



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 11:34 AM UTC

PDB ID : 4PKN / pdb_00004pkn
Title : Crystal structure of the football-shaped GroEL-GroES2-(ADPBeFx)₁₄ complex containing substrate Rubisco
Authors : Fei, X.; Ye, X.; Laronde-Leblanc, N.; Lorimer, G.H.
Deposited on : 2014-05-15
Resolution : 3.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

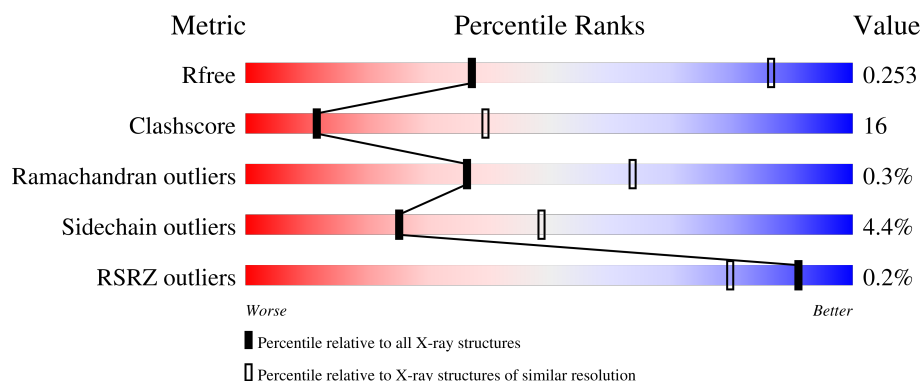
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.66 Å.

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



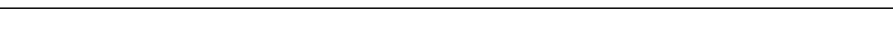
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	

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Mol	Chain	Length	Quality of chain
1	F	548	
1	G	548	
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	
2	1	97	
2	2	97	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	
2	V	97	
2	W	97	
2	X	97	
2	Y	97	
2	Z	97	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BEF	B	602	-	-	X	-
4	BEF	E	602	-	-	X	-
4	BEF	G	602	-	-	X	-
4	BEF	J	602	-	-	X	-
4	BEF	K	602	-	-	X	-
4	BEF	L	602	-	-	X	-
4	BEF	N	602	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 64579 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

- Molecule 2 is a protein called 10 kDa chaperonin.

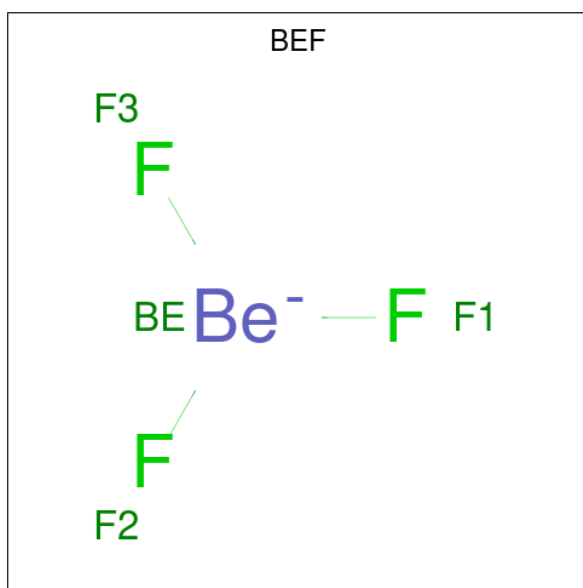
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	P	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	Q	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	U	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	T	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	R	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	S	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	X	95	Total	C	N	O	S	0	0	0
			714	446	125	142	1			
2	W	96	Total	C	N	O	S	0	0	0
			719	449	126	143	1			
2	V	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Y	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Z	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	2	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	1	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total 4	Be 1	F 3	0	0
4	A	1	Total 4	Be 1	F 3	0	0
4	B	1	Total 4	Be 1	F 3	0	0
4	F	1	Total 4	Be 1	F 3	0	0
4	E	1	Total 4	Be 1	F 3	0	0
4	C	1	Total 4	Be 1	F 3	0	0
4	D	1	Total 4	Be 1	F 3	0	0
4	K	1	Total 4	Be 1	F 3	0	0
4	J	1	Total 4	Be 1	F 3	0	0
4	I	1	Total 4	Be 1	F 3	0	0
4	L	1	Total 4	Be 1	F 3	0	0
4	M	1	Total 4	Be 1	F 3	0	0
4	H	1	Total 4	Be 1	F 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	N	1	Total	Be	F	0	0
			4	1	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	N	1	Total	Mg	0	0
			1	1		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	K	0	0
			1	1		
6	A	1	Total	K	0	0
			1	1		

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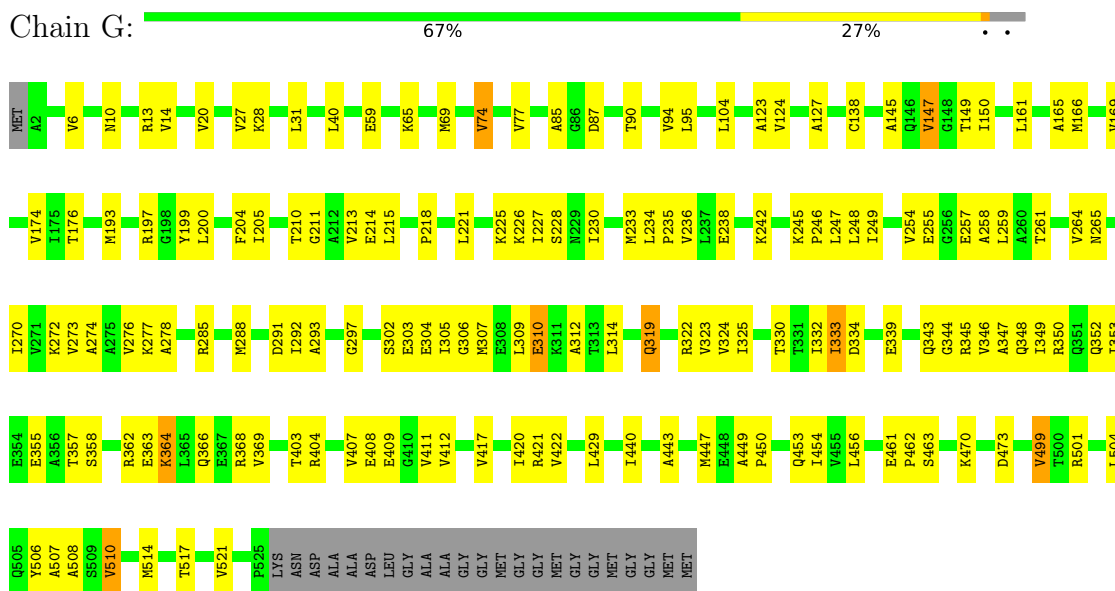
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	K 1	0	0
6	F	1	Total 1	K 1	0	0
6	E	1	Total 1	K 1	0	0
6	C	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	K	1	Total 1	K 1	0	0
6	J	1	Total 1	K 1	0	0
6	I	1	Total 1	K 1	0	0
6	L	1	Total 1	K 1	0	0
6	M	1	Total 1	K 1	0	0
6	H	1	Total 1	K 1	0	0
6	N	1	Total 1	K 1	0	0

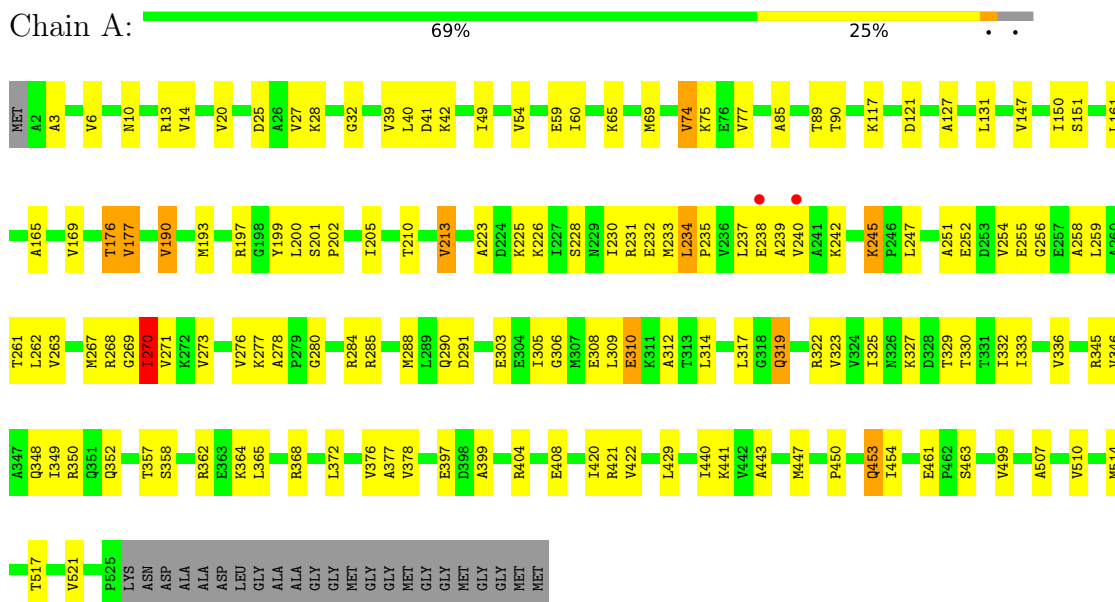
3 Residue-property plots

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

• Molecule 1: 60 kDa chaperonin

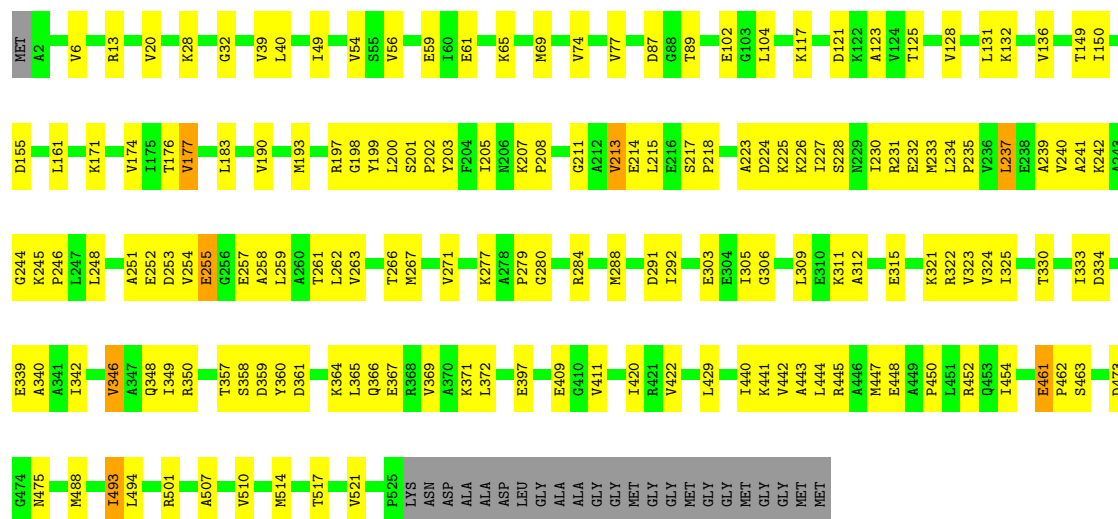


• Molecule 1: 60 kDa chaperonin



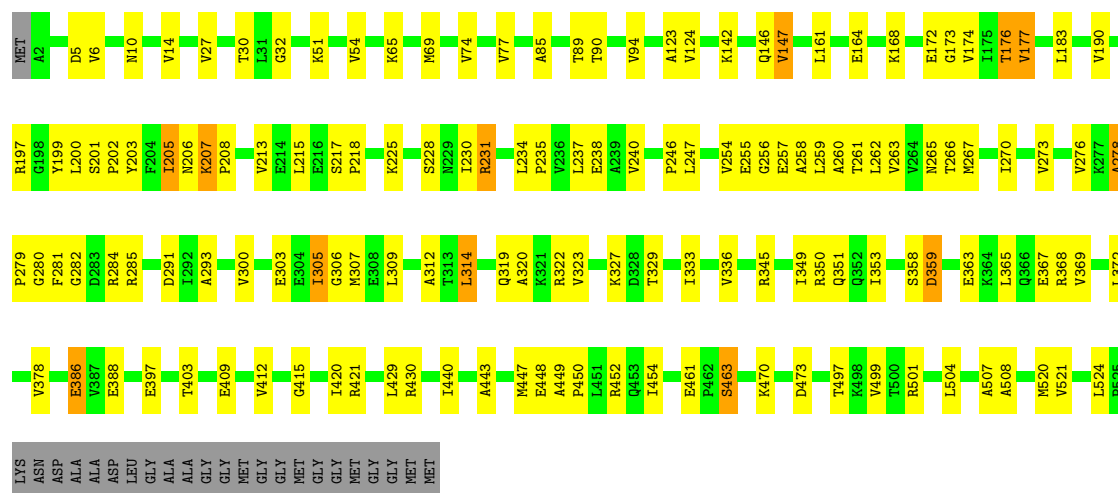
- Molecule 1: 60 kDa chaperonin

Chain B:  66% 28%



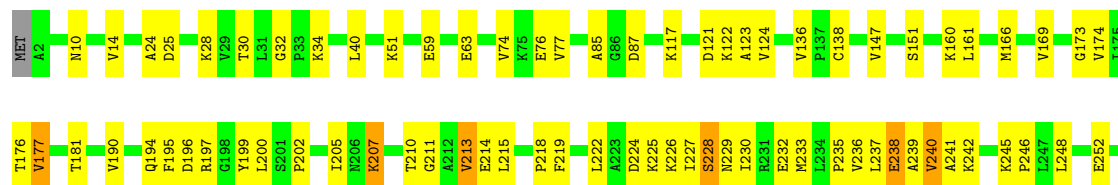
- Molecule 1: 60 kDa chaperonin

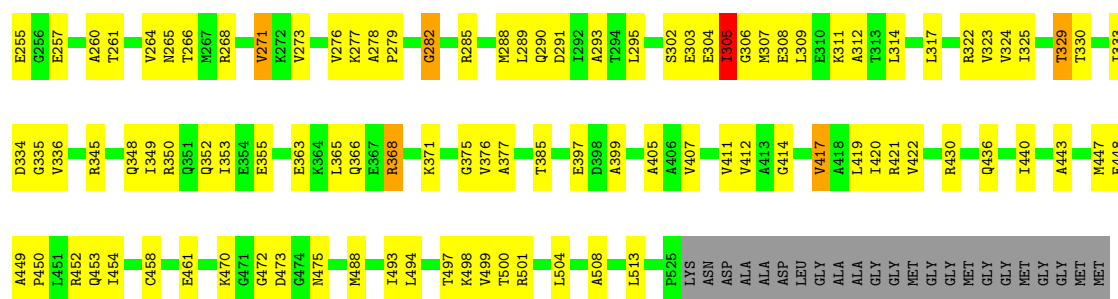
Chain F:  69% 24%



- Molecule 1: 60 kDa chaperonin

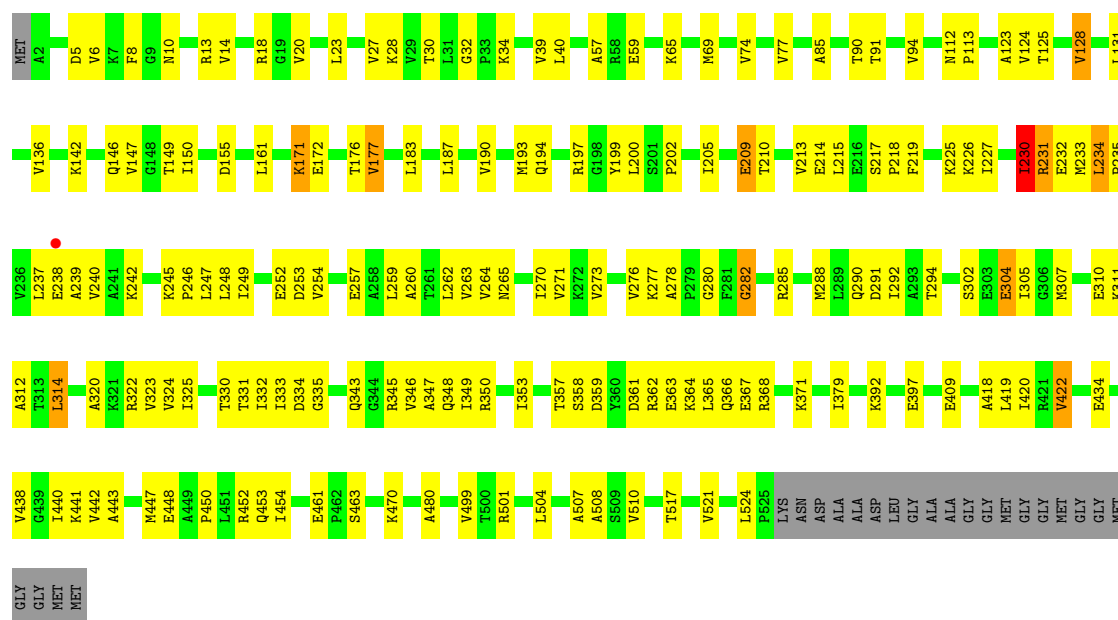
Chain E:  64% 30%





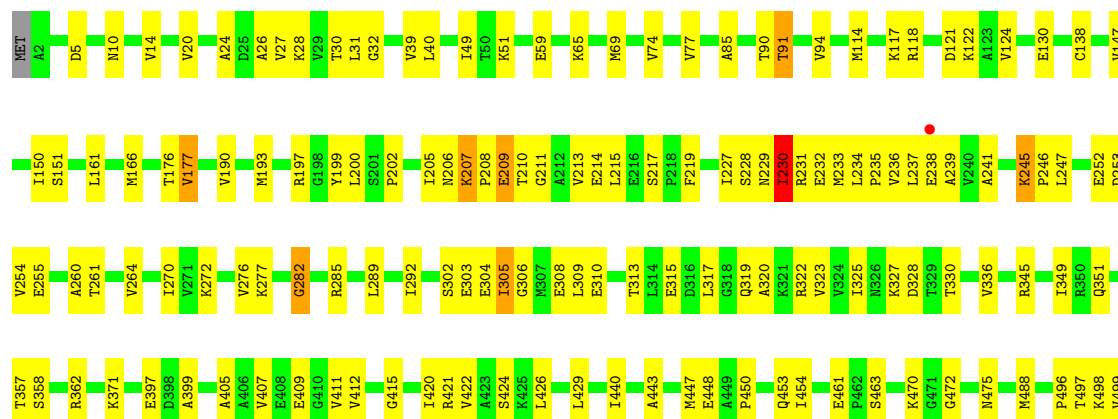
• Molecule 1: 60 kDa chaperonin

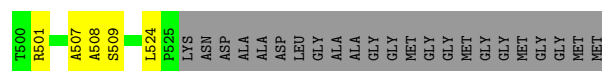
Chain C: 63% 30%



• Molecule 1: 60 kDa chaperonin

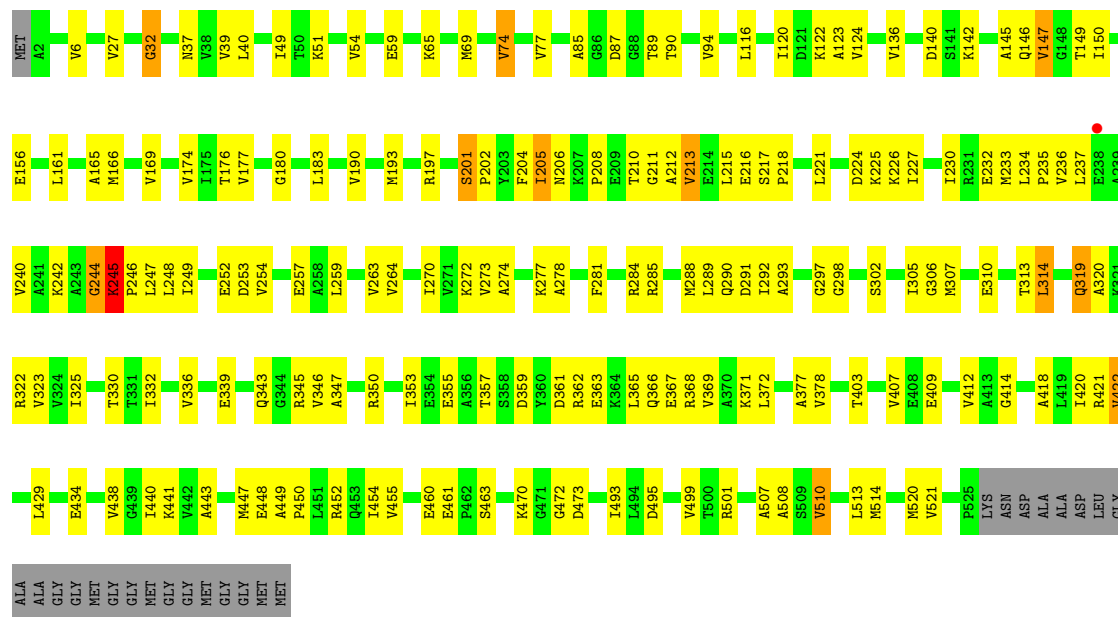
Chain D: 68% 26%





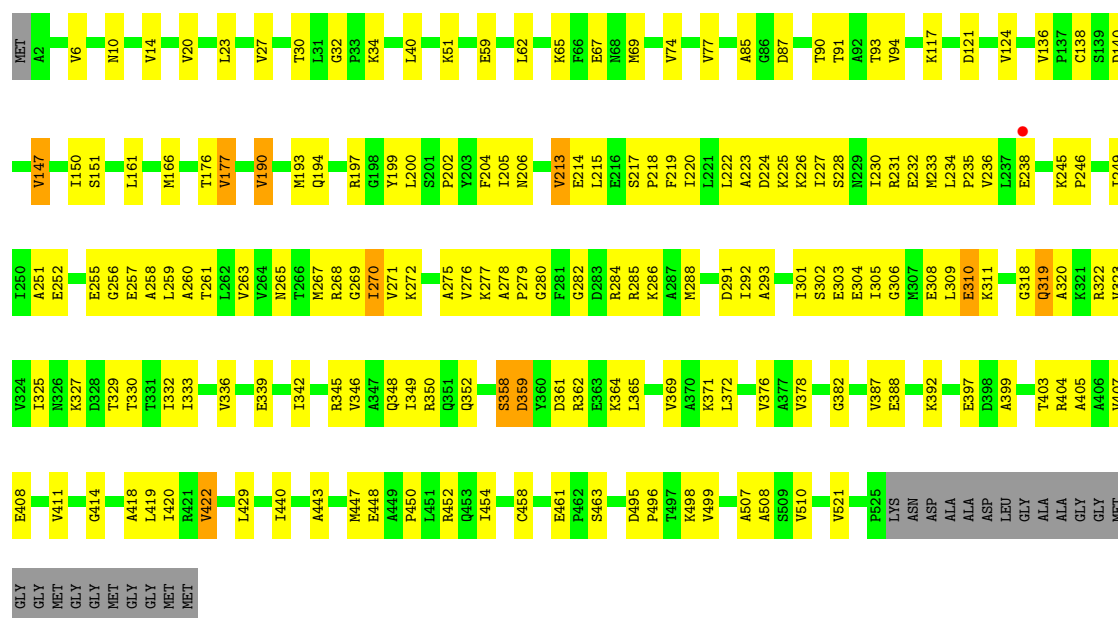
- Molecule 1: 60 kDa chaperonin

Chain K: 63% 30%



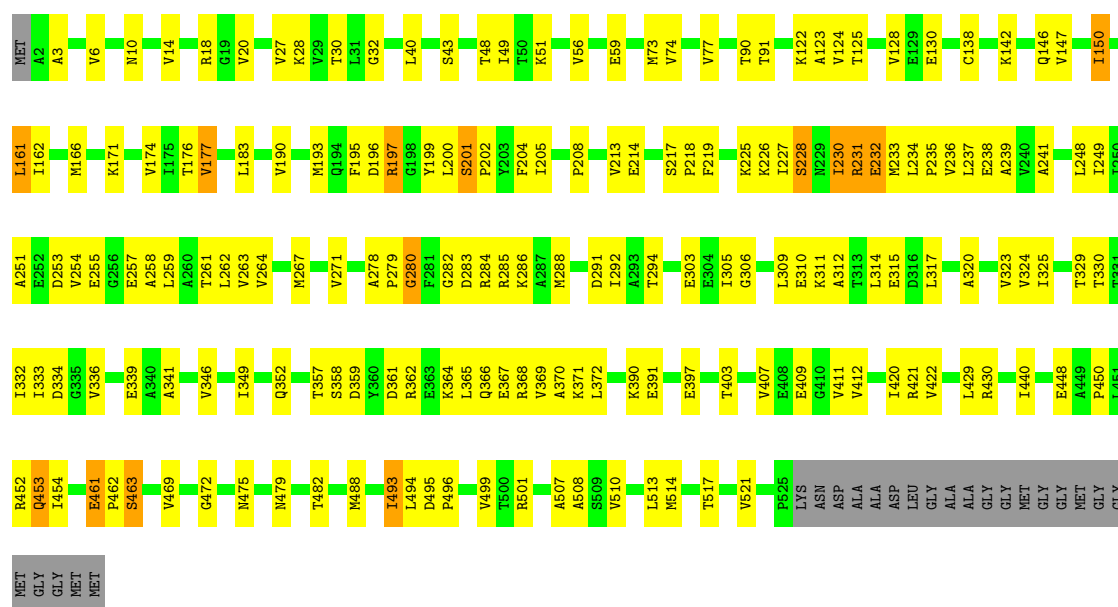
- Molecule 1: 60 kDa chaperonin

Chain J: 63% 31%



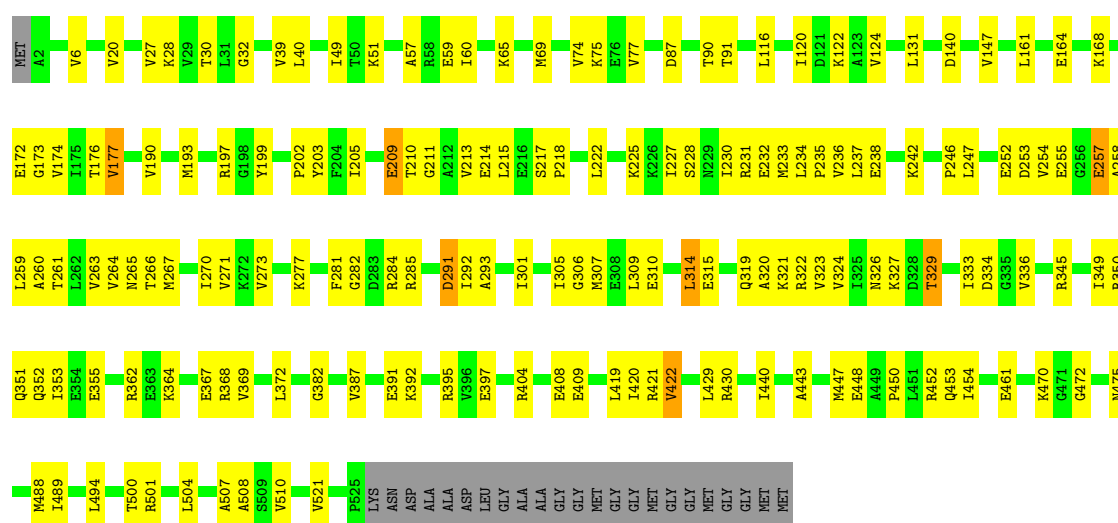
- Molecule 1: 60 kDa chaperonin

Chain I:  63% 30%



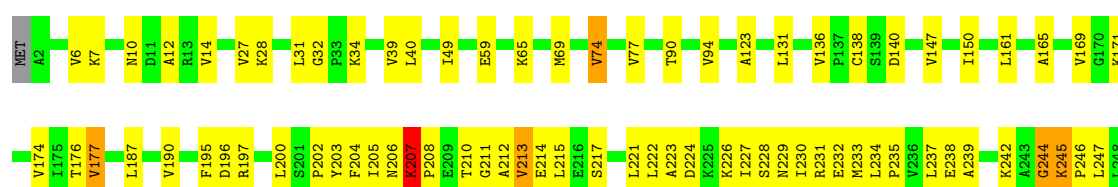
• Molecule 1: 60 kDa chaperonin

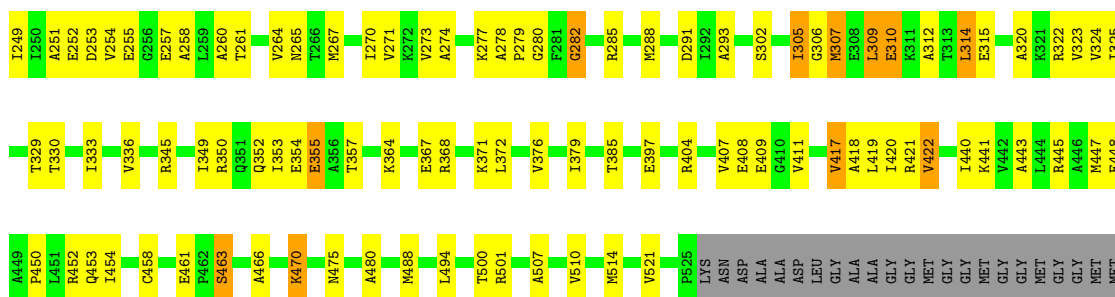
Chain L:  66% 28%



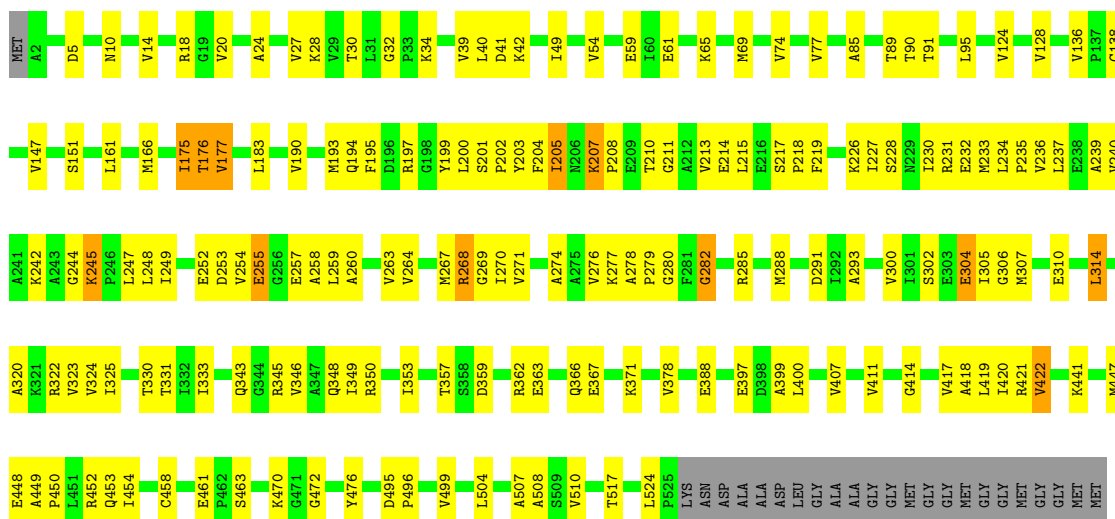
• Molecule 1: 60 kDa chaperonin

Chain M:  64% 28%

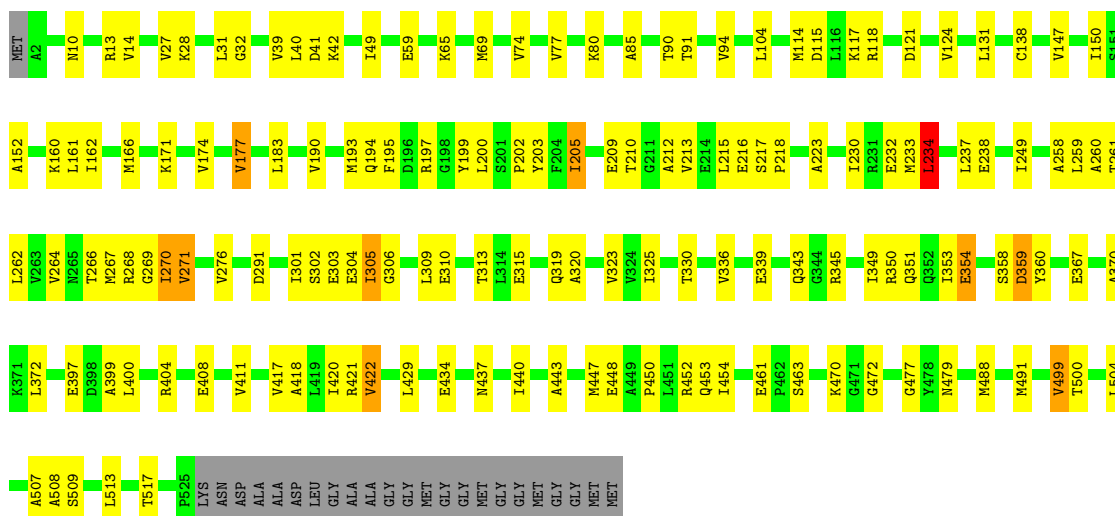




- Molecule 1: 60 kDa chaperonin



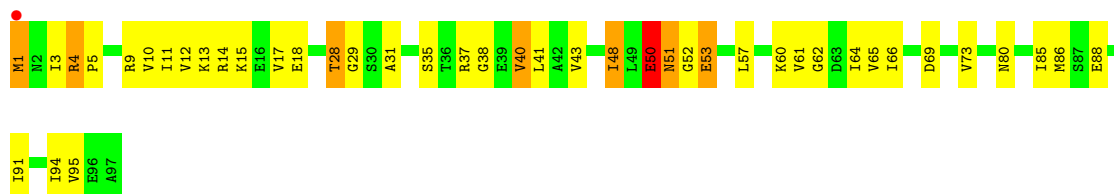
- Molecule 1: 60 kDa chaperonin



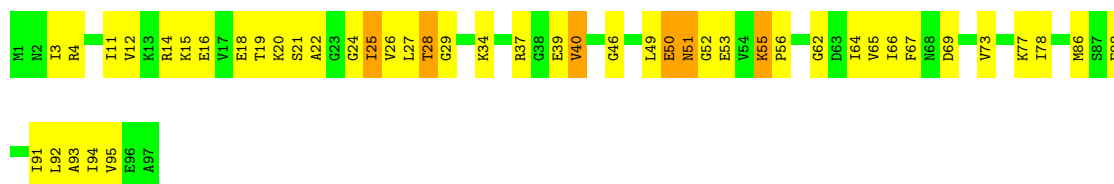
- Molecule 2: 10 kDa chaperonin



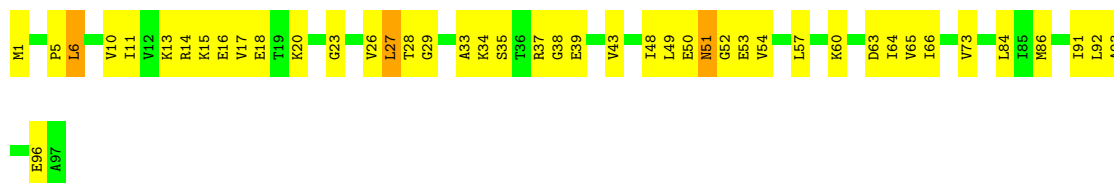
- Molecule 2: 10 kDa chaperonin



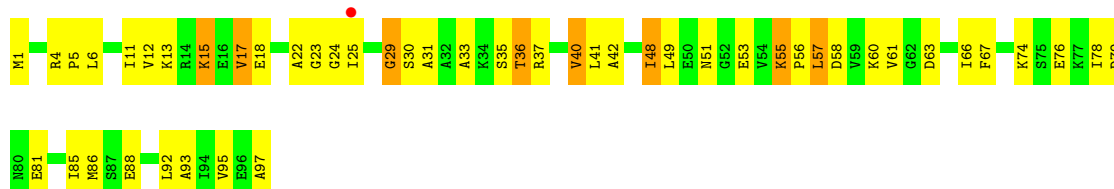
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin

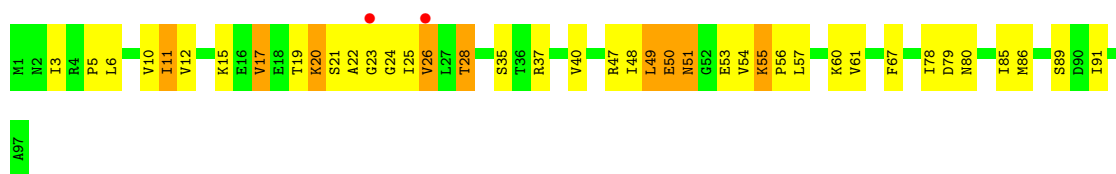


- Molecule 2: 10 kDa chaperonin

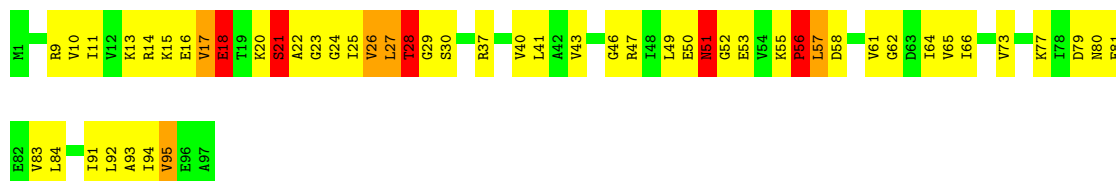


- Molecule 2: 10 kDa chaperonin

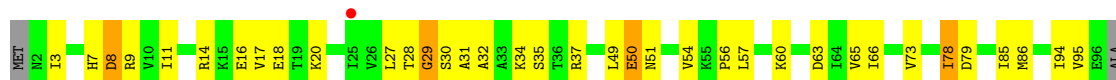




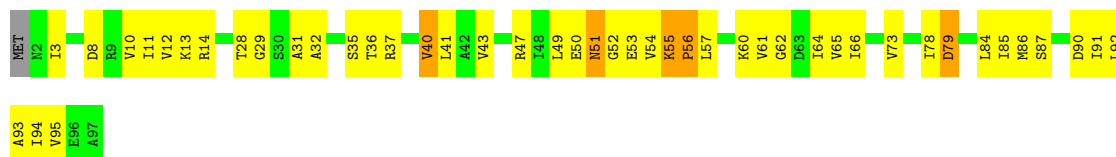
- Molecule 2: 10 kDa chaperonin



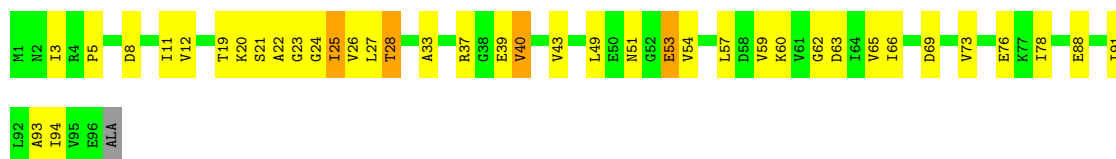
- Molecule 2: 10 kDa chaperonin



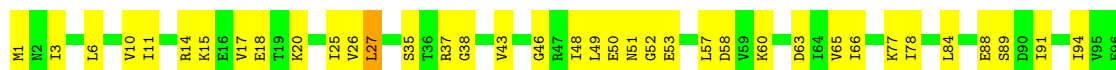
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin

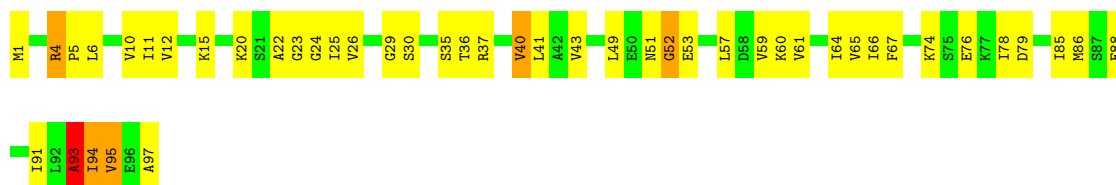


- Molecule 2: 10 kDa chaperonin

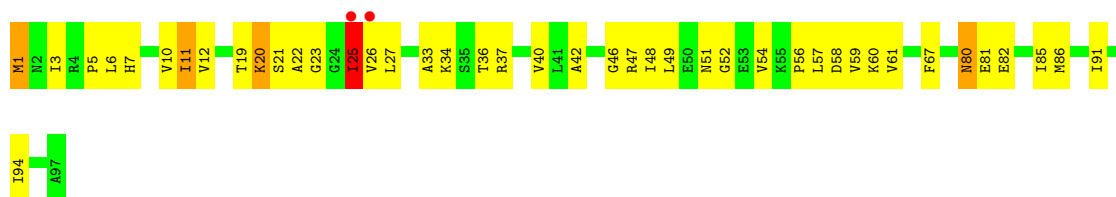


ALA

- Molecule 2: 10 kDa chaperonin

Chain Z:  53% 41% 5% •

- Molecule 2: 10 kDa chaperonin

Chain 2:  2% 56% 39% • •

- Molecule 2: 10 kDa chaperonin

Chain 1:  52% 43% 5%

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.95Å 173.65Å 411.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.19 – 3.66 122.19 – 3.66	Depositor EDS
% Data completeness (in resolution range)	99.5 (122.19-3.66) 99.6 (122.19-3.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.188 , 0.241 0.198 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	87.5	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 93.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.190 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	64579	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	0/3883	0.90	6/5243 (0.1%)
1	B	0.43	0/3883	0.88	11/5243 (0.2%)
1	C	0.46	0/3883	0.93	8/5243 (0.2%)
1	D	0.48	0/3883	0.92	8/5243 (0.2%)
1	E	0.46	0/3883	0.91	6/5243 (0.1%)
1	F	0.47	0/3883	0.91	12/5243 (0.2%)
1	G	0.48	0/3883	0.88	3/5243 (0.1%)
1	H	0.46	0/3883	0.92	9/5243 (0.2%)
1	I	0.43	0/3883	0.91	9/5243 (0.2%)
1	J	0.45	0/3883	0.90	4/5243 (0.1%)
1	K	0.46	0/3883	0.93	11/5243 (0.2%)
1	L	0.45	0/3883	0.89	5/5243 (0.1%)
1	M	0.45	0/3883	0.95	12/5243 (0.2%)
1	N	0.48	0/3883	0.92	7/5243 (0.1%)
2	1	0.44	0/731	1.04	2/983 (0.2%)
2	2	0.44	0/731	1.06	6/983 (0.6%)
2	O	0.42	0/731	1.07	4/983 (0.4%)
2	P	0.47	0/731	1.12	6/983 (0.6%)
2	Q	0.43	0/731	1.10	6/983 (0.6%)
2	R	0.44	0/731	1.14	6/983 (0.6%)
2	S	0.55	0/731	1.24	7/983 (0.7%)
2	T	0.42	0/731	1.12	7/983 (0.7%)
2	U	0.40	0/731	0.96	0/983
2	V	0.38	0/726	1.02	5/976 (0.5%)
2	W	0.44	0/723	1.06	1/973 (0.1%)
2	X	0.47	0/718	0.98	1/966 (0.1%)
2	Y	0.41	0/726	1.06	0/976
2	Z	0.42	0/731	1.10	6/983 (0.6%)
All	All	0.46	0/64565	0.94	168/87123 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
1	K	0	1
2	2	0	1
2	O	0	1
2	P	0	1
2	Q	0	1
2	S	0	4
2	T	0	1
2	W	0	1
2	X	0	1
2	Z	0	1
All	All	0	15

There are no bond length outliers.

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	227	ILE	N-CA-C	-10.46	102.60	111.91
1	H	282	GLY	N-CA-C	10.28	125.08	112.64
1	H	245	LYS	N-CA-C	10.14	120.02	108.25
1	C	282	GLY	N-CA-C	9.37	123.98	112.64
1	D	245	LYS	N-CA-C	8.78	118.23	108.14
2	Q	46	GLY	N-CA-C	8.32	121.88	110.56
1	E	282	GLY	N-CA-C	8.20	122.56	112.64
1	I	32	GLY	CA-C-N	8.11	127.69	118.85
1	I	32	GLY	C-N-CA	8.11	127.69	118.85
1	J	32	GLY	CA-C-N	7.95	127.62	119.19
1	J	32	GLY	C-N-CA	7.95	127.62	119.19
1	A	245	LYS	N-CA-C	7.74	115.10	108.13
1	C	231	ARG	N-CA-C	-7.62	103.08	112.38
1	F	358	SER	CB-CA-C	-7.35	108.09	116.54
1	K	201	SER	CA-C-N	7.22	127.38	119.87
1	K	201	SER	C-N-CA	7.22	127.38	119.87
1	M	282	GLY	N-CA-C	7.21	121.36	112.64
2	2	25	ILE	N-CA-C	7.20	118.39	108.89
1	I	231	ARG	N-CA-C	-7.13	104.14	112.92
1	N	234	LEU	N-CA-C	7.11	122.49	113.25
2	X	16	GLU	CB-CA-C	-7.08	108.42	116.63
1	F	358	SER	N-CA-C	7.06	119.04	108.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	282	GLY	N-CA-C	7.01	121.12	112.64
2	P	48	ILE	N-CA-C	6.96	118.93	107.24
2	2	52	GLY	N-CA-C	-6.88	96.87	113.18
2	R	17	VAL	N-CA-C	6.86	119.62	112.83
2	P	4	ARG	CA-C-N	6.86	126.78	119.85
2	P	4	ARG	C-N-CA	6.86	126.78	119.85
2	V	54	VAL	N-CA-C	6.81	117.44	107.37
1	K	347	ALA	N-CA-C	6.79	118.76	111.36
1	C	210	THR	N-CA-C	-6.76	105.06	113.38
1	H	32	GLY	CA-C-N	6.75	126.35	119.19
1	H	32	GLY	C-N-CA	6.75	126.35	119.19
1	M	245	LYS	N-CA-C	6.72	114.18	108.13
2	1	23	GLY	N-CA-C	-6.66	106.56	115.21
1	C	304	GLU	N-CA-C	-6.65	105.04	113.02
2	V	25	ILE	N-CA-C	6.59	118.56	111.58
1	B	201	SER	CA-C-N	6.59	126.21	119.56
1	B	201	SER	C-N-CA	6.59	126.21	119.56
2	V	53	GLU	N-CA-C	6.55	116.71	108.45
1	F	278	ALA	CA-C-N	6.55	126.32	119.05
1	F	278	ALA	C-N-CA	6.55	126.32	119.05
2	Q	55	LYS	CA-C-N	6.50	126.19	119.82
2	Q	55	LYS	C-N-CA	6.50	126.19	119.82
1	K	32	GLY	CA-C-N	6.47	126.05	119.19
1	K	32	GLY	C-N-CA	6.47	126.05	119.19
2	S	27	LEU	N-CA-C	6.46	118.86	111.11
1	L	282	GLY	N-CA-C	6.45	120.45	112.64
1	B	32	GLY	CA-C-N	6.45	125.88	118.85
1	B	32	GLY	C-N-CA	6.45	125.88	118.85
2	Z	93	ALA	CB-CA-C	-6.41	107.44	115.89
1	I	230	ILE	N-CA-C	6.40	116.61	106.88
1	I	43	SER	N-CA-C	6.38	117.89	111.07
1	K	205	ILE	N-CA-C	6.38	117.98	109.37
1	D	32	GLY	CA-C-N	6.33	125.74	118.85
1	D	32	GLY	C-N-CA	6.33	125.74	118.85
1	E	207	LYS	CA-C-N	-6.30	113.79	120.03
1	E	207	LYS	C-N-CA	-6.30	113.79	120.03
1	N	305	ILE	N-CA-C	-6.27	101.17	108.82
2	R	49	LEU	N-CA-C	6.25	119.31	108.76
2	O	16	GLU	CB-CA-C	-6.23	107.62	116.34
2	S	21	SER	N-CA-C	6.21	118.58	108.76
2	T	55	LYS	CA-C-N	6.18	126.51	119.83
2	T	55	LYS	C-N-CA	6.18	126.51	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	309	LEU	N-CA-C	6.17	118.01	111.28
1	M	244	GLY	N-CA-C	6.17	127.79	113.18
2	S	55	LYS	CA-C-N	6.15	127.80	120.23
2	S	55	LYS	C-N-CA	6.15	127.80	120.23
1	M	32	GLY	CA-C-N	6.12	125.67	119.19
1	M	32	GLY	C-N-CA	6.12	125.67	119.19
1	F	173	GLY	N-CA-C	6.11	119.05	112.33
1	G	347	ALA	N-CA-C	6.10	118.01	111.36
1	J	310	GLU	N-CA-C	6.09	118.00	111.36
2	P	51	ASN	CA-C-N	6.07	132.62	121.70
2	P	51	ASN	C-N-CA	6.07	132.62	121.70
1	M	207	LYS	CA-C-N	-6.02	114.07	120.03
1	M	207	LYS	C-N-CA	-6.02	114.07	120.03
1	A	234	LEU	N-CA-C	6.02	120.94	112.75
1	E	32	GLY	CA-C-N	6.00	125.39	118.85
1	E	32	GLY	C-N-CA	6.00	125.39	118.85
2	S	51	ASN	N-CA-C	5.96	122.57	113.51
2	2	7	HIS	CB-CA-C	-5.96	109.68	116.54
1	D	207	LYS	CA-C-N	-5.91	112.45	119.84
1	D	207	LYS	C-N-CA	-5.91	112.45	119.84
2	R	20	LYS	CA-C-N	5.91	132.34	121.70
2	R	20	LYS	C-N-CA	5.91	132.34	121.70
1	N	205	ILE	N-CA-C	5.90	116.90	108.93
1	I	232	GLU	N-CA-C	-5.90	104.98	111.82
1	B	340	ALA	N-CA-C	-5.89	104.77	111.07
1	C	32	GLY	CA-C-N	5.88	125.42	119.19
1	C	32	GLY	C-N-CA	5.88	125.42	119.19
1	F	32	GLY	CA-C-N	5.86	125.24	118.85
1	F	32	GLY	C-N-CA	5.86	125.24	118.85
1	D	234	LEU	N-CA-C	5.84	120.69	112.75
1	M	280	GLY	N-CA-C	5.84	119.80	112.79
2	Z	93	ALA	N-CA-C	5.80	118.76	109.02
1	B	280	GLY	N-CA-C	5.79	119.74	112.79
2	S	18	GLU	N-CA-C	5.79	117.81	107.80
1	J	246	PRO	N-CA-C	5.72	119.60	110.40
1	N	269	GLY	N-CA-C	-5.69	106.89	115.32
2	T	48	ILE	N-CA-C	5.68	116.31	107.28
2	Q	25	ILE	N-CA-C	5.66	117.58	111.58
1	G	310	GLU	N-CA-C	-5.63	105.14	111.28
1	I	280	GLY	N-CA-C	5.63	119.55	112.79
2	W	32	ALA	N-CA-C	-5.62	104.33	110.91
1	D	282	GLY	N-CA-C	5.59	119.41	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	234	LEU	N-CA-C	5.59	120.35	112.75
2	O	7	HIS	CB-CA-C	-5.57	110.17	116.63
1	K	211	GLY	N-CA-C	-5.55	101.80	111.62
2	Q	51	ASN	N-CA-C	-5.54	104.42	110.91
1	K	245	LYS	CA-C-N	-5.52	112.94	119.84
1	K	245	LYS	C-N-CA	-5.52	112.94	119.84
1	A	32	GLY	CA-C-N	5.50	125.02	119.19
1	A	32	GLY	C-N-CA	5.50	125.02	119.19
2	Q	14	ARG	N-CA-C	5.49	117.64	109.25
2	1	54	VAL	N-CA-C	5.47	114.62	106.85
1	B	346	VAL	N-CA-C	-5.46	105.21	110.72
1	L	32	GLY	CA-C-N	5.45	124.79	118.85
1	L	32	GLY	C-N-CA	5.45	124.79	118.85
1	N	32	GLY	CA-C-N	5.45	124.78	118.85
1	N	32	GLY	C-N-CA	5.45	124.78	118.85
2	P	53	GLU	CB-CA-C	-5.43	109.84	117.23
2	T	29	GLY	N-CA-C	5.42	118.83	111.72
2	O	16	GLU	N-CA-C	5.40	115.99	108.00
1	N	359	ASP	CB-CA-C	-5.39	109.89	117.23
1	F	207	LYS	CA-C-N	5.37	125.37	120.21
1	F	207	LYS	C-N-CA	5.37	125.37	120.21
1	M	229	ASN	N-CA-C	-5.36	106.59	113.02
2	V	51	ASN	N-CA-C	-5.35	106.60	113.02
1	E	305	ILE	N-CA-C	5.33	120.42	109.34
1	G	344	GLY	N-CA-C	-5.31	106.36	112.73
1	H	201	SER	CA-C-N	5.31	124.92	119.56
1	H	201	SER	C-N-CA	5.31	124.92	119.56
2	Z	94	ILE	N-CA-C	5.31	116.37	108.46
2	Z	52	GLY	N-CA-C	-5.31	100.61	113.18
1	A	310	GLU	N-CA-C	5.30	116.86	111.14
1	K	180	GLY	N-CA-C	5.29	125.71	113.18
1	C	358	SER	CB-CA-C	-5.28	110.04	117.23
1	D	305	ILE	N-CA-C	-5.28	102.38	108.82
2	R	55	LYS	CA-C-N	5.28	125.53	119.83
2	R	55	LYS	C-N-CA	5.28	125.53	119.83
1	L	60	ILE	N-CA-C	5.24	116.13	108.58
2	T	23	GLY	N-CA-C	-5.22	108.63	115.47
1	B	28	LYS	N-CA-C	5.21	116.96	111.28
1	K	244	GLY	N-CA-C	5.21	124.67	115.61
1	B	207	LYS	CA-C-N	-5.20	115.22	120.21
1	B	207	LYS	C-N-CA	-5.20	115.22	120.21
1	H	207	LYS	CA-C-N	5.20	125.28	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	207	LYS	C-N-CA	5.20	125.28	119.87
1	M	258	ALA	N-CA-C	-5.19	105.07	111.40
1	F	205	ILE	N-CA-C	5.18	116.37	109.37
2	2	81	GLU	N-CA-C	5.17	117.59	108.75
1	C	234	LEU	N-CA-C	5.17	121.23	109.81
2	S	56	PRO	N-CA-C	5.14	118.58	110.50
2	Z	4	ARG	CA-C-N	5.13	125.41	119.92
2	Z	4	ARG	C-N-CA	5.13	125.41	119.92
2	V	23	GLY	N-CA-C	-5.12	108.83	115.59
2	T	36	THR	N-CA-C	-5.12	106.81	113.16
1	L	173	GLY	N-CA-C	5.09	117.93	112.33
2	O	17	VAL	N-CA-C	5.09	115.37	107.28
1	I	201	SER	CA-C-N	5.09	125.16	119.87
1	I	201	SER	C-N-CA	5.09	125.16	119.87
2	2	20	LYS	CA-C-N	5.08	130.84	121.70
2	2	20	LYS	C-N-CA	5.08	130.84	121.70
1	A	210	THR	N-CA-C	-5.05	106.41	112.58
1	B	244	GLY	N-CA-C	5.04	122.25	115.00
2	T	78	ILE	N-CA-C	-5.01	101.43	109.20
1	F	305	ILE	N-CA-C	-5.00	102.72	108.82

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	56	PRO	Peptide
1	E	228	SER	Peptide
1	E	305	ILE	Peptide
1	K	208	PRO	Peptide
2	O	29	GLY	Peptide
2	P	50	GLU	Peptide
2	Q	51	ASN	Peptide
2	S	18	GLU	Peptide
2	S	28	THR	Peptide
2	S	51	ASN	Peptide
2	S	56	PRO	Peptide
2	T	15	LYS	Peptide
2	W	56	PRO	Peptide
2	X	29	GLY	Peptide
2	Z	93	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3974	112	0
1	B	3855	0	3976	124	0
1	C	3855	0	3975	130	0
1	D	3855	0	3976	108	0
1	E	3855	0	3976	135	0
1	F	3855	0	3975	100	0
1	G	3855	0	3975	119	0
1	H	3855	0	3976	129	0
1	I	3855	0	3975	133	0
1	J	3855	0	3975	137	0
1	K	3855	0	3974	128	0
1	L	3855	0	3975	111	0
1	M	3855	0	3975	133	0
1	N	3855	0	3976	98	0
2	1	727	0	762	43	0
2	2	727	0	762	43	0
2	O	727	0	762	24	0
2	P	727	0	762	43	0
2	Q	727	0	762	40	0
2	R	727	0	762	34	0
2	S	727	0	762	60	0
2	T	727	0	762	40	0
2	U	727	0	762	43	0
2	V	722	0	757	27	0
2	W	719	0	750	38	0
2	X	714	0	745	19	0
2	Y	722	0	757	28	0
2	Z	727	0	762	37	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	3	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
3	G	27	0	12	2	0
3	H	27	0	12	2	0
3	I	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	27	0	12	3	0
3	K	27	0	12	2	0
3	L	27	0	12	2	0
3	M	27	0	12	3	0
3	N	27	0	12	2	0
4	A	4	0	0	0	0
4	B	4	0	0	3	0
4	C	4	0	0	1	0
4	D	4	0	0	1	0
4	E	4	0	0	2	0
4	F	4	0	0	1	0
4	G	4	0	0	3	0
4	H	4	0	0	1	0
4	I	4	0	0	1	0
4	J	4	0	0	2	0
4	K	4	0	0	2	0
4	L	4	0	0	2	0
4	M	4	0	0	1	0
4	N	4	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
All	All	64579	0	66450	2087	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 (2087) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LYS:HG2	1:C:252:GLU:HG2	1.39	1.03
1:C:239:ALA:HA	2:Q:25:ILE:HD11	1.43	1.01
1:E:238:GLU:HB2	2:S:22:ALA:HB1	1.45	0.97
2:S:28:THR:HG22	2:S:29:GLY:HA3	1.49	0.94
1:B:291:ASP:HB3	1:B:372:LEU:HD21	1.50	0.93
2:X:18:GLU:HB3	2:X:28:THR:HB	1.52	0.92
1:G:234:LEU:HD13	1:G:309:LEU:HB2	1.51	0.91
1:J:200:LEU:HD11	1:J:277:LYS:HG3	1.54	0.88
1:D:205:ILE:HG22	1:D:207:LYS:H	1.39	0.87
2:V:20:LYS:HG3	2:V:28:THR:HG23	1.56	0.87
1:K:236:VAL:HG13	1:K:237:LEU:HD12	1.56	0.86
2:S:46:GLY:HA2	2:S:57:LEU:HG	1.59	0.85
1:I:231:ARG:HH12	2:W:31:ALA:HB2	1.40	0.85
1:L:205:ILE:HA	1:L:213:VAL:HG22	1.59	0.85
1:F:237:LEU:HD21	1:F:312:ALA:HB3	1.60	0.83
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.59	0.83
2:O:37:ARG:HG2	2:O:66:ILE:HG12	1.61	0.83
1:N:205:ILE:HA	1:N:213:VAL:HG22	1.60	0.82
2:2:48:ILE:HG12	2:2:54:VAL:HG12	1.59	0.82
1:L:284:ARG:HB3	1:L:364:LYS:HE2	1.62	0.82
2:Z:65:VAL:HG12	2:Z:94:ILE:HG22	1.61	0.82
1:C:227:ILE:HD11	1:C:254:VAL:HG22	1.59	0.82
1:C:367:GLU:HG2	1:C:371:LYS:HE2	1.62	0.82
1:M:231:ARG:HD3	1:M:261:THR:HG21	1.61	0.81
2:1:37:ARG:HG2	2:1:66:ILE:HG22	1.62	0.81
2:S:50:GLU:O	2:S:51:ASN:ND2	2.12	0.81
2:2:20:LYS:HD3	2:2:22:ALA:HB2	1.60	0.81
1:I:294:THR:HB	1:I:341:ALA:HB1	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ALA:HB1	1:B:271:VAL:HG11	1.62	0.81
1:J:228:SER:HB2	1:J:255:GLU:HB3	1.62	0.81
1:D:228:SER:HB2	1:D:255:GLU:HB2	1.61	0.80
1:I:197:ARG:HH11	1:I:279:PRO:HG3	1.47	0.80
2:R:48:ILE:HG12	2:R:54:VAL:HG12	1.63	0.80
2:S:37:ARG:HG2	2:S:66:ILE:HG22	1.64	0.80
1:G:358:SER:HA	1:G:362:ARG:HE	1.46	0.79
1:N:232:GLU:HG2	1:N:309:LEU:HB3	1.63	0.79
1:C:322:ARG:HB3	1:C:333:ILE:HD12	1.65	0.78
2:2:20:LYS:HA	2:2:21:SER:HB3	1.65	0.78
1:C:278:ALA:HB3	1:C:285:ARG:HD2	1.64	0.78
2:R:78:ILE:HG13	2:R:79:ASP:H	1.48	0.77
1:G:234:LEU:HD21	1:G:310:GLU:HG3	1.64	0.77
1:G:350:ARG:HA	1:G:353:ILE:HG12	1.67	0.77
1:L:420:ILE:HD13	1:L:448:GLU:HG2	1.67	0.77
2:S:15:LYS:HG3	2:S:16:GLU:H	1.50	0.77
2:1:79:ASP:O	2:1:80:ASN:ND2	2.14	0.77
1:M:350:ARG:HA	1:M:353:ILE:HG23	1.68	0.76
1:A:200:LEU:HD11	1:A:277:LYS:HG3	1.65	0.76
2:T:35:SER:OG	2:T:37:ARG:O	2.04	0.76
1:M:411:VAL:HG21	1:M:494:LEU:HD23	1.67	0.76
2:W:50:GLU:O	2:W:51:ASN:ND2	2.19	0.76
1:D:420:ILE:HD13	1:D:448:GLU:HG2	1.67	0.76
1:E:322:ARG:HB3	1:E:333:ILE:HD12	1.68	0.76
1:G:261:THR:O	1:G:265:ASN:ND2	2.17	0.76
2:S:22:ALA:HB2	2:S:25:ILE:H	1.51	0.75
2:2:20:LYS:HB3	2:2:22:ALA:N	2.00	0.75
1:I:411:VAL:HG21	1:I:494:LEU:HD23	1.68	0.75
1:H:322:ARG:HB3	1:H:333:ILE:HD12	1.68	0.75
1:E:304:GLU:C	1:E:306:GLY:HA2	2.12	0.74
2:T:5:PRO:HB3	2:T:11:ILE:HG23	1.67	0.74
1:I:214:GLU:HG2	1:I:324:VAL:HG22	1.69	0.74
1:H:230:ILE:HG22	1:H:257:GLU:HG3	1.69	0.74
1:K:357:THR:HG22	1:K:359:ASP:HB2	1.67	0.74
2:Z:91:ILE:HG22	2:Z:93:ALA:H	1.51	0.74
2:Q:37:ARG:HG2	2:Q:66:ILE:HG12	1.69	0.74
1:I:226:LYS:HE3	1:I:253:ASP:HB3	1.67	0.74
1:H:278:ALA:HB3	1:H:285:ARG:HD2	1.68	0.74
1:E:228:SER:HA	1:E:255:GLU:HB2	1.68	0.74
1:E:200:LEU:HD11	1:E:277:LYS:HG3	1.68	0.74
1:K:355:GLU:O	1:K:362:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:241:ALA:HA	1:I:271:VAL:HG11	1.69	0.74
1:E:278:ALA:HB3	1:E:285:ARG:HD2	1.70	0.73
2:P:14:ARG:HG2	2:P:35:SER:HB3	1.70	0.73
1:I:174:VAL:HG21	1:I:367:GLU:HA	1.70	0.73
1:I:236:VAL:HG21	1:I:312:ALA:HB3	1.69	0.73
1:A:291:ASP:HB3	1:A:372:LEU:HD21	1.69	0.73
1:B:321:LYS:HB2	1:B:334:ASP:HB2	1.69	0.73
1:D:228:SER:CB	1:D:255:GLU:HB2	2.18	0.73
1:K:242:LYS:HZ2	2:Y:25:ILE:H	1.35	0.73
1:J:495:ASP:OD1	3:J:601:ADP:O2'	2.04	0.73
1:C:448:GLU:OE1	1:C:452:ARG:NH1	2.22	0.73
1:D:358:SER:O	1:D:362:ARG:NH1	2.21	0.73
2:T:57:LEU:HD23	2:T:88:GLU:HB2	1.71	0.73
1:K:205:ILE:HA	1:K:213:VAL:HG12	1.70	0.73
2:2:1:MET:N	2:2:1:MET:SD	2.61	0.73
2:1:25:ILE:HG13	2:1:26:VAL:HG23	1.70	0.73
1:M:227:ILE:HG23	1:M:230:ILE:HB	1.68	0.73
1:K:323:VAL:HG12	1:K:332:ILE:HG12	1.71	0.73
1:G:366:GLN:HA	1:G:369:VAL:HG12	1.69	0.73
1:E:291:ASP:OD1	1:E:345:ARG:NH2	2.21	0.73
1:A:291:ASP:OD1	1:A:345:ARG:NH2	2.22	0.72
1:B:226:LYS:HG3	1:B:253:ASP:HB3	1.72	0.72
1:B:228:SER:HA	1:B:255:GLU:HB2	1.71	0.72
1:B:333:ILE:HG13	1:B:334:ASP:H	1.54	0.72
1:H:205:ILE:HA	1:H:213:VAL:HG22	1.72	0.72
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.70	0.72
1:K:305:ILE:HG23	1:J:267:MET:HG3	1.70	0.72
1:H:367:GLU:HG2	1:H:371:LYS:HE2	1.72	0.72
2:V:37:ARG:HG2	2:V:66:ILE:HG12	1.71	0.72
2:2:60:LYS:HG2	2:2:61:VAL:H	1.55	0.72
1:C:234:LEU:O	1:C:237:LEU:N	2.21	0.72
2:P:18:GLU:HB2	2:P:28:THR:HB	1.72	0.72
1:H:242:LYS:HE3	1:H:270:ILE:HD11	1.70	0.71
1:N:237:LEU:HD22	2:2:27:LEU:HD11	1.72	0.71
1:C:171:LYS:HG2	1:C:172:GLU:H	1.54	0.71
1:M:325:ILE:HG12	1:M:330:THR:HG23	1.71	0.71
1:K:216:GLU:OE2	1:K:322:ARG:NH1	2.23	0.71
1:H:230:ILE:HA	1:H:257:GLU:HB3	1.72	0.71
1:B:225:LYS:HB2	1:B:303:GLU:HG3	1.73	0.71
2:W:49:LEU:H	2:W:52:GLY:HA2	1.55	0.71
2:W:53:GLU:HG3	2:W:54:VAL:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:64:ILE:HG23	2:1:95:VAL:HG13	1.70	0.71
2:X:17:VAL:HG23	2:X:34:LYS:HA	1.73	0.71
1:G:333:ILE:HG22	1:G:334:ASP:H	1.56	0.70
1:J:166:MET:HE1	1:J:407:VAL:HG21	1.73	0.70
1:H:228:SER:HA	1:H:255:GLU:HB2	1.73	0.70
1:I:305:ILE:HG22	1:I:306:GLY:H	1.56	0.70
1:G:322:ARG:HB3	1:G:333:ILE:HG13	1.73	0.70
1:H:242:LYS:HD3	2:V:25:ILE:HD12	1.74	0.70
1:A:200:LEU:HD13	1:A:276:VAL:HA	1.73	0.70
1:E:117:LYS:NZ	1:E:121:ASP:OD2	2.24	0.70
2:Z:57:LEU:HD23	2:Z:88:GLU:HB2	1.74	0.70
3:G:601:ADP:O3B	4:G:602:BEF:F3	2.00	0.70
2:S:22:ALA:HA	2:S:26:VAL:HB	1.74	0.70
2:S:64:ILE:HG23	2:S:95:VAL:HG13	1.74	0.70
2:2:49:LEU:HD13	2:1:51:ASN:H	1.56	0.70
1:A:197:ARG:HD2	1:A:277:LYS:HB2	1.74	0.70
1:H:166:MET:HE1	1:H:407:VAL:HG21	1.74	0.70
1:M:210:THR:HG23	1:N:351:GLN:HG2	1.74	0.69
1:M:265:ASN:HD21	2:1:27:LEU:HD13	1.57	0.69
1:H:232:GLU:HG3	1:H:233:MET:H	1.57	0.69
1:M:278:ALA:HB3	1:M:285:ARG:HD2	1.74	0.69
1:I:333:ILE:HG13	1:I:334:ASP:H	1.58	0.69
1:A:284:ARG:HA	1:A:364:LYS:HZ1	1.58	0.69
1:D:229:ASN:C	1:D:231:ARG:H	1.98	0.69
2:P:51:ASN:HB3	2:P:52:GLY:HA2	1.74	0.69
1:M:291:ASP:OD1	1:M:345:ARG:NH2	2.23	0.69
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.75	0.69
1:G:227:ILE:HD13	1:G:254:VAL:HG22	1.74	0.69
1:N:420:ILE:HD13	1:N:448:GLU:HG2	1.73	0.69
2:W:37:ARG:HG2	2:W:66:ILE:HG12	1.75	0.69
1:K:325:ILE:HG12	1:K:330:THR:HG23	1.74	0.69
1:M:420:ILE:HD13	1:M:448:GLU:HG2	1.73	0.69
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.74	0.69
1:E:225:LYS:HD2	1:E:303:GLU:HG3	1.74	0.69
1:J:197:ARG:HD2	1:J:277:LYS:HB2	1.75	0.69
1:B:305:ILE:HG22	1:B:306:GLY:H	1.57	0.68
1:B:197:ARG:HH11	1:B:198:GLY:H	1.39	0.68
1:A:325:ILE:HG13	1:A:330:THR:HG23	1.73	0.68
1:B:227:ILE:O	1:B:230:ILE:HG22	1.94	0.68
1:A:230:ILE:O	1:A:233:MET:HG2	1.93	0.68
1:H:197:ARG:HG2	1:H:277:LYS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:3:ILE:HD11	2:Q:78:ILE:HG12	1.75	0.68
1:L:40:LEU:HD13	1:L:59:GLU:HG3	1.76	0.68
2:1:21:SER:HA	2:1:26:VAL:O	1.93	0.68
1:N:117:LYS:NZ	1:N:121:ASP:OD2	2.27	0.68
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.75	0.67
1:L:122:LYS:HE2	1:L:429:LEU:HD11	1.76	0.67
2:T:85:ILE:HD11	2:S:92:LEU:HD13	1.75	0.67
1:J:305:ILE:HG22	1:J:306:GLY:H	1.59	0.67
1:A:213:VAL:HG22	1:A:325:ILE:HB	1.77	0.67
2:Y:51:ASN:N	2:Y:52:GLY:HA2	2.09	0.67
2:Z:67:PHE:HB2	2:Z:86:MET:HE1	1.74	0.67
1:F:228:SER:HB2	1:F:255:GLU:HB2	1.77	0.67
1:M:40:LEU:HD13	1:M:59:GLU:HG3	1.77	0.67
1:H:236:VAL:HG13	1:H:237:LEU:HD12	1.76	0.67
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.77	0.67
1:D:206:ASN:OD1	1:D:208:PRO:HD3	1.95	0.67
1:J:27:VAL:HG21	1:J:93:THR:HG21	1.77	0.67
1:K:227:ILE:HD13	1:K:254:VAL:HG22	1.77	0.67
1:J:6:VAL:HG12	1:J:521:VAL:HG22	1.77	0.67
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.76	0.67
1:J:269:GLY:C	1:J:271:VAL:H	2.03	0.67
1:J:291:ASP:OD1	1:J:345:ARG:NH2	2.27	0.67
1:A:305:ILE:HG22	1:A:306:GLY:H	1.59	0.67
1:K:234:LEU:HG	1:K:235:PRO:HD3	1.76	0.67
1:I:227:ILE:HD13	1:I:254:VAL:HG22	1.77	0.67
1:F:420:ILE:HD13	1:F:448:GLU:HG2	1.76	0.66
1:K:230:ILE:HG23	1:K:233:MET:HG3	1.76	0.66
1:L:291:ASP:OD1	1:L:291:ASP:N	2.24	0.66
1:E:420:ILE:HD13	1:E:448:GLU:HG2	1.75	0.66
1:B:258:ALA:O	1:B:261:THR:OG1	2.13	0.66
2:U:37:ARG:HB3	2:U:66:ILE:HG12	1.77	0.66
1:L:228:SER:HB2	1:L:255:GLU:HB2	1.78	0.66
1:L:231:ARG:NH1	1:L:257:GLU:O	2.28	0.66
1:L:238:GLU:HG3	2:Z:23:GLY:HA3	1.77	0.66
1:M:200:LEU:HD11	1:M:277:LYS:HG3	1.76	0.66
1:B:40:LEU:HD13	1:B:59:GLU:HG3	1.78	0.66
1:I:452:ARG:HH21	1:I:463:SER:HA	1.61	0.66
2:R:17:VAL:HG23	2:R:19:THR:H	1.60	0.66
2:S:22:ALA:HB3	2:S:24:GLY:N	2.11	0.65
2:R:50:GLU:O	2:R:51:ASN:ND2	2.28	0.65
2:R:60:LYS:HG2	2:R:61:VAL:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:SER:H	1:K:307:MET:HE3	1.61	0.65
1:M:282:GLY:HA2	1:M:285:ARG:HH21	1.61	0.65
1:A:85:ALA:HB1	1:A:499:VAL:HG22	1.79	0.65
3:E:601:ADP:O2B	4:E:602:BEF:F1	2.04	0.65
1:M:235:PRO:HB3	2:1:25:ILE:O	1.97	0.65
1:I:231:ARG:NH1	2:W:31:ALA:HB2	2.10	0.65
1:A:349:ILE:HG23	1:A:365:LEU:HD22	1.79	0.65
1:E:350:ARG:HA	1:E:353:ILE:HG23	1.77	0.65
2:S:10:VAL:HG21	2:S:91:ILE:HD11	1.77	0.65
1:K:166:MET:HE1	1:K:407:VAL:HG21	1.79	0.65
1:M:242:LYS:HE2	2:1:24:GLY:HA3	1.78	0.65
1:A:235:PRO:HA	1:A:238:GLU:HB3	1.79	0.65
1:F:225:LYS:HD2	1:F:230:ILE:HD11	1.77	0.65
2:S:22:ALA:CB	2:S:25:ILE:H	2.10	0.65
1:I:166:MET:HE1	1:I:407:VAL:HG21	1.79	0.65
1:H:177:VAL:HG11	1:H:397:GLU:HG2	1.77	0.65
1:D:206:ASN:ND2	1:D:214:GLU:H	1.93	0.65
2:R:10:VAL:HG21	2:R:91:ILE:HD11	1.78	0.65
1:H:419:LEU:HB3	1:H:447:MET:HB3	1.78	0.65
1:N:77:VAL:HG21	1:N:507:ALA:HA	1.79	0.65
1:F:319:GLN:HB2	1:F:336:VAL:HG11	1.77	0.64
1:C:420:ILE:HD11	1:C:470:LYS:HG3	1.78	0.64
2:P:11:ILE:HG12	2:P:85:ILE:HG12	1.79	0.64
2:U:17:VAL:HA	2:U:35:SER:HB3	1.79	0.64
1:L:172:GLU:HG2	1:L:350:ARG:HH22	1.62	0.64
2:Z:12:VAL:HG12	2:Z:40:VAL:HA	1.77	0.64
1:G:420:ILE:HD11	1:G:470:LYS:HG3	1.80	0.64
2:Q:93:ALA:HB2	2:R:5:PRO:HA	1.80	0.64
1:M:195:PHE:CE1	1:M:279:PRO:HG3	2.33	0.64
1:B:237:LEU:HD11	1:B:312:ALA:HB3	1.78	0.64
2:P:37:ARG:HG2	2:P:66:ILE:HG12	1.79	0.64
1:K:247:LEU:HD12	1:K:273:VAL:HG13	1.78	0.64
1:N:238:GLU:OE2	2:2:23:GLY:N	2.25	0.64
1:A:177:VAL:HG11	1:A:397:GLU:HG2	1.78	0.64
1:A:327:LYS:H	1:A:327:LYS:HD3	1.62	0.64
1:H:207:LYS:HE3	1:H:208:PRO:HD2	1.80	0.64
1:A:237:LEU:HD13	1:A:317:LEU:HD11	1.79	0.64
1:D:206:ASN:HD21	1:D:214:GLU:H	1.46	0.64
1:K:213:VAL:HG22	1:K:325:ILE:HB	1.79	0.64
1:L:327:LYS:H	1:L:327:LYS:HD3	1.63	0.64
1:G:214:GLU:HG2	1:G:324:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HD2	1:A:261:THR:HG21	1.78	0.64
1:E:122:LYS:NZ	1:E:430:ARG:O	2.30	0.64
1:J:319:GLN:HG2	1:J:336:VAL:HG21	1.80	0.64
2:P:37:ARG:HH12	2:Q:78:ILE:HD13	1.62	0.64
1:I:367:GLU:HG2	1:I:371:LYS:HE2	1.80	0.64
1:C:419:LEU:HB3	1:C:447:MET:HB3	1.80	0.63
1:G:278:ALA:HB1	1:G:285:ARG:HB2	1.81	0.63
2:Y:15:LYS:HG2	2:Y:38:GLY:HA2	1.80	0.63
2:1:60:LYS:HG2	2:1:61:VAL:H	1.63	0.63
1:I:225:LYS:HB2	1:I:303:GLU:HG3	1.80	0.63
1:I:258:ALA:O	1:I:261:THR:OG1	2.16	0.63
1:G:40:LEU:HD13	1:G:59:GLU:HG3	1.81	0.63
1:C:197:ARG:HG2	1:C:277:LYS:HB2	1.79	0.63
1:D:319:GLN:HB2	1:D:336:VAL:HG11	1.80	0.63
3:N:601:ADP:O3B	4:N:602:BEF:F1	2.06	0.63
1:C:74:VAL:O	1:C:77:VAL:HG12	1.99	0.63
1:B:230:ILE:O	1:B:233:MET:HG2	1.99	0.63
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.81	0.63
1:C:240:VAL:HG11	1:C:314:LEU:HB3	1.80	0.63
1:D:77:VAL:HG21	1:D:507:ALA:HA	1.80	0.63
1:M:261:THR:HG22	2:1:29:GLY:HA2	1.79	0.63
2:Z:35:SER:OG	2:Z:37:ARG:O	2.15	0.63
2:R:37:ARG:NH2	2:S:77:LYS:O	2.31	0.63
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.80	0.63
1:D:200:LEU:HD13	1:D:276:VAL:HA	1.80	0.63
1:D:429:LEU:HG	1:D:440:ILE:HD13	1.81	0.63
1:G:247:LEU:HD12	1:G:273:VAL:HG13	1.81	0.62
1:F:30:THR:OG1	1:F:51:LYS:O	2.17	0.62
2:P:15:LYS:HG2	2:P:38:GLY:HA2	1.81	0.62
1:J:224:ASP:OD1	1:J:286:LYS:NZ	2.32	0.62
1:N:209:GLU:O	1:N:210:THR:OG1	2.12	0.62
1:E:236:VAL:HG21	1:E:312:ALA:HB3	1.79	0.62
1:K:39:VAL:HG22	1:K:49:ILE:HG12	1.81	0.62
1:M:215:LEU:HB2	1:M:323:VAL:HG22	1.81	0.62
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.80	0.62
1:E:261:THR:O	1:E:265:ASN:ND2	2.26	0.62
3:K:601:ADP:O2B	4:K:602:BEF:F3	2.08	0.62
2:Y:51:ASN:H	2:Y:52:GLY:HA2	1.64	0.62
1:C:270:ILE:HG12	2:Q:26:VAL:HG22	1.81	0.62
1:L:225:LYS:HD2	1:L:309:LEU:HD11	1.81	0.62
2:V:49:LEU:HB2	2:V:53:GLU:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:HG13	1:A:376:VAL:HB	1.79	0.62
2:O:93:ALA:HB2	2:P:5:PRO:HA	1.80	0.62
2:R:53:GLU:OE1	2:S:52:GLY:N	2.32	0.62
1:I:230:ILE:HD13	1:I:309:LEU:HD22	1.82	0.62
1:L:6:VAL:HG12	1:L:521:VAL:HG22	1.82	0.62
1:K:122:LYS:HE2	1:K:429:LEU:HD11	1.81	0.62
1:A:268:ARG:N	1:A:269:GLY:HA2	2.15	0.62
1:K:205:ILE:HG23	1:K:212:ALA:H	1.65	0.62
1:L:74:VAL:O	1:L:77:VAL:HG12	2.00	0.62
2:Z:11:ILE:HG22	2:Z:85:ILE:HG22	1.80	0.62
1:A:270:ILE:HD12	2:O:25:ILE:HB	1.81	0.62
1:B:231:ARG:HH22	2:P:28:THR:HG22	1.64	0.62
1:C:125:THR:O	1:C:128:VAL:HG12	2.00	0.62
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.80	0.62
1:J:206:ASN:ND2	1:J:214:GLU:O	2.32	0.62
1:J:280:GLY:HA3	1:J:284:ARG:HD2	1.81	0.62
1:M:232:GLU:O	1:M:235:PRO:HD2	2.00	0.62
1:H:40:LEU:HD13	1:H:59:GLU:HG3	1.81	0.62
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.82	0.62
1:J:261:THR:O	1:J:265:ASN:ND2	2.27	0.61
1:N:232:GLU:CG	1:N:309:LEU:HB3	2.29	0.61
1:D:443:ALA:O	1:D:447:MET:HG3	2.00	0.61
1:A:237:LEU:HD23	1:A:312:ALA:HB3	1.82	0.61
1:J:232:GLU:O	1:J:235:PRO:HD2	2.00	0.61
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.79	0.61
2:U:15:LYS:HB2	2:U:38:GLY:HA2	1.81	0.61
1:N:339:GLU:O	1:N:343:GLN:NE2	2.32	0.61
1:G:305:ILE:HG22	1:G:306:GLY:H	1.66	0.61
1:A:284:ARG:HA	1:A:364:LYS:NZ	2.16	0.61
1:E:214:GLU:HG2	1:E:324:VAL:HG22	1.81	0.61
1:H:210:THR:HG23	1:H:211:GLY:H	1.64	0.61
1:G:352:GLN:O	1:G:355:GLU:HG2	2.00	0.61
1:D:233:MET:HG2	1:D:309:LEU:HB3	1.82	0.61
1:K:363:GLU:O	1:K:366:GLN:HG2	2.00	0.61
1:M:226:LYS:HG3	1:M:252:GLU:HG2	1.83	0.61
1:H:77:VAL:HG21	1:H:507:ALA:HA	1.83	0.61
1:J:268:ARG:N	1:J:269:GLY:HA2	2.15	0.61
1:I:177:VAL:HG11	1:I:397:GLU:HG2	1.83	0.61
2:Z:36:THR:O	2:Z:66:ILE:HG12	2.01	0.61
2:U:15:LYS:HG3	2:U:16:GLU:H	1.65	0.61
1:N:40:LEU:HD13	1:N:59:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:353:ILE:O	1:L:362:ARG:HG2	2.01	0.60
2:V:88:GLU:O	2:V:91:ILE:HG22	2.01	0.60
1:A:74:VAL:O	1:A:77:VAL:HG12	2.01	0.60
1:N:305:ILE:HG22	1:N:306:GLY:H	1.65	0.60
2:2:12:VAL:HG12	2:2:40:VAL:HA	1.84	0.60
1:C:193:MET:HE2	1:C:292:ILE:HG12	1.84	0.60
2:P:51:ASN:HB3	2:P:52:GLY:CA	2.30	0.60
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.83	0.60
1:N:114:MET:O	1:N:118:ARG:HG3	2.01	0.60
1:B:411:VAL:HG21	1:B:494:LEU:HD23	1.82	0.60
1:C:305:ILE:HG13	1:C:307:MET:HG2	1.84	0.60
2:T:17:VAL:HG23	2:T:33:ALA:HB2	1.83	0.60
1:H:213:VAL:O	1:H:324:VAL:HA	2.01	0.60
1:F:177:VAL:HG11	1:F:397:GLU:HG2	1.83	0.60
2:P:37:ARG:HH22	2:Q:78:ILE:HB	1.67	0.60
1:E:411:VAL:HG21	1:E:494:LEU:HD23	1.82	0.60
1:D:202:PRO:O	1:D:205:ILE:HG12	2.01	0.60
1:J:325:ILE:HG13	1:J:330:THR:HG23	1.83	0.60
1:I:325:ILE:HG13	1:I:330:THR:HG23	1.82	0.60
1:C:240:VAL:CG1	1:C:314:LEU:HB3	2.32	0.60
1:K:420:ILE:HD11	1:K:470:LYS:HG3	1.82	0.60
1:G:278:ALA:HB3	1:G:285:ARG:HD3	1.84	0.60
3:I:601:ADP:O3B	4:I:602:BEF:F1	2.09	0.60
1:M:206:ASN:ND2	1:M:214:GLU:O	2.35	0.60
1:G:288:MET:HA	1:G:291:ASP:OD2	2.01	0.59
1:H:420:ILE:HD11	1:H:470:LYS:HG3	1.84	0.59
2:X:95:VAL:HA	2:W:3:ILE:HG22	1.83	0.59
2:S:20:LYS:HG3	2:S:21:SER:H	1.67	0.59
1:I:352:GLN:HB3	1:I:365:LEU:HD11	1.84	0.59
1:G:221:LEU:HB3	1:G:249:ILE:HD13	1.84	0.59
1:G:238:GLU:OE1	1:G:238:GLU:N	2.35	0.59
1:B:232:GLU:O	1:B:235:PRO:HD2	2.02	0.59
1:B:325:ILE:HG13	1:B:330:THR:HG23	1.84	0.59
1:C:226:LYS:HA	1:C:252:GLU:HB3	1.84	0.59
1:D:117:LYS:NZ	1:D:121:ASP:OD2	2.35	0.59
2:S:50:GLU:C	2:S:52:GLY:HA2	2.27	0.59
1:K:74:VAL:O	1:K:77:VAL:HG12	2.02	0.59
1:J:176:THR:HG23	1:J:378:VAL:HG22	1.83	0.59
1:J:308:GLU:CD	1:J:308:GLU:H	2.10	0.59
2:2:11:ILE:HB	2:2:85:ILE:HD13	1.84	0.59
1:E:241:ALA:HA	1:E:271:VAL:HG11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:GLU:O	1:G:343:GLN:HB2	2.01	0.59
1:A:269:GLY:C	1:A:271:VAL:H	2.10	0.59
1:B:202:PRO:O	1:B:205:ILE:HG12	2.02	0.59
1:D:238:GLU:HA	1:D:241:ALA:HB3	1.84	0.59
1:I:228:SER:HB3	1:I:255:GLU:HB2	1.85	0.59
1:I:429:LEU:HG	1:I:440:ILE:HD13	1.85	0.59
2:2:36:THR:HG23	2:2:37:ARG:HG3	1.84	0.59
1:B:74:VAL:O	1:B:77:VAL:HG12	2.02	0.59
1:B:230:ILE:HG21	1:B:309:LEU:HD13	1.84	0.59
2:R:25:ILE:HG22	2:R:26:VAL:H	1.67	0.59
1:I:284:ARG:HG2	1:I:288:MET:HE2	1.84	0.59
1:G:74:VAL:O	1:G:77:VAL:HG12	2.02	0.59
1:C:77:VAL:HB	1:C:510:VAL:HG21	1.85	0.59
1:C:252:GLU:OE1	1:C:285:ARG:NH2	2.35	0.59
2:T:29:GLY:HA2	2:T:31:ALA:N	2.18	0.59
2:R:12:VAL:HG12	2:R:40:VAL:HA	1.84	0.59
1:D:122:LYS:HE2	1:D:429:LEU:HD11	1.83	0.59
1:L:39:VAL:HG22	1:L:49:ILE:HG12	1.84	0.59
1:M:226:LYS:H	1:M:226:LYS:HD2	1.68	0.59
1:N:117:LYS:HE2	1:N:513:LEU:HG	1.82	0.59
1:B:6:VAL:HG12	1:B:521:VAL:HG22	1.85	0.59
1:E:225:LYS:HB2	1:E:303:GLU:HB2	1.83	0.59
1:E:266:THR:HG22	1:E:273:VAL:H	1.66	0.59
2:R:11:ILE:HB	2:R:85:ILE:HD13	1.83	0.59
1:K:40:LEU:HD13	1:K:59:GLU:HG3	1.84	0.59
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.85	0.59
1:H:74:VAL:O	1:H:77:VAL:HG12	2.03	0.59
1:F:293:ALA:HB2	1:F:300:VAL:HG23	1.85	0.59
1:C:235:PRO:HA	1:C:238:GLU:HB2	1.84	0.59
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.84	0.59
2:U:43:VAL:HG23	2:U:57:LEU:HD12	1.85	0.59
1:K:291:ASP:HB3	1:K:372:LEU:HD21	1.85	0.59
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.84	0.59
1:D:233:MET:SD	1:D:309:LEU:HB3	2.43	0.58
1:L:489:ILE:HG23	1:L:494:LEU:HD21	1.85	0.58
1:H:248:LEU:HD12	1:H:323:VAL:HG21	1.85	0.58
1:L:230:ILE:HG23	1:L:233:MET:HB2	1.84	0.58
1:L:409:GLU:CD	1:L:501:ARG:HH21	2.10	0.58
1:A:319:GLN:HG2	1:A:336:VAL:HG21	1.84	0.58
1:G:13:ARG:NH1	1:G:517:THR:O	2.37	0.58
1:G:242:LYS:HD2	1:G:247:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:HD13	1:E:276:VAL:HA	1.85	0.58
1:K:6:VAL:HG12	1:K:521:VAL:HG22	1.84	0.58
1:J:263:VAL:HG22	1:J:267:MET:HE3	1.85	0.58
1:I:349:ILE:HD12	1:I:368:ARG:HE	1.69	0.58
1:L:20:VAL:HG13	1:L:74:VAL:HG11	1.86	0.58
2:1:57:LEU:HD23	2:1:88:GLU:HB2	1.85	0.58
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.85	0.58
1:D:252:GLU:OE1	1:D:285:ARG:NH2	2.36	0.58
1:H:305:ILE:HG22	1:H:306:GLY:H	1.67	0.58
2:1:16:GLU:HG2	2:1:17:VAL:N	2.18	0.58
1:F:247:LEU:HB3	1:F:273:VAL:HG13	1.85	0.58
1:D:230:ILE:HG12	1:D:233:MET:HE2	1.85	0.58
2:Q:55:LYS:HD3	2:Q:56:PRO:HD2	1.84	0.58
2:R:49:LEU:HD13	2:S:50:GLU:HA	1.84	0.58
2:S:18:GLU:OE1	2:S:20:LYS:HD3	2.04	0.58
1:K:288:MET:HA	1:K:291:ASP:OD2	2.04	0.58
1:J:233:MET:HG2	1:J:310:GLU:HA	1.86	0.58
1:L:421:ARG:NH1	1:L:472:GLY:O	2.37	0.58
2:W:93:ALA:HB2	2:V:5:PRO:HA	1.85	0.58
1:G:349:ILE:HG12	1:G:368:ARG:HH21	1.68	0.58
1:J:74:VAL:O	1:J:77:VAL:HG12	2.04	0.58
1:I:91:THR:OG1	3:I:601:ADP:O2B	2.21	0.58
1:M:221:LEU:HD23	1:M:249:ILE:HG12	1.85	0.58
1:F:27:VAL:O	1:F:30:THR:HG22	2.03	0.58
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.85	0.58
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.86	0.58
1:G:363:GLU:O	1:G:366:GLN:HG2	2.04	0.58
1:I:125:THR:O	1:I:128:VAL:HG12	2.04	0.58
1:L:87:ASP:OD1	4:L:602:BEF:F3	2.12	0.58
1:L:177:VAL:HG11	1:L:397:GLU:HG2	1.86	0.58
2:X:11:ILE:HG12	2:X:85:ILE:HG12	1.84	0.58
1:E:219:PHE:HB3	1:E:317:LEU:HD13	1.86	0.57
1:D:205:ILE:HG22	1:D:207:LYS:N	2.15	0.57
1:F:225:LYS:HE2	1:F:303:GLU:HB2	1.85	0.57
2:T:12:VAL:HG12	2:T:40:VAL:HA	1.86	0.57
1:J:269:GLY:O	1:J:270:ILE:HG13	2.04	0.57
1:I:30:THR:HB	1:I:51:LYS:HG3	1.86	0.57
1:L:353:ILE:HD11	1:L:369:VAL:HG21	1.85	0.57
1:M:239:ALA:O	1:M:242:LYS:HG2	2.04	0.57
1:M:420:ILE:HD11	1:M:470:LYS:HG3	1.85	0.57
1:N:74:VAL:O	1:N:77:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:GLU:OE2	1:F:350:ARG:NH2	2.32	0.57
1:J:231:ARG:NH2	1:J:257:GLU:HB3	2.19	0.57
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.86	0.57
1:I:193:MET:HE2	1:I:292:ILE:HG12	1.86	0.57
2:Z:85:ILE:HD11	2:1:92:LEU:HD13	1.85	0.57
1:B:89:THR:OG1	4:B:602:BEF:F2	2.13	0.57
2:T:36:THR:O	2:T:66:ILE:HG12	2.04	0.57
2:T:57:LEU:H	2:T:57:LEU:HD12	1.68	0.57
1:F:305:ILE:HG22	1:F:306:GLY:H	1.70	0.57
1:D:420:ILE:HD11	1:D:470:LYS:HD3	1.86	0.57
1:K:74:VAL:HG12	1:K:514:MET:HE1	1.86	0.57
1:L:27:VAL:O	1:L:30:THR:HG22	2.05	0.57
1:N:223:ALA:HA	1:N:301:ILE:HG13	1.86	0.57
2:Y:48:ILE:HG22	2:Y:53:GLU:O	2.04	0.57
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.87	0.57
1:E:222:LEU:HD22	1:E:293:ALA:HB2	1.86	0.57
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.86	0.57
1:E:215:LEU:HB2	1:E:323:VAL:HG22	1.87	0.57
1:K:319:GLN:HG2	1:K:336:VAL:HG21	1.87	0.57
1:I:130:GLU:HB3	1:I:422:VAL:HG13	1.86	0.57
1:M:409:GLU:OE2	1:M:501:ARG:NH2	2.38	0.57
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.35	0.57
1:A:269:GLY:O	1:A:270:ILE:HG12	2.04	0.57
1:E:232:GLU:O	1:E:235:PRO:HD2	2.04	0.57
1:G:218:PRO:HG3	1:G:323:VAL:HG22	1.87	0.56
1:A:232:GLU:O	1:A:235:PRO:HD2	2.05	0.56
1:C:213:VAL:O	1:C:324:VAL:HA	2.05	0.56
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.88	0.56
2:Z:5:PRO:HB3	2:Z:11:ILE:HG23	1.86	0.56
1:B:254:VAL:HG12	1:B:259:LEU:HG	1.87	0.56
1:G:95:LEU:HD13	1:G:504:LEU:HD23	1.86	0.56
1:G:193:MET:HE2	1:G:292:ILE:HG12	1.87	0.56
1:A:323:VAL:HG12	1:A:332:ILE:HG12	1.87	0.56
1:B:193:MET:HE2	1:B:292:ILE:HG12	1.87	0.56
1:F:327:LYS:HD3	1:F:327:LYS:H	1.70	0.56
1:E:87:ASP:OD1	4:E:602:BEF:F3	2.13	0.56
1:C:177:VAL:HG11	1:C:397:GLU:HG2	1.88	0.56
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.87	0.56
1:I:122:LYS:HE2	1:I:429:LEU:HD11	1.88	0.56
2:V:12:VAL:HG23	2:V:39:GLU:C	2.30	0.56
2:P:10:VAL:HG22	2:P:43:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:1:MET:HA	2:T:97:ALA:HB2	1.87	0.56
1:M:367:GLU:HG2	1:M:371:LYS:HE2	1.88	0.56
1:E:419:LEU:HD11	1:E:500:THR:HG23	1.88	0.56
1:C:10:ASN:O	1:C:14:VAL:HG23	2.06	0.56
2:T:29:GLY:HA2	2:T:30:SER:C	2.29	0.56
2:R:89:SER:O	2:S:9:ARG:NH2	2.38	0.56
1:I:74:VAL:O	1:I:77:VAL:HG12	2.05	0.56
1:H:232:GLU:HG3	1:H:233:MET:N	2.19	0.56
2:W:36:THR:HG21	2:V:76:GLU:OE2	2.06	0.56
1:F:461:GLU:OE1	1:M:452:ARG:NH2	2.38	0.56
1:C:91:THR:OG1	3:C:601:ADP:O2B	2.23	0.56
1:C:349:ILE:HD13	1:C:368:ARG:HD2	1.87	0.56
2:T:11:ILE:HG22	2:T:85:ILE:HG22	1.87	0.56
1:C:27:VAL:O	1:C:30:THR:HG22	2.04	0.56
2:S:65:VAL:HG12	2:S:94:ILE:HG22	1.88	0.56
1:K:210:THR:HA	1:L:351:GLN:HB3	1.88	0.56
1:K:217:SER:O	1:K:245:LYS:NZ	2.31	0.56
1:K:278:ALA:HB1	1:K:285:ARG:HB2	1.88	0.56
1:I:6:VAL:HG12	1:I:521:VAL:HG22	1.88	0.56
1:L:232:GLU:OE1	2:Y:77:LYS:NZ	2.39	0.56
2:X:37:ARG:HG2	2:X:66:ILE:HG12	1.88	0.56
2:X:78:ILE:HG13	2:X:79:ASP:N	2.19	0.56
1:G:305:ILE:HG23	1:A:267:MET:HG3	1.88	0.56
2:S:53:GLU:OE1	2:S:53:GLU:N	2.38	0.56
1:B:197:ARG:HG2	1:B:277:LYS:HB3	1.86	0.56
1:F:291:ASP:OD1	1:F:345:ARG:NE	2.29	0.56
1:C:217:SER:HA	1:C:320:ALA:O	2.06	0.56
1:D:304:GLU:C	1:D:305:ILE:HD12	2.31	0.56
1:H:231:ARG:HB2	1:H:258:ALA:HA	1.88	0.56
1:N:303:GLU:OE1	1:N:303:GLU:N	2.39	0.56
1:J:233:MET:HA	1:J:310:GLU:HA	1.87	0.56
1:I:361:ASP:O	1:I:365:LEU:HB3	2.06	0.56
2:W:55:LYS:HA	2:W:55:LYS:HE3	1.87	0.56
2:Y:20:LYS:HG2	2:Y:27:LEU:HD12	1.87	0.56
2:Z:20:LYS:HG3	2:Z:22:ALA:H	1.71	0.56
1:G:174:VAL:HG22	1:G:366:GLN:HG3	1.88	0.55
1:A:6:VAL:HG12	1:A:521:VAL:HG22	1.87	0.55
1:B:65:LYS:O	1:B:69:MET:HG3	2.06	0.55
1:E:279:PRO:HG2	1:E:288:MET:HE2	1.88	0.55
2:O:78:ILE:HG22	2:U:37:ARG:HH22	1.70	0.55
1:K:350:ARG:HA	1:K:353:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:278:ALA:HB1	1:J:285:ARG:HB2	1.88	0.55
2:Z:4:ARG:O	2:1:93:ALA:HB1	2.05	0.55
1:F:124:VAL:HG22	1:F:504:LEU:HD11	1.88	0.55
1:D:74:VAL:O	1:D:77:VAL:HG12	2.05	0.55
2:Q:22:ALA:C	2:Q:24:GLY:H	2.13	0.55
1:I:349:ILE:HG21	1:I:369:VAL:HG22	1.87	0.55
2:1:18:GLU:CG	2:1:19:THR:H	2.20	0.55
1:A:280:GLY:HA3	1:A:284:ARG:HD2	1.89	0.55
1:B:203:TYR:HB3	1:B:267:MET:HE2	1.88	0.55
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.89	0.55
1:K:197:ARG:NH1	1:K:277:LYS:HD2	2.22	0.55
1:K:264:VAL:HG12	1:L:305:ILE:HG23	1.89	0.55
1:I:475:ASN:O	1:I:488:MET:HG2	2.06	0.55
1:B:237:LEU:O	1:B:240:VAL:HG12	2.07	0.55
1:E:199:TYR:HA	1:E:276:VAL:HG12	1.87	0.55
2:Q:88:GLU:O	2:Q:91:ILE:HG22	2.05	0.55
1:M:196:ASP:O	1:M:197:ARG:HG2	2.06	0.55
1:N:304:GLU:C	1:N:305:ILE:HD12	2.32	0.55
2:X:8:ASP:HA	2:X:57:LEU:HD11	1.87	0.55
2:1:57:LEU:H	2:1:57:LEU:HD12	1.70	0.55
2:1:73:VAL:HG21	2:1:84:LEU:HD23	1.89	0.55
1:E:233:MET:O	1:E:236:VAL:HG12	2.06	0.55
2:S:21:SER:HB3	2:S:23:GLY:HA2	1.88	0.55
1:L:270:ILE:HG21	2:Z:26:VAL:HG22	1.88	0.55
1:N:203:TYR:HB3	1:N:267:MET:HE3	1.87	0.55
1:N:249:ILE:HD12	1:N:262:LEU:HD21	1.89	0.55
1:G:197:ARG:NH1	1:G:277:LYS:HD2	2.21	0.55
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.89	0.55
2:P:50:GLU:OE1	2:Q:50:GLU:HG3	2.07	0.55
1:I:197:ARG:HD3	1:I:279:PRO:HA	1.88	0.55
1:M:237:LEU:HD21	1:M:312:ALA:HB3	1.89	0.55
1:F:240:VAL:HG11	1:F:314:LEU:HB3	1.89	0.55
2:Q:19:THR:HA	2:Q:27:LEU:HD23	1.88	0.55
2:U:18:GLU:OE1	2:U:33:ALA:HB3	2.07	0.55
1:K:278:ALA:HB3	1:K:285:ARG:HD3	1.87	0.55
1:J:190:VAL:HG13	1:J:376:VAL:HB	1.87	0.55
1:M:244:GLY:O	1:M:245:LYS:HG2	2.06	0.55
1:H:345:ARG:O	1:H:349:ILE:HG13	2.07	0.55
1:E:226:LYS:HE3	1:E:252:GLU:HG2	1.88	0.55
1:E:238:GLU:HG2	1:E:239:ALA:N	2.21	0.55
1:K:290:GLN:OE1	1:K:345:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:57:LEU:HD23	2:Y:88:GLU:HB2	1.89	0.55
1:F:123:ALA:HB2	1:F:440:ILE:HG23	1.88	0.55
1:E:138:CYS:HB2	1:E:411:VAL:HG13	1.87	0.55
1:E:205:ILE:HD13	1:E:211:GLY:HA2	1.89	0.55
2:V:22:ALA:C	2:V:24:GLY:H	2.13	0.55
1:C:155:ASP:OD2	1:C:392:LYS:NZ	2.40	0.55
1:D:233:MET:CG	1:D:309:LEU:HB3	2.37	0.55
1:D:313:THR:CG2	1:D:315:GLU:HG2	2.37	0.55
2:Y:37:ARG:HG2	2:Y:66:ILE:HG12	1.87	0.55
1:B:361:ASP:O	1:B:365:LEU:HB3	2.06	0.54
1:E:257:GLU:O	2:S:30:SER:OG	2.24	0.54
1:J:205:ILE:HA	1:J:213:VAL:HG12	1.89	0.54
1:J:302:SER:HB2	1:J:305:ILE:HD13	1.88	0.54
1:L:291:ASP:HB2	1:L:372:LEU:HD21	1.89	0.54
1:L:321:LYS:HB2	1:L:334:ASP:HB3	1.89	0.54
1:L:326:ASN:HD21	1:L:329:THR:HG22	1.72	0.54
1:H:91:THR:OG1	3:H:601:ADP:O2B	2.25	0.54
1:H:218:PRO:HG3	1:H:323:VAL:HG22	1.89	0.54
1:B:87:ASP:OD1	4:B:602:BEF:F3	2.14	0.54
1:J:30:THR:HB	1:J:51:LYS:HG3	1.89	0.54
1:M:350:ARG:O	1:M:353:ILE:HG12	2.06	0.54
1:B:125:THR:O	1:B:128:VAL:HG12	2.07	0.54
1:F:77:VAL:HG21	1:F:507:ALA:HA	1.88	0.54
1:J:319:GLN:HG3	1:J:320:ALA:N	2.21	0.54
1:M:279:PRO:HD2	1:M:285:ARG:HG3	1.89	0.54
1:H:293:ALA:HB2	1:H:300:VAL:HG23	1.89	0.54
2:2:22:ALA:O	2:2:27:LEU:HB2	2.08	0.54
1:B:233:MET:SD	1:B:309:LEU:HB3	2.47	0.54
1:E:420:ILE:HD11	1:E:470:LYS:HG2	1.89	0.54
1:C:237:LEU:HD21	1:C:312:ALA:HB3	1.89	0.54
1:J:218:PRO:HG3	1:J:323:VAL:HG22	1.88	0.54
1:J:304:GLU:C	1:J:305:ILE:HD12	2.33	0.54
1:H:239:ALA:HA	2:V:25:ILE:HD11	1.88	0.54
1:B:174:VAL:HG21	1:B:367:GLU:HA	1.90	0.54
1:E:169:VAL:HG21	1:E:377:ALA:HB2	1.89	0.54
1:C:345:ARG:O	1:C:349:ILE:HG13	2.08	0.54
3:J:601:ADP:O3B	4:J:602:BEF:F2	2.16	0.54
1:M:230:ILE:HD12	1:M:309:LEU:HD21	1.89	0.54
2:Y:65:VAL:HG12	2:Y:94:ILE:HG12	1.87	0.54
1:A:197:ARG:HG3	1:A:277:LYS:O	2.08	0.54
1:B:234:LEU:O	1:B:237:LEU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:420:ILE:HD11	1:F:470:LYS:HD3	1.88	0.54
1:I:421:ARG:NH1	1:I:472:GLY:O	2.41	0.54
1:M:208:PRO:HB2	1:M:212:ALA:HB3	1.89	0.54
1:H:450:PRO:O	1:H:454:ILE:HG13	2.07	0.54
1:N:420:ILE:HD11	1:N:470:LYS:HD3	1.89	0.54
2:2:21:SER:N	2:2:27:LEU:O	2.41	0.54
1:A:28:LYS:HE2	1:A:453:GLN:OE1	2.06	0.54
1:J:327:LYS:H	1:J:327:LYS:HD3	1.73	0.54
1:H:305:ILE:HG22	1:H:306:GLY:N	2.22	0.54
1:N:448:GLU:OE1	1:N:452:ARG:NH1	2.40	0.54
1:A:176:THR:HG23	1:A:378:VAL:HG22	1.90	0.54
1:F:278:ALA:HB1	1:F:279:PRO:HD2	1.90	0.54
1:L:217:SER:HA	1:L:320:ALA:O	2.08	0.54
1:H:217:SER:HA	1:H:320:ALA:O	2.07	0.54
1:N:429:LEU:HG	1:N:440:ILE:HD13	1.90	0.54
1:G:74:VAL:HG12	1:G:514:MET:HE1	1.90	0.54
1:E:239:ALA:CB	1:E:314:LEU:HD11	2.38	0.54
2:S:27:LEU:HD12	2:S:28:THR:N	2.23	0.54
1:K:204:PHE:CD2	1:K:274:ALA:HA	2.43	0.54
1:K:443:ALA:O	1:K:447:MET:HG3	2.08	0.54
1:L:209:GLU:O	1:L:210:THR:OG1	2.23	0.54
1:L:247:LEU:HB3	1:L:273:VAL:HG13	1.88	0.54
1:M:10:ASN:O	1:M:14:VAL:HG23	2.08	0.54
1:M:74:VAL:O	1:M:77:VAL:HG12	2.08	0.54
1:M:203:TYR:HB3	1:M:267:MET:HE3	1.89	0.54
2:1:18:GLU:HG2	2:1:19:THR:H	1.73	0.54
2:1:48:ILE:HA	2:1:53:GLU:O	2.08	0.54
1:G:228:SER:HA	1:G:255:GLU:HB2	1.90	0.54
1:E:226:LYS:HG3	1:E:252:GLU:HB3	1.90	0.54
1:C:288:MET:HA	1:C:291:ASP:OD2	2.08	0.54
1:C:290:GLN:HE21	1:C:294:THR:HG23	1.72	0.54
1:K:206:ASN:N	1:K:212:ALA:O	2.37	0.54
1:H:359:ASP:O	1:H:363:GLU:HG3	2.08	0.54
1:A:77:VAL:HG21	1:A:507:ALA:HA	1.91	0.53
1:F:238:GLU:N	1:F:238:GLU:OE2	2.41	0.53
1:K:248:LEU:HD21	1:K:325:ILE:HD11	1.90	0.53
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.89	0.53
1:L:199:TYR:OH	1:L:327:LYS:HG3	2.08	0.53
2:X:14:ARG:NH1	2:X:35:SER:O	2.40	0.53
1:J:10:ASN:O	1:J:14:VAL:HG23	2.08	0.53
1:I:40:LEU:HD21	1:I:56:VAL:HG22	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:304:GLU:C	1:H:305:ILE:HD12	2.33	0.53
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.90	0.53
1:A:25:ASP:HA	1:A:28:LYS:HD2	1.89	0.53
1:A:193:MET:HB3	1:A:332:ILE:HB	1.89	0.53
1:B:208:PRO:HG2	1:B:214:GLU:HG3	1.90	0.53
1:F:388:GLU:HA	1:E:513:LEU:HD11	1.90	0.53
1:D:313:THR:HG22	1:D:315:GLU:H	1.73	0.53
1:L:281:PHE:HA	1:L:285:ARG:HH21	1.74	0.53
2:2:3:ILE:HD11	2:2:11:ILE:HD12	1.90	0.53
2:Q:40:VAL:HG13	2:Q:62:GLY:N	2.24	0.53
2:T:51:ASN:HD22	2:S:51:ASN:ND2	2.06	0.53
1:L:305:ILE:HG22	1:L:306:GLY:H	1.73	0.53
2:2:20:LYS:HB3	2:2:22:ALA:H	1.73	0.53
1:A:303:GLU:HB2	1:A:309:LEU:HD21	1.89	0.53
1:D:245:LYS:HB3	1:D:246:PRO:HD2	1.90	0.53
2:P:17:VAL:HG12	2:P:35:SER:HB2	1.91	0.53
2:T:74:LYS:NZ	2:T:76:GLU:OE2	2.33	0.53
1:N:230:ILE:HG12	1:N:261:THR:HG21	1.89	0.53
1:B:346:VAL:O	1:B:350:ARG:HG3	2.09	0.53
1:F:74:VAL:O	1:F:77:VAL:HG12	2.08	0.53
1:C:245:LYS:HE2	1:C:246:PRO:HD2	1.91	0.53
1:H:288:MET:HA	1:H:291:ASP:OD2	2.09	0.53
2:X:65:VAL:HG12	2:X:94:ILE:HG22	1.89	0.53
2:V:43:VAL:HG23	2:V:57:LEU:HD12	1.91	0.53
1:B:231:ARG:HD2	1:B:257:GLU:HG3	1.91	0.53
1:F:231:ARG:NH2	1:F:257:GLU:OE2	2.42	0.53
1:D:305:ILE:HG22	1:D:306:GLY:H	1.73	0.53
1:J:308:GLU:N	1:J:308:GLU:OE2	2.42	0.53
1:M:228:SER:HB3	1:M:255:GLU:HB2	1.91	0.53
1:A:205:ILE:HA	1:A:213:VAL:HG12	1.89	0.53
1:D:209:GLU:HG2	1:D:210:THR:N	2.24	0.53
2:R:3:ILE:HD11	2:R:11:ILE:HD12	1.89	0.53
1:I:239:ALA:HB1	1:I:314:LEU:HD11	1.90	0.53
1:L:164:GLU:OE2	1:L:168:LYS:NZ	2.41	0.53
1:M:310:GLU:OE1	1:M:310:GLU:N	2.42	0.53
1:H:219:PHE:CZ	1:H:245:LYS:HG3	2.44	0.53
1:N:174:VAL:HG21	1:N:367:GLU:HA	1.91	0.53
1:N:230:ILE:HG13	1:N:234:LEU:HD23	1.90	0.53
1:F:176:THR:HB	1:F:378:VAL:HG22	1.90	0.53
1:F:281:PHE:HB2	1:F:284:ARG:HH11	1.74	0.53
1:E:450:PRO:O	1:E:454:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:20:LYS:HG3	2:Q:28:THR:HG23	1.90	0.53
2:U:39:GLU:HA	2:U:64:ILE:HA	1.91	0.53
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.90	0.53
1:G:77:VAL:HG21	1:G:507:ALA:HA	1.91	0.53
1:B:117:LYS:NZ	1:B:121:ASP:OD2	2.41	0.53
1:E:169:VAL:HG12	1:E:173:GLY:HA3	1.90	0.53
1:C:353:ILE:HG23	1:C:366:GLN:HE22	1.74	0.53
1:J:278:ALA:HB3	1:J:285:ARG:HD3	1.91	0.53
1:L:215:LEU:HB2	1:L:323:VAL:HG22	1.91	0.53
1:L:236:VAL:HG21	1:L:310:GLU:O	2.09	0.53
2:Z:57:LEU:H	2:Z:57:LEU:HD12	1.72	0.53
1:B:218:PRO:HG3	1:B:323:VAL:HG22	1.91	0.52
1:I:197:ARG:NH1	1:I:279:PRO:HG3	2.20	0.52
1:L:450:PRO:O	1:L:454:ILE:HG13	2.09	0.52
1:G:147:VAL:HG22	1:G:403:THR:HG22	1.90	0.52
1:G:197:ARG:HH11	1:G:277:LYS:HD2	1.74	0.52
1:D:261:THR:HG23	2:R:28:THR:O	2.09	0.52
1:J:305:ILE:HG22	1:J:306:GLY:N	2.25	0.52
1:J:443:ALA:O	1:J:447:MET:HG3	2.09	0.52
1:M:213:VAL:O	1:M:324:VAL:HA	2.09	0.52
1:H:253:ASP:OD1	1:H:277:LYS:NZ	2.38	0.52
1:H:302:SER:HB2	1:H:305:ILE:HD13	1.90	0.52
1:F:280:GLY:O	1:F:285:ARG:NE	2.41	0.52
1:C:237:LEU:HD11	1:C:312:ALA:HB3	1.91	0.52
1:D:209:GLU:HG2	1:D:210:THR:HG23	1.92	0.52
1:K:218:PRO:HG3	1:K:323:VAL:HG22	1.90	0.52
1:I:305:ILE:HG22	1:I:306:GLY:N	2.23	0.52
2:X:7:HIS:NE2	2:Y:58:ASP:OD2	2.43	0.52
1:G:87:ASP:OD1	4:G:602:BEF:F1	2.17	0.52
1:B:284:ARG:HG2	1:B:288:MET:HE2	1.92	0.52
1:C:77:VAL:HG21	1:C:507:ALA:HA	1.90	0.52
2:P:60:LYS:HG2	2:P:61:VAL:H	1.74	0.52
1:M:77:VAL:HG21	1:M:507:ALA:HA	1.91	0.52
1:G:358:SER:HA	1:G:362:ARG:NE	2.20	0.52
1:A:322:ARG:HB2	1:A:333:ILE:HD12	1.92	0.52
1:F:215:LEU:HB2	1:F:323:VAL:HG22	1.92	0.52
1:K:197:ARG:HH11	1:K:277:LYS:HD2	1.74	0.52
1:J:220:ILE:N	1:J:318:GLY:O	2.30	0.52
1:M:443:ALA:O	1:M:447:MET:HG3	2.10	0.52
1:N:39:VAL:HG22	1:N:49:ILE:HG12	1.91	0.52
1:G:443:ALA:O	1:G:447:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:22:ALA:HB1	2:R:23:GLY:HA2	1.91	0.52
1:H:240:VAL:HB	1:H:314:LEU:HD23	1.91	0.52
2:Y:10:VAL:HG11	2:Y:91:ILE:HD11	1.90	0.52
2:2:59:VAL:HG22	2:2:94:ILE:HD11	1.92	0.52
3:D:601:ADP:O3B	4:D:602:BEF:F3	2.18	0.52
2:Q:25:ILE:HG13	2:Q:26:VAL:HG23	1.91	0.52
1:M:202:PRO:O	1:M:205:ILE:HG13	2.09	0.52
1:M:302:SER:HB2	1:M:305:ILE:HG22	1.90	0.52
3:M:601:ADP:O2B	4:M:602:BEF:F1	2.18	0.52
1:H:248:LEU:HD23	1:H:249:ILE:N	2.25	0.52
1:E:268:ARG:HG3	2:S:27:LEU:HD21	1.91	0.52
1:E:304:GLU:CD	1:E:305:ILE:H	2.17	0.52
2:S:28:THR:HG22	2:S:29:GLY:CA	2.33	0.52
1:M:291:ASP:OD2	1:M:368:ARG:HD3	2.09	0.52
1:A:278:ALA:HB1	1:A:285:ARG:HB2	1.92	0.52
1:E:123:ALA:HB2	1:E:440:ILE:HG23	1.92	0.52
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.92	0.52
1:K:409:GLU:CD	1:K:501:ARG:HH21	2.16	0.52
1:L:199:TYR:CE1	1:L:202:PRO:HA	2.44	0.52
1:L:319:GLN:HB2	1:L:336:VAL:HG11	1.92	0.52
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.91	0.52
1:H:217:SER:O	1:H:245:LYS:HD2	2.09	0.52
1:N:65:LYS:O	1:N:69:MET:HG3	2.10	0.52
1:E:151:SER:HB3	1:E:399:ALA:HA	1.92	0.52
1:D:237:LEU:HD11	1:D:317:LEU:HD21	1.90	0.52
2:S:18:GLU:HB2	2:S:20:LYS:HB2	1.92	0.52
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.40	0.52
1:K:232:GLU:O	1:K:235:PRO:HD2	2.10	0.52
1:L:77:VAL:HG21	1:L:507:ALA:HA	1.92	0.52
1:M:448:GLU:O	1:M:452:ARG:HG3	2.09	0.52
2:2:67:PHE:HB2	2:2:86:MET:HE1	1.92	0.52
1:B:215:LEU:HD13	1:B:246:PRO:HB2	1.91	0.51
1:B:315:GLU:OE1	1:B:315:GLU:N	2.44	0.51
1:F:215:LEU:HD23	1:F:246:PRO:HB2	1.93	0.51
1:E:224:ASP:HB2	1:E:302:SER:HA	1.91	0.51
1:E:261:THR:HG22	2:S:29:GLY:HA2	1.92	0.51
2:S:20:LYS:HB3	2:S:27:LEU:O	2.10	0.51
1:M:39:VAL:HG22	1:M:49:ILE:HG12	1.92	0.51
2:1:65:VAL:HG12	2:1:94:ILE:HG22	1.93	0.51
1:G:261:THR:HG22	2:U:29:GLY:HA3	1.92	0.51
1:G:333:ILE:HG22	1:G:334:ASP:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:VAL:O	1:B:349:ILE:HG22	2.09	0.51
1:E:169:VAL:HG13	1:E:375:GLY:O	2.10	0.51
1:C:215:LEU:HB2	1:C:323:VAL:HG22	1.92	0.51
2:T:48:ILE:HA	2:T:53:GLU:O	2.10	0.51
2:S:27:LEU:HD12	2:S:28:THR:H	1.74	0.51
1:J:138:CYS:HB2	1:J:411:VAL:HG13	1.91	0.51
1:N:205:ILE:HG23	1:N:212:ALA:O	2.11	0.51
1:A:25:ASP:HA	1:A:28:LYS:CD	2.41	0.51
1:C:233:MET:C	1:C:235:PRO:HD2	2.35	0.51
1:D:260:ALA:O	1:D:264:VAL:HG23	2.11	0.51
1:J:199:TYR:HB2	1:J:204:PHE:HD2	1.74	0.51
1:J:269:GLY:O	1:J:271:VAL:N	2.35	0.51
1:C:6:VAL:HG12	1:C:521:VAL:HG22	1.92	0.51
1:M:278:ALA:CB	1:M:285:ARG:HD2	2.41	0.51
1:A:200:LEU:HB3	1:A:259:LEU:HD11	1.92	0.51
2:Q:28:THR:OG1	2:Q:29:GLY:N	2.41	0.51
1:I:315:GLU:N	1:I:315:GLU:OE1	2.43	0.51
1:I:450:PRO:O	1:I:454:ILE:HG13	2.11	0.51
1:M:177:VAL:HG11	1:M:397:GLU:HG2	1.92	0.51
1:N:138:CYS:HB2	1:N:411:VAL:HG13	1.92	0.51
1:G:242:LYS:HE2	1:G:242:LYS:HA	1.92	0.51
1:F:174:VAL:HG21	1:F:367:GLU:HA	1.92	0.51
1:F:409:GLU:CD	1:F:501:ARG:HH21	2.19	0.51
1:E:285:ARG:HA	1:E:288:MET:HG2	1.92	0.51
2:P:57:LEU:HD12	2:P:57:LEU:H	1.76	0.51
1:K:174:VAL:HG22	1:K:366:GLN:HG3	1.93	0.51
1:I:196:ASP:HA	1:I:329:THR:HG22	1.93	0.51
1:M:205:ILE:HD13	1:M:211:GLY:HA2	1.91	0.51
1:N:450:PRO:O	1:N:454:ILE:HG13	2.11	0.51
1:E:10:ASN:O	1:E:14:VAL:HG23	2.10	0.51
1:D:229:ASN:C	1:D:231:ARG:N	2.66	0.51
1:K:361:ASP:O	1:K:365:LEU:HB2	2.10	0.51
1:H:199:TYR:HA	1:H:276:VAL:HG12	1.92	0.51
1:N:10:ASN:O	1:N:14:VAL:HG23	2.10	0.51
2:Y:49:LEU:O	2:Y:51:ASN:N	2.42	0.51
2:1:61:VAL:HG22	2:1:62:GLY:H	1.75	0.51
1:F:199:TYR:CE1	1:F:202:PRO:HA	2.46	0.51
1:C:282:GLY:HA2	1:C:285:ARG:HH21	1.76	0.51
2:P:65:VAL:HG12	2:P:94:ILE:HG22	1.93	0.51
2:T:51:ASN:HD22	2:S:51:ASN:CG	2.18	0.51
1:J:230:ILE:HG22	1:J:233:MET:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:234:LEU:HD22	1:J:238:GLU:HG2	1.93	0.51
1:L:264:VAL:HG21	1:M:306:GLY:HA3	1.92	0.51
1:H:263:VAL:O	1:H:267:MET:HG2	2.11	0.51
1:H:420:ILE:HD11	1:H:470:LYS:CG	2.40	0.51
2:Y:6:LEU:HD23	2:Z:93:ALA:HB2	1.92	0.51
1:G:355:GLU:HG3	1:G:362:ARG:HA	1.93	0.51
1:B:227:ILE:HD12	1:B:228:SER:N	2.26	0.51
1:F:234:LEU:N	1:F:235:PRO:HD2	2.26	0.51
1:E:166:MET:HE1	1:E:407:VAL:HG21	1.93	0.51
2:O:28:THR:HG22	2:O:29:GLY:H	1.75	0.51
2:U:5:PRO:HA	2:T:93:ALA:HB2	1.92	0.51
1:J:40:LEU:HD13	1:J:59:GLU:HG3	1.92	0.51
1:M:217:SER:HA	1:M:320:ALA:O	2.11	0.51
1:M:235:PRO:HA	1:M:238:GLU:HB2	1.92	0.51
2:Z:5:PRO:HA	2:1:93:ALA:HB2	1.92	0.51
1:G:238:GLU:OE2	1:G:312:ALA:HB3	2.10	0.51
1:A:65:LYS:O	1:A:69:MET:HG3	2.11	0.51
1:B:367:GLU:HG2	1:B:371:LYS:HE2	1.92	0.51
1:B:409:GLU:CD	1:B:501:ARG:HH21	2.18	0.51
1:D:270:ILE:HD13	2:R:26:VAL:O	2.10	0.51
2:Z:60:LYS:HE3	2:Z:61:VAL:HG22	1.92	0.51
1:G:145:ALA:O	1:G:149:THR:HG23	2.11	0.50
1:G:420:ILE:HD11	1:G:470:LYS:CG	2.41	0.50
1:F:448:GLU:O	1:F:452:ARG:HG3	2.11	0.50
1:E:498:LYS:HG3	1:E:501:ARG:NH2	2.26	0.50
2:P:57:LEU:HD23	2:P:88:GLU:HB2	1.92	0.50
2:Z:11:ILE:HG13	2:Z:41:LEU:HB2	1.94	0.50
1:F:409:GLU:OE2	1:F:501:ARG:NH2	2.43	0.50
1:D:205:ILE:HG21	1:D:211:GLY:HA2	1.92	0.50
2:R:20:LYS:HA	2:R:21:SER:HB2	1.93	0.50
1:K:244:GLY:O	1:K:245:LYS:HB2	2.11	0.50
1:I:323:VAL:HG12	1:I:332:ILE:HG12	1.93	0.50
1:L:225:LYS:CD	1:L:309:LEU:HD11	2.41	0.50
1:M:260:ALA:O	1:M:264:VAL:HG23	2.12	0.50
1:M:404:ARG:O	1:M:407:VAL:HG12	2.12	0.50
2:Y:14:ARG:NH2	2:Y:84:LEU:HD21	2.26	0.50
1:B:420:ILE:HG22	1:B:448:GLU:HA	1.92	0.50
1:F:199:TYR:OH	1:F:327:LYS:HG3	2.11	0.50
2:P:37:ARG:NH2	2:Q:77:LYS:O	2.44	0.50
2:R:47:ARG:O	2:R:54:VAL:HA	2.10	0.50
1:K:87:ASP:OD1	4:K:602:BEF:F2	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:450:PRO:O	1:J:454:ILE:HG13	2.11	0.50
1:M:65:LYS:O	1:M:69:MET:HG3	2.12	0.50
1:H:282:GLY:HA2	1:H:285:ARG:HH21	1.76	0.50
1:N:162:ILE:O	1:N:166:MET:HG3	2.11	0.50
2:W:91:ILE:HG22	2:W:92:LEU:O	2.11	0.50
2:1:15:LYS:HG3	2:1:16:GLU:H	1.77	0.50
1:B:348:GLN:HG3	1:C:209:GLU:HA	1.93	0.50
2:O:50:GLU:HG3	2:U:50:GLU:OE1	2.12	0.50
1:K:305:ILE:HG22	1:K:306:GLY:H	1.77	0.50
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.92	0.50
1:C:85:ALA:HB1	1:C:499:VAL:HG22	1.93	0.50
1:D:236:VAL:HG21	1:D:310:GLU:O	2.10	0.50
1:J:34:LYS:HG3	1:J:458:CYS:SG	2.52	0.50
1:I:202:PRO:O	1:I:205:ILE:HG12	2.10	0.50
1:A:308:GLU:H	1:A:308:GLU:CD	2.19	0.50
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.42	0.50
1:E:385:THR:HG22	1:D:509:SER:OG	2.12	0.50
1:D:246:PRO:HB3	1:D:272:LYS:HB2	1.93	0.50
2:T:49:LEU:O	2:T:53:GLU:HB2	2.10	0.50
1:J:200:LEU:HD13	1:J:276:VAL:HA	1.94	0.50
1:L:234:LEU:HD22	1:L:237:LEU:HD23	1.94	0.50
1:D:219:PHE:HE1	1:D:319:GLN:HE21	1.60	0.50
1:I:195:PHE:HD1	1:I:371:LYS:HE3	1.76	0.50
1:B:305:ILE:HG22	1:B:306:GLY:N	2.25	0.50
1:F:215:LEU:HD13	1:F:323:VAL:HG23	1.94	0.50
1:C:363:GLU:O	1:C:367:GLU:HB2	2.12	0.50
2:U:48:ILE:HD12	2:T:55:LYS:HD3	1.94	0.50
1:L:193:MET:HE2	1:L:292:ILE:HG12	1.93	0.50
1:L:443:ALA:O	1:L:447:MET:HG3	2.12	0.50
1:H:472:GLY:HA3	1:H:476:TYR:HD2	1.76	0.50
2:W:10:VAL:HG22	2:W:43:VAL:HG12	1.93	0.50
1:E:419:LEU:HB3	1:E:447:MET:HB3	1.93	0.50
1:C:225:LYS:HG2	1:C:226:LYS:O	2.12	0.50
1:J:232:GLU:C	1:J:235:PRO:HD2	2.37	0.50
1:I:199:TYR:CE1	1:I:202:PRO:HA	2.47	0.50
1:M:195:PHE:HB3	1:M:330:THR:HB	1.94	0.50
1:H:95:LEU:HD13	1:H:504:LEU:HD23	1.93	0.50
1:G:10:ASN:O	1:G:14:VAL:HG23	2.11	0.49
1:G:200:LEU:HD13	1:G:276:VAL:HA	1.92	0.49
1:G:305:ILE:HD12	1:A:267:MET:SD	2.52	0.49
1:C:249:ILE:HD12	1:C:262:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:14:ARG:HG2	2:U:35:SER:OG	2.12	0.49
2:W:14:ARG:HG2	2:W:35:SER:HB3	1.92	0.49
2:W:60:LYS:HG2	2:W:61:VAL:H	1.77	0.49
2:Y:49:LEU:C	2:Y:51:ASN:H	2.20	0.49
1:G:343:GLN:O	1:G:346:VAL:HG22	2.12	0.49
1:B:475:ASN:O	1:B:488:MET:HG2	2.12	0.49
1:F:228:SER:CB	1:F:255:GLU:HB2	2.40	0.49
1:C:171:LYS:HG2	1:C:172:GLU:N	2.23	0.49
1:C:359:ASP:O	1:C:363:GLU:HG3	2.12	0.49
2:U:63:ASP:OD1	2:U:63:ASP:N	2.39	0.49
1:J:202:PRO:O	1:J:205:ILE:HG12	2.12	0.49
1:J:233:MET:SD	1:J:309:LEU:HB3	2.52	0.49
1:E:352:GLN:HA	1:E:355:GLU:HG2	1.94	0.49
1:D:217:SER:HA	1:D:320:ALA:O	2.13	0.49
2:O:93:ALA:CB	2:P:5:PRO:HA	2.42	0.49
1:J:193:MET:SD	1:J:371:LYS:HB3	2.52	0.49
1:I:233:MET:HG3	1:I:309:LEU:O	2.11	0.49
1:M:253:ASP:OD1	1:M:254:VAL:N	2.45	0.49
1:H:190:VAL:HG11	1:H:194:GLN:HE22	1.75	0.49
1:G:124:VAL:HG21	1:G:508:ALA:HB2	1.94	0.49
1:E:305:ILE:HG12	1:E:307:MET:HG3	1.93	0.49
1:I:346:VAL:O	1:I:349:ILE:HG22	2.13	0.49
1:H:208:PRO:C	1:H:210:THR:H	2.19	0.49
1:G:65:LYS:O	1:G:69:MET:HG3	2.13	0.49
1:A:233:MET:HB2	1:A:310:GLU:HA	1.95	0.49
1:E:245:LYS:HE2	1:E:246:PRO:HD2	1.93	0.49
1:D:232:GLU:O	1:D:235:PRO:HD2	2.13	0.49
1:K:418:ALA:O	1:K:422:VAL:HG13	2.13	0.49
2:1:91:ILE:HG22	2:1:92:LEU:O	2.13	0.49
1:E:174:VAL:HG13	1:E:376:VAL:HG13	1.94	0.49
1:H:20:VAL:HG13	1:H:74:VAL:HG11	1.94	0.49
1:G:264:VAL:HG12	1:F:305:ILE:HG23	1.93	0.49
1:G:305:ILE:HG22	1:G:306:GLY:N	2.28	0.49
1:A:247:LEU:HB3	1:A:273:VAL:HG13	1.94	0.49
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.93	0.49
1:D:303:GLU:OE1	1:D:303:GLU:N	2.46	0.49
2:P:12:VAL:HG22	2:P:40:VAL:HA	1.94	0.49
1:J:284:ARG:HA	1:J:364:LYS:NZ	2.28	0.49
1:I:208:PRO:HG2	1:I:214:GLU:HG3	1.95	0.49
1:A:255:GLU:HG3	1:A:256:GLY:H	1.78	0.49
1:B:128:VAL:HG23	1:B:501:ARG:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HB3	1:B:258:ALA:HB2	1.94	0.49
1:F:65:LYS:O	1:F:69:MET:HG3	2.12	0.49
1:E:229:ASN:HB2	1:E:257:GLU:HB3	1.95	0.49
1:C:218:PRO:HG3	1:C:323:VAL:HG22	1.94	0.49
2:U:10:VAL:HG11	2:U:91:ILE:HD11	1.95	0.49
2:R:48:ILE:HA	2:R:53:GLU:O	2.12	0.49
1:J:117:LYS:NZ	1:J:121:ASP:OD2	2.41	0.49
1:J:199:TYR:CZ	1:J:205:ILE:HD11	2.46	0.49
1:I:124:VAL:HG21	1:I:508:ALA:CB	2.42	0.49
1:I:248:LEU:HD12	1:I:323:VAL:HG21	1.95	0.49
1:L:124:VAL:HG22	1:L:504:LEU:HD11	1.94	0.49
1:L:260:ALA:O	1:L:264:VAL:HG23	2.12	0.49
1:M:232:GLU:OE1	1:M:232:GLU:N	2.42	0.49
1:H:280:GLY:O	1:H:285:ARG:HD3	2.13	0.49
2:X:49:LEU:HG	2:X:50:GLU:H	1.78	0.49
1:E:213:VAL:O	1:E:324:VAL:HA	2.12	0.49
1:D:91:THR:OG1	3:D:601:ADP:O2B	2.30	0.49
1:L:261:THR:O	1:L:265:ASN:ND2	2.29	0.49
1:L:266:THR:HA	1:L:271:VAL:O	2.12	0.49
1:M:138:CYS:HB2	1:M:411:VAL:HG13	1.95	0.49
1:H:306:GLY:HA3	1:N:268:ARG:HH22	1.78	0.49
1:H:448:GLU:O	1:H:452:ARG:HG3	2.13	0.49
1:A:117:LYS:NZ	1:A:121:ASP:OD2	2.45	0.49
1:A:443:ALA:O	1:A:447:MET:HG3	2.13	0.49
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.43	0.49
1:D:130:GLU:HG3	1:D:426:LEU:HD21	1.95	0.49
1:M:28:LYS:HG2	1:M:94:VAL:HG22	1.94	0.49
1:H:10:ASN:O	1:H:14:VAL:HG23	2.12	0.49
1:H:322:ARG:HD2	1:H:333:ILE:HD12	1.95	0.49
1:C:242:LYS:HB2	2:Q:25:ILE:HD12	1.95	0.48
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.95	0.48
2:Q:64:ILE:O	2:Q:95:VAL:N	2.41	0.48
1:I:77:VAL:HB	1:I:510:VAL:HG21	1.93	0.48
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.95	0.48
1:I:124:VAL:HG21	1:I:508:ALA:HB2	1.95	0.48
1:I:257:GLU:OE1	2:W:31:ALA:HA	2.13	0.48
1:L:352:GLN:O	1:L:355:GLU:HG2	2.13	0.48
1:M:244:GLY:C	1:M:245:LYS:HG2	2.38	0.48
3:H:601:ADP:O3B	4:H:602:BEF:F2	2.20	0.48
1:N:209:GLU:H	1:N:209:GLU:CD	2.21	0.48
2:Y:6:LEU:HB3	2:Z:93:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ASN:O	1:F:14:VAL:HG23	2.13	0.48
1:C:282:GLY:HA2	1:C:285:ARG:HE	1.77	0.48
1:D:114:MET:O	1:D:118:ARG:HG3	2.13	0.48
2:P:69:ASP:HA	2:P:73:VAL:HG21	1.95	0.48
2:T:5:PRO:HA	2:S:93:ALA:HB2	1.94	0.48
1:K:366:GLN:HA	1:K:369:VAL:HG12	1.96	0.48
1:I:10:ASN:O	1:I:14:VAL:HG23	2.12	0.48
1:L:222:LEU:HD22	1:L:293:ALA:HB2	1.95	0.48
1:H:305:ILE:HD11	1:N:203:TYR:CE2	2.48	0.48
1:A:404:ARG:O	1:A:408:GLU:HG3	2.13	0.48
1:B:177:VAL:HG11	1:B:397:GLU:HG2	1.95	0.48
1:F:305:ILE:C	1:F:307:MET:H	2.21	0.48
1:D:39:VAL:HG22	1:D:49:ILE:HG12	1.95	0.48
1:D:229:ASN:O	1:D:231:ARG:N	2.46	0.48
1:K:227:ILE:HA	1:K:230:ILE:HB	1.95	0.48
1:K:448:GLU:OE1	1:K:452:ARG:NH1	2.46	0.48
1:I:174:VAL:HG23	1:I:370:ALA:HB2	1.95	0.48
1:B:199:TYR:CE1	1:B:202:PRO:HA	2.48	0.48
1:E:405:ALA:HB1	1:E:498:LYS:HB3	1.95	0.48
1:C:187:LEU:HD13	1:C:379:ILE:HG12	1.94	0.48
1:D:325:ILE:HG13	1:D:330:THR:HG23	1.94	0.48
1:I:291:ASP:HB3	1:I:372:LEU:HD21	1.95	0.48
1:H:237:LEU:O	1:H:240:VAL:HG22	2.14	0.48
2:2:57:LEU:C	2:2:59:VAL:H	2.21	0.48
2:1:66:ILE:HG13	2:1:92:LEU:HB2	1.94	0.48
1:G:204:PHE:CD2	1:G:274:ALA:HA	2.49	0.48
1:A:39:VAL:HG22	1:A:49:ILE:HG12	1.95	0.48
1:A:305:ILE:HG22	1:A:306:GLY:N	2.28	0.48
1:A:358:SER:O	1:A:362:ARG:HG2	2.14	0.48
1:F:225:LYS:HD2	1:F:230:ILE:CD1	2.42	0.48
1:F:240:VAL:CG1	1:F:314:LEU:HB3	2.43	0.48
1:C:199:TYR:CE1	1:C:202:PRO:HA	2.48	0.48
2:S:73:VAL:HG21	2:S:84:LEU:HD23	1.95	0.48
1:I:232:GLU:O	1:I:235:PRO:HD2	2.14	0.48
1:L:355:GLU:O	1:L:362:ARG:NH2	2.46	0.48
1:A:10:ASN:HA	1:A:13:ARG:HB2	1.95	0.48
1:E:345:ARG:O	1:E:349:ILE:HG13	2.13	0.48
1:C:190:VAL:HG11	1:C:194:GLN:HE22	1.78	0.48
2:U:50:GLU:C	2:U:52:GLY:H	2.20	0.48
2:S:20:LYS:HG3	2:S:21:SER:N	2.28	0.48
1:J:91:THR:OG1	3:J:601:ADP:O2B	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:305:ILE:HG23	1:N:267:MET:SD	2.53	0.48
1:N:345:ARG:O	1:N:349:ILE:HG12	2.14	0.48
1:G:193:MET:HB3	1:G:332:ILE:CG1	2.43	0.48
1:B:230:ILE:C	1:B:232:GLU:H	2.22	0.48
2:Q:21:SER:H	2:Q:27:LEU:HG	1.79	0.48
1:K:176:THR:HG23	1:K:378:VAL:HG22	1.96	0.48
1:J:405:ALA:HB1	1:J:498:LYS:HB3	1.96	0.48
1:M:215:LEU:O	1:M:322:ARG:HA	2.14	0.48
1:H:176:THR:OG1	1:H:378:VAL:HG22	2.14	0.48
2:W:11:ILE:HG12	2:W:85:ILE:HG12	1.95	0.48
1:G:210:THR:H	1:F:351:GLN:HG3	1.79	0.48
1:E:260:ALA:O	1:E:264:VAL:HG23	2.14	0.48
1:C:230:ILE:C	1:C:232:GLU:N	2.70	0.48
1:M:247:LEU:O	1:M:273:VAL:HA	2.13	0.48
2:V:8:ASP:HA	2:V:57:LEU:HD21	1.95	0.48
2:V:93:ALA:HB2	2:2:5:PRO:HA	1.96	0.48
1:F:412:VAL:HG13	1:F:497:THR:OG1	2.13	0.48
1:E:202:PRO:O	1:E:205:ILE:HG13	2.14	0.48
1:E:314:LEU:H	1:E:314:LEU:HD12	1.78	0.48
2:U:60:LYS:NZ	2:U:63:ASP:HB3	2.29	0.48
2:S:46:GLY:HA3	2:S:56:PRO:HA	1.96	0.48
1:K:227:ILE:HG22	1:K:227:ILE:O	2.14	0.48
1:I:49:ILE:O	1:I:391:GLU:HB2	2.14	0.48
1:I:230:ILE:CD1	1:I:309:LEU:HD22	2.43	0.48
1:I:234:LEU:N	1:I:235:PRO:HD2	2.29	0.48
1:I:349:ILE:HD12	1:I:368:ARG:NE	2.28	0.48
2:X:28:THR:HG22	2:X:29:GLY:H	1.78	0.48
1:A:228:SER:OG	1:A:255:GLU:HB3	2.14	0.48
1:B:199:TYR:CZ	1:B:205:ILE:HD11	2.49	0.48
1:B:339:GLU:HA	1:B:342:ILE:HB	1.96	0.48
1:B:440:ILE:O	1:B:444:LEU:HG	2.14	0.48
1:F:6:VAL:HG12	1:F:521:VAL:HG22	1.95	0.48
1:E:282:GLY:HA2	1:E:285:ARG:NH2	2.29	0.48
1:D:233:MET:HG3	1:D:310:GLU:CD	2.38	0.48
1:D:253:ASP:OD1	1:D:254:VAL:N	2.46	0.48
1:D:415:GLY:HA2	3:D:601:ADP:H1'	1.95	0.48
2:O:65:VAL:HG12	2:O:94:ILE:HG22	1.96	0.48
2:Q:65:VAL:HG12	2:Q:94:ILE:HG22	1.95	0.48
2:T:1:MET:HE1	2:T:79:ASP:HB2	1.95	0.48
2:T:11:ILE:HG13	2:T:41:LEU:HB2	1.96	0.48
2:Z:51:ASN:C	2:Z:53:GLU:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:LEU:N	1:G:235:PRO:HD2	2.28	0.47
1:G:302:SER:H	1:G:307:MET:HE3	1.79	0.47
1:C:5:ASP:HB2	1:C:524:LEU:HD23	1.94	0.47
2:P:50:GLU:O	2:P:51:ASN:HB2	2.13	0.47
2:U:50:GLU:HB3	2:U:51:ASN:H	1.53	0.47
1:L:252:GLU:O	1:L:277:LYS:HG3	2.14	0.47
2:Y:43:VAL:HG23	2:Y:57:LEU:HD22	1.96	0.47
1:A:223:ALA:O	1:A:251:ALA:HA	2.14	0.47
1:B:149:THR:HG23	1:B:155:ASP:C	2.40	0.47
1:C:230:ILE:HA	1:C:230:ILE:HD12	1.71	0.47
2:S:14:ARG:HG3	2:S:84:LEU:HD13	1.96	0.47
1:J:77:VAL:HG21	1:J:507:ALA:HA	1.96	0.47
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.94	0.47
1:N:443:ALA:O	1:N:447:MET:HG3	2.14	0.47
2:X:54:VAL:O	2:X:56:PRO:HD3	2.13	0.47
2:W:13:LYS:HB2	2:W:41:LEU:HD11	1.95	0.47
1:F:322:ARG:H	1:F:333:ILE:HG22	1.79	0.47
1:E:239:ALA:HB1	1:E:314:LEU:HD11	1.97	0.47
1:E:368:ARG:HH12	1:E:371:LYS:HD2	1.79	0.47
1:D:230:ILE:O	1:D:233:MET:HB3	2.15	0.47
2:U:48:ILE:HA	2:U:53:GLU:O	2.13	0.47
1:M:419:LEU:HB3	1:M:447:MET:HB3	1.96	0.47
1:H:18:ARG:HB3	1:H:18:ARG:NH1	2.29	0.47
1:N:266:THR:HA	1:N:271:VAL:O	2.13	0.47
1:N:421:ARG:NH1	1:N:472:GLY:O	2.47	0.47
1:C:200:LEU:HB3	1:C:259:LEU:HD11	1.96	0.47
1:C:323:VAL:HG12	1:C:332:ILE:HG12	1.95	0.47
1:D:227:ILE:O	1:D:230:ILE:HG22	2.14	0.47
1:K:414:GLY:HA3	1:K:493:ILE:HG22	1.96	0.47
1:J:361:ASP:O	1:J:365:LEU:HB2	2.14	0.47
1:I:231:ARG:HD2	1:I:261:THR:HG21	1.96	0.47
1:A:255:GLU:HG3	1:A:256:GLY:N	2.29	0.47
1:B:215:LEU:HB2	1:B:323:VAL:HG22	1.95	0.47
1:B:233:MET:HG3	1:B:234:LEU:HD22	1.97	0.47
1:D:496:PRO:O	1:D:499:VAL:HG22	2.15	0.47
2:T:22:ALA:C	2:T:24:GLY:H	2.21	0.47
1:J:256:GLY:O	1:J:259:LEU:N	2.47	0.47
1:I:195:PHE:CD1	1:I:371:LYS:HE3	2.49	0.47
2:2:49:LEU:C	2:2:51:ASN:H	2.22	0.47
1:B:443:ALA:O	1:B:447:MET:HG3	2.13	0.47
1:F:201:SER:HB3	1:F:259:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:VAL:HG13	1:E:497:THR:OG1	2.15	0.47
1:C:367:GLU:O	1:C:371:LYS:HG3	2.13	0.47
1:D:302:SER:OG	1:D:305:ILE:HD13	2.14	0.47
2:U:20:LYS:HB3	2:U:27:LEU:HD12	1.97	0.47
1:K:201:SER:HB3	1:K:259:LEU:HD22	1.97	0.47
1:K:281:PHE:H	1:K:284:ARG:HD2	1.79	0.47
1:L:28:LYS:HD2	1:L:453:GLN:CD	2.40	0.47
1:L:382:GLY:O	1:L:392:LYS:NZ	2.47	0.47
1:M:226:LYS:HE3	1:M:252:GLU:HG2	1.95	0.47
1:H:350:ARG:HA	1:H:353:ILE:HG13	1.96	0.47
1:H:363:GLU:O	1:H:367:GLU:HB2	2.15	0.47
2:W:65:VAL:HG12	2:W:94:ILE:HG22	1.96	0.47
2:Z:5:PRO:HA	2:1:93:ALA:CB	2.44	0.47
1:G:234:LEU:HD23	1:G:234:LEU:HA	1.42	0.47
1:A:10:ASN:O	1:A:14:VAL:HG23	2.14	0.47
1:F:415:GLY:N	3:F:601:ADP:O2'	2.40	0.47
1:E:304:GLU:O	1:E:306:GLY:HA2	2.15	0.47
2:U:17:VAL:HG13	2:U:35:SER:N	2.29	0.47
2:R:67:PHE:CD2	2:R:86:MET:HE1	2.49	0.47
1:K:343:GLN:O	1:K:346:VAL:HG22	2.13	0.47
1:J:419:LEU:HD12	1:J:447:MET:HE2	1.96	0.47
1:I:142:LYS:O	1:I:146:GLN:HG3	2.15	0.47
1:L:57:ALA:O	1:L:75:LYS:HE2	2.15	0.47
1:L:253:ASP:OD1	1:L:254:VAL:N	2.46	0.47
1:L:265:ASN:HA	1:L:270:ILE:HD13	1.96	0.47
1:M:270:ILE:HG22	1:M:271:VAL:HG13	1.96	0.47
1:M:302:SER:O	1:M:305:ILE:HG22	2.15	0.47
1:M:417:VAL:HA	1:M:420:ILE:HG22	1.96	0.47
1:H:226:LYS:HG2	1:H:252:GLU:HG2	1.96	0.47
1:H:418:ALA:O	1:H:422:VAL:HG13	2.14	0.47
1:N:358:SER:OG	1:N:359:ASP:N	2.45	0.47
2:Z:24:GLY:HA2	2:Z:25:ILE:HA	1.60	0.47
1:G:409:GLU:OE2	1:G:501:ARG:NH2	2.33	0.47
1:A:308:GLU:N	1:A:308:GLU:OE2	2.47	0.47
1:B:77:VAL:HB	1:B:510:VAL:HG21	1.97	0.47
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.96	0.47
2:P:51:ASN:CB	2:P:52:GLY:HA2	2.45	0.47
1:J:225:LYS:HE3	1:J:226:LYS:HG2	1.96	0.47
1:I:279:PRO:HB2	1:I:288:MET:HE3	1.97	0.47
2:V:19:THR:HG23	2:V:27:LEU:HD21	1.97	0.47
2:Z:29:GLY:HA2	2:Z:30:SER:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ALA:HA	1:E:271:VAL:CG1	2.45	0.47
1:C:227:ILE:HG12	1:C:253:ASP:O	2.14	0.47
1:D:229:ASN:OD1	1:D:230:ILE:N	2.42	0.47
1:D:313:THR:HG21	1:D:315:GLU:HG2	1.96	0.47
2:P:10:VAL:HG12	2:P:12:VAL:HG23	1.96	0.47
2:T:24:GLY:HA2	2:T:25:ILE:HA	1.57	0.47
1:K:245:LYS:HB3	1:K:246:PRO:HD2	1.96	0.47
1:K:305:ILE:HG22	1:K:306:GLY:N	2.29	0.47
1:J:90:THR:O	1:J:94:VAL:HG23	2.15	0.47
1:J:245:LYS:HB2	1:J:245:LYS:HE3	1.68	0.47
1:I:448:GLU:O	1:I:452:ARG:HG3	2.15	0.47
1:M:6:VAL:HG12	1:M:521:VAL:HG22	1.96	0.47
1:M:261:THR:O	1:M:265:ASN:ND2	2.38	0.47
1:M:404:ARG:O	1:M:408:GLU:HG2	2.15	0.47
1:N:305:ILE:HG22	1:N:306:GLY:N	2.28	0.47
2:W:28:THR:HG22	2:W:29:GLY:H	1.79	0.47
1:G:20:VAL:HG13	1:G:74:VAL:HG11	1.96	0.47
1:G:225:LYS:HD2	1:G:226:LYS:H	1.80	0.47
1:A:169:VAL:HG11	1:A:377:ALA:HB2	1.97	0.47
1:A:240:VAL:HG23	1:A:314:LEU:HD13	1.96	0.47
1:B:77:VAL:HG21	1:B:507:ALA:HA	1.97	0.47
1:F:265:ASN:HA	1:F:270:ILE:HD13	1.97	0.47
1:D:475:ASN:O	1:D:488:MET:HG2	2.15	0.47
2:O:11:ILE:HG12	2:O:85:ILE:HG12	1.97	0.47
1:K:215:LEU:HB3	1:K:218:PRO:HB3	1.97	0.47
1:K:513:LEU:HD11	1:J:388:GLU:HA	1.96	0.47
1:J:429:LEU:HG	1:J:440:ILE:HD13	1.97	0.47
1:I:40:LEU:HD13	1:I:59:GLU:HG3	1.97	0.47
1:I:138:CYS:HB2	1:I:411:VAL:HG13	1.97	0.47
1:I:420:ILE:HD11	1:I:469:VAL:HG12	1.97	0.47
1:N:90:THR:OG1	4:N:602:BEF:F3	2.23	0.47
2:X:18:GLU:OE2	2:X:30:SER:HA	2.16	0.47
1:G:238:GLU:O	1:G:242:LYS:HG2	2.14	0.46
1:B:20:VAL:HG13	1:B:74:VAL:HG11	1.97	0.46
1:F:359:ASP:O	1:F:363:GLU:HG3	2.15	0.46
1:C:231:ARG:NH1	1:C:257:GLU:HB3	2.30	0.46
2:U:20:LYS:HE2	2:U:27:LEU:HB2	1.97	0.46
2:S:22:ALA:H	2:S:23:GLY:C	2.23	0.46
1:J:199:TYR:CE1	1:J:202:PRO:HA	2.50	0.46
1:M:239:ALA:HA	1:M:242:LYS:HE3	1.98	0.46
1:G:257:GLU:O	1:G:261:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:LYS:HD2	1:E:160:LYS:HA	1.65	0.46
1:D:322:ARG:HG2	1:D:323:VAL:N	2.31	0.46
1:D:450:PRO:O	1:D:454:ILE:HG13	2.14	0.46
2:U:6:LEU:HD22	2:T:93:ALA:HA	1.95	0.46
2:S:91:ILE:HG22	2:S:92:LEU:O	2.14	0.46
1:K:145:ALA:O	1:K:149:THR:HG23	2.15	0.46
1:J:228:SER:CB	1:J:255:GLU:HB3	2.41	0.46
1:I:231:ARG:HA	1:I:234:LEU:HD13	1.97	0.46
1:I:282:GLY:O	1:I:286:LYS:HG2	2.16	0.46
1:I:288:MET:HG2	1:I:368:ARG:HD2	1.96	0.46
1:I:349:ILE:HD13	1:I:369:VAL:CG2	2.45	0.46
1:L:281:PHE:HB2	1:L:284:ARG:HH11	1.80	0.46
1:N:28:LYS:HG2	1:N:94:VAL:HG22	1.97	0.46
2:Y:1:MET:HG3	2:Z:97:ALA:HB2	1.98	0.46
1:G:246:PRO:HB3	1:G:272:LYS:HB2	1.97	0.46
1:E:215:LEU:O	1:E:322:ARG:HA	2.15	0.46
1:E:308:GLU:HB2	1:E:311:LYS:HE3	1.96	0.46
1:C:450:PRO:O	1:C:454:ILE:HG13	2.16	0.46
1:J:322:ARG:HB3	1:J:333:ILE:HD12	1.98	0.46
3:L:601:ADP:O1B	4:L:602:BEF:F2	2.23	0.46
1:N:434:GLU:O	1:N:437:ASN:HB2	2.15	0.46
2:1:77:LYS:HD3	2:1:82:GLU:HA	1.97	0.46
1:B:231:ARG:NH1	2:P:31:ALA:HB2	2.31	0.46
1:C:265:ASN:O	1:C:270:ILE:HG22	2.15	0.46
1:C:441:LYS:HD3	1:C:441:LYS:HA	1.67	0.46
1:D:421:ARG:HD3	1:D:421:ARG:HA	1.78	0.46
2:O:5:PRO:HA	2:U:93:ALA:HB2	1.97	0.46
1:J:323:VAL:HG12	1:J:332:ILE:HG12	1.98	0.46
1:I:237:LEU:O	1:I:241:ALA:N	2.48	0.46
1:L:65:LYS:O	1:L:69:MET:HG3	2.15	0.46
1:L:234:LEU:N	1:L:235:PRO:HD2	2.30	0.46
1:L:305:ILE:HG22	1:L:306:GLY:N	2.30	0.46
1:M:322:ARG:HB3	1:M:333:ILE:HD12	1.97	0.46
2:W:53:GLU:CG	2:W:54:VAL:H	2.26	0.46
1:G:138:CYS:HB2	1:G:411:VAL:HG13	1.97	0.46
1:B:225:LYS:CB	1:B:303:GLU:HG3	2.42	0.46
1:E:24:ALA:O	1:E:28:LYS:HG3	2.15	0.46
1:E:417:VAL:HA	1:E:420:ILE:HG22	1.97	0.46
1:C:362:ARG:O	1:C:366:GLN:HB2	2.15	0.46
2:O:50:GLU:HA	2:U:49:LEU:HD21	1.98	0.46
1:K:319:GLN:HG3	1:K:320:ALA:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:349:ILE:HD13	1:L:368:ARG:HD2	1.98	0.46
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.97	0.46
1:H:343:GLN:HA	1:H:346:VAL:HG22	1.98	0.46
1:N:183:LEU:H	1:N:183:LEU:HD12	1.80	0.46
2:2:49:LEU:HD13	2:1:51:ASN:N	2.27	0.46
1:G:404:ARG:O	1:G:408:GLU:HG2	2.16	0.46
1:B:510:VAL:O	1:B:514:MET:HB2	2.15	0.46
1:F:266:THR:HG22	1:F:273:VAL:H	1.81	0.46
1:D:421:ARG:NH1	1:D:472:GLY:O	2.49	0.46
2:S:17:VAL:HG22	2:S:18:GLU:N	2.31	0.46
1:K:236:VAL:HG11	1:K:310:GLU:O	2.15	0.46
1:I:3:ALA:HA	1:H:61:GLU:HG2	1.98	0.46
1:M:419:LEU:HD11	1:M:500:THR:HG23	1.98	0.46
1:H:54:VAL:HB	1:H:89:THR:HG21	1.97	0.46
1:H:234:LEU:N	1:H:235:PRO:HD2	2.30	0.46
1:H:242:LYS:HA	1:H:271:VAL:HG11	1.98	0.46
2:V:65:VAL:HG12	2:V:94:ILE:HG23	1.98	0.46
1:D:239:ALA:CB	2:R:24:GLY:HA2	2.45	0.46
1:D:305:ILE:HG22	1:D:306:GLY:N	2.31	0.46
1:K:183:LEU:H	1:K:183:LEU:HD12	1.80	0.46
1:J:269:GLY:C	1:J:271:VAL:N	2.72	0.46
1:J:291:ASP:HB3	1:J:372:LEU:HD21	1.98	0.46
1:L:227:ILE:O	1:L:227:ILE:HG22	2.16	0.46
1:H:175:ILE:HG13	1:H:400:LEU:HD21	1.98	0.46
1:H:205:ILE:HD12	1:H:210:THR:HA	1.97	0.46
1:H:307:MET:HE2	1:H:307:MET:HB3	1.81	0.46
1:N:124:VAL:HG21	1:N:508:ALA:CB	2.46	0.46
1:N:350:ARG:HA	1:N:353:ILE:HD12	1.98	0.46
1:A:237:LEU:O	1:A:240:VAL:HG22	2.16	0.46
1:F:429:LEU:HG	1:F:440:ILE:HD13	1.97	0.46
3:F:601:ADP:O3B	4:F:602:BEF:F2	2.24	0.46
1:J:65:LYS:O	1:J:69:MET:HG3	2.16	0.46
1:J:217:SER:O	1:J:245:LYS:NZ	2.41	0.46
2:W:61:VAL:HG12	2:W:62:GLY:N	2.31	0.46
2:W:64:ILE:HG23	2:W:95:VAL:HB	1.98	0.46
2:Z:49:LEU:O	2:Z:52:GLY:N	2.48	0.46
2:2:20:LYS:HE2	2:1:77:LYS:HG3	1.98	0.46
2:2:46:GLY:HA2	2:2:57:LEU:HG	1.98	0.46
1:G:228:SER:HB3	1:G:255:GLU:OE1	2.16	0.46
1:G:233:MET:O	1:G:236:VAL:HG22	2.15	0.46
1:B:171:LYS:HD3	1:B:171:LYS:HA	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:LEU:O	1:F:263:VAL:HG23	2.16	0.46
1:F:365:LEU:O	1:F:368:ARG:HG2	2.15	0.46
1:D:421:ARG:O	1:D:424:SER:OG	2.27	0.46
2:T:67:PHE:HB2	2:T:86:MET:HE1	1.97	0.46
1:L:131:LEU:HD23	1:L:131:LEU:HA	1.78	0.46
1:M:74:VAL:HG12	1:M:514:MET:HE1	1.98	0.46
1:M:171:LYS:HD2	1:M:407:VAL:HG21	1.97	0.46
1:H:278:ALA:CB	1:H:285:ARG:HD2	2.44	0.46
2:V:59:VAL:HG12	2:V:94:ILE:HD11	1.98	0.46
1:A:303:GLU:OE1	1:A:309:LEU:HD11	2.16	0.46
1:E:195:PHE:CE1	1:E:279:PRO:HG3	2.51	0.46
1:E:350:ARG:O	1:E:353:ILE:HG12	2.16	0.46
2:U:13:LYS:HG2	2:U:14:ARG:O	2.16	0.46
2:T:4:ARG:CZ	2:S:94:ILE:HD11	2.46	0.46
1:J:197:ARG:HG3	1:J:277:LYS:O	2.16	0.46
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.98	0.46
1:I:73:MET:SD	1:H:49:ILE:HD11	2.56	0.46
1:M:354:GLU:O	1:M:355:GLU:HG2	2.16	0.46
1:M:450:PRO:O	1:M:454:ILE:HG13	2.16	0.46
1:A:259:LEU:O	1:A:263:VAL:HG23	2.16	0.45
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.98	0.45
1:C:280:GLY:O	1:C:285:ARG:HD3	2.15	0.45
1:D:193:MET:SD	1:D:371:LYS:HB3	2.56	0.45
2:U:14:ARG:HG2	2:U:35:SER:HG	1.81	0.45
2:U:23:GLY:O	2:U:26:VAL:HG12	2.16	0.45
2:R:78:ILE:HG13	2:R:79:ASP:N	2.22	0.45
1:K:77:VAL:HG21	1:K:507:ALA:HA	1.98	0.45
1:J:448:GLU:O	1:J:452:ARG:HG3	2.16	0.45
1:I:305:ILE:HD11	1:H:203:TYR:CE2	2.52	0.45
1:I:362:ARG:O	1:I:366:GLN:HB2	2.15	0.45
1:L:419:LEU:HD11	1:L:500:THR:HG23	1.98	0.45
1:M:452:ARG:HH21	1:M:463:SER:HA	1.79	0.45
1:H:260:ALA:O	1:H:264:VAL:HG23	2.16	0.45
1:N:232:GLU:HG3	1:N:310:GLU:CD	2.41	0.45
1:G:349:ILE:HG12	1:G:368:ARG:NH2	2.32	0.45
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.98	0.45
1:E:305:ILE:N	1:E:306:GLY:HA2	2.30	0.45
1:E:448:GLU:O	1:E:452:ARG:HG3	2.16	0.45
2:R:11:ILE:HB	2:R:85:ILE:CD1	2.45	0.45
2:R:53:GLU:CD	2:S:52:GLY:H	2.24	0.45
1:K:353:ILE:O	1:K:362:ARG:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:308:GLU:OE1	1:J:311:LYS:HB2	2.15	0.45
1:N:115:ASP:OD1	1:N:118:ARG:HD2	2.17	0.45
1:A:199:TYR:CE1	1:A:202:PRO:HA	2.52	0.45
1:B:197:ARG:NH1	1:B:198:GLY:H	2.10	0.45
1:F:421:ARG:HD3	1:F:421:ARG:HA	1.71	0.45
1:D:138:CYS:HB2	1:D:411:VAL:HG13	1.97	0.45
1:D:177:VAL:HG11	1:D:397:GLU:HG2	1.98	0.45
2:Q:91:ILE:HG23	2:R:6:LEU:HD21	1.98	0.45
1:K:176:THR:CG2	1:K:378:VAL:HG22	2.46	0.45
1:M:288:MET:HA	1:M:291:ASP:OD2	2.17	0.45
1:N:319:GLN:HB2	1:N:336:VAL:HG11	1.98	0.45
2:V:21:SER:H	2:V:27:LEU:HG	1.80	0.45
1:G:345:ARG:O	1:G:348:GLN:NE2	2.48	0.45
1:G:364:LYS:HB3	1:G:364:LYS:HE2	1.56	0.45
1:A:450:PRO:O	1:A:454:ILE:HG13	2.16	0.45
1:B:150:ILE:HG12	1:B:493:ILE:HA	1.99	0.45
1:E:278:ALA:CB	1:E:285:ARG:HD2	2.41	0.45
1:E:443:ALA:O	1:E:447:MET:HG3	2.17	0.45
1:K:339:GLU:O	1:K:343:GLN:HB2	2.17	0.45
1:H:302:SER:CB	1:H:305:ILE:HD13	2.46	0.45
1:G:166:MET:HE1	1:G:407:VAL:HG21	1.98	0.45
1:F:450:PRO:O	1:F:454:ILE:HG13	2.16	0.45
1:E:229:ASN:HB2	1:E:257:GLU:CB	2.46	0.45
1:C:443:ALA:O	1:C:447:MET:HG3	2.17	0.45
1:D:308:GLU:HG2	1:D:310:GLU:OE1	2.15	0.45
2:U:5:PRO:HA	2:T:93:ALA:CB	2.47	0.45
1:L:209:GLU:C	1:L:211:GLY:H	2.24	0.45
1:M:291:ASP:HB3	1:M:372:LEU:HD21	1.98	0.45
1:H:268:ARG:N	1:H:269:GLY:HA2	2.32	0.45
1:G:248:LEU:HD21	1:G:325:ILE:HD11	1.99	0.45
1:B:232:GLU:C	1:B:235:PRO:HD2	2.41	0.45
1:B:241:ALA:CB	1:B:271:VAL:HG11	2.39	0.45
1:E:252:GLU:OE1	1:E:285:ARG:NH2	2.50	0.45
1:C:345:ARG:O	1:C:348:GLN:HG3	2.17	0.45
2:U:91:ILE:HG22	2:U:92:LEU:O	2.16	0.45
1:K:240:VAL:HG11	1:K:314:LEU:HB3	1.98	0.45
1:K:420:ILE:HD11	1:K:470:LYS:CG	2.46	0.45
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.98	0.45
1:M:165:ALA:O	1:M:169:VAL:HG22	2.17	0.45
1:M:257:GLU:HG3	2:1:30:SER:HB2	1.99	0.45
1:M:421:ARG:HD3	1:M:421:ARG:HA	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:80:LYS:HD3	1:N:80:LYS:HA	1.71	0.45
1:N:421:ARG:HD3	1:N:421:ARG:HA	1.75	0.45
1:G:6:VAL:HG12	1:G:521:VAL:HG22	1.99	0.45
1:E:295:LEU:HD23	1:E:335:GLY:HA3	1.98	0.45
1:K:201:SER:HA	1:K:202:PRO:HD2	1.83	0.45
1:J:228:SER:HA	1:J:258:ALA:HB2	1.98	0.45
1:J:252:GLU:HA	1:J:285:ARG:HH11	1.81	0.45
1:M:409:GLU:CD	1:M:501:ARG:HH21	2.24	0.45
2:W:86:MET:HE3	2:W:91:ILE:HG12	1.99	0.45
2:2:19:THR:HG22	2:2:20:LYS:H	1.81	0.45
2:2:57:LEU:O	2:2:59:VAL:N	2.50	0.45
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.99	0.45
1:A:202:PRO:O	1:A:205:ILE:HG12	2.17	0.45
1:A:348:GLN:OE1	1:A:352:GLN:NE2	2.50	0.45
1:E:34:LYS:HG3	1:E:458:CYS:SG	2.57	0.45
1:C:214:GLU:HG2	1:C:324:VAL:HG22	1.99	0.45
1:D:327:LYS:HG3	1:D:328:ASP:OD1	2.17	0.45
1:K:193:MET:HE1	1:K:288:MET:HE2	1.99	0.45
1:J:278:ALA:CB	1:J:285:ARG:HB2	2.47	0.45
1:L:420:ILE:HD11	1:L:470:LYS:HD3	1.99	0.45
1:M:345:ARG:O	1:M:349:ILE:HG13	2.17	0.45
1:N:417:VAL:HG11	1:N:488:MET:HG3	1.98	0.45
2:2:25:ILE:H	2:2:25:ILE:HG13	1.58	0.45
1:A:245:LYS:HB2	1:A:245:LYS:HE3	1.63	0.45
1:A:288:MET:HA	1:A:291:ASP:OD2	2.17	0.45
1:F:206:ASN:HB2	1:F:213:VAL:HA	1.99	0.45
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.98	0.45
1:D:282:GLY:HA2	1:D:285:ARG:CZ	2.46	0.45
2:P:86:MET:HE3	2:P:91:ILE:HG12	1.99	0.45
2:U:14:ARG:NH2	2:U:84:LEU:HD21	2.31	0.45
1:K:65:LYS:O	1:K:69:MET:HG3	2.17	0.45
1:I:128:VAL:HG23	1:I:501:ARG:HG2	1.99	0.45
1:M:206:ASN:OD1	1:M:207:LYS:N	2.41	0.45
1:M:265:ASN:ND2	2:1:27:LEU:HD13	2.27	0.45
1:M:302:SER:HB2	1:M:305:ILE:CG2	2.47	0.45
1:H:414:GLY:HA2	1:H:495:ASP:OD2	2.16	0.45
1:N:258:ALA:O	1:N:262:LEU:HB2	2.16	0.45
2:1:3:ILE:HG12	2:1:78:ILE:HD13	1.98	0.45
1:A:310:GLU:OE1	1:A:310:GLU:N	2.50	0.45
1:B:197:ARG:HD2	1:B:197:ARG:HA	1.62	0.45
1:F:231:ARG:HE	1:F:261:THR:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.98	0.45
1:C:65:LYS:O	1:C:69:MET:HG3	2.17	0.45
1:C:260:ALA:O	1:C:264:VAL:HG23	2.17	0.45
1:C:347:ALA:HA	1:C:350:ARG:HG3	1.99	0.45
1:D:28:LYS:HG2	1:D:94:VAL:HG22	1.98	0.45
2:O:94:ILE:HD11	2:P:4:ARG:HH11	1.81	0.45
2:P:61:VAL:HG12	2:P:62:GLY:N	2.31	0.45
2:S:22:ALA:N	2:S:23:GLY:C	2.75	0.45
1:K:441:LYS:HD3	1:K:441:LYS:HA	1.67	0.45
1:J:345:ARG:O	1:J:349:ILE:HG13	2.17	0.45
1:J:358:SER:O	1:J:362:ARG:HG2	2.17	0.45
1:I:280:GLY:H	1:I:285:ARG:HB3	1.82	0.45
1:I:309:LEU:HD12	1:I:310:GLU:N	2.32	0.45
1:L:230:ILE:CG2	1:L:233:MET:HB2	2.46	0.45
1:M:187:LEU:HD13	1:M:379:ILE:HG12	1.99	0.45
1:M:247:LEU:HD12	1:M:273:VAL:HG13	1.98	0.45
1:M:314:LEU:HD12	1:M:315:GLU:N	2.32	0.45
1:M:385:THR:HG22	1:N:509:SER:OG	2.17	0.45
1:H:197:ARG:HD3	1:H:197:ARG:HA	1.71	0.45
1:N:174:VAL:HG23	1:N:370:ALA:HB2	1.99	0.45
1:A:239:ALA:O	1:A:242:LYS:HG2	2.16	0.44
1:F:260:ALA:HB1	1:E:306:GLY:N	2.32	0.44
1:E:196:ASP:O	1:E:197:ARG:NH1	2.48	0.44
1:E:219:PHE:O	1:E:248:LEU:N	2.47	0.44
1:D:232:GLU:C	1:D:235:PRO:HD2	2.42	0.44
1:K:149:THR:CG2	1:K:156:GLU:HA	2.47	0.44
1:K:165:ALA:O	1:K:169:VAL:HG22	2.17	0.44
1:I:513:LEU:HD11	1:H:388:GLU:HA	1.98	0.44
1:M:204:PHE:CE2	1:M:274:ALA:HA	2.53	0.44
1:H:254:VAL:HG12	1:H:259:LEU:HG	1.99	0.44
2:Y:14:ARG:HG2	2:Y:35:SER:OG	2.17	0.44
1:G:270:ILE:CD1	2:U:27:LEU:HB3	2.47	0.44
1:G:417:VAL:O	1:G:421:ARG:HB2	2.17	0.44
1:B:262:LEU:O	1:B:266:THR:HG23	2.16	0.44
1:B:441:LYS:O	1:B:445:ARG:HB2	2.17	0.44
1:C:14:VAL:O	1:C:18:ARG:HG3	2.16	0.44
2:Q:12:VAL:HG23	2:Q:39:GLU:C	2.42	0.44
1:K:225:LYS:HD2	1:K:226:LYS:H	1.82	0.44
1:J:310:GLU:OE1	1:J:310:GLU:N	2.50	0.44
1:I:196:ASP:O	1:I:197:ARG:HG3	2.17	0.44
1:M:322:ARG:HG2	1:M:323:VAL:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:GLU:OE1	1:H:285:ARG:NH2	2.50	0.44
1:N:477:GLY:C	1:N:488:MET:HE3	2.42	0.44
1:A:305:ILE:HD12	1:B:263:VAL:HG11	2.00	0.44
1:E:264:VAL:HG12	2:S:27:LEU:HD21	1.99	0.44
1:C:232:GLU:HG2	1:C:233:MET:H	1.82	0.44
2:S:15:LYS:HG3	2:S:16:GLU:N	2.25	0.44
1:J:352:GLN:HB3	1:J:365:LEU:HD11	1.99	0.44
1:J:418:ALA:O	1:J:422:VAL:HG13	2.17	0.44
1:H:242:LYS:O	1:H:242:LYS:HG2	2.17	0.44
1:H:441:LYS:HD3	1:H:441:LYS:HA	1.57	0.44
1:N:194:GLN:HG3	1:N:330:THR:O	2.17	0.44
1:N:313:THR:CG2	1:N:315:GLU:HG2	2.47	0.44
2:Z:43:VAL:HG11	2:Z:59:VAL:O	2.17	0.44
1:E:345:ARG:O	1:E:348:GLN:HG3	2.17	0.44
1:E:475:ASN:O	1:E:488:MET:HG2	2.16	0.44
2:Q:49:LEU:O	2:Q:52:GLY:HA2	2.18	0.44
2:Q:49:LEU:HB2	2:Q:53:GLU:HB2	1.97	0.44
1:K:169:VAL:HG11	1:K:377:ALA:HB2	1.99	0.44
1:J:177:VAL:HG11	1:J:397:GLU:HG2	1.99	0.44
1:I:218:PRO:HG3	1:I:323:VAL:HG22	1.99	0.44
1:L:301:ILE:HG21	1:L:309:LEU:HD23	2.00	0.44
1:H:305:ILE:HD11	1:N:203:TYR:CZ	2.53	0.44
2:2:80:ASN:O	2:2:80:ASN:ND2	2.41	0.44
1:A:225:LYS:HD2	1:A:226:LYS:H	1.83	0.44
1:B:233:MET:HG3	1:B:234:LEU:N	2.32	0.44
1:B:322:ARG:O	1:B:333:ILE:HG12	2.17	0.44
1:B:450:PRO:O	1:B:454:ILE:HG13	2.18	0.44
1:F:353:ILE:HD11	1:F:369:VAL:HG21	1.98	0.44
1:J:77:VAL:HB	1:J:510:VAL:HG21	2.00	0.44
1:L:91:THR:OG1	3:L:601:ADP:O3B	2.32	0.44
1:L:174:VAL:HG21	1:L:367:GLU:HA	1.99	0.44
1:N:193:MET:HE3	1:N:195:PHE:HD2	1.83	0.44
2:W:14:ARG:NH1	2:W:84:LEU:HD21	2.33	0.44
2:Z:76:GLU:OE2	2:1:36:THR:OG1	2.32	0.44
1:G:199:TYR:HA	1:G:276:VAL:HG12	2.00	0.44
1:B:205:ILE:HD12	1:B:211:GLY:C	2.43	0.44
1:F:278:ALA:HB3	1:F:285:ARG:HD3	2.00	0.44
1:E:227:ILE:HG22	1:E:227:ILE:O	2.17	0.44
1:C:128:VAL:HG23	1:C:501:ARG:HG2	2.00	0.44
1:C:142:LYS:O	1:C:146:GLN:HG3	2.17	0.44
1:C:227:ILE:HD12	1:C:230:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:89:SER:O	2:P:9:ARG:NH2	2.50	0.44
2:Q:69:ASP:CB	2:Q:73:VAL:HG11	2.48	0.44
1:K:116:LEU:O	1:K:120:ILE:HG13	2.16	0.44
1:J:23:LEU:O	1:J:27:VAL:HG22	2.17	0.44
1:H:195:PHE:HB2	1:H:279:PRO:HB3	2.00	0.44
1:H:421:ARG:HA	1:H:421:ARG:HD3	1.86	0.44
2:X:9:ARG:NH2	2:Y:89:SER:O	2.51	0.44
1:A:199:TYR:CZ	1:A:205:ILE:HD11	2.52	0.44
1:A:200:LEU:HD23	1:A:254:VAL:HB	2.00	0.44
1:A:226:LYS:HE2	1:A:252:GLU:HG2	2.00	0.44
1:E:368:ARG:HA	1:E:368:ARG:CZ	2.47	0.44
1:D:412:VAL:HG13	1:D:497:THR:OG1	2.18	0.44
2:U:5:PRO:HG2	2:U:43:VAL:C	2.43	0.44
2:T:4:ARG:O	2:S:93:ALA:HB1	2.18	0.44
2:T:13:LYS:HD2	2:T:81:GLU:OE1	2.17	0.44
2:S:57:LEU:HD23	2:S:57:LEU:HA	1.64	0.44
2:W:73:VAL:HG22	2:W:86:MET:HB3	1.99	0.44
2:Y:3:ILE:HD11	2:Y:78:ILE:HG21	2.00	0.44
1:G:197:ARG:HD3	1:G:197:ARG:HA	1.82	0.44
3:G:601:ADP:O1A	4:G:602:BEF:F2	2.26	0.44
1:B:311:LYS:O	1:B:311:LYS:HD3	2.17	0.44
1:F:254:VAL:HG12	1:F:259:LEU:HD12	1.98	0.44
1:F:305:ILE:HG22	1:F:306:GLY:N	2.31	0.44
1:E:412:VAL:HG13	1:E:497:THR:HG1	1.83	0.44
1:C:420:ILE:HD11	1:C:470:LYS:CG	2.46	0.44
1:K:54:VAL:HB	1:K:89:THR:HG21	1.99	0.44
1:K:421:ARG:HD3	1:K:421:ARG:HA	1.84	0.44
1:K:450:PRO:O	1:K:454:ILE:HG13	2.16	0.44
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.98	0.44
1:I:333:ILE:HG13	1:I:334:ASP:N	2.31	0.44
1:L:387:VAL:HG21	1:M:510:VAL:HG12	2.00	0.44
1:B:358:SER:OG	1:B:359:ASP:N	2.42	0.44
1:E:226:LYS:HD2	1:E:226:LYS:H	1.83	0.44
1:C:343:GLN:HA	1:C:346:VAL:HG22	2.00	0.44
1:D:151:SER:HB3	1:D:399:ALA:HA	2.00	0.44
2:U:14:ARG:NH1	2:U:34:LYS:HB2	2.33	0.44
2:S:13:LYS:HB2	2:S:41:LEU:HD11	1.99	0.44
1:K:246:PRO:HB3	1:K:272:LYS:HE3	1.99	0.44
1:J:345:ARG:O	1:J:348:GLN:HG3	2.18	0.44
1:I:283:ASP:HA	1:I:286:LYS:HE2	2.00	0.44
1:L:124:VAL:HG21	1:L:508:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:418:ALA:O	1:M:422:VAL:HG13	2.18	0.44
1:H:34:LYS:HG3	1:H:458:CYS:SG	2.58	0.44
1:H:183:LEU:H	1:H:183:LEU:HD12	1.83	0.44
2:W:54:VAL:O	2:W:56:PRO:HD3	2.18	0.44
1:G:215:LEU:HB2	1:G:323:VAL:HG22	1.99	0.43
1:G:409:GLU:CD	1:G:501:ARG:HH21	2.24	0.43
1:A:346:VAL:O	1:A:350:ARG:HG3	2.18	0.43
1:E:218:PRO:HA	1:E:246:PRO:HG2	1.99	0.43
1:C:90:THR:O	1:C:94:VAL:HG23	2.18	0.43
1:C:282:GLY:HA2	1:C:285:ARG:NH2	2.33	0.43
1:C:438:VAL:O	1:C:442:VAL:HG23	2.18	0.43
2:O:91:ILE:HG22	2:O:92:LEU:O	2.17	0.43
2:Q:93:ALA:CB	2:R:5:PRO:HA	2.48	0.43
1:K:149:THR:HG22	1:K:156:GLU:HA	2.00	0.43
1:J:249:ILE:HB	1:J:275:ALA:HA	2.00	0.43
1:J:282:GLY:O	1:J:285:ARG:HG2	2.18	0.43
1:J:303:GLU:HB2	1:J:309:LEU:HD21	2.00	0.43
1:I:18:ARG:NH1	1:I:18:ARG:HB3	2.33	0.43
1:M:310:GLU:H	1:M:310:GLU:CD	2.26	0.43
1:N:197:ARG:HA	1:N:197:ARG:HD3	1.82	0.43
2:W:52:GLY:HA3	2:W:53:GLU:HA	1.46	0.43
2:1:14:ARG:HG3	2:1:84:LEU:HD13	2.00	0.43
1:B:429:LEU:HG	1:B:440:ILE:HD13	2.00	0.43
1:F:218:PRO:HB3	1:F:246:PRO:HG2	2.00	0.43
1:E:213:VAL:CG1	1:E:325:ILE:HB	2.49	0.43
2:O:95:VAL:HA	2:P:3:ILE:HG22	2.00	0.43
1:J:124:VAL:HG21	1:J:508:ALA:CB	2.47	0.43
1:J:222:LEU:HD22	1:J:293:ALA:HB2	2.00	0.43
1:J:358:SER:HB3	1:J:359:ASP:H	1.58	0.43
1:H:151:SER:HB3	1:H:399:ALA:HA	1.98	0.43
1:H:193:MET:SD	1:H:371:LYS:HB3	2.58	0.43
1:N:177:VAL:HG11	1:N:397:GLU:HG2	2.00	0.43
1:N:479:ASN:HB2	1:N:491:MET:HE1	1.99	0.43
2:X:73:VAL:HG12	2:X:86:MET:HB3	1.99	0.43
1:G:227:ILE:HA	1:G:230:ILE:HD11	2.00	0.43
1:A:269:GLY:C	1:A:271:VAL:N	2.77	0.43
1:B:348:GLN:HA	1:C:209:GLU:HB2	1.99	0.43
1:E:436:GLN:O	1:E:440:ILE:HG13	2.18	0.43
1:K:270:ILE:HG21	2:Y:26:VAL:HG13	2.00	0.43
1:J:365:LEU:HD23	1:J:365:LEU:HA	1.69	0.43
1:I:225:LYS:CB	1:I:303:GLU:HG3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:ASP:HB2	1:H:524:LEU:HD23	2.00	0.43
1:H:24:ALA:O	1:H:28:LYS:HG3	2.18	0.43
1:N:162:ILE:HD13	1:N:400:LEU:HA	2.00	0.43
1:N:354:GLU:O	1:N:354:GLU:HG2	2.17	0.43
2:V:40:VAL:HG13	2:V:62:GLY:N	2.33	0.43
2:2:20:LYS:NZ	2:1:77:LYS:HE2	2.32	0.43
1:G:225:LYS:HD3	1:G:303:GLU:OE1	2.18	0.43
1:B:253:ASP:OD1	1:B:254:VAL:N	2.48	0.43
1:F:215:LEU:O	1:F:322:ARG:HA	2.19	0.43
1:E:30:THR:HB	1:E:51:LYS:HG3	1.99	0.43
1:E:228:SER:CA	1:E:255:GLU:HB2	2.44	0.43
1:D:10:ASN:O	1:D:14:VAL:HG23	2.18	0.43
1:D:231:ARG:O	1:D:235:PRO:HD3	2.18	0.43
2:P:50:GLU:HB2	2:Q:50:GLU:HB2	1.99	0.43
1:K:224:ASP:O	1:K:252:GLU:HB2	2.18	0.43
1:L:350:ARG:HA	1:L:353:ILE:HD12	2.01	0.43
1:M:213:VAL:CG1	1:M:325:ILE:HB	2.48	0.43
1:M:222:LEU:HD22	1:M:293:ALA:HB2	2.01	0.43
2:W:93:ALA:CB	2:V:5:PRO:HA	2.48	0.43
1:F:217:SER:HA	1:F:320:ALA:O	2.18	0.43
1:F:281:PHE:HB2	1:F:284:ARG:NH1	2.32	0.43
1:E:266:THR:CG2	1:E:273:VAL:H	2.32	0.43
1:C:13:ARG:NH1	1:C:517:THR:O	2.51	0.43
2:O:47:ARG:O	2:O:54:VAL:HA	2.18	0.43
1:J:260:ALA:HA	1:J:263:VAL:HG12	2.00	0.43
1:J:288:MET:HA	1:J:291:ASP:OD2	2.18	0.43
1:I:421:ARG:HD3	1:I:421:ARG:HA	1.76	0.43
1:H:65:LYS:O	1:H:69:MET:HG3	2.17	0.43
1:N:325:ILE:HG13	1:N:330:THR:HG23	2.01	0.43
2:W:61:VAL:HG12	2:W:62:GLY:H	1.83	0.43
2:2:47:ARG:O	2:2:54:VAL:HA	2.18	0.43
2:2:49:LEU:HD12	2:2:49:LEU:O	2.18	0.43
1:G:261:THR:HG22	2:U:29:GLY:CA	2.49	0.43
1:B:230:ILE:C	1:B:232:GLU:N	2.75	0.43
1:E:230:ILE:HD13	1:E:309:LEU:HD21	2.01	0.43
1:E:232:GLU:C	1:E:235:PRO:HD2	2.44	0.43
1:E:421:ARG:HD3	1:E:421:ARG:HA	1.75	0.43
1:C:270:ILE:HG23	1:C:271:VAL:H	1.84	0.43
2:O:15:LYS:HG2	2:O:38:GLY:HA2	2.01	0.43
2:Q:16:GLU:HG3	2:Q:18:GLU:HG2	2.00	0.43
2:S:47:ARG:HG2	2:S:49:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:240:VAL:CG1	1:K:314:LEU:HB3	2.48	0.43
1:K:293:ALA:HB1	1:K:298:GLY:O	2.19	0.43
1:J:219:PHE:CE2	1:J:245:LYS:HD3	2.53	0.43
1:I:183:LEU:H	1:I:183:LEU:HD12	1.84	0.43
1:I:217:SER:HA	1:I:320:ALA:O	2.18	0.43
1:I:349:ILE:HD11	1:I:365:LEU:HG	2.00	0.43
1:L:140:ASP:N	1:L:140:ASP:OD1	2.52	0.43
1:H:124:VAL:HG21	1:H:508:ALA:CB	2.48	0.43
1:H:244:GLY:C	1:H:245:LYS:HG2	2.43	0.43
1:H:259:LEU:O	1:H:263:VAL:HG23	2.18	0.43
1:N:31:LEU:HD23	1:N:453:GLN:HB3	2.00	0.43
2:2:22:ALA:HA	2:2:23:GLY:HA2	1.73	0.43
2:2:49:LEU:C	2:2:51:ASN:N	2.76	0.43
1:A:199:TYR:HA	1:A:276:VAL:HG12	2.00	0.43
1:F:164:GLU:OE2	1:F:168:LYS:NZ	2.52	0.43
1:F:270:ILE:HD12	1:F:270:ILE:H	1.83	0.43
1:E:308:GLU:HB2	1:E:311:LYS:HB3	1.99	0.43
1:D:199:TYR:CE1	1:D:202:PRO:HA	2.54	0.43
1:D:199:TYR:CE2	1:D:205:ILE:HD11	2.54	0.43
2:O:16:GLU:HB3	2:O:17:VAL:H	1.50	0.43
2:U:6:LEU:H	2:U:6:LEU:CD2	2.32	0.43
1:J:147:VAL:HG22	1:J:403:THR:HG22	2.00	0.43
1:J:272:LYS:HD3	1:J:272:LYS:HA	1.89	0.43
1:L:259:LEU:O	1:L:263:VAL:HG23	2.19	0.43
1:L:404:ARG:O	1:L:408:GLU:HG2	2.19	0.43
1:L:429:LEU:HG	1:L:440:ILE:HD13	2.00	0.43
1:M:31:LEU:HD23	1:M:453:GLN:HB3	2.01	0.43
1:H:194:GLN:HB2	1:H:331:THR:HG22	2.00	0.43
1:H:232:GLU:CG	1:H:233:MET:H	2.27	0.43
1:H:417:VAL:O	1:H:421:ARG:HB2	2.18	0.43
2:W:12:VAL:HG22	2:W:40:VAL:HA	2.00	0.43
2:2:10:VAL:HG21	2:2:91:ILE:HD11	1.99	0.43
1:A:365:LEU:HA	1:A:365:LEU:HD23	1.76	0.43
1:A:421:ARG:HD3	1:A:421:ARG:HA	1.69	0.43
1:B:279:PRO:HB2	1:B:288:MET:HE3	1.99	0.43
1:F:322:ARG:HB2	1:F:333:ILE:HG21	2.01	0.43
1:J:382:GLY:O	1:J:392:LYS:NZ	2.51	0.43
1:J:414:GLY:HA2	1:J:495:ASP:OD2	2.19	0.43
1:L:122:LYS:NZ	1:L:430:ARG:O	2.51	0.43
2:V:91:ILE:HG23	2:2:6:LEU:HD21	2.01	0.43
2:Z:6:LEU:HB2	2:1:93:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.99	0.43
1:B:227:ILE:HD11	1:B:254:VAL:HG13	2.00	0.43
1:F:54:VAL:HB	1:F:89:THR:HG21	2.00	0.43
1:F:90:THR:O	1:F:94:VAL:HG23	2.18	0.43
1:F:200:LEU:HD13	1:F:276:VAL:HA	2.00	0.43
1:F:278:ALA:CB	1:F:285:ARG:HD3	2.49	0.43
1:E:257:GLU:H	1:E:257:GLU:CD	2.27	0.43
1:C:197:ARG:HD3	1:C:197:ARG:HA	1.75	0.43
1:C:232:GLU:HG2	1:C:233:MET:N	2.34	0.43
1:J:306:GLY:HA3	1:I:264:VAL:HG21	2.01	0.43
1:I:150:ILE:HD11	1:I:493:ILE:HG22	2.01	0.43
1:L:203:TYR:HB3	1:L:267:MET:HE3	2.00	0.43
1:M:233:MET:SD	1:M:310:GLU:HB3	2.58	0.43
1:N:199:TYR:CE1	1:N:202:PRO:HA	2.54	0.43
2:Y:20:LYS:HA	2:Y:27:LEU:HD12	2.01	0.43
2:Z:78:ILE:HD12	2:Z:79:ASP:O	2.19	0.43
1:G:234:LEU:HD21	1:G:310:GLU:CG	2.42	0.43
1:A:269:GLY:O	1:A:271:VAL:N	2.41	0.43
1:F:258:ALA:O	1:F:262:LEU:HB2	2.18	0.43
1:E:363:GLU:O	1:E:366:GLN:HG2	2.19	0.43
1:C:253:ASP:OD1	1:C:254:VAL:N	2.52	0.43
2:T:60:LYS:HE3	2:T:61:VAL:HG22	2.00	0.43
1:M:195:PHE:HE2	1:M:197:ARG:HB2	1.84	0.43
1:M:252:GLU:OE1	1:M:285:ARG:NH2	2.52	0.43
1:M:364:LYS:O	1:M:367:GLU:HB3	2.19	0.43
1:N:217:SER:HA	1:N:320:ALA:O	2.19	0.43
1:A:226:LYS:HG2	1:A:252:GLU:HG2	2.01	0.42
1:B:231:ARG:HH21	1:B:261:THR:CG2	2.32	0.42
1:B:305:ILE:CG2	1:B:306:GLY:H	2.31	0.42
1:F:429:LEU:HD12	1:F:430:ARG:H	1.83	0.42
1:C:302:SER:C	1:C:304:GLU:H	2.27	0.42
2:U:15:LYS:HG3	2:U:16:GLU:N	2.33	0.42
2:T:15:LYS:HD3	2:T:37:ARG:CB	2.49	0.42
2:T:57:LEU:O	2:T:58:ASP:HB2	2.19	0.42
2:S:17:VAL:HG22	2:S:18:GLU:H	1.83	0.42
1:K:37:ASN:OD1	1:K:51:LYS:HB2	2.19	0.42
1:J:235:PRO:HA	1:J:238:GLU:CG	2.49	0.42
1:I:496:PRO:O	1:I:499:VAL:HG22	2.19	0.42
1:I:510:VAL:O	1:I:514:MET:HB2	2.19	0.42
1:L:254:VAL:HG12	1:L:259:LEU:HG	2.01	0.42
1:M:171:LYS:HA	1:M:171:LYS:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:171:LYS:HA	1:N:171:LYS:HD3	1.71	0.42
2:X:20:LYS:HB3	2:X:27:LEU:HG	2.01	0.42
2:W:94:ILE:O	2:V:3:ILE:HG23	2.19	0.42
1:A:41:ASP:OD1	1:A:42:LYS:N	2.52	0.42
1:A:197:ARG:HA	1:A:197:ARG:HD3	1.89	0.42
1:B:349:ILE:HD13	1:B:369:VAL:HG22	2.01	0.42
1:F:345:ARG:O	1:F:349:ILE:HG13	2.20	0.42
1:C:131:LEU:HD23	1:C:131:LEU:HA	1.78	0.42
1:C:183:LEU:H	1:C:183:LEU:HD12	1.85	0.42
1:D:289:LEU:HA	1:D:292:ILE:HG22	2.02	0.42
2:O:67:PHE:CE2	2:O:86:MET:HE1	2.54	0.42
2:S:61:VAL:HG22	2:S:62:GLY:N	2.34	0.42
1:K:6:VAL:HA	1:K:520:MET:O	2.18	0.42
1:K:147:VAL:HG22	1:K:403:THR:HG22	2.00	0.42
1:K:357:THR:HG21	1:K:361:ASP:HB2	2.01	0.42
1:J:140:ASP:OD1	1:J:140:ASP:N	2.52	0.42
1:I:238:GLU:HA	1:I:241:ALA:HB3	2.00	0.42
1:I:261:THR:HG22	2:W:29:GLY:N	2.34	0.42
1:L:345:ARG:O	1:L:349:ILE:HG13	2.18	0.42
1:N:218:PRO:HG3	1:N:323:VAL:HG22	2.00	0.42
1:A:54:VAL:HB	1:A:89:THR:HG21	2.01	0.42
1:B:217:SER:O	1:B:245:LYS:HD2	2.20	0.42
1:B:517:THR:HG23	1:C:39:VAL:HG23	2.01	0.42
1:F:207:LYS:HA	1:F:208:PRO:HD2	1.94	0.42
1:E:289:LEU:HD12	1:E:290:GLN:N	2.34	0.42
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.27	0.42
1:K:293:ALA:O	1:K:297:GLY:N	2.52	0.42
1:I:219:PHE:HB3	1:I:317:LEU:HD13	2.00	0.42
1:L:349:ILE:O	1:L:353:ILE:HG13	2.19	0.42
1:M:197:ARG:HD3	1:M:197:ARG:HA	1.90	0.42
1:H:199:TYR:CE1	1:H:202:PRO:HA	2.54	0.42
1:H:496:PRO:O	1:H:499:VAL:HG22	2.19	0.42
1:N:131:LEU:HA	1:N:131:LEU:HD23	1.80	0.42
2:X:60:LYS:HB2	2:X:63:ASP:OD2	2.19	0.42
2:Z:74:LYS:HB3	2:Z:85:ILE:HD11	2.01	0.42
1:B:223:ALA:O	1:B:251:ALA:HA	2.20	0.42
1:C:124:VAL:HG21	1:C:508:ALA:HB2	2.01	0.42
1:C:193:MET:SD	1:C:371:LYS:HB3	2.59	0.42
1:D:90:THR:O	1:D:94:VAL:HG23	2.20	0.42
2:Q:67:PHE:HA	2:Q:92:LEU:HD13	2.01	0.42
1:K:336:VAL:HG12	1:K:336:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:LYS:HD2	1:I:453:GLN:CD	2.44	0.42
1:L:475:ASN:O	1:L:488:MET:HG2	2.20	0.42
1:M:352:GLN:O	1:M:355:GLU:HB3	2.19	0.42
1:N:28:LYS:HD2	1:N:453:GLN:NE2	2.34	0.42
2:W:37:ARG:HH22	2:V:78:ILE:HD13	1.84	0.42
2:2:19:THR:OG1	2:2:33:ALA:HB1	2.19	0.42
1:A:151:SER:HB3	1:A:399:ALA:HA	2.01	0.42
1:B:261:THR:HG22	2:P:29:GLY:N	2.34	0.42
1:C:259:LEU:O	1:C:263:VAL:HG23	2.19	0.42
1:C:334:ASP:OD1	1:C:335:GLY:N	2.52	0.42
1:D:345:ARG:O	1:D:349:ILE:HG12	2.19	0.42
2:O:78:ILE:HG22	2:U:37:ARG:NH2	2.35	0.42
2:Q:65:VAL:HA	2:Q:94:ILE:HA	2.01	0.42
2:Q:69:ASP:HB2	2:Q:73:VAL:HG11	2.00	0.42
2:R:5:PRO:HG3	2:R:11:ILE:HG22	2.02	0.42
1:K:221:LEU:HB3	1:K:249:ILE:HD13	2.01	0.42
1:K:290:GLN:HB3	1:K:345:ARG:HH22	1.83	0.42
1:K:367:GLU:O	1:K:371:LYS:HG3	2.19	0.42
1:I:48:THR:HG22	1:I:390:LYS:NZ	2.34	0.42
1:I:231:ARG:HB2	1:I:234:LEU:HD22	2.02	0.42
1:I:251:ALA:O	1:I:278:ALA:N	2.53	0.42
1:L:30:THR:OG1	1:L:51:LYS:O	2.31	0.42
2:W:53:GLU:HG3	2:W:54:VAL:N	2.29	0.42
2:2:25:ILE:HA	2:2:26:VAL:HA	1.68	0.42
2:1:18:GLU:HG2	2:1:19:THR:N	2.34	0.42
1:G:127:ALA:HB1	1:G:447:MET:HE1	2.01	0.42
1:G:193:MET:HB3	1:G:332:ILE:HD11	2.01	0.42
1:A:177:VAL:CG1	1:A:397:GLU:HG2	2.47	0.42
1:A:336:VAL:O	1:A:336:VAL:HG12	2.19	0.42
1:B:213:VAL:O	1:B:324:VAL:HA	2.20	0.42
1:B:237:LEU:CD1	1:B:312:ALA:HB3	2.46	0.42
1:F:256:GLY:O	1:F:259:LEU:N	2.53	0.42
1:C:418:ALA:O	1:C:422:VAL:HG13	2.20	0.42
2:P:1:MET:SD	2:P:1:MET:N	2.90	0.42
1:I:311:LYS:O	1:I:311:LYS:HD3	2.19	0.42
1:L:267:MET:SD	1:M:305:ILE:HD11	2.59	0.42
1:M:336:VAL:O	1:M:336:VAL:HG12	2.20	0.42
1:H:77:VAL:HB	1:H:510:VAL:HG21	2.02	0.42
2:Z:10:VAL:HG22	2:Z:43:VAL:HG12	2.01	0.42
2:2:19:THR:HG22	2:2:20:LYS:N	2.34	0.42
1:G:227:ILE:O	1:G:227:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:303:GLU:HG3	1:G:304:GLU:N	2.35	0.42
1:G:506:TYR:O	1:G:510:VAL:HG23	2.20	0.42
1:A:60:ILE:O	1:A:75:LYS:NZ	2.52	0.42
1:A:165:ALA:O	1:A:169:VAL:HG22	2.19	0.42
1:B:224:ASP:O	1:B:252:GLU:HB2	2.20	0.42
1:F:197:ARG:HA	1:F:197:ARG:HD3	1.86	0.42
1:E:177:VAL:HG11	1:E:397:GLU:HG2	2.01	0.42
1:E:210:THR:HG23	1:D:351:GLN:CD	2.45	0.42
1:D:30:THR:HB	1:D:51:LYS:HG3	2.02	0.42
2:Q:4:ARG:HD3	2:Q:4:ARG:HA	1.72	0.42
2:T:5:PRO:HG3	2:T:42:ALA:C	2.44	0.42
1:I:77:VAL:HG21	1:I:507:ALA:HA	2.02	0.42
1:M:245:LYS:HB3	1:M:246:PRO:HD2	2.01	0.42
1:N:160:LYS:HD2	1:N:160:LYS:HA	1.88	0.42
1:N:291:ASP:HB3	1:N:372:LEU:HD21	2.01	0.42
1:G:124:VAL:HG22	1:G:504:LEU:HD11	2.02	0.42
1:G:449:ALA:HB3	1:G:450:PRO:HD3	2.00	0.42
1:G:450:PRO:O	1:G:454:ILE:HG13	2.19	0.42
1:A:290:GLN:OE1	1:A:290:GLN:N	2.41	0.42
1:B:183:LEU:HD12	1:B:183:LEU:H	1.84	0.42
1:E:449:ALA:HB3	1:E:450:PRO:HD3	2.02	0.42
1:C:28:LYS:HD2	1:C:453:GLN:CD	2.44	0.42
1:C:310:GLU:OE1	1:C:310:GLU:N	2.52	0.42
1:D:197:ARG:HH11	1:D:277:LYS:HD3	1.84	0.42
2:P:15:LYS:HD2	2:P:15:LYS:HA	1.84	0.42
2:P:51:ASN:C	2:P:53:GLU:H	2.26	0.42
2:S:14:ARG:NE	2:S:84:LEU:HD11	2.34	0.42
1:J:414:GLY:HA2	1:J:495:ASP:CG	2.44	0.42
1:I:204:PHE:CZ	1:I:262:LEU:HD23	2.55	0.42
1:I:461:GLU:HA	1:I:462:PRO:HD3	1.91	0.42
1:L:218:PRO:HB3	1:L:246:PRO:HG2	2.01	0.42
1:M:34:LYS:HE2	1:M:480:ALA:O	2.19	0.42
2:2:11:ILE:CG2	2:2:42:ALA:HB3	2.50	0.42
1:G:28:LYS:HD2	1:G:453:GLN:NE2	2.35	0.42
1:G:90:THR:O	1:G:94:VAL:HG23	2.19	0.42
1:G:293:ALA:O	1:G:297:GLY:N	2.53	0.42
1:A:349:ILE:HD13	1:A:368:ARG:HD2	2.01	0.42
1:A:514:MET:O	1:A:517:THR:HG23	2.20	0.42
1:B:102:GLU:HB2	1:B:442:VAL:HG13	2.02	0.42
1:B:214:GLU:HG2	1:B:324:VAL:HG22	2.00	0.42
1:F:203:TYR:HB3	1:F:267:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:ARG:NH2	1:F:463:SER:HA	2.35	0.42
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.50	0.42
1:E:268:ARG:HG3	2:S:27:LEU:CD2	2.49	0.42
1:C:282:GLY:HA2	1:C:285:ARG:NE	2.35	0.42
1:K:259:LEU:O	1:K:263:VAL:HG23	2.20	0.42
1:J:342:ILE:O	1:J:346:VAL:HG23	2.19	0.42
1:L:314:LEU:HD12	1:L:315:GLU:N	2.35	0.42
1:L:391:GLU:OE2	1:L:395:ARG:NE	2.53	0.42
1:M:7:LYS:HB3	1:M:12:ALA:HB2	2.02	0.42
1:M:305:ILE:C	1:M:307:MET:H	2.27	0.42
1:H:322:ARG:HG2	1:H:323:VAL:N	2.35	0.42
1:H:367:GLU:O	1:H:371:LYS:HG3	2.20	0.42
2:Z:15:LYS:HD3	2:Z:37:ARG:CB	2.50	0.42
1:G:165:ALA:O	1:G:169:VAL:HG22	2.20	0.42
1:F:142:LYS:HE2	1:F:146:GLN:NE2	2.35	0.42
1:F:443:ALA:O	1:F:447:MET:HG3	2.20	0.42
1:E:414:GLY:HA3	1:E:493:ILE:HG22	2.01	0.42
1:C:28:LYS:HG2	1:C:94:VAL:HG22	2.02	0.42
2:S:79:ASP:C	2:S:81:GLU:H	2.28	0.42
1:J:346:VAL:O	1:J:350:ARG:HG3	2.20	0.42
1:J:365:LEU:O	1:J:369:VAL:HG23	2.19	0.42
1:J:404:ARG:O	1:J:408:GLU:HG3	2.19	0.42
1:J:496:PRO:O	1:J:499:VAL:HG22	2.20	0.42
1:I:358:SER:OG	1:I:359:ASP:N	2.50	0.42
1:L:215:LEU:HB2	1:L:323:VAL:CG2	2.50	0.42
1:H:138:CYS:HB2	1:H:411:VAL:HG13	2.02	0.42
1:N:404:ARG:O	1:N:408:GLU:HG3	2.20	0.42
2:V:20:LYS:NZ	2:V:33:ALA:HB3	2.35	0.42
2:Y:46:GLY:HA2	2:Y:57:LEU:HD12	2.02	0.42
1:B:13:ARG:HD2	1:B:104:LEU:HD22	2.01	0.41
1:B:39:VAL:HG22	1:B:49:ILE:HG12	2.02	0.41
1:B:248:LEU:HD12	1:B:323:VAL:HG21	2.02	0.41
1:B:333:ILE:HG13	1:B:334:ASP:N	2.27	0.41
1:E:336:VAL:O	1:E:336:VAL:HG12	2.20	0.41
1:C:123:ALA:HB2	1:C:440:ILE:HG23	2.02	0.41
1:C:364:LYS:HA	1:C:367:GLU:HB3	2.02	0.41
1:C:434:GLU:O	1:C:438:VAL:HG23	2.20	0.41
2:O:73:VAL:HG12	2:O:86:MET:HB3	2.02	0.41
2:U:6:LEU:H	2:U:6:LEU:HD23	1.85	0.41
1:K:142:LYS:O	1:K:146:GLN:HG3	2.20	0.41
1:K:291:ASP:OD2	1:K:368:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:SER:HB2	1:I:259:LEU:HD22	2.02	0.41
1:L:230:ILE:HG22	1:L:230:ILE:O	2.20	0.41
1:L:231:ARG:HH11	1:L:258:ALA:HA	1.85	0.41
1:H:214:GLU:HG2	1:H:324:VAL:HG22	2.01	0.41
1:H:345:ARG:HA	1:H:348:GLN:HG3	2.02	0.41
2:2:57:LEU:HA	2:2:57:LEU:HD23	1.80	0.41
1:G:205:ILE:HD13	1:G:211:GLY:HA2	2.02	0.41
1:A:127:ALA:HB1	1:A:447:MET:HE1	2.02	0.41
1:A:429:LEU:HG	1:A:440:ILE:HD13	2.02	0.41
1:B:197:ARG:CG	1:B:277:LYS:HB3	2.49	0.41
1:B:200:LEU:HD22	1:B:254:VAL:HB	2.01	0.41
1:E:365:LEU:O	1:E:368:ARG:HB3	2.19	0.41
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.50	0.41
2:P:13:LYS:HB2	2:P:41:LEU:HD11	2.03	0.41
1:K:510:VAL:HG13	1:J:387:VAL:HG21	2.01	0.41
1:I:336:VAL:O	1:I:336:VAL:HG12	2.20	0.41
1:L:197:ARG:HD2	1:L:277:LYS:HB3	2.02	0.41
1:M:140:ASP:OD1	1:M:140:ASP:N	2.53	0.41
1:H:517:THR:HG23	1:N:39:VAL:HG23	2.01	0.41
1:N:13:ARG:HD2	1:N:104:LEU:HD22	2.02	0.41
1:N:91:THR:OG1	3:N:601:ADP:O2B	2.38	0.41
2:V:25:ILE:HG13	2:V:26:VAL:HG23	2.02	0.41
2:Z:85:ILE:CD1	2:1:92:LEU:HD13	2.48	0.41
1:G:456:LEU:HD13	1:G:462:PRO:HG3	2.03	0.41
1:A:278:ALA:HB3	1:A:285:ARG:HD3	2.01	0.41
1:B:54:VAL:HB	1:B:89:THR:HG21	2.01	0.41
1:B:227:ILE:H	1:B:227:ILE:HG13	1.71	0.41
1:B:239:ALA:O	1:B:242:LYS:HG2	2.20	0.41
1:E:124:VAL:HG22	1:E:504:LEU:HD11	2.00	0.41
1:E:195:PHE:HE2	1:E:197:ARG:HB2	1.85	0.41
1:D:405:ALA:HB1	1:D:498:LYS:HB3	2.02	0.41
2:O:57:LEU:HD23	2:O:57:LEU:HA	1.87	0.41
2:P:4:ARG:HA	2:P:5:PRO:HD2	1.94	0.41
2:P:14:ARG:NH2	2:P:69:ASP:OD2	2.54	0.41
2:P:64:ILE:HG23	2:P:95:VAL:HB	2.01	0.41
2:T:40:VAL:HG12	2:T:63:ASP:O	2.19	0.41
2:T:55:LYS:HA	2:T:56:PRO:HD3	1.74	0.41
1:K:210:THR:HA	1:L:351:GLN:CB	2.50	0.41
1:K:290:GLN:C	1:K:345:ARG:HH12	2.28	0.41
1:J:215:LEU:HB2	1:J:323:VAL:CG2	2.50	0.41
1:L:214:GLU:HG2	1:L:324:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:PHE:CE2	1:H:274:ALA:HA	2.55	0.41
1:H:325:ILE:HG12	1:H:330:THR:HG23	2.02	0.41
1:N:41:ASP:OD1	1:N:42:LYS:N	2.53	0.41
2:Y:60:LYS:HB2	2:Y:63:ASP:OD2	2.20	0.41
2:2:49:LEU:O	2:2:51:ASN:N	2.53	0.41
1:G:429:LEU:HG	1:G:440:ILE:HD13	2.02	0.41
1:G:517:THR:HG23	1:A:39:VAL:HG23	2.03	0.41
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.88	0.41
1:B:123:ALA:HB2	1:B:440:ILE:HG23	2.02	0.41
1:F:386:GLU:HG2	1:E:76:GLU:OE2	2.20	0.41
1:C:8:PHE:HE2	1:D:26:ALA:HA	1.85	0.41
1:C:237:LEU:HD21	1:C:312:ALA:CB	2.51	0.41
1:C:361:ASP:OD2	1:C:365:LEU:HD22	2.20	0.41
1:D:24:ALA:O	1:D:28:LYS:HG3	2.20	0.41
2:Q:12:VAL:HG23	2:Q:39:GLU:O	2.21	0.41
2:T:22:ALA:C	2:T:24:GLY:N	2.79	0.41
2:S:43:VAL:CG2	2:S:57:LEU:HD13	2.50	0.41
1:K:226:LYS:O	1:K:230:ILE:HD12	2.20	0.41
1:K:232:GLU:HG2	1:K:233:MET:N	2.35	0.41
1:J:87:ASP:OD1	4:J:602:BEF:F3	2.28	0.41
1:J:197:ARG:HG2	1:J:279:PRO:HA	2.02	0.41
1:J:255:GLU:HG3	1:J:256:GLY:N	2.35	0.41
1:L:230:ILE:HD12	1:L:230:ILE:N	2.35	0.41
1:H:41:ASP:OD1	1:H:42:LYS:N	2.53	0.41
1:A:278:ALA:CB	1:A:285:ARG:HB2	2.50	0.41
1:C:112:ASN:HA	1:C:113:PRO:HD3	1.93	0.41
1:C:124:VAL:HG22	1:C:504:LEU:HD11	2.02	0.41
1:C:247:LEU:HB3	1:C:273:VAL:HG13	2.02	0.41
1:D:166:MET:HE1	1:D:407:VAL:HG21	2.01	0.41
1:D:206:ASN:C	1:D:207:LYS:HG2	2.45	0.41
2:O:23:GLY:N	2:P:80:ASN:OD1	2.39	0.41
2:S:17:VAL:HG22	2:S:18:GLU:HG2	2.02	0.41
1:K:90:THR:O	1:K:94:VAL:HG23	2.21	0.41
1:K:290:GLN:HB3	1:K:345:ARG:NH2	2.35	0.41
1:J:213:VAL:HG22	1:J:325:ILE:HB	2.02	0.41
1:L:264:VAL:HG21	1:M:306:GLY:CA	2.50	0.41
1:L:420:ILE:HD11	1:L:470:LYS:HG2	2.02	0.41
1:M:34:LYS:HG3	1:M:458:CYS:SG	2.60	0.41
1:N:152:ALA:HB2	1:N:399:ALA:HB2	2.01	0.41
2:Z:4:ARG:NH2	2:1:94:ILE:HD11	2.35	0.41
1:G:245:LYS:HB3	1:G:246:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HB	1:A:510:VAL:HG21	2.03	0.41
3:B:601:ADP:O3A	4:B:602:BEF:F1	2.28	0.41
1:F:147:VAL:HG22	1:F:403:THR:HG22	2.03	0.41
1:E:230:ILE:HG22	1:E:233:MET:H	1.84	0.41
1:C:199:TYR:HA	1:C:276:VAL:HG12	2.03	0.41
1:C:322:ARG:HG2	1:C:323:VAL:N	2.36	0.41
1:D:215:LEU:HB2	1:D:323:VAL:CG2	2.51	0.41
1:K:434:GLU:O	1:K:438:VAL:HG23	2.21	0.41
1:I:409:GLU:CD	1:I:501:ARG:HH21	2.29	0.41
1:M:31:LEU:HD12	3:M:601:ADP:O2A	2.20	0.41
1:M:288:MET:HE1	1:M:371:LYS:HD2	2.01	0.41
1:M:475:ASN:O	1:M:488:MET:HG2	2.21	0.41
1:N:302:SER:HB2	1:N:305:ILE:HD13	2.03	0.41
1:N:488:MET:HE2	1:N:488:MET:HA	2.03	0.41
2:V:93:ALA:CB	2:2:5:PRO:HA	2.51	0.41
2:2:34:LYS:HD2	2:2:34:LYS:HA	1.86	0.41
1:A:258:ALA:O	1:A:262:LEU:HB2	2.20	0.41
1:A:441:LYS:HA	1:A:441:LYS:HD2	1.84	0.41
1:B:226:LYS:HZ2	1:B:255:GLU:CD	2.28	0.41
1:F:5:ASP:HB2	1:F:524:LEU:HD23	2.02	0.41
1:D:219:PHE:HB2	1:D:247:LEU:HD23	2.02	0.41
2:T:66:ILE:O	2:T:92:LEU:HB2	2.20	0.41
1:K:140:ASP:N	1:K:140:ASP:OD1	2.54	0.41
1:J:226:LYS:O	1:J:227:ILE:HD13	2.21	0.41
1:I:166:MET:HE2	1:I:166:MET:HB3	1.95	0.41
1:I:479:ASN:CG	1:I:482:THR:HG22	2.46	0.41
1:L:314:LEU:H	1:L:314:LEU:HG	1.72	0.41
1:N:268:ARG:HB2	1:N:270:ILE:HG13	2.02	0.41
2:Y:17:VAL:HG22	2:Y:18:GLU:OE1	2.21	0.41
1:G:31:LEU:HD23	1:G:453:GLN:HB3	2.02	0.41
1:G:123:ALA:HB2	1:G:440:ILE:HG23	2.03	0.41
1:A:201:SER:HB2	1:A:259:LEU:HD21	2.03	0.41
1:C:194:GLN:HB2	1:C:331:THR:HG22	2.03	0.41
1:C:311:LYS:O	1:C:311:LYS:HD3	2.21	0.41
1:K:205:ILE:HG22	1:K:206:ASN:O	2.21	0.41
1:K:449:ALA:HB3	1:K:450:PRO:HD3	2.02	0.41
1:J:224:ASP:HB2	1:J:301:ILE:O	2.21	0.41
1:J:282:GLY:O	1:J:286:LYS:HG3	2.21	0.41
1:I:20:VAL:HG13	1:I:74:VAL:HG11	2.03	0.41
1:I:248:LEU:HD23	1:I:249:ILE:N	2.36	0.41
1:L:77:VAL:HB	1:L:510:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:322:ARG:HB2	1:L:333:ILE:HG21	2.02	0.41
1:H:166:MET:HE2	1:H:166:MET:HB3	1.93	0.41
1:N:200:LEU:HD13	1:N:276:VAL:HA	2.02	0.41
2:W:87:SER:O	2:W:90:ASP:HB2	2.21	0.41
2:1:61:VAL:HG22	2:1:62:GLY:N	2.35	0.41
1:G:258:ALA:O	1:G:261:THR:OG1	2.32	0.41
1:G:288:MET:O	1:G:292:ILE:HG13	2.20	0.41
1:A:3:ALA:HA	1:B:61:GLU:HG2	2.03	0.41
1:B:366:GLN:O	1:B:369:VAL:HB	2.21	0.41
1:F:231:ARG:NE	1:F:261:THR:HG21	2.35	0.41
1:F:520:MET:HE2	1:F:520:MET:HB3	1.94	0.41
1:E:74:VAL:O	1:E:77:VAL:HG12	2.20	0.41
1:E:237:LEU:HA	1:E:240:VAL:HG13	2.03	0.41
1:E:421:ARG:NH1	1:E:472:GLY:O	2.53	0.41
1:C:23:LEU:HD21	1:C:57:ALA:HA	2.02	0.41
1:C:219:PHE:CZ	1:C:245:LYS:HG3	2.56	0.41
3:C:601:ADP:O3B	4:C:602:BEF:F2	2.29	0.41
2:O:87:SER:O	2:O:90:ASP:N	2.51	0.41
2:Q:40:VAL:HG13	2:Q:62:GLY:H	1.86	0.41
2:U:73:VAL:HG12	2:U:86:MET:HB3	2.02	0.41
1:K:226:LYS:HA	1:K:253:ASP:O	2.21	0.41
1:J:193:MET:HB3	1:J:332:ILE:HB	2.03	0.41
1:J:231:ARG:HH22	1:J:257:GLU:HB3	1.84	0.41
1:I:162:ILE:HG21	1:I:403:THR:HG21	2.02	0.41
1:I:171:LYS:HA	1:I:171:LYS:HD3	1.76	0.41
1:I:200:LEU:HD23	1:I:200:LEU:HA	1.84	0.41
1:I:495:ASP:OD1	3:I:601:ADP:O2'	2.30	0.41
1:I:517:THR:HG23	1:H:39:VAL:HG23	2.02	0.41
1:L:116:LEU:O	1:L:120:ILE:HG13	2.20	0.41
1:L:307:MET:HB3	1:L:307:MET:HE2	1.85	0.41
1:M:131:LEU:HA	1:M:131:LEU:HD23	1.86	0.41
1:M:174:VAL:HG13	1:M:376:VAL:HG13	2.02	0.41
1:H:268:ARG:H	1:H:268:ARG:HG2	1.54	0.41
1:H:310:GLU:OE1	1:H:310:GLU:N	2.53	0.41
1:H:345:ARG:HA	1:H:348:GLN:CG	2.51	0.41
1:N:124:VAL:HG22	1:N:504:LEU:HD11	2.02	0.41
1:N:259:LEU:HA	1:N:259:LEU:HD23	1.87	0.41
2:W:8:ASP:HB3	2:W:47:ARG:HG2	2.03	0.41
2:Y:57:LEU:HD12	2:Y:57:LEU:H	1.86	0.41
1:G:13:ARG:CD	1:G:104:LEU:HD22	2.51	0.41
1:G:245:LYS:NZ	1:G:319:GLN:OE1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:HE2	1:C:480:ALA:O	2.21	0.41
1:C:149:THR:HG23	1:C:155:ASP:C	2.46	0.41
2:U:17:VAL:C	2:U:18:GLU:HG2	2.46	0.41
2:U:28:THR:HG22	2:U:29:GLY:H	1.85	0.41
1:K:414:GLY:HA2	1:K:495:ASP:OD2	2.21	0.41
1:M:441:LYS:O	1:M:445:ARG:HB2	2.21	0.41
1:M:466:ALA:O	1:M:470:LYS:HB2	2.20	0.41
2:W:49:LEU:HD21	2:W:55:LYS:HB2	2.03	0.41
2:V:69:ASP:HB2	2:V:73:VAL:HG11	2.03	0.41
2:Z:64:ILE:HB	2:Z:95:VAL:HG13	2.03	0.41
1:G:309:LEU:H	1:G:309:LEU:HD12	1.86	0.40
1:B:284:ARG:NH2	1:B:364:LYS:HZ2	2.18	0.40
1:D:65:LYS:O	1:D:69:MET:HG3	2.21	0.40
2:Q:67:PHE:CD2	2:Q:86:MET:HE1	2.56	0.40
2:R:15:LYS:O	2:R:35:SER:OG	2.33	0.40
2:R:55:LYS:HA	2:R:56:PRO:HD2	1.93	0.40
2:S:25:ILE:HB	2:S:26:VAL:H	1.66	0.40
1:K:289:LEU:HD23	1:K:292:ILE:HD12	2.03	0.40
1:J:176:THR:O	1:J:378:VAL:HA	2.21	0.40
1:A:233:MET:HE3	1:A:309:LEU:O	2.21	0.40
1:B:128:VAL:O	1:B:132:LYS:HG3	2.20	0.40
1:E:197:ARG:HG3	1:E:277:LYS:HB2	2.04	0.40
1:E:242:LYS:HE2	1:E:242:LYS:HB3	1.60	0.40
1:E:322:ARG:HG2	1:E:323:VAL:N	2.36	0.40
1:C:248:LEU:HD21	1:C:325:ILE:HD11	2.03	0.40
2:P:48:ILE:HG12	2:P:53:GLU:O	2.21	0.40
1:K:421:ARG:NH1	1:K:472:GLY:O	2.55	0.40
1:J:151:SER:HB3	1:J:399:ALA:HA	2.02	0.40
1:J:270:ILE:HD12	1:J:271:VAL:HG12	2.04	0.40
1:J:288:MET:O	1:J:292:ILE:HG13	2.21	0.40
1:J:419:LEU:HB3	1:J:447:MET:HB3	2.03	0.40
1:I:161:LEU:HD12	1:I:161:LEU:HA	1.94	0.40
1:I:233:MET:C	1:I:235:PRO:HD2	2.47	0.40
1:I:349:ILE:HD12	1:I:368:ARG:HH21	1.85	0.40
1:M:305:ILE:HG12	1:M:306:GLY:H	1.85	0.40
1:H:85:ALA:HB1	1:H:499:VAL:HG12	2.02	0.40
2:Z:67:PHE:CB	2:Z:86:MET:HE1	2.48	0.40
2:1:74:LYS:HD2	2:1:74:LYS:HA	1.92	0.40
1:B:218:PRO:HB3	1:B:246:PRO:HG2	2.03	0.40
1:B:360:TYR:CE1	1:B:364:LYS:HD2	2.57	0.40
1:B:461:GLU:HA	1:B:462:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:GLU:CD	1:C:501:ARG:HH21	2.29	0.40
2:P:61:VAL:HG12	2:P:62:GLY:H	1.85	0.40
1:I:364:LYS:HB2	1:I:364:LYS:HE3	1.89	0.40
1:I:429:LEU:HD12	1:I:430:ARG:H	1.86	0.40
1:M:208:PRO:HG2	1:M:214:GLU:HG3	2.03	0.40
1:H:207:LYS:HB3	1:H:208:PRO:HD2	2.03	0.40
1:H:247:LEU:HD23	1:H:248:LEU:N	2.36	0.40
1:H:449:ALA:HB3	1:H:450:PRO:HD3	2.03	0.40
1:H:472:GLY:HA3	1:H:476:TYR:CD2	2.55	0.40
2:X:31:ALA:O	2:X:32:ALA:HB3	2.21	0.40
2:W:78:ILE:HG22	2:W:79:ASP:OD2	2.21	0.40
2:V:60:LYS:NZ	2:V:63:ASP:HB3	2.36	0.40
1:G:420:ILE:HD13	1:G:420:ILE:HG21	1.86	0.40
1:B:40:LEU:HD11	1:B:56:VAL:HA	2.02	0.40
1:B:230:ILE:O	1:B:232:GLU:N	2.54	0.40
1:F:205:ILE:HG22	1:F:206:ASN:O	2.21	0.40
1:F:291:ASP:HB3	1:F:372:LEU:HD21	2.03	0.40
1:E:28:LYS:HD2	1:E:453:GLN:CD	2.47	0.40
1:E:194:GLN:NE2	1:E:329:THR:HG21	2.36	0.40
1:E:225:LYS:HD3	1:E:309:LEU:HD11	2.04	0.40
1:E:290:GLN:O	1:E:293:ALA:HB3	2.22	0.40
2:T:6:LEU:HD12	2:T:6:LEU:HA	1.84	0.40
1:K:32:GLY:H	3:K:601:ADP:H5'2	1.86	0.40
1:J:260:ALA:O	1:J:263:VAL:HG12	2.20	0.40
1:H:362:ARG:O	1:H:366:GLN:HB2	2.22	0.40
1:N:260:ALA:O	1:N:264:VAL:HG23	2.22	0.40
1:N:418:ALA:O	1:N:422:VAL:HG12	2.21	0.40
2:1:20:LYS:HA	2:1:20:LYS:HD3	1.80	0.40
1:G:254:VAL:HG12	1:G:259:LEU:HG	2.04	0.40
1:A:20:VAL:HG13	1:A:74:VAL:HG11	2.03	0.40
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.93	0.40
1:D:5:ASP:HB2	1:D:524:LEU:CD2	2.51	0.40
1:D:239:ALA:HB2	2:R:24:GLY:HA2	2.02	0.40
2:Q:15:LYS:HA	2:Q:16:GLU:HA	1.84	0.40
2:Q:34:LYS:HD3	2:Q:69:ASP:OD2	2.20	0.40
2:Q:49:LEU:HD13	2:Q:53:GLU:HG2	2.03	0.40
2:Q:50:GLU:OE1	2:R:50:GLU:HG2	2.21	0.40
2:T:5:PRO:HA	2:S:93:ALA:CB	2.50	0.40
2:R:57:LEU:H	2:R:57:LEU:HD22	1.86	0.40
2:S:14:ARG:HG3	2:S:84:LEU:CD1	2.52	0.40
1:K:217:SER:HA	1:K:320:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:247:LEU:O	1:K:273:VAL:HA	2.21	0.40
1:K:288:MET:O	1:K:292:ILE:HG13	2.20	0.40
1:J:20:VAL:HG13	1:J:74:VAL:HG11	2.03	0.40
1:J:62:LEU:HD23	1:J:67:GLU:HB3	2.03	0.40
1:I:263:VAL:O	1:I:267:MET:HG2	2.21	0.40
1:L:419:LEU:O	1:L:422:VAL:HG22	2.21	0.40
1:M:39:VAL:HG23	1:N:517:THR:HG23	2.04	0.40
1:M:264:VAL:HG21	1:N:306:GLY:HA3	2.03	0.40
3:M:601:ADP:PB	3:M:601:ADP:H5'1	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/548 (95%)	506 (97%)	15 (3%)	1 (0%)	43	70
1	B	522/548 (95%)	502 (96%)	20 (4%)	0	100	100
1	C	522/548 (95%)	501 (96%)	20 (4%)	1 (0%)	43	70
1	D	522/548 (95%)	498 (95%)	23 (4%)	1 (0%)	43	70
1	E	522/548 (95%)	505 (97%)	16 (3%)	1 (0%)	43	70
1	F	522/548 (95%)	500 (96%)	21 (4%)	1 (0%)	43	70
1	G	522/548 (95%)	503 (96%)	18 (3%)	1 (0%)	43	70
1	H	522/548 (95%)	501 (96%)	21 (4%)	0	100	100
1	I	522/548 (95%)	503 (96%)	19 (4%)	0	100	100
1	J	522/548 (95%)	500 (96%)	20 (4%)	2 (0%)	30	58
1	K	522/548 (95%)	505 (97%)	17 (3%)	0	100	100
1	L	522/548 (95%)	508 (97%)	14 (3%)	0	100	100
1	M	522/548 (95%)	502 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	522/548 (95%)	505 (97%)	17 (3%)	0	100	100
2	1	95/97 (98%)	83 (87%)	12 (13%)	0	100	100
2	2	95/97 (98%)	82 (86%)	12 (13%)	1 (1%)	11	39
2	O	95/97 (98%)	86 (90%)	8 (8%)	1 (1%)	11	39
2	P	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
2	Q	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
2	R	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	5	28
2	S	95/97 (98%)	77 (81%)	14 (15%)	4 (4%)	2	16
2	T	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	11	39
2	U	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	11	39
2	V	94/97 (97%)	84 (89%)	10 (11%)	0	100	100
2	W	94/97 (97%)	78 (83%)	15 (16%)	1 (1%)	11	39
2	X	93/97 (96%)	81 (87%)	10 (11%)	2 (2%)	5	27
2	Y	94/97 (97%)	86 (92%)	7 (7%)	1 (1%)	11	39
2	Z	95/97 (98%)	88 (93%)	7 (7%)	0	100	100
All	All	8633/9030 (96%)	8209 (95%)	402 (5%)	22 (0%)	36	64

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE
1	E	305	ILE
1	C	230	ILE
1	D	230	ILE
2	S	26	VAL
1	J	270	ILE
2	R	51	ASN
2	X	51	ASN
2	T	57	LEU
2	R	50	GLU
2	Y	50	GLU
2	2	58	ASP
1	F	359	ASP
2	O	51	ASN
2	U	51	ASN
2	S	17	VAL
2	S	57	LEU

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Mol	Chain	Res	Type
2	S	58	ASP
2	W	51	ASN
1	J	359	ASP
2	X	3	ILE
1	G	333	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/415 (97%)	386 (96%)	18 (4%)	24	48
1	B	404/415 (97%)	389 (96%)	15 (4%)	30	52
1	C	404/415 (97%)	389 (96%)	15 (4%)	30	52
1	D	404/415 (97%)	391 (97%)	13 (3%)	34	54
1	E	404/415 (97%)	383 (95%)	21 (5%)	21	46
1	F	404/415 (97%)	391 (97%)	13 (3%)	34	54
1	G	404/415 (97%)	388 (96%)	16 (4%)	28	50
1	H	404/415 (97%)	386 (96%)	18 (4%)	24	48
1	I	404/415 (97%)	388 (96%)	16 (4%)	28	50
1	J	404/415 (97%)	387 (96%)	17 (4%)	26	49
1	K	404/415 (97%)	385 (95%)	19 (5%)	23	47
1	L	404/415 (97%)	390 (96%)	14 (4%)	32	53
1	M	404/415 (97%)	381 (94%)	23 (6%)	18	43
1	N	404/415 (97%)	387 (96%)	17 (4%)	26	49
2	1	80/80 (100%)	71 (89%)	9 (11%)	5	24
2	2	80/80 (100%)	75 (94%)	5 (6%)	16	41
2	O	80/80 (100%)	78 (98%)	2 (2%)	42	59
2	P	80/80 (100%)	76 (95%)	4 (5%)	22	46
2	Q	80/80 (100%)	76 (95%)	4 (5%)	22	46
2	R	80/80 (100%)	76 (95%)	4 (5%)	22	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	80/80 (100%)	73 (91%)	7 (9%)	9	31
2	T	80/80 (100%)	76 (95%)	4 (5%)	22	46
2	U	80/80 (100%)	74 (92%)	6 (8%)	12	37
2	V	80/80 (100%)	77 (96%)	3 (4%)	29	51
2	W	79/80 (99%)	75 (95%)	4 (5%)	21	46
2	X	79/80 (99%)	76 (96%)	3 (4%)	29	51
2	Y	80/80 (100%)	78 (98%)	2 (2%)	42	59
2	Z	80/80 (100%)	77 (96%)	3 (4%)	29	51
All	All	6774/6930 (98%)	6479 (96%)	295 (4%)	25	49

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	74	VAL
1	G	147	VAL
1	G	150	ILE
1	G	161	LEU
1	G	176	THR
1	G	314	LEU
1	G	319	GLN
1	G	357	THR
1	G	364	LYS
1	G	412	VAL
1	G	422	VAL
1	G	461	GLU
1	G	463	SER
1	G	473	ASP
1	G	499	VAL
1	G	510	VAL
1	A	74	VAL
1	A	147	VAL
1	A	150	ILE
1	A	161	LEU
1	A	176	THR
1	A	177	VAL
1	A	190	VAL
1	A	213	VAL
1	A	234	LEU
1	A	270	ILE

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Mol	Chain	Res	Type
1	A	319	GLN
1	A	329	THR
1	A	357	THR
1	A	420	ILE
1	A	422	VAL
1	A	453	GLN
1	A	461	GLU
1	A	463	SER
1	B	136	VAL
1	B	161	LEU
1	B	176	THR
1	B	177	VAL
1	B	190	VAL
1	B	213	VAL
1	B	237	LEU
1	B	255	GLU
1	B	357	THR
1	B	422	VAL
1	B	452	ARG
1	B	461	GLU
1	B	463	SER
1	B	473	ASP
1	B	493	ILE
1	F	147	VAL
1	F	161	LEU
1	F	176	THR
1	F	177	VAL
1	F	183	LEU
1	F	190	VAL
1	F	231	ARG
1	F	309	LEU
1	F	314	LEU
1	F	329	THR
1	F	386	GLU
1	F	463	SER
1	F	473	ASP
1	E	63	GLU
1	E	136	VAL
1	E	147	VAL
1	E	161	LEU
1	E	176	THR
1	E	177	VAL

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Mol	Chain	Res	Type
1	E	181	THR
1	E	190	VAL
1	E	207	LYS
1	E	213	VAL
1	E	238	GLU
1	E	240	VAL
1	E	271	VAL
1	E	305	ILE
1	E	329	THR
1	E	334	ASP
1	E	368	ARG
1	E	417	VAL
1	E	422	VAL
1	E	461	GLU
1	E	473	ASP
1	C	128	VAL
1	C	136	VAL
1	C	147	VAL
1	C	150	ILE
1	C	161	LEU
1	C	171	LYS
1	C	176	THR
1	C	177	VAL
1	C	209	GLU
1	C	230	ILE
1	C	314	LEU
1	C	357	THR
1	C	422	VAL
1	C	461	GLU
1	C	463	SER
1	D	91	THR
1	D	147	VAL
1	D	150	ILE
1	D	161	LEU
1	D	176	THR
1	D	177	VAL
1	D	190	VAL
1	D	209	GLU
1	D	230	ILE
1	D	357	THR
1	D	422	VAL
1	D	461	GLU

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Mol	Chain	Res	Type
1	D	463	SER
2	O	28	THR
2	O	50	GLU
2	P	1	MET
2	P	28	THR
2	P	40	VAL
2	P	50	GLU
2	Q	11	ILE
2	Q	28	THR
2	Q	40	VAL
2	Q	50	GLU
2	U	6	LEU
2	U	11	ILE
2	U	27	LEU
2	U	54	VAL
2	U	65	VAL
2	U	96	GLU
2	T	17	VAL
2	T	18	GLU
2	T	40	VAL
2	T	95	VAL
2	R	11	ILE
2	R	26	VAL
2	R	28	THR
2	R	80	ASN
2	S	11	ILE
2	S	21	SER
2	S	28	THR
2	S	40	VAL
2	S	80	ASN
2	S	83	VAL
2	S	95	VAL
1	K	74	VAL
1	K	136	VAL
1	K	147	VAL
1	K	150	ILE
1	K	161	LEU
1	K	177	VAL
1	K	190	VAL
1	K	213	VAL
1	K	245	LYS
1	K	257	GLU

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Mol	Chain	Res	Type
1	K	313	THR
1	K	314	LEU
1	K	319	GLN
1	K	412	VAL
1	K	422	VAL
1	K	461	GLU
1	K	463	SER
1	K	473	ASP
1	K	510	VAL
1	J	136	VAL
1	J	147	VAL
1	J	150	ILE
1	J	161	LEU
1	J	177	VAL
1	J	190	VAL
1	J	194	GLN
1	J	213	VAL
1	J	236	VAL
1	J	319	GLN
1	J	329	THR
1	J	339	GLU
1	J	358	SER
1	J	420	ILE
1	J	422	VAL
1	J	461	GLU
1	J	463	SER
1	I	147	VAL
1	I	150	ILE
1	I	161	LEU
1	I	176	THR
1	I	177	VAL
1	I	190	VAL
1	I	197	ARG
1	I	213	VAL
1	I	228	SER
1	I	339	GLU
1	I	357	THR
1	I	412	VAL
1	I	453	GLN
1	I	461	GLU
1	I	463	SER
1	I	493	ILE

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Mol	Chain	Res	Type
1	L	147	VAL
1	L	161	LEU
1	L	176	THR
1	L	177	VAL
1	L	190	VAL
1	L	209	GLU
1	L	242	LYS
1	L	257	GLU
1	L	291	ASP
1	L	314	LEU
1	L	329	THR
1	L	422	VAL
1	L	452	ARG
1	L	461	GLU
1	M	74	VAL
1	M	136	VAL
1	M	147	VAL
1	M	150	ILE
1	M	161	LEU
1	M	176	THR
1	M	177	VAL
1	M	190	VAL
1	M	207	LYS
1	M	213	VAL
1	M	224	ASP
1	M	305	ILE
1	M	307	MET
1	M	310	GLU
1	M	314	LEU
1	M	329	THR
1	M	355	GLU
1	M	357	THR
1	M	417	VAL
1	M	422	VAL
1	M	461	GLU
1	M	463	SER
1	M	470	LYS
1	H	30	THR
1	H	128	VAL
1	H	136	VAL
1	H	147	VAL
1	H	161	LEU

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Mol	Chain	Res	Type
1	H	175	ILE
1	H	176	THR
1	H	177	VAL
1	H	205	ILE
1	H	255	GLU
1	H	268	ARG
1	H	304	GLU
1	H	314	LEU
1	H	357	THR
1	H	422	VAL
1	H	453	GLN
1	H	461	GLU
1	H	463	SER
1	N	147	VAL
1	N	150	ILE
1	N	161	LEU
1	N	177	VAL
1	N	190	VAL
1	N	216	GLU
1	N	233	MET
1	N	234	LEU
1	N	270	ILE
1	N	271	VAL
1	N	354	GLU
1	N	360	TYR
1	N	422	VAL
1	N	461	GLU
1	N	463	SER
1	N	499	VAL
1	N	500	THR
2	X	8	ASP
2	X	50	GLU
2	X	78	ILE
2	W	40	VAL
2	W	55	LYS
2	W	57	LEU
2	W	79	ASP
2	V	11	ILE
2	V	28	THR
2	V	40	VAL
2	Y	11	ILE
2	Y	27	LEU

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Mol	Chain	Res	Type
2	Z	1	MET
2	Z	40	VAL
2	Z	95	VAL
2	2	1	MET
2	2	11	ILE
2	2	25	ILE
2	2	80	ASN
2	2	82	GLU
2	1	11	ILE
2	1	16	GLU
2	1	21	SER
2	1	27	LEU
2	1	40	VAL
2	1	50	GLU
2	1	80	ASN
2	1	83	VAL
2	1	95	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	457	ASN
1	A	10	ASN
1	A	352	GLN
1	B	351	GLN
1	B	366	GLN
1	F	146	GLN
1	F	229	ASN
1	F	453	GLN
1	E	10	ASN
1	E	146	GLN
1	E	229	ASN
1	C	290	GLN
1	D	505	GLN
2	T	51	ASN
2	R	7	HIS
2	R	45	ASN
2	R	80	ASN
1	K	351	GLN
1	K	457	ASN
1	J	72	GLN
1	J	146	GLN

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Mol	Chain	Res	Type
1	J	206	ASN
1	I	453	GLN
1	L	505	GLN
1	M	505	GLN
1	N	153	ASN
2	X	51	ASN
2	W	7	HIS
2	V	51	ASN
2	Y	7	HIS
2	Y	45	ASN
2	Y	68	ASN
2	Z	51	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 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
3	ADP	B	601	5,6	28,29,29	1.37	4 (14%)	43,45,45	1.93	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	D	601	5,6	28,29,29	1.42	5 (17%)	43,45,45	1.81	10 (23%)
4	BEF	E	602	-	0,3,3	-	-	-		
4	BEF	H	602	-	0,3,3	-	-	-		
3	ADP	K	601	5,6	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)
4	BEF	J	602	-	0,3,3	-	-	-		
4	BEF	N	602	-	0,3,3	-	-	-		
3	ADP	L	601	5,6	28,29,29	1.41	4 (14%)	43,45,45	1.83	10 (23%)
4	BEF	G	602	-	0,3,3	-	-	-		
4	BEF	D	602	-	0,3,3	-	-	-		
4	BEF	L	602	-	0,3,3	-	-	-		
3	ADP	E	601	5,6	28,29,29	1.39	4 (14%)	43,45,45	1.84	9 (20%)
3	ADP	J	601	5,6	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
4	BEF	M	602	-	0,3,3	-	-	-		
3	ADP	C	601	5,6	28,29,29	1.39	4 (14%)	43,45,45	1.79	7 (16%)
4	BEF	F	602	-	0,3,3	-	-	-		
3	ADP	H	601	5,6	28,29,29	1.39	5 (17%)	43,45,45	1.80	8 (18%)
4	BEF	A	602	-	0,3,3	-	-	-		
3	ADP	G	601	5,6	28,29,29	1.37	4 (14%)	43,45,45	1.91	9 (20%)
3	ADP	N	601	5,6	28,29,29	1.40	5 (17%)	43,45,45	1.84	11 (25%)
4	BEF	B	602	-	0,3,3	-	-	-		
3	ADP	I	601	5,6	28,29,29	1.37	5 (17%)	43,45,45	1.88	10 (23%)
4	BEF	C	602	-	0,3,3	-	-	-		
3	ADP	M	601	5,6	28,29,29	1.46	5 (17%)	43,45,45	1.83	8 (18%)
3	ADP	F	601	5,6	28,29,29	1.34	4 (14%)	43,45,45	1.95	11 (25%)
4	BEF	I	602	-	0,3,3	-	-	-		
4	BEF	K	602	-	0,3,3	-	-	-		
3	ADP	A	601	5,6	28,29,29	1.35	4 (14%)	43,45,45	1.97	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	M	601	5,6	-	8/16/32/32	0/3/3/3
3	ADP	F	601	5,6	-	4/16/32/32	0/3/3/3
3	ADP	L	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	H	601	5,6	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	G	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	D	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	K	601	5,6	-	2/16/32/32	0/3/3/3
3	ADP	N	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	I	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	J	601	5,6	-	7/16/32/32	0/3/3/3
3	ADP	E	601	5,6	-	4/16/32/32	0/3/3/3
3	ADP	A	601	5,6	-	4/16/32/32	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	601	ADP	C5-C4	4.69	1.47	1.39
3	D	601	ADP	C5-C4	4.67	1.47	1.39
3	L	601	ADP	C5-C4	4.60	1.47	1.39
3	C	601	ADP	C5-C4	4.60	1.47	1.39
3	K	601	ADP	C5-C4	4.54	1.47	1.39
3	H	601	ADP	C5-C4	4.53	1.47	1.39
3	B	601	ADP	C5-C4	4.53	1.47	1.39
3	J	601	ADP	C5-C4	4.52	1.47	1.39
3	E	601	ADP	C5-C4	4.52	1.47	1.39
3	I	601	ADP	C5-C4	4.51	1.47	1.39
3	F	601	ADP	C5-C4	4.33	1.46	1.39
3	N	601	ADP	C5-C4	4.31	1.46	1.39
3	G	601	ADP	C5-C4	4.27	1.46	1.39
3	A	601	ADP	C5-C4	4.27	1.46	1.39
3	K	601	ADP	C5-C6	2.73	1.48	1.41
3	L	601	ADP	C5-C6	2.71	1.48	1.41
3	H	601	ADP	C5-C6	2.67	1.48	1.41
3	N	601	ADP	C4-N9	-2.67	1.32	1.37
3	E	601	ADP	C5-C6	2.63	1.48	1.41
3	A	601	ADP	C5-C6	2.62	1.48	1.41
3	M	601	ADP	C5-C6	2.60	1.48	1.41
3	C	601	ADP	C5-C6	2.60	1.48	1.41
3	G	601	ADP	C5-C6	2.59	1.48	1.41
3	I	601	ADP	C5-C6	2.57	1.48	1.41
3	F	601	ADP	C5-C6	2.56	1.48	1.41
3	D	601	ADP	C5-C6	2.56	1.48	1.41
3	J	601	ADP	C5-C6	2.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	ADP	C5-C6	2.49	1.47	1.41
3	J	601	ADP	C5-N7	-2.47	1.34	1.39
3	M	601	ADP	C8-N7	2.46	1.36	1.31
3	N	601	ADP	C5-C6	2.43	1.47	1.41
3	E	601	ADP	C8-N7	2.42	1.36	1.31
3	G	601	ADP	C5-N7	-2.42	1.34	1.39
3	D	601	ADP	C8-N7	2.40	1.36	1.31
3	C	601	ADP	C8-N7	2.39	1.36	1.31
3	M	601	ADP	C5-N7	-2.39	1.34	1.39
3	F	601	ADP	C5-N7	-2.38	1.34	1.39
3	K	601	ADP	C8-N7	2.36	1.36	1.31
3	B	601	ADP	C5-N7	-2.34	1.34	1.39
3	L	601	ADP	C5-N7	-2.34	1.34	1.39
3	A	601	ADP	C5-N7	-2.33	1.34	1.39
3	L	601	ADP	C8-N7	2.32	1.36	1.31
3	N	601	ADP	C5-N7	-2.31	1.34	1.39
3	C	601	ADP	C5-N7	-2.31	1.34	1.39
3	E	601	ADP	C5-N7	-2.29	1.34	1.39
3	H	601	ADP	C5-N7	-2.29	1.34	1.39
3	B	601	ADP	C8-N7	2.28	1.36	1.31
3	M	601	ADP	PA-O3A	2.28	1.62	1.59
3	I	601	ADP	C5-N7	-2.28	1.34	1.39
3	N	601	ADP	C8-N7	2.25	1.36	1.31
3	I	601	ADP	C8-N7	2.25	1.36	1.31
3	D	601	ADP	C5-N7	-2.24	1.35	1.39
3	J	601	ADP	C8-N7	2.24	1.36	1.31
3	G	601	ADP	C8-N7	2.23	1.36	1.31
3	H	601	ADP	C8-N7	2.22	1.36	1.31
3	K	601	ADP	C5-N7	-2.22	1.35	1.39
3	D	601	ADP	C4-N9	-2.21	1.33	1.37
3	A	601	ADP	C8-N7	2.18	1.35	1.31
3	F	601	ADP	C8-N7	2.17	1.35	1.31
3	I	601	ADP	C4-N9	-2.11	1.33	1.37
3	H	601	ADP	C4-N9	-2.04	1.33	1.37

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	601	ADP	C5-C4-N3	-6.07	118.35	126.72
3	F	601	ADP	C5-C4-N3	-6.07	118.36	126.72
3	A	601	ADP	C5-C4-N3	-6.03	118.41	126.72
3	K	601	ADP	C5-C4-N3	-6.03	118.41	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	601	ADP	C5-C4-N3	-5.94	118.54	126.72
3	C	601	ADP	C5-C4-N3	-5.92	118.56	126.72
3	M	601	ADP	C5-C4-N3	-5.91	118.58	126.72
3	B	601	ADP	C5-C4-N3	-5.89	118.61	126.72
3	E	601	ADP	C5-C4-N3	-5.77	118.78	126.72
3	H	601	ADP	C5-C4-N3	-5.69	118.89	126.72
3	L	601	ADP	C5-C4-N3	-5.59	119.03	126.72
3	I	601	ADP	C5-C4-N3	-5.48	119.17	126.72
3	D	601	ADP	C5-C4-N3	-5.37	119.33	126.72
3	A	601	ADP	N3-C4-N9	4.95	135.59	127.17
3	B	601	ADP	N3-C4-N9	4.94	135.56	127.17
3	G	601	ADP	N3-C4-N9	4.90	135.50	127.17
3	F	601	ADP	N3-C4-N9	4.85	135.42	127.17
3	K	601	ADP	N3-C4-N9	4.79	135.31	127.17
3	N	601	ADP	C5-C4-N3	-4.78	120.13	126.72
3	J	601	ADP	N3-C4-N9	4.77	135.27	127.17
3	C	601	ADP	N3-C4-N9	4.68	135.13	127.17
3	I	601	ADP	N3-C4-N9	4.68	135.13	127.17
3	E	601	ADP	N3-C4-N9	4.60	134.99	127.17
3	H	601	ADP	N3-C4-N9	4.54	134.88	127.17
3	L	601	ADP	N3-C4-N9	4.46	134.75	127.17
3	M	601	ADP	N3-C4-N9	4.45	134.74	127.17
3	D	601	ADP	N3-C4-N9	4.30	134.48	127.17
3	N	601	ADP	N3-C4-N9	4.18	134.27	127.17
3	N	601	ADP	C4-N9-C8	4.07	110.01	105.74
3	G	601	ADP	C2-N3-C4	3.98	121.55	111.83
3	K	601	ADP	C2-N3-C4	3.89	121.33	111.83
3	F	601	ADP	C2-N3-C4	3.86	121.27	111.83
3	A	601	ADP	C2-N3-C4	3.86	121.26	111.83
3	B	601	ADP	C2-N3-C4	3.76	121.01	111.83
3	C	601	ADP	C2-N3-C4	3.72	120.91	111.83
3	J	601	ADP	C2-N3-C4	3.66	120.78	111.83
3	E	601	ADP	C2-N3-C4	3.64	120.72	111.83
3	L	601	ADP	C2-N3-C4	3.62	120.68	111.83
3	M	601	ADP	C2-N3-C4	3.62	120.68	111.83
3	H	601	ADP	C2-N3-C4	3.58	120.58	111.83
3	M	601	ADP	C4-C5-N7	-3.58	106.49	110.58
3	I	601	ADP	C4-N9-C8	3.57	109.49	105.74
3	I	601	ADP	C2-N3-C4	3.50	120.38	111.83
3	N	601	ADP	N3-C2-N1	-3.47	123.33	128.58
3	A	601	ADP	C4-C5-N7	-3.45	106.64	110.58
3	H	601	ADP	C4-C5-N7	-3.44	106.65	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	ADP	C4-C5-N7	-3.44	106.65	110.58
3	G	601	ADP	N3-C2-N1	-3.42	123.41	128.58
3	D	601	ADP	C2-N3-C4	3.40	120.14	111.83
3	N	601	ADP	C2-N3-C4	3.39	120.11	111.83
3	G	601	ADP	C4-C5-N7	-3.38	106.72	110.58
3	F	601	ADP	C4-C5-N7	-3.37	106.73	110.58
3	L	601	ADP	C4-C5-N7	-3.36	106.74	110.58
3	K	601	ADP	C4-C5-N7	-3.32	106.78	110.58
3	J	601	ADP	C4-C5-N7	-3.31	106.80	110.58
3	K	601	ADP	N3-C2-N1	-3.30	123.59	128.58
3	C	601	ADP	C4-C5-N7	-3.28	106.83	110.58
3	I	601	ADP	C4-C5-N7	-3.27	106.84	110.58
3	L	601	ADP	N3-C2-N1	-3.27	123.63	128.58
3	F	601	ADP	N3-C2-N1	-3.25	123.66	128.58
3	B	601	ADP	N3-C2-N1	-3.24	123.67	128.58
3	D	601	ADP	C4-C5-N7	-3.22	106.90	110.58
3	A	601	ADP	N3-C2-N1	-3.22	123.70	128.58
3	C	601	ADP	N3-C2-N1	-3.16	123.80	128.58
3	I	601	ADP	N3-C2-N1	-3.16	123.81	128.58
3	N	601	ADP	C4-C5-N7	-3.15	106.97	110.58
3	A	601	ADP	C4-N9-C8	3.12	109.02	105.74
3	E	601	ADP	N3-C2-N1	-3.12	123.86	128.58
3	B	601	ADP	C4-C5-N7	-3.12	107.02	110.58
3	J	601	ADP	N3-C2-N1	-3.06	123.94	128.58
3	H	601	ADP	N3-C2-N1	-3.04	123.97	128.58
3	B	601	ADP	C4-N9-C8	3.02	108.91	105.74
3	M	601	ADP	N3-C2-N1	-2.97	124.09	128.58
3	E	601	ADP	C4-N9-C8	2.94	108.83	105.74
3	G	601	ADP	C4-N9-C8	2.94	108.82	105.74
3	D	601	ADP	N3-C2-N1	-2.91	124.17	128.58
3	D	601	ADP	C4-N9-C8	2.89	108.78	105.74
3	H	601	ADP	C4-N9-C8	2.85	108.73	105.74
3	F	601	ADP	C4-N9-C8	2.79	108.67	105.74
3	A	601	ADP	C5-N7-C8	2.72	107.73	103.45
3	N	601	ADP	N9-C8-N7	-2.68	110.13	113.94
3	L	601	ADP	C4-N9-C8	2.68	108.55	105.74
3	J	601	ADP	C4-N9-C8	2.67	108.54	105.74
3	K	601	ADP	C4-N9-C8	2.59	108.46	105.74
3	B	601	ADP	C2'-C1'-N9	-2.59	106.86	113.30
3	I	601	ADP	C5-N7-C8	2.59	107.52	103.45
3	E	601	ADP	C5-N7-C8	2.58	107.50	103.45
3	G	601	ADP	C5-N7-C8	2.57	107.49	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	601	ADP	C5-N7-C8	2.52	107.42	103.45
3	H	601	ADP	C5-N7-C8	2.52	107.41	103.45
3	F	601	ADP	C5-N7-C8	2.52	107.41	103.45
3	I	601	ADP	C2'-C1'-N9	-2.50	107.10	113.30
3	C	601	ADP	C4-N9-C8	2.48	108.34	105.74
3	M	601	ADP	C5-N7-C8	2.48	107.34	103.45
3	J	601	ADP	C5-N7-C8	2.47	107.34	103.45
3	K	601	ADP	C5-N7-C8	2.45	107.30	103.45
3	I	601	ADP	N9-C8-N7	-2.45	110.46	113.94
3	C	601	ADP	C5-N7-C8	2.44	107.28	103.45
3	N	601	ADP	C5-N7-C8	2.44	107.28	103.45
3	B	601	ADP	C5-N7-C8	2.40	107.22	103.45
3	F	601	ADP	C3'-C2'-C1'	2.36	105.93	101.46
3	A	601	ADP	N9-C8-N7	-2.34	110.62	113.94
3	L	601	ADP	O3'-C3'-C2'	-2.33	104.35	111.82
3	J	601	ADP	C3'-C2'-C1'	2.30	105.82	101.46
3	D	601	ADP	C5-N7-C8	2.29	107.05	103.45
3	M	601	ADP	C4-N9-C8	2.27	108.12	105.74
3	N	601	ADP	C6-C5-N7	2.25	136.43	132.09
3	A	601	ADP	O3'-C3'-C2'	-2.23	104.66	111.82
3	E	601	ADP	N9-C8-N7	-2.23	110.78	113.94
3	G	601	ADP	N9-C8-N7	-2.20	110.82	113.94
3	G	601	ADP	C6-C5-N7	2.20	136.33	132.09
3	F	601	ADP	C2'-C3'-C4'	2.19	106.85	102.61
3	A	601	ADP	C6-C5-N7	2.15	136.23	132.09
3	B	601	ADP	O5'-C5'-C4'	2.13	116.23	108.99
3	M	601	ADP	O4'-C1'-N9	2.12	112.16	108.09
3	K	601	ADP	C6-C5-N7	2.12	136.17	132.09
3	N	601	ADP	C2'-C1'-N9	-2.10	108.08	113.30
3	B	601	ADP	C3'-C2'-C1'	2.10	105.43	101.46
3	F	601	ADP	N9-C8-N7	-2.09	110.98	113.94
3	H	601	ADP	N9-C8-N7	-2.08	110.98	113.94
3	N	601	ADP	C2-N1-C6	2.07	122.14	118.73
3	D	601	ADP	C2'-C1'-N9	-2.07	108.16	113.30
3	I	601	ADP	C3'-C2'-C1'	2.06	105.36	101.46
3	B	601	ADP	N9-C8-N7	-2.05	111.03	113.94
3	E	601	ADP	C6-C5-N7	2.04	136.01	132.09
3	D	601	ADP	C6-C5-N7	2.03	136.01	132.09
3	F	601	ADP	C6-C5-N7	2.02	135.99	132.09
3	L	601	ADP	N9-C8-N7	-2.02	111.07	113.94
3	L	601	ADP	C6-C5-N7	2.02	135.97	132.09
3	D	601	ADP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	C5'-O5'-PA-O1A
3	F	601	ADP	O4'-C4'-C5'-O5'
3	F	601	ADP	C3'-C4'-C5'-O5'
3	E	601	ADP	PA-O3A-PB-O3B
3	E	601	ADP	C5'-O5'-PA-O1A
3	C	601	ADP	PB-O3A-PA-O5'
3	K	601	ADP	C5'-O5'-PA-O1A
3	J	601	ADP	PB-O3A-PA-O5'
3	J	601	ADP	C5'-O5'-PA-O2A
3	I	601	ADP	C5'-O5'-PA-O3A
3	L	601	ADP	C5'-O5'-PA-O1A
3	L	601	ADP	C5'-O5'-PA-O2A
3	L	601	ADP	C5'-O5'-PA-O3A
3	M	601	ADP	C5'-O5'-PA-O1A
3	M	601	ADP	C5'-O5'-PA-O2A
3	H	601	ADP	PB-O3A-PA-O5'
3	H	601	ADP	C5'-O5'-PA-O3A
3	J	601	ADP	C3'-C4'-C5'-O5'
3	H	601	ADP	C3'-C4'-C5'-O5'
3	J	601	ADP	O4'-C4'-C5'-O5'
3	H	601	ADP	O4'-C4'-C5'-O5'
3	C	601	ADP	C3'-C4'-C5'-O5'
3	N	601	ADP	O4'-C4'-C5'-O5'
3	N	601	ADP	C3'-C4'-C5'-O5'
3	C	601	ADP	O4'-C4'-C5'-O5'
3	G	601	ADP	O4'-C4'-C5'-O5'
3	G	601	ADP	C3'-C4'-C5'-O5'
3	G	601	ADP	PB-O3A-PA-O5'
3	A	601	ADP	PB-O3A-PA-O5'
3	B	601	ADP	PB-O3A-PA-O5'
3	F	601	ADP	PB-O3A-PA-O5'
3	D	601	ADP	PB-O3A-PA-O5'
3	K	601	ADP	PB-O3A-PA-O5'
3	I	601	ADP	PB-O3A-PA-O5'
3	M	601	ADP	PA-O3A-PB-O1B
3	B	601	ADP	O4'-C4'-C5'-O5'
3	M	601	ADP	C3'-C4'-C5'-O5'
3	J	601	ADP	C2'-C1'-N9-C8
3	G	601	ADP	C5'-O5'-PA-O1A
3	B	601	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	F	601	ADP	C5'-O5'-PA-O3A
3	E	601	ADP	C5'-O5'-PA-O2A
3	E	601	ADP	C5'-O5'-PA-O3A
3	J	601	ADP	C5'-O5'-PA-O3A
3	I	601	ADP	C5'-O5'-PA-O1A
3	M	601	ADP	C5'-O5'-PA-O3A
3	H	601	ADP	C5'-O5'-PA-O1A
3	N	601	ADP	C5'-O5'-PA-O1A
3	B	601	ADP	C3'-C4'-C5'-O5'
3	M	601	ADP	O4'-C4'-C5'-O5'
3	N	601	ADP	PB-O3A-PA-O5'
3	D	601	ADP	O4'-C4'-C5'-O5'
3	M	601	ADP	PA-O3A-PB-O2B
3	M	601	ADP	PA-O3A-PB-O3B
3	G	601	ADP	PB-O3A-PA-O2A
3	A	601	ADP	PB-O3A-PA-O1A
3	B	601	ADP	PB-O3A-PA-O1A
3	J	601	ADP	PB-O3A-PA-O1A
3	A	601	ADP	C2'-C1'-N9-C8
3	D	601	ADP	C3'-C4'-C5'-O5'
3	N	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

26 monomers are involved in 36 short contacts:

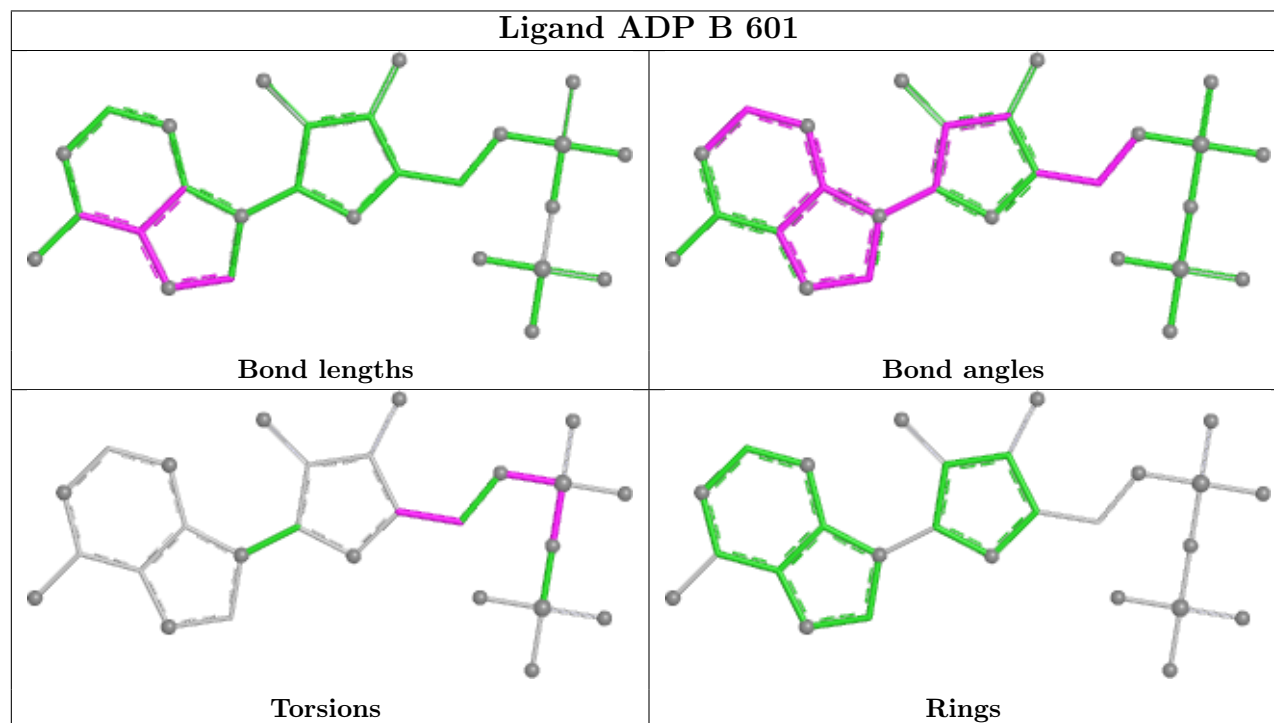
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ADP	1	0
3	D	601	ADP	3	0
4	E	602	BEF	2	0
4	H	602	BEF	1	0
3	K	601	ADP	2	0
4	J	602	BEF	2	0
4	N	602	BEF	2	0
3	L	601	ADP	2	0
4	G	602	BEF	3	0
4	D	602	BEF	1	0
4	L	602	BEF	2	0
3	E	601	ADP	1	0
3	J	601	ADP	3	0
4	M	602	BEF	1	0
3	C	601	ADP	2	0
4	F	602	BEF	1	0

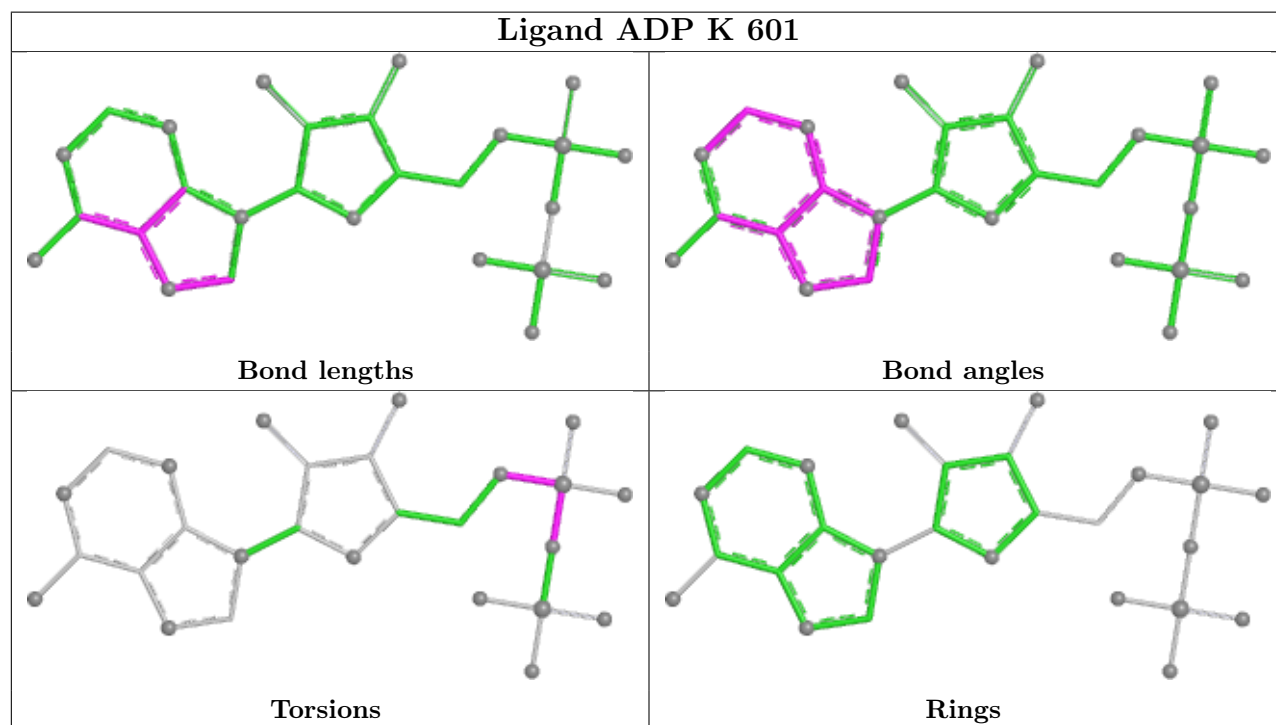
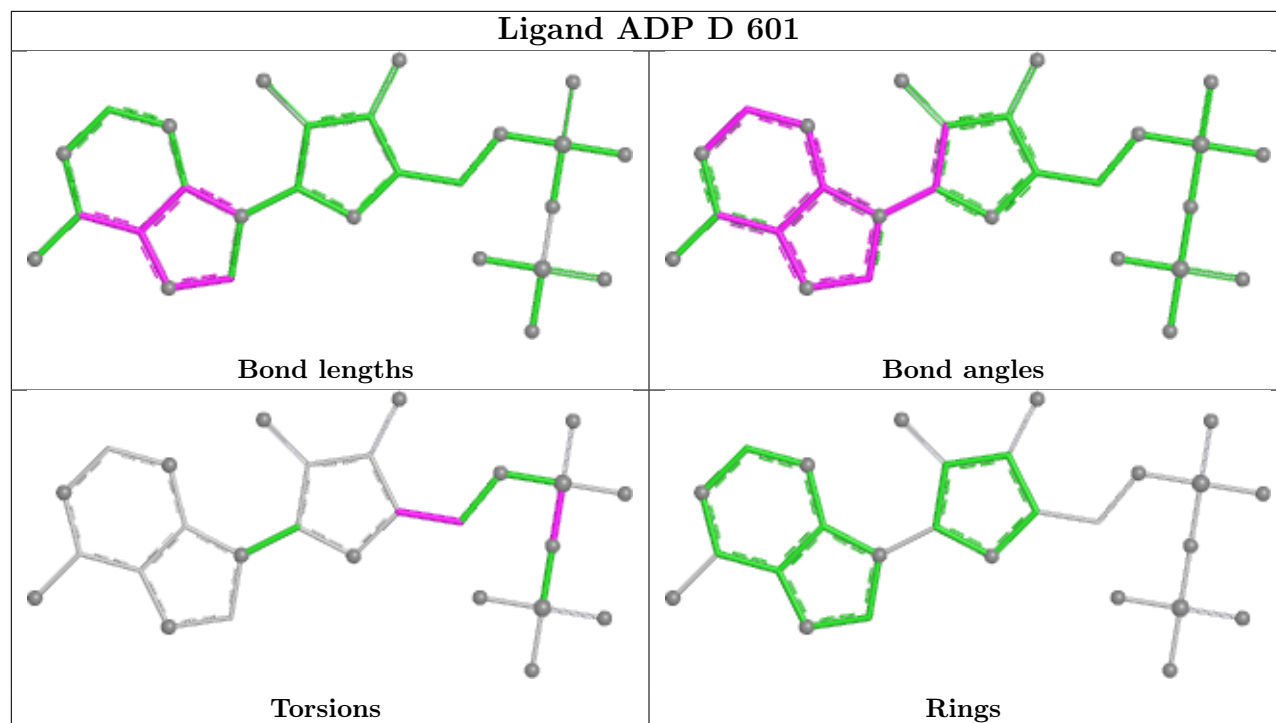
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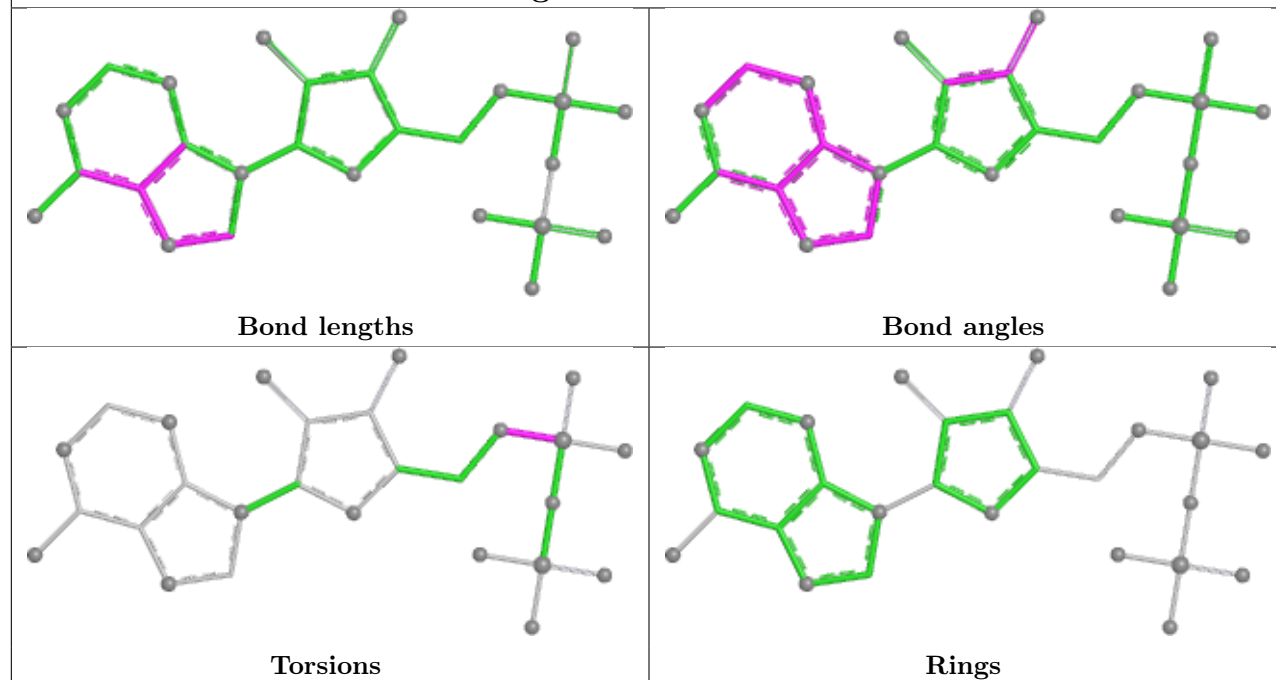
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	601	ADP	2	0
3	G	601	ADP	2	0
3	N	601	ADP	2	0
4	B	602	BEF	3	0
3	I	601	ADP	3	0
4	C	602	BEF	1	0
3	M	601	ADP	3	0
3	F	601	ADP	2	0
4	I	602	BEF	1	0
4	K	602	BEF	2	0

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

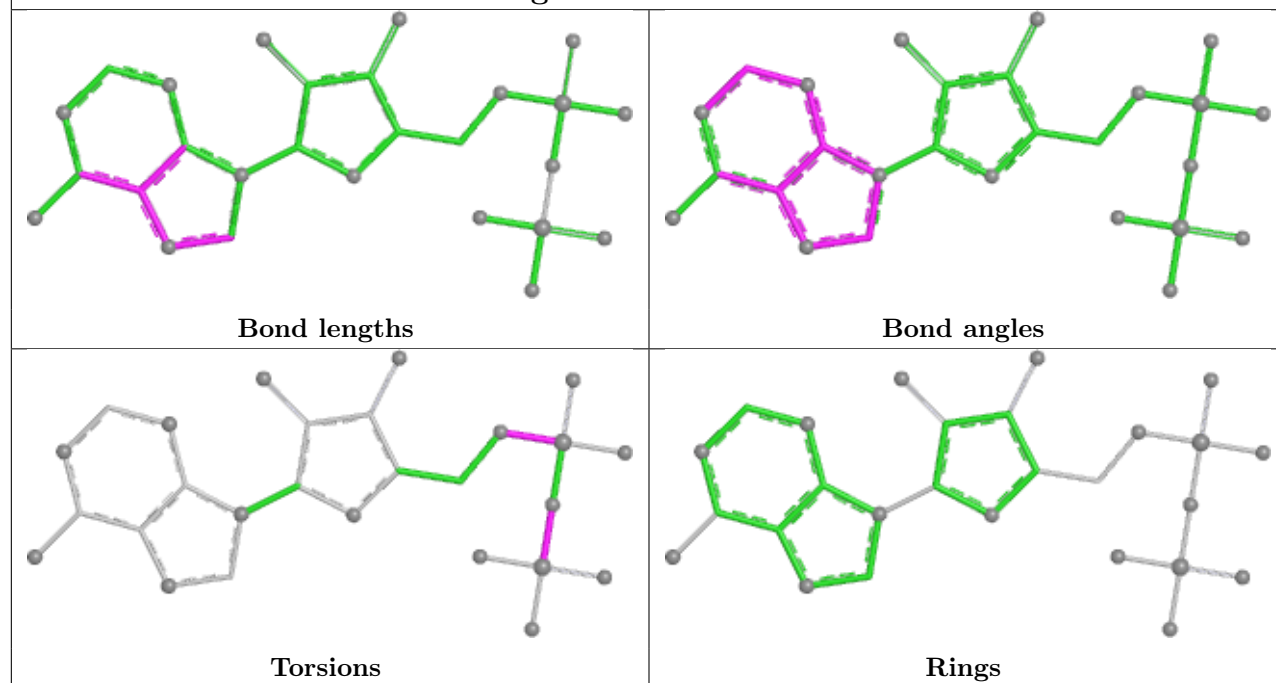




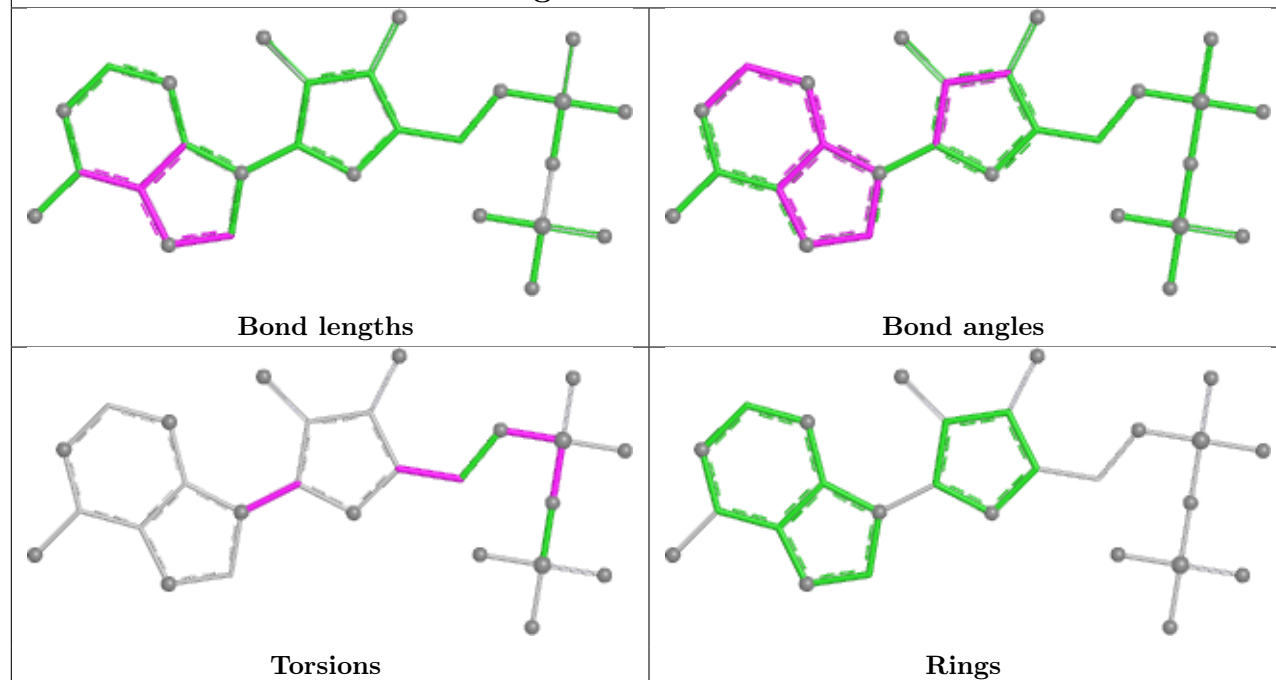
Ligand ADP L 601



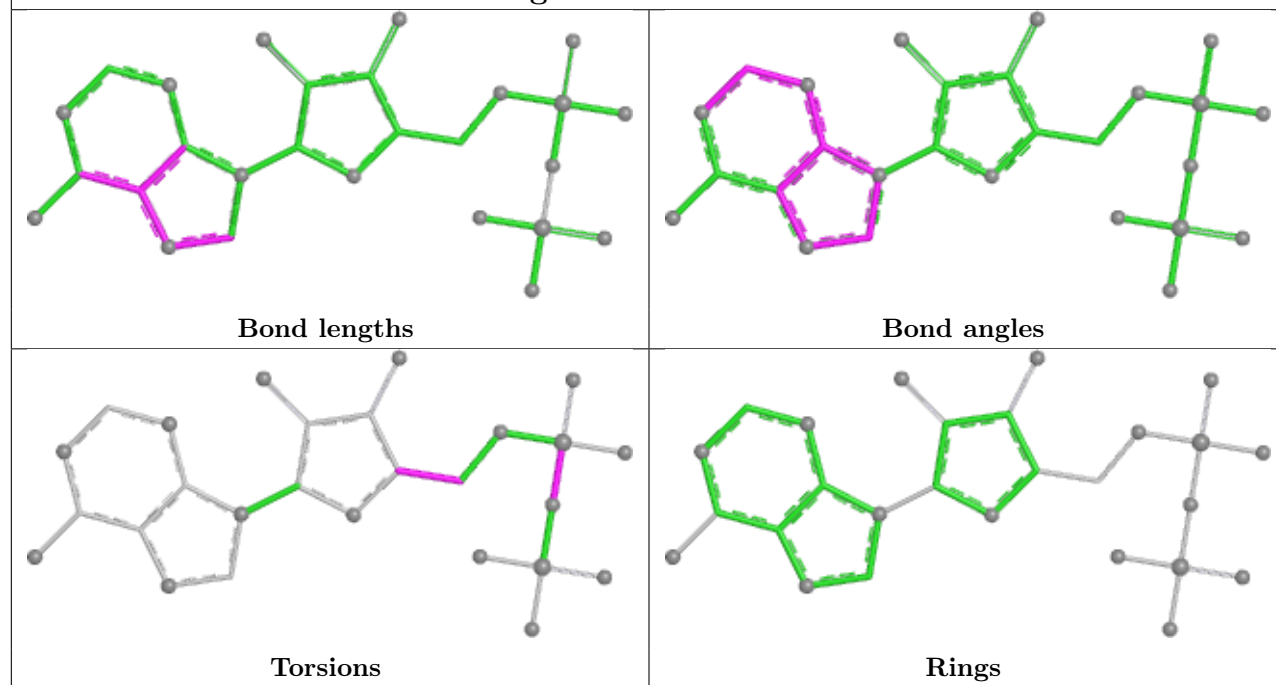
Ligand ADP E 601

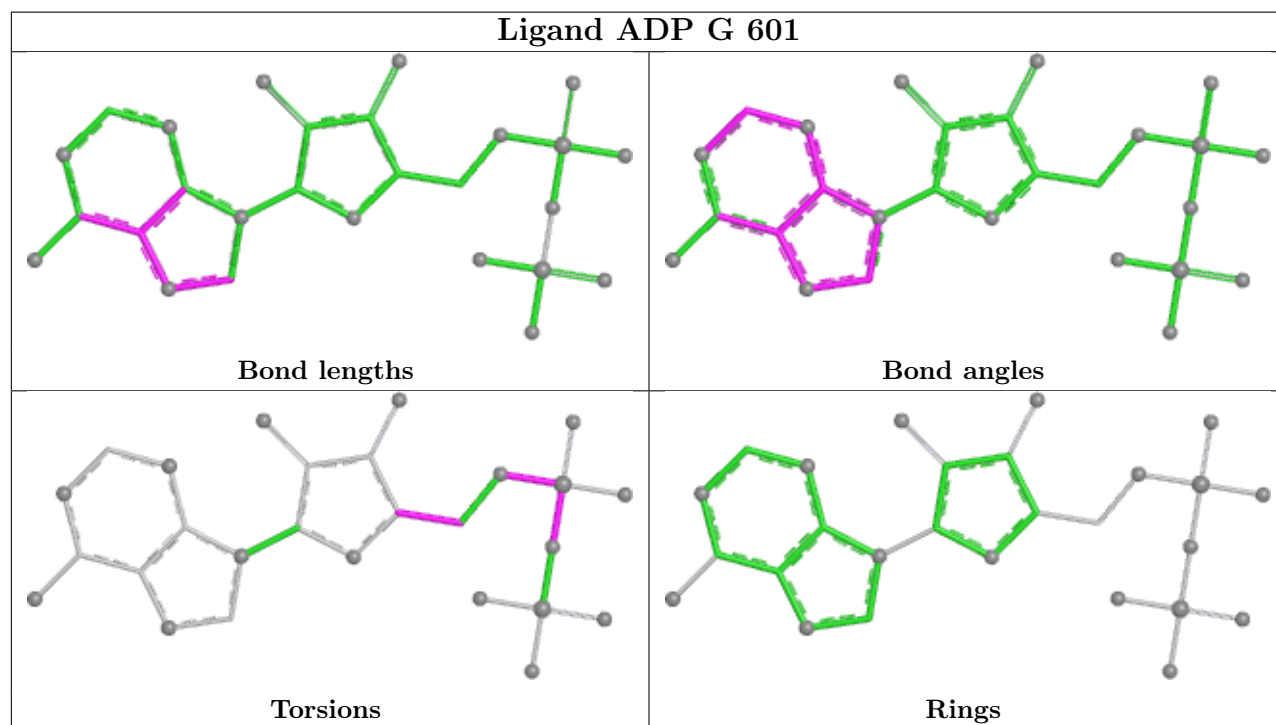
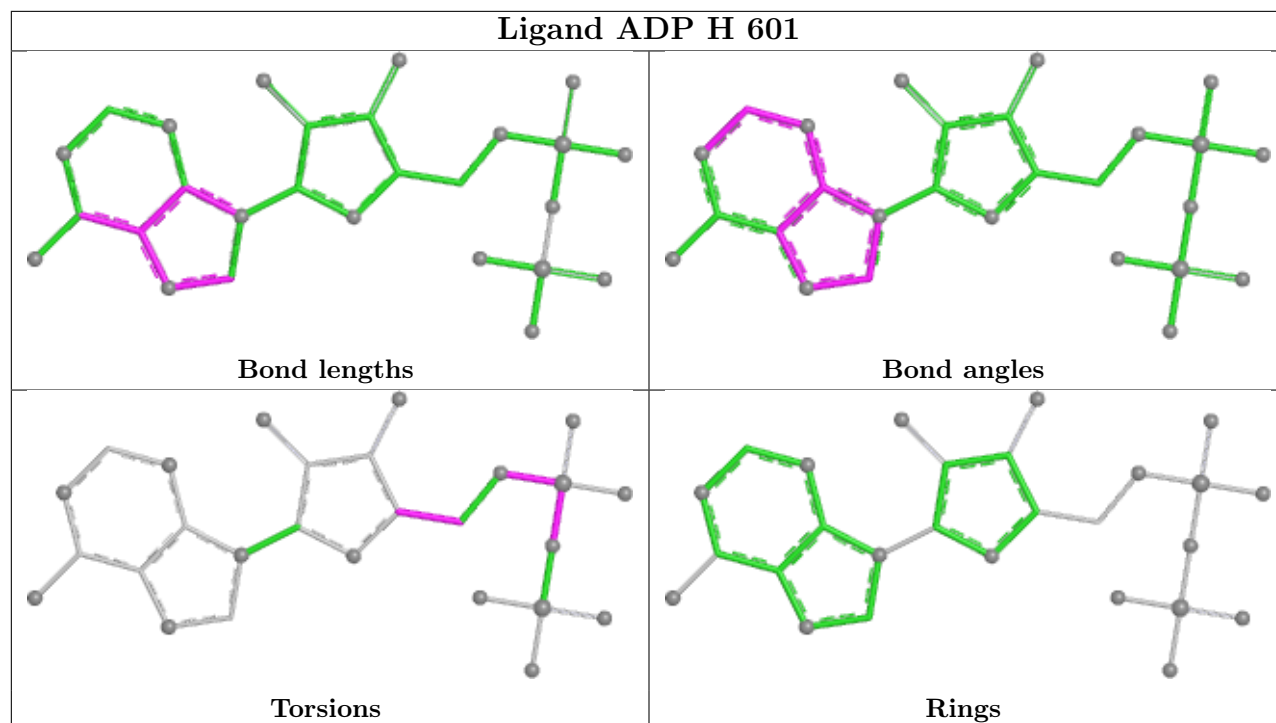


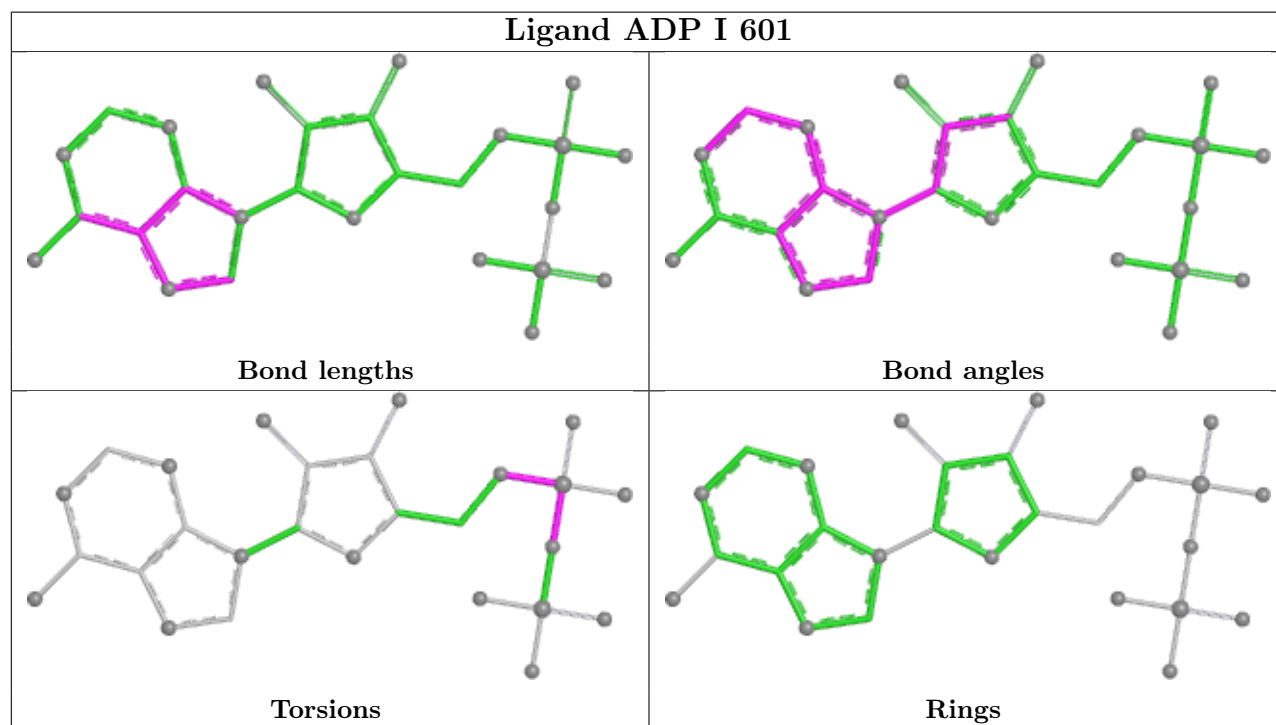
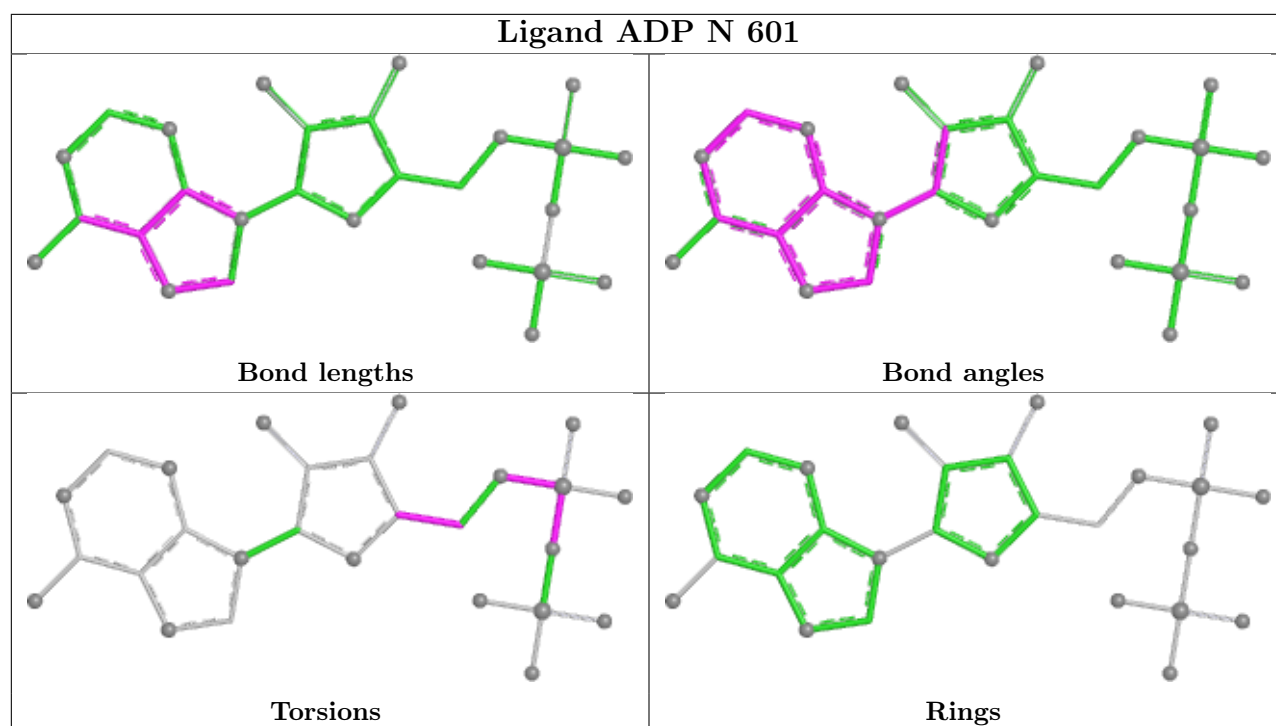
Ligand ADP J 601

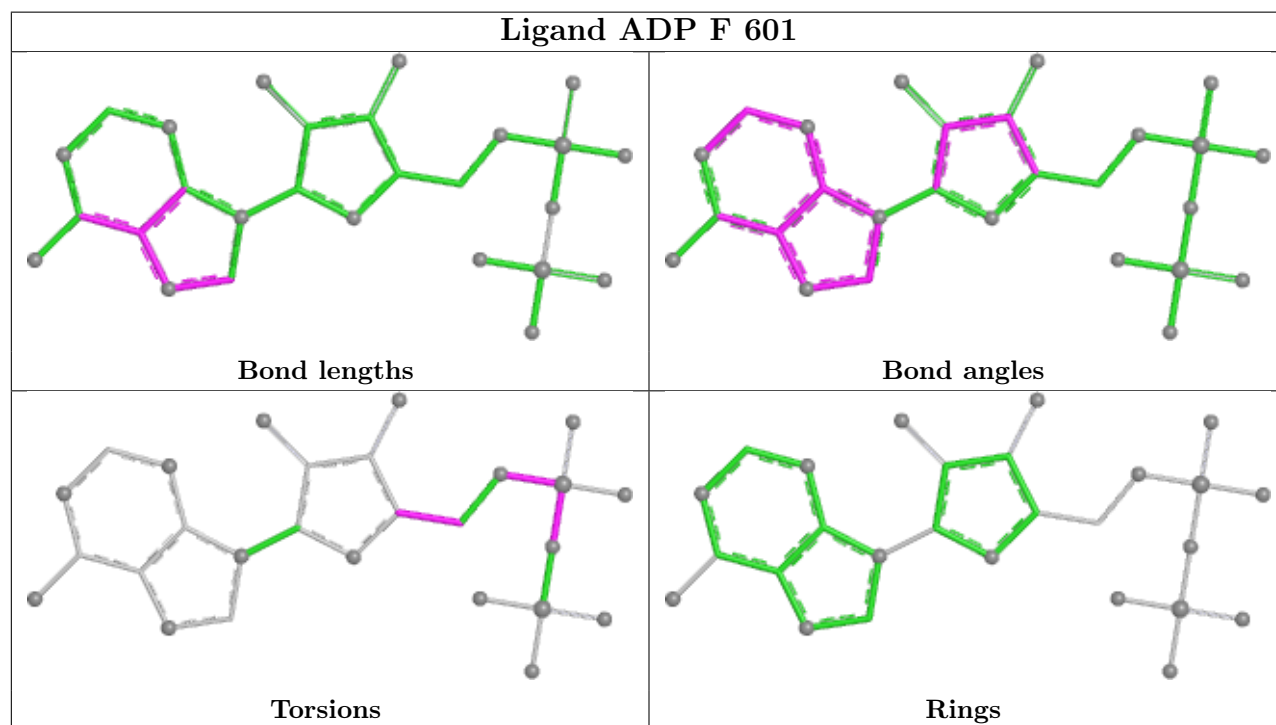
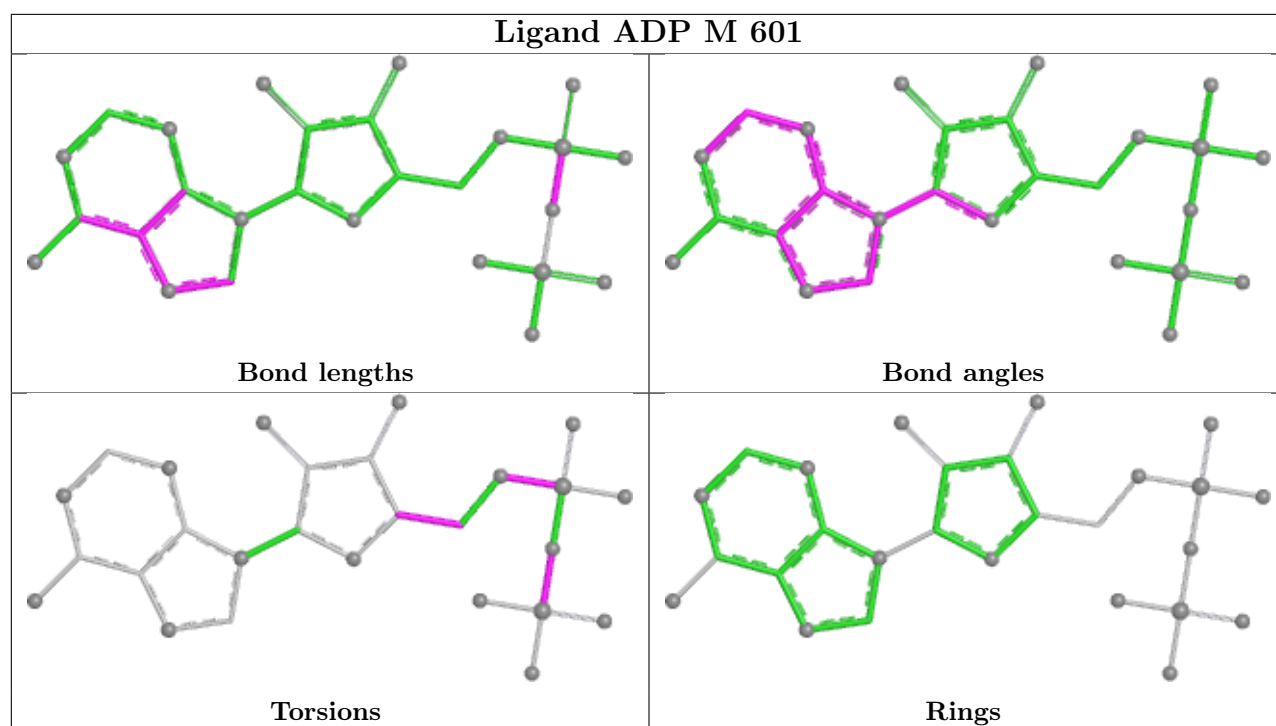


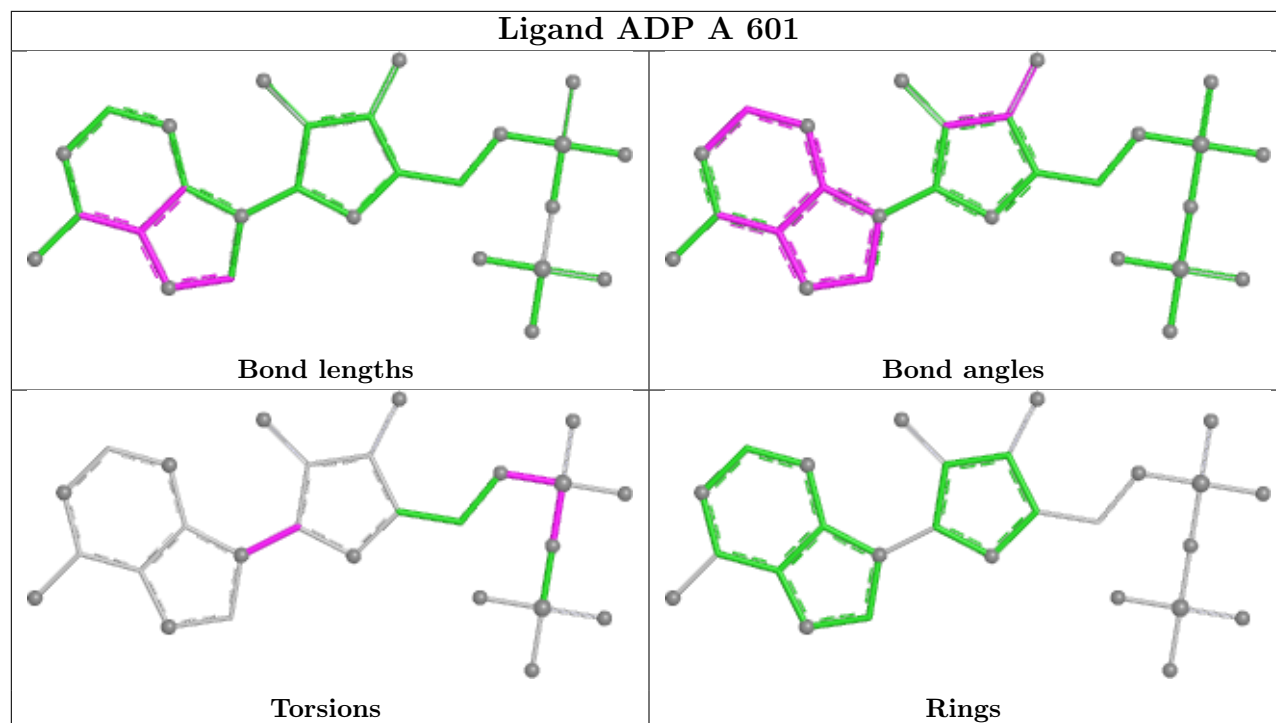
Ligand ADP C 601











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/548 (95%)	-0.15	2 (0%) 88 71	48, 77, 200, 288	0
1	B	524/548 (95%)	-0.25	0 100 100	52, 85, 190, 249	0
1	C	524/548 (95%)	-0.25	1 (0%) 91 80	42, 86, 191, 259	0
1	D	524/548 (95%)	-0.23	1 (0%) 91 80	47, 75, 147, 200	0
1	E	524/548 (95%)	-0.25	0 100 100	51, 88, 197, 270	0
1	F	524/548 (95%)	-0.26	0 100 100	42, 81, 185, 243	0
1	G	524/548 (95%)	-0.24	0 100 100	36, 72, 192, 265	0
1	H	524/548 (95%)	-0.25	0 100 100	43, 89, 210, 243	0
1	I	524/548 (95%)	-0.22	0 100 100	55, 97, 207, 273	0
1	J	524/548 (95%)	-0.15	1 (0%) 91 80	50, 86, 206, 254	0
1	K	524/548 (95%)	-0.21	1 (0%) 91 80	43, 80, 200, 293	0
1	L	524/548 (95%)	-0.30	0 100 100	46, 86, 193, 240	0
1	M	524/548 (95%)	-0.26	0 100 100	45, 85, 198, 281	0
1	N	524/548 (95%)	-0.25	0 100 100	40, 75, 135, 186	0
2	1	97/97 (100%)	-0.01	0 100 100	81, 119, 204, 255	0
2	2	97/97 (100%)	-0.10	2 (2%) 63 38	73, 112, 188, 247	0
2	O	97/97 (100%)	0.01	2 (2%) 63 38	63, 100, 224, 270	0
2	P	97/97 (100%)	-0.09	1 (1%) 79 54	67, 102, 214, 254	0
2	Q	97/97 (100%)	-0.18	0 100 100	84, 122, 244, 275	0
2	R	97/97 (100%)	-0.02	2 (2%) 63 38	82, 121, 182, 198	0
2	S	97/97 (100%)	0.04	0 100 100	82, 132, 211, 243	0
2	T	97/97 (100%)	-0.01	1 (1%) 79 54	91, 144, 202, 233	0
2	U	97/97 (100%)	-0.07	0 100 100	88, 128, 223, 240	0
2	V	96/97 (98%)	-0.15	0 100 100	71, 125, 230, 288	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	96/97 (98%)	-0.11	0 100 100	63, 104, 204, 227	0
2	X	95/97 (97%)	-0.10	1 (1%) 78 52	56, 105, 213, 250	0
2	Y	96/97 (98%)	-0.18	0 100 100	83, 123, 214, 292	0
2	Z	97/97 (100%)	0.01	0 100 100	85, 127, 212, 253	0
All	All	8689/9030 (96%)	-0.21	15 (0%) 91 80	36, 91, 200, 293	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	97	ALA	3.7
1	K	238	GLU	3.5
2	2	25	ILE	3.0
2	T	25	ILE	2.9
2	2	26	VAL	2.8
2	R	26	VAL	2.8
2	P	1	MET	2.6
2	X	25	ILE	2.6
1	C	238	GLU	2.4
1	A	238	GLU	2.3
1	A	240	VAL	2.3
2	R	23	GLY	2.2
1	J	238	GLU	2.0
2	O	26	VAL	2.0
1	D	238	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

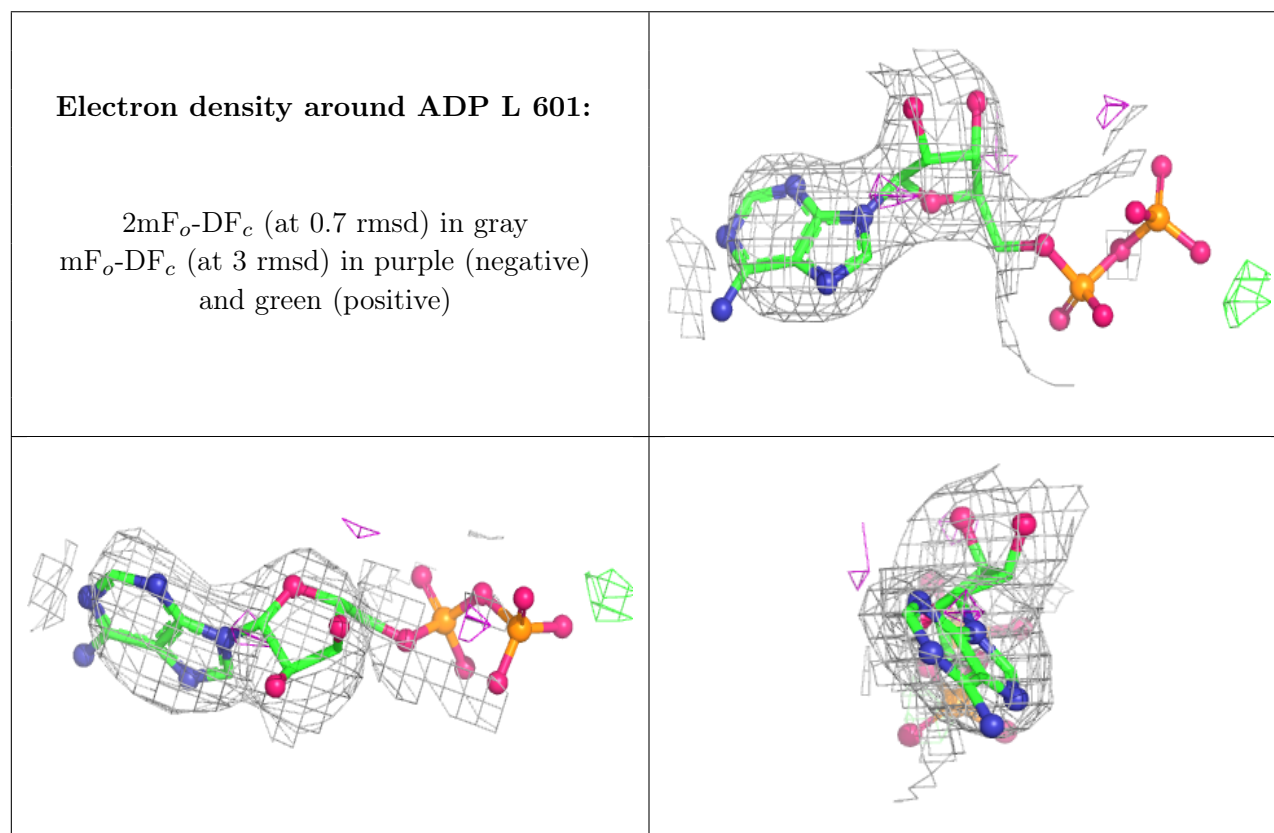
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	K	B	604	1/1	0.82	0.11	115,115,115,115	0
6	K	H	604	1/1	0.88	0.12	162,162,162,162	0
6	K	N	604	1/1	0.90	0.11	123,123,123,123	0
4	BEF	A	602	4/4	0.92	0.09	41,46,52,62	0
4	BEF	M	602	4/4	0.93	0.08	37,56,59,69	0
4	BEF	L	602	4/4	0.94	0.10	31,60,69,211	0
6	K	J	604	1/1	0.94	0.06	99,99,99,99	0
6	K	A	604	1/1	0.95	0.07	76,76,76,76	0
4	BEF	F	602	4/4	0.95	0.07	44,58,60,65	0
6	K	E	604	1/1	0.95	0.07	87,87,87,87	0
4	BEF	I	602	4/4	0.95	0.08	39,77,92,141	0
5	MG	A	603	1/1	0.95	0.10	27,27,27,27	0
5	MG	L	603	1/1	0.95	0.11	53,53,53,53	0
4	BEF	J	602	4/4	0.96	0.07	18,31,49,90	0
3	ADP	L	601	27/27	0.96	0.08	45,70,77,85	0
3	ADP	M	601	27/27	0.96	0.07	26,47,57,70	0
4	BEF	E	602	4/4	0.97	0.07	13,27,53,65	0
4	BEF	C	602	4/4	0.97	0.06	9,45,68,69	0
3	ADP	C	601	27/27	0.97	0.05	29,55,68,72	0
3	ADP	D	601	27/27	0.97	0.06	33,44,59,63	0
3	ADP	K	601	27/27	0.97	0.06	29,50,57,71	0
3	ADP	J	601	27/27	0.97	0.07	11,46,74,80	0
3	ADP	I	601	27/27	0.97	0.06	2,60,73,75	0
3	ADP	A	601	27/27	0.97	0.07	31,50,65,75	0
3	ADP	B	601	27/27	0.97	0.07	26,57,65,66	0
3	ADP	N	601	27/27	0.97	0.07	35,42,48,61	0
4	BEF	G	602	4/4	0.97	0.08	19,29,42,121	0
3	ADP	F	601	27/27	0.97	0.06	30,53,62,71	0
6	K	I	604	1/1	0.97	0.06	67,67,67,67	0
6	K	L	604	1/1	0.97	0.04	65,65,65,65	0
6	K	M	604	1/1	0.97	0.04	51,51,51,51	0
4	BEF	B	602	4/4	0.97	0.06	7,12,25,66	0
3	ADP	E	601	27/27	0.97	0.06	29,50,59,69	0
5	MG	M	603	1/1	0.98	0.06	8,8,8,8	0
6	K	G	604	1/1	0.98	0.04	51,51,51,51	0
4	BEF	D	602	4/4	0.98	0.05	30,30,35,51	0
4	BEF	K	602	4/4	0.98	0.07	19,25,82,105	0
6	K	F	604	1/1	0.98	0.05	81,81,81,81	0
4	BEF	H	602	4/4	0.98	0.05	12,21,33,89	0
6	K	D	604	1/1	0.98	0.07	63,63,63,63	0
4	BEF	N	602	4/4	0.98	0.07	12,28,34,74	0
5	MG	G	603	1/1	0.98	0.04	41,41,41,41	0
3	ADP	H	601	27/27	0.98	0.05	36,58,64,84	0

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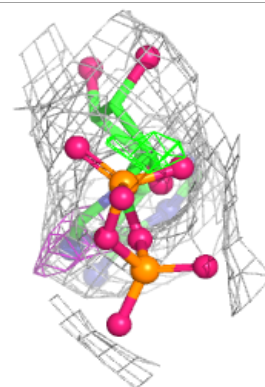
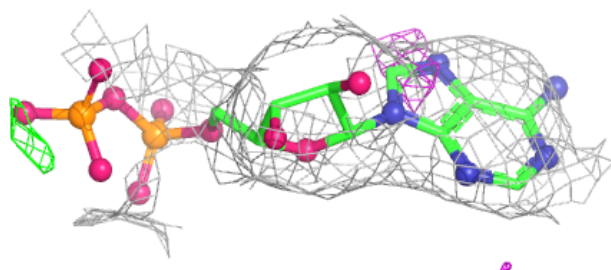
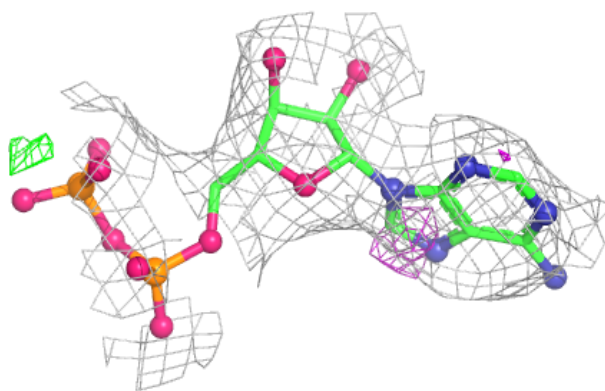
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	D	603	1/1	0.98	0.05	16,16,16,16	0
5	MG	J	603	1/1	0.98	0.07	51,51,51,51	0
3	ADP	G	601	27/27	0.98	0.05	20,43,54,57	0
6	K	C	604	1/1	0.99	0.04	64,64,64,64	0
5	MG	H	603	1/1	0.99	0.02	44,44,44,44	0
6	K	K	604	1/1	0.99	0.04	47,47,47,47	0
5	MG	N	603	1/1	0.99	0.07	11,11,11,11	0
5	MG	K	603	1/1	0.99	0.05	44,44,44,44	0
5	MG	E	603	1/1	0.99	0.04	11,11,11,11	0
5	MG	I	603	1/1	0.99	0.03	17,17,17,17	0
5	MG	C	603	1/1	0.99	0.04	21,21,21,21	0
5	MG	B	603	1/1	0.99	0.04	32,32,32,32	0
5	MG	F	603	1/1	1.00	0.03	33,33,33,33	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.

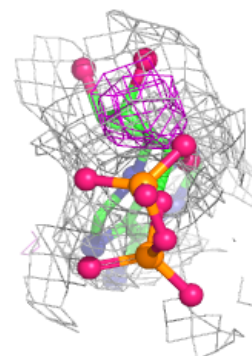
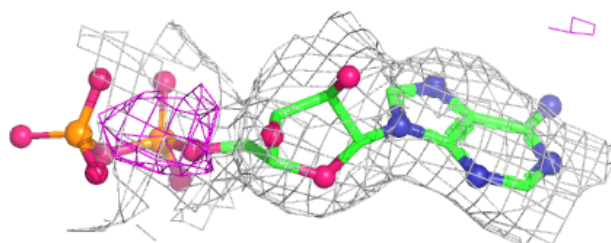
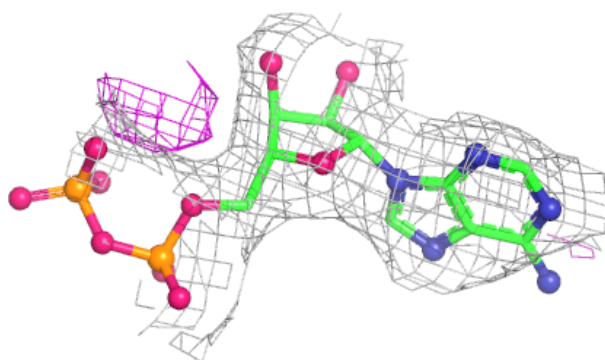


Electron density around ADP M 601:

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

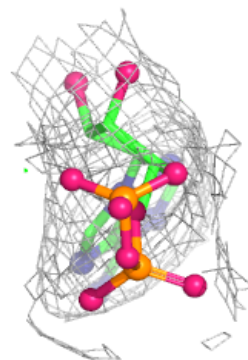
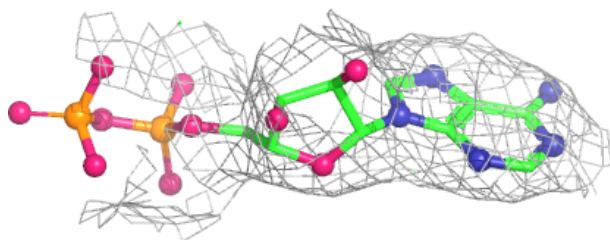
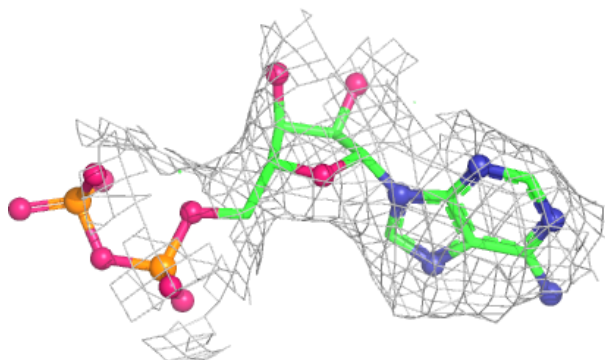
**Electron density around ADP C 601:**

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

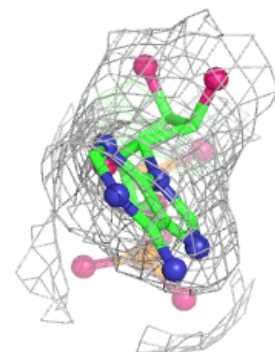
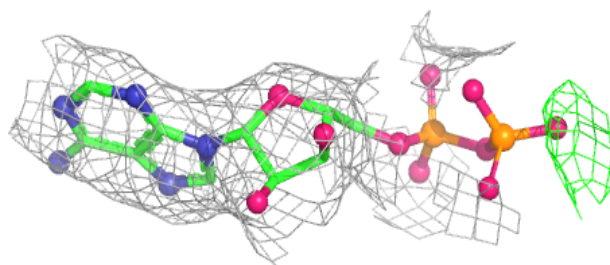
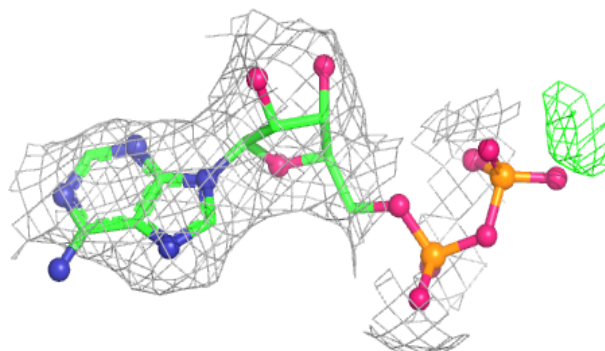


Electron density around ADP D 601:

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

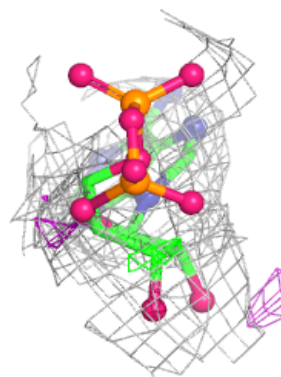
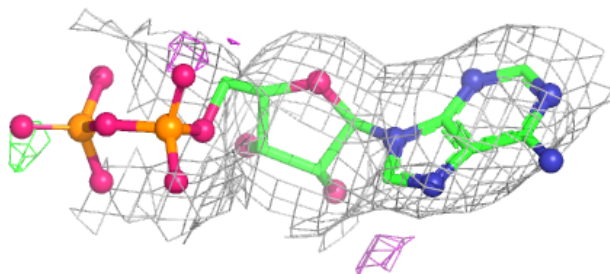
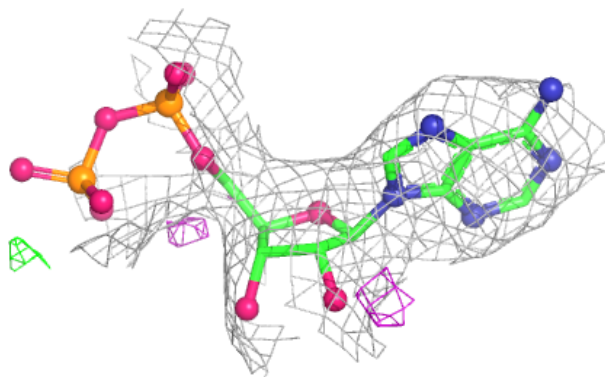
**Electron density around ADP K 601:**

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

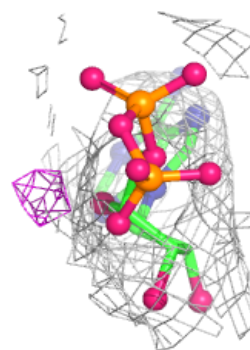
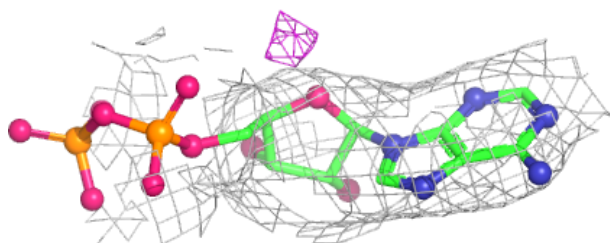
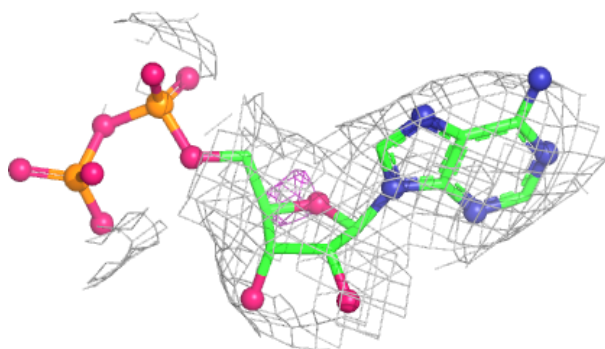


Electron density around ADP J 601:

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

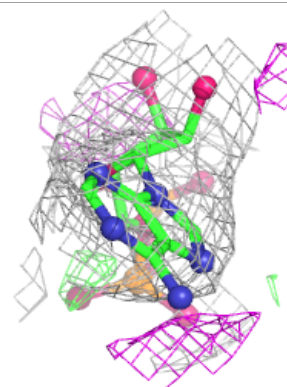
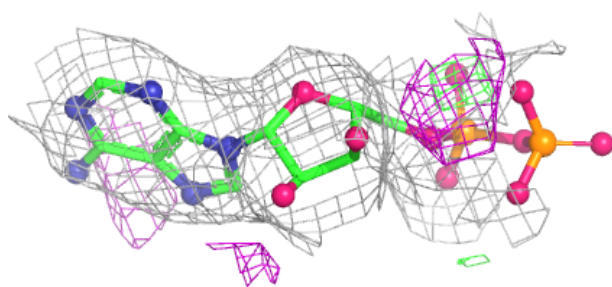
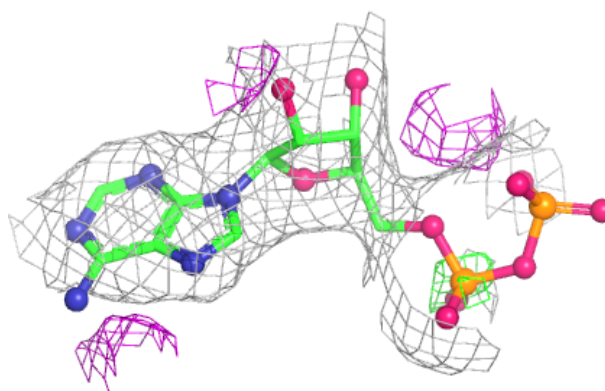
**Electron density around ADP I 601:**

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

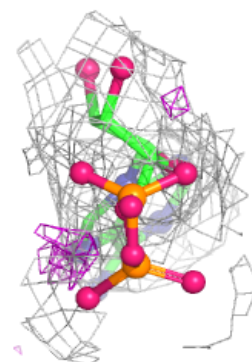
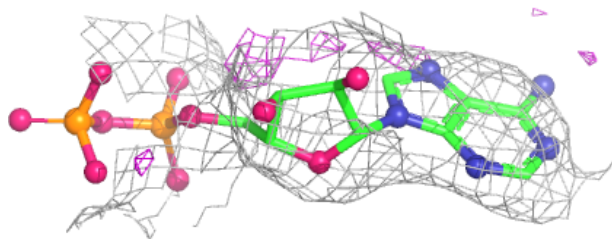
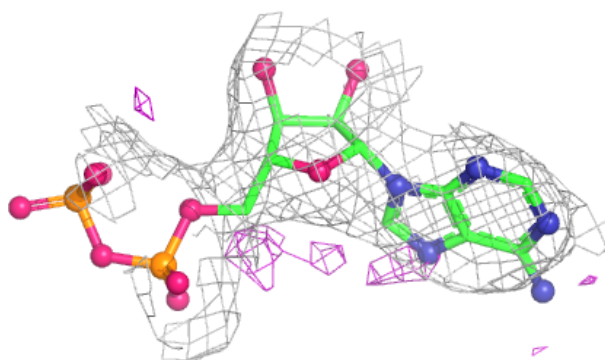


Electron density around ADP A 601:

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

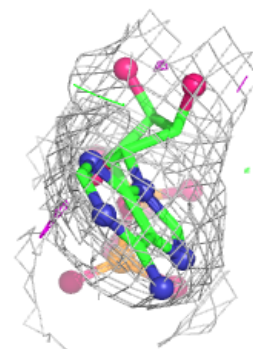
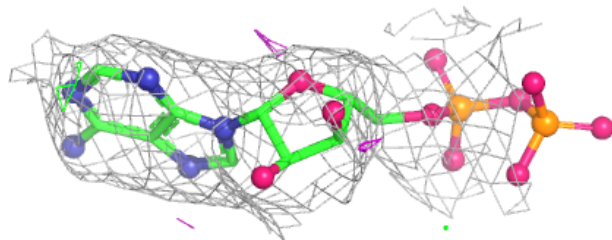
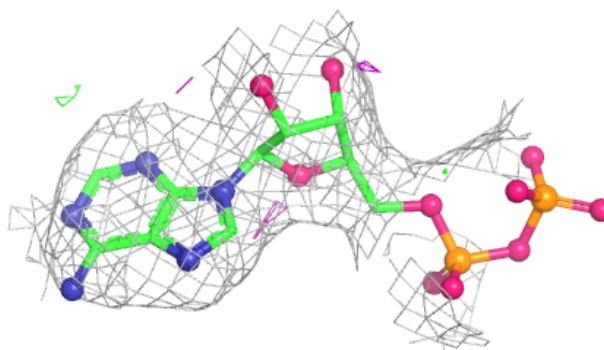
**Electron density around ADP B 601:**

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

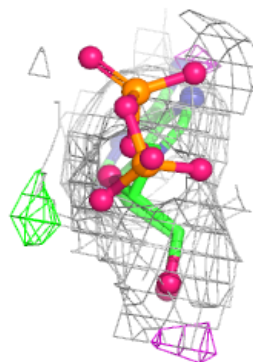
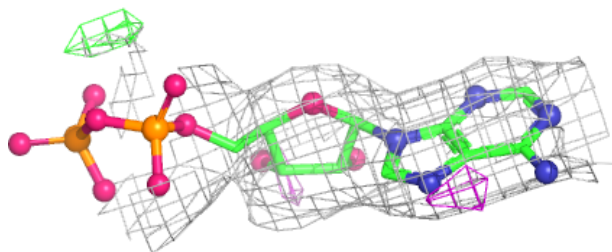
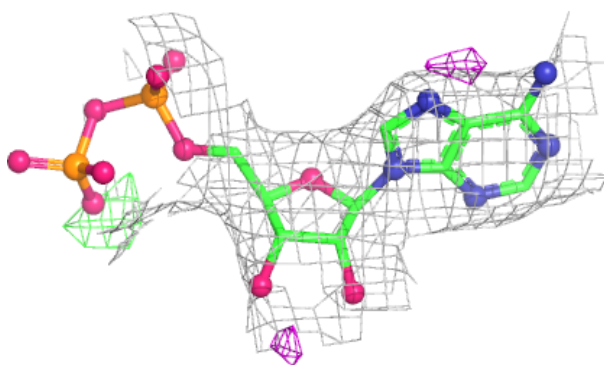


Electron density around ADP N 601:

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

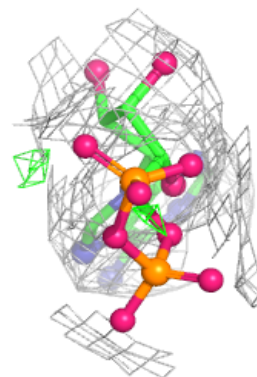
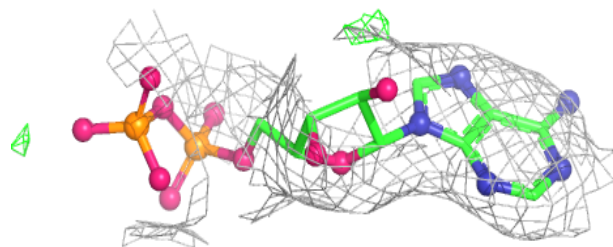
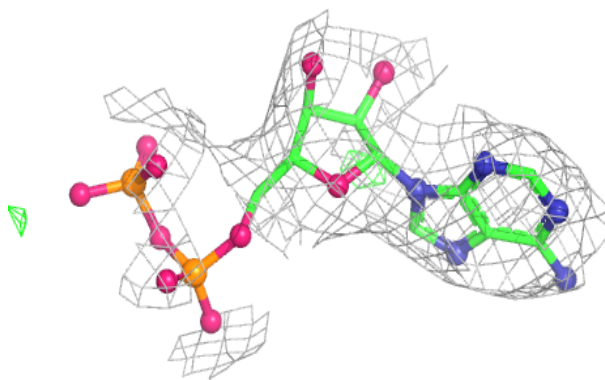
**Electron density around ADP F 601:**

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

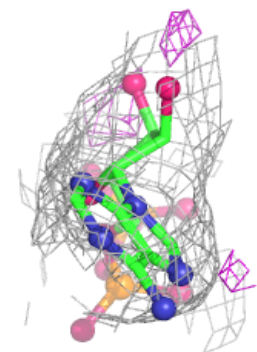
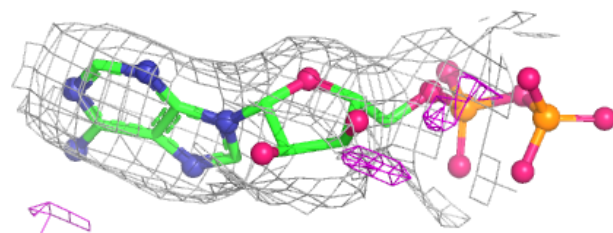
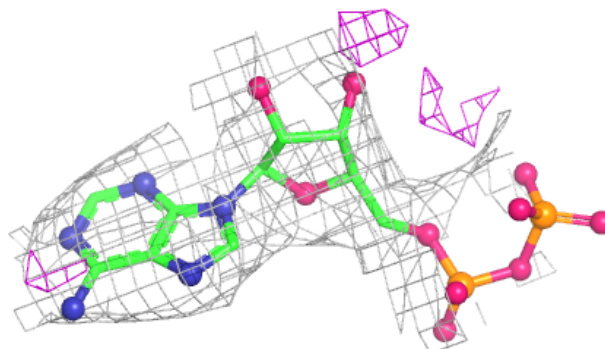


Electron density around ADP E 601:

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

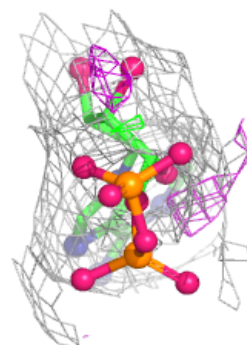
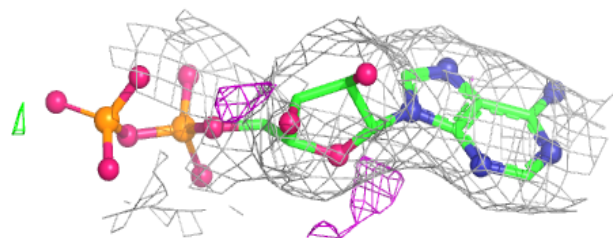
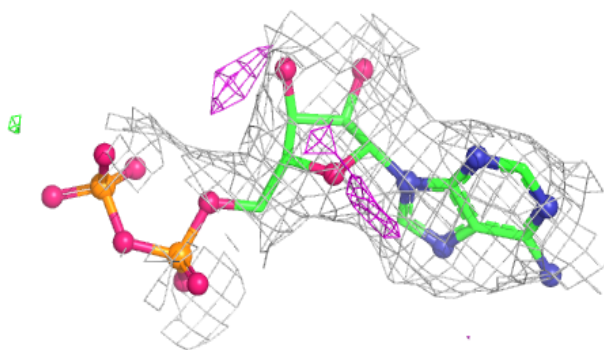
**Electron density around ADP H 601:**

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



Electron density around ADP G 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.