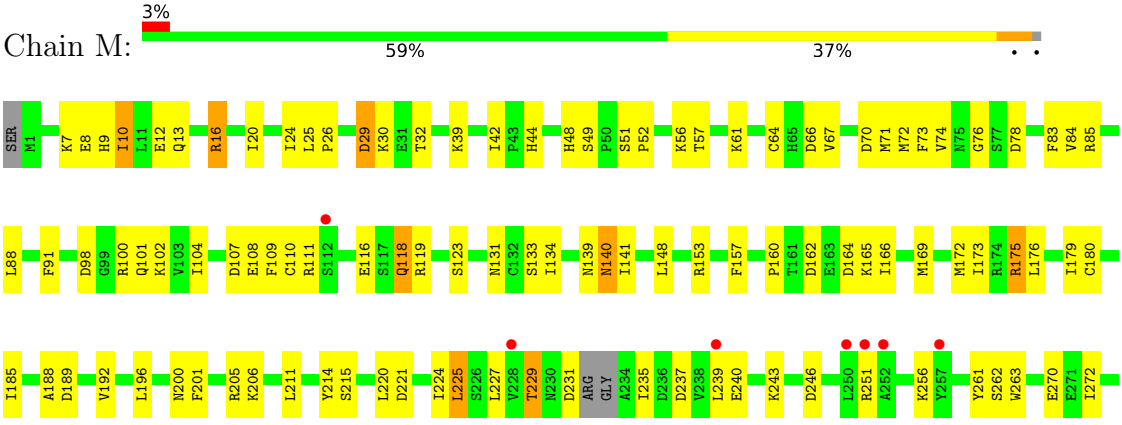
• Molecule 2: Sliding-clamp-loader large subunit

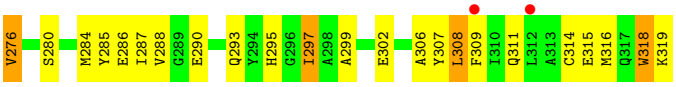
Chain L:



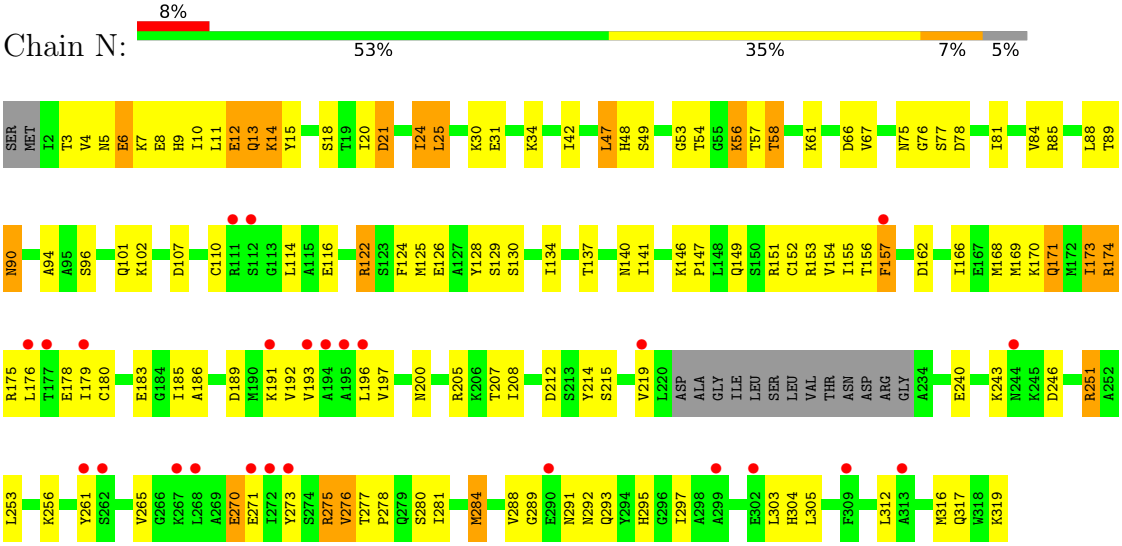
• Molecule 2: Sliding-clamp-loader large subunit

Chain M:

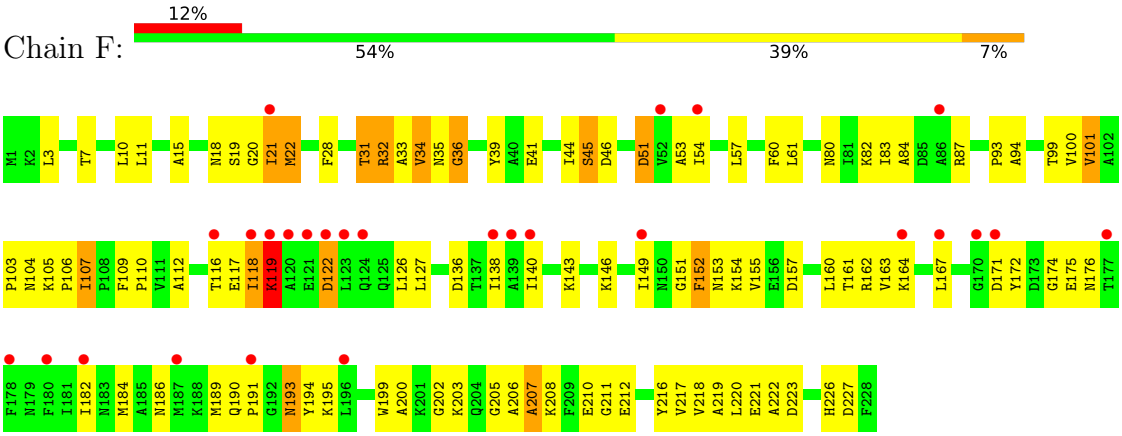




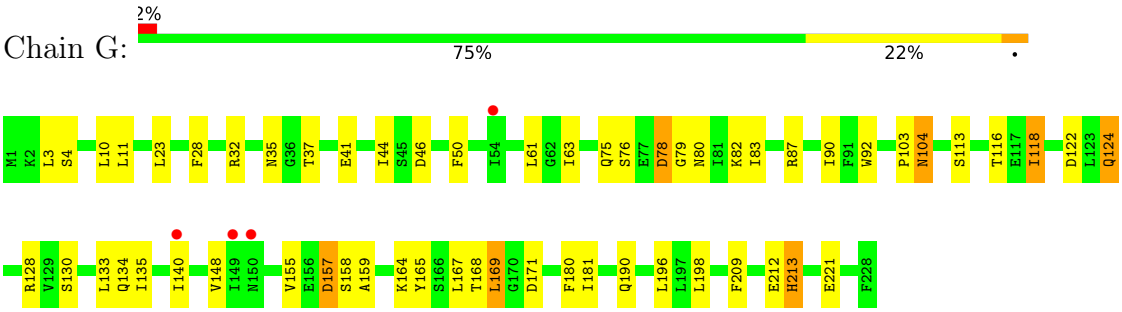
• Molecule 2: Sliding-clamp-loader large subunit



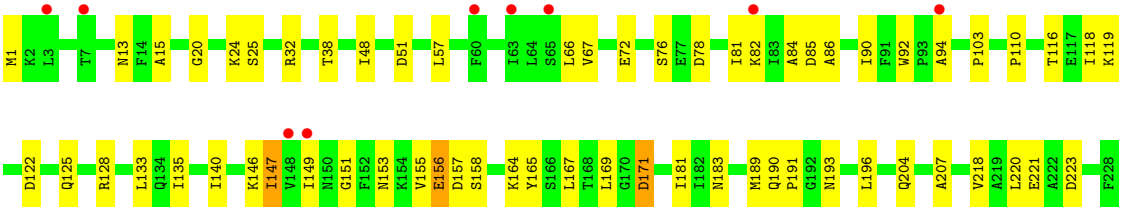
• Molecule 3: Sliding clamp



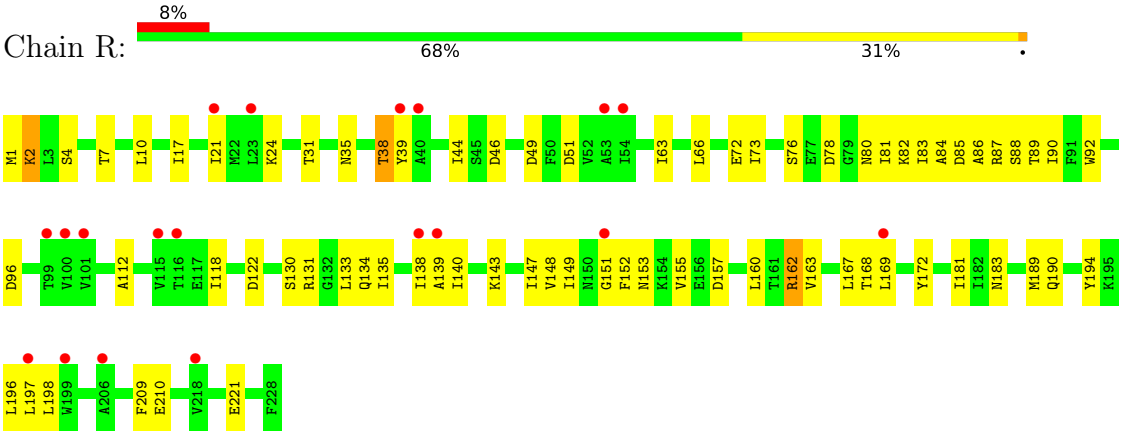
• Molecule 3: Sliding clamp



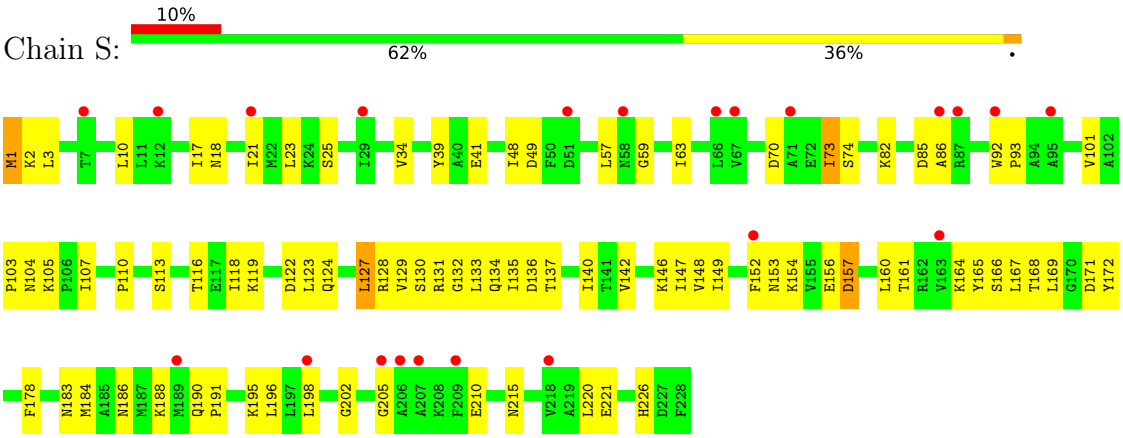
• Molecule 3: Sliding clamp



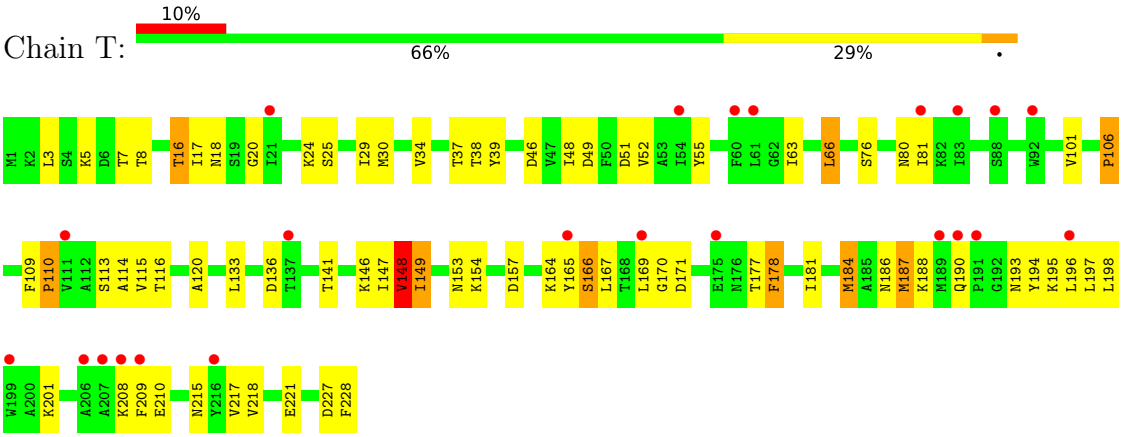
• Molecule 3: Sliding clamp



• Molecule 3: Sliding clamp

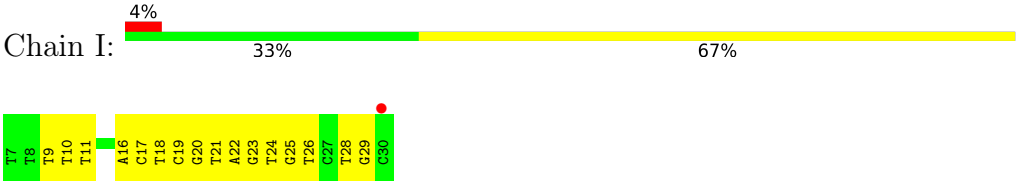


• Molecule 3: Sliding clamp



• Molecule 4: DNA template

Chain I:



• Molecule 4: DNA template

Chain O:

• Molecule 5: DNA primer

Chain J:

• Molecule 5: DNA primer

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.24Å 231.99Å 264.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.10 48.13 – 3.10	Depositor EDS
% Data completeness (in resolution range)	71.3 (48.13-3.10) 71.3 (48.13-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.253 , 0.265 0.253 , 0.264	Depositor DCC
R_{free} test set	1999 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å^2)	95.1	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	35422	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, AF3

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	0.24	0/1505	0.45	0/2025
1	Q	0.27	0/1495	0.48	0/2011
2	B	0.27	0/2551	0.47	0/3438
2	C	0.24	0/2557	0.47	0/3446
2	D	0.26	0/2543	0.48	0/3428
2	E	0.29	0/2543	0.52	0/3428
2	K	0.25	0/2551	0.48	0/3438
2	L	0.25	0/2557	0.47	0/3446
2	M	0.25	0/2535	0.47	0/3416
2	N	0.25	0/2450	0.49	0/3300
3	F	0.25	0/1779	0.48	0/2410
3	G	0.25	0/1779	0.46	0/2410
3	H	0.25	0/1779	0.45	0/2410
3	R	0.25	0/1779	0.49	0/2410
3	S	0.25	0/1779	0.47	0/2410
3	T	0.25	0/1779	0.51	0/2410
4	I	0.53	0/544	1.07	0/838
4	O	0.51	0/544	1.04	0/838
5	J	0.50	0/459	0.85	0/706
5	P	0.48	0/459	0.82	0/706
All	All	0.28	0/35967	0.52	0/48924

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1
3	T	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	21	ASP	Peptide
3	T	148	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1474	0	1491	61	0
1	Q	1469	0	1502	60	0
2	B	2507	0	2538	76	0
2	C	2513	0	2543	72	0
2	D	2499	0	2526	98	0
2	E	2499	0	2523	147	0
2	K	2507	0	2539	76	0
2	L	2513	0	2543	80	0
2	M	2492	0	2521	91	0
2	N	2407	0	2434	95	0
3	F	1750	0	1755	77	0
3	G	1750	0	1755	34	0
3	H	1750	0	1755	33	0
3	R	1750	0	1755	51	0
3	S	1750	0	1755	59	0
3	T	1750	0	1755	52	0
4	I	489	0	277	17	0
4	O	489	0	277	17	0
5	J	408	0	225	10	0
5	P	408	0	225	10	0
6	B	4	0	0	4	0
6	C	4	0	0	1	0
6	D	4	0	0	0	0
6	K	4	0	0	2	0
6	L	4	0	0	2	0
6	M	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	27	0	12	8	0
7	C	27	0	12	6	0
7	D	27	0	12	5	0
7	E	27	0	12	6	0
7	K	27	0	12	4	0
7	L	27	0	12	4	0
7	M	27	0	12	8	0
7	N	27	0	12	5	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	35422	0	34790	1084	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 16.

All (1084) 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:E:250:LEU:HD22	2:E:309:PHE:HB3	1.41	1.02
3:F:190:GLN:HB3	3:F:191:PRO:HD2	1.46	0.96
2:C:145:ILE:HG13	2:C:147:PRO:HD2	1.52	0.92
2:L:12:GLU:OE2	2:M:153:ARG:NH1	2.08	0.85
1:A:134:ASN:HD22	2:E:111:ARG:NH2	1.74	0.85
3:F:140:ILE:HG22	3:F:149:ILE:HG22	1.58	0.84
1:A:7:ASP:OD2	3:F:32:ARG:NH2	2.10	0.83
1:A:134:ASN:ND2	2:E:111:ARG:CZ	2.42	0.82
3:H:146:LYS:HA	3:H:171:ASP:HA	1.61	0.82
2:E:223:GLY:O	2:E:226:SER:OG	1.96	0.81
2:N:12:GLU:HG3	7:N:401:ADP:H4'	1.61	0.81
2:E:231:ASP:HA	2:E:235:ILE:HG22	1.63	0.81
6:K:402:AF3:F3	7:K:403:ADP:O2B	1.88	0.80
2:C:116:GLU:OE2	2:C:119:ARG:NH1	2.14	0.80
2:N:122:ARG:O	2:N:151:ARG:NH1	2.14	0.80
3:F:194:TYR:HB3	3:F:210:GLU:O	1.83	0.79
2:E:233:GLY:HA3	2:E:267:LYS:NZ	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:LEU:HD13	2:E:265:VAL:HG12	1.64	0.77
3:R:87:ARG:HH12	3:S:119:LYS:HD3	1.49	0.76
2:L:299:ALA:H	2:M:295:HIS:HE1	1.32	0.76
1:A:134:ASN:ND2	2:E:111:ARG:NH2	2.34	0.75
1:A:33:LYS:HA	2:B:119:ARG:HD3	1.68	0.75
2:B:16:ARG:HH21	7:B:902:ADP:H5'1	1.51	0.75
1:A:139:ILE:HD13	2:E:256:LYS:HE3	1.68	0.75
2:E:12:GLU:O	7:E:401:ADP:O3'	2.05	0.75
2:K:108:GLU:OE2	6:K:402:AF3:F3	1.94	0.74
3:S:2:LYS:HE2	3:S:70:ASP:HA	1.68	0.74
2:L:46:ILE:HG12	2:L:136:ILE:HB	1.70	0.74
2:D:12:GLU:O	7:D:403:ADP:O3'	2.05	0.73
3:R:122:ASP:HB3	3:R:167:LEU:HD21	1.70	0.73
2:D:46:ILE:HG12	2:D:136:ILE:HB	1.71	0.73
3:G:78:ASP:O	3:G:80:ASN:N	2.20	0.73
2:C:297:ILE:HD12	2:D:297:ILE:HD11	1.71	0.72
2:K:111:ARG:HH12	2:L:116:GLU:HB3	1.54	0.72
2:C:75:ASN:HD22	2:D:123:SER:HB3	1.54	0.72
3:F:22:MET:HB2	3:F:53:ALA:HA	1.70	0.72
3:S:1:MET:HG2	3:S:48:ILE:HA	1.72	0.71
2:M:205:ARG:HE	7:M:403:ADP:H5'1	1.55	0.71
2:E:219:VAL:HG22	2:E:221:ASP:H	1.54	0.71
2:B:213:SER:HB2	2:C:153:ARG:HH21	1.56	0.71
3:T:141:THR:H	3:T:148:VAL:HG11	1.55	0.71
2:L:280:SER:OG	2:L:316:MET:SD	2.49	0.70
1:Q:22:TRP:HA	1:Q:25:VAL:HG12	1.74	0.70
2:M:280:SER:OG	2:M:316:MET:SD	2.50	0.69
2:E:225:LEU:HA	2:E:229:THR:HG23	1.74	0.69
3:R:4:SER:N	3:R:46:ASP:OD2	2.25	0.69
2:D:240:GLU:HA	2:D:243:LYS:HB3	1.73	0.69
2:B:261:TYR:OH	2:B:291:ASN:ND2	2.26	0.69
2:D:88:LEU:HG	2:D:104:ILE:HD13	1.74	0.69
2:E:58:THR:HG23	7:E:401:ADP:O2A	1.93	0.69
2:C:192:VAL:HG22	2:C:225:LEU:HB2	1.74	0.69
2:D:11:LEU:HD22	2:D:212:ASP:HB2	1.75	0.69
3:T:18:ASN:ND2	3:T:20:GLY:O	2.22	0.69
2:E:233:GLY:HA3	2:E:267:LYS:HZ2	1.57	0.69
2:E:273:TYR:HE1	2:E:281:ILE:CG2	2.06	0.69
2:M:290:GLU:HA	2:M:293:GLN:HG2	1.73	0.69
2:N:212:ASP:OD1	1:Q:148:ASN:ND2	2.26	0.68
2:E:243:LYS:O	2:E:245:LYS:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:70:ASP:HB3	2:M:102:LYS:HG2	1.75	0.68
2:M:188:ALA:HB3	2:M:221:ASP:HA	1.74	0.68
2:D:6:GLU:O	2:D:8:GLU:N	2.27	0.68
2:C:176:LEU:HD22	2:C:211:LEU:HD22	1.76	0.68
2:K:45:ILE:HG22	2:K:153:ARG:HB2	1.75	0.68
2:D:235:ILE:HD13	2:D:268:LEU:HA	1.76	0.68
2:E:16:ARG:HH21	7:E:401:ADP:H5'2	1.59	0.68
2:E:233:GLY:CA	2:E:267:LYS:NZ	2.56	0.68
2:B:24:ILE:HD11	2:B:175:ARG:HG3	1.77	0.67
3:F:176:ASN:HB2	3:F:227:ASP:OD2	1.95	0.67
2:E:24:ILE:HD12	2:E:171:GLN:HB3	1.76	0.67
2:K:5:ASN:O	2:K:7:LYS:N	2.27	0.67
2:B:304:HIS:HE1	2:C:293:GLN:HE21	1.40	0.67
3:G:133:LEU:HD13	3:G:164:LYS:HG2	1.76	0.67
2:N:240:GLU:HA	2:N:243:LYS:HE3	1.77	0.67
2:B:141:ILE:HG12	2:B:141:ILE:O	1.94	0.67
2:D:176:LEU:HD22	2:D:211:LEU:HD22	1.76	0.66
2:M:88:LEU:HG	2:M:104:ILE:HD13	1.77	0.66
2:E:237:ASP:HB2	2:E:253:LEU:HD21	1.76	0.66
2:M:110:CYS:SG	2:M:139:ASN:N	2.68	0.66
2:D:276:VAL:O	2:D:280:SER:OG	2.13	0.66
3:S:146:LYS:HD3	3:S:171:ASP:HB3	1.78	0.66
1:A:144:ILE:O	1:A:148:ASN:ND2	2.29	0.66
2:B:251:ARG:HH22	2:C:270:GLU:HG3	1.61	0.66
2:L:49:SER:O	2:L:51:SER:N	2.29	0.66
2:D:110:CYS:HB3	2:D:138:ALA:HB1	1.78	0.66
3:F:189:MET:HA	3:F:216:TYR:HE2	1.61	0.66
1:A:123:ILE:HD11	1:A:155:LEU:HD21	1.78	0.65
2:L:300:ASN:ND2	2:M:262:SER:O	2.29	0.65
2:K:176:LEU:HD22	2:K:211:LEU:HD22	1.79	0.65
2:D:161:THR:HG23	2:D:164:ASP:H	1.61	0.65
4:I:28:DT:H2"	4:I:29:DG:OP2	1.95	0.65
2:M:85:ARG:NH2	4:O:17:DC:OP1	2.29	0.65
2:B:10:ILE:O	2:B:12:GLU:N	2.30	0.65
3:R:63:ILE:HD11	3:S:132:GLY:HA3	1.79	0.65
3:R:118:ILE:HG22	3:R:169:LEU:HD22	1.78	0.65
2:E:46:ILE:HG12	2:E:136:ILE:HB	1.78	0.64
2:M:206:LYS:NZ	2:N:152:CYS:O	2.31	0.64
3:S:146:LYS:HA	3:S:171:ASP:HA	1.79	0.64
2:D:24:ILE:O	7:D:403:ADP:N6	2.29	0.64
2:M:284:MET:HE2	2:M:288:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:108:GLU:OE1	2:L:122:ARG:NE	2.29	0.64
2:L:212:ASP:OD1	2:M:39:LYS:NZ	2.31	0.64
2:N:20:ILE:O	2:N:30:LYS:NZ	2.29	0.64
2:C:11:LEU:HD22	2:C:212:ASP:HB2	1.80	0.64
4:I:24:DT:H2"	4:I:25:DG:OP2	1.97	0.64
2:L:200:ASN:N	2:L:200:ASN:OD1	2.30	0.64
3:S:134:GLN:O	3:S:153:ASN:ND2	2.31	0.64
3:S:149:ILE:HB	3:S:167:LEU:HB3	1.79	0.64
2:E:273:TYR:HD1	2:E:281:ILE:HD12	1.61	0.64
3:S:17:ILE:HG13	3:S:188:LYS:HD2	1.80	0.64
1:A:19:SER:HB3	3:F:34:VAL:HG21	1.80	0.63
4:O:9:DT:H72	1:Q:41:PHE:H	1.63	0.63
1:Q:3:LEU:HD13	1:Q:4:PHE:H	1.63	0.63
1:A:48:ASN:HB2	1:A:105:GLY:HA2	1.80	0.63
2:C:12:GLU:O	7:C:403:ADP:O3'	2.15	0.63
2:L:119:ARG:HA	2:L:122:ARG:HD3	1.79	0.63
3:S:137:THR:HG22	3:S:183:ASN:HA	1.79	0.63
3:F:193:ASN:N	3:F:193:ASN:HD22	1.97	0.63
2:L:254:ALA:HB3	2:L:255:PRO:HD3	1.80	0.63
2:B:200:ASN:HD21	2:B:210:GLU:HG3	1.63	0.63
2:E:272:ILE:HG21	2:E:284:MET:HE2	1.79	0.63
2:K:275:ARG:HB3	2:K:319:LYS:OXT	1.98	0.63
2:K:110:CYS:SG	2:L:122:ARG:NH2	2.70	0.63
1:A:111:TRP:HZ3	4:I:10:DT:H5'	1.64	0.63
2:N:153:ARG:HH11	2:N:155:ILE:HD11	1.64	0.63
1:A:92:GLU:OE2	1:A:96:ASN:ND2	2.32	0.62
2:D:24:ILE:HD11	2:D:175:ARG:HG3	1.80	0.62
3:H:72:GLU:HB3	3:H:84:ALA:HB3	1.80	0.62
3:R:85:ASP:OD1	3:R:86:ALA:N	2.32	0.62
2:E:235:ILE:HG23	2:E:235:ILE:O	1.99	0.62
3:T:210:GLU:HA	3:T:215:ASN:HA	1.82	0.62
3:H:85:ASP:OD1	3:H:86:ALA:N	2.32	0.62
2:C:5:ASN:O	2:C:7:LYS:N	2.29	0.62
2:E:278:PRO:HA	2:E:281:ILE:HB	1.81	0.62
3:F:221:GLU:O	3:F:223:ASP:N	2.33	0.62
1:A:26:GLN:NE2	1:A:30:ASP:OD1	2.31	0.62
6:M:402:AF3:F1	2:N:151:ARG:NH2	2.23	0.62
2:N:9:HIS:HD2	1:Q:154:VAL:HG22	1.63	0.62
1:Q:185:LEU:HD12	1:Q:186:GLU:HG3	1.80	0.62
4:O:24:DT:H2"	4:O:25:DG:OP2	1.99	0.62
2:N:12:GLU:HG2	2:N:13:GLN:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:72:GLU:HB2	3:R:84:ALA:HB3	1.80	0.62
2:E:96:SER:OG	2:E:99:GLY:O	2.15	0.62
5:P:1:DG:H2"	5:P:2:DC:OP2	2.00	0.62
1:Q:131:TYR:HB2	1:Q:133:VAL:HG23	1.82	0.62
3:T:24:LYS:HA	3:T:51:ASP:HB3	1.81	0.62
1:A:159:LYS:NZ	3:H:94:ALA:O	2.32	0.62
3:F:15:ALA:HB2	3:F:57:LEU:HD23	1.82	0.62
2:N:12:GLU:O	7:N:401:ADP:O3'	2.18	0.62
2:B:242:LEU:HB3	2:B:318:TRP:HZ2	1.65	0.61
2:M:110:CYS:SG	2:M:140:ASN:N	2.73	0.61
1:Q:130:ARG:HG3	1:Q:131:TYR:CE1	2.35	0.61
1:A:45:GLY:O	1:A:49:ASN:HB2	2.00	0.61
2:E:190:MET:O	2:E:192:VAL:N	2.33	0.61
2:E:230:ASN:ND2	2:E:230:ASN:H	1.98	0.61
2:K:20:ILE:HD11	2:K:63:LEU:HG	1.82	0.61
2:M:131:ASN:ND2	3:R:96:ASP:OD2	2.30	0.61
2:N:153:ARG:NH1	2:N:155:ILE:HD11	2.16	0.61
1:Q:162:VAL:HG21	1:Q:183:LEU:HD13	1.83	0.61
3:S:133:LEU:HG	3:S:164:LYS:HD3	1.81	0.61
2:E:228:VAL:HG23	2:E:228:VAL:O	2.00	0.61
3:F:136:ASP:HB2	3:F:154:LYS:HG2	1.82	0.61
3:R:87:ARG:HD3	3:S:122:ASP:OD2	2.01	0.61
2:M:10:ILE:HG23	2:M:12:GLU:HG2	1.81	0.60
3:S:1:MET:HG3	3:S:49:ASP:OD2	2.01	0.60
2:D:2:ILE:N	2:D:22:GLU:OE2	2.34	0.60
3:G:113:SER:N	3:G:198:LEU:O	2.33	0.60
5:P:3:DA:H2"	5:P:4:DG:OP2	2.01	0.60
3:T:197:LEU:HB2	3:T:208:LYS:HB3	1.83	0.60
1:Q:55:ILE:HG21	1:Q:95:PHE:CE1	2.37	0.60
3:T:195:LYS:HB3	3:T:210:GLU:OE2	2.00	0.60
2:E:241:SER:O	2:E:246:ASP:OD1	2.20	0.60
3:T:147:ILE:HG13	3:T:148:VAL:H	1.67	0.60
2:E:16:ARG:HE	2:E:58:THR:HG22	1.65	0.60
2:L:145:ILE:HB	2:L:147:PRO:HD2	1.84	0.59
2:M:205:ARG:NH2	7:M:403:ADP:O2B	2.36	0.59
2:N:171:GLN:HG2	2:N:174:ARG:HH21	1.67	0.59
1:A:72:PHE:HB3	1:A:74:GLU:OE2	2.02	0.59
2:C:85:ARG:NH2	4:I:19:DC:OP1	2.33	0.59
2:L:45:ILE:HG22	2:L:153:ARG:HB2	1.84	0.59
2:B:93:SER:HA	3:F:99:THR:HG21	1.83	0.59
2:E:3:THR:HG21	2:E:18:SER:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:181:ILE:HB	3:G:221:GLU:HB2	1.84	0.59
3:F:116:THR:OG1	3:F:117:GLU:N	2.36	0.59
2:B:233:GLY:HA2	2:B:236:ASP:OD2	2.02	0.59
6:B:901:AF3:F3	7:B:902:ADP:PB	2.50	0.59
2:B:12:GLU:O	7:B:902:ADP:O3'	2.16	0.59
2:C:110:CYS:HB3	2:C:138:ALA:HB1	1.85	0.59
3:R:21:ILE:HG13	3:R:31:THR:HB	1.85	0.59
3:R:134:GLN:O	3:R:153:ASN:ND2	2.36	0.59
2:E:24:ILE:N	7:E:401:ADP:N1	2.47	0.59
2:L:251:ARG:NH2	2:M:270:GLU:OE1	2.36	0.59
2:M:57:THR:OG1	7:M:403:ADP:O3B	2.21	0.59
2:M:176:LEU:HD22	2:M:211:LEU:HD22	1.85	0.59
2:E:173:ILE:HD11	2:E:194:ALA:HA	1.84	0.58
2:L:200:ASN:HD22	2:L:206:LYS:HG3	1.68	0.58
1:A:150:LYS:HD2	1:A:153:LEU:HD12	1.85	0.58
2:K:201:PHE:HB3	2:K:202:PRO:HD3	1.85	0.58
2:B:25:LEU:HD21	2:B:59:VAL:HG21	1.84	0.58
3:R:76:SER:HB3	3:R:82:LYS:HB2	1.84	0.58
1:A:124:ILE:HD12	1:A:139:ILE:HA	1.84	0.58
2:N:21:ASP:OD2	2:N:34:LYS:NZ	2.36	0.58
2:D:241:SER:HB3	2:D:250:LEU:HB3	1.84	0.58
2:E:104:ILE:HB	2:E:134:ILE:HG12	1.85	0.58
2:K:83:PHE:HA	2:K:87:PRO:HD2	1.85	0.58
2:L:220:LEU:HA	2:L:224:ILE:HD12	1.85	0.58
3:S:39:TYR:HE2	3:S:103:PRO:HB3	1.67	0.58
2:C:8:GLU:OE2	2:D:129:SER:OG	2.22	0.58
2:D:297:ILE:HD13	2:E:297:ILE:HD11	1.84	0.58
3:F:33:ALA:O	3:F:35:ASN:N	2.36	0.58
3:F:109:PHE:HZ	3:F:112:ALA:HB2	1.68	0.58
4:I:10:DT:H2"	4:I:11:DT:C5	2.38	0.58
2:E:121:LEU:HA	2:E:124:PHE:HB3	1.85	0.58
3:F:193:ASN:HD22	3:F:193:ASN:H	1.50	0.58
3:H:67:VAL:HA	3:H:85:ASP:OD2	2.04	0.58
2:L:312:LEU:O	2:L:316:MET:HB2	2.03	0.58
2:M:272:ILE:HG21	2:M:284:MET:HG3	1.86	0.58
1:Q:167:LEU:HD13	1:Q:179:GLN:O	2.04	0.58
3:T:114:ALA:HB3	3:T:198:LEU:HD13	1.86	0.58
2:C:204:PHE:HB2	7:C:403:ADP:C8	2.39	0.58
3:G:122:ASP:HB3	3:G:167:LEU:HD21	1.86	0.58
3:H:122:ASP:HB3	3:H:167:LEU:HD21	1.86	0.58
3:H:133:LEU:HG	3:H:164:LYS:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:165:ASP:OD1	1:Q:165:ASP:N	2.31	0.58
3:T:147:ILE:HG21	3:T:170:GLY:H	1.69	0.58
1:Q:164:ASP:HA	1:Q:167:LEU:HD12	1.85	0.57
3:F:190:GLN:HB3	3:F:191:PRO:CD	2.29	0.57
2:C:5:ASN:HB2	2:C:14:LYS:HA	1.85	0.57
2:K:104:ILE:HB	2:K:134:ILE:HG13	1.85	0.57
2:K:192:VAL:HG22	2:K:225:LEU:HB2	1.86	0.57
3:G:87:ARG:HH12	3:H:119:LYS:HD2	1.68	0.57
2:N:58:THR:N	7:N:401:ADP:O1A	2.38	0.57
3:S:113:SER:N	3:S:198:LEU:O	2.38	0.57
2:E:273:TYR:HE1	2:E:281:ILE:HG23	1.68	0.57
5:P:2:DC:H2"	5:P:3:DA:C8	2.39	0.57
2:B:56:LYS:NZ	6:B:901:AF3:F2	2.28	0.57
2:C:84:VAL:O	2:C:89:THR:OG1	2.22	0.57
2:K:282:ILE:O	2:K:286:GLU:HB2	2.05	0.57
2:M:98:ASP:OD1	2:M:98:ASP:N	2.38	0.57
3:H:38:THR:HG22	3:H:218:VAL:HG12	1.86	0.57
1:A:55:ILE:HD13	1:A:60:TYR:HD2	1.70	0.57
2:B:42:ILE:HD11	2:B:67:VAL:HG21	1.87	0.57
2:N:96:SER:HB3	2:N:102:LYS:HE2	1.87	0.57
3:H:135:ILE:HD13	3:H:151:GLY:HA3	1.87	0.57
2:L:110:CYS:HB3	2:L:138:ALA:HB1	1.87	0.57
2:B:53:GLY:O	2:B:204:PHE:N	2.35	0.56
3:F:82:LYS:HE2	3:F:84:ALA:HB2	1.86	0.56
2:K:119:ARG:HD3	1:Q:33:LYS:HA	1.87	0.56
2:K:316:MET:HB3	2:K:318:TRP:HB2	1.86	0.56
2:M:52:PRO:HB3	2:N:147:PRO:HA	1.86	0.56
2:D:293:GLN:HE21	2:D:294:TYR:HE1	1.53	0.56
4:I:22:DA:H2"	4:I:23:DG:C8	2.40	0.56
3:R:1:MET:HG2	3:R:49:ASP:HB2	1.87	0.56
3:S:92:TRP:HD1	3:S:93:PRO:HD2	1.69	0.56
2:K:145:ILE:HG12	2:K:147:PRO:HD2	1.86	0.56
2:N:125:MET:HG2	2:N:134:ILE:HD12	1.88	0.56
3:F:39:TYR:HB3	3:F:217:VAL:HB	1.87	0.56
2:M:192:VAL:HG21	2:M:220:LEU:HB3	1.86	0.56
3:T:136:ASP:HB3	3:T:154:LYS:H	1.71	0.56
2:M:52:PRO:HG3	2:N:146:LYS:HB3	1.87	0.56
2:B:88:LEU:HD21	2:B:104:ILE:HG21	1.86	0.56
2:D:303:LEU:HD13	2:E:265:VAL:CG1	2.33	0.56
5:P:7:DA:OP2	5:P:7:DA:H8	1.89	0.56
2:B:111:ARG:NH2	2:C:116:GLU:OE1	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:LEU:HG	2:E:104:ILE:HD13	1.88	0.56
2:E:243:LYS:O	2:E:245:LYS:N	2.39	0.56
2:K:46:ILE:HG12	2:K:136:ILE:HB	1.88	0.56
2:M:72:MET:HE2	3:S:156:GLU:HA	1.87	0.56
3:T:7:THR:HG21	3:T:46:ASP:OD2	2.06	0.56
2:D:246:ASP:OD2	2:D:249:GLN:HB3	2.06	0.56
3:G:148:VAL:HG12	3:G:168:THR:HA	1.88	0.56
3:H:116:THR:HG21	3:H:147:ILE:HD11	1.87	0.55
2:L:44:HIS:HB3	2:L:152:CYS:HB3	1.87	0.55
2:N:9:HIS:CD2	1:Q:154:VAL:HG22	2.41	0.55
3:R:17:ILE:HG13	3:R:38:THR:HG23	1.87	0.55
2:E:11:LEU:HD23	2:E:179:ILE:HD11	1.87	0.55
3:F:182:ILE:HA	3:F:221:GLU:OE2	2.06	0.55
2:C:175:ARG:O	2:C:179:ILE:HG12	2.07	0.55
2:D:173:ILE:HD11	2:D:194:ALA:HA	1.87	0.55
3:S:21:ILE:HB	3:S:57:LEU:HD22	1.89	0.55
3:T:208:LYS:HD2	3:T:217:VAL:HG12	1.88	0.55
2:E:234:ALA:HA	2:E:238:VAL:HG21	1.87	0.55
3:R:10:LEU:HD22	3:R:44:ILE:HD13	1.89	0.55
3:T:147:ILE:HG12	3:T:169:LEU:HB3	1.88	0.55
2:B:293:GLN:HG2	2:E:297:ILE:HG23	1.88	0.55
2:N:278:PRO:HA	2:N:281:ILE:HB	1.87	0.55
2:E:107:ASP:HA	2:E:137:THR:HB	1.88	0.55
2:E:205:ARG:HD2	7:E:401:ADP:H5'1	1.88	0.55
3:F:122:ASP:O	3:F:126:LEU:N	2.38	0.55
2:M:12:GLU:O	7:M:403:ADP:O3'	2.25	0.55
2:C:304:HIS:CD2	2:D:293:GLN:HB3	2.42	0.55
2:D:273:TYR:HA	2:D:281:ILE:HD11	1.88	0.55
2:N:205:ARG:HD3	7:N:401:ADP:H5'1	1.89	0.55
5:P:18:DA:H2"	5:P:19:DT:H5"	1.88	0.55
3:S:190:GLN:OE1	3:S:190:GLN:N	2.40	0.55
2:B:16:ARG:HG3	2:B:58:THR:HG22	1.88	0.55
2:B:96:SER:HB3	2:B:102:LYS:HE3	1.88	0.55
2:K:26:PRO:O	2:K:28:PHE:N	2.40	0.54
1:Q:40:PHE:HE2	1:Q:65:VAL:HG12	1.72	0.54
3:R:87:ARG:O	3:S:168:THR:OG1	2.22	0.54
3:G:133:LEU:HD22	3:G:164:LYS:HE2	1.89	0.54
1:A:139:ILE:CD1	2:E:256:LYS:HE3	2.37	0.54
1:A:148:ASN:HB3	2:E:213:SER:H	1.72	0.54
2:M:108:GLU:HB3	2:N:122:ARG:NH1	2.23	0.54
2:M:175:ARG:O	2:M:179:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:195:LYS:HE2	3:T:197:LEU:HD21	1.90	0.54
2:B:16:ARG:NH2	7:B:902:ADP:H5'1	2.22	0.54
2:E:233:GLY:CA	2:E:267:LYS:HZ3	2.19	0.54
2:M:101:GLN:NE2	2:M:133:SER:OG	2.41	0.54
2:N:124:PHE:HE2	2:N:134:ILE:HD11	1.73	0.54
2:E:166:ILE:O	2:E:170:LYS:NZ	2.40	0.54
2:L:88:LEU:HG	2:L:104:ILE:HD13	1.89	0.54
2:E:273:TYR:HE1	2:E:281:ILE:HG21	1.71	0.54
3:H:66:LEU:HD11	3:H:90:ILE:HD11	1.89	0.54
3:T:146:LYS:NZ	3:T:171:ASP:OD1	2.29	0.54
2:E:141:ILE:HG12	2:E:149:GLN:HE22	1.72	0.54
2:E:293:GLN:HE21	2:E:294:TYR:HE1	1.56	0.54
3:G:118:ILE:HG22	3:G:169:LEU:HD11	1.89	0.54
1:Q:124:ILE:HD13	1:Q:139:ILE:HG12	1.90	0.54
1:A:148:ASN:HB3	2:E:213:SER:HA	1.90	0.53
2:D:108:GLU:HG3	2:E:122:ARG:HG3	1.89	0.53
2:M:42:ILE:HG13	2:M:67:VAL:HG21	1.90	0.53
3:T:37:THR:OG1	3:T:186:ASN:ND2	2.41	0.53
3:T:120:ALA:N	3:T:193:ASN:OD1	2.40	0.53
2:D:49:SER:HB3	2:D:157:PHE:HB2	1.91	0.53
3:F:153:ASN:H	3:F:164:LYS:HZ3	1.54	0.53
2:L:297:ILE:HD13	2:M:297:ILE:HD11	1.89	0.53
2:N:276:VAL:O	2:N:319:LYS:NZ	2.40	0.53
3:R:130:SER:HA	3:R:135:ILE:HB	1.89	0.53
3:S:118:ILE:HD13	3:S:169:LEU:HD22	1.91	0.53
2:B:49:SER:HB3	2:B:157:PHE:HB2	1.91	0.53
2:E:190:MET:SD	2:E:191:LYS:N	2.82	0.53
2:E:233:GLY:CA	2:E:267:LYS:HZ2	2.18	0.53
3:F:122:ASP:OD2	3:F:167:LEU:HD11	2.08	0.53
3:G:76:SER:HB2	3:G:82:LYS:HB2	1.90	0.53
2:M:116:GLU:OE2	2:M:119:ARG:NH1	2.41	0.53
2:B:304:HIS:CE1	2:C:293:GLN:HE21	2.26	0.53
2:C:235:ILE:O	2:C:237:ASP:N	2.42	0.53
2:K:4:VAL:HG12	2:K:6:GLU:H	1.74	0.53
2:M:235:ILE:HD11	2:M:263:TRP:HH2	1.73	0.53
2:B:250:LEU:HD13	2:B:309:PHE:HB3	1.90	0.53
2:C:17:PRO:HD2	2:C:58:THR:HG21	1.90	0.53
2:D:104:ILE:HB	2:D:134:ILE:HG12	1.90	0.53
2:E:15:TYR:CZ	2:E:179:ILE:HG13	2.43	0.53
2:K:162:ASP:OD1	2:K:162:ASP:N	2.41	0.53
2:M:24:ILE:O	7:M:403:ADP:N6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:HG23	1:A:166:PHE:HB2	1.91	0.53
3:H:207:ALA:HB2	3:H:220:LEU:HD21	1.91	0.53
3:R:162:ARG:HD3	3:R:163:VAL:O	2.09	0.53
2:D:175:ARG:O	2:D:179:ILE:HG12	2.08	0.53
2:D:304:HIS:HE1	2:E:293:GLN:HG3	1.73	0.53
7:K:403:ADP:H5'1	7:K:403:ADP:H8	1.73	0.53
3:R:24:LYS:HA	3:R:51:ASP:HB3	1.91	0.53
1:A:55:ILE:HG23	1:A:56:ALA:H	1.74	0.53
2:B:303:LEU:HD13	2:C:265:VAL:HG12	1.91	0.53
2:L:272:ILE:HG21	2:L:284:MET:HG3	1.90	0.53
2:M:13:GLN:HE22	2:M:16:ARG:HH11	1.57	0.53
2:N:24:ILE:HG13	7:N:401:ADP:N1	2.24	0.53
2:K:27:ALA:HB2	2:K:167:GLU:OE2	2.09	0.52
2:N:303:LEU:HD13	1:Q:83:ASN:HB2	1.92	0.52
2:M:237:ASP:OD2	2:M:256:LYS:NZ	2.36	0.52
2:B:242:LEU:HB3	2:B:318:TRP:CZ2	2.45	0.52
2:E:268:LEU:HD22	2:E:268:LEU:O	2.09	0.52
2:L:186:ALA:HB3	2:L:219:VAL:HG22	1.90	0.52
3:S:123:LEU:HD23	3:S:191:PRO:HA	1.92	0.52
2:B:176:LEU:HD22	2:B:211:LEU:HD13	1.91	0.52
2:L:308:LEU:O	2:L:312:LEU:HB2	2.09	0.52
1:Q:155:LEU:HG	1:Q:183:LEU:HD21	1.91	0.52
3:R:89:THR:N	3:S:166:SER:O	2.43	0.52
3:T:29:ILE:HD12	3:T:30:MET:H	1.74	0.52
3:T:63:ILE:HA	3:T:66:LEU:HD23	1.91	0.52
3:G:11:LEU:HB3	3:G:61:LEU:HD11	1.91	0.52
4:O:25:DG:H2"	4:O:26:DT:OP2	2.09	0.52
1:A:60:TYR:OH	1:A:94:HIS:ND1	2.38	0.52
1:A:111:TRP:CZ3	4:I:10:DT:H5'	2.45	0.52
2:B:37:THR:HG22	2:B:67:VAL:HG23	1.92	0.52
2:D:9:HIS:CD2	2:E:41:LYS:HB3	2.44	0.52
2:M:276:VAL:HA	2:M:318:TRP:HB2	1.91	0.52
2:L:25:LEU:HD21	2:L:59:VAL:HG21	1.90	0.52
3:R:1:MET:HB3	3:R:73:ILE:H	1.74	0.52
2:N:57:THR:HG22	2:N:61:LYS:HD2	1.92	0.52
1:A:19:SER:HA	3:F:19:SER:OG	2.10	0.52
3:F:122:ASP:OD2	3:F:167:LEU:CD1	2.58	0.52
2:L:188:ALA:HB3	2:L:221:ASP:HA	1.91	0.52
2:C:42:ILE:HD12	2:C:103:VAL:HG21	1.92	0.51
2:E:255:PRO:HG3	2:E:302:GLU:OE2	2.10	0.51
2:K:141:ILE:HG13	2:K:149:GLN:OE1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:265:VAL:HG11	2:C:292:ASN:HB2	1.92	0.51
2:D:10:ILE:O	2:D:12:GLU:N	2.43	0.51
2:E:108:GLU:OE1	2:E:139:ASN:ND2	2.35	0.51
3:G:83:ILE:HB	3:G:90:ILE:HB	1.92	0.51
2:N:303:LEU:HD21	1:Q:79:VAL:HG12	1.91	0.51
1:A:73:PRO:HG3	2:E:247:VAL:HG11	1.92	0.51
2:B:200:ASN:ND2	2:B:210:GLU:HG3	2.26	0.51
2:B:280:SER:HB3	2:B:316:MET:HE3	1.92	0.51
2:K:19:THR:HG22	2:K:22:GLU:H	1.75	0.51
3:R:140:ILE:HD13	3:R:198:LEU:HD11	1.92	0.51
6:C:402:AF3:F1	7:C:403:ADP:O2B	2.19	0.51
2:E:255:PRO:C	2:E:257:TYR:H	2.14	0.51
2:B:162:ASP:O	2:B:166:ILE:HG12	2.10	0.51
2:D:291:ASN:O	2:D:304:HIS:NE2	2.40	0.51
2:N:312:LEU:O	2:N:316:MET:HG2	2.10	0.51
3:R:1:MET:O	3:R:72:GLU:HA	2.10	0.51
3:T:181:ILE:HG13	3:T:221:GLU:HB2	1.92	0.51
2:L:176:LEU:HD22	2:L:211:LEU:HD22	1.92	0.51
1:Q:38:ASN:OD1	1:Q:38:ASN:N	2.43	0.51
3:R:1:MET:CG	3:R:49:ASP:HB2	2.41	0.51
3:R:181:ILE:HG13	3:R:221:GLU:HB2	1.92	0.51
3:S:1:MET:N	3:S:73:ILE:O	2.43	0.51
2:C:91:PHE:HB2	3:G:35:ASN:HB2	1.92	0.51
2:M:251:ARG:HH22	2:N:270:GLU:HG2	1.76	0.51
3:R:189:MET:HB3	3:R:194:TYR:HE2	1.76	0.51
2:E:33:PHE:HB3	2:E:63:LEU:HD21	1.91	0.51
2:K:277:THR:HG21	2:K:317:GLN:HB2	1.92	0.51
2:N:48:HIS:HE1	2:N:156:THR:HG22	1.76	0.51
2:E:280:SER:HB3	2:E:316:MET:SD	2.51	0.51
2:K:249:GLN:HG2	2:K:253:LEU:HD23	1.93	0.51
3:T:52:VAL:HG21	3:T:81:ILE:HD11	1.93	0.51
2:B:5:ASN:O	2:B:7:LYS:N	2.40	0.50
2:B:238:VAL:HG11	2:B:264:PHE:HZ	1.77	0.50
2:N:48:HIS:CE1	2:N:156:THR:HG22	2.47	0.50
2:B:206:LYS:HD2	2:C:150:SER:HA	1.93	0.50
2:C:15:TYR:OH	2:C:183:GLU:OE1	2.26	0.50
3:T:148:VAL:O	3:T:149:ILE:HG12	2.11	0.50
2:B:206:LYS:NZ	2:C:153:ARG:HH12	2.08	0.50
3:F:160:LEU:H	3:F:160:LEU:HD23	1.76	0.50
3:G:190:GLN:NE2	3:G:213:HIS:HE1	2.09	0.50
2:N:81:ILE:HG23	2:N:85:ARG:HH12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:85:ASP:OD1	3:S:86:ALA:N	2.45	0.50
2:K:226:SER:O	2:K:230:ASN:HB2	2.11	0.50
2:M:306:ALA:HA	2:M:309:PHE:HB2	1.94	0.50
3:S:34:VAL:HG22	3:S:101:VAL:HG21	1.94	0.50
3:T:25:SER:HA	3:T:48:ILE:HG13	1.93	0.50
1:A:72:PHE:CZ	1:A:108:TYR:HB2	2.47	0.50
3:G:165:TYR:HE2	3:G:167:LEU:HB2	1.76	0.50
2:L:239:LEU:O	2:L:243:LYS:HG3	2.12	0.50
2:M:251:ARG:NH2	2:N:270:GLU:HG2	2.26	0.50
2:N:20:ILE:HG22	2:N:66:ASP:OD2	2.12	0.50
1:Q:11:ASN:O	1:Q:14:GLN:N	2.41	0.50
4:I:25:DG:H2"	4:I:26:DT:OP2	2.12	0.50
1:Q:135:THR:O	1:Q:139:ILE:N	2.44	0.50
2:E:225:LEU:HD23	2:E:225:LEU:H	1.76	0.50
2:E:264:PHE:CD1	2:E:264:PHE:C	2.84	0.50
3:F:18:ASN:ND2	3:F:101:VAL:O	2.45	0.50
3:F:136:ASP:O	3:F:184:MET:HB2	2.12	0.50
3:G:32:ARG:HB2	3:G:103:PRO:HG3	1.93	0.50
2:K:268:LEU:O	2:K:272:ILE:HG12	2.11	0.50
2:M:118:GLN:HG2	2:M:148:LEU:HD12	1.94	0.50
4:O:22:DA:H2"	4:O:23:DG:C8	2.47	0.50
1:Q:156:LYS:HA	1:Q:159:LYS:HB3	1.92	0.50
3:S:105:LYS:HG3	3:S:107:ILE:HG23	1.94	0.50
2:D:4:VAL:HG12	2:D:15:TYR:CE1	2.47	0.50
2:D:126:GLU:OE2	2:D:151:ARG:NH2	2.42	0.50
2:D:293:GLN:HG3	2:D:294:TYR:CD1	2.47	0.50
2:E:273:TYR:CD1	2:E:281:ILE:HD12	2.44	0.50
2:L:261:TYR:OH	2:L:291:ASN:OD1	2.21	0.50
3:R:140:ILE:HA	3:R:149:ILE:HA	1.93	0.50
3:S:157:ASP:CG	3:S:161:THR:H	2.14	0.50
2:E:230:ASN:ND2	2:E:235:ILE:HB	2.27	0.49
2:E:272:ILE:HG21	2:E:284:MET:CE	2.42	0.49
2:K:17:PRO:HB3	2:K:22:GLU:HG3	1.94	0.49
2:L:53:GLY:N	7:L:403:ADP:O1B	2.42	0.49
2:E:170:LYS:HA	2:E:173:ILE:HB	1.93	0.49
2:K:164:ASP:HA	2:K:167:GLU:HG2	1.93	0.49
2:L:47:LEU:HD22	2:L:157:PHE:HE2	1.77	0.49
2:M:49:SER:HB3	2:M:157:PHE:HB2	1.95	0.49
2:N:4:VAL:HG13	2:N:15:TYR:HE1	1.76	0.49
1:A:178:LYS:O	1:A:182:LYS:HB2	2.12	0.49
2:B:118:GLN:OE1	2:B:145:ILE:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:148:VAL:HG12	3:R:168:THR:HA	1.94	0.49
1:A:15:VAL:O	1:A:19:SER:OG	2.30	0.49
2:D:242:LEU:HD22	2:D:312:LEU:HB3	1.94	0.49
2:E:225:LEU:HA	2:E:229:THR:CG2	2.40	0.49
3:H:140:ILE:HG12	3:H:149:ILE:HG12	1.94	0.49
2:L:46:ILE:HG13	2:L:152:CYS:SG	2.53	0.49
1:A:130:ARG:NH1	1:A:130:ARG:O	2.41	0.49
2:D:16:ARG:NH2	7:D:403:ADP:H5'1	2.27	0.49
3:F:153:ASN:H	3:F:164:LYS:NZ	2.10	0.49
1:Q:40:PHE:O	1:Q:43:ILE:HB	2.12	0.49
3:T:210:GLU:N	3:T:210:GLU:OE1	2.45	0.49
1:A:76:MET:N	1:A:77:PRO:HD2	2.28	0.49
2:M:84:VAL:HA	2:M:88:LEU:HB2	1.93	0.49
2:C:176:LEU:HD21	2:C:208:ILE:HD13	1.94	0.49
2:D:98:ASP:OD1	2:D:98:ASP:N	2.33	0.49
2:E:16:ARG:NE	2:E:58:THR:HG22	2.27	0.49
3:F:35:ASN:OD1	3:F:36:GLY:N	2.43	0.49
2:B:46:ILE:HG12	2:B:136:ILE:HB	1.94	0.49
2:D:110:CYS:SG	2:E:122:ARG:NH2	2.85	0.49
2:E:161:THR:HG22	2:E:164:ASP:OD2	2.13	0.49
5:J:7:DA:H2'	5:J:7:DA:OP2	2.12	0.49
2:C:8:GLU:HG2	2:C:13:GLN:HB2	1.94	0.49
3:F:199:TRP:HE3	3:F:206:ALA:H	1.61	0.49
3:G:50:PHE:CD2	3:G:75:GLN:HB2	2.48	0.49
2:M:91:PHE:CE2	2:M:102:LYS:HB3	2.48	0.49
3:R:81:ILE:HB	3:R:92:TRP:HB3	1.95	0.49
2:D:84:VAL:O	2:D:89:THR:HG23	2.13	0.48
2:D:204:PHE:HB2	7:D:403:ADP:C8	2.47	0.48
2:E:308:LEU:O	2:E:312:LEU:HB2	2.13	0.48
5:J:6:DC:H2"	5:J:7:DA:H8	1.77	0.48
3:F:11:LEU:HB3	3:F:61:LEU:HD11	1.94	0.48
3:F:189:MET:HG3	3:F:216:TYR:CD2	2.48	0.48
3:G:80:ASN:HB3	3:G:92:TRP:O	2.13	0.48
2:N:77:SER:HA	2:N:114:LEU:HD11	1.94	0.48
3:R:51:ASP:OD1	3:R:51:ASP:N	2.43	0.48
2:E:176:LEU:HA	2:E:179:ILE:HG22	1.95	0.48
2:K:243:LYS:HD3	2:K:318:TRP:O	2.13	0.48
2:M:26:PRO:HG3	2:M:160:PRO:HB3	1.94	0.48
3:R:7:THR:HA	3:R:44:ILE:HG12	1.96	0.48
3:S:202:GLY:H	3:S:226:HIS:HE1	1.59	0.48
2:E:187:ILE:HG23	2:E:220:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:157:ASP:O	3:G:159:ALA:N	2.46	0.48
4:I:25:DG:OP2	4:I:25:DG:H8	1.96	0.48
2:K:42:ILE:HD12	2:K:135:ILE:HD11	1.94	0.48
2:L:111:ARG:NE	2:M:116:GLU:OE1	2.46	0.48
3:R:138:ILE:HA	3:R:151:GLY:HA2	1.94	0.48
3:S:41:GLU:HG3	3:S:215:ASN:HB2	1.95	0.48
2:D:303:LEU:CD1	2:E:265:VAL:HG12	2.39	0.48
2:E:232:ARG:HA	2:E:232:ARG:HD3	1.46	0.48
5:J:4:DG:H2"	5:J:5:DA:OP2	2.12	0.48
2:L:290:GLU:OE2	2:M:293:GLN:NE2	2.32	0.48
1:A:12:GLU:OE1	1:A:12:GLU:N	2.44	0.48
2:C:307:TYR:CE1	2:D:286:GLU:HA	2.49	0.48
2:D:242:LEU:HD13	2:D:312:LEU:HD23	1.95	0.48
2:E:119:ARG:HB3	2:E:122:ARG:NH1	2.28	0.48
2:K:25:LEU:HB2	2:K:30:LYS:HB2	1.95	0.48
2:M:111:ARG:HH11	2:N:116:GLU:HB3	1.79	0.48
1:Q:43:ILE:HG13	1:Q:55:ILE:HD13	1.95	0.48
3:R:63:ILE:HD12	3:S:129:VAL:HA	1.94	0.48
5:J:6:DC:H2"	5:J:7:DA:OP2	2.13	0.48
2:N:5:ASN:C	2:N:7:LYS:H	2.17	0.48
2:N:76:GLY:N	2:N:107:ASP:O	2.45	0.48
3:F:3:LEU:HA	3:F:46:ASP:OD2	2.14	0.48
5:J:6:DC:H2"	5:J:7:DA:C8	2.48	0.48
5:J:11:DC:H2"	5:J:12:DG:C8	2.49	0.48
2:K:176:LEU:HD23	2:K:179:ILE:HD12	1.96	0.48
2:M:308:LEU:HA	2:M:311:GLN:HB2	1.96	0.48
1:Q:75:CYS:SG	1:Q:103:PRO:HG3	2.54	0.48
2:B:44:HIS:HD1	2:B:134:ILE:H	1.61	0.48
3:R:88:SER:HA	3:S:167:LEU:HA	1.96	0.48
2:C:104:ILE:HB	2:C:134:ILE:HG12	1.94	0.47
2:M:56:LYS:NZ	7:M:403:ADP:O1B	2.33	0.47
2:D:270:GLU:N	2:D:270:GLU:OE1	2.47	0.47
3:F:136:ASP:HB3	3:F:154:LYS:HZ3	1.78	0.47
3:H:1:MET:HB3	3:H:48:ILE:HA	1.94	0.47
3:H:181:ILE:HD12	3:H:223:ASP:HB2	1.96	0.47
2:L:237:ASP:OD2	2:L:256:LYS:NZ	2.42	0.47
3:T:39:TYR:HB3	3:T:217:VAL:HG22	1.95	0.47
3:F:7:THR:HG23	3:F:44:ILE:HG21	1.96	0.47
2:K:81:ILE:HD11	2:K:120:HIS:CD2	2.50	0.47
2:K:108:GLU:HG3	2:L:122:ARG:HG3	1.95	0.47
2:L:14:LYS:HE2	2:L:15:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:16:THR:OG1	3:T:16:THR:O	2.22	0.47
3:T:209:PHE:HE2	3:T:218:VAL:HB	1.80	0.47
1:A:19:SER:C	1:A:21:ASP:H	2.16	0.47
2:B:20:ILE:HG12	2:B:33:PHE:HB3	1.96	0.47
2:D:121:LEU:HA	2:D:124:PHE:HB3	1.96	0.47
2:D:235:ILE:HD11	2:D:271:GLU:HB2	1.96	0.47
2:E:199:LYS:HE3	2:E:229:THR:CG2	2.43	0.47
3:G:63:ILE:HG13	3:G:92:TRP:HZ3	1.80	0.47
2:M:297:ILE:HG21	2:N:297:ILE:HG12	1.96	0.47
2:B:44:HIS:CE1	2:B:133:SER:HA	2.49	0.47
2:M:314:CYS:SG	2:M:315:GLU:HG3	2.55	0.47
2:N:205:ARG:HA	2:N:208:ILE:HG12	1.97	0.47
2:D:84:VAL:HA	2:D:88:LEU:HB2	1.95	0.47
3:T:17:ILE:HG12	3:T:188:LYS:HE3	1.97	0.47
3:T:116:THR:O	3:T:196:LEU:N	2.48	0.47
2:B:42:ILE:HG21	2:B:135:ILE:HD11	1.96	0.47
2:B:84:VAL:HA	2:B:88:LEU:HD12	1.96	0.47
2:C:288:VAL:HG22	2:C:308:LEU:HD11	1.96	0.47
2:D:33:PHE:CZ	2:D:59:VAL:HG11	2.50	0.47
2:D:89:THR:HG22	2:D:124:PHE:HE2	1.79	0.47
2:E:190:MET:HB2	2:E:193:VAL:HB	1.96	0.47
3:F:44:ILE:HG13	3:F:45:SER:H	1.79	0.47
3:F:109:PHE:CD1	3:F:208:LYS:HD2	2.48	0.47
2:L:49:SER:HB3	2:L:56:LYS:HD3	1.96	0.47
2:M:76:GLY:N	2:M:107:ASP:O	2.45	0.47
2:M:139:ASN:ND2	6:M:402:AF3:F2	2.26	0.47
1:Q:14:GLN:HB3	1:Q:18:TYR:CE2	2.50	0.47
1:Q:76:MET:N	1:Q:77:PRO:HD2	2.30	0.47
3:R:90:ILE:HG12	3:S:165:TYR:HD1	1.79	0.47
3:S:116:THR:HG21	3:S:147:ILE:HD11	1.96	0.47
2:M:169:MET:O	2:M:173:ILE:HG12	2.14	0.47
5:P:6:DC:H2"	5:P:7:DA:C8	2.49	0.47
3:R:189:MET:HB3	3:R:194:TYR:CE2	2.50	0.47
2:E:20:ILE:HG22	2:E:66:ASP:OD2	2.15	0.47
2:E:230:ASN:ND2	2:E:230:ASN:N	2.60	0.47
2:E:264:PHE:HE1	2:E:268:LEU:HD12	1.79	0.47
3:H:81:ILE:HG13	3:H:92:TRP:HB3	1.96	0.47
2:K:81:ILE:HD13	2:K:116:GLU:HG3	1.97	0.47
2:K:165:LYS:HG3	2:K:201:PHE:CZ	2.50	0.47
2:K:297:ILE:HG21	2:L:297:ILE:HG13	1.97	0.47
2:L:45:ILE:HG13	2:L:135:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:277:THR:HG23	2:E:280:SER:H	1.80	0.47
2:K:290:GLU:O	2:K:294:TYR:HD2	1.98	0.47
5:P:3:DA:H1'	5:P:4:DG:H5'	1.97	0.47
1:Q:150:LYS:O	1:Q:154:VAL:HG23	2.14	0.47
3:S:124:GLN:HG3	3:S:128:ARG:HD2	1.97	0.47
3:T:49:ASP:OD1	3:T:49:ASP:N	2.47	0.47
1:A:14:GLN:HG2	2:B:127:ALA:HA	1.96	0.46
2:B:45:ILE:HB	2:B:135:ILE:HD13	1.96	0.46
2:B:139:ASN:ND2	6:B:901:AF3:F2	2.34	0.46
2:D:81:ILE:HG21	4:I:16:DA:H3'	1.97	0.46
2:E:267:LYS:O	2:E:267:LYS:HG2	2.15	0.46
2:E:273:TYR:CE1	2:E:281:ILE:HG23	2.48	0.46
3:F:189:MET:HG3	3:F:216:TYR:HD2	1.80	0.46
1:A:55:ILE:O	1:A:57:GLN:N	2.48	0.46
4:O:9:DT:H5'	1:Q:111:TRP:CE3	2.50	0.46
1:Q:76:MET:HA	1:Q:79:VAL:HB	1.97	0.46
3:T:178:PHE:HB3	3:T:227:ASP:HB2	1.96	0.46
3:F:193:ASN:N	3:F:193:ASN:ND2	2.64	0.46
7:B:902:ADP:O1A	7:B:902:ADP:O1B	2.33	0.46
2:C:45:ILE:HG22	2:C:153:ARG:HB2	1.97	0.46
3:H:20:GLY:HA2	3:H:57:LEU:HB2	1.97	0.46
2:M:299:ALA:HB2	2:N:295:HIS:ND1	2.30	0.46
2:N:261:TYR:CZ	2:N:265:VAL:HG21	2.51	0.46
1:A:55:ILE:O	1:A:57:GLN:NE2	2.49	0.46
2:B:214:TYR:CE2	2:B:228:VAL:HG22	2.51	0.46
2:C:299:ALA:HB2	2:D:295:HIS:HB3	1.97	0.46
5:J:8:DC:H2"	5:J:9:DT:OP2	2.16	0.46
2:L:2:ILE:HA	2:L:22:GLU:OE2	2.15	0.46
3:R:73:ILE:HG23	3:R:83:ILE:HD13	1.98	0.46
3:S:142:VAL:HA	3:S:147:ILE:HA	1.98	0.46
3:F:207:ALA:O	3:F:218:VAL:HG22	2.16	0.46
3:H:190:GLN:HB2	3:H:191:PRO:HD2	1.97	0.46
2:L:299:ALA:H	2:M:295:HIS:CE1	2.21	0.46
2:B:142:ASP:C	2:B:144:ILE:N	2.69	0.46
2:N:291:ASN:O	2:N:304:HIS:NE2	2.32	0.46
2:B:3:THR:OG1	2:B:22:GLU:OE2	2.32	0.46
2:D:232:ARG:HA	2:D:263:TRP:CH2	2.51	0.46
2:E:288:VAL:HG22	2:E:308:LEU:HD11	1.97	0.46
2:K:246:ASP:OD1	2:K:246:ASP:N	2.49	0.46
2:L:306:ALA:O	2:L:310:ILE:HG12	2.16	0.46
2:N:265:VAL:HG11	2:N:292:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:4:DG:H2"	5:P:5:DA:OP2	2.15	0.46
3:S:127:LEU:HD22	3:S:131:ARG:HH11	1.80	0.46
1:A:155:LEU:HD22	1:A:186:GLU:OE2	2.16	0.46
2:C:16:ARG:NH2	7:C:403:ADP:O2A	2.49	0.46
2:C:255:PRO:HG3	2:C:302:GLU:OE2	2.15	0.46
2:E:234:ALA:HA	2:E:238:VAL:CG2	2.46	0.46
3:F:21:ILE:HB	3:F:31:THR:HB	1.98	0.46
3:G:3:LEU:HA	3:G:46:ASP:OD2	2.15	0.46
3:H:171:ASP:OD1	3:H:171:ASP:N	2.41	0.46
2:K:277:THR:OG1	2:K:278:PRO:HD2	2.15	0.46
2:N:84:VAL:HA	2:N:88:LEU:HD13	1.98	0.46
1:Q:155:LEU:HD11	1:Q:183:LEU:HD11	1.98	0.46
2:C:119:ARG:HA	2:C:122:ARG:HH11	1.81	0.45
2:E:260:ASP:OD1	2:E:260:ASP:N	2.46	0.45
3:F:146:LYS:HG2	3:F:171:ASP:HA	1.98	0.45
3:F:200:ALA:HA	3:F:205:GLY:HA2	1.98	0.45
4:I:17:DC:H42	5:J:14:DG:H1	1.63	0.45
2:M:185:ILE:HD12	2:M:215:SER:HB2	1.98	0.45
2:N:191:LYS:N	2:N:191:LYS:HD2	2.31	0.45
3:S:129:VAL:HG21	3:S:165:TYR:CD1	2.50	0.45
2:E:272:ILE:N	2:E:272:ILE:CD1	2.78	0.45
3:F:51:ASP:OD1	3:F:51:ASP:N	2.40	0.45
2:L:214:TYR:C	2:L:216:SER:H	2.19	0.45
2:C:307:TYR:HE1	2:D:286:GLU:HA	1.82	0.45
2:D:20:ILE:HG22	2:D:66:ASP:OD2	2.17	0.45
2:D:269:ALA:HA	2:D:272:ILE:HG22	1.98	0.45
2:N:56:LYS:HZ3	2:N:157:PHE:HE2	1.64	0.45
1:Q:61:SER:O	1:Q:63:PHE:N	2.49	0.45
1:Q:130:ARG:HG3	1:Q:131:TYR:CD1	2.52	0.45
3:S:2:LYS:NZ	3:S:3:LEU:O	2.39	0.45
3:S:148:VAL:HG12	3:S:168:THR:HA	1.99	0.45
6:B:901:AF3:F3	7:B:902:ADP:O2B	2.22	0.45
2:C:242:LEU:HD23	2:C:313:ALA:HB2	1.98	0.45
2:E:146:LYS:HA	2:E:149:GLN:HG3	1.99	0.45
2:K:286:GLU:HA	1:Q:85:ILE:HD13	1.98	0.45
2:B:108:GLU:HB3	2:C:122:ARG:NH2	2.31	0.45
2:D:288:VAL:HG22	2:D:308:LEU:HD11	1.99	0.45
2:K:139:ASN:HB2	2:L:122:ARG:NH2	2.30	0.45
3:T:115:VAL:HG22	3:T:197:LEU:HD22	1.98	0.45
1:A:41[B]:PHE:CE1	4:I:9:DT:H6	2.35	0.45
2:E:17:PRO:HB3	2:E:22:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:ILE:HB	2:E:149:GLN:HE21	1.81	0.45
2:E:289:GLY:O	2:E:293:GLN:HB2	2.17	0.45
3:F:44:ILE:HD12	3:F:44:ILE:HA	1.82	0.45
1:Q:40:PHE:CZ	1:Q:44:ILE:HD11	2.51	0.45
3:R:92:TRP:CZ3	3:S:133:LEU:HD13	2.52	0.45
2:B:180:CYS:SG	2:B:211:LEU:HD11	2.56	0.45
2:C:44:HIS:O	2:C:153:ARG:HG2	2.16	0.45
3:F:138:ILE:HA	3:F:151:GLY:HA3	1.99	0.45
3:F:194:TYR:CD1	3:F:211:GLY:HA2	2.52	0.45
2:K:81:ILE:HG21	4:O:20:DG:H3'	1.98	0.45
2:L:108:GLU:H	2:L:137:THR:HB	1.80	0.45
2:M:165:LYS:HE2	2:M:201:PHE:CE2	2.52	0.45
2:N:271:GLU:O	2:N:275:ARG:HG3	2.16	0.45
4:O:8:DT:H5"	4:O:8:DT:H6	1.81	0.45
2:D:70:ASP:O	2:D:91:PHE:HZ	1.98	0.45
2:E:243:LYS:C	2:E:245:LYS:H	2.20	0.45
2:E:254:ALA:HB3	2:E:255:PRO:HD3	1.99	0.45
2:M:9:HIS:CE1	2:N:101:GLN:HE22	2.34	0.45
1:A:71:GLN:HG3	1:A:111:TRP:HA	1.99	0.45
1:A:176:GLU:O	1:A:180:LEU:HB2	2.15	0.45
3:F:119:LYS:CB	3:F:122:ASP:HB3	2.46	0.45
3:F:190:GLN:CB	3:F:191:PRO:HD2	2.32	0.45
2:K:57:THR:HG23	7:K:403:ADP:O2B	2.17	0.45
2:M:25:LEU:HB2	2:M:30:LYS:HB2	1.98	0.45
2:M:98:ASP:OD2	2:M:100:ARG:NE	2.47	0.45
2:M:307:TYR:CD1	2:N:289:GLY:HA3	2.51	0.45
2:N:146:LYS:HA	2:N:146:LYS:HD3	1.74	0.45
2:D:161:THR:HG22	2:D:164:ASP:OD2	2.17	0.45
2:E:197:VAL:O	2:E:201:PHE:HA	2.17	0.45
3:F:32:ARG:H	3:F:103:PRO:HD3	1.80	0.45
1:Q:151:LEU:N	1:Q:152:PRO:HD2	2.32	0.45
2:D:162:ASP:O	2:D:166:ILE:HG12	2.17	0.44
2:D:192:VAL:HG22	2:D:225:LEU:HB2	1.98	0.44
2:D:304:HIS:CE1	2:E:293:GLN:HG3	2.51	0.44
3:F:28:PHE:CE1	3:F:41:GLU:HB2	2.52	0.44
2:K:157:PHE:O	2:K:159:GLN:N	2.43	0.44
2:K:273:TYR:HE1	2:K:281:ILE:HG12	1.82	0.44
2:N:11:LEU:HD12	2:N:14:LYS:HB3	1.99	0.44
1:A:148:ASN:HB3	2:E:213:SER:CA	2.47	0.44
2:D:44:HIS:CE1	2:D:133:SER:HA	2.52	0.44
2:E:306:ALA:O	2:E:310:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:49:SER:HB3	2:K:157:PHE:HB2	1.99	0.44
2:N:305:LEU:HD13	2:N:305:LEU:HA	1.83	0.44
3:R:80:ASN:HB3	3:R:92:TRP:O	2.18	0.44
3:S:74:SER:HB3	3:S:82:LYS:HE2	1.98	0.44
1:A:125:LYS:HA	1:A:125:LYS:HD2	1.80	0.44
2:B:121:LEU:HD11	2:B:134:ILE:HD13	2.00	0.44
2:E:230:ASN:HB2	2:E:234:ALA:HB3	1.98	0.44
2:K:293:GLN:OE1	1:Q:85:ILE:HA	2.17	0.44
3:F:172:TYR:CZ	3:F:174:GLY:HA3	2.52	0.44
2:K:280:SER:HB3	2:K:316:MET:SD	2.57	0.44
2:L:109:PHE:HB3	2:L:136:ILE:HG23	2.00	0.44
2:N:4:VAL:HG13	2:N:15:TYR:CE1	2.51	0.44
1:A:171:THR:HB	1:A:173:ASN:HD21	1.82	0.44
2:B:82:ASP:HA	2:B:85:ARG:HG2	2.00	0.44
2:D:44:HIS:CG	2:D:125:MET:HE3	2.53	0.44
2:E:230:ASN:N	2:E:230:ASN:HD22	2.14	0.44
3:F:157:ASP:OD1	3:F:162:ARG:NH1	2.42	0.44
3:G:4:SER:N	3:G:46:ASP:OD2	2.41	0.44
5:J:2:DC:H2"	5:J:3:DA:C8	2.51	0.44
2:L:91:PHE:HD1	3:R:35:ASN:HB2	1.83	0.44
2:L:178:GLU:OE2	2:L:181:LYS:HE2	2.18	0.44
2:L:235:ILE:HD11	2:L:263:TRP:CH2	2.53	0.44
3:T:113:SER:HB3	3:T:228:PHE:CZ	2.53	0.44
2:C:116:GLU:HG3	4:I:18:DT:H4'	1.98	0.44
2:D:307:TYR:HE1	2:E:286:GLU:HA	1.83	0.44
2:E:161:THR:HG23	2:E:164:ASP:H	1.83	0.44
2:K:256:LYS:HB3	2:K:256:LYS:HE2	1.81	0.44
2:M:104:ILE:HB	2:M:134:ILE:HG12	2.00	0.44
2:N:75:ASN:HB3	2:N:78:ASP:HB2	2.00	0.44
1:Q:71:GLN:HE22	1:Q:112:ALA:HB2	1.83	0.44
3:R:7:THR:HG23	3:R:44:ILE:HG21	2.00	0.44
2:D:13:GLN:HG2	2:E:129:SER:OG	2.18	0.44
2:E:16:ARG:NH2	7:E:401:ADP:H5'2	2.31	0.44
2:E:198:LYS:HE2	2:E:198:LYS:HB3	1.60	0.44
3:G:104:ASN:OD1	3:G:104:ASN:N	2.50	0.44
2:L:85:ARG:NH2	4:O:19:DC:OP1	2.39	0.44
2:N:3:THR:HG21	2:N:18:SER:OG	2.17	0.44
2:N:125:MET:O	2:N:129:SER:HB2	2.18	0.44
1:Q:151:LEU:O	1:Q:155:LEU:N	2.39	0.44
3:T:190:GLN:O	3:T:194:TYR:OH	2.13	0.44
2:D:237:ASP:OD1	2:D:237:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:PRO:O	2:E:45:ILE:HG13	2.17	0.44
2:E:146:LYS:N	2:E:147:PRO:HD2	2.33	0.44
2:L:242:LEU:HD12	2:L:250:LEU:HD11	2.00	0.44
2:N:126:GLU:HG3	2:N:151:ARG:NH1	2.33	0.44
3:R:66:LEU:HD13	3:S:128:ARG:HB3	2.00	0.44
3:S:59:GLY:O	3:S:63:ILE:HG12	2.18	0.44
2:C:48:HIS:CE1	2:C:141:ILE:HG12	2.53	0.44
3:F:60:PHE:HE1	3:F:83:ILE:HD11	1.82	0.44
3:F:152:PHE:HA	3:F:164:LYS:HZ3	1.83	0.44
2:K:285:TYR:HB2	1:Q:97:TYR:CE1	2.53	0.44
2:L:25:LEU:HB2	2:L:30:LYS:HB2	1.99	0.44
2:L:254:ALA:HB1	2:L:302:GLU:HB3	1.99	0.44
2:N:94:ALA:O	2:N:102:LYS:HE3	2.17	0.44
5:P:4:DG:H2"	5:P:5:DA:C8	2.53	0.44
3:S:130:SER:HB2	3:S:135:ILE:HB	1.98	0.44
3:S:140:ILE:HD13	3:S:196:LEU:HD21	1.99	0.44
2:C:257:TYR:HB2	2:C:305:LEU:HD21	2.00	0.43
2:E:307:TYR:O	2:E:311:GLN:HG2	2.18	0.43
3:H:183:ASN:HB2	3:H:221:GLU:OE2	2.18	0.43
2:K:214:TYR:CE2	2:K:228:VAL:HG22	2.53	0.43
2:N:110:CYS:SG	2:N:140:ASN:N	2.91	0.43
2:N:186:ALA:HB3	2:N:219:VAL:HG12	1.99	0.43
2:N:276:VAL:HG11	2:N:316:MET:HE1	1.99	0.43
1:Q:43:ILE:HG23	1:Q:95:PHE:CD2	2.53	0.43
3:R:139:ALA:HB2	3:R:181:ILE:HG22	1.99	0.43
2:B:5:ASN:C	2:B:7:LYS:H	2.20	0.43
2:C:283:ARG:NH1	2:C:286:GLU:OE1	2.51	0.43
3:T:133:LEU:O	3:T:164:LYS:NZ	2.31	0.43
2:D:109:PHE:HB3	2:D:136:ILE:HG23	2.00	0.43
2:D:276:VAL:O	2:D:277:THR:OG1	2.35	0.43
2:E:300:ASN:ND2	2:E:303:LEU:HD13	2.33	0.43
2:L:235:ILE:HG22	2:L:238:VAL:HB	2.01	0.43
2:L:271:GLU:O	2:L:275:ARG:HG2	2.19	0.43
2:N:90:ASN:OD1	3:S:186:ASN:ND2	2.39	0.43
2:N:281:ILE:O	2:N:284:MET:HG3	2.17	0.43
3:T:165:TYR:CG	3:T:166:SER:N	2.86	0.43
2:B:81:ILE:HG21	4:I:20:DG:H3'	1.99	0.43
3:F:143:LYS:HE3	3:F:143:LYS:HB3	1.76	0.43
3:G:28:PHE:HE1	3:G:41:GLU:HB2	1.83	0.43
1:A:70:SER:OG	2:E:251:ARG:NE	2.35	0.43
2:B:268:LEU:O	2:B:272:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:PRO:O	2:D:281:ILE:HG22	2.18	0.43
3:F:28:PHE:HE2	3:F:106:PRO:HB3	1.82	0.43
2:K:273:TYR:O	2:K:275:ARG:N	2.52	0.43
2:L:24:ILE:O	7:L:403:ADP:N6	2.52	0.43
2:M:287:ILE:HD12	2:M:311:GLN:HB3	2.00	0.43
2:N:162:ASP:N	2:N:162:ASP:OD1	2.51	0.43
1:Q:147:LYS:HB2	1:Q:148:ASN:H	1.63	0.43
2:C:20:ILE:HG22	2:C:66:ASP:OD2	2.18	0.43
2:D:108:GLU:HB3	2:E:122:ARG:CZ	2.49	0.43
2:D:299:ALA:HB2	2:E:295:HIS:HD1	1.84	0.43
2:K:57:THR:OG1	7:K:403:ADP:O2A	2.31	0.43
2:L:205:ARG:NH2	6:L:402:AF3:F1	2.25	0.43
2:M:74:VAL:HG21	2:M:83:PHE:CE1	2.53	0.43
1:Q:43:ILE:HG23	1:Q:95:PHE:CE2	2.53	0.43
3:R:112:ALA:HB2	3:R:197:LEU:HB3	2.00	0.43
3:S:18:ASN:HD21	3:S:101:VAL:HB	1.84	0.43
2:C:8:GLU:HG2	2:C:13:GLN:CB	2.49	0.43
2:E:284:MET:HE1	2:E:288:VAL:HG21	2.00	0.43
3:G:28:PHE:CE1	3:G:41:GLU:HB2	2.54	0.43
2:K:67:VAL:HG11	2:K:101:GLN:OE1	2.19	0.43
2:K:75:ASN:HB3	2:K:78:ASP:HB2	2.00	0.43
2:K:111:ARG:NH1	2:L:116:GLU:HB3	2.29	0.43
2:L:41:LYS:NZ	2:L:101:GLN:HB2	2.33	0.43
2:L:108:GLU:OE2	6:L:402:AF3:F3	2.27	0.43
2:L:297:ILE:HG23	2:M:295:HIS:O	2.19	0.43
2:M:44:HIS:CE1	2:M:133:SER:HA	2.53	0.43
2:M:61:LYS:HE2	2:M:73:PHE:CD1	2.53	0.43
2:N:25:LEU:HD13	2:N:30:LYS:HB2	2.00	0.43
2:N:42:ILE:HD13	2:N:67:VAL:HG21	2.01	0.43
1:Q:4:PHE:HZ	3:T:39:TYR:CG	2.37	0.43
3:S:136:ASP:HB2	3:S:154:LYS:H	1.84	0.43
2:B:205:ARG:NH2	7:B:902:ADP:O3B	2.52	0.43
2:M:189:ASP:OD2	2:M:225:LEU:HD12	2.19	0.43
2:N:183:GLU:HG3	2:N:185:ILE:HG13	2.01	0.43
2:C:255:PRO:HG3	2:C:302:GLU:CD	2.39	0.43
2:D:168:MET:HE3	2:D:201:PHE:HZ	1.82	0.43
2:D:231:ASP:OD1	2:D:232:ARG:N	2.41	0.43
2:M:20:ILE:O	2:M:30:LYS:NZ	2.51	0.43
2:N:47:LEU:HB2	2:N:56:LYS:NZ	2.34	0.43
1:Q:163:THR:O	1:Q:167:LEU:HG	2.19	0.43
3:R:24:LYS:HE3	3:R:24:LYS:HB3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TRP:CZ3	4:I:9:DT:H4'	2.53	0.43
2:C:297:ILE:H	2:C:297:ILE:HG12	1.63	0.43
2:D:47:LEU:HD23	2:D:155:ILE:HB	2.01	0.43
2:D:77:SER:HA	2:D:111:ARG:HH11	1.82	0.43
2:D:89:THR:HG22	2:D:124:PHE:CE2	2.54	0.43
3:H:32:ARG:HD3	3:H:103:PRO:HA	2.00	0.43
2:L:214:TYR:HD2	2:L:224:ILE:HG23	1.84	0.43
2:M:172:MET:SD	2:M:175:ARG:HD3	2.59	0.43
2:N:155:ILE:HD13	2:N:155:ILE:HA	1.73	0.43
2:N:175:ARG:O	2:N:179:ILE:N	2.44	0.43
2:E:48:HIS:HB2	2:E:138:ALA:HB3	2.00	0.42
3:G:10:LEU:HD13	3:G:190:GLN:NE2	2.34	0.42
2:M:243:LYS:HA	2:M:318:TRP:HZ2	1.83	0.42
2:N:280:SER:HB3	2:N:316:MET:SD	2.59	0.42
1:Q:20:LYS:HE3	3:T:55:TYR:CZ	2.54	0.42
3:S:25:SER:HA	3:S:48:ILE:HG22	2.01	0.42
1:A:183:LEU:HG	1:A:186:GLU:HG3	2.00	0.42
2:B:191:LYS:HB2	2:B:225:LEU:HD11	2.01	0.42
2:C:185:ILE:HD12	2:C:215:SER:HB2	2.00	0.42
2:E:227:LEU:HD23	2:E:227:LEU:HA	1.77	0.42
3:G:116:THR:HG23	3:G:196:LEU:HB3	2.01	0.42
6:M:402:AF3:F3	7:M:403:ADP:PB	2.67	0.42
4:O:27:DC:H2"	4:O:28:DT:H72	2.01	0.42
1:A:118:SER:OG	1:A:179:GLN:NE2	2.48	0.42
1:A:159:LYS:HD2	1:A:187:TRP:HE3	1.84	0.42
2:B:242:LEU:HD13	2:B:242:LEU:HA	1.84	0.42
2:C:122:ARG:HD2	2:C:147:PRO:HB2	2.01	0.42
2:D:261:TYR:CE2	2:D:305:LEU:HG	2.54	0.42
2:E:261:TYR:CZ	2:E:265:VAL:HG21	2.54	0.42
3:F:20:GLY:O	3:F:100:VAL:HG21	2.18	0.42
3:F:109:PHE:HA	3:F:208:LYS:NZ	2.33	0.42
2:K:164:ASP:OD1	2:K:164:ASP:N	2.52	0.42
2:L:231:ASP:HA	2:L:263:TRP:NE1	2.34	0.42
2:N:251:ARG:HD2	1:Q:71:GLN:NE2	2.34	0.42
4:O:11:DT:H2'	4:O:12:DA:C8	2.54	0.42
2:C:57:THR:HB	7:C:403:ADP:O2A	2.20	0.42
2:D:277:THR:OG1	2:D:280:SER:OG	2.35	0.42
3:G:140:ILE:HG23	3:G:180:PHE:HB2	2.00	0.42
2:K:285:TYR:HB2	1:Q:97:TYR:HE1	1.83	0.42
2:M:148:LEU:HD23	2:M:148:LEU:HA	1.84	0.42
5:P:3:DA:H2"	5:P:4:DG:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:146:LYS:HD2	3:T:146:LYS:HA	1.62	0.42
2:C:48:HIS:CE1	2:C:156:THR:HG23	2.55	0.42
2:D:263:TRP:O	2:D:267:LYS:HG2	2.20	0.42
2:E:272:ILE:N	2:E:272:ILE:HD13	2.34	0.42
3:F:195:LYS:HE2	3:F:195:LYS:HB3	1.91	0.42
3:G:87:ARG:NH1	3:H:122:ASP:OD2	2.52	0.42
4:I:21:DT:H2"	4:I:22:DA:C8	2.55	0.42
5:J:1:DG:H2"	5:J:2:DC:OP2	2.16	0.42
2:M:162:ASP:O	2:M:166:ILE:HG12	2.19	0.42
2:B:118:GLN:HG2	2:B:145:ILE:HG12	2.01	0.42
2:D:116:GLU:OE1	2:D:119:ARG:NH1	2.53	0.42
2:E:115:ALA:O	2:E:119:ARG:HG3	2.20	0.42
3:F:208:LYS:HE2	3:F:208:LYS:HB3	1.77	0.42
2:N:200:ASN:HB2	2:N:207:THR:HB	2.02	0.42
2:N:277:THR:HG22	2:N:317:GLN:O	2.20	0.42
4:O:21:DT:H2"	4:O:22:DA:C8	2.54	0.42
3:S:147:ILE:HG23	3:S:172:TYR:HB2	2.02	0.42
2:B:239:LEU:HD11	2:B:272:ILE:HG12	2.01	0.42
2:E:199:LYS:NZ	2:E:210:GLU:OE2	2.48	0.42
2:E:268:LEU:HD22	2:E:272:ILE:HG12	2.02	0.42
3:H:76:SER:HA	3:H:82:LYS:HE3	2.00	0.42
2:L:5:ASN:C	2:L:7:LYS:H	2.22	0.42
2:L:212:ASP:OD2	2:M:153:ARG:NH2	2.53	0.42
2:M:243:LYS:HA	2:M:318:TRP:CZ2	2.54	0.42
2:N:193:VAL:O	2:N:197:VAL:HG22	2.20	0.42
3:R:183:ASN:HB2	3:R:221:GLU:OE2	2.19	0.42
3:T:39:TYR:OH	3:T:106:PRO:HA	2.19	0.42
2:E:169:MET:O	2:E:173:ILE:HG12	2.20	0.42
2:E:276:VAL:HG22	2:E:277:THR:H	1.85	0.42
3:F:34:VAL:O	3:F:101:VAL:HG21	2.20	0.42
2:K:224:ILE:O	2:K:228:VAL:HG23	2.20	0.42
2:N:89:THR:HG23	2:N:128:TYR:CE2	2.55	0.42
3:S:10:LEU:HD22	3:S:190:GLN:NE2	2.35	0.42
3:T:63:ILE:O	3:T:66:LEU:HB2	2.19	0.42
3:T:153:ASN:O	3:T:157:ASP:N	2.53	0.42
1:A:159:LYS:HD2	1:A:187:TRP:CE3	2.55	0.42
2:C:25:LEU:HD21	2:C:59:VAL:HG21	2.01	0.42
2:C:86:GLY:HA3	2:C:87:PRO:HD3	1.93	0.42
2:C:186:ALA:HB3	2:C:219:VAL:HG22	2.02	0.42
2:E:233:GLY:HA3	2:E:267:LYS:HD3	2.02	0.42
3:G:212:GLU:HG2	3:G:213:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:15:ALA:HB2	3:H:57:LEU:HD23	2.02	0.42
2:K:261:TYR:CZ	2:K:265:VAL:HG11	2.54	0.42
2:N:256:LYS:HB3	2:N:256:LYS:HE2	1.80	0.42
1:Q:177:GLN:O	1:Q:181:LYS:HG3	2.20	0.42
3:S:149:ILE:O	3:S:166:SER:HA	2.19	0.42
3:S:205:GLY:HA3	3:S:220:LEU:HD12	2.02	0.42
2:B:116:GLU:CD	2:B:119:ARG:HH12	2.23	0.42
2:C:78:ASP:OD1	2:D:85:ARG:NE	2.46	0.42
2:D:90:ASN:HB3	3:H:156:GLU:OE2	2.20	0.42
2:E:118:GLN:OE1	2:E:144:ILE:HA	2.20	0.42
2:E:268:LEU:HD23	2:E:268:LEU:HA	1.61	0.42
3:F:110:PRO:HB2	3:F:199:TRP:CD1	2.55	0.42
3:H:118:ILE:HA	3:H:169:LEU:HD22	2.00	0.42
2:N:169:MET:O	2:N:173:ILE:HG12	2.19	0.42
3:S:183:ASN:HB2	3:S:221:GLU:OE2	2.20	0.42
1:A:2:SER:OG	3:F:219:ALA:HA	2.20	0.41
1:A:164:ASP:OD1	1:A:164:ASP:N	2.53	0.41
2:C:294:TYR:HB3	2:D:293:GLN:HB2	2.02	0.41
2:K:141:ILE:HD12	2:K:141:ILE:HA	1.76	0.41
2:K:167:GLU:HG3	2:K:168:MET:N	2.34	0.41
2:K:243:LYS:HA	2:K:243:LYS:HD2	1.68	0.41
2:L:48:HIS:O	2:L:157:PHE:HB2	2.19	0.41
2:E:272:ILE:HD12	2:E:272:ILE:HA	1.73	0.41
3:F:80:ASN:OD1	3:F:93:PRO:HA	2.19	0.41
3:F:105:LYS:C	3:F:107:ILE:H	2.22	0.41
3:G:196:LEU:HD13	3:G:209:PHE:CE2	2.55	0.41
3:H:153:ASN:O	3:H:157:ASP:N	2.52	0.41
2:L:56:LYS:HE3	2:L:56:LYS:HB2	1.71	0.41
2:N:175:ARG:HA	2:N:178:GLU:HB3	2.02	0.41
2:N:289:GLY:O	2:N:293:GLN:HB2	2.20	0.41
1:A:10:LEU:HB2	1:A:14:GLN:HB2	2.02	0.41
2:B:8:GLU:O	2:B:10:ILE:N	2.53	0.41
2:E:255:PRO:C	2:E:257:TYR:N	2.73	0.41
2:L:48:HIS:CG	2:L:141:ILE:HG12	2.54	0.41
2:L:288:VAL:HG22	2:L:308:LEU:HD11	2.01	0.41
2:M:111:ARG:NH1	2:N:116:GLU:HB3	2.35	0.41
2:N:189:ASP:O	2:N:192:VAL:HG12	2.21	0.41
3:R:196:LEU:HD13	3:R:209:PHE:CE1	2.55	0.41
1:A:184:ALA:O	1:A:186:GLU:N	2.53	0.41
2:B:122:ARG:HA	2:B:125:MET:HE2	2.01	0.41
2:C:237:ASP:OD2	2:C:256:LYS:NZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:LEU:HD23	2:D:176:LEU:HA	1.87	0.41
3:F:118:ILE:HB	3:F:119:LYS:H	1.78	0.41
3:H:116:THR:O	3:H:196:LEU:N	2.53	0.41
2:K:15:TYR:CE2	2:K:179:ILE:HG23	2.55	0.41
2:K:273:TYR:C	2:K:275:ARG:H	2.22	0.41
2:L:192:VAL:HG22	2:L:225:LEU:HB2	2.01	0.41
2:N:8:GLU:OE2	1:Q:130:ARG:NH2	2.54	0.41
2:N:85:ARG:NH2	4:O:15:DT:OP1	2.53	0.41
3:T:16:THR:HG23	3:T:188:LYS:HZ3	1.85	0.41
1:A:145:LEU:HD21	1:A:154:VAL:HG21	2.01	0.41
1:A:151:LEU:O	1:A:155:LEU:HD12	2.21	0.41
2:B:12:GLU:H	2:B:12:GLU:HG3	1.59	0.41
2:C:235:ILE:HD11	2:C:271:GLU:HG3	2.01	0.41
2:D:206:LYS:HE2	2:E:152:CYS:O	2.20	0.41
2:E:99:GLY:O	2:E:100:ARG:HG2	2.19	0.41
3:F:189:MET:HA	3:F:216:TYR:CE2	2.49	0.41
3:H:25:SER:N	3:H:51:ASP:OD1	2.51	0.41
2:K:235:ILE:HD12	2:K:239:LEU:HD21	2.02	0.41
2:L:39:LYS:HE2	2:L:39:LYS:HB3	1.69	0.41
2:B:11:LEU:HD22	2:B:212:ASP:HB2	2.03	0.41
2:C:188:ALA:HB3	2:C:221:ASP:HA	2.01	0.41
2:D:10:ILE:O	2:D:12:GLU:HG2	2.21	0.41
2:D:206:LYS:O	2:D:210:GLU:HG2	2.20	0.41
2:E:15:TYR:CE2	2:E:179:ILE:HG13	2.56	0.41
2:E:56:LYS:HB3	2:E:137:THR:HG23	2.02	0.41
2:E:283:ARG:HD2	2:E:283:ARG:HA	1.85	0.41
3:G:130:SER:HA	3:G:135:ILE:HB	2.02	0.41
2:L:59:VAL:O	2:L:63:LEU:HB2	2.20	0.41
3:R:90:ILE:HG12	3:S:165:TYR:CD1	2.54	0.41
3:S:152:PHE:HB2	3:S:160:LEU:HD23	2.02	0.41
3:S:195:LYS:HB2	3:S:210:GLU:HB3	2.02	0.41
3:T:177:THR:N	3:T:227:ASP:OD2	2.53	0.41
2:C:16:ARG:HH21	7:C:403:ADP:H5'1	1.84	0.41
4:I:10:DT:OP2	4:I:10:DT:H71	2.20	0.41
1:Q:4:PHE:HZ	3:T:39:TYR:CD1	2.39	0.41
3:T:76:SER:OG	3:T:80:ASN:N	2.42	0.41
1:A:175:LYS:O	1:A:179:GLN:N	2.54	0.41
2:C:108:GLU:HB3	2:D:122:ARG:NH2	2.36	0.41
2:E:243:LYS:HD3	2:E:244:ASN:H	1.85	0.41
2:E:312:LEU:O	2:E:316:MET:HG2	2.21	0.41
3:G:124:GLN:O	3:G:128:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:110:CYS:HB2	2:K:140:ASN:OD1	2.21	0.41
2:L:8:GLU:HB2	2:L:14:LYS:HB2	2.03	0.41
2:M:51:SER:HA	2:M:52:PRO:HD3	1.92	0.41
2:N:168:MET:HA	2:N:171:GLN:HG3	2.03	0.41
2:N:169:MET:HE3	2:N:169:MET:HA	2.01	0.41
1:Q:181:LYS:O	1:Q:185:LEU:HG	2.20	0.41
3:R:194:TYR:HA	3:R:210:GLU:O	2.20	0.41
2:B:84:VAL:O	2:B:89:THR:HG23	2.21	0.41
2:B:201:PHE:HB3	2:B:202:PRO:HD3	2.02	0.41
2:D:84:VAL:HG22	2:D:88:LEU:HD22	2.01	0.41
3:F:7:THR:HA	3:F:44:ILE:HG12	2.02	0.41
3:F:162:ARG:HB3	3:F:163:VAL:H	1.69	0.41
3:F:194:TYR:HE1	3:F:212:GLU:HG2	1.86	0.41
3:H:125:GLN:OE1	3:H:165:TYR:OH	2.18	0.41
2:K:10:ILE:HG23	2:K:13:GLN:HB2	2.02	0.41
2:L:307:TYR:HE1	2:M:286:GLU:HA	1.86	0.41
2:N:137:THR:O	2:N:137:THR:OG1	2.38	0.41
2:N:278:PRO:HA	2:N:281:ILE:HD12	2.03	0.41
1:Q:44:ILE:H	1:Q:44:ILE:HG13	1.68	0.41
1:Q:176:GLU:HA	1:Q:179:GLN:HB2	2.03	0.41
3:S:178:PHE:HA	3:S:226:HIS:HA	2.03	0.41
3:T:210:GLU:HB2	3:T:215:ASN:OD1	2.21	0.41
2:B:77:SER:HA	2:B:111:ARG:HD3	2.02	0.41
2:D:306:ALA:O	2:D:310:ILE:HG12	2.20	0.41
2:E:99:GLY:N	3:H:204:GLN:HB3	2.36	0.41
3:G:190:GLN:HE21	3:G:213:HIS:HE1	1.69	0.41
2:M:8:GLU:HG2	2:M:13:GLN:HB3	2.03	0.41
2:C:121:LEU:HA	2:C:124:PHE:HB3	2.03	0.40
2:C:142:ASP:OD1	2:C:142:ASP:N	2.52	0.40
2:E:243:LYS:C	2:E:245:LYS:N	2.74	0.40
2:L:12:GLU:O	7:L:403:ADP:O3'	2.29	0.40
2:N:246:ASP:OD1	2:N:246:ASP:N	2.53	0.40
4:O:22:DA:H2"	4:O:23:DG:H8	1.85	0.40
2:B:56:LYS:HE3	7:B:902:ADP:O1B	2.21	0.40
2:B:189:ASP:OD2	2:B:225:LEU:HD12	2.21	0.40
2:B:265:VAL:HG11	2:B:292:ASN:HB2	2.02	0.40
2:C:235:ILE:H	2:C:235:ILE:HG12	1.59	0.40
2:D:186:ALA:HB3	2:D:219:VAL:HG23	2.03	0.40
3:F:39:TYR:CE1	3:F:41:GLU:HB3	2.57	0.40
3:F:184:MET:C	3:F:186:ASN:H	2.25	0.40
2:K:242:LEU:HD23	2:K:250:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:64:CYS:SG	2:M:71:MET:HG3	2.61	0.40
2:N:4:VAL:HG12	2:N:6:GLU:HG2	2.03	0.40
4:O:8:DT:O2	1:Q:107:ARG:NH1	2.54	0.40
1:A:144:ILE:HG23	1:A:148:ASN:HD21	1.86	0.40
2:B:111:ARG:HG2	2:C:119:ARG:HD3	2.02	0.40
2:D:201:PHE:HB3	2:D:202:PRO:HD3	2.03	0.40
2:D:204:PHE:HD2	7:D:403:ADP:C5	2.40	0.40
2:D:307:TYR:CD1	2:E:289:GLY:HA3	2.57	0.40
3:H:24:LYS:O	3:H:48:ILE:HD11	2.21	0.40
2:K:11:LEU:HD22	2:K:212:ASP:HB2	2.03	0.40
2:K:217:LYS:HA	2:K:217:LYS:HD3	1.70	0.40
2:L:148:LEU:HD23	2:L:148:LEU:HA	1.88	0.40
2:M:10:ILE:HG22	2:M:13:GLN:HB3	2.03	0.40
2:M:29:ASP:N	2:M:29:ASP:OD1	2.55	0.40
2:M:29:ASP:O	2:M:32:THR:OG1	2.32	0.40
2:N:170:LYS:O	2:N:174:ARG:HB2	2.21	0.40
4:O:7:DT:O2	4:O:7:DT:H2'	2.21	0.40
1:Q:50:LYS:HA	1:Q:50:LYS:HD3	1.87	0.40
3:T:3:LEU:HD23	3:T:8:THR:HG22	2.03	0.40
3:T:34:VAL:HA	3:T:101:VAL:HG11	2.03	0.40
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.88	0.40
2:E:224:ILE:C	2:E:226:SER:H	2.25	0.40
2:K:26:PRO:HG2	2:K:29:ASP:HB2	2.04	0.40
2:K:235:ILE:O	2:K:239:LEU:HG	2.21	0.40
3:R:147:ILE:HB	3:R:172:TYR:HB2	2.03	0.40
3:T:109:PHE:HD1	3:T:110:PRO:HD2	1.85	0.40
3:T:188:LYS:HE3	3:T:188:LYS:HB3	1.93	0.40
1:A:148:ASN:HB3	2:E:213:SER:N	2.35	0.40
2:B:7:LYS:O	2:C:130:SER:HB3	2.22	0.40
2:D:197:VAL:O	2:D:201:PHE:HA	2.22	0.40
2:E:176:LEU:HD22	2:E:211:LEU:HD12	2.04	0.40
3:F:10:LEU:HD22	3:F:190:GLN:NE2	2.37	0.40
3:F:80:ASN:HA	3:F:94:ALA:HB2	2.03	0.40
2:L:24:ILE:N	7:L:403:ADP:HN62	2.20	0.40
2:M:180:CYS:HB3	2:M:185:ILE:HB	2.03	0.40
2:M:196:LEU:HD21	2:M:214:TYR:HD2	1.86	0.40
2:M:205:ARG:HG3	7:M:403:ADP:H4'	2.04	0.40
2:M:229:THR:OG1	2:M:231:ASP:HB2	2.21	0.40
4:O:9:DT:H72	1:Q:40:PHE:N	2.36	0.40
1:Q:82:MET:HE2	1:Q:94:HIS:HA	2.03	0.40
3:R:152:PHE:HD2	3:R:157:ASP:OD2	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:184:MET:HA	3:T:187:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	179/187 (96%)	142 (79%)	21 (12%)	16 (9%)	1 4
1	Q	179/187 (96%)	140 (78%)	28 (16%)	11 (6%)	1 9
2	B	317/320 (99%)	291 (92%)	19 (6%)	7 (2%)	6 29
2	C	318/320 (99%)	290 (91%)	22 (7%)	6 (2%)	8 33
2	D	316/320 (99%)	287 (91%)	20 (6%)	9 (3%)	5 25
2	E	316/320 (99%)	281 (89%)	26 (8%)	9 (3%)	5 25
2	K	317/320 (99%)	289 (91%)	21 (7%)	7 (2%)	6 29
2	L	318/320 (99%)	286 (90%)	25 (8%)	7 (2%)	6 29
2	M	313/320 (98%)	289 (92%)	23 (7%)	1 (0%)	41 73
2	N	301/320 (94%)	266 (88%)	32 (11%)	3 (1%)	15 49
3	F	226/228 (99%)	181 (80%)	37 (16%)	8 (4%)	3 20
3	G	226/228 (99%)	208 (92%)	14 (6%)	4 (2%)	8 34
3	H	226/228 (99%)	205 (91%)	19 (8%)	2 (1%)	17 52
3	R	226/228 (99%)	207 (92%)	18 (8%)	1 (0%)	34 69
3	S	226/228 (99%)	201 (89%)	23 (10%)	2 (1%)	17 52
3	T	226/228 (99%)	195 (86%)	24 (11%)	7 (3%)	4 23
All	All	4230/4302 (98%)	3758 (89%)	372 (9%)	100 (2%)	6 27

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO
2	B	201	PHE
2	D	11	LEU
2	E	191	LYS
3	F	34	VAL
3	G	79	GLY
2	K	6	GLU
2	K	27	ALA
2	K	201	PHE
2	L	49	SER
2	L	50	PRO
2	N	130	SER
1	Q	12	GLU
1	Q	35	LYS
1	Q	103	PRO
1	Q	180	LEU
1	A	5	LYS
1	A	49	ASN
1	A	56	ALA
1	A	149	GLY
1	A	150	LYS
1	A	172	LYS
1	A	173	ASN
2	B	6	GLU
2	B	11	LEU
2	B	233	GLY
2	C	230	ASN
2	C	236	ASP
2	D	7	LYS
2	E	100	ARG
2	E	123	SER
2	E	244	ASN
3	F	107	ILE
3	F	222	ALA
3	G	78	ASP
3	G	158	SER
2	L	219	VAL
1	Q	33	LYS
1	Q	150	LYS
3	S	104	ASN
3	T	110	PRO
3	T	149	ILE
3	T	178	PHE

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Mol	Chain	Res	Type
1	A	40	PHE
2	C	6	GLU
2	C	11	LEU
2	D	231	ASP
2	D	276	VAL
2	E	189	ASP
3	F	119	LYS
3	H	110	PRO
2	L	216	SER
2	N	6	GLU
1	Q	37	GLU
1	Q	62	LYS
1	Q	173	ASN
1	A	20	LYS
1	A	185	LEU
2	B	9	HIS
2	B	234	ALA
2	C	231	ASP
2	D	236	ASP
2	E	256	LYS
2	E	296	GLY
2	E	298	ALA
3	F	202	GLY
3	G	213	HIS
2	K	274	SER
2	L	6	GLU
2	L	314	CYS
2	N	53	GLY
1	Q	110	LYS
3	R	2	LYS
1	A	41[A]	PHE
1	A	41[B]	PHE
1	A	171	THR
1	A	174	VAL
2	B	112	SER
2	C	1	MET
2	D	230	ASN
2	D	278	PRO
2	E	315	GLU
3	F	207	ALA
2	K	70	ASP
2	M	140	ASN

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Mol	Chain	Res	Type
3	S	110	PRO
3	T	148	VAL
3	T	201	LYS
3	F	155	VAL
3	H	158	SER
1	Q	147	LYS
3	T	166	SER
2	D	235	ILE
2	K	158	GLY
2	L	310	ILE
2	K	235	ILE
3	T	106	PRO
1	A	55	ILE
2	D	277	THR
3	F	36	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	160/163 (98%)	132 (82%)	28 (18%)	2 8
1	Q	159/163 (98%)	123 (77%)	36 (23%)	1 3
2	B	277/278 (100%)	264 (95%)	13 (5%)	26 59
2	C	278/278 (100%)	258 (93%)	20 (7%)	14 44
2	D	276/278 (99%)	263 (95%)	13 (5%)	26 59
2	E	276/278 (99%)	251 (91%)	25 (9%)	9 33
2	K	277/278 (100%)	259 (94%)	18 (6%)	17 47
2	L	278/278 (100%)	260 (94%)	18 (6%)	17 47
2	M	276/278 (99%)	247 (90%)	29 (10%)	7 26
2	N	266/278 (96%)	230 (86%)	36 (14%)	4 16
3	F	189/189 (100%)	168 (89%)	21 (11%)	6 24
3	G	189/189 (100%)	178 (94%)	11 (6%)	20 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	H	189/189 (100%)	180 (95%)	9 (5%)	25 58
3	R	189/189 (100%)	178 (94%)	11 (6%)	20 51
3	S	189/189 (100%)	183 (97%)	6 (3%)	39 69
3	T	189/189 (100%)	182 (96%)	7 (4%)	34 66
All	All	3657/3684 (99%)	3356 (92%)	301 (8%)	11 38

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	ASP
1	A	10	LEU
1	A	19	SER
1	A	21	ASP
1	A	39	GLU
1	A	40	PHE
1	A	49	ASN
1	A	55	ILE
1	A	63	PHE
1	A	87	SER
1	A	95	PHE
1	A	107	ARG
1	A	117	ASP
1	A	119	THR
1	A	121	VAL
1	A	150	LYS
1	A	155	LEU
1	A	159	LYS
1	A	161	LEU
1	A	162	VAL
1	A	163	THR
1	A	164	ASP
1	A	166	PHE
1	A	167	LEU
1	A	168	LYS
1	A	179	GLN
1	A	180	LEU
2	B	25	LEU
2	B	32	THR
2	B	98	ASP
2	B	123	SER

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Mol	Chain	Res	Type
2	B	141	ILE
2	B	179	ILE
2	B	200	ASN
2	B	206	LYS
2	B	225	LEU
2	B	236	ASP
2	B	242	LEU
2	B	276	VAL
2	B	311	GLN
2	C	1	MET
2	C	8	GLU
2	C	16	ARG
2	C	32	THR
2	C	45	ILE
2	C	66	ASP
2	C	71	MET
2	C	72	MET
2	C	79	CYS
2	C	89	THR
2	C	93	SER
2	C	105	VAL
2	C	131	ASN
2	C	141	ILE
2	C	153	ARG
2	C	161	THR
2	C	235	ILE
2	C	293	GLN
2	C	297	ILE
2	C	316	MET
2	D	5	ASN
2	D	20	ILE
2	D	21	ASP
2	D	25	LEU
2	D	88	LEU
2	D	97	PHE
2	D	111	ARG
2	D	141	ILE
2	D	175	ARG
2	D	229	THR
2	D	231	ASP
2	D	240	GLU
2	D	284	MET

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Mol	Chain	Res	Type
2	E	28	PHE
2	E	35	SER
2	E	48	HIS
2	E	66	ASP
2	E	109	PHE
2	E	122	ARG
2	E	130	SER
2	E	150	SER
2	E	212	ASP
2	E	227	LEU
2	E	229	THR
2	E	230	ASN
2	E	232	ARG
2	E	235	ILE
2	E	238	VAL
2	E	242	LEU
2	E	243	LYS
2	E	253	LEU
2	E	268	LEU
2	E	271	GLU
2	E	272	ILE
2	E	273	TYR
2	E	305	LEU
2	E	312	LEU
2	E	315	GLU
3	F	21	ILE
3	F	22	MET
3	F	31	THR
3	F	32	ARG
3	F	45	SER
3	F	51	ASP
3	F	54	ILE
3	F	87	ARG
3	F	101	VAL
3	F	104	ASN
3	F	118	ILE
3	F	119	LYS
3	F	122	ASP
3	F	127	LEU
3	F	152	PHE
3	F	161	THR
3	F	175	GLU

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Mol	Chain	Res	Type
3	F	193	ASN
3	F	203	LYS
3	F	220	LEU
3	F	226	HIS
3	G	23	LEU
3	G	37	THR
3	G	44	ILE
3	G	104	ASN
3	G	118	ILE
3	G	124	GLN
3	G	134	GLN
3	G	155	VAL
3	G	157	ASP
3	G	169	LEU
3	G	171	ASP
3	H	13	ASN
3	H	78	ASP
3	H	128	ARG
3	H	147	ILE
3	H	155	VAL
3	H	156	GLU
3	H	171	ASP
3	H	189	MET
3	H	193	ASN
2	K	3	THR
2	K	7	LYS
2	K	10	ILE
2	K	11	LEU
2	K	19	THR
2	K	21	ASP
2	K	35	SER
2	K	71	MET
2	K	72	MET
2	K	79	CYS
2	K	88	LEU
2	K	105	VAL
2	K	109	PHE
2	K	141	ILE
2	K	156	THR
2	K	286	GLU
2	K	293	GLN
2	K	319	LYS

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Mol	Chain	Res	Type
2	L	11	LEU
2	L	67	VAL
2	L	114	LEU
2	L	122	ARG
2	L	141	ILE
2	L	152	CYS
2	L	156	THR
2	L	182	HIS
2	L	191	LYS
2	L	200	ASN
2	L	206	LYS
2	L	244	ASN
2	L	253	LEU
2	L	273	TYR
2	L	276	VAL
2	L	283	ARG
2	L	311	GLN
2	L	312	LEU
2	M	7	LYS
2	M	10	ILE
2	M	16	ARG
2	M	29	ASP
2	M	48	HIS
2	M	66	ASP
2	M	78	ASP
2	M	109	PHE
2	M	118	GLN
2	M	123	SER
2	M	141	ILE
2	M	164	ASP
2	M	175	ARG
2	M	200	ASN
2	M	224	ILE
2	M	225	LEU
2	M	227	LEU
2	M	229	THR
2	M	239	LEU
2	M	240	GLU
2	M	246	ASP
2	M	261	TYR
2	M	276	VAL
2	M	285	TYR

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Mol	Chain	Res	Type
2	M	297	ILE
2	M	302	GLU
2	M	308	LEU
2	M	318	TRP
2	M	319	LYS
2	N	10	ILE
2	N	12	GLU
2	N	13	GLN
2	N	14	LYS
2	N	21	ASP
2	N	24	ILE
2	N	25	LEU
2	N	31	GLU
2	N	47	LEU
2	N	49	SER
2	N	54	THR
2	N	56	LYS
2	N	58	THR
2	N	90	ASN
2	N	122	ARG
2	N	141	ILE
2	N	149	GLN
2	N	154	VAL
2	N	157	PHE
2	N	166	ILE
2	N	171	GLN
2	N	173	ILE
2	N	174	ARG
2	N	176	LEU
2	N	180	CYS
2	N	196	LEU
2	N	214	TYR
2	N	215	SER
2	N	251	ARG
2	N	253	LEU
2	N	270	GLU
2	N	273	TYR
2	N	275	ARG
2	N	276	VAL
2	N	284	MET
2	N	288	VAL
1	Q	3	LEU

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Mol	Chain	Res	Type
1	Q	8	ILE
1	Q	32	PHE
1	Q	37	GLU
1	Q	38	ASN
1	Q	40	PHE
1	Q	48	ASN
1	Q	51	THR
1	Q	52	LYS
1	Q	62	LYS
1	Q	67	ASN
1	Q	83	ASN
1	Q	84	LEU
1	Q	85	ILE
1	Q	92	GLU
1	Q	96	ASN
1	Q	102	VAL
1	Q	111	TRP
1	Q	113	LYS
1	Q	114	LEU
1	Q	117	ASP
1	Q	118	SER
1	Q	121	VAL
1	Q	142	LYS
1	Q	146	THR
1	Q	147	LYS
1	Q	151	LEU
1	Q	154	VAL
1	Q	161	LEU
1	Q	165	ASP
1	Q	170	VAL
1	Q	175	LYS
1	Q	176	GLU
1	Q	179	GLN
1	Q	183	LEU
1	Q	185	LEU
3	R	2	LYS
3	R	38	THR
3	R	39	TYR
3	R	78	ASP
3	R	131	ARG
3	R	133	LEU
3	R	143	LYS

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Mol	Chain	Res	Type
3	R	155	VAL
3	R	160	LEU
3	R	162	ARG
3	R	190	GLN
3	S	1	MET
3	S	23	LEU
3	S	73	ILE
3	S	127	LEU
3	S	157	ASP
3	S	184	MET
3	T	5	LYS
3	T	16	THR
3	T	38	THR
3	T	66	LEU
3	T	167	LEU
3	T	184	MET
3	T	187	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	134	ASN
2	B	291	ASN
2	C	293	GLN
2	E	230	ASN
3	F	193	ASN
3	G	190	GLN
3	G	213	HIS
2	K	120	HIS
2	M	295	HIS
2	M	304	HIS
2	N	48	HIS
2	N	101	GLN
2	N	171	GLN
2	N	293	GLN
1	Q	48	ASN
1	Q	71	GLN
1	Q	148	ASN
3	R	153	ASN
3	R	186	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
7	ADP	N	401	8	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
7	ADP	K	403	8	24,29,29	0.97	1 (4%)	29,45,45	1.48	4 (13%)
7	ADP	M	403	8	24,29,29	0.97	1 (4%)	29,45,45	1.50	4 (13%)
6	AF3	C	402	-	0,3,3	-	-	-		
7	ADP	L	403	8	24,29,29	0.97	1 (4%)	29,45,45	1.44	4 (13%)
6	AF3	K	402	-	0,3,3	-	-	-		
6	AF3	D	402	-	0,3,3	-	-	-		
6	AF3	M	402	-	0,3,3	-	-	-		
6	AF3	L	402	-	0,3,3	-	-	-		
7	ADP	C	403	8	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
7	ADP	B	902	8	24,29,29	0.96	1 (4%)	29,45,45	1.56	4 (13%)
7	ADP	E	401	8	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)
6	AF3	B	901	-	0,3,3	-	-	-		
7	ADP	D	403	8	24,29,29	0.96	1 (4%)	29,45,45	1.54	4 (13%)

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
7	ADP	N	401	8	-	4/12/32/32	0/3/3/3
7	ADP	K	403	8	-	4/12/32/32	0/3/3/3
7	ADP	M	403	8	-	5/12/32/32	0/3/3/3
7	ADP	L	403	8	-	5/12/32/32	0/3/3/3
7	ADP	C	403	8	-	0/12/32/32	0/3/3/3
7	ADP	B	902	8	-	2/12/32/32	0/3/3/3
7	ADP	E	401	8	-	4/12/32/32	0/3/3/3
7	ADP	D	403	8	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	403	ADP	C5-C4	2.60	1.47	1.40
7	B	902	ADP	C5-C4	2.56	1.47	1.40
7	E	401	ADP	C5-C4	2.52	1.47	1.40
7	D	403	ADP	C5-C4	2.51	1.47	1.40
7	N	401	ADP	C5-C4	2.51	1.47	1.40
7	C	403	ADP	C5-C4	2.51	1.47	1.40
7	L	403	ADP	C5-C4	2.46	1.47	1.40
7	M	403	ADP	C5-C4	2.44	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	401	ADP	PA-O3A-PB	-3.93	119.35	132.83
7	B	902	ADP	C3'-C2'-C1'	3.81	106.71	100.98
7	D	403	ADP	PA-O3A-PB	-3.70	120.12	132.83
7	M	403	ADP	C3'-C2'-C1'	3.68	106.52	100.98
7	K	403	ADP	C3'-C2'-C1'	3.67	106.50	100.98
7	N	401	ADP	PA-O3A-PB	-3.59	120.50	132.83
7	C	403	ADP	C3'-C2'-C1'	3.58	106.36	100.98
7	N	401	ADP	C3'-C2'-C1'	3.51	106.26	100.98
7	D	403	ADP	C3'-C2'-C1'	3.50	106.25	100.98
7	B	902	ADP	PA-O3A-PB	-3.46	120.97	132.83
7	N	401	ADP	N3-C2-N1	-3.45	123.29	128.68
7	E	401	ADP	C3'-C2'-C1'	3.41	106.11	100.98
7	L	403	ADP	PA-O3A-PB	-3.38	121.24	132.83
7	K	403	ADP	PA-O3A-PB	-3.34	121.35	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	403	ADP	PA-O3A-PB	-3.34	121.38	132.83
7	L	403	ADP	C3'-C2'-C1'	3.28	105.92	100.98
7	E	401	ADP	N3-C2-N1	-3.17	123.72	128.68
7	C	403	ADP	PA-O3A-PB	-3.16	122.00	132.83
7	L	403	ADP	N3-C2-N1	-3.12	123.80	128.68
7	K	403	ADP	N3-C2-N1	-3.08	123.86	128.68
7	B	902	ADP	N3-C2-N1	-3.08	123.86	128.68
7	C	403	ADP	N3-C2-N1	-3.04	123.92	128.68
7	D	403	ADP	N3-C2-N1	-3.01	123.97	128.68
7	M	403	ADP	N3-C2-N1	-2.97	124.03	128.68
7	B	902	ADP	C4-C5-N7	-2.71	106.58	109.40
7	C	403	ADP	C4-C5-N7	-2.67	106.62	109.40
7	D	403	ADP	C4-C5-N7	-2.61	106.68	109.40
7	K	403	ADP	C4-C5-N7	-2.58	106.71	109.40
7	L	403	ADP	C4-C5-N7	-2.56	106.73	109.40
7	E	401	ADP	C4-C5-N7	-2.55	106.74	109.40
7	M	403	ADP	C4-C5-N7	-2.49	106.81	109.40
7	N	401	ADP	C4-C5-N7	-2.47	106.82	109.40

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	902	ADP	C5'-O5'-PA-O3A
7	E	401	ADP	C5'-O5'-PA-O1A
7	E	401	ADP	C5'-O5'-PA-O2A
7	K	403	ADP	PA-O3A-PB-O2B
7	K	403	ADP	PA-O3A-PB-O3B
7	L	403	ADP	C5'-O5'-PA-O1A
7	L	403	ADP	C5'-O5'-PA-O2A
7	L	403	ADP	O4'-C4'-C5'-O5'
7	M	403	ADP	PA-O3A-PB-O3B
7	M	403	ADP	C5'-O5'-PA-O2A
7	N	401	ADP	C5'-O5'-PA-O3A
7	K	403	ADP	O4'-C4'-C5'-O5'
7	L	403	ADP	C3'-C4'-C5'-O5'
7	K	403	ADP	C3'-C4'-C5'-O5'
7	M	403	ADP	C5'-O5'-PA-O3A
7	N	401	ADP	PB-O3A-PA-O2A
7	B	902	ADP	C5'-O5'-PA-O1A
7	M	403	ADP	C5'-O5'-PA-O1A
7	N	401	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
7	N	401	ADP	PB-O3A-PA-O1A
7	E	401	ADP	O4'-C4'-C5'-O5'
7	M	403	ADP	PA-O3A-PB-O2B
7	E	401	ADP	C5'-O5'-PA-O3A
7	L	403	ADP	C5'-O5'-PA-O3A

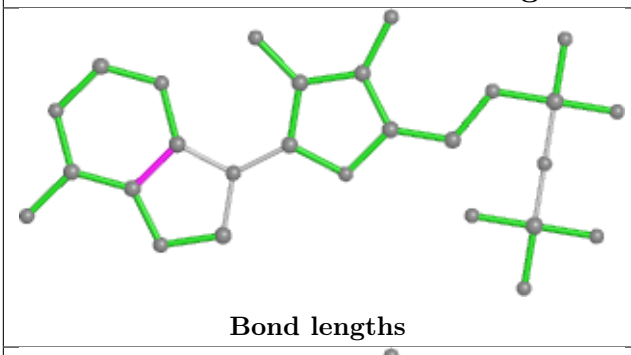
There are no ring outliers.

13 monomers are involved in 53 short contacts:

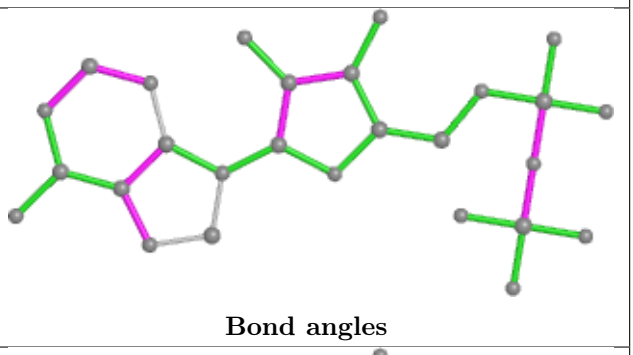
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	401	ADP	5	0
7	K	403	ADP	4	0
7	M	403	ADP	8	0
6	C	402	AF3	1	0
7	L	403	ADP	4	0
6	K	402	AF3	2	0
6	M	402	AF3	3	0
6	L	402	AF3	2	0
7	C	403	ADP	6	0
7	B	902	ADP	8	0
7	E	401	ADP	6	0
6	B	901	AF3	4	0
7	D	403	ADP	5	0

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

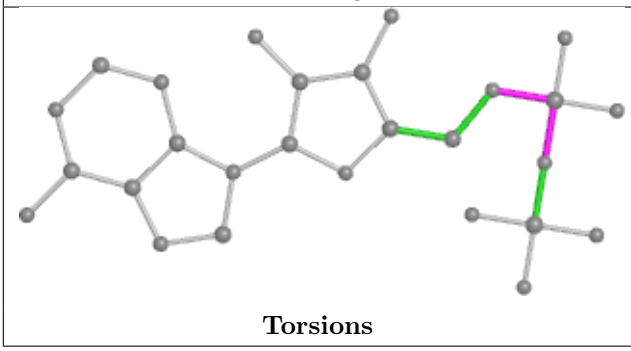
Ligand ADP N 401



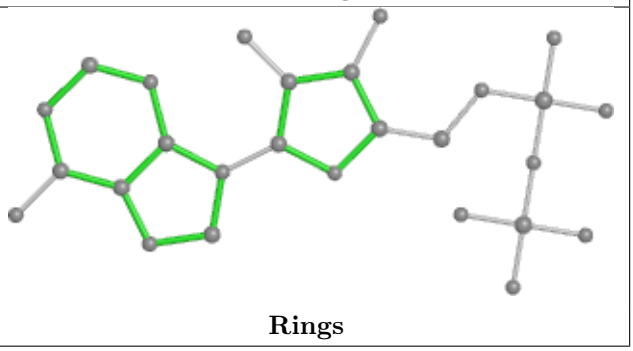
Bond lengths



Bond angles

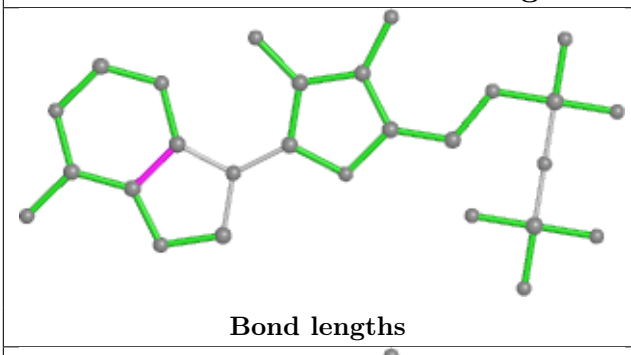


Torsions

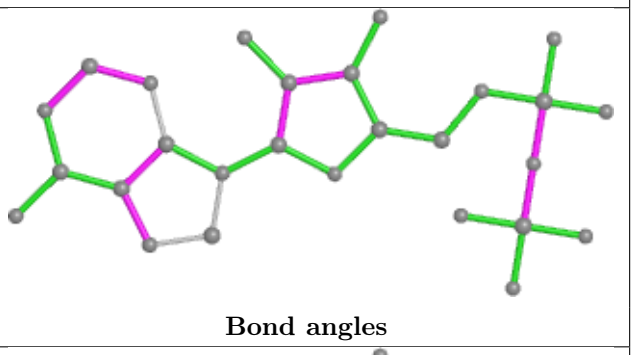


Rings

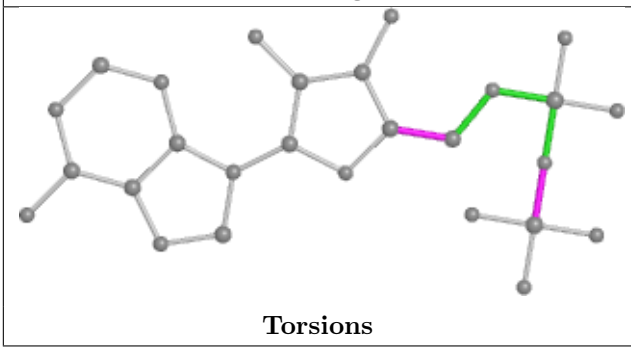
Ligand ADP K 403



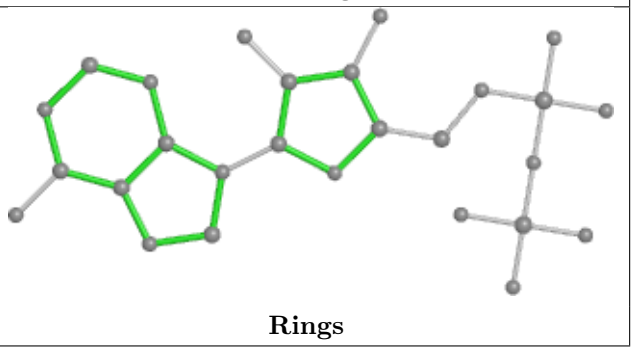
Bond lengths



Bond angles

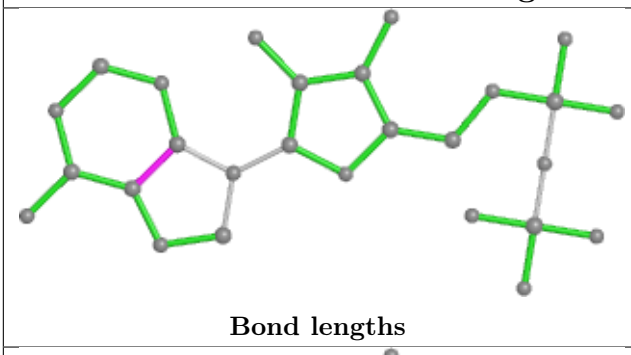


Torsions

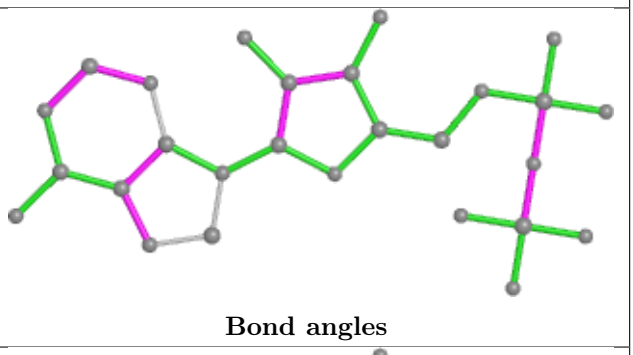


Rings

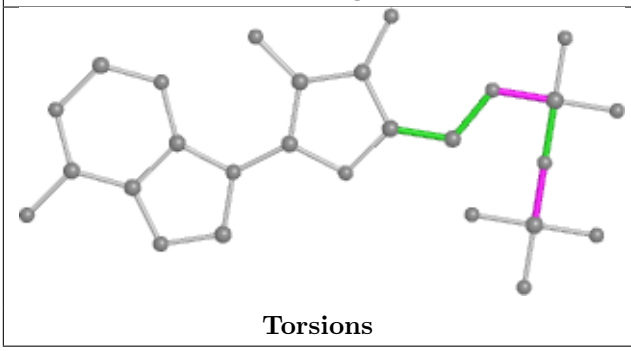
Ligand ADP M 403



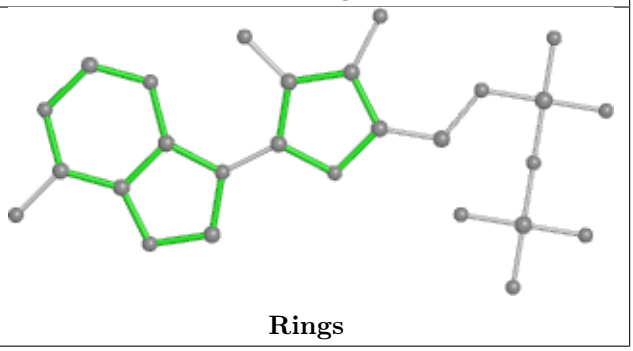
Bond lengths



Bond angles

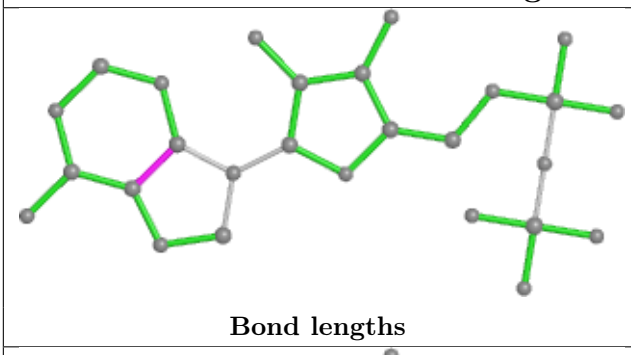


Torsions

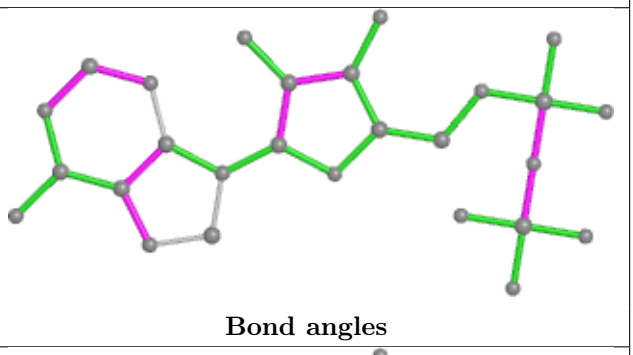


Rings

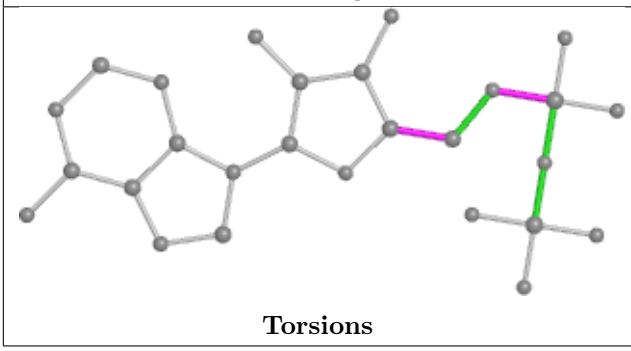
Ligand ADP L 403



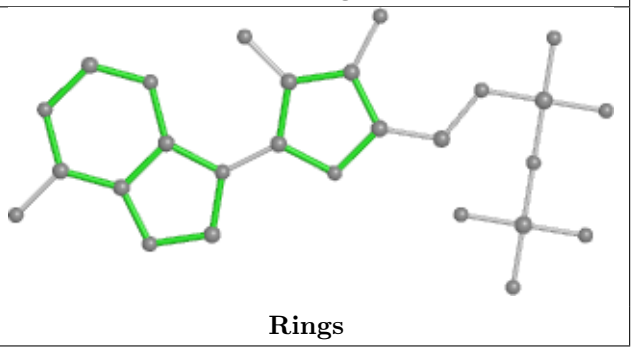
Bond lengths



Bond angles

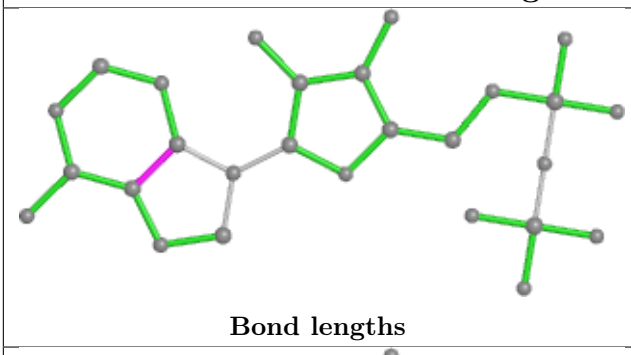


Torsions

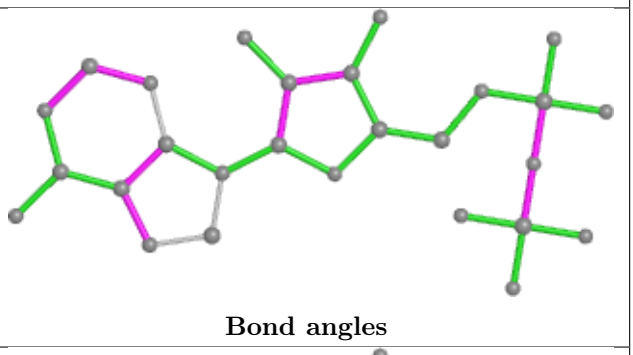


Rings

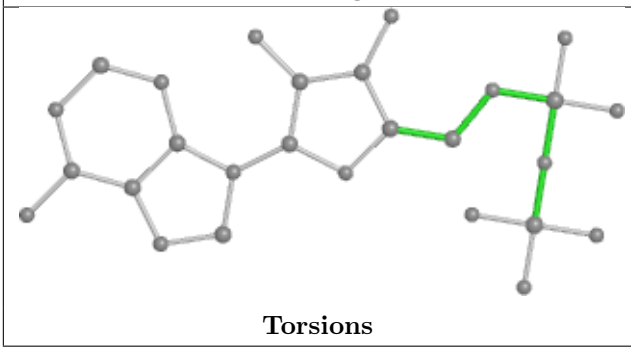
Ligand ADP C 403



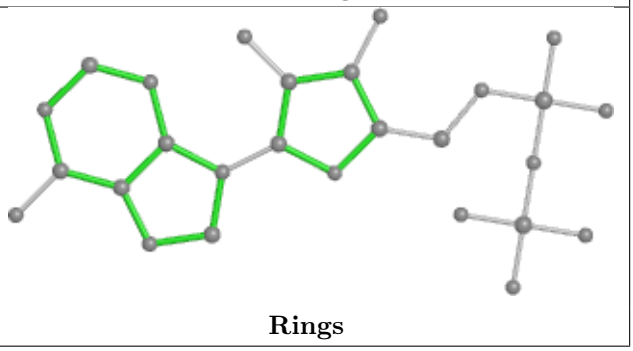
Bond lengths



Bond angles

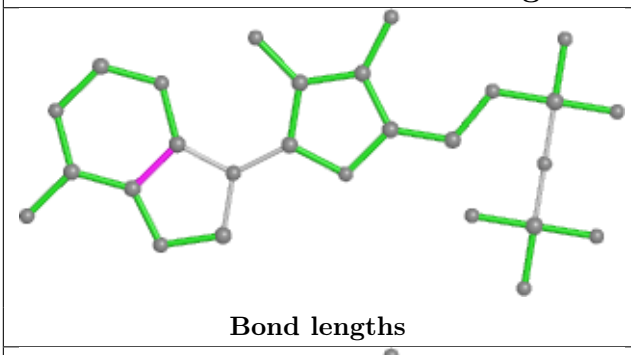


Torsions

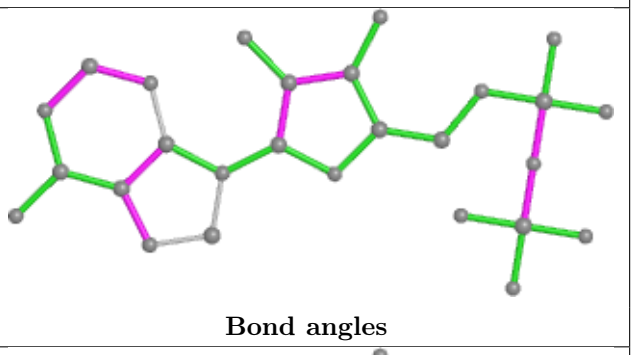


Rings

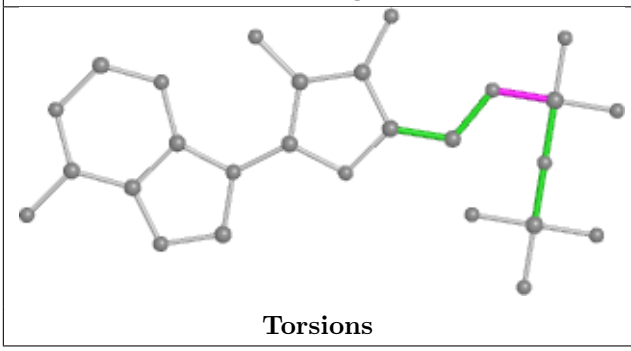
Ligand ADP B 902



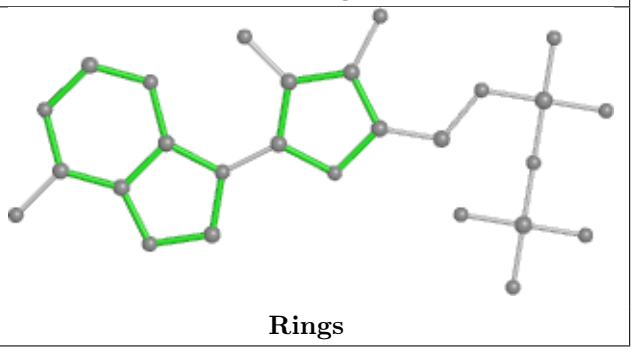
Bond lengths



Bond angles

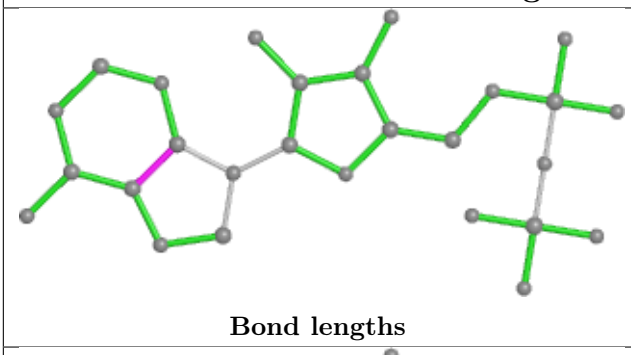


Torsions

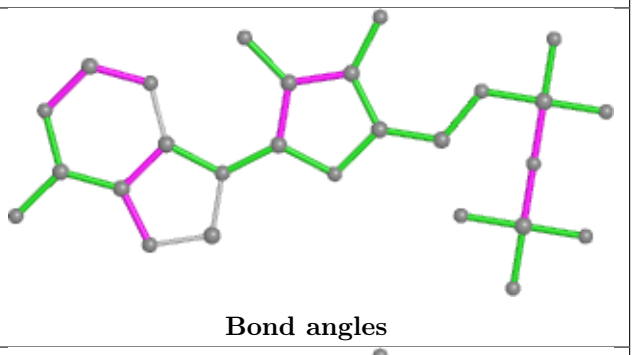


Rings

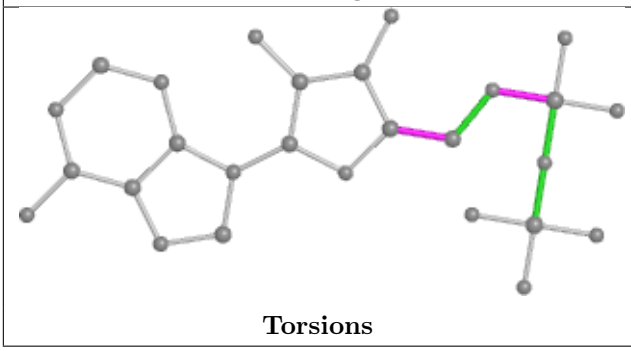
Ligand ADP E 401



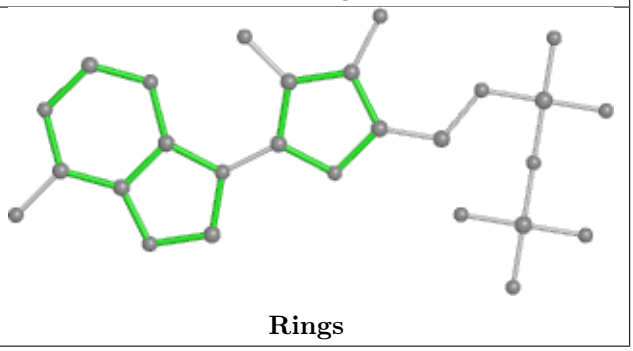
Bond lengths



Bond angles

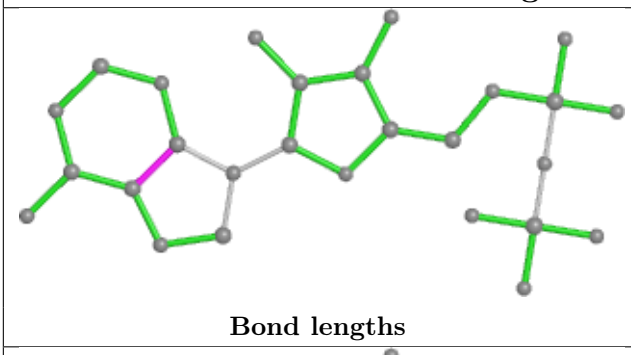


Torsions

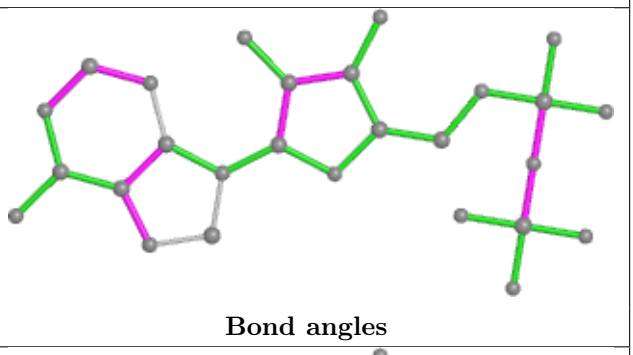


Rings

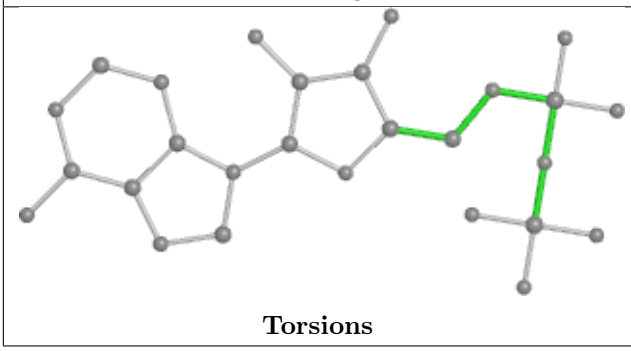
Ligand ADP D 403



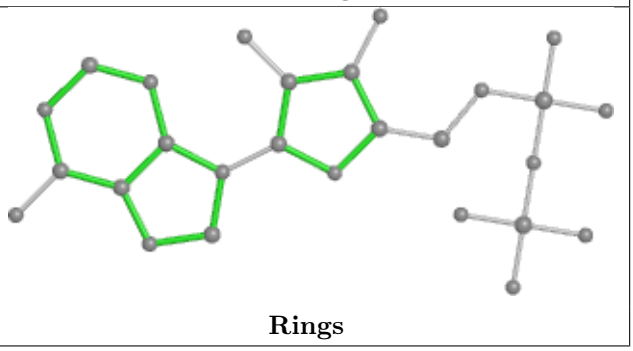
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	182/187 (97%)	0.26	13 (7%) 16 6	99, 139, 167, 176	0
1	Q	183/187 (97%)	0.80	34 (18%) 1 0	119, 185, 203, 213	0
2	B	319/320 (99%)	-0.15	0 100 100	59, 89, 109, 139	0
2	C	320/320 (100%)	-0.15	0 100 100	53, 80, 142, 152	0
2	D	318/320 (99%)	-0.14	1 (0%) 94 88	53, 86, 168, 191	0
2	E	318/320 (99%)	-0.09	6 (1%) 66 46	60, 119, 168, 188	0
2	K	319/320 (99%)	0.15	13 (4%) 37 18	102, 138, 186, 199	0
2	L	320/320 (100%)	0.01	9 (2%) 53 30	89, 116, 197, 206	0
2	M	317/320 (99%)	0.09	9 (2%) 53 30	80, 119, 192, 202	0
2	N	305/320 (95%)	0.41	25 (8%) 11 4	92, 169, 219, 236	0
3	F	228/228 (100%)	0.35	27 (11%) 4 2	110, 144, 189, 213	0
3	G	228/228 (100%)	-0.19	4 (1%) 68 47	75, 105, 128, 151	0
3	H	228/228 (100%)	0.05	9 (3%) 39 20	92, 125, 172, 180	0
3	R	228/228 (100%)	0.25	19 (8%) 11 4	131, 158, 174, 186	0
3	S	228/228 (100%)	0.18	22 (9%) 8 2	124, 158, 181, 193	0
3	T	228/228 (100%)	0.40	23 (10%) 7 2	144, 176, 190, 202	0
4	I	24/24 (100%)	-0.14	1 (4%) 36 18	80, 160, 248, 304	0
4	O	24/24 (100%)	-0.30	0 100 100	106, 187, 271, 291	0
5	J	20/20 (100%)	-0.42	0 100 100	86, 130, 310, 339	0
5	P	20/20 (100%)	-0.05	3 (15%) 2 1	132, 214, 282, 306	0
All	All	4357/4390 (99%)	0.10	218 (5%) 28 13	53, 131, 192, 339	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	171	THR	8.5
2	N	195	ALA	8.1
1	Q	160	GLY	7.0
3	T	191	PRO	6.6
1	Q	161	LEU	6.6
2	N	196	LEU	6.5
1	A	53	CYS	6.4
3	F	118	ILE	6.4
3	R	21	ILE	6.2
3	F	21	ILE	5.5
3	F	120	ALA	5.5
1	Q	61	SER	5.5
3	T	111	VAL	5.4
1	Q	69	LEU	5.2
2	N	267	LYS	5.1
3	F	119	LYS	5.1
3	H	149	ILE	5.1
3	F	139	ALA	5.0
3	F	170	GLY	5.0
1	Q	162	VAL	4.9
3	F	54	ILE	4.7
3	S	67	VAL	4.7
1	Q	103	PRO	4.7
1	A	36	ALA	4.7
1	Q	104	ARG	4.7
1	Q	163	THR	4.7
2	K	318	TRP	4.6
1	A	37	GLU	4.5
3	T	60	PHE	4.4
3	T	83	ILE	4.3
2	N	268	LEU	4.2
2	N	112	SER	4.2
3	R	54	ILE	4.2
2	N	179	ILE	4.2
3	F	138	ILE	4.1
2	E	270	GLU	4.1
3	T	189	MET	4.0
2	N	177	THR	4.0
2	L	235	ILE	4.0
1	Q	174	VAL	4.0
3	T	21	ILE	4.0
2	N	299	ALA	3.9
3	R	151	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
3	S	66	LEU	3.8
3	F	177	THR	3.8
3	S	92	TRP	3.7
3	S	207	ALA	3.7
1	A	162	VAL	3.6
2	K	272	ILE	3.6
3	R	139	ALA	3.6
2	K	285	TYR	3.6
3	T	81	ILE	3.6
3	F	180	PHE	3.6
1	Q	55	ILE	3.6
3	R	199	TRP	3.6
3	R	40	ALA	3.5
2	L	285	TYR	3.5
3	T	209	PHE	3.5
3	R	138	ILE	3.5
1	Q	164	ASP	3.4
1	A	55	ILE	3.4
1	Q	179	GLN	3.4
3	F	178	PHE	3.4
3	S	206	ALA	3.4
2	E	269	ALA	3.4
2	K	269	ALA	3.3
2	N	194	ALA	3.3
3	F	124	GLN	3.3
1	Q	168	LYS	3.3
3	H	3	LEU	3.3
2	L	288	VAL	3.3
5	P	20	DA	3.3
1	Q	42	GLU	3.3
1	Q	177	GLN	3.2
3	R	101	VAL	3.2
4	I	30	DC	3.2
3	R	206	ALA	3.2
1	A	187	TRP	3.2
1	Q	85	ILE	3.2
1	Q	95	PHE	3.2
1	Q	82	MET	3.2
3	H	148	VAL	3.2
3	F	121	GLU	3.2
3	R	39	TYR	3.2
2	N	157	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
3	T	199	TRP	3.1
3	T	206	ALA	3.1
2	K	287	ILE	3.1
3	H	60	PHE	3.1
2	N	309	PHE	3.1
3	F	182	ILE	3.0
2	N	273	TYR	3.0
1	Q	86	GLY	3.0
2	N	193	VAL	3.0
3	H	63	ILE	3.0
3	H	7	THR	3.0
1	A	161	LEU	2.9
3	R	23	LEU	2.9
3	T	137	THR	2.9
3	T	175	GLU	2.9
1	A	54	SER	2.9
2	K	270	GLU	2.9
1	Q	126	LEU	2.9
2	E	229	THR	2.9
2	K	284	MET	2.8
1	A	43	ILE	2.8
2	M	312	LEU	2.8
2	N	261	TYR	2.8
3	S	86	ALA	2.8
3	T	165	TYR	2.8
1	Q	181	LYS	2.8
2	N	272	ILE	2.8
3	F	171	ASP	2.8
3	R	116	THR	2.8
2	M	257	TYR	2.8
2	N	313	ALA	2.8
5	P	19	DT	2.8
1	Q	170	VAL	2.8
2	N	290	GLU	2.7
3	F	122	ASP	2.7
3	T	61	LEU	2.7
3	S	58	ASN	2.7
1	Q	158	LEU	2.7
3	T	169	LEU	2.7
3	S	71	ALA	2.7
3	S	87	ARG	2.7
3	T	207	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	2	SER	2.7
2	L	256	LYS	2.7
2	N	191	LYS	2.6
3	F	196	LEU	2.6
3	T	216	TYR	2.6
3	R	218	VAL	2.6
3	G	149	ILE	2.6
2	N	244	ASN	2.6
1	Q	97	TYR	2.6
1	Q	165	ASP	2.6
2	K	268	LEU	2.6
3	H	94	ALA	2.6
1	Q	94	HIS	2.6
2	K	294	TYR	2.6
3	S	21	ILE	2.6
2	M	112	SER	2.6
2	M	251	ARG	2.6
3	F	116	THR	2.6
3	S	205	GLY	2.5
2	M	239	LEU	2.5
3	S	152	PHE	2.5
1	Q	75	CYS	2.5
3	G	150	ASN	2.5
1	Q	185	LEU	2.5
3	S	218	VAL	2.5
3	G	140	ILE	2.5
2	K	312	LEU	2.5
3	R	53	ALA	2.4
2	N	111	ARG	2.4
1	A	39	GLU	2.4
3	S	51	ASP	2.4
1	A	52	LYS	2.4
2	K	222	ALA	2.4
3	T	88	SER	2.4
1	Q	38	ASN	2.4
1	Q	57	GLN	2.4
3	R	99	THR	2.4
2	M	252	ALA	2.4
2	L	236	ASP	2.4
2	N	271	GLU	2.3
2	K	273	TYR	2.3
3	H	65	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	310	ILE	2.3
3	S	209	PHE	2.3
5	P	18	DA	2.3
3	F	123	LEU	2.3
2	M	309	PHE	2.3
2	L	253	LEU	2.3
1	A	95	PHE	2.3
3	S	189	MET	2.3
2	E	268	LEU	2.3
2	M	250	LEU	2.3
3	S	12	LYS	2.3
3	T	54	ILE	2.3
3	G	54	ILE	2.3
2	L	201	PHE	2.2
3	F	167	LEU	2.2
3	R	100	VAL	2.2
3	T	190	GLN	2.2
3	F	164	LYS	2.2
1	Q	62	LYS	2.2
2	K	247	VAL	2.2
2	N	262	SER	2.2
3	S	163	VAL	2.2
2	M	228	VAL	2.2
2	N	176	LEU	2.2
2	E	281	ILE	2.2
3	F	149	ILE	2.2
3	F	187	MET	2.2
3	T	92	TRP	2.2
1	Q	166	PHE	2.2
3	R	115	VAL	2.2
3	F	140	ILE	2.1
2	N	219	VAL	2.1
2	L	219	VAL	2.1
3	S	29	ILE	2.1
1	Q	98	LEU	2.1
3	H	82	LYS	2.1
3	S	7	THR	2.1
2	E	309	PHE	2.1
3	T	196	LEU	2.1
3	T	208	LYS	2.0
3	F	86	ALA	2.0
3	R	197	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	R	169	LEU	2.0
3	S	95	ALA	2.0
3	F	191	PRO	2.0
3	F	52	VAL	2.0
2	D	251	ARG	2.0
2	N	302	GLU	2.0
3	S	198	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ADP	N	401	27/27	0.86	0.18	148,168,177,180	0
7	ADP	K	403	27/27	0.91	0.26	103,115,122,124	0
7	ADP	E	401	27/27	0.92	0.18	84,102,106,113	0
7	ADP	D	403	27/27	0.95	0.25	56,66,74,80	0
7	ADP	M	403	27/27	0.95	0.27	87,96,107,116	0
7	ADP	B	902	27/27	0.95	0.24	69,71,75,76	0
8	MG	N	402	1/1	0.95	0.55	140,140,140,140	0
7	ADP	L	403	27/27	0.96	0.21	89,97,102,103	0
7	ADP	C	403	27/27	0.96	0.24	54,61,66,67	0
6	AF3	K	402	4/4	0.97	0.35	100,100,101,102	0
6	AF3	B	901	4/4	0.97	0.25	66,67,68,68	0
6	AF3	C	402	4/4	0.98	0.23	54,55,55,55	0
6	AF3	L	402	4/4	0.98	0.23	85,85,86,87	0
8	MG	B	903	1/1	0.98	0.35	64,64,64,64	0
8	MG	D	401	1/1	0.98	0.35	59,59,59,59	0
8	MG	E	402	1/1	0.98	0.56	79,79,79,79	0

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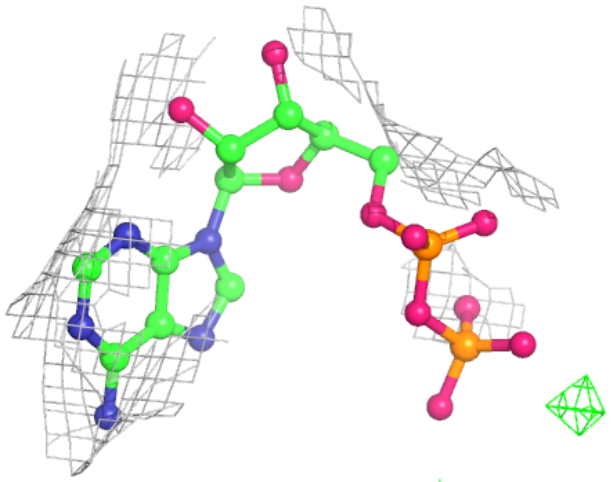
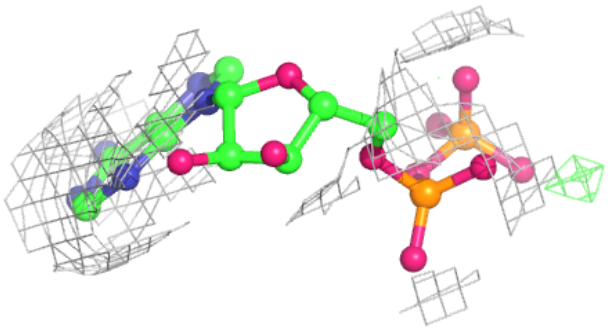
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	K	401	1/1	0.98	0.43	96,96,96,96	0
6	AF3	M	402	4/4	0.98	0.38	83,84,84,85	0
6	AF3	D	402	4/4	0.99	0.28	52,56,62,70	0
8	MG	L	401	1/1	0.99	0.23	84,84,84,84	0
8	MG	M	401	1/1	0.99	0.51	84,84,84,84	0
8	MG	C	401	1/1	0.99	0.41	48,48,48,48	0

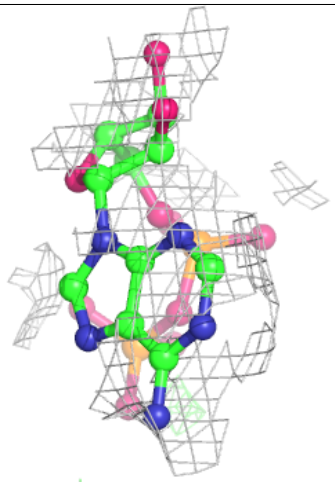
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP N 401:

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

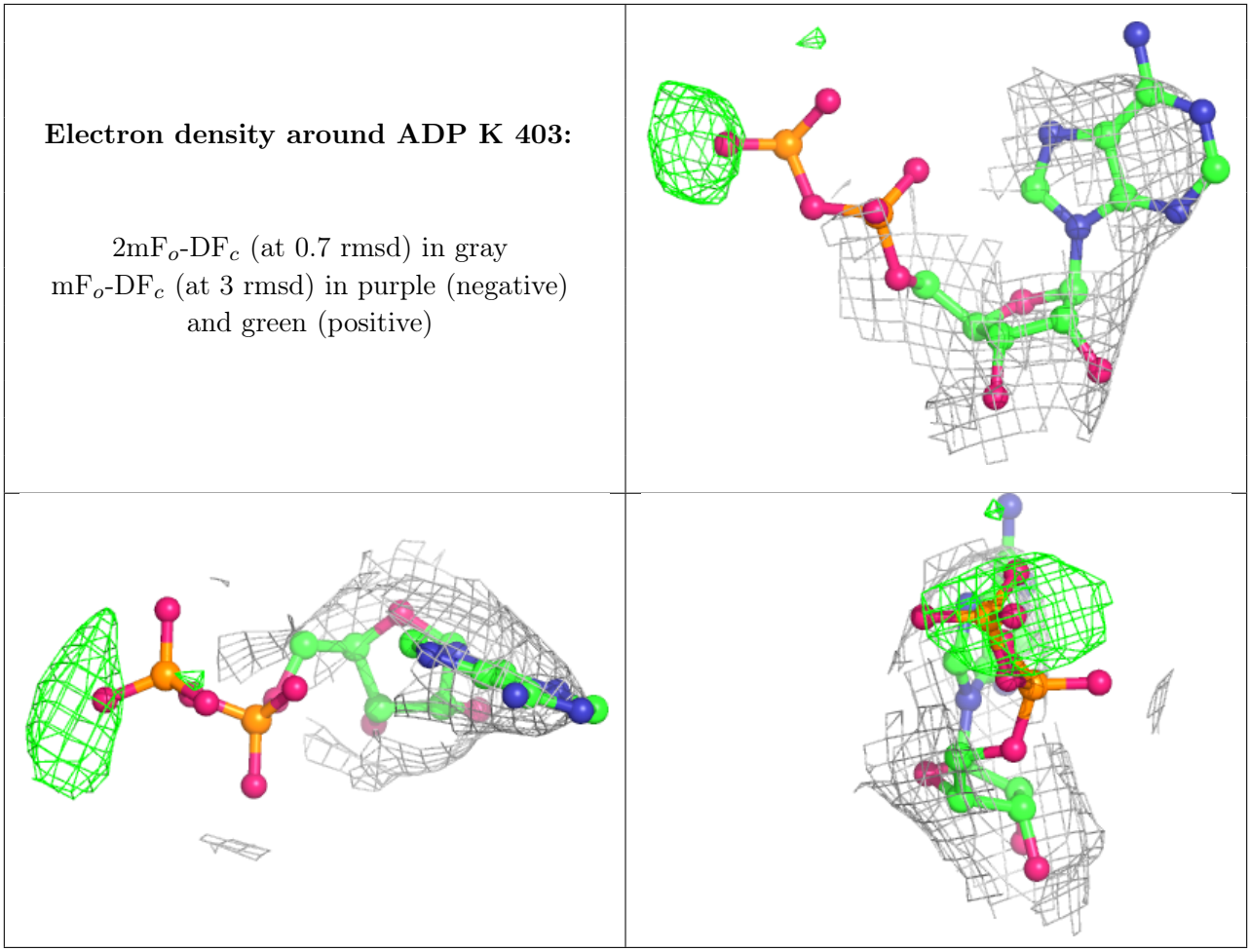






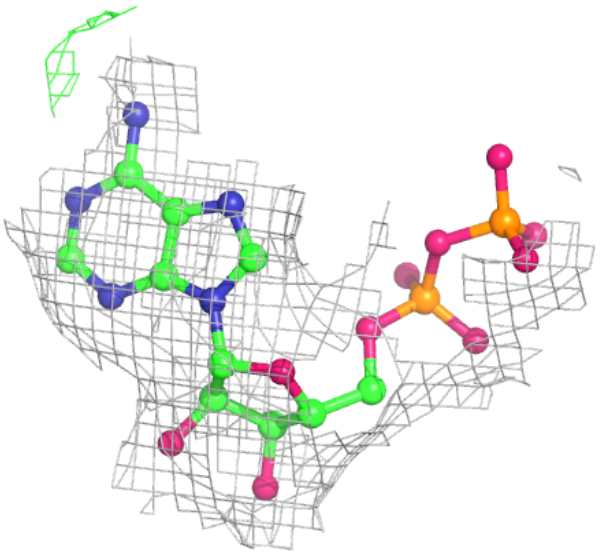
Electron density around ADP K 403:

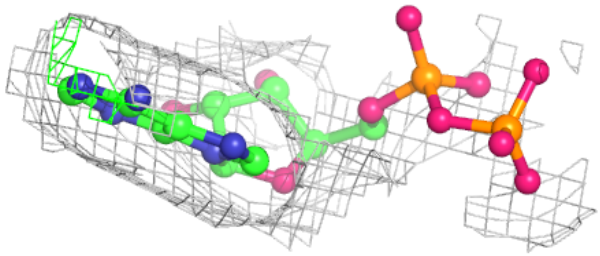
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

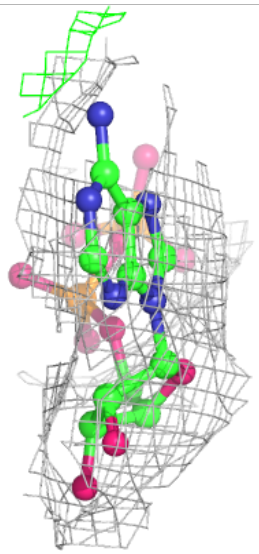


Electron density around ADP E 401:

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

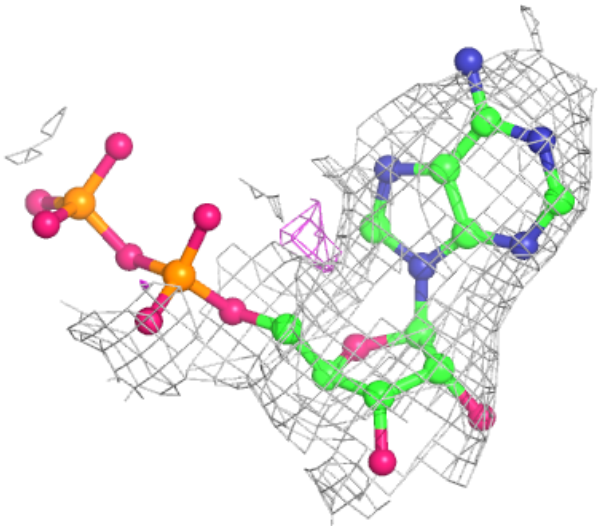


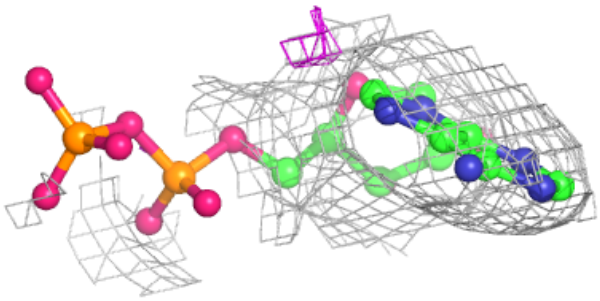


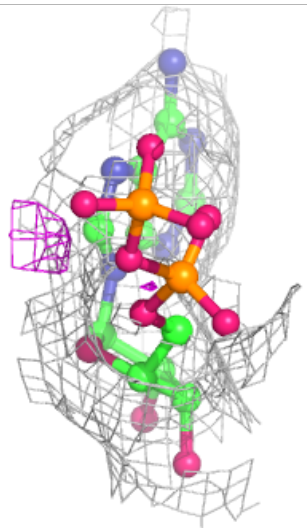


Electron density around ADP D 403:

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

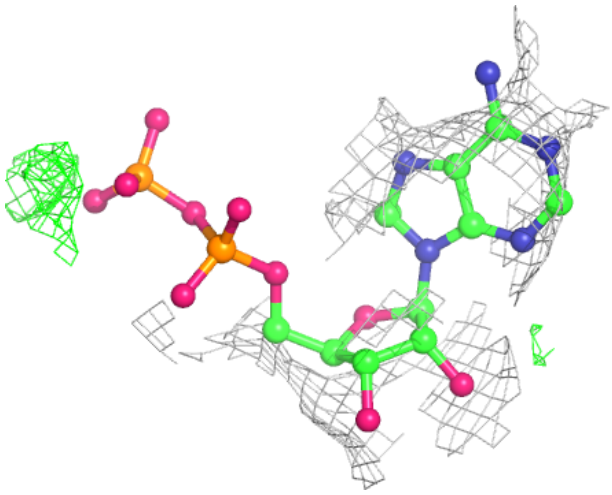


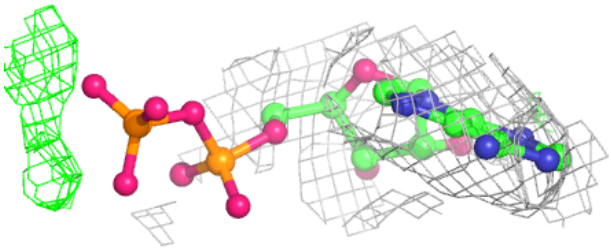


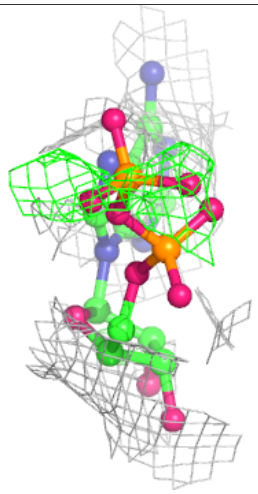


Electron density around ADP M 403:

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

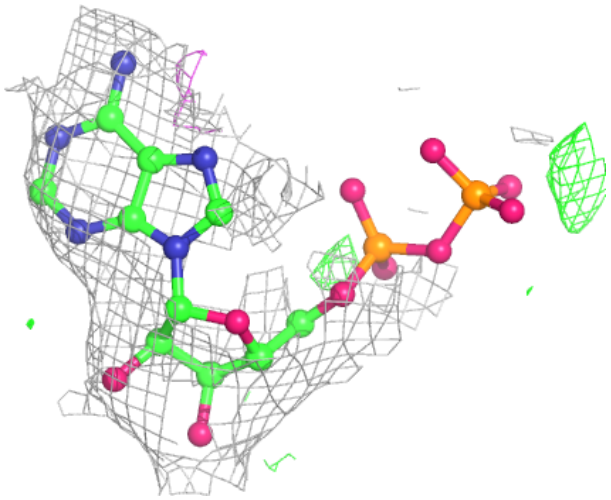


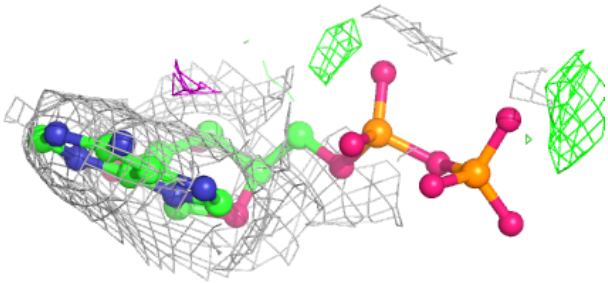


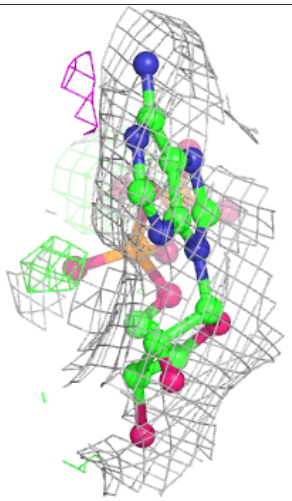


Electron density around ADP B 902:

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

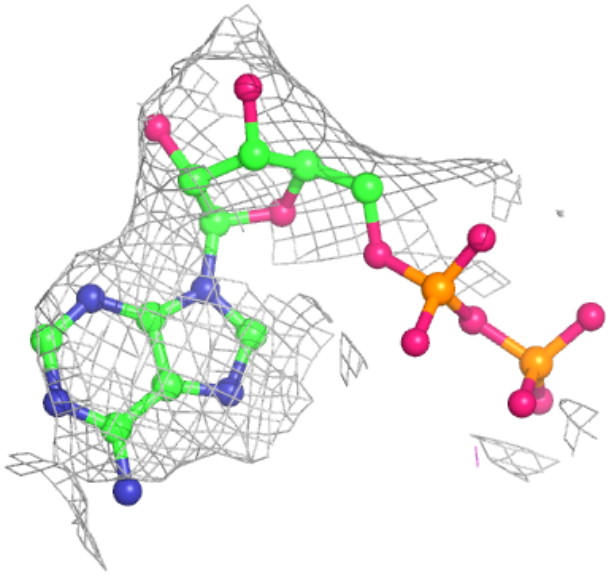


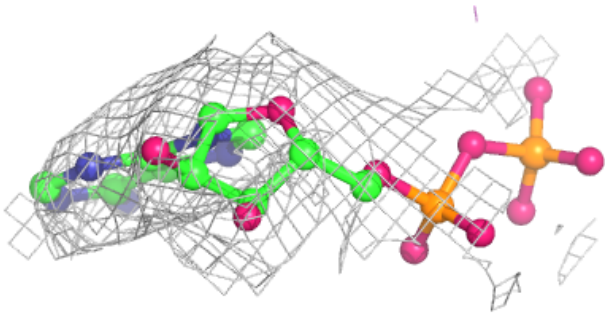


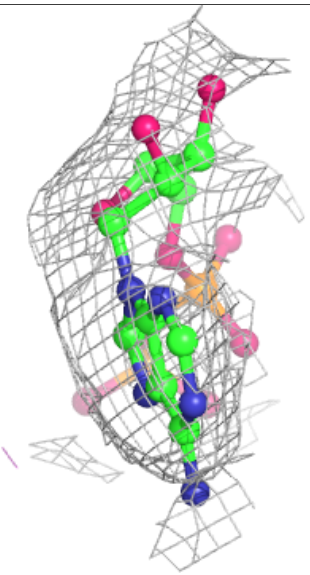


Electron density around ADP L 403:

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

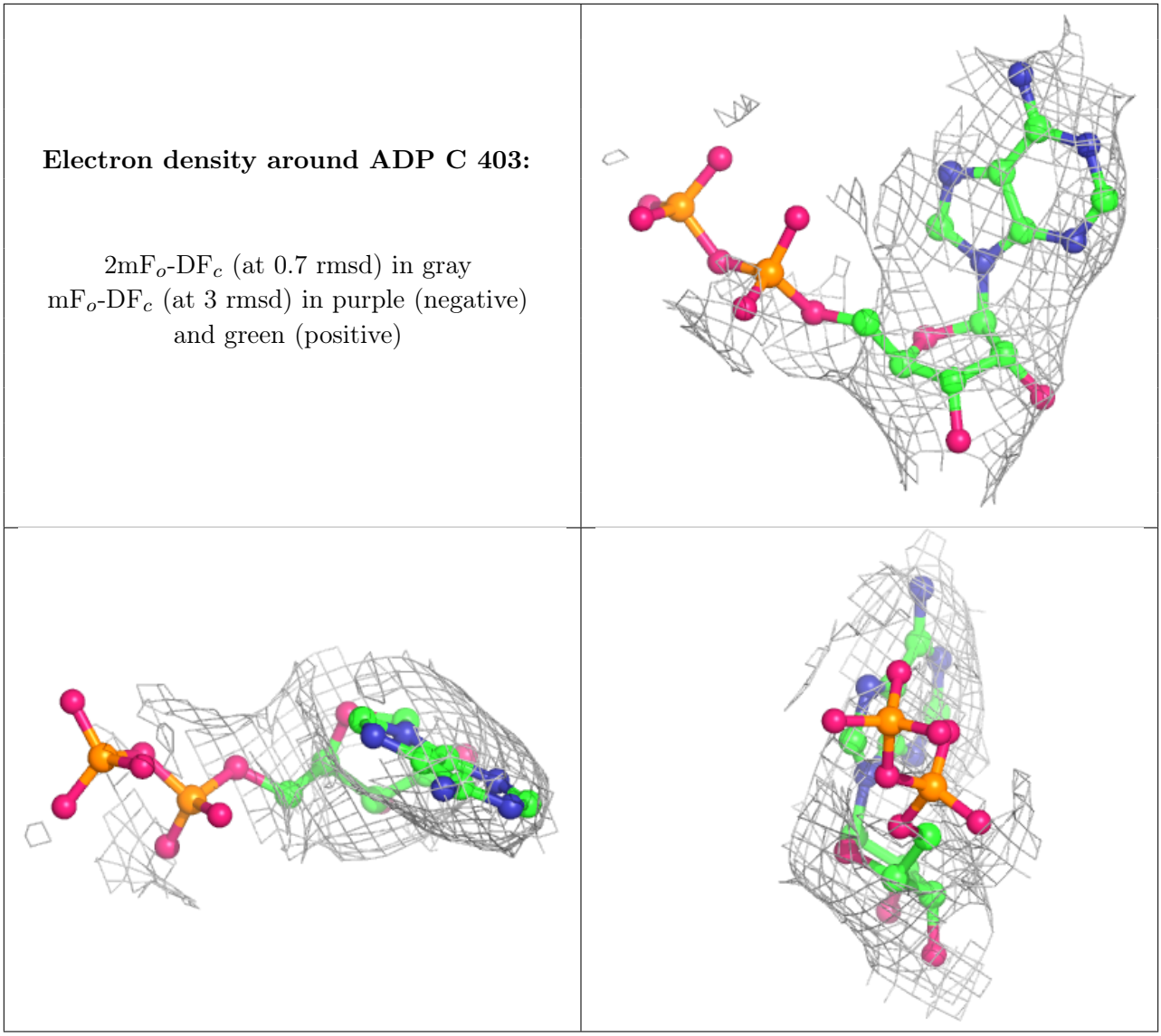






Electron density around ADP C 403:

$2mF_o$-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.