



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:22 PM UTC

PDB ID : 1SX4 / pdb_00001sx4
Title : GroEL-GroES-ADP7
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.
Deposited on : 2004-03-30
Resolution : 3.00 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

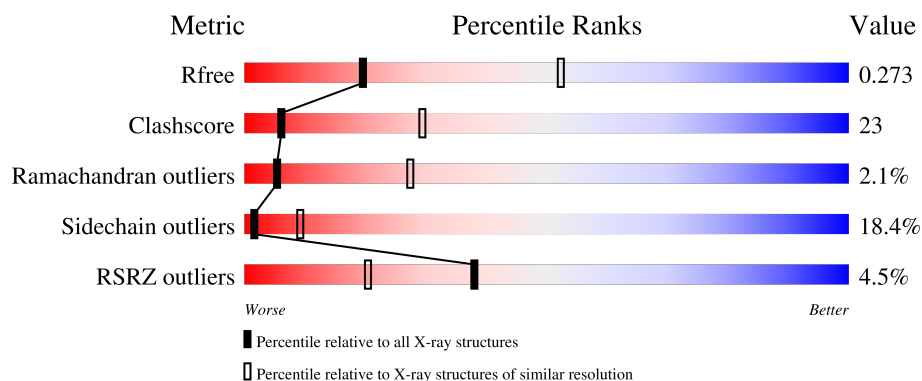
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	524	3% 50% 37% 11% .
1	B	524	4% 52% 36% 11% .
1	C	524	4% 48% 41% 10% .
1	D	524	4% 49% 39% 10% .
1	E	524	7% 52% 37% 10% .

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Mol	Chain	Length	Quality of chain
1	F	524	
1	G	524	
1	H	524	
1	I	524	
1	J	524	
1	K	524	
1	L	524	
1	M	524	
1	N	524	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 59457 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	B	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	C	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	D	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	E	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	F	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	G	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	H	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	I	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	J	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	K	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	L	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	M	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	N	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			

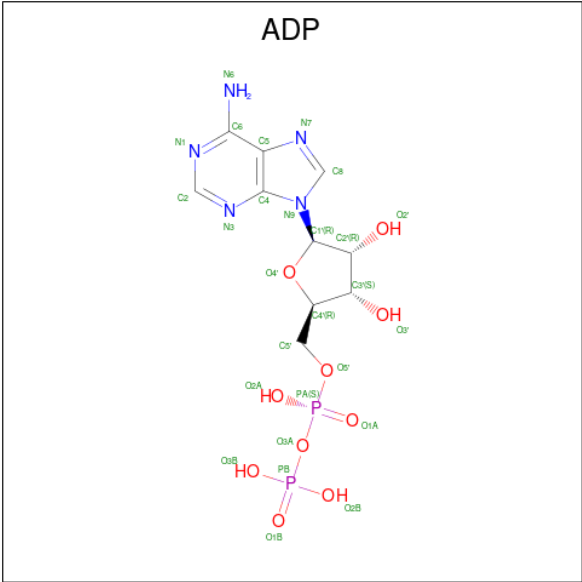
- Molecule 2 is a protein called groES protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	P	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	Q	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	R	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	S	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	T	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	U	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	10	Total	O	0	0
			10	10		
5	C	11	Total	O	0	0
			11	11		
5	D	11	Total	O	0	0
			11	11		
5	E	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	8	Total 8	O 8	0	0
5	G	13	Total 13	O 13	0	0
5	H	12	Total 12	O 12	0	0
5	I	19	Total 19	O 19	0	0
5	J	14	Total 14	O 14	0	0
5	K	14	Total 14	O 14	0	0
5	L	16	Total 16	O 16	0	0
5	M	10	Total 10	O 10	0	0
5	N	21	Total 21	O 21	0	0

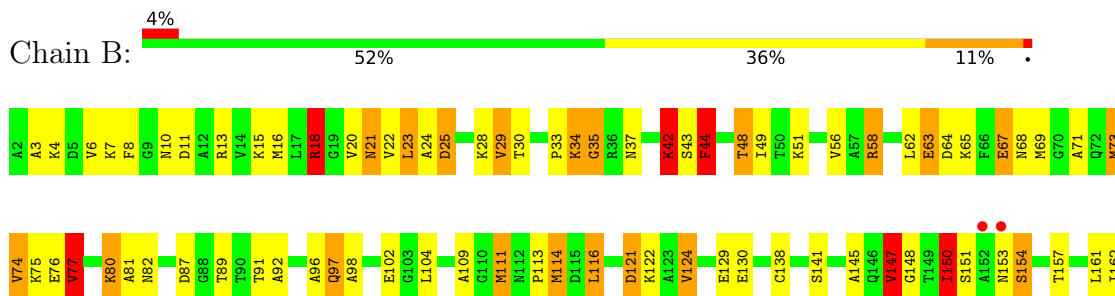
3 Residue-property plots

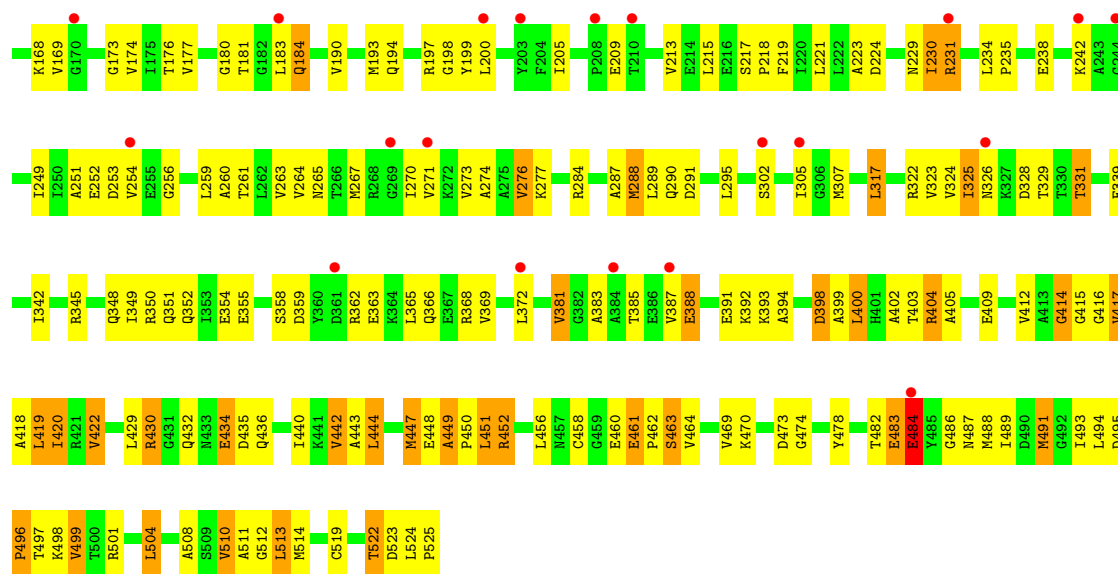
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: groEL protein

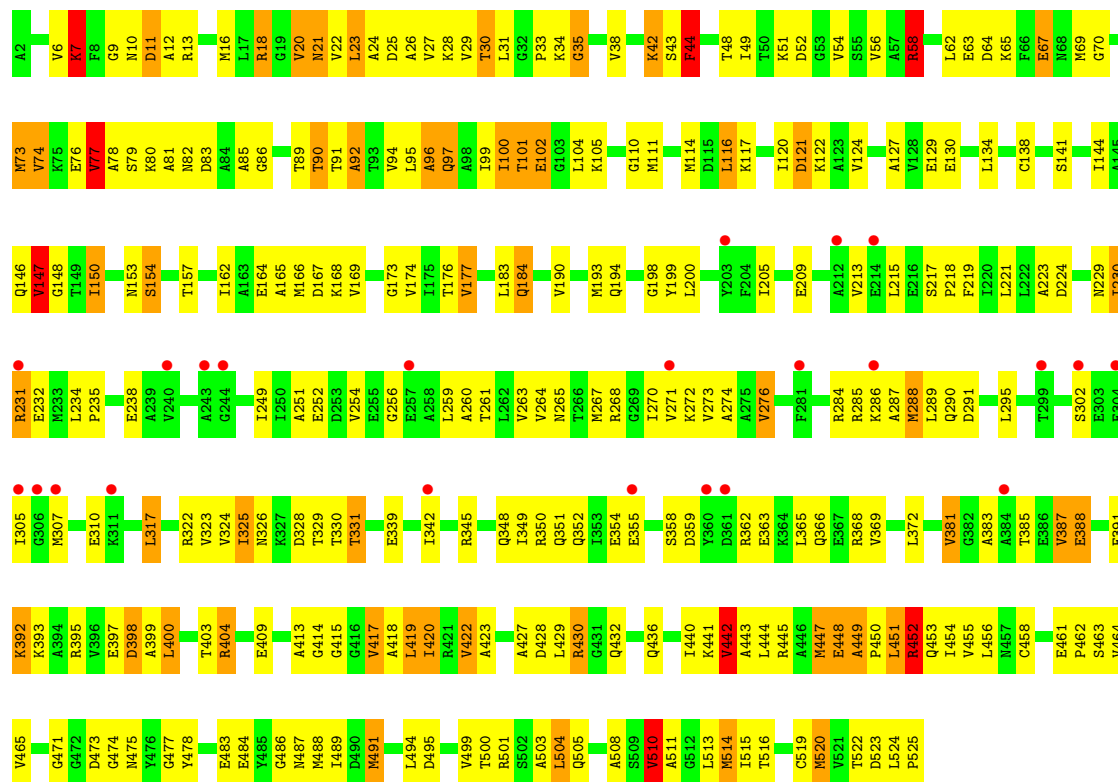


• Molecule 1: groEL protein

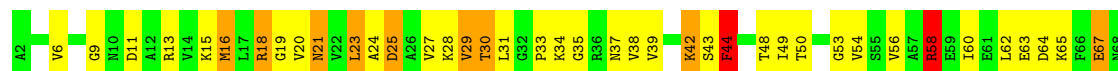


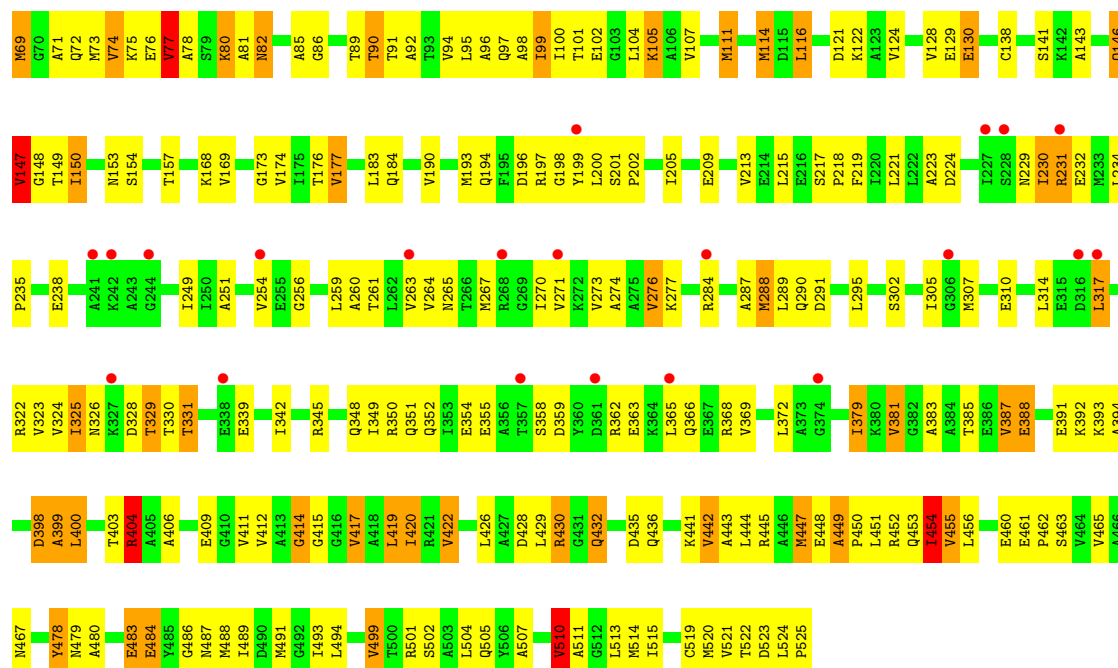


• Molecule 1: groEL protein

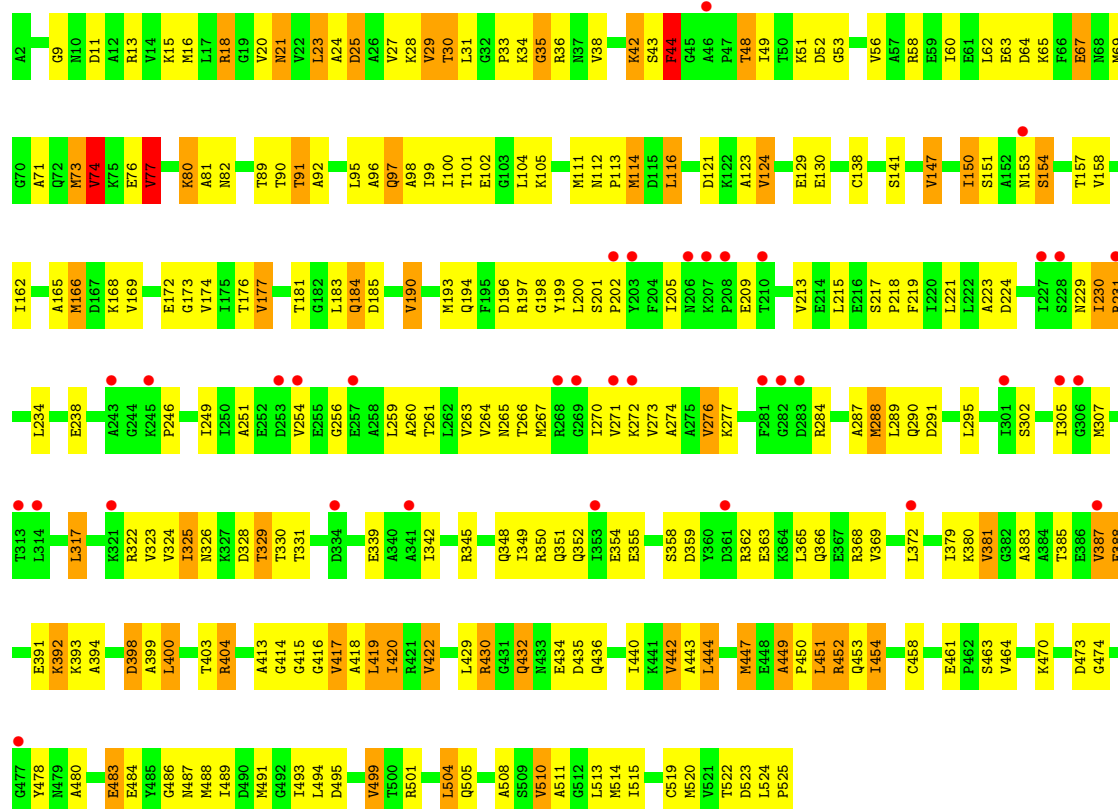


• Molecule 1: groEL protein

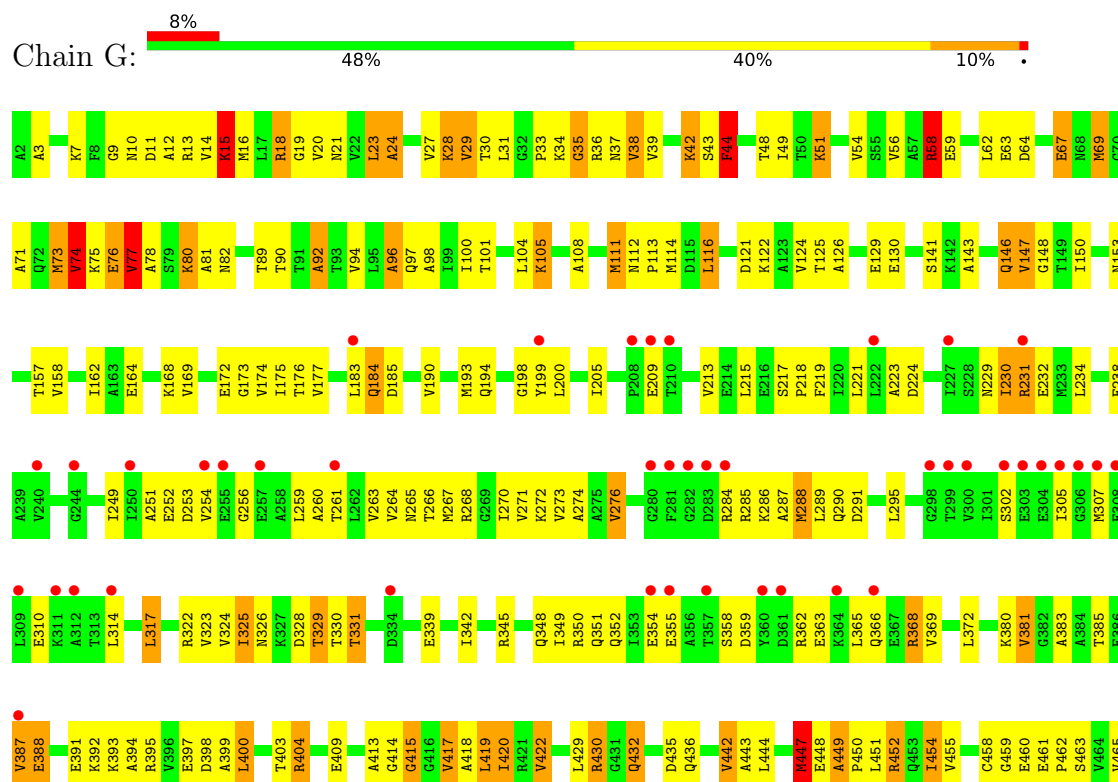
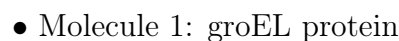




• Molecule 1: groEL protein

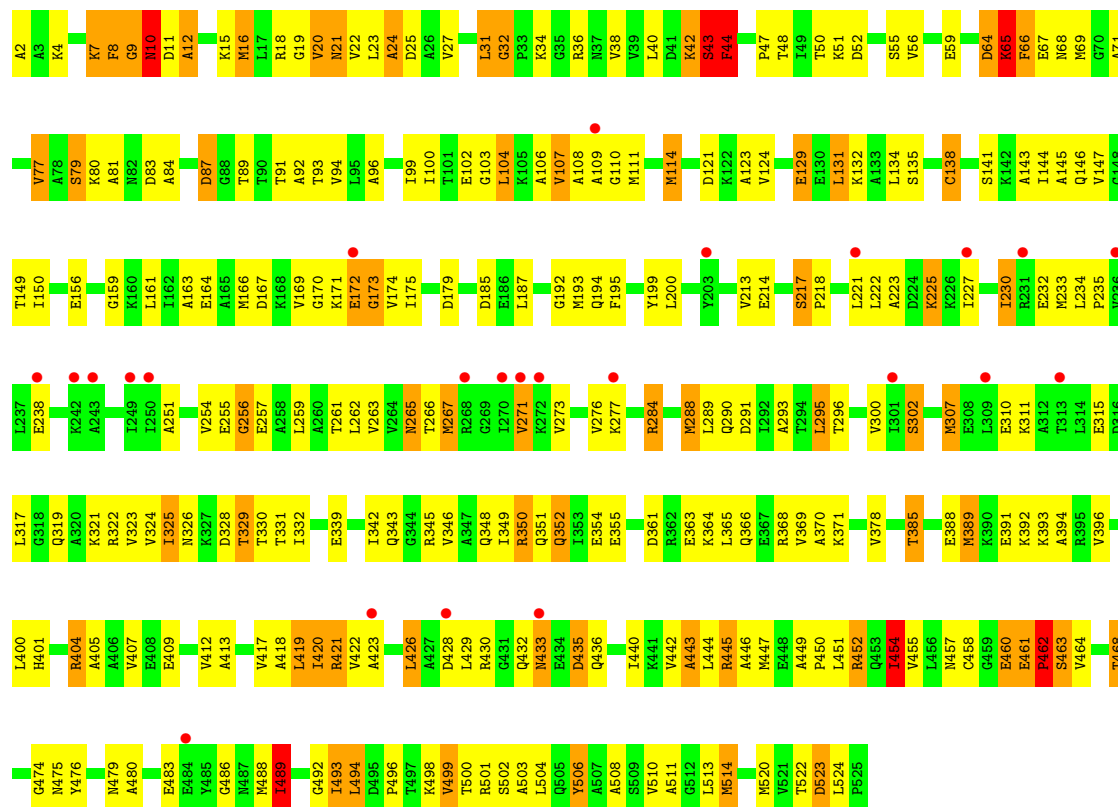


• Molecule 1: groEL protein

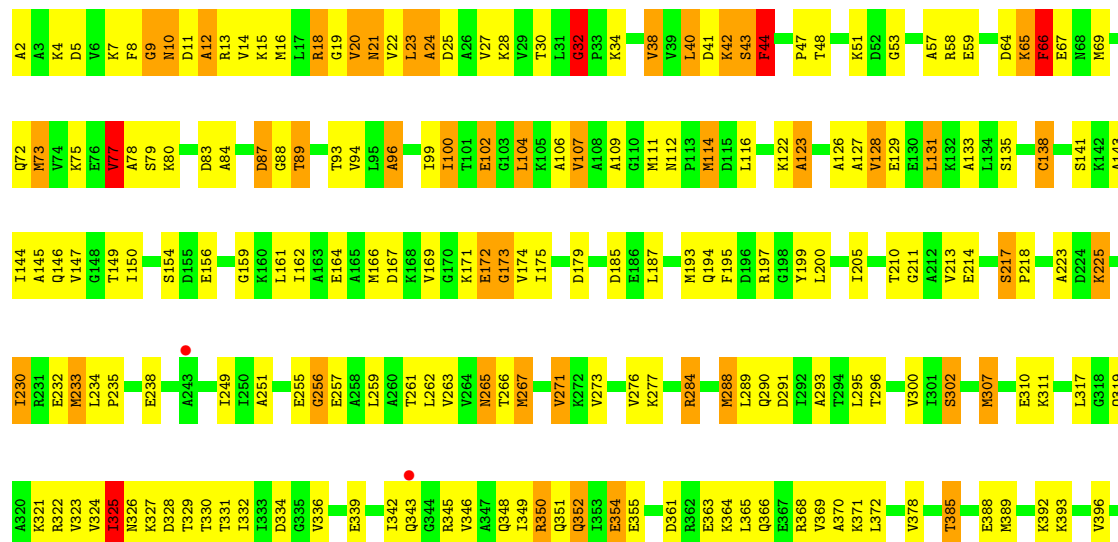


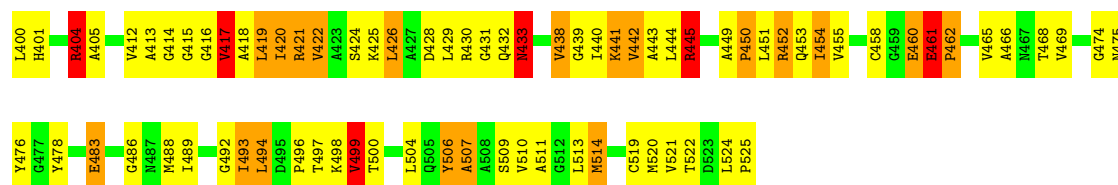


• Molecule 1: groEL protein

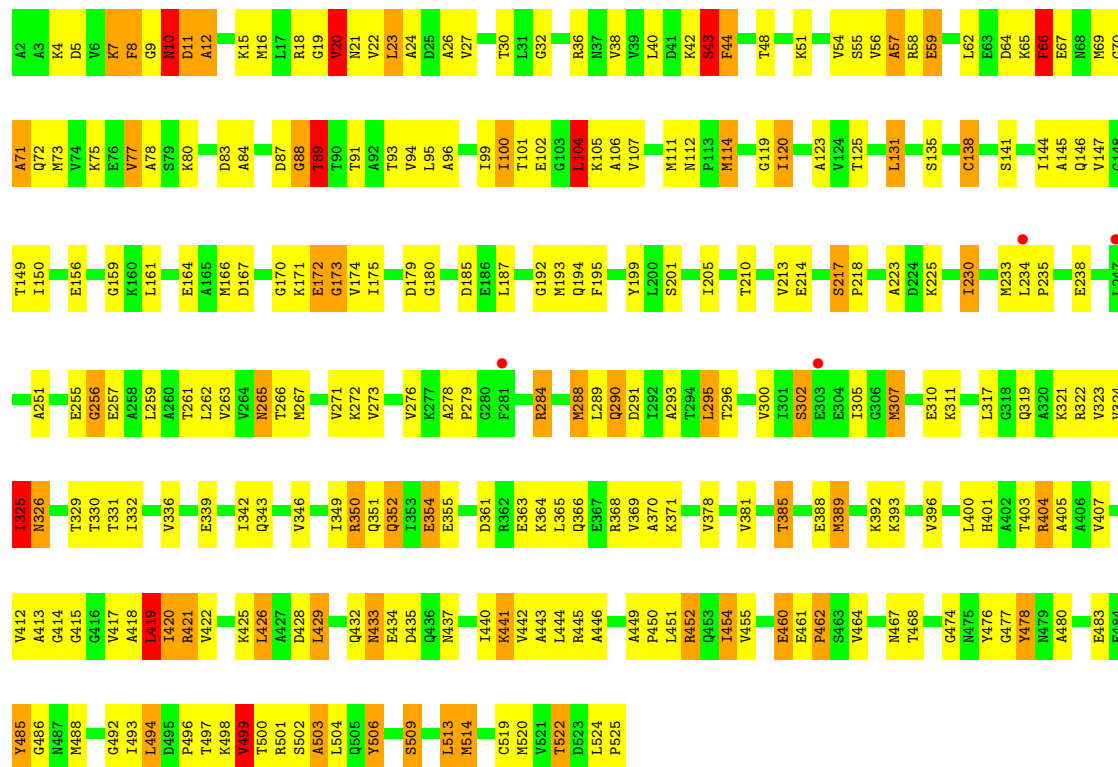


• Molecule 1: groEL protein

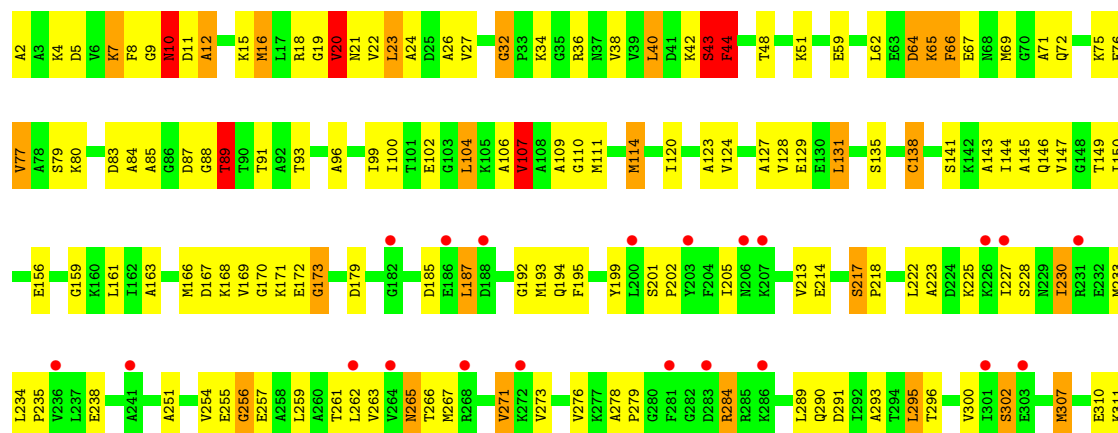


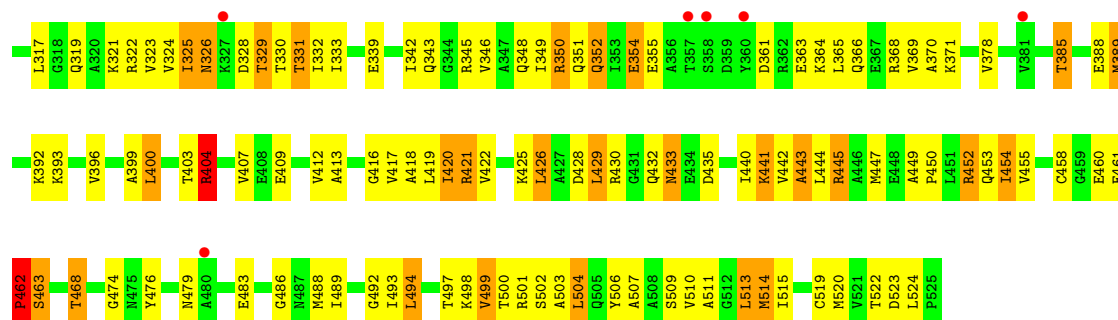


• Molecule 1: groEL protein

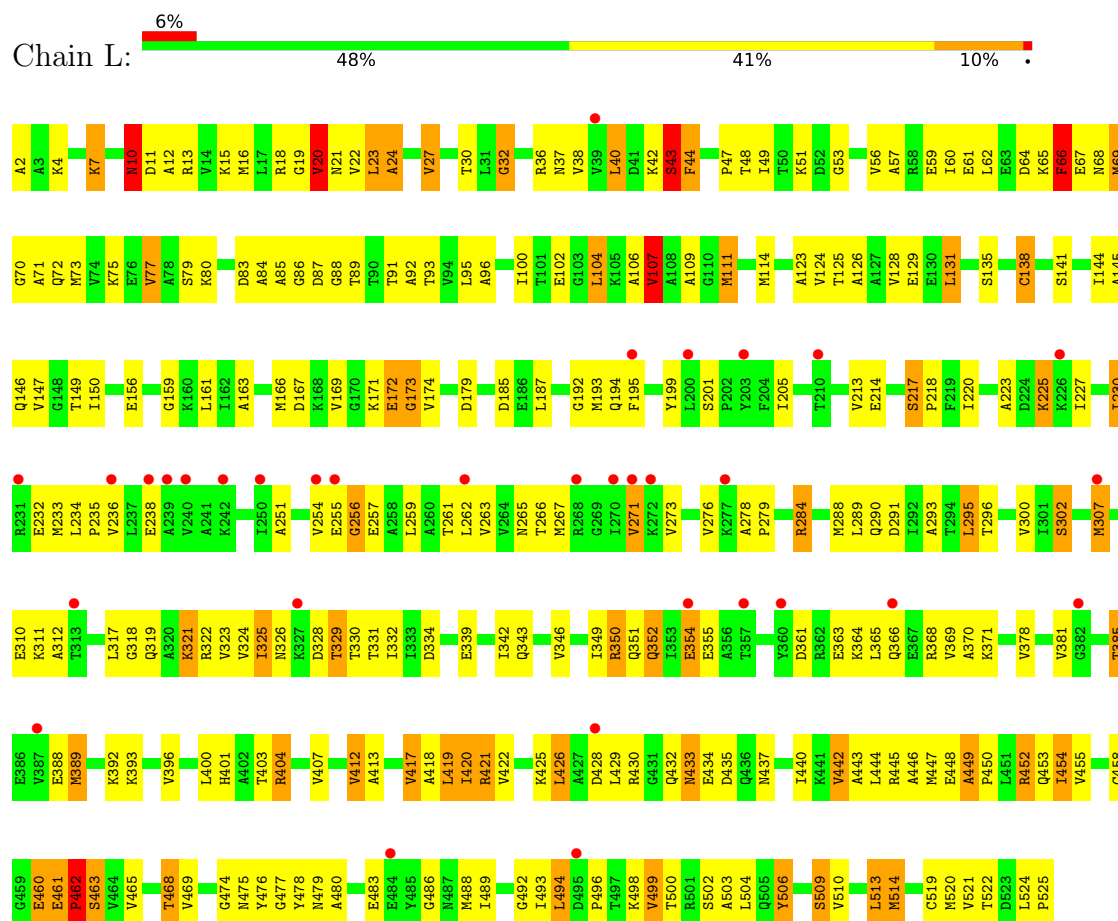


• Molecule 1: groEL protein

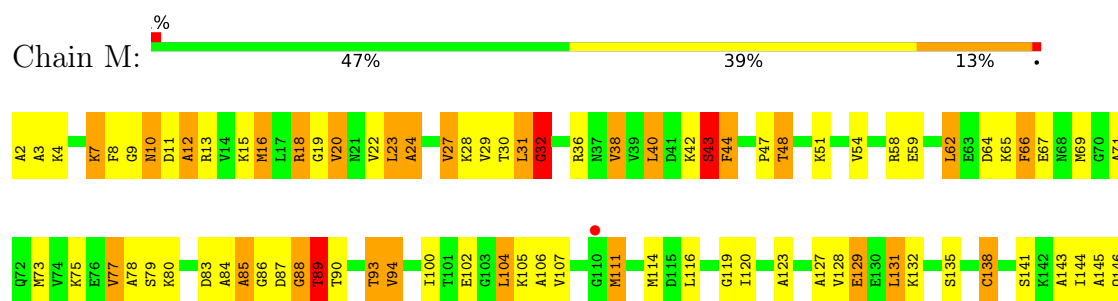


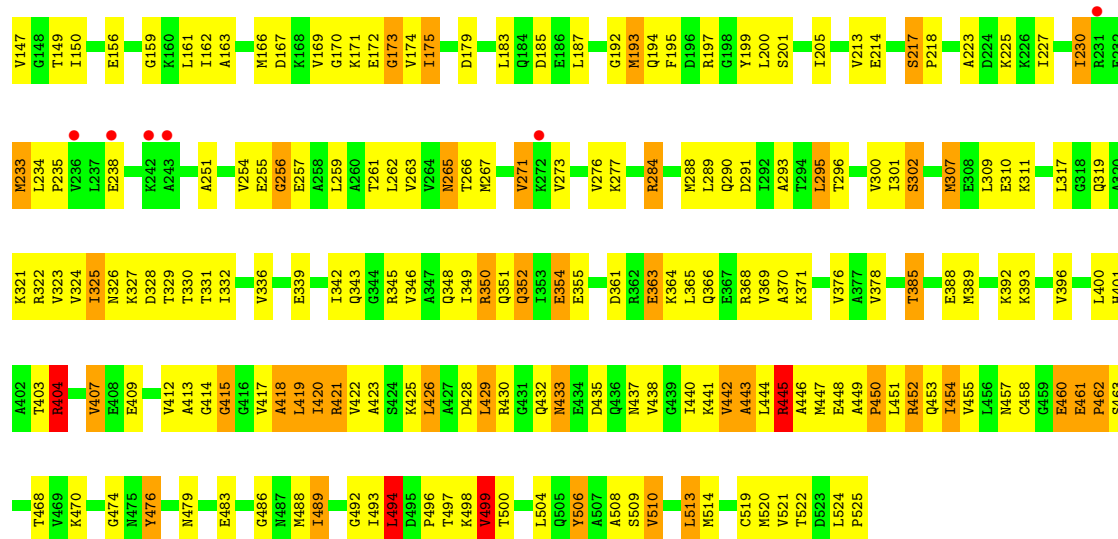


• Molecule 1: groEL protein

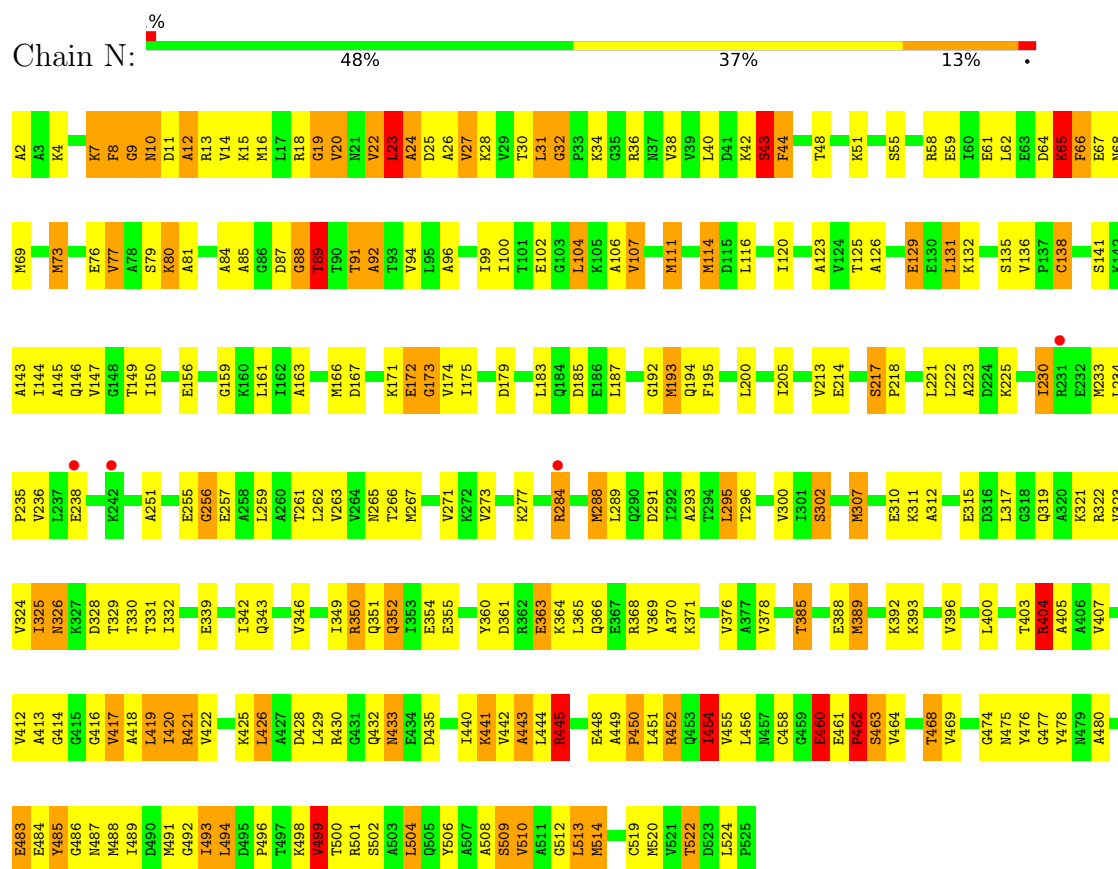


• Molecule 1: groEL protein

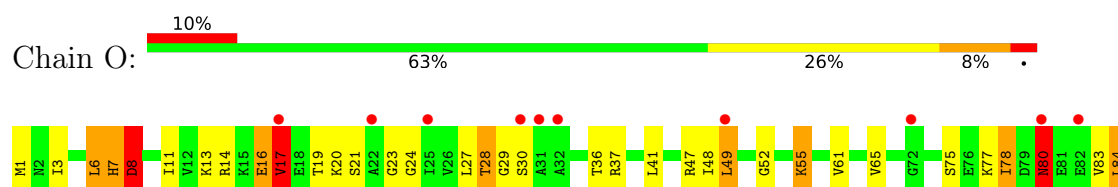




• Molecule 1: groEL protein

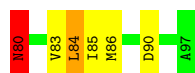


• Molecule 2: groES protein

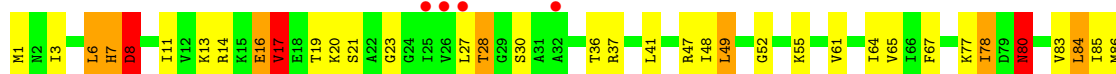




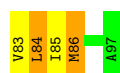
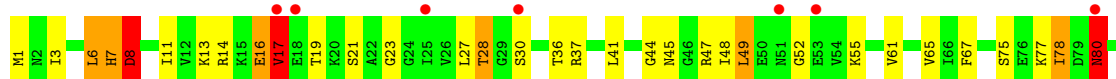
- Molecule 2: groES protein



- Molecule 2: groES protein



- Molecule 2: groES protein

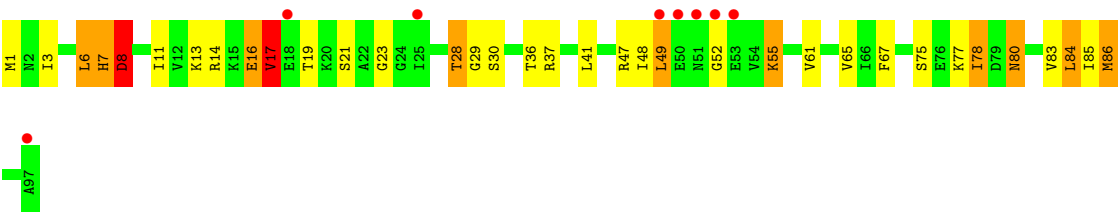


- Molecule 2: groES protein



- Molecule 2: groES protein





● Molecule 2: groES protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	255.26Å 265.25Å 184.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 97.0 (40.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC refmac_5.1.19	Depositor
R, R_{free}	0.258 , 0.287 0.246 , 0.273	Depositor DCC
R_{free} test set	12081 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 86.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	59457	wwPDB-VP
Average B, all atoms (Å ²)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: ADP, MG

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	1.55	39/3884 (1.0%)	1.51	31/5243 (0.6%)
1	B	1.38	25/3884 (0.6%)	1.40	27/5243 (0.5%)
1	C	1.53	34/3884 (0.9%)	1.51	44/5243 (0.8%)
1	D	1.53	37/3884 (1.0%)	1.47	31/5243 (0.6%)
1	E	1.30	19/3884 (0.5%)	1.35	22/5243 (0.4%)
1	F	1.24	18/3884 (0.5%)	1.32	19/5243 (0.4%)
1	G	1.47	39/3884 (1.0%)	1.43	32/5243 (0.6%)
1	H	1.37	24/3884 (0.6%)	1.42	33/5243 (0.6%)
1	I	1.50	40/3884 (1.0%)	1.48	35/5243 (0.7%)
1	J	1.43	26/3884 (0.7%)	1.45	30/5243 (0.6%)
1	K	1.24	13/3884 (0.3%)	1.32	16/5243 (0.3%)
1	L	1.16	11/3884 (0.3%)	1.29	13/5243 (0.2%)
1	M	1.42	31/3884 (0.8%)	1.42	22/5243 (0.4%)
1	N	1.42	34/3884 (0.9%)	1.41	32/5243 (0.6%)
2	O	0.90	1/732 (0.1%)	1.07	2/983 (0.2%)
2	P	0.86	1/732 (0.1%)	1.07	2/983 (0.2%)
2	Q	0.90	1/732 (0.1%)	1.12	2/983 (0.2%)
2	R	0.99	2/732 (0.3%)	1.10	2/983 (0.2%)
2	S	0.94	2/732 (0.3%)	1.10	2/983 (0.2%)
2	T	0.92	2/732 (0.3%)	1.09	2/983 (0.2%)
2	U	0.90	1/732 (0.1%)	1.09	2/983 (0.2%)
All	All	1.37	400/59500 (0.7%)	1.39	401/80283 (0.5%)

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	I	0	2
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
All	All	0	4

All (400) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	MET	SD-CE	17.03	2.22	1.79
1	N	514	MET	SD-CE	16.68	2.21	1.79
1	J	114	MET	SD-CE	16.38	2.20	1.79
1	D	111	MET	SD-CE	14.66	2.16	1.79
1	F	111	MET	SD-CE	14.31	2.15	1.79
1	E	114	MET	SD-CE	14.03	2.14	1.79
1	K	114	MET	SD-CE	13.45	2.13	1.79
1	J	514	MET	SD-CE	12.50	2.10	1.79
1	M	111	MET	SD-CE	11.91	2.09	1.79
1	G	491	MET	SD-CE	-11.87	1.49	1.79
1	N	114	MET	SD-CE	11.77	2.08	1.79
1	D	71	ALA	CA-CB	-11.21	1.35	1.53
1	K	514	MET	SD-CE	10.87	2.06	1.79
1	G	520	MET	SD-CE	-10.82	1.52	1.79
1	C	78	ALA	CA-CB	-10.56	1.36	1.53
1	C	520	MET	SD-CE	-10.41	1.53	1.79
1	B	114	MET	SD-CE	10.29	2.05	1.79
1	H	114	MET	SD-CE	9.84	2.04	1.79
1	B	71	ALA	CA-CB	-9.77	1.37	1.53
1	C	20	VAL	CA-CB	-9.35	1.43	1.54
1	A	16	MET	SD-CE	9.33	2.02	1.79
1	J	288	MET	SD-CE	9.26	2.02	1.79
1	I	114	MET	SD-CE	9.06	2.02	1.79
1	A	73	MET	SD-CE	8.86	2.01	1.79
1	C	508	ALA	CA-CB	-8.84	1.39	1.53
1	E	520	MET	SD-CE	-8.79	1.57	1.79
1	F	520	MET	SD-CE	-8.74	1.57	1.79
1	G	76	GLU	C-O	8.71	1.35	1.24
1	E	71	ALA	CA-CB	-8.68	1.39	1.53
1	F	69	MET	SD-CE	-8.62	1.58	1.79
1	M	114	MET	SD-CE	8.55	2.00	1.79
1	E	111	MET	SD-CE	8.50	2.00	1.79
1	N	454	ILE	CA-CB	-8.45	1.45	1.54
1	I	73	MET	CG-SD	8.31	2.01	1.80
1	J	94	VAL	C-O	8.28	1.33	1.24
1	H	288	MET	SD-CE	8.25	2.00	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	MET	SD-CE	8.23	2.00	1.79
1	H	12	ALA	CA-CB	-8.20	1.40	1.53
1	C	491	MET	SD-CE	-8.14	1.59	1.79
1	C	449	ALA	CA-CB	-8.12	1.43	1.53
1	M	94	VAL	C-O	8.12	1.33	1.24
1	N	499	VAL	CA-CB	8.09	1.64	1.54
1	D	105	LYS	C-O	8.08	1.34	1.24
1	E	73	MET	SD-CE	7.95	1.99	1.79
1	L	111	MET	SD-CE	7.91	1.99	1.79
1	D	449	ALA	CA-CB	-7.89	1.43	1.53
1	G	105	LYS	C-O	7.89	1.34	1.24
1	D	116	LEU	CA-C	-7.86	1.42	1.52
1	A	116	LEU	CA-C	-7.85	1.42	1.52
1	I	405	ALA	CA-CB	-7.77	1.41	1.53
1	M	506	TYR	CA-C	-7.73	1.42	1.52
1	A	105	LYS	C-O	7.67	1.33	1.24
1	M	16	MET	SD-CE	7.66	1.98	1.79
1	G	71	ALA	CA-CB	-7.58	1.40	1.53
1	D	521	VAL	C-O	-7.58	1.16	1.24
1	C	77	VAL	C-O	7.55	1.32	1.24
1	F	508	ALA	CA-CB	-7.51	1.41	1.53
1	M	27	VAL	CA-CB	-7.51	1.44	1.54
1	A	114	MET	CG-SD	7.43	1.99	1.80
1	M	508	ALA	CA-CB	-7.41	1.41	1.53
1	D	16	MET	SD-CE	7.40	1.98	1.79
1	K	468	THR	CA-CB	7.40	1.65	1.53
1	A	514	MET	SD-CE	7.35	1.98	1.79
1	D	520	MET	SD-CE	-7.32	1.61	1.79
1	E	449	ALA	CA-CB	-7.31	1.43	1.53
1	H	87	ASP	CA-C	-7.30	1.44	1.52
1	G	478	TYR	CA-C	-7.30	1.44	1.52
1	I	506	TYR	CA-C	-7.28	1.42	1.52
1	G	69	MET	SD-CE	-7.24	1.61	1.79
1	A	78	ALA	CA-CB	-7.22	1.41	1.53
1	J	443	ALA	CA-CB	-7.22	1.42	1.53
1	E	166	MET	SD-CE	7.21	1.97	1.79
1	G	116	LEU	CA-C	-7.21	1.43	1.52
1	A	449	ALA	CA-CB	-7.19	1.44	1.53
1	J	12	ALA	CA-CB	-7.17	1.42	1.53
1	H	446	ALA	C-O	-7.15	1.15	1.24
1	N	94	VAL	C-O	7.12	1.32	1.24
1	G	111	MET	SD-CE	7.12	1.97	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	114	MET	SD-CE	7.11	1.97	1.79
1	J	446	ALA	C-O	-7.07	1.15	1.24
1	C	31	LEU	CA-C	-7.05	1.44	1.52
1	A	106	ALA	CA-CB	-7.03	1.42	1.53
1	I	417	VAL	CA-CB	-7.02	1.45	1.54
1	H	508	ALA	CA-CB	-7.02	1.41	1.53
1	C	464	VAL	CA-CB	-6.98	1.45	1.54
1	N	111	MET	SD-CE	6.91	1.96	1.79
1	L	514	MET	SD-CE	6.88	1.96	1.79
1	F	16	MET	SD-CE	6.87	1.96	1.79
1	A	412	VAL	CA-C	-6.87	1.45	1.52
1	H	468	THR	CA-CB	6.86	1.64	1.53
1	I	18	ARG	CA-C	-6.86	1.44	1.52
1	C	477	GLY	C-O	-6.84	1.17	1.23
1	D	114	MET	SD-CE	6.83	1.96	1.79
1	M	12	ALA	CA-CB	-6.81	1.43	1.53
1	M	88	GLY	C-O	-6.80	1.14	1.24
1	J	54	VAL	CA-CB	-6.79	1.45	1.54
1	A	71	ALA	CA-CB	-6.76	1.42	1.53
1	E	454	ILE	CA-CB	-6.73	1.46	1.54
1	J	499	VAL	CA-CB	6.72	1.63	1.54
1	C	177	VAL	CA-CB	6.71	1.63	1.54
1	A	452	ARG	NE-CZ	6.71	1.40	1.33
1	A	39	VAL	CA-CB	-6.69	1.46	1.54
1	A	506	TYR	CA-C	-6.66	1.44	1.52
1	N	288	MET	SD-CE	6.61	1.96	1.79
1	H	443	ALA	CA-CB	-6.61	1.42	1.53
1	G	113	PRO	C-O	6.61	1.32	1.24
1	J	100	ILE	C-O	-6.60	1.16	1.24
1	J	480	ALA	CA-CB	-6.60	1.42	1.53
1	G	449	ALA	CA-CB	-6.59	1.45	1.53
1	D	99	ILE	CA-CB	-6.57	1.46	1.54
1	H	523	ASP	CA-C	-6.57	1.44	1.53
1	N	443	ALA	CA-CB	-6.57	1.43	1.53
1	A	520	MET	SD-CE	-6.55	1.63	1.79
1	D	78	ALA	CA-CB	-6.51	1.42	1.53
1	L	468	THR	CA-CB	6.50	1.63	1.53
1	L	506	TYR	CA-C	-6.50	1.44	1.52
1	N	26	ALA	C-O	-6.50	1.15	1.24
1	D	29	VAL	CA-C	-6.47	1.42	1.52
1	C	92	ALA	CA-CB	-6.43	1.42	1.53
1	G	471	GLY	C-O	-6.43	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	445	ARG	NE-CZ	6.43	1.40	1.33
1	G	73	MET	SD-CE	6.41	1.95	1.79
1	B	34	LYS	CA-C	6.39	1.61	1.52
1	L	69	MET	SD-CE	-6.37	1.63	1.79
2	O	17	VAL	CA-CB	6.36	1.63	1.54
1	N	91	THR	C-O	-6.35	1.16	1.24
1	M	18	ARG	NE-CZ	6.35	1.40	1.33
1	B	124	VAL	CA-C	6.34	1.60	1.52
1	H	94	VAL	C-O	6.34	1.31	1.24
1	M	414	GLY	C-O	6.34	1.31	1.23
1	I	233	MET	SD-CE	6.33	1.95	1.79
1	F	10	ASN	CA-C	6.33	1.60	1.52
1	N	417	VAL	CA-CB	-6.33	1.45	1.54
1	L	506	TYR	C-O	-6.30	1.16	1.24
1	I	422	VAL	C-O	-6.30	1.16	1.24
1	I	514	MET	SD-CE	6.29	1.95	1.79
1	F	29	VAL	CA-CB	-6.29	1.44	1.54
1	M	407	VAL	CA-CB	-6.29	1.47	1.54
1	D	379	ILE	CA-CB	-6.29	1.46	1.54
1	C	116	LEU	CA-C	-6.28	1.44	1.52
1	C	11	ASP	C-O	-6.27	1.16	1.24
1	E	36	ARG	C-O	-6.27	1.15	1.23
1	M	443	ALA	CA-CB	-6.24	1.43	1.53
1	C	510	VAL	CA-C	6.24	1.60	1.52
1	G	113	PRO	CA-C	6.23	1.61	1.52
1	H	514	MET	SD-CE	6.22	1.95	1.79
1	J	104	LEU	CA-C	-6.21	1.44	1.52
1	F	111	MET	CG-SD	-6.20	1.65	1.80
1	H	56	VAL	CA-CB	-6.20	1.47	1.54
2	T	86	MET	SD-CE	-6.20	1.64	1.79
1	D	105	LYS	N-CA	-6.19	1.38	1.46
1	B	449	ALA	CA-CB	-6.18	1.45	1.53
1	H	454	ILE	CA-CB	-6.17	1.47	1.54
1	G	500	THR	CA-CB	-6.17	1.43	1.53
1	I	57	ALA	CA-CB	-6.16	1.43	1.53
1	N	445	ARG	NE-CZ	6.16	1.39	1.33
1	I	112	ASN	C-O	-6.15	1.16	1.24
1	E	29	VAL	CA-CB	-6.14	1.44	1.54
2	R	17	VAL	CA-CB	6.14	1.62	1.54
1	F	464	VAL	CA-CB	-6.13	1.46	1.54
1	L	73	MET	CG-SD	6.12	1.96	1.80
1	C	445	ARG	NE-CZ	6.10	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	418	ALA	CA-CB	6.10	1.62	1.53
1	I	66	PHE	N-CA	6.10	1.54	1.46
1	I	499	VAL	CA-CB	6.10	1.62	1.54
1	B	75	LYS	CA-C	6.10	1.61	1.52
1	N	480	ALA	CA-CB	-6.09	1.43	1.53
1	D	177	VAL	CA-CB	6.08	1.62	1.54
1	D	82	ASN	CA-C	6.07	1.61	1.52
1	I	38	VAL	C-O	-6.07	1.17	1.24
1	A	177	VAL	CA-C	6.06	1.59	1.52
1	F	78	ALA	CA-CB	-6.06	1.43	1.53
1	I	18	ARG	CZ-NH2	6.04	1.41	1.33
1	G	29	VAL	CA-C	-6.03	1.43	1.52
1	B	29	VAL	CA-CB	-6.00	1.46	1.54
1	G	56	VAL	CA-CB	-6.00	1.47	1.54
1	A	99	ILE	CA-CB	-6.00	1.47	1.54
1	H	423	ALA	CA-CB	-5.99	1.44	1.53
1	M	85	ALA	CA-CB	5.97	1.62	1.54
1	F	12	ALA	CA-CB	-5.97	1.44	1.53
1	K	12	ALA	CA-CB	-5.96	1.44	1.53
1	E	31	LEU	CA-C	-5.92	1.45	1.52
1	M	415	GLY	C-O	-5.91	1.17	1.24
1	B	22	VAL	CA-CB	-5.88	1.47	1.54
1	F	449	ALA	CA-CB	-5.88	1.45	1.53
1	G	105	LYS	CD-CE	5.88	1.70	1.52
1	C	452	ARG	C-O	5.87	1.31	1.24
1	I	507	ALA	C-O	-5.87	1.17	1.24
1	J	503	ALA	C-O	-5.86	1.17	1.24
1	L	449	ALA	C-O	-5.85	1.19	1.24
1	J	405	ALA	CA-CB	-5.84	1.43	1.53
1	G	38	VAL	C-O	-5.84	1.18	1.24
1	A	459	GLY	C-O	-5.83	1.15	1.23
1	D	130	GLU	CD-OE1	5.83	1.36	1.25
1	D	34	LYS	CA-C	5.83	1.60	1.52
1	C	127	ALA	C-O	-5.83	1.17	1.24
1	M	58	ARG	N-CA	-5.83	1.39	1.46
1	N	31	LEU	C-O	5.82	1.30	1.24
1	K	18	ARG	NE-CZ	5.82	1.39	1.33
1	K	445	ARG	NE-CZ	5.82	1.39	1.33
1	G	447	MET	SD-CE	-5.81	1.65	1.79
1	J	94	VAL	CA-CB	-5.81	1.47	1.54
1	A	405	ALA	CA-CB	-5.81	1.44	1.53
1	C	52	ASP	CA-C	-5.81	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	499	VAL	CA-CB	5.81	1.61	1.54
1	N	16	MET	CG-SD	-5.80	1.66	1.80
1	B	42	LYS	CA-C	5.80	1.58	1.52
1	N	12	ALA	CA-CB	-5.80	1.43	1.53
1	D	404	ARG	NE-CZ	5.79	1.39	1.33
1	A	75	LYS	CA-C	5.79	1.61	1.52
1	D	90	THR	CA-CB	-5.78	1.44	1.53
1	A	85	ALA	CA-CB	-5.78	1.44	1.53
1	G	24	ALA	C-O	-5.78	1.17	1.24
1	H	21	ASN	CA-C	5.76	1.60	1.52
1	J	506	TYR	CA-C	-5.76	1.45	1.52
1	A	418	ALA	CA-CB	-5.75	1.44	1.53
1	M	105	LYS	CA-C	-5.75	1.45	1.52
1	I	445	ARG	NE-CZ	5.75	1.39	1.33
1	A	6	VAL	CA-CB	-5.75	1.47	1.54
1	D	15	LYS	N-CA	-5.75	1.39	1.46
1	D	114	MET	CG-SD	5.75	1.95	1.80
1	G	3	ALA	CA-CB	-5.75	1.44	1.53
1	F	449	ALA	C-O	-5.75	1.19	1.24
1	H	108	ALA	CA-CB	-5.75	1.43	1.53
1	I	267	MET	SD-CE	5.75	1.94	1.79
1	B	150	ILE	CA-CB	-5.74	1.47	1.54
1	G	108	ALA	CA-CB	-5.73	1.43	1.53
1	I	288	MET	SD-CE	5.73	1.93	1.79
2	T	17	VAL	CA-CB	5.73	1.62	1.54
1	G	31	LEU	CA-C	-5.72	1.45	1.52
1	L	68	ASN	C-O	-5.71	1.17	1.24
1	B	109	ALA	CA-CB	-5.71	1.43	1.53
1	B	10	ASN	CA-C	5.70	1.60	1.52
1	A	503	ALA	CA-CB	-5.70	1.44	1.53
1	C	503	ALA	N-CA	5.70	1.52	1.46
1	M	31	LEU	C-O	5.69	1.30	1.24
1	E	60	ILE	CA-CB	-5.69	1.47	1.54
1	C	423	ALA	CA-CB	-5.68	1.44	1.53
1	G	78	ALA	CA-CB	-5.67	1.44	1.53
1	G	111	MET	CG-SD	-5.67	1.66	1.80
1	C	427	ALA	CA-CB	-5.66	1.43	1.53
1	D	399	ALA	CA-CB	-5.66	1.44	1.53
1	A	94	VAL	N-CA	-5.65	1.40	1.46
1	I	73	MET	SD-CE	-5.65	1.65	1.79
1	I	511	ALA	CA-CB	-5.65	1.44	1.53
1	C	413	ALA	CA-CB	-5.64	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	74	VAL	CA-C	-5.63	1.44	1.52
1	J	26	ALA	C-O	-5.63	1.16	1.24
1	J	58	ARG	NE-CZ	5.62	1.39	1.33
1	C	515	ILE	C-O	5.62	1.30	1.24
1	G	466	ALA	CA-CB	-5.61	1.44	1.53
1	D	515	ILE	N-CA	-5.61	1.40	1.46
1	A	30	THR	C-O	-5.61	1.16	1.24
1	G	503	ALA	C-O	-5.60	1.17	1.24
1	N	508	ALA	CA-CB	-5.59	1.44	1.53
1	A	419	LEU	CA-C	5.59	1.60	1.52
1	I	461	GLU	CD-OE1	5.58	1.35	1.25
1	F	177	VAL	CA-CB	5.57	1.62	1.54
1	E	116	LEU	CA-C	-5.57	1.45	1.52
1	N	73	MET	C-O	-5.57	1.17	1.24
1	M	494	LEU	CA-C	5.56	1.59	1.52
1	H	506	TYR	CA-C	-5.56	1.45	1.52
1	B	513	LEU	CA-C	-5.56	1.45	1.52
1	J	446	ALA	CA-C	-5.55	1.45	1.52
1	N	468	THR	CA-CB	5.55	1.62	1.53
1	G	112	ASN	C-O	-5.55	1.17	1.24
1	G	503	ALA	CA-CB	-5.54	1.44	1.53
1	N	136	VAL	CA-CB	-5.54	1.47	1.54
1	I	414	GLY	C-O	5.54	1.30	1.23
2	U	17	VAL	CA-CB	5.54	1.61	1.54
1	D	60	ILE	CA-CB	-5.54	1.47	1.54
1	I	12	ALA	CA-CB	-5.54	1.44	1.53
1	M	38	VAL	C-O	-5.53	1.18	1.24
1	N	14	VAL	CA-CB	-5.53	1.48	1.54
1	C	105	LYS	C-O	5.53	1.31	1.24
1	D	69	MET	SD-CE	-5.53	1.65	1.79
1	C	503	ALA	C-O	-5.52	1.17	1.24
1	I	58	ARG	CZ-NH2	5.51	1.40	1.33
1	G	488	MET	SD-CE	-5.50	1.65	1.79
1	K	5	ASP	N-CA	-5.50	1.39	1.46
1	N	76	GLU	C-O	5.50	1.30	1.24
1	D	454	ILE	CA-C	-5.50	1.45	1.52
1	J	5	ASP	N-CA	-5.50	1.39	1.46
1	B	7	LYS	C-O	-5.49	1.17	1.24
1	H	71	ALA	CA-CB	-5.49	1.44	1.53
1	B	461	GLU	CA-C	5.48	1.59	1.52
1	M	446	ALA	C-O	-5.47	1.17	1.24
1	C	478	TYR	CA-C	-5.47	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	82	ASN	C-O	5.47	1.31	1.24
1	F	22	VAL	CA-CB	-5.47	1.48	1.54
1	D	478	TYR	CA-C	-5.45	1.46	1.52
1	C	475	ASN	CA-C	-5.44	1.45	1.52
1	A	114	MET	SD-CE	5.44	1.93	1.79
1	G	515	ILE	C-O	5.44	1.30	1.24
2	P	17	VAL	CA-CB	5.44	1.61	1.54
1	A	141	SER	C-O	-5.43	1.17	1.24
1	I	102	GLU	C-O	5.42	1.31	1.24
1	G	74	VAL	CA-C	-5.42	1.45	1.52
1	N	38	VAL	CA-CB	-5.42	1.47	1.54
1	I	133	ALA	CA-CB	-5.41	1.44	1.53
1	N	61	GLU	C-O	-5.40	1.17	1.23
1	G	508	ALA	CA-CB	-5.39	1.44	1.53
1	B	67	GLU	C-O	-5.39	1.17	1.24
1	C	56	VAL	CA-CB	-5.38	1.48	1.54
1	N	73	MET	CG-SD	5.38	1.94	1.80
1	B	3	ALA	CA-CB	-5.38	1.44	1.53
1	H	267	MET	SD-CE	5.37	1.93	1.79
1	J	522	THR	C-O	-5.36	1.18	1.24
1	M	54	VAL	CA-CB	-5.36	1.47	1.54
1	D	412	VAL	CA-C	-5.35	1.48	1.52
1	H	405	ALA	CA-CB	-5.35	1.44	1.53
1	A	90	THR	CB-CG2	5.34	1.70	1.52
1	J	94	VAL	N-CA	-5.34	1.40	1.46
1	N	58	ARG	N-CA	-5.34	1.39	1.46
1	N	522	THR	C-O	-5.34	1.18	1.23
1	G	507	ALA	CA-C	-5.34	1.46	1.52
1	D	149	THR	CA-C	-5.33	1.45	1.52
2	S	59	VAL	CA-CB	5.33	1.61	1.54
1	I	77	VAL	CA-CB	-5.32	1.47	1.54
1	M	423	ALA	CA-CB	-5.32	1.44	1.53
1	M	423	ALA	CA-C	5.32	1.59	1.52
1	I	87	ASP	CA-C	-5.31	1.46	1.52
1	N	92	ALA	CA-CB	5.31	1.61	1.53
1	M	476	TYR	CA-C	-5.30	1.46	1.52
1	B	491	MET	SD-CE	-5.30	1.66	1.79
1	K	16	MET	SD-CE	5.30	1.92	1.79
1	B	73	MET	SD-CE	5.28	1.92	1.79
1	H	22	VAL	CA-CB	-5.28	1.47	1.54
1	I	506	TYR	CA-CB	-5.28	1.44	1.53
1	B	412	VAL	CA-C	-5.28	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	VAL	CA-CB	-5.27	1.46	1.54
1	K	71	ALA	CA-C	-5.26	1.46	1.52
1	N	26	ALA	CA-C	-5.26	1.45	1.52
1	D	29	VAL	CA-CB	-5.26	1.46	1.54
1	I	123	ALA	CA-C	-5.26	1.46	1.52
1	C	440	ILE	CA-CB	-5.25	1.48	1.54
1	J	95	LEU	C-O	-5.24	1.17	1.24
1	I	443	ALA	CA-CB	-5.23	1.45	1.53
2	Q	17	VAL	CA-CB	5.23	1.61	1.54
1	K	20	VAL	CA-C	5.21	1.59	1.52
1	I	466	ALA	CA-CB	-5.20	1.45	1.53
1	B	478	TYR	C-O	-5.19	1.17	1.24
1	A	511	ALA	CA-CB	-5.19	1.44	1.53
1	G	459	GLY	C-O	-5.19	1.17	1.24
1	D	411	VAL	C-O	5.18	1.29	1.23
1	M	233	MET	SD-CE	5.18	1.92	1.79
1	D	502	SER	C-O	-5.17	1.18	1.24
1	F	114	MET	CG-SD	5.17	1.93	1.80
1	L	66	PHE	N-CA	5.16	1.52	1.46
1	I	413	ALA	N-CA	-5.16	1.39	1.46
1	I	5	ASP	CA-C	-5.15	1.46	1.52
2	R	86	MET	SD-CE	-5.15	1.66	1.79
1	E	81	ALA	CA-CB	5.14	1.62	1.53
1	G	94	VAL	C-O	5.14	1.30	1.24
1	I	514	MET	CA-C	5.14	1.59	1.52
1	B	145	ALA	CA-CB	-5.14	1.45	1.53
1	E	105	LYS	CD-CE	5.13	1.67	1.52
1	K	26	ALA	CA-CB	-5.13	1.45	1.53
1	A	502	SER	C-O	-5.13	1.18	1.24
1	N	22	VAL	C-O	-5.13	1.18	1.24
1	N	483	GLU	CD-OE2	5.12	1.35	1.25
1	C	90	THR	C-O	-5.12	1.18	1.24
1	N	491	MET	SD-CE	-5.11	1.66	1.79
1	I	100	ILE	CA-CB	-5.11	1.48	1.54
1	E	177	VAL	CA-CB	5.11	1.61	1.54
1	E	77	VAL	CA-CB	5.11	1.60	1.54
1	C	448	GLU	C-O	5.10	1.30	1.24
1	I	128	VAL	CA-CB	-5.10	1.48	1.54
1	D	521	VAL	CA-CB	-5.10	1.48	1.54
1	G	100	ILE	CA-CB	-5.10	1.48	1.54
1	D	94	VAL	N-CA	-5.09	1.40	1.46
1	J	66	PHE	N-CA	5.09	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	THR	CA-CB	-5.09	1.45	1.53
1	I	433	ASN	CG-OD1	5.09	1.33	1.23
1	J	5	ASP	CA-C	-5.09	1.46	1.52
1	C	111	MET	SD-CE	5.08	1.92	1.79
2	S	17	VAL	CA-CB	5.08	1.61	1.54
1	F	521	VAL	C-O	-5.08	1.18	1.24
1	H	18	ARG	CZ-NH1	5.08	1.39	1.32
1	K	76	GLU	C-O	5.07	1.30	1.24
1	D	406	ALA	CA-CB	-5.07	1.45	1.53
1	A	141	SER	CA-C	-5.06	1.45	1.52
1	G	75	LYS	CA-C	5.06	1.59	1.52
1	A	427	ALA	CA-CB	-5.06	1.44	1.53
1	J	57	ALA	CA-CB	-5.06	1.45	1.53
1	K	443	ALA	CA-CB	-5.05	1.45	1.53
1	B	508	ALA	CA-CB	-5.05	1.45	1.53
1	H	16	MET	SD-CE	5.04	1.92	1.79
1	I	41	ASP	CA-C	-5.04	1.46	1.53
1	N	487	ASN	CA-C	-5.03	1.46	1.52
1	A	22	VAL	CA-CB	-5.02	1.48	1.54
1	A	517	THR	C-O	5.02	1.29	1.23
1	B	440	ILE	CA-C	5.02	1.58	1.52
1	H	64	ASP	CA-C	-5.02	1.46	1.52
1	A	90	THR	C-O	-5.01	1.18	1.24
1	M	78	ALA	CA-CB	-5.01	1.45	1.53
1	E	508	ALA	CA-CB	-5.01	1.45	1.53
1	M	10	ASN	C-O	-5.01	1.18	1.24
1	N	405	ALA	CA-CB	-5.00	1.45	1.53
1	F	42	LYS	CD-CE	5.00	1.67	1.52

All (401) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	GLU	N-CA-C	-12.33	97.92	111.36
1	A	116	LEU	N-CA-C	-11.95	98.34	111.36
1	D	454	ILE	N-CA-C	-11.39	99.22	110.72
1	A	77	VAL	N-CA-C	-11.30	99.91	110.53
1	G	77	VAL	N-CA-C	-11.20	100.00	110.53
1	B	77	VAL	N-CA-C	-10.20	100.83	110.42
1	D	56	VAL	N-CA-C	-10.10	101.03	110.53
1	C	77	VAL	N-CA-C	-10.08	100.94	110.42
1	D	77	VAL	N-CA-C	-10.06	100.03	111.00
1	F	77	VAL	N-CA-C	-10.01	101.11	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	77	VAL	N-CA-C	-9.98	101.15	110.53
1	A	415	GLY	N-CA-C	-9.89	99.68	114.90
1	B	21	ASN	N-CA-C	9.84	121.60	111.07
1	A	454	ILE	N-CA-C	-9.55	100.88	110.62
1	M	10	ASN	N-CA-C	9.31	121.12	110.97
1	C	442	VAL	CA-C-O	-9.20	111.70	121.27
1	G	67	GLU	N-CA-C	-8.78	101.71	111.28
1	M	462	PRO	N-CD-CG	-8.60	90.29	103.20
1	C	510	VAL	N-CA-C	8.45	119.26	110.72
1	D	146	GLN	CA-C-N	-8.42	109.78	120.56
1	D	146	GLN	C-N-CA	-8.42	109.78	120.56
1	D	415	GLY	N-CA-C	-8.33	103.31	115.30
1	E	67	GLU	N-CA-C	-8.31	102.22	111.28
1	K	10	ASN	N-CA-C	8.25	119.90	111.07
1	D	21	ASN	N-CA-C	8.24	119.88	111.07
1	G	21	ASN	N-CA-C	8.23	120.98	111.11
1	H	462	PRO	N-CD-CG	-8.23	90.86	103.20
1	B	67	GLU	N-CA-C	-8.22	102.32	111.28
1	F	415	GLY	N-CA-C	-8.21	102.25	114.90
1	L	462	PRO	N-CD-CG	-8.21	90.88	103.20
1	C	96	ALA	N-CA-C	-8.20	101.40	111.40
1	C	26	ALA	N-CA-C	-8.19	102.54	112.54
1	E	415	GLY	N-CA-C	-8.18	102.30	114.90
1	I	462	PRO	N-CD-CG	-8.12	91.03	103.20
1	B	25	ASP	N-CA-C	8.07	120.08	111.28
1	N	10	ASN	N-CA-C	7.97	119.66	110.97
1	E	116	LEU	N-CA-C	-7.96	102.60	111.28
1	D	107	VAL	N-CA-C	-7.94	102.34	111.00
1	G	126	ALA	N-CA-C	-7.92	101.95	111.69
1	E	21	ASN	N-CA-C	7.89	119.88	111.28
1	A	21	ASN	N-CA-C	7.87	120.62	111.02
1	B	451	LEU	N-CA-C	-7.87	102.65	111.07
1	A	67	GLU	N-CA-C	-7.85	102.72	111.28
1	A	146	GLN	CA-C-N	-7.85	110.51	120.56
1	A	146	GLN	C-N-CA	-7.85	110.51	120.56
1	A	15	LYS	N-CA-C	-7.80	102.72	111.07
2	Q	16	GLU	N-CA-C	7.80	121.06	109.59
1	J	10	ASN	N-CA-C	7.76	119.43	110.97
1	G	415	GLY	N-CA-C	-7.73	103.00	114.90
2	U	16	GLU	N-CA-C	7.73	120.95	109.59
2	R	16	GLU	N-CA-C	7.69	120.90	109.59
1	C	67	GLU	N-CA-C	-7.67	102.92	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	LEU	N-CA-C	-7.67	102.92	111.28
1	E	56	VAL	N-CA-C	-7.67	102.80	110.62
1	D	116	LEU	N-CA-C	-7.62	102.97	111.28
1	A	444	LEU	N-CA-C	-7.58	102.99	111.71
1	G	56	VAL	N-CA-C	-7.55	103.17	110.42
1	M	438	VAL	N-CA-C	-7.48	102.99	110.62
1	D	147	VAL	N-CA-CB	7.47	120.14	110.57
1	B	469	VAL	N-CA-C	-7.44	103.20	110.72
1	D	53	GLY	N-CA-C	7.41	121.87	112.83
1	H	10	ASN	N-CA-C	7.41	119.04	110.97
1	F	116	LEU	N-CA-C	-7.40	103.15	111.07
2	S	16	GLU	N-CA-C	7.38	120.44	109.59
2	O	16	GLU	N-CA-C	7.33	120.37	109.59
1	L	107	VAL	N-CA-C	-7.31	103.17	110.62
1	K	71	ALA	N-CA-C	-7.30	103.25	111.14
1	E	35	GLY	N-CA-C	-7.29	102.75	112.82
2	T	16	GLU	N-CA-C	7.19	120.16	109.59
2	P	16	GLU	N-CA-C	7.18	120.15	109.59
1	C	83	ASP	N-CA-C	-7.18	103.99	112.89
1	C	415	GLY	N-CA-C	-7.17	103.86	114.90
1	F	25	ASP	N-CA-C	7.16	119.09	111.28
1	J	59	GLU	CA-C-N	-7.16	111.78	121.80
1	J	59	GLU	C-N-CA	-7.16	111.78	121.80
1	D	124	VAL	N-CA-C	7.15	117.94	110.72
1	L	10	ASN	N-CA-C	7.14	118.86	111.14
1	A	35	GLY	N-CA-C	-7.14	103.40	112.54
1	G	116	LEU	N-CA-C	-7.13	103.44	111.07
1	I	96	ALA	N-CA-C	-7.10	103.63	111.36
1	H	21	ASN	N-CA-C	7.05	119.57	111.11
1	C	91	THR	N-CA-C	-7.03	103.31	110.97
1	I	116	LEU	N-CA-C	-7.02	103.71	111.36
1	G	146	GLN	CA-C-N	-7.01	111.59	120.56
1	G	146	GLN	C-N-CA	-7.01	111.59	120.56
1	C	117	LYS	N-CA-C	6.96	118.52	111.07
1	M	116	LEU	N-CA-C	-6.96	103.62	111.14
1	A	414	GLY	N-CA-C	6.92	123.32	112.31
1	N	462	PRO	N-CD-CG	-6.88	92.88	103.20
1	D	515	ILE	N-CA-C	-6.88	104.39	112.98
1	J	71	ALA	N-CA-C	-6.88	103.79	111.28
1	C	514	MET	CA-C-N	-6.86	111.65	121.52
1	C	514	MET	C-N-CA	-6.86	111.65	121.52
1	L	53	GLY	N-CA-C	6.84	122.36	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	464	VAL	N-CA-C	6.80	116.93	110.53
1	G	515	ILE	N-CA-C	-6.79	104.99	112.80
1	C	451	LEU	N-CA-C	-6.79	103.97	111.36
1	C	121	ASP	N-CA-CB	6.78	119.91	110.07
1	G	397	GLU	CA-C-N	6.76	129.66	120.54
1	G	397	GLU	C-N-CA	6.76	129.66	120.54
1	E	451	LEU	N-CA-C	-6.72	104.04	111.36
1	L	109	ALA	N-CA-C	-6.72	105.08	113.28
1	A	124	VAL	N-CA-C	6.70	117.49	110.72
1	A	442	VAL	CA-C-O	-6.69	114.45	121.41
1	B	68	ASN	N-CA-C	6.67	118.20	111.07
1	E	91	THR	N-CA-C	-6.65	103.72	110.97
1	N	175	ILE	N-CA-C	6.61	117.41	107.75
1	D	455	VAL	N-CA-C	6.60	117.38	110.72
1	N	404	ARG	N-CA-C	-6.58	104.11	111.28
1	H	460	GLU	CA-C-N	6.57	129.47	120.67
1	H	460	GLU	C-N-CA	6.57	129.47	120.67
1	C	22	VAL	N-CA-C	-6.56	104.12	110.42
1	B	415	GLY	N-CA-C	-6.56	104.80	114.90
1	J	8	PHE	N-CA-C	6.55	120.20	109.72
1	B	124	VAL	N-CA-C	6.54	116.70	110.42
1	C	116	LEU	N-CA-C	-6.52	103.29	111.11
1	I	414	GLY	CA-C-N	-6.51	108.65	121.41
1	I	414	GLY	C-N-CA	-6.51	108.65	121.41
1	H	8	PHE	N-CA-C	6.50	120.12	109.72
1	I	22	VAL	N-CA-C	-6.49	104.16	110.72
1	I	24	ALA	N-CA-C	6.49	119.18	111.33
1	G	514	MET	CA-C-N	-6.48	112.18	121.52
1	G	514	MET	C-N-CA	-6.48	112.18	121.52
1	D	25	ASP	N-CA-C	6.46	119.31	111.82
1	I	450	PRO	N-CD-CG	-6.46	93.52	103.20
1	H	20	VAL	N-CA-C	6.42	117.10	110.36
1	B	444	LEU	N-CA-C	-6.41	104.29	111.28
1	C	35	GLY	N-CA-C	-6.39	105.30	112.33
1	I	175	ILE	N-CA-C	6.38	117.42	107.28
1	G	15	LYS	N-CA-C	-6.38	104.25	111.07
1	C	471	GLY	N-CA-C	6.36	121.45	114.40
1	K	107	VAL	N-CA-C	-6.34	104.16	110.62
1	F	56	VAL	N-CA-C	-6.32	104.35	110.42
1	F	21	ASN	N-CA-C	6.31	118.68	111.11
1	J	5	ASP	N-CA-C	-6.31	98.13	108.41
1	E	124	VAL	N-CA-C	6.27	116.44	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	404	ARG	N-CA-C	-6.25	104.57	111.82
1	D	105	LYS	N-CA-C	-6.25	104.57	111.82
1	J	462	PRO	N-CD-CG	-6.24	93.83	103.20
1	C	146	GLN	CA-C-N	-6.23	111.83	120.74
1	C	146	GLN	C-N-CA	-6.23	111.83	120.74
1	G	125	THR	N-CA-C	-6.23	104.78	112.38
1	K	404	ARG	N-CA-C	-6.20	104.52	111.28
1	H	489	ILE	N-CA-C	-6.20	104.81	110.82
1	I	404	ARG	N-CA-C	-6.20	104.53	111.28
1	J	112	ASN	N-CA-C	6.16	119.50	108.47
1	D	72	GLN	N-CA-C	-6.15	105.74	113.18
1	J	21	ASN	N-CA-C	6.13	118.46	111.11
1	E	53	GLY	N-CA-C	6.10	120.02	112.64
1	D	484	GLU	N-CA-C	6.09	119.12	109.50
1	L	21	ASN	N-CA-C	6.09	118.41	111.11
2	U	65	VAL	N-CA-C	6.09	117.46	108.45
1	D	35	GLY	N-CA-C	-6.08	104.75	112.54
1	M	510	VAL	N-CA-C	-6.08	104.05	112.50
1	J	88	GLY	N-CA-C	-6.07	107.09	113.58
1	N	116	LEU	N-CA-C	-6.06	104.68	111.28
1	K	64	ASP	N-CA-C	-6.06	100.69	109.59
1	I	10	ASN	N-CA-C	6.05	117.68	111.14
1	B	111	MET	N-CA-C	6.03	119.00	110.50
1	I	94	VAL	N-CA-C	6.02	117.49	110.62
1	A	434	GLU	N-CA-C	6.02	117.84	111.28
1	A	515	ILE	N-CA-C	-6.02	105.88	112.80
1	A	484	GLU	N-CA-C	6.00	118.53	109.23
2	Q	65	VAL	N-CA-C	6.00	117.40	108.46
1	C	21	ASN	N-CA-C	5.99	117.89	111.36
1	I	438	VAL	N-CA-C	-5.99	104.52	110.62
1	G	92	ALA	N-CA-C	-5.98	103.72	111.02
2	S	65	VAL	N-CA-C	5.97	117.35	108.46
1	I	42	LYS	N-CA-C	-5.96	97.75	108.48
1	A	451	LEU	N-CA-C	-5.96	104.87	111.36
1	B	461	GLU	CB-CA-C	5.96	116.07	110.17
1	B	65	LYS	CD-CE-NZ	-5.95	92.86	111.90
1	B	35	GLY	N-CA-C	-5.94	104.93	112.54
1	K	26	ALA	N-CA-C	-5.94	105.11	112.90
1	N	450	PRO	N-CD-CG	-5.94	94.29	103.20
1	G	454	ILE	N-CA-C	-5.94	104.56	110.62
1	I	65	LYS	N-CA-C	-5.93	103.12	110.41
1	G	96	ALA	N-CA-C	-5.93	104.40	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	329	THR	N-CA-C	5.93	117.13	107.23
1	K	5	ASP	N-CA-C	-5.93	98.75	108.41
1	M	79	SER	N-CA-C	5.91	117.73	111.28
1	E	158	VAL	N-CA-C	-5.91	104.97	110.53
1	B	56	VAL	N-CA-C	-5.89	104.77	110.72
1	H	31	LEU	N-CA-C	5.89	118.58	111.40
1	F	434	GLU	N-CA-C	5.89	117.70	111.28
1	N	484	GLU	N-CA-C	5.88	118.48	108.90
1	I	88	GLY	N-CA-C	-5.88	107.49	114.48
1	A	147	VAL	CB-CA-C	5.86	119.70	112.02
1	J	478	TYR	N-CA-C	-5.85	99.36	108.90
2	T	65	VAL	N-CA-C	5.85	117.17	108.46
2	R	65	VAL	N-CA-C	5.83	117.09	108.45
1	K	20	VAL	N-CA-C	5.82	116.47	110.36
1	L	510	VAL	N-CA-C	-5.82	103.64	111.44
1	H	55	SER	CA-C-O	-5.79	114.70	120.90
1	C	25	ASP	N-CA-C	5.78	117.58	111.28
1	C	110	GLY	N-CA-C	-5.78	106.54	116.01
1	D	510	VAL	N-CA-C	5.77	115.99	110.74
1	F	147	VAL	N-CA-CB	5.76	117.94	110.57
2	O	65	VAL	N-CA-C	5.76	117.04	108.46
1	B	75	LYS	CA-C-O	5.75	126.40	119.61
1	I	44	PHE	N-CA-C	-5.75	101.17	110.32
1	A	105	LYS	N-CA-C	-5.75	104.99	112.23
1	I	24	ALA	CA-C-N	-5.75	111.57	120.31
1	I	24	ALA	C-N-CA	-5.75	111.57	120.31
1	N	485	TYR	N-CA-C	-5.74	102.81	110.55
1	F	451	LEU	N-CA-C	-5.73	105.12	111.36
1	M	450	PRO	N-CD-CG	-5.72	94.62	103.20
1	A	329	THR	N-CA-C	5.72	117.56	107.61
1	A	56	VAL	N-CA-C	-5.71	104.95	110.72
1	A	158	VAL	N-CA-C	-5.71	105.16	110.53
1	G	36	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	K	462	PRO	N-CD-CG	-5.70	94.66	103.20
1	H	87	ASP	CA-C-O	-5.69	114.89	121.26
1	D	15	LYS	N-CA-C	-5.68	104.99	111.07
1	C	120	ILE	CA-C-N	-5.67	112.72	120.44
1	C	120	ILE	C-N-CA	-5.67	112.72	120.44
1	C	494	LEU	N-CA-C	5.67	118.49	109.24
1	H	170	GLY	CA-C-O	-5.67	118.04	122.52
1	B	414	GLY	N-CA-C	5.67	121.22	111.98
1	B	8	PHE	N-CA-C	5.65	118.90	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	MET	N-CA-C	5.65	117.98	110.53
1	F	65	LYS	CD-CE-NZ	-5.65	93.83	111.90
1	A	514	MET	CG-SD-CE	-5.64	88.48	100.90
1	N	456	LEU	CA-C-N	5.64	128.11	120.38
1	N	456	LEU	C-N-CA	5.64	128.11	120.38
1	B	18	ARG	N-CA-C	-5.63	105.23	111.71
1	F	67	GLU	N-CA-C	-5.62	105.24	111.71
1	G	101	THR	OG1-CB-CG2	-5.62	98.06	109.30
1	M	93	THR	N-CA-C	5.62	118.13	111.33
1	B	147	VAL	N-CA-CB	5.61	117.75	110.57
1	J	26	ALA	CA-C-N	-5.61	113.58	121.55
1	J	26	ALA	C-N-CA	-5.61	113.58	121.55
2	P	65	VAL	N-CA-C	5.61	116.82	108.46
1	C	397	GLU	CA-C-N	5.61	128.11	120.54
1	C	397	GLU	C-N-CA	5.61	128.11	120.54
1	M	29	VAL	N-CA-C	-5.60	105.46	113.07
1	N	414	GLY	CA-C-N	-5.59	112.76	122.83
1	N	414	GLY	C-N-CA	-5.59	112.76	122.83
1	M	175	ILE	N-CA-C	5.59	115.92	107.75
1	J	20	VAL	N-CA-C	5.59	116.32	110.62
1	N	24	ALA	N-CA-C	5.58	117.36	111.28
1	C	484	GLU	N-CA-C	5.58	117.66	109.24
1	N	509	SER	N-CA-C	-5.57	105.12	111.14
1	D	499	VAL	N-CA-CB	5.56	119.85	110.56
1	H	24	ALA	CA-C-N	-5.55	111.24	120.68
1	H	24	ALA	C-N-CA	-5.55	111.24	120.68
1	J	78	ALA	N-CA-C	-5.55	105.31	111.36
1	I	89	THR	CA-C-N	-5.54	112.43	120.29
1	I	89	THR	C-N-CA	-5.54	112.43	120.29
1	C	79	SER	N-CA-C	5.53	117.39	111.36
1	H	20	VAL	CA-C-N	-5.53	113.08	120.54
1	H	20	VAL	C-N-CA	-5.53	113.08	120.54
1	C	147	VAL	N-CA-CB	5.52	118.47	110.52
1	C	101	THR	O-C-N	5.52	127.97	122.12
1	H	44	PHE	N-CA-C	-5.52	101.54	110.32
1	N	23	LEU	CB-CA-C	-5.52	102.14	110.92
1	H	464	VAL	N-CA-C	5.52	115.72	110.53
1	K	44	PHE	N-CA-C	-5.50	101.57	110.32
1	M	489	ILE	N-CA-C	-5.50	105.74	110.74
1	J	4	LYS	N-CA-C	5.49	118.59	110.46
1	H	64	ASP	N-CA-C	-5.49	101.52	109.59
1	I	21	ASN	N-CA-C	5.48	117.69	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	VAL	N-CA-C	5.47	115.67	110.42
1	H	329	THR	N-CA-C	5.47	118.01	108.76
1	C	100	ILE	N-CA-C	5.47	115.67	110.42
1	G	71	ALA	N-CA-C	-5.46	105.49	111.82
1	E	25	ASP	N-CA-C	5.46	117.98	111.71
1	I	431	GLY	CA-C-O	-5.45	116.48	121.72
1	J	170	GLY	CA-C-O	-5.45	118.68	122.22
1	B	522	THR	OG1-CB-CG2	-5.45	98.41	109.30
1	N	8	PHE	N-CA-C	5.44	118.42	109.72
1	C	77	VAL	N-CA-CB	5.43	116.78	110.65
1	M	58	ARG	N-CA-C	-5.42	105.48	111.71
1	M	170	GLY	CA-C-O	-5.42	118.24	122.52
1	A	164	GLU	N-CA-C	5.41	116.85	111.07
1	M	461	GLU	N-CA-CB	-5.40	101.47	109.90
1	M	32	GLY	N-CA-C	5.40	123.36	112.34
1	C	30	THR	CA-C-N	-5.40	114.61	122.65
1	C	30	THR	C-N-CA	-5.40	114.61	122.65
1	N	65	LYS	N-CA-C	-5.40	103.36	110.33
1	J	509	SER	N-CA-C	-5.38	105.33	111.14
1	C	428	ASP	N-CA-C	5.36	119.93	113.17
1	J	175	ILE	N-CA-C	5.36	115.58	107.75
1	M	48	THR	OG1-CB-CG2	-5.36	98.58	109.30
1	H	109	ALA	N-CA-C	-5.36	106.75	113.28
1	J	419	LEU	N-CA-C	-5.36	105.52	111.36
1	I	5	ASP	N-CA-C	-5.35	99.69	108.41
1	D	196	ASP	N-CA-C	5.34	119.99	112.72
1	G	442	VAL	CA-C-O	-5.34	115.72	121.27
1	I	499	VAL	N-CA-CB	5.33	119.47	110.56
1	E	36	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	I	162	ILE	N-CA-C	-5.33	105.30	110.42
1	L	24	ALA	N-CA-C	5.33	117.78	111.33
1	I	372	LEU	N-CA-C	5.33	117.90	111.40
1	K	170	GLY	CA-C-O	-5.32	118.31	122.52
1	N	510	VAL	N-CA-C	-5.32	104.44	111.09
1	I	483	GLU	N-CA-C	5.32	118.92	111.90
1	E	329	THR	N-CA-C	5.32	116.86	107.61
1	B	121	ASP	N-CA-CB	5.31	118.03	110.16
1	K	333	ILE	N-CA-C	5.30	115.49	107.80
1	F	445	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	H	511	ALA	N-CA-C	-5.30	105.17	111.69
1	A	500	THR	N-CA-C	-5.29	105.52	111.28
1	A	412	VAL	N-CA-C	-5.29	100.67	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	65	LYS	CA-C-O	-5.28	115.97	121.99
1	E	444	LEU	N-CA-C	-5.28	105.53	111.28
1	H	65	LYS	CA-C-O	-5.28	116.07	122.03
1	N	499	VAL	N-CA-CB	5.28	117.33	110.57
1	I	506	TYR	N-CA-C	-5.28	105.58	112.23
1	C	110	GLY	CA-C-O	5.26	123.72	118.77
1	M	20	VAL	N-CA-C	5.26	115.99	110.62
1	A	417	VAL	N-CA-C	5.26	115.48	110.53
1	H	114	MET	N-CA-C	-5.26	105.62	111.36
1	K	416	GLY	N-CA-C	-5.26	107.25	114.67
1	B	484	GLU	N-CA-C	5.26	117.38	109.23
1	N	19	GLY	CA-C-N	-5.26	113.25	120.46
1	N	19	GLY	C-N-CA	-5.26	113.25	120.46
1	H	423	ALA	N-CA-C	5.26	116.70	111.07
1	I	325	ILE	N-CA-C	5.25	116.94	108.85
1	G	35	GLY	N-CA-C	-5.25	105.81	112.54
1	J	414	GLY	CA-C-N	-5.25	111.11	121.41
1	J	414	GLY	C-N-CA	-5.25	111.11	121.41
1	F	27	VAL	N-CA-C	5.25	116.72	111.00
1	A	150	ILE	CA-C-N	5.24	127.82	120.28
1	A	150	ILE	C-N-CA	5.24	127.82	120.28
1	G	29	VAL	N-CA-C	-5.23	104.36	111.89
1	H	510	VAL	N-CA-C	-5.23	105.23	112.50
1	N	416	GLY	N-CA-C	-5.22	107.46	114.25
1	K	326	ASN	CB-CA-C	-5.22	101.51	111.48
1	C	515	ILE	N-CA-C	-5.21	106.80	112.80
1	L	20	VAL	CB-CA-C	5.21	118.64	111.97
1	L	329	THR	N-CA-C	5.21	117.94	109.24
1	L	86	GLY	N-CA-C	-5.21	107.50	115.00
1	J	499	VAL	N-CA-CB	5.20	118.39	110.58
1	E	65	LYS	CD-CE-NZ	-5.20	95.25	111.90
1	D	30	THR	CB-CA-C	-5.20	101.77	110.56
1	D	50	THR	OG1-CB-CG2	-5.19	98.92	109.30
1	F	35	GLY	N-CA-C	-5.19	106.62	112.33
1	I	78	ALA	N-CA-C	-5.19	105.69	112.23
1	H	50	THR	OG1-CB-CG2	-5.18	98.94	109.30
1	I	109	ALA	N-CA-C	-5.18	106.96	113.28
1	L	509	SER	N-CA-C	-5.18	105.54	111.14
1	E	121	ASP	N-CA-CB	5.17	117.82	110.16
1	N	460	GLU	CA-C-N	5.17	128.44	121.20
1	N	460	GLU	C-N-CA	5.17	128.44	121.20
1	N	36	ARG	N-CA-C	-5.17	102.54	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	146	GLN	CA-C-N	-5.16	113.95	120.56
1	F	146	GLN	C-N-CA	-5.16	113.95	120.56
1	B	496	PRO	N-CD-CG	-5.16	95.46	103.20
1	J	112	ASN	CA-C-O	5.16	122.64	119.29
1	N	499	VAL	CB-CA-C	5.16	118.78	112.02
1	G	36	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	H	175	ILE	N-CA-C	5.16	115.28	107.80
1	J	104	LEU	N-CA-C	-5.16	106.50	112.89
1	D	111	MET	N-CA-C	5.15	117.77	110.50
1	C	7	LYS	N-CA-C	5.15	117.80	109.40
1	D	414	GLY	O-C-N	-5.15	118.69	122.71
1	H	99	ILE	N-CA-C	-5.15	105.69	110.53
1	E	499	VAL	N-CA-CB	5.15	117.93	110.52
1	N	55	SER	CA-C-O	-5.13	115.41	120.90
1	G	158	VAL	N-CA-C	-5.12	105.72	110.53
1	E	30	THR	N-CA-C	5.10	118.65	112.93
1	F	470	LYS	N-CA-C	-5.10	105.80	111.36
1	J	55	SER	N-CA-C	5.09	117.22	111.11
1	M	16	MET	CG-SD-CE	-5.09	89.70	100.90
1	G	74	VAL	N-CA-C	-5.09	104.69	111.05
1	B	499	VAL	N-CA-CB	5.08	119.05	110.56
1	G	413	ALA	N-CA-C	5.08	117.06	109.59
1	J	485	TYR	N-CA-C	-5.08	103.69	110.55
1	M	24	ALA	CA-C-N	-5.08	112.60	120.31
1	M	24	ALA	C-N-CA	-5.08	112.60	120.31
1	N	20	VAL	CA-C-O	-5.07	115.67	120.95
1	A	522	THR	OG1-CB-CG2	-5.07	99.16	109.30
1	D	467	ASN	N-CA-C	5.07	117.20	111.11
1	C	500	THR	N-CA-C	-5.07	105.88	111.71
1	N	464	VAL	N-CA-C	5.07	115.19	110.42
1	J	326	ASN	CB-CA-C	-5.07	101.80	111.48
1	C	134	LEU	CB-CG-CD2	-5.07	95.50	110.70
1	N	88	GLY	N-CA-C	-5.06	107.99	114.37
1	H	435	ASP	N-CA-C	-5.06	105.86	112.23
1	D	329	THR	N-CA-C	5.05	116.41	107.61
1	E	15	LYS	N-CA-C	-5.05	105.66	111.07
1	K	109	ALA	N-CA-C	-5.05	107.11	113.28
1	N	326	ASN	CB-CA-C	-5.05	101.83	111.48
1	L	468	THR	N-CA-CB	5.05	117.63	110.16
1	F	412	VAL	N-CA-C	-5.03	102.39	108.53
1	I	122	LYS	CA-C-N	5.03	126.98	120.44
1	I	122	LYS	C-N-CA	5.03	126.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	GLU	N-CA-C	5.03	117.14	111.11
1	N	183	LEU	N-CA-C	-5.03	107.32	113.50
1	J	325	ILE	N-CA-C	5.02	116.58	108.85
1	H	134	LEU	CA-C-N	5.02	128.23	121.05
1	H	134	LEU	C-N-CA	5.02	128.23	121.05
1	C	56	VAL	N-CA-C	-5.02	105.60	110.42
1	E	196	ASP	N-CA-C	5.02	119.54	112.72
1	G	28	LYS	CD-CE-NZ	-5.02	95.84	111.90
1	F	522	THR	OG1-CB-CG2	-5.01	99.27	109.30
1	G	514	MET	CG-SD-CE	-5.01	89.87	100.90
1	M	71	ALA	N-CA-C	-5.01	105.81	111.28
1	H	79	SER	N-CA-C	5.01	116.82	111.36
1	K	329	THR	N-CA-C	5.01	117.23	108.76

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	32	GLY	Peptide
1	I	415	GLY	Peptide
1	J	415	GLY	Peptide
1	M	415	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3976	207	0
1	B	3856	0	3976	192	0
1	C	3856	0	3976	203	0
1	D	3856	0	3976	197	0
1	E	3856	0	3976	185	0
1	F	3856	0	3976	182	0
1	G	3856	0	3976	195	0
1	H	3856	0	3976	178	0
1	I	3856	0	3976	182	0
1	J	3856	0	3976	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3856	0	3976	188	0
1	L	3856	0	3976	202	1
1	M	3856	0	3976	206	0
1	N	3856	0	3976	187	0
2	O	728	0	762	24	0
2	P	728	0	762	22	0
2	Q	728	0	762	21	0
2	R	728	0	762	18	0
2	S	728	0	762	17	0
2	T	728	0	762	17	0
2	U	728	0	762	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	2	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	0	0
4	G	27	0	12	1	0
5	A	12	0	0	1	0
5	B	10	0	0	6	0
5	C	11	0	0	1	0
5	D	11	0	0	2	0
5	E	10	0	0	2	0
5	F	8	0	0	1	0
5	G	13	0	0	2	0
5	H	12	0	0	7	0
5	I	19	0	0	3	0
5	J	14	0	0	4	0
5	K	14	0	0	2	0
5	L	16	0	0	3	0
5	M	10	0	0	2	0
5	N	21	0	0	8	0
All	All	59457	0	61082	2724	1

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 23.

All (2724) 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:I:73:MET:CG	1:I:73:MET:SD	2.01	1.48
1:A:73:MET:CE	1:A:73:MET:SD	2.01	1.46
1:J:288:MET:CE	1:J:288:MET:SD	2.02	1.46
1:I:114:MET:CE	1:I:114:MET:SD	2.02	1.46
1:A:16:MET:CE	1:A:16:MET:SD	2.02	1.45
1:B:114:MET:CE	1:B:114:MET:SD	2.05	1.45
1:H:114:MET:SD	1:H:114:MET:CE	2.04	1.45
1:K:514:MET:CE	1:K:514:MET:SD	2.06	1.42
1:M:111:MET:CE	1:M:111:MET:SD	2.09	1.39
1:N:114:MET:CE	1:N:114:MET:SD	2.09	1.39
1:J:514:MET:SD	1:J:514:MET:CE	2.10	1.37
1:K:114:MET:CE	1:K:114:MET:SD	2.13	1.36
1:E:114:MET:SD	1:E:114:MET:CE	2.14	1.35
1:F:111:MET:CE	1:F:111:MET:SD	2.15	1.33
1:D:111:MET:CE	1:D:111:MET:SD	2.16	1.33
1:J:114:MET:CE	1:J:114:MET:SD	2.20	1.30
1:N:514:MET:CE	1:N:514:MET:SD	2.21	1.27
1:C:73:MET:CE	1:C:73:MET:SD	2.22	1.27
4:A:600:ADP:O3B	5:A:610:HOH:O	1.52	1.24
4:B:600:ADP:O3B	5:B:605:HOH:O	1.59	1.18
1:B:18:ARG:CG	1:B:18:ARG:HH11	1.62	1.11
1:F:18:ARG:HH11	1:F:18:ARG:CG	1.64	1.09
1:G:414:GLY:O	1:G:417:VAL:HG12	1.54	1.08
1:D:18:ARG:HB3	1:D:18:ARG:HH11	1.20	1.07
1:M:452:ARG:HH11	1:M:452:ARG:HG2	1.15	1.07
1:F:18:ARG:HH11	1:F:18:ARG:HG2	1.18	1.06
1:F:414:GLY:O	1:F:417:VAL:HG12	1.56	1.06
1:J:419:LEU:HD21	1:J:500:THR:CG2	1.86	1.05
1:D:430:ARG:HG2	1:D:430:ARG:HH11	1.22	1.04
1:D:510:VAL:HG23	1:D:514:MET:HE2	1.40	1.03
1:B:18:ARG:HH11	1:B:18:ARG:HG2	1.23	1.02
1:B:414:GLY:O	1:B:417:VAL:HG12	1.58	1.02
1:B:44:PHE:HD1	1:B:44:PHE:H	1.08	1.01
1:N:452:ARG:HG2	1:N:452:ARG:HH11	1.25	1.01
1:A:510:VAL:HG23	1:A:514:MET:HE2	1.42	1.01
1:G:510:VAL:HG23	1:G:514:MET:HE2	1.40	1.01
1:D:18:ARG:HH11	1:D:18:ARG:CB	1.74	1.00
1:D:414:GLY:O	1:D:417:VAL:HG12	1.61	1.00
1:I:131:LEU:CD1	1:I:422:VAL:HG11	1.92	1.00
1:K:419:LEU:HD21	1:K:500:THR:CG2	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:LYS:O	1:M:66:PHE:HB2	1.58	1.00
1:H:452:ARG:HG2	1:H:452:ARG:HH11	1.27	1.00
4:D:600:ADP:O3B	5:D:604:HOH:O	1.80	0.99
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.27	0.99
1:K:419:LEU:CD2	1:K:500:THR:CG2	2.40	0.99
1:H:419:LEU:HD21	1:H:500:THR:CG2	1.94	0.98
1:N:65:LYS:O	1:N:66:PHE:HB2	1.63	0.97
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.28	0.97
1:A:414:GLY:O	1:A:417:VAL:HG12	1.65	0.97
1:C:18:ARG:HH11	1:C:18:ARG:CG	1.77	0.97
1:G:33:PRO:HA	1:G:153:ASN:HD21	1.28	0.97
1:J:131:LEU:CD1	1:J:422:VAL:HG11	1.94	0.97
4:C:600:ADP:O3B	5:C:607:HOH:O	1.82	0.97
1:G:18:ARG:CG	1:G:18:ARG:HH11	1.78	0.96
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.29	0.96
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.27	0.95
1:B:18:ARG:HG2	1:B:18:ARG:NH1	1.76	0.95
1:B:463:SER:HB3	5:H:537:HOH:O	1.66	0.95
1:C:18:ARG:HH11	1:C:18:ARG:CB	1.78	0.95
1:E:33:PRO:HA	1:E:153:ASN:HD21	1.27	0.95
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.31	0.95
1:J:419:LEU:CD2	1:J:500:THR:CG2	2.44	0.95
1:C:414:GLY:O	1:C:417:VAL:HG12	1.66	0.95
1:B:18:ARG:HH11	1:B:18:ARG:CB	1.79	0.95
1:M:131:LEU:CD1	1:M:422:VAL:HG11	1.96	0.95
1:J:65:LYS:O	1:J:66:PHE:HB2	1.65	0.94
1:I:419:LEU:HD21	1:I:500:THR:CG2	1.97	0.94
1:C:44:PHE:HD1	1:C:44:PHE:H	1.09	0.94
1:F:18:ARG:HG2	1:F:18:ARG:NH1	1.76	0.94
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.49	0.93
1:H:419:LEU:CD2	1:H:500:THR:CG2	2.45	0.93
1:K:65:LYS:O	1:K:66:PHE:HB2	1.66	0.93
1:F:33:PRO:HA	1:F:153:ASN:HD21	1.32	0.93
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.48	0.93
1:E:414:GLY:O	1:E:417:VAL:HG12	1.68	0.93
1:C:18:ARG:HH11	1:C:18:ARG:HB3	1.33	0.93
1:A:44:PHE:H	1:A:44:PHE:HD1	1.11	0.93
1:B:510:VAL:HG23	1:B:514:MET:HE2	1.49	0.92
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.49	0.92
1:G:18:ARG:HH11	1:G:18:ARG:HG2	1.32	0.92
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.51	0.92
1:M:419:LEU:HD21	1:M:500:THR:CG2	2.00	0.92
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.34	0.92
1:A:18:ARG:HH11	1:A:18:ARG:HB3	1.35	0.91
1:D:432:GLN:NE2	1:D:436:GLN:HE22	1.69	0.91
1:E:44:PHE:HD1	1:E:44:PHE:H	1.13	0.91
1:F:430:ARG:HG2	1:F:430:ARG:HH11	1.35	0.90
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.51	0.90
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.53	0.90
1:E:430:ARG:HH11	1:E:430:ARG:HG2	1.35	0.89
1:F:510:VAL:HG23	1:F:514:MET:HE2	1.53	0.89
1:K:452:ARG:HG2	1:K:452:ARG:HH11	1.35	0.89
1:N:419:LEU:CD2	1:N:500:THR:CG2	2.49	0.89
1:J:125:THR:O	5:J:531:HOH:O	1.89	0.89
1:L:131:LEU:CD1	1:L:422:VAL:HG11	2.01	0.89
1:H:65:LYS:O	1:H:66:PHE:HB2	1.70	0.89
1:L:452:ARG:HG2	1:L:452:ARG:HH11	1.35	0.89
1:F:486:GLY:HA3	1:F:491:MET:HE2	1.53	0.88
1:E:18:ARG:HH11	1:E:18:ARG:CG	1.86	0.88
1:D:44:PHE:H	1:D:44:PHE:HD1	1.14	0.88
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.52	0.88
1:H:69:MET:HE1	1:H:522:THR:HB	1.54	0.87
1:I:23:LEU:HD11	1:I:75:LYS:HG3	1.55	0.87
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.36	0.87
1:N:419:LEU:HD21	1:N:500:THR:CG2	2.04	0.87
1:I:149:THR:HG23	1:I:159:GLY:HA3	1.56	0.87
1:A:404:ARG:HH11	1:A:404:ARG:HG3	1.39	0.87
1:H:131:LEU:CD1	1:H:422:VAL:HG11	2.04	0.87
1:N:291:ASP:OD2	1:N:368:ARG:HD2	1.75	0.87
1:E:18:ARG:HH11	1:E:18:ARG:CB	1.87	0.87
1:C:33:PRO:HA	1:C:153:ASN:ND2	1.90	0.87
1:C:114:MET:HE3	1:C:114:MET:O	1.75	0.86
1:G:44:PHE:HD1	1:G:44:PHE:H	1.20	0.86
1:B:305:ILE:HG12	1:C:267:MET:HE3	1.57	0.86
1:D:18:ARG:HH11	1:D:18:ARG:CG	1.88	0.86
1:C:510:VAL:HG23	1:C:514:MET:HE2	1.55	0.86
1:L:131:LEU:HD12	1:L:422:VAL:HG11	1.54	0.86
1:L:69:MET:HE1	1:L:522:THR:HB	1.55	0.86
1:I:452:ARG:HG2	1:I:452:ARG:HH11	1.39	0.86
1:H:149:THR:HG23	1:H:159:GLY:HA3	1.58	0.85
1:L:419:LEU:HD21	1:L:500:THR:CG2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:419:LEU:HD21	1:N:500:THR:HG23	1.56	0.85
1:F:18:ARG:HH11	1:F:18:ARG:CB	1.87	0.85
1:B:33:PRO:HA	1:B:153:ASN:HD21	1.41	0.85
1:B:234:LEU:O	1:B:238:GLU:HG3	1.76	0.85
1:F:44:PHE:HD1	1:F:44:PHE:H	1.22	0.85
1:A:18:ARG:HH11	1:A:18:ARG:CB	1.89	0.85
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.38	0.85
1:D:69:MET:O	1:D:73:MET:HG3	1.77	0.85
1:K:131:LEU:CD1	1:K:422:VAL:HG11	2.06	0.85
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.58	0.85
1:E:349:ILE:HA	1:E:352:GLN:CG	2.07	0.84
1:G:349:ILE:HA	1:G:352:GLN:CG	2.07	0.84
1:I:65:LYS:O	1:I:66:PHE:HB2	1.74	0.84
1:M:131:LEU:HD12	1:M:422:VAL:HG11	1.57	0.84
1:A:414:GLY:O	1:A:417:VAL:CG1	2.25	0.84
1:L:37:ASN:OD1	5:L:538:HOH:O	1.95	0.84
1:C:349:ILE:HA	1:C:352:GLN:CG	2.07	0.84
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.41	0.84
1:A:74:VAL:O	1:A:77:VAL:HG13	1.76	0.84
1:J:65:LYS:HG3	5:J:536:HOH:O	1.76	0.84
1:J:149:THR:HG23	1:J:159:GLY:HA3	1.57	0.84
1:A:486:GLY:HA3	1:A:491:MET:HE2	1.60	0.83
1:B:486:GLY:HA3	1:B:491:MET:HE2	1.57	0.83
1:C:519:CYS:HB3	1:D:38:VAL:HG13	1.60	0.83
1:D:74:VAL:O	1:D:77:VAL:HG13	1.77	0.83
1:M:100:ILE:O	1:M:104:LEU:HB2	1.79	0.83
1:A:20:VAL:HG13	1:A:74:VAL:HG11	1.61	0.83
1:E:510:VAL:HG23	1:E:514:MET:HE2	1.60	0.83
1:J:131:LEU:HD12	1:J:422:VAL:HG11	1.59	0.83
1:F:349:ILE:HA	1:F:352:GLN:CG	2.09	0.82
1:K:149:THR:HG23	1:K:159:GLY:HA3	1.59	0.82
1:M:419:LEU:CD2	1:M:500:THR:CG2	2.58	0.82
1:J:291:ASP:OD2	1:J:368:ARG:HD2	1.79	0.82
1:M:452:ARG:HG2	1:M:452:ARG:NH1	1.89	0.82
1:A:224:ASP:HB3	1:A:302:SER:HB3	1.61	0.82
1:B:224:ASP:HB3	1:B:302:SER:HB3	1.62	0.82
1:J:69:MET:HE1	1:J:522:THR:HB	1.58	0.82
1:I:419:LEU:CD2	1:I:500:THR:CG2	2.57	0.82
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.62	0.82
1:N:149:THR:HG23	1:N:159:GLY:HA3	1.61	0.82
1:J:419:LEU:HD21	1:J:500:THR:HG22	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:291:ASP:OD2	1:M:368:ARG:HD2	1.79	0.82
1:C:224:ASP:HB3	1:C:302:SER:HB3	1.62	0.81
1:D:18:ARG:HB3	1:D:18:ARG:NH1	1.95	0.81
1:I:131:LEU:HD12	1:I:422:VAL:HG11	1.61	0.81
1:A:349:ILE:HA	1:A:352:GLN:CG	2.10	0.81
1:I:291:ASP:OD2	1:I:368:ARG:HD2	1.79	0.81
1:E:18:ARG:HH11	1:E:18:ARG:HB3	1.44	0.81
1:G:414:GLY:O	1:G:417:VAL:CG1	2.28	0.81
1:B:349:ILE:HA	1:B:352:GLN:CG	2.10	0.81
1:G:224:ASP:HB3	1:G:302:SER:HB3	1.63	0.81
1:M:149:THR:HG23	1:M:159:GLY:HA3	1.61	0.81
1:D:349:ILE:HA	1:D:352:GLN:CG	2.10	0.81
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.63	0.81
1:I:75:LYS:NZ	5:I:537:HOH:O	2.10	0.81
1:D:432:GLN:HE21	1:D:436:GLN:HE22	1.26	0.81
4:E:600:ADP:O3B	5:E:608:HOH:O	2.00	0.80
1:J:404:ARG:HG2	1:J:404:ARG:HH11	1.44	0.80
1:A:234:LEU:O	1:A:238:GLU:HG3	1.81	0.80
1:L:64:ASP:HB3	1:L:67:GLU:HB2	1.63	0.80
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.64	0.80
1:E:234:LEU:O	1:E:238:GLU:HG3	1.81	0.80
1:E:486:GLY:HA3	1:E:491:MET:HE2	1.64	0.79
1:K:419:LEU:HD21	1:K:500:THR:HG23	1.62	0.79
1:B:74:VAL:O	1:B:77:VAL:HG13	1.82	0.79
1:E:224:ASP:HB3	1:E:302:SER:HB3	1.64	0.79
1:L:291:ASP:OD2	1:L:368:ARG:HD2	1.82	0.79
1:A:114:MET:O	1:A:114:MET:HE3	1.82	0.79
1:B:18:ARG:CG	1:B:18:ARG:NH1	2.33	0.79
1:D:234:LEU:O	1:D:238:GLU:HG3	1.81	0.79
1:G:510:VAL:CG2	1:G:514:MET:HE2	2.11	0.79
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.64	0.79
1:N:452:ARG:HG2	1:N:452:ARG:NH1	1.96	0.79
1:E:265:ASN:HA	1:E:270:ILE:HD12	1.65	0.79
1:L:65:LYS:O	1:L:66:PHE:HB2	1.80	0.79
1:G:417:VAL:HG11	1:G:488:MET:HG3	1.65	0.79
1:K:494:LEU:O	1:K:494:LEU:HD23	1.82	0.78
1:C:265:ASN:HA	1:C:270:ILE:HD12	1.65	0.78
1:E:417:VAL:HG11	1:E:488:MET:HG3	1.65	0.78
2:R:13:LYS:HB3	2:R:41:LEU:HD11	1.65	0.78
1:B:74:VAL:HG13	1:B:514:MET:HE1	1.65	0.78
1:F:417:VAL:HG11	1:F:488:MET:HG3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:MET:CE	1:H:522:THR:HB	2.13	0.78
1:I:404:ARG:HG2	1:I:404:ARG:HH11	1.47	0.78
1:D:414:GLY:O	1:D:417:VAL:CG1	2.31	0.78
1:B:18:ARG:HH11	1:B:18:ARG:HB3	1.47	0.78
1:H:291:ASP:OD2	1:H:368:ARG:HD2	1.82	0.78
1:B:414:GLY:O	1:B:417:VAL:CG1	2.32	0.78
1:L:419:LEU:CD2	1:L:500:THR:CG2	2.61	0.78
1:A:18:ARG:HH11	1:A:18:ARG:CG	1.95	0.77
1:F:224:ASP:HB3	1:F:302:SER:HB3	1.66	0.77
1:H:494:LEU:HD23	1:H:494:LEU:O	1.83	0.77
1:I:149:THR:CG2	1:I:159:GLY:HA3	2.13	0.77
1:H:419:LEU:HD21	1:H:500:THR:HG23	1.64	0.77
1:F:33:PRO:HA	1:F:153:ASN:ND2	2.00	0.77
1:B:366:GLN:O	1:B:369:VAL:HG22	1.84	0.77
1:I:494:LEU:O	1:I:494:LEU:HD23	1.85	0.77
1:K:100:ILE:O	1:K:104:LEU:HB2	1.85	0.77
1:K:146:GLN:HE21	1:K:150:ILE:HD11	1.49	0.77
1:M:69:MET:HE1	1:M:522:THR:HB	1.65	0.77
1:N:69:MET:HE1	1:N:522:THR:HB	1.65	0.77
1:B:417:VAL:O	1:B:420:ILE:HG22	1.85	0.77
1:C:234:LEU:O	1:C:238:GLU:HG3	1.84	0.77
1:E:33:PRO:HA	1:E:153:ASN:ND2	1.98	0.77
1:N:284:ARG:HH11	1:N:364:LYS:HD2	1.50	0.77
1:C:366:GLN:O	1:C:369:VAL:HG22	1.85	0.76
1:K:213:VAL:HB	1:K:325:ILE:HG12	1.65	0.76
1:M:173:GLY:O	1:M:404:ARG:NH2	2.17	0.76
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.68	0.76
1:E:432:GLN:NE2	1:E:436:GLN:HE22	1.83	0.76
1:G:510:VAL:HG23	1:G:514:MET:CE	2.14	0.76
2:T:13:LYS:HB3	2:T:41:LEU:HD11	1.65	0.76
1:N:100:ILE:O	1:N:104:LEU:HB2	1.84	0.76
1:G:234:LEU:O	1:G:238:GLU:HG3	1.86	0.76
1:D:224:ASP:HB3	1:D:302:SER:HB3	1.67	0.76
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.67	0.76
1:H:452:ARG:HG2	1:H:452:ARG:NH1	1.98	0.76
1:L:69:MET:CE	1:L:522:THR:HB	2.15	0.76
1:A:417:VAL:O	1:A:420:ILE:HG22	1.87	0.75
1:A:417:VAL:HG11	1:A:488:MET:HG3	1.68	0.75
1:G:359:ASP:O	1:G:363:GLU:OE2	2.05	0.75
1:I:173:GLY:O	1:I:404:ARG:NH2	2.19	0.75
1:B:359:ASP:O	1:B:363:GLU:OE2	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:ASP:O	1:F:363:GLU:OE2	2.04	0.75
1:C:18:ARG:HH11	1:C:18:ARG:HG2	1.50	0.75
1:J:149:THR:CG2	1:J:159:GLY:HA3	2.15	0.75
1:C:102:GLU:HB3	1:C:442:VAL:HG22	1.69	0.75
1:D:33:PRO:HA	1:D:153:ASN:HD21	1.52	0.75
1:F:234:LEU:O	1:F:238:GLU:HG3	1.85	0.75
4:G:600:ADP:O3B	5:G:607:HOH:O	2.04	0.75
1:H:96:ALA:O	1:H:100:ILE:HG13	1.85	0.75
1:N:65:LYS:O	1:N:66:PHE:CB	2.33	0.75
1:B:381:VAL:CG1	1:B:392:LYS:CG	2.65	0.75
1:C:359:ASP:O	1:C:363:GLU:OE2	2.04	0.75
1:D:366:GLN:O	1:D:369:VAL:HG22	1.85	0.75
1:J:284:ARG:HH11	1:J:364:LYS:HD2	1.52	0.75
1:N:87:ASP:HB3	1:N:499:VAL:HG21	1.67	0.75
1:B:381:VAL:HG11	1:B:392:LYS:HG3	1.67	0.74
1:I:2:ALA:O	1:I:4:LYS:HE3	1.87	0.74
1:N:419:LEU:CD2	1:N:500:THR:HG23	2.14	0.74
1:D:486:GLY:HA3	1:D:491:MET:HE2	1.69	0.74
1:C:417:VAL:O	1:C:420:ILE:HG22	1.86	0.74
2:Q:13:LYS:HB3	2:Q:41:LEU:HD11	1.69	0.74
1:J:419:LEU:CD2	1:J:500:THR:HG21	2.17	0.74
1:A:510:VAL:HG23	1:A:514:MET:CE	2.18	0.74
1:G:33:PRO:HA	1:G:153:ASN:ND2	2.01	0.74
1:A:265:ASN:HA	1:A:270:ILE:HD12	1.70	0.74
1:D:404:ARG:HH11	1:D:404:ARG:HG3	1.52	0.74
1:E:366:GLN:O	1:E:369:VAL:HG22	1.86	0.74
1:C:305:ILE:HG12	1:D:267:MET:HE3	1.70	0.74
1:H:64:ASP:HB3	1:H:67:GLU:HB2	1.70	0.74
1:K:131:LEU:HD12	1:K:422:VAL:HG11	1.68	0.74
1:B:265:ASN:HA	1:B:270:ILE:HD12	1.70	0.74
1:G:18:ARG:HG2	1:G:18:ARG:NH1	1.94	0.73
1:M:69:MET:CE	1:M:522:THR:HB	2.18	0.73
1:J:433:ASN:OD1	5:J:533:HOH:O	2.05	0.73
1:K:149:THR:CG2	1:K:159:GLY:HA3	2.19	0.73
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.69	0.73
1:B:229:ASN:HB3	1:B:231:ARG:HG3	1.71	0.73
1:C:18:ARG:HG2	1:C:18:ARG:NH1	2.02	0.73
1:E:74:VAL:HG13	1:E:514:MET:HE1	1.70	0.73
1:I:69:MET:HE1	1:I:522:THR:HB	1.71	0.73
1:N:404:ARG:HG2	1:N:404:ARG:HH11	1.53	0.73
1:C:74:VAL:O	1:C:77:VAL:HG13	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:LEU:HD13	1:I:422:VAL:HG11	1.70	0.73
1:A:359:ASP:O	1:A:363:GLU:OE2	2.07	0.73
1:C:18:ARG:CG	1:C:18:ARG:NH1	2.46	0.72
1:G:452:ARG:HG2	1:G:452:ARG:HH11	1.53	0.72
1:L:434:GLU:HB2	5:L:528:HOH:O	1.89	0.72
1:I:84:ALA:O	1:I:498:LYS:HE2	1.90	0.72
1:B:510:VAL:CG2	1:B:514:MET:HE2	2.17	0.72
1:C:417:VAL:HG11	1:C:488:MET:HG3	1.69	0.72
1:G:74:VAL:O	1:G:77:VAL:HG13	1.90	0.72
1:D:114:MET:O	1:D:114:MET:HE3	1.89	0.72
1:D:265:ASN:HA	1:D:270:ILE:HD12	1.71	0.72
1:H:131:LEU:HD12	1:H:422:VAL:HG11	1.70	0.72
1:H:149:THR:CG2	1:H:159:GLY:HA3	2.19	0.72
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.54	0.72
1:E:380:LYS:HD3	5:E:606:HOH:O	1.90	0.72
1:F:510:VAL:CG2	1:F:514:MET:HE2	2.20	0.72
1:J:16:MET:O	1:J:20:VAL:HG12	1.90	0.72
1:J:32:GLY:HA2	1:J:454:ILE:HD13	1.71	0.72
1:L:149:THR:CG2	1:L:159:GLY:HA3	2.17	0.72
1:B:381:VAL:CG1	1:B:392:LYS:HG3	2.19	0.72
1:F:265:ASN:HA	1:F:270:ILE:HD12	1.72	0.72
1:N:174:VAL:HG21	1:N:194:GLN:HB3	1.72	0.72
1:A:409:GLU:OE2	1:A:501:ARG:NH2	2.19	0.72
1:F:366:GLN:O	1:F:369:VAL:HG22	1.88	0.72
1:L:284:ARG:HH11	1:L:364:LYS:HD2	1.55	0.72
1:N:11:ASP:O	1:N:12:ALA:C	2.31	0.72
1:C:486:GLY:HA3	1:C:491:MET:HE2	1.71	0.72
1:F:414:GLY:O	1:F:417:VAL:CG1	2.36	0.72
1:F:443:ALA:O	1:F:447:MET:HE3	1.88	0.72
1:H:284:ARG:HH11	1:H:364:LYS:HD2	1.54	0.72
1:D:489:ILE:HD13	1:D:494:LEU:HD22	1.70	0.72
1:G:18:ARG:HH11	1:G:18:ARG:CB	2.03	0.72
1:G:366:GLN:O	1:G:369:VAL:HG22	1.89	0.71
1:J:452:ARG:HG2	1:J:452:ARG:NH1	2.01	0.71
1:M:149:THR:CG2	1:M:159:GLY:HA3	2.19	0.71
1:C:18:ARG:HB3	1:C:18:ARG:NH1	2.05	0.71
1:I:419:LEU:HD21	1:I:500:THR:HG23	1.71	0.71
1:L:166:MET:HE2	1:L:171:LYS:HA	1.72	0.71
1:D:510:VAL:CG2	1:D:514:MET:HE2	2.17	0.71
1:G:23:LEU:CD1	1:G:23:LEU:C	2.63	0.71
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:494:LEU:HD23	1:J:494:LEU:O	1.90	0.71
1:C:510:VAL:CG2	1:C:514:MET:HE2	2.20	0.71
1:K:106:ALA:HA	1:K:111:MET:HE3	1.72	0.71
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.54	0.71
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.70	0.71
1:H:84:ALA:O	1:H:498:LYS:HE2	1.90	0.71
1:J:69:MET:CE	1:J:522:THR:HB	2.19	0.71
1:K:32:GLY:HA2	1:K:454:ILE:HD13	1.71	0.71
1:K:291:ASP:OD2	1:K:368:ARG:HD2	1.90	0.71
1:B:381:VAL:HG12	1:B:392:LYS:HG2	1.71	0.71
1:D:381:VAL:HG11	1:D:392:LYS:HG3	1.73	0.71
1:D:489:ILE:HD13	1:D:494:LEU:CD2	2.21	0.71
1:E:359:ASP:O	1:E:363:GLU:OE2	2.08	0.71
1:F:74:VAL:O	1:F:77:VAL:HG13	1.91	0.71
1:K:419:LEU:CD2	1:K:500:THR:HG21	2.19	0.71
1:L:47:PRO:HG2	1:M:73:MET:HG3	1.72	0.71
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.72	0.71
1:J:434:GLU:HB2	5:J:532:HOH:O	1.89	0.71
1:C:365:LEU:O	1:C:369:VAL:HG13	1.91	0.71
1:G:265:ASN:HA	1:G:270:ILE:HD12	1.72	0.71
1:H:179:ASP:OD1	1:H:393:LYS:HD2	1.90	0.71
2:U:13:LYS:HB3	2:U:41:LEU:HD11	1.73	0.71
1:B:33:PRO:HA	1:B:153:ASN:ND2	2.04	0.71
1:K:419:LEU:CD2	1:K:500:THR:HG23	2.18	0.71
1:H:102:GLU:OE2	1:H:445:ARG:NH1	2.24	0.71
1:M:494:LEU:HD23	1:M:494:LEU:O	1.91	0.71
1:N:66:PHE:H	1:N:69:MET:HG3	1.56	0.71
1:I:64:ASP:HB3	1:I:67:GLU:HB2	1.73	0.70
1:I:404:ARG:HH11	1:I:404:ARG:CG	2.03	0.70
1:L:38:VAL:HG22	1:M:519:CYS:HB3	1.73	0.70
1:E:18:ARG:HH11	1:E:18:ARG:HG2	1.55	0.70
1:M:404:ARG:HH11	1:M:404:ARG:CG	2.00	0.70
1:H:100:ILE:O	1:H:104:LEU:HB2	1.90	0.70
1:N:259:LEU:O	1:N:263:VAL:HG23	1.91	0.70
2:O:13:LYS:HB3	2:O:41:LEU:HD11	1.74	0.70
1:D:345:ARG:HA	1:D:348:GLN:HE21	1.56	0.70
1:F:452:ARG:HG2	1:F:452:ARG:HH11	1.56	0.70
1:H:65:LYS:O	1:H:66:PHE:CB	2.40	0.70
1:J:131:LEU:HD13	1:J:422:VAL:HG11	1.73	0.70
1:N:106:ALA:HA	1:N:111:MET:HE3	1.71	0.70
1:I:100:ILE:O	1:I:104:LEU:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:13:LYS:HB3	2:P:41:LEU:HD11	1.73	0.70
1:C:381:VAL:CG1	1:C:392:LYS:HG2	2.22	0.70
1:E:74:VAL:O	1:E:77:VAL:HG13	1.91	0.70
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.74	0.70
1:A:510:VAL:CG2	1:A:514:MET:HE2	2.18	0.70
1:C:404:ARG:HH11	1:C:404:ARG:HG3	1.57	0.69
1:D:359:ASP:O	1:D:363:GLU:OE2	2.09	0.69
1:K:284:ARG:HH11	1:K:364:LYS:HD2	1.57	0.69
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.72	0.69
1:F:18:ARG:CG	1:F:18:ARG:NH1	2.35	0.69
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.74	0.69
1:K:166:MET:HE2	1:K:171:LYS:HA	1.74	0.69
1:M:27:VAL:HG11	1:M:93:THR:HG21	1.74	0.69
1:C:451:LEU:HD23	1:C:451:LEU:C	2.17	0.69
1:D:417:VAL:O	1:D:420:ILE:HG22	1.92	0.69
1:C:16:MET:O	1:C:20:VAL:HG23	1.93	0.69
1:D:381:VAL:CG1	1:D:392:LYS:CG	2.70	0.69
1:D:417:VAL:HG11	1:D:488:MET:HG3	1.73	0.69
1:H:131:LEU:HD13	1:H:422:VAL:HG11	1.73	0.69
1:J:64:ASP:HB3	1:J:67:GLU:HB2	1.74	0.69
1:A:430:ARG:HG2	1:A:430:ARG:NH1	2.03	0.69
1:F:381:VAL:HG11	1:F:392:LYS:HG3	1.73	0.69
1:G:365:LEU:O	1:G:369:VAL:HG13	1.92	0.69
1:G:443:ALA:O	1:G:447:MET:HE3	1.92	0.69
1:G:487:ASN:O	1:G:491:MET:HG3	1.93	0.69
1:A:381:VAL:CG1	1:A:392:LYS:HG3	2.23	0.69
1:A:381:VAL:HG11	1:A:392:LYS:HG3	1.74	0.69
1:C:487:ASN:O	1:C:491:MET:HG3	1.93	0.69
1:E:44:PHE:CD1	1:E:44:PHE:N	2.59	0.69
1:I:65:LYS:O	1:I:66:PHE:CB	2.40	0.69
1:J:100:ILE:O	1:J:104:LEU:HB2	1.92	0.69
1:J:166:MET:HE2	1:J:171:LYS:HA	1.75	0.69
1:K:84:ALA:O	1:K:498:LYS:HE2	1.91	0.69
1:H:2:ALA:O	1:H:4:LYS:HE3	1.93	0.69
1:J:106:ALA:HA	1:J:111:MET:HE3	1.75	0.69
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.75	0.69
1:K:96:ALA:O	1:K:100:ILE:HG13	1.90	0.69
1:C:432:GLN:NE2	1:C:436:GLN:HE22	1.90	0.68
1:I:166:MET:HE2	1:I:171:LYS:HA	1.75	0.68
1:J:174:VAL:HG21	1:J:194:GLN:HB3	1.75	0.68
1:L:494:LEU:O	1:L:494:LEU:HD23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:7:HIS:O	2:S:8:ASP:HB3	1.92	0.68
1:F:74:VAL:HG13	1:F:514:MET:HE1	1.75	0.68
1:L:404:ARG:HH11	1:L:404:ARG:CG	2.06	0.68
1:F:111:MET:HG2	1:F:435:ASP:OD1	1.92	0.68
1:K:179:ASP:OD1	1:K:393:LYS:HD2	1.93	0.68
1:A:366:GLN:O	1:A:369:VAL:HG22	1.93	0.68
1:F:365:LEU:O	1:F:369:VAL:HG13	1.93	0.68
2:S:13:LYS:HB3	2:S:41:LEU:HD11	1.74	0.68
1:B:417:VAL:HG11	1:B:488:MET:HG3	1.76	0.68
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.75	0.68
1:D:381:VAL:HG12	1:D:392:LYS:HG2	1.75	0.68
1:J:65:LYS:O	1:J:66:PHE:CB	2.36	0.68
1:A:24:ALA:O	1:A:28:LYS:HG3	1.94	0.68
1:C:516:THR:OG1	1:D:37:ASN:ND2	2.27	0.68
1:I:259:LEU:O	1:I:263:VAL:HG23	1.94	0.68
1:M:83:ASP:OD2	1:M:327:LYS:HE2	1.94	0.68
1:M:84:ALA:O	1:M:498:LYS:HE2	1.94	0.68
1:M:106:ALA:HA	1:M:111:MET:HE3	1.75	0.68
1:D:381:VAL:CG1	1:D:392:LYS:HG3	2.24	0.68
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.75	0.68
1:A:365:LEU:O	1:A:369:VAL:HG13	1.93	0.68
1:E:18:ARG:HG2	1:E:18:ARG:NH1	2.07	0.68
1:F:409:GLU:OE2	1:F:501:ARG:NH2	2.26	0.68
1:G:404:ARG:HG3	1:G:404:ARG:HH11	1.59	0.68
1:G:430:ARG:HG2	1:G:430:ARG:NH1	2.05	0.68
1:M:16:MET:SD	1:M:514:MET:HG2	2.34	0.68
1:F:18:ARG:HH11	1:F:18:ARG:HB3	1.59	0.68
1:M:87:ASP:HB3	1:M:499:VAL:HG21	1.76	0.68
1:E:365:LEU:O	1:E:369:VAL:HG13	1.95	0.67
1:N:149:THR:CG2	1:N:159:GLY:HA3	2.24	0.67
1:A:38:VAL:HG13	1:G:519:CYS:HB3	1.74	0.67
1:B:76:GLU:OE1	1:C:387:VAL:HG22	1.94	0.67
1:F:381:VAL:CG1	1:F:392:LYS:CG	2.71	0.67
1:H:32:GLY:HA2	1:H:454:ILE:HD13	1.75	0.67
2:Q:7:HIS:O	2:Q:8:ASP:HB3	1.95	0.67
2:P:7:HIS:O	2:P:8:ASP:HB3	1.94	0.67
2:T:7:HIS:O	2:T:8:ASP:HB3	1.93	0.67
1:B:16:MET:HE1	1:B:514:MET:HB3	1.74	0.67
1:K:452:ARG:HG2	1:K:452:ARG:NH1	2.10	0.67
1:N:326:ASN:HB2	1:N:329:THR:H	1.59	0.67
1:G:381:VAL:CG1	1:G:392:LYS:HG3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:66:PHE:H	1:J:69:MET:HG3	1.59	0.67
1:L:100:ILE:O	1:L:104:LEU:HB2	1.95	0.67
1:A:238:GLU:OE2	2:O:23:GLY:C	2.38	0.67
1:B:16:MET:O	1:B:20:VAL:HG23	1.94	0.67
1:M:90:THR:O	1:M:94:VAL:HG23	1.94	0.67
1:E:381:VAL:HG11	1:E:392:LYS:HG3	1.77	0.67
1:F:381:VAL:HG12	1:F:392:LYS:HG2	1.76	0.67
1:D:64:ASP:HB3	1:D:67:GLU:HB2	1.76	0.67
1:H:419:LEU:CD2	1:H:500:THR:HG23	2.21	0.67
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.77	0.67
1:B:147:VAL:HG22	1:B:403:THR:HG22	1.77	0.67
1:B:365:LEU:O	1:B:369:VAL:HG13	1.94	0.67
1:B:381:VAL:CG1	1:B:392:LYS:HG2	2.24	0.67
1:H:146:GLN:HE21	1:H:150:ILE:HD11	1.60	0.67
1:K:131:LEU:HD13	1:K:422:VAL:HG11	1.77	0.67
1:M:421:ARG:HD2	1:M:474:GLY:O	1.94	0.67
1:B:452:ARG:HG2	1:B:452:ARG:HH11	1.60	0.66
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.77	0.66
1:C:452:ARG:HG2	1:C:452:ARG:HH11	1.60	0.66
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.77	0.66
1:K:259:LEU:O	1:K:263:VAL:HG23	1.95	0.66
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.77	0.66
1:C:381:VAL:CG1	1:C:392:LYS:CG	2.72	0.66
1:I:461:GLU:OE2	5:I:541:HOH:O	2.12	0.66
1:K:102:GLU:OE2	1:K:445:ARG:NH1	2.28	0.66
1:N:131:LEU:CD1	1:N:422:VAL:HG11	2.25	0.66
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.76	0.66
1:M:419:LEU:HD21	1:M:500:THR:HG23	1.74	0.66
1:N:166:MET:HE2	1:N:171:LYS:HA	1.77	0.66
1:B:385:THR:OG1	1:B:388:GLU:HB2	1.96	0.66
1:D:450:PRO:O	1:D:454:ILE:HG13	1.95	0.66
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.77	0.66
1:F:381:VAL:CG1	1:F:392:LYS:HG3	2.25	0.66
1:H:66:PHE:HD1	1:H:520:MET:HE2	1.61	0.66
1:D:305:ILE:HG12	1:E:267:MET:HE3	1.77	0.66
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.76	0.66
1:J:419:LEU:HD21	1:J:500:THR:HG23	1.74	0.66
1:B:44:PHE:CD1	1:B:44:PHE:N	2.57	0.66
1:C:77:VAL:HG23	1:C:92:ALA:HB1	1.78	0.66
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.78	0.66
1:E:522:THR:OG1	1:E:523:ASP:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:284:ARG:HH11	1:M:364:LYS:HD2	1.61	0.66
1:N:125:THR:O	5:N:537:HOH:O	2.13	0.66
2:R:7:HIS:O	2:R:8:ASP:HB3	1.95	0.66
1:C:23:LEU:CD1	1:C:23:LEU:C	2.68	0.66
1:L:146:GLN:HE21	1:L:150:ILE:HD11	1.61	0.66
1:A:432:GLN:NE2	1:A:436:GLN:HE22	1.94	0.66
1:B:18:ARG:NH1	1:B:18:ARG:HB3	2.10	0.66
1:G:417:VAL:O	1:G:420:ILE:HG22	1.96	0.66
1:H:66:PHE:H	1:H:69:MET:HG3	1.61	0.66
1:J:179:ASP:OD1	1:J:393:LYS:HD2	1.95	0.66
1:D:82:ASN:HB2	1:D:89:THR:CG2	2.25	0.65
1:D:254:VAL:HG12	1:D:259:LEU:HB2	1.77	0.65
1:M:193:MET:CE	1:M:195:PHE:HD1	2.08	0.65
1:D:430:ARG:HG2	1:D:430:ARG:NH1	1.99	0.65
1:J:193:MET:CE	1:J:195:PHE:HD1	2.09	0.65
1:C:510:VAL:HG12	1:D:385:THR:HG21	1.78	0.65
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.55	0.65
1:D:430:ARG:HH11	1:D:430:ARG:CG	2.02	0.65
1:I:179:ASP:OD1	1:I:393:LYS:HD2	1.96	0.65
1:A:385:THR:HG21	1:G:510:VAL:HG12	1.79	0.65
1:C:381:VAL:HG12	1:C:392:LYS:HG2	1.78	0.65
1:G:162:ILE:HG21	1:G:403:THR:HG21	1.79	0.65
1:I:106:ALA:HA	1:I:111:MET:HE3	1.78	0.65
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.77	0.65
1:C:229:ASN:HB3	1:C:231:ARG:HG3	1.78	0.65
1:E:288:MET:HG3	1:E:368:ARG:HD2	1.78	0.65
1:H:259:LEU:O	1:H:263:VAL:HG23	1.96	0.65
1:L:179:ASP:OD1	1:L:393:LYS:HD2	1.97	0.65
1:D:365:LEU:O	1:D:369:VAL:HG13	1.97	0.65
1:E:385:THR:OG1	1:E:388:GLU:HB2	1.97	0.65
1:G:24:ALA:O	1:G:28:LYS:HG3	1.97	0.65
1:I:492:GLY:C	1:I:493:ILE:HD13	2.22	0.65
1:L:452:ARG:HG2	1:L:452:ARG:NH1	2.09	0.65
1:M:66:PHE:HD1	1:M:520:MET:HE2	1.62	0.65
1:N:69:MET:CE	1:N:522:THR:HB	2.27	0.65
1:J:149:THR:CG2	1:J:156:GLU:HA	2.26	0.65
1:K:326:ASN:HB2	1:K:329:THR:H	1.61	0.65
1:F:417:VAL:O	1:F:420:ILE:HG22	1.96	0.64
1:M:131:LEU:HD13	1:M:422:VAL:HG11	1.79	0.64
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.78	0.64
1:B:432:GLN:NE2	1:B:436:GLN:HE22	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.78	0.64
1:E:381:VAL:CG1	1:E:392:LYS:HG3	2.28	0.64
1:G:381:VAL:HG11	1:G:392:LYS:HG3	1.79	0.64
1:N:179:ASP:OD1	1:N:393:LYS:HD2	1.97	0.64
1:N:418:ALA:O	1:N:422:VAL:HG13	1.95	0.64
2:O:7:HIS:O	2:O:8:ASP:HB3	1.97	0.64
1:A:451:LEU:C	1:A:451:LEU:HD23	2.22	0.64
1:C:64:ASP:HB3	1:C:67:GLU:HB2	1.78	0.64
1:D:82:ASN:HB2	1:D:89:THR:HG21	1.77	0.64
1:L:19:GLY:HA3	1:L:67:GLU:O	1.96	0.64
1:L:49:ILE:HD11	1:M:73:MET:HE3	1.78	0.64
1:A:42:LYS:HG2	1:A:44:PHE:CE2	2.32	0.64
1:C:44:PHE:CD1	1:C:44:PHE:N	2.58	0.64
1:D:24:ALA:O	1:D:28:LYS:HG3	1.97	0.64
1:D:510:VAL:HG23	1:D:514:MET:CE	2.23	0.64
1:F:486:GLY:CA	1:F:491:MET:HE2	2.25	0.64
1:F:114:MET:HE3	1:F:114:MET:O	1.98	0.64
1:M:47:PRO:HG2	1:N:73:MET:HG3	1.78	0.64
1:M:64:ASP:HB3	1:M:67:GLU:HB2	1.78	0.64
1:I:73:MET:CG	1:I:73:MET:CE	2.75	0.64
1:K:27:VAL:HG11	1:K:93:THR:HG21	1.79	0.64
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.80	0.64
1:J:326:ASN:HB2	1:J:329:THR:H	1.63	0.64
1:J:421:ARG:HD2	1:J:474:GLY:O	1.98	0.64
1:B:404:ARG:HG3	1:B:404:ARG:HH11	1.63	0.64
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.78	0.64
1:D:432:GLN:HE21	1:D:436:GLN:NE2	1.96	0.64
1:F:305:ILE:HG12	1:G:267:MET:HE3	1.79	0.64
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.80	0.64
1:I:30:THR:HB	1:I:51:LYS:O	1.98	0.64
1:I:65:LYS:HG3	5:I:533:HOH:O	1.98	0.64
1:N:138:CYS:SG	1:N:144:ILE:HD13	2.38	0.64
1:F:288:MET:HG3	1:F:368:ARG:HD2	1.79	0.63
1:L:417:VAL:HG21	1:L:488:MET:HG3	1.80	0.63
1:M:146:GLN:HE21	1:M:150:ILE:HD11	1.62	0.63
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.80	0.63
1:I:452:ARG:HG2	1:I:452:ARG:NH1	2.12	0.63
1:F:229:ASN:HB3	1:F:231:ARG:HG3	1.79	0.63
1:G:345:ARG:HA	1:G:348:GLN:HE21	1.62	0.63
1:K:417:VAL:HG21	1:K:488:MET:HG3	1.80	0.63
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:451:LEU:HD23	1:G:451:LEU:C	2.22	0.63
1:I:69:MET:CE	1:I:522:THR:HB	2.28	0.63
1:M:66:PHE:H	1:M:69:MET:HG3	1.63	0.63
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.80	0.63
1:C:430:ARG:HG2	1:C:430:ARG:NH1	2.06	0.63
1:D:489:ILE:CD1	1:D:494:LEU:HD22	2.28	0.63
1:G:20:VAL:HG13	1:G:74:VAL:HG11	1.80	0.63
1:H:166:MET:HE2	1:H:171:LYS:HA	1.79	0.63
1:N:149:THR:CG2	1:N:156:GLU:HA	2.28	0.63
1:A:49:ILE:HD13	1:G:513:LEU:HB3	1.81	0.63
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.80	0.63
1:B:462:PRO:HD2	5:B:611:HOH:O	1.97	0.63
1:C:414:GLY:O	1:C:417:VAL:CG1	2.44	0.63
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.81	0.63
1:I:421:ARG:HD2	1:I:474:GLY:O	1.99	0.63
1:N:96:ALA:O	1:N:100:ILE:HG13	1.99	0.63
1:D:381:VAL:CG1	1:D:392:LYS:HG2	2.29	0.63
1:E:260:ALA:O	1:E:264:VAL:HG23	1.99	0.63
1:E:414:GLY:O	1:E:417:VAL:CG1	2.44	0.63
1:J:43:SER:HB3	1:J:44:PHE:CD1	2.33	0.63
1:J:138:CYS:SG	1:J:144:ILE:HD13	2.39	0.63
1:N:193:MET:CE	1:N:195:PHE:HD1	2.11	0.63
1:B:288:MET:HG3	1:B:368:ARG:HD2	1.79	0.62
1:B:487:ASN:O	1:B:491:MET:HG3	1.99	0.62
1:F:147:VAL:HG22	1:F:403:THR:HG22	1.81	0.62
1:G:28:LYS:O	1:G:29:VAL:C	2.40	0.62
1:G:254:VAL:HG12	1:G:259:LEU:HB2	1.80	0.62
1:C:254:VAL:HG12	1:C:259:LEU:HB2	1.81	0.62
1:I:494:LEU:HD23	1:I:494:LEU:C	2.23	0.62
1:A:345:ARG:HA	1:A:348:GLN:HE21	1.63	0.62
1:C:345:ARG:HA	1:C:348:GLN:HE21	1.64	0.62
1:D:260:ALA:O	1:D:264:VAL:HG23	1.99	0.62
1:E:345:ARG:HA	1:E:348:GLN:HE21	1.64	0.62
1:E:381:VAL:CG1	1:E:392:LYS:CG	2.76	0.62
2:R:23:GLY:H	2:S:80:ASN:ND2	1.97	0.62
1:H:11:ASP:O	1:H:12:ALA:C	2.38	0.62
1:H:149:THR:CG2	1:H:156:GLU:HA	2.30	0.62
1:J:146:GLN:HE21	1:J:150:ILE:HD11	1.64	0.62
1:L:32:GLY:HA2	1:L:454:ILE:HD13	1.81	0.62
1:M:2:ALA:O	1:M:4:LYS:HE3	2.00	0.62
1:M:166:MET:HE2	1:M:171:LYS:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:VAL:CG1	1:A:392:LYS:CG	2.77	0.62
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.81	0.62
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.81	0.62
1:H:419:LEU:CD2	1:H:500:THR:HG21	2.26	0.62
1:A:288:MET:HG3	1:A:368:ARG:HD2	1.80	0.62
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.81	0.62
1:M:385:THR:HG23	1:M:388:GLU:HB2	1.81	0.62
1:D:229:ASN:HB3	1:D:231:ARG:HG3	1.82	0.62
1:F:430:ARG:HG2	1:F:430:ARG:NH1	2.06	0.62
1:J:392:LYS:O	1:J:396:VAL:HG23	1.99	0.62
1:K:2:ALA:O	1:K:4:LYS:HE3	1.99	0.62
1:M:419:LEU:CD2	1:M:500:THR:HG21	2.28	0.62
1:N:64:ASP:HB3	1:N:67:GLU:HB2	1.81	0.62
1:G:229:ASN:HB3	1:G:231:ARG:HG3	1.81	0.62
1:H:419:LEU:HD21	1:H:500:THR:HG22	1.79	0.62
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.82	0.62
1:M:492:GLY:C	1:M:493:ILE:HD13	2.24	0.62
1:L:16:MET:O	1:L:20:VAL:HG12	2.00	0.62
1:L:106:ALA:HA	1:L:111:MET:HE3	1.81	0.62
1:A:37:ASN:ND2	1:G:516:THR:OG1	2.32	0.62
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.81	0.62
1:E:381:VAL:HG12	1:E:392:LYS:HG2	1.81	0.62
1:E:430:ARG:HG2	1:E:430:ARG:NH1	2.09	0.62
1:F:260:ALA:O	1:F:264:VAL:HG23	2.00	0.62
1:F:450:PRO:O	1:F:454:ILE:HG13	1.99	0.62
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.81	0.62
1:D:6:VAL:HG23	1:D:6:VAL:O	2.00	0.61
1:D:522:THR:OG1	1:D:523:ASP:N	2.25	0.61
1:M:259:LEU:O	1:M:263:VAL:HG23	2.00	0.61
1:A:229:ASN:HB3	1:A:231:ARG:HG3	1.82	0.61
1:D:288:MET:HG3	1:D:368:ARG:HD2	1.81	0.61
1:G:409:GLU:OE2	1:G:501:ARG:NH2	2.22	0.61
1:B:345:ARG:HA	1:B:348:GLN:HE21	1.65	0.61
1:L:326:ASN:HB2	1:L:329:THR:H	1.64	0.61
1:A:381:VAL:HG12	1:A:392:LYS:HG2	1.81	0.61
1:E:417:VAL:O	1:E:420:ILE:HG22	1.99	0.61
1:L:11:ASP:O	1:L:12:ALA:C	2.41	0.61
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.82	0.61
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.82	0.61
1:K:419:LEU:HD21	1:K:500:THR:HG22	1.77	0.61
1:N:84:ALA:O	1:N:498:LYS:HE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLN:HA	1:A:354:GLU:HG2	1.82	0.61
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.82	0.61
1:K:421:ARG:HD2	1:K:474:GLY:O	2.01	0.61
1:L:66:PHE:HD1	1:L:520:MET:HE2	1.65	0.61
1:N:146:GLN:HE21	1:N:150:ILE:HD11	1.65	0.61
1:A:44:PHE:CD1	1:A:44:PHE:N	2.57	0.61
1:E:147:VAL:HG22	1:E:403:THR:HG22	1.81	0.61
1:I:296:THR:HB	1:I:319:GLN:H	1.65	0.61
1:N:417:VAL:HG21	1:N:488:MET:HG3	1.83	0.61
2:U:7:HIS:O	2:U:8:ASP:HB3	1.99	0.61
1:H:65:LYS:HA	5:H:528:HOH:O	1.99	0.61
1:I:146:GLN:HE21	1:I:150:ILE:HD11	1.65	0.61
1:L:462:PRO:O	1:L:463:SER:C	2.43	0.61
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.82	0.61
1:E:82:ASN:HB2	1:E:89:THR:HG21	1.82	0.61
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.81	0.61
2:R:84:LEU:N	2:R:84:LEU:HD12	2.15	0.61
1:A:162:ILE:HG21	1:A:403:THR:HG21	1.83	0.61
1:A:270:ILE:HG12	2:O:27:LEU:HD13	1.81	0.61
1:C:381:VAL:HG11	1:C:392:LYS:HG3	1.83	0.61
1:D:121:ASP:OD1	5:D:610:HOH:O	2.16	0.61
1:G:288:MET:HG3	1:G:368:ARG:HD2	1.82	0.61
1:M:452:ARG:NH1	1:M:452:ARG:CG	2.58	0.61
1:A:504:LEU:O	1:A:504:LEU:HD22	2.00	0.60
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.82	0.60
1:M:192:GLY:HA2	1:M:295:LEU:HD11	1.83	0.60
1:D:409:GLU:OE2	1:D:501:ARG:NH2	2.26	0.60
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.82	0.60
1:G:381:VAL:CG1	1:G:392:LYS:CG	2.79	0.60
1:M:106:ALA:CA	1:M:111:MET:HE3	2.30	0.60
1:B:34:LYS:HD2	1:B:458:CYS:SG	2.41	0.60
1:E:432:GLN:HE21	1:E:436:GLN:HE22	1.46	0.60
1:G:450:PRO:O	1:G:454:ILE:HG13	2.01	0.60
1:I:80:LYS:HA	1:I:83:ASP:HB2	1.82	0.60
1:I:496:PRO:HB2	1:I:499:VAL:HG13	1.83	0.60
1:H:193:MET:CE	1:H:195:PHE:HD1	2.14	0.60
1:I:493:ILE:HD13	1:I:493:ILE:N	2.16	0.60
1:M:325:ILE:HG22	1:M:330:THR:HA	1.82	0.60
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.84	0.60
1:N:476:TYR:HA	1:N:486:GLY:O	2.02	0.60
1:C:260:ALA:O	1:C:264:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:GLN:HA	1:F:354:GLU:HG2	1.83	0.60
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.83	0.60
1:N:296:THR:HB	1:N:319:GLN:H	1.66	0.60
1:A:18:ARG:NH1	1:A:18:ARG:HG2	2.17	0.60
1:C:520:MET:HG2	1:D:39:VAL:HB	1.81	0.60
1:L:84:ALA:O	1:L:498:LYS:HE2	2.01	0.60
1:N:428:ASP:HB2	5:N:529:HOH:O	2.01	0.60
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.84	0.60
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.61	0.60
1:C:76:GLU:OE1	1:D:387:VAL:HG22	2.01	0.60
1:E:510:VAL:HG23	1:E:514:MET:CE	2.30	0.60
1:F:111:MET:CE	1:F:111:MET:CG	2.78	0.60
1:C:114:MET:HE3	1:C:114:MET:C	2.27	0.60
1:M:441:LYS:O	1:M:442:VAL:C	2.45	0.60
1:B:64:ASP:HB3	1:B:67:GLU:HB2	1.82	0.60
1:B:162:ILE:HG21	1:B:403:THR:HG21	1.84	0.60
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.84	0.60
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.54	0.60
1:F:381:VAL:CG1	1:F:392:LYS:HG2	2.30	0.60
1:I:326:ASN:HB2	1:I:329:THR:H	1.67	0.60
1:D:429:LEU:O	1:D:430:ARG:HG2	2.02	0.60
1:J:87:ASP:HB3	1:J:499:VAL:HG21	1.84	0.60
1:J:259:LEU:O	1:J:263:VAL:HG23	2.02	0.60
1:G:23:LEU:C	1:G:23:LEU:HD13	2.25	0.59
1:H:323:VAL:HG12	1:H:332:ILE:HA	1.84	0.59
1:I:21:ASN:O	1:I:25:ASP:N	2.29	0.59
1:K:323:VAL:HG12	1:K:332:ILE:HA	1.83	0.59
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.84	0.59
1:D:198:GLY:O	1:D:276:VAL:HG12	2.02	0.59
1:D:451:LEU:C	1:D:451:LEU:HD23	2.26	0.59
1:E:162:ILE:HG21	1:E:403:THR:HG21	1.82	0.59
1:E:229:ASN:HB3	1:E:231:ARG:HG3	1.84	0.59
1:N:419:LEU:CD2	1:N:500:THR:HG21	2.32	0.59
1:D:194:GLN:HB2	1:D:331:THR:HB	1.85	0.59
1:N:421:ARG:HD2	1:N:474:GLY:O	2.02	0.59
1:H:496:PRO:HB2	1:H:499:VAL:HG13	1.84	0.59
1:I:73:MET:SD	1:I:73:MET:CB	2.90	0.59
1:J:404:ARG:HH11	1:J:404:ARG:CG	2.15	0.59
1:B:260:ALA:O	1:B:264:VAL:HG23	2.02	0.59
1:C:351:GLN:HA	1:C:354:GLU:HG2	1.83	0.59
1:F:77:VAL:HG23	1:F:92:ALA:HB1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.42	0.59
1:A:486:GLY:CA	1:A:491:MET:HE2	2.32	0.59
1:C:28:LYS:HD2	1:C:453:GLN:CD	2.28	0.59
1:E:91:THR:O	1:E:92:ALA:C	2.44	0.59
1:C:288:MET:HG3	1:C:368:ARG:HD2	1.83	0.59
1:C:486:GLY:CA	1:C:491:MET:HE2	2.32	0.59
1:D:383:ALA:HB1	1:D:388:GLU:HB3	1.85	0.59
1:H:428:ASP:O	1:H:429:LEU:C	2.45	0.59
1:J:123:ALA:HB2	1:J:440:ILE:HG23	1.85	0.59
1:K:296:THR:HB	1:K:319:GLN:H	1.67	0.59
1:L:72:GLN:HA	1:L:72:GLN:NE2	2.17	0.59
1:L:223:ALA:O	1:L:251:ALA:HA	2.03	0.59
2:O:84:LEU:N	2:O:84:LEU:HD12	2.17	0.59
1:A:489:ILE:HD13	1:A:494:LEU:HD22	1.83	0.59
1:C:153:ASN:O	1:C:154:SER:HB2	2.03	0.59
1:C:302:SER:H	1:C:307:MET:HE3	1.68	0.59
1:C:409:GLU:OE2	1:C:501:ARG:NH2	2.27	0.59
1:C:409:GLU:CD	1:C:501:ARG:HH21	2.10	0.59
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.83	0.59
1:G:198:GLY:O	1:G:276:VAL:HG12	2.02	0.59
1:G:486:GLY:HA3	1:G:491:MET:HE2	1.85	0.59
1:I:284:ARG:HH11	1:I:364:LYS:HD2	1.67	0.59
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.83	0.59
1:E:18:ARG:HB3	1:E:18:ARG:NH1	2.15	0.59
1:F:345:ARG:HA	1:F:348:GLN:HE21	1.67	0.59
1:G:452:ARG:HG2	1:G:452:ARG:NH1	2.18	0.59
2:Q:16:GLU:HB2	2:Q:19:THR:OG1	2.03	0.59
1:H:284:ARG:O	1:H:288:MET:HG3	2.02	0.59
1:I:149:THR:CG2	1:I:156:GLU:HA	2.32	0.59
1:I:319:GLN:O	1:I:336:VAL:HG23	2.03	0.59
1:N:131:LEU:HD12	1:N:422:VAL:HG11	1.84	0.59
2:Q:47:ARG:HD2	2:Q:49:LEU:HB2	1.85	0.59
1:A:18:ARG:HB3	1:A:18:ARG:NH1	2.13	0.58
1:C:147:VAL:HG22	1:C:403:THR:HG22	1.83	0.58
1:I:223:ALA:O	1:I:251:ALA:HA	2.02	0.58
1:J:302:SER:H	1:J:307:MET:HE3	1.68	0.58
1:L:2:ALA:O	1:L:4:LYS:HE3	2.03	0.58
1:M:23:LEU:HD11	1:M:75:LYS:HG3	1.85	0.58
1:N:433:ASN:OD1	1:N:435:ASP:HB2	2.03	0.58
1:B:486:GLY:HA3	1:B:491:MET:CE	2.33	0.58
1:D:486:GLY:CA	1:D:491:MET:HE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:VAL:HG13	1:E:74:VAL:HG11	1.85	0.58
1:J:213:VAL:HB	1:J:325:ILE:CG1	2.32	0.58
1:L:64:ASP:C	1:L:65:LYS:O	2.39	0.58
1:D:23:LEU:C	1:D:23:LEU:CD1	2.76	0.58
1:F:76:GLU:OE1	1:G:387:VAL:HG22	2.02	0.58
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.85	0.58
1:E:351:GLN:HA	1:E:354:GLU:HG2	1.85	0.58
1:H:106:ALA:HA	1:H:111:MET:HE3	1.83	0.58
1:I:87:ASP:HB3	1:I:499:VAL:HG21	1.84	0.58
1:I:138:CYS:SG	1:I:144:ILE:HD13	2.44	0.58
1:J:8:PHE:O	1:J:9:GLY:C	2.45	0.58
1:K:66:PHE:H	1:K:69:MET:HG3	1.67	0.58
1:K:149:THR:CG2	1:K:156:GLU:HA	2.33	0.58
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.68	0.58
1:K:65:LYS:O	1:K:66:PHE:CB	2.36	0.58
1:L:149:THR:CG2	1:L:156:GLU:HA	2.33	0.58
1:L:419:LEU:HD21	1:L:500:THR:HG23	1.86	0.58
1:A:130:GLU:HB3	1:A:422:VAL:HB	1.86	0.58
1:B:261:THR:HG23	2:P:29:GLY:H	1.68	0.58
1:D:147:VAL:HG22	1:D:403:THR:HG22	1.83	0.58
1:F:69:MET:O	1:F:73:MET:HG3	2.04	0.58
1:K:69:MET:CE	1:K:522:THR:HB	2.34	0.58
1:L:421:ARG:HD2	1:L:474:GLY:O	2.03	0.58
1:M:138:CYS:SG	1:M:144:ILE:HD13	2.43	0.58
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.86	0.58
1:B:394:ALA:O	1:B:398:ASP:HB2	2.04	0.58
1:I:193:MET:CE	1:I:195:PHE:HD1	2.17	0.58
1:K:102:GLU:HB3	1:K:442:VAL:HG22	1.86	0.58
1:K:325:ILE:HG22	1:K:330:THR:HA	1.85	0.58
1:L:259:LEU:O	1:L:263:VAL:HG23	2.03	0.58
1:N:65:LYS:HA	5:N:532:HOH:O	2.03	0.58
1:K:217:SER:N	1:K:218:PRO:CD	2.67	0.58
1:L:96:ALA:O	1:L:100:ILE:HG13	2.04	0.58
1:N:223:ALA:O	1:N:251:ALA:HA	2.03	0.58
1:E:443:ALA:O	1:E:447:MET:HE3	2.04	0.58
1:F:20:VAL:HG13	1:F:74:VAL:HG11	1.86	0.58
1:I:419:LEU:CD2	1:I:500:THR:HG21	2.33	0.58
1:J:145:ALA:O	1:J:149:THR:HG23	2.02	0.58
1:K:193:MET:CE	1:K:195:PHE:HD1	2.17	0.58
2:T:47:ARG:HD2	2:T:49:LEU:HB2	1.86	0.58
1:F:486:GLY:HA3	1:F:491:MET:CE	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:429:LEU:O	1:G:430:ARG:HG2	2.04	0.57
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.86	0.57
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.86	0.57
1:B:497:THR:N	5:B:606:HOH:O	2.36	0.57
1:C:54:VAL:O	1:C:58:ARG:HG2	2.03	0.57
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.85	0.57
1:G:510:VAL:CG2	1:G:514:MET:CE	2.80	0.57
1:H:123:ALA:HB2	1:H:440:ILE:HG23	1.86	0.57
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.85	0.57
1:E:394:ALA:O	1:E:398:ASP:HB2	2.04	0.57
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.85	0.57
1:H:385:THR:HG23	1:H:388:GLU:HB2	1.86	0.57
1:H:412:VAL:HG23	1:H:418:ALA:HB2	1.86	0.57
1:L:173:GLY:O	1:L:404:ARG:NH2	2.36	0.57
1:N:15:LYS:HB3	1:N:66:PHE:HB3	1.86	0.57
1:A:268:ARG:HH22	2:O:20:LYS:HZ2	1.52	0.57
1:M:179:ASP:OD1	1:M:393:LYS:HD2	2.05	0.57
1:N:418:ALA:HB3	5:N:538:HOH:O	2.04	0.57
2:S:84:LEU:HD12	2:S:84:LEU:N	2.18	0.57
1:A:383:ALA:HB1	1:A:388:GLU:HB3	1.85	0.57
1:B:383:ALA:HB1	1:B:388:GLU:HB3	1.85	0.57
1:B:430:ARG:HG2	1:B:430:ARG:NH1	2.00	0.57
1:E:150:ILE:HD13	1:E:493:ILE:HA	1.87	0.57
1:G:510:VAL:O	1:G:511:ALA:C	2.47	0.57
1:H:145:ALA:O	1:H:149:THR:HG23	2.04	0.57
1:A:194:GLN:HB2	1:A:331:THR:HB	1.87	0.57
1:F:414:GLY:HA2	1:F:495:ASP:OD2	2.04	0.57
1:H:143:ALA:O	1:H:146:GLN:HB3	2.04	0.57
1:I:497:THR:O	1:I:498:LYS:C	2.47	0.57
1:L:77:VAL:HG22	1:L:506:TYR:HD1	1.70	0.57
1:A:394:ALA:O	1:A:398:ASP:HB2	2.04	0.57
1:C:28:LYS:O	1:C:29:VAL:C	2.45	0.57
1:G:28:LYS:C	1:G:30:THR:N	2.56	0.57
1:L:43:SER:HB3	1:L:44:PHE:CD1	2.39	0.57
1:L:428:ASP:O	1:L:429:LEU:C	2.48	0.57
1:M:65:LYS:O	1:M:66:PHE:CB	2.30	0.57
1:E:77:VAL:HG23	1:E:92:ALA:HB1	1.86	0.57
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.87	0.57
1:H:43:SER:HB3	1:H:44:PHE:CD1	2.40	0.57
1:A:16:MET:CE	1:A:16:MET:CG	2.82	0.57
1:B:63:GLU:HG3	1:B:63:GLU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:VAL:CG2	1:E:514:MET:HE2	2.32	0.57
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.87	0.57
1:F:522:THR:OG1	1:F:523:ASP:N	2.33	0.57
1:H:326:ASN:HB2	1:H:329:THR:H	1.69	0.57
1:J:476:TYR:HA	1:J:486:GLY:O	2.04	0.57
1:L:125:THR:HA	5:L:529:HOH:O	2.04	0.57
1:M:38:VAL:HG22	1:N:519:CYS:HB3	1.86	0.57
1:B:114:MET:O	1:B:114:MET:HE3	2.05	0.57
1:D:324:VAL:HB	1:D:331:THR:HG23	1.87	0.57
1:E:404:ARG:HH11	1:E:404:ARG:HG3	1.70	0.57
1:H:124:VAL:HB	5:H:527:HOH:O	2.04	0.57
1:J:217:SER:N	1:J:218:PRO:CD	2.68	0.57
1:L:49:ILE:CD1	1:M:73:MET:HE3	2.34	0.57
1:M:223:ALA:O	1:M:251:ALA:HA	2.05	0.57
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.86	0.56
1:D:18:ARG:NH1	1:D:18:ARG:HG2	2.20	0.56
1:D:150:ILE:HD13	1:D:493:ILE:HA	1.87	0.56
1:D:419:LEU:HG	1:D:447:MET:HG2	1.86	0.56
1:F:16:MET:O	1:F:20:VAL:HG23	2.05	0.56
1:M:11:ASP:O	1:M:12:ALA:C	2.46	0.56
2:U:47:ARG:HD2	2:U:49:LEU:HB2	1.86	0.56
1:D:33:PRO:HA	1:D:153:ASN:ND2	2.18	0.56
2:S:41:LEU:O	2:S:61:VAL:HG13	2.05	0.56
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.88	0.56
1:A:419:LEU:HG	1:A:447:MET:HG2	1.88	0.56
1:C:74:VAL:HG13	1:C:514:MET:HE1	1.88	0.56
1:C:429:LEU:O	1:C:430:ARG:HG2	2.05	0.56
1:D:16:MET:O	1:D:20:VAL:HG23	2.05	0.56
1:E:419:LEU:HG	1:E:447:MET:HG2	1.87	0.56
1:E:451:LEU:HD23	1:E:451:LEU:C	2.31	0.56
1:G:28:LYS:O	1:G:30:THR:N	2.38	0.56
1:G:432:GLN:NE2	1:G:436:GLN:HE22	2.04	0.56
1:I:32:GLY:HA2	1:I:454:ILE:HG23	1.86	0.56
1:M:413:ALA:HB1	1:M:417:VAL:HB	1.85	0.56
1:N:13:ARG:HD2	1:N:104:LEU:HD11	1.88	0.56
1:N:66:PHE:N	5:N:532:HOH:O	2.34	0.56
1:B:351:GLN:HA	1:B:354:GLU:HG2	1.86	0.56
1:D:100:ILE:O	1:D:101:THR:C	2.44	0.56
1:D:326:ASN:HD22	1:D:329:THR:HB	1.71	0.56
1:F:404:ARG:HH11	1:F:404:ARG:HG3	1.69	0.56
1:G:260:ALA:O	1:G:264:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:LYS:HB3	1:I:66:PHE:HB3	1.88	0.56
1:J:43:SER:HB3	1:J:44:PHE:HD1	1.71	0.56
1:J:223:ALA:O	1:J:251:ALA:HA	2.05	0.56
2:P:16:GLU:HB2	2:P:19:THR:OG1	2.06	0.56
2:U:16:GLU:HB2	2:U:19:THR:OG1	2.06	0.56
1:C:381:VAL:HG11	1:C:392:LYS:CG	2.35	0.56
1:C:383:ALA:HB1	1:C:388:GLU:HB3	1.88	0.56
1:D:351:GLN:HA	1:D:354:GLU:HG2	1.87	0.56
1:F:417:VAL:O	1:F:418:ALA:C	2.47	0.56
1:G:18:ARG:HH11	1:G:18:ARG:HB3	1.71	0.56
1:G:351:GLN:HA	1:G:354:GLU:HG2	1.88	0.56
2:U:78:ILE:HD13	2:U:83:VAL:HG21	1.87	0.56
1:H:443:ALA:O	1:H:447:MET:HG3	2.05	0.56
1:L:47:PRO:CG	1:M:73:MET:HG3	2.35	0.56
1:B:23:LEU:CD1	1:B:23:LEU:C	2.79	0.56
1:B:198:GLY:O	1:B:276:VAL:HG12	2.06	0.56
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.87	0.56
1:D:510:VAL:O	1:D:511:ALA:C	2.46	0.56
1:H:66:PHE:N	5:H:528:HOH:O	2.37	0.56
1:B:324:VAL:HB	1:B:331:THR:HG23	1.87	0.56
1:G:414:GLY:HA2	1:G:495:ASP:OD2	2.06	0.56
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.87	0.56
1:L:433:ASN:OD1	1:L:435:ASP:HB2	2.06	0.56
1:M:218:PRO:HG3	1:M:323:VAL:HG22	1.88	0.56
1:M:428:ASP:O	1:M:429:LEU:C	2.48	0.56
1:N:32:GLY:HA2	1:N:454:ILE:HG23	1.88	0.56
2:T:16:GLU:HB2	2:T:19:THR:OG1	2.06	0.56
1:B:510:VAL:HG12	1:C:385:THR:HG21	1.88	0.56
1:H:173:GLY:O	1:H:404:ARG:NH2	2.38	0.56
1:M:102:GLU:OE2	1:M:445:ARG:NH1	2.39	0.56
1:C:324:VAL:HB	1:C:331:THR:HG23	1.88	0.56
1:F:394:ALA:O	1:F:398:ASP:HB2	2.04	0.56
1:G:42:LYS:HG2	1:G:44:PHE:CE2	2.41	0.56
1:G:383:ALA:HB1	1:G:388:GLU:HB3	1.87	0.55
1:H:24:ALA:HA	1:H:27:VAL:HG12	1.88	0.55
1:K:19:GLY:HA3	1:K:67:GLU:O	2.06	0.55
1:N:323:VAL:HG12	1:N:332:ILE:HA	1.88	0.55
1:G:18:ARG:CG	1:G:18:ARG:NH1	2.50	0.55
1:H:494:LEU:HD23	1:H:494:LEU:C	2.30	0.55
1:J:24:ALA:HA	1:J:27:VAL:HG12	1.88	0.55
1:K:262:LEU:HD22	1:K:273:VAL:HG11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ARG:HG2	1:B:452:ARG:NH1	2.21	0.55
1:I:145:ALA:O	1:I:149:THR:HG23	2.05	0.55
1:J:15:LYS:HB3	1:J:66:PHE:HB3	1.89	0.55
1:J:30:THR:HB	1:J:51:LYS:O	2.06	0.55
1:A:385:THR:OG1	1:A:388:GLU:HB2	2.07	0.55
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.89	0.55
1:D:105:LYS:HD3	1:K:110:GLY:O	2.07	0.55
1:I:66:PHE:H	1:I:69:MET:HG3	1.72	0.55
1:A:16:MET:O	1:A:20:VAL:HG23	2.07	0.55
1:A:456:LEU:HD13	1:A:462:PRO:CG	2.36	0.55
1:C:381:VAL:CG1	1:C:392:LYS:HG3	2.36	0.55
1:E:153:ASN:O	1:E:154:SER:HB2	2.06	0.55
1:F:473:ASP:O	1:F:474:GLY:C	2.47	0.55
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.87	0.55
1:I:16:MET:SD	1:I:514:MET:HG2	2.47	0.55
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.88	0.55
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.88	0.55
1:D:452:ARG:HG2	1:D:452:ARG:HH11	1.71	0.55
1:H:16:MET:HG3	1:H:520:MET:SD	2.46	0.55
1:K:428:ASP:O	1:K:429:LEU:C	2.49	0.55
1:L:131:LEU:HD13	1:L:422:VAL:HG11	1.87	0.55
1:L:392:LYS:O	1:L:396:VAL:HG23	2.07	0.55
1:C:121:ASP:O	1:C:122:LYS:C	2.44	0.55
1:E:383:ALA:HB1	1:E:388:GLU:HB3	1.88	0.55
1:G:381:VAL:HG12	1:G:392:LYS:HG2	1.89	0.55
1:L:419:LEU:HD21	1:L:500:THR:HG22	1.85	0.55
1:M:149:THR:CG2	1:M:156:GLU:HA	2.37	0.55
2:P:84:LEU:HD12	2:P:84:LEU:N	2.22	0.55
1:D:18:ARG:HH11	1:D:18:ARG:HG2	1.72	0.55
1:D:80:LYS:O	1:D:81:ALA:C	2.49	0.55
1:D:501:ARG:HD3	1:D:505:GLN:OE1	2.07	0.55
1:F:504:LEU:O	1:F:504:LEU:HD22	2.07	0.55
1:J:173:GLY:O	1:J:404:ARG:NH2	2.37	0.55
1:K:145:ALA:O	1:K:149:THR:HG23	2.07	0.55
1:N:366:GLN:HA	1:N:369:VAL:HG22	1.88	0.55
1:G:324:VAL:HB	1:G:331:THR:HG23	1.88	0.55
1:G:419:LEU:HG	1:G:447:MET:HG2	1.88	0.55
1:H:47:PRO:HG2	1:I:73:MET:HG3	1.89	0.55
1:C:95:LEU:O	1:C:99:ILE:HG13	2.07	0.55
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.42	0.55
1:F:44:PHE:HD1	1:F:44:PHE:N	1.99	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:ASP:O	5:H:527:HOH:O	2.18	0.55
1:L:193:MET:CE	1:L:195:PHE:HD1	2.20	0.55
1:L:296:THR:HB	1:L:319:GLN:H	1.72	0.55
1:N:30:THR:HB	1:N:51:LYS:O	2.07	0.55
1:N:102:GLU:OE2	1:N:445:ARG:NH1	2.39	0.55
1:F:510:VAL:HG12	1:G:385:THR:HG21	1.88	0.54
1:I:419:LEU:HD21	1:I:500:THR:HG22	1.85	0.54
1:J:32:GLY:HA2	1:J:454:ILE:CD1	2.37	0.54
1:M:30:THR:HB	1:M:51:LYS:O	2.08	0.54
1:N:69:MET:HG3	5:N:532:HOH:O	2.05	0.54
1:A:305:ILE:O	1:A:305:ILE:HG22	2.06	0.54
1:A:450:PRO:O	1:A:454:ILE:HG13	2.07	0.54
1:J:149:THR:HG21	1:J:156:GLU:HA	1.88	0.54
1:N:451:LEU:O	1:N:452:ARG:C	2.47	0.54
1:D:111:MET:CE	1:D:111:MET:CG	2.84	0.54
1:E:381:VAL:CG1	1:E:392:LYS:HG2	2.37	0.54
1:N:214:GLU:HG3	1:N:324:VAL:HG22	1.88	0.54
2:S:47:ARG:HD2	2:S:49:LEU:HB2	1.88	0.54
1:A:217:SER:N	1:A:218:PRO:HD3	2.23	0.54
1:C:198:GLY:O	1:C:276:VAL:HG12	2.07	0.54
1:C:287:ALA:O	1:C:290:GLN:HB3	2.07	0.54
1:L:214:GLU:HG3	1:L:324:VAL:HG22	1.89	0.54
1:L:426:LEU:CD1	1:L:444:LEU:HD21	2.36	0.54
1:A:267:MET:HE3	1:G:305:ILE:HG12	1.90	0.54
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.90	0.54
1:B:223:ALA:O	1:B:251:ALA:HA	2.07	0.54
1:E:487:ASN:O	1:E:491:MET:HG3	2.06	0.54
1:F:34:LYS:HD2	1:F:458:CYS:SG	2.48	0.54
1:G:64:ASP:HB3	1:G:67:GLU:HB2	1.89	0.54
1:L:36:ARG:O	1:L:51:LYS:HG2	2.06	0.54
1:L:262:LEU:HD22	1:L:273:VAL:HG11	1.88	0.54
1:L:385:THR:HG23	1:L:388:GLU:HB2	1.88	0.54
1:C:23:LEU:C	1:C:23:LEU:HD13	2.31	0.54
1:G:130:GLU:HB3	1:G:422:VAL:HB	1.90	0.54
1:I:11:ASP:O	1:I:12:ALA:C	2.48	0.54
1:J:296:THR:HB	1:J:319:GLN:H	1.73	0.54
1:N:32:GLY:HA2	1:N:454:ILE:HD13	1.89	0.54
2:R:16:GLU:HB2	2:R:19:THR:OG1	2.07	0.54
1:A:74:VAL:HG13	1:A:514:MET:HE1	1.88	0.54
1:D:44:PHE:CD1	1:D:44:PHE:N	2.61	0.54
1:E:16:MET:O	1:E:20:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:SER:H	1:F:307:MET:HE3	1.73	0.54
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.90	0.54
1:A:6:VAL:O	1:A:6:VAL:HG23	2.07	0.54
1:A:80:LYS:O	1:A:81:ALA:C	2.50	0.54
1:A:510:VAL:O	1:A:511:ALA:C	2.50	0.54
1:C:194:GLN:HB2	1:C:331:THR:HB	1.90	0.54
1:C:305:ILE:HG22	1:C:305:ILE:O	2.08	0.54
1:C:501:ARG:HD3	1:C:505:GLN:OE1	2.06	0.54
1:D:143:ALA:HA	1:D:146:GLN:NE2	2.22	0.54
1:E:302:SER:H	1:E:307:MET:HE3	1.73	0.54
1:G:114:MET:O	1:G:114:MET:HE3	2.07	0.54
1:H:476:TYR:HA	1:H:486:GLY:O	2.07	0.54
1:L:66:PHE:H	1:L:69:MET:HG3	1.72	0.54
1:M:32:GLY:HA2	1:M:454:ILE:HD13	1.88	0.54
1:N:173:GLY:O	1:N:404:ARG:NH2	2.41	0.54
1:N:217:SER:N	1:N:218:PRO:CD	2.71	0.54
1:A:252:GLU:OE1	1:A:285:ARG:NH1	2.41	0.54
1:B:130:GLU:HB3	1:B:422:VAL:HB	1.90	0.54
1:E:524:LEU:CD2	1:E:525:PRO:HD2	2.38	0.54
1:F:326:ASN:HD22	1:F:329:THR:HB	1.72	0.54
1:H:192:GLY:HA2	1:H:295:LEU:HD11	1.90	0.54
1:I:72:GLN:HE22	1:I:75:LYS:NZ	2.06	0.54
1:L:47:PRO:HG2	1:M:73:MET:CG	2.38	0.54
1:M:145:ALA:O	1:M:149:THR:HG23	2.08	0.54
1:B:443:ALA:O	1:B:447:MET:HE3	2.08	0.54
1:D:452:ARG:HG2	1:D:452:ARG:NH1	2.23	0.54
1:G:184:GLN:CD	1:G:184:GLN:H	2.15	0.54
1:I:385:THR:HG23	1:I:388:GLU:HB2	1.88	0.54
1:K:24:ALA:HA	1:K:27:VAL:HG12	1.89	0.54
1:L:102:GLU:OE2	1:L:445:ARG:NH1	2.42	0.54
1:L:342:ILE:O	1:L:346:VAL:HG23	2.08	0.54
1:N:385:THR:HG23	1:N:388:GLU:HB2	1.89	0.54
1:B:77:VAL:HG23	1:B:92:ALA:HB1	1.89	0.53
1:E:190:VAL:HG11	1:E:194:GLN:NE2	2.22	0.53
1:J:426:LEU:CD1	1:J:444:LEU:HD21	2.37	0.53
1:L:476:TYR:HA	1:L:486:GLY:O	2.07	0.53
1:N:433:ASN:CG	1:N:435:ASP:HB2	2.33	0.53
1:B:302:SER:H	1:B:307:MET:HE3	1.72	0.53
1:H:421:ARG:HD2	1:H:474:GLY:O	2.07	0.53
1:K:429:LEU:HB3	1:K:440:ILE:HG21	1.90	0.53
1:K:455:VAL:HG11	1:K:462:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:GLY:HA3	1:N:67:GLU:O	2.08	0.53
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.90	0.53
1:A:39:VAL:HB	1:G:520:MET:HG2	1.90	0.53
1:D:217:SER:N	1:D:218:PRO:HD3	2.23	0.53
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.13	0.53
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.90	0.53
1:F:385:THR:OG1	1:F:388:GLU:HB2	2.08	0.53
1:L:65:LYS:O	1:L:66:PHE:CB	2.49	0.53
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.16	0.53
1:M:169:VAL:HG13	1:M:173:GLY:HA3	1.91	0.53
1:N:429:LEU:HB3	1:N:440:ILE:HG21	1.91	0.53
2:P:47:ARG:HD2	2:P:49:LEU:HB2	1.90	0.53
1:F:18:ARG:HB2	1:F:67:GLU:HG2	1.90	0.53
1:G:121:ASP:O	1:G:122:LYS:C	2.51	0.53
1:G:194:GLN:HB2	1:G:331:THR:HB	1.91	0.53
1:H:233:MET:C	1:H:235:PRO:HD2	2.34	0.53
1:J:19:GLY:HA3	1:J:67:GLU:O	2.08	0.53
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.90	0.53
1:H:302:SER:H	1:H:307:MET:HE3	1.73	0.53
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.89	0.53
1:M:85:ALA:HB1	1:M:499:VAL:HB	1.90	0.53
1:N:66:PHE:HD1	1:N:520:MET:HE2	1.73	0.53
1:D:305:ILE:O	1:D:305:ILE:HG22	2.09	0.53
1:E:324:VAL:HB	1:E:331:THR:HG23	1.90	0.53
1:F:383:ALA:HB1	1:F:388:GLU:HB3	1.90	0.53
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.91	0.53
1:H:214:GLU:HG3	1:H:324:VAL:HG22	1.90	0.53
1:I:302:SER:H	1:I:307:MET:HE3	1.72	0.53
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.91	0.53
1:K:223:ALA:O	1:K:251:ALA:HA	2.08	0.53
1:K:494:LEU:HD23	1:K:494:LEU:C	2.32	0.53
1:B:486:GLY:CA	1:B:491:MET:HE2	2.35	0.53
1:E:82:ASN:HB2	1:E:89:THR:CG2	2.39	0.53
1:G:147:VAL:HG22	1:G:403:THR:HG22	1.91	0.53
1:I:262:LEU:HD22	1:I:273:VAL:HG11	1.90	0.53
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.90	0.53
1:M:22:VAL:HG11	1:M:62:LEU:HD21	1.90	0.53
1:B:180:GLY:CA	5:B:604:HOH:O	2.56	0.53
1:C:100:ILE:HD11	1:C:514:MET:CE	2.38	0.53
1:C:199:TYR:HB3	1:C:325:ILE:HD11	1.91	0.53
1:C:268:ARG:HH22	2:Q:20:LYS:HZ2	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:LEU:HD23	1:C:525:PRO:HD2	1.90	0.53
1:F:261:THR:HG23	2:T:29:GLY:H	1.74	0.53
1:J:514:MET:CE	1:J:514:MET:CG	2.85	0.53
1:L:100:ILE:HD13	1:L:514:MET:SD	2.49	0.53
1:A:28:LYS:HD2	1:A:453:GLN:CD	2.34	0.53
1:B:6:VAL:HG23	1:B:6:VAL:O	2.08	0.53
1:E:35:GLY:HA3	1:E:51:LYS:HE2	1.90	0.53
1:E:217:SER:N	1:E:218:PRO:HD3	2.24	0.53
1:F:217:SER:N	1:F:218:PRO:HD3	2.24	0.53
1:H:217:SER:N	1:H:218:PRO:CD	2.72	0.53
1:I:218:PRO:HG3	1:I:323:VAL:HG22	1.90	0.53
1:L:102:GLU:HB3	1:L:442:VAL:HG22	1.91	0.53
1:A:113:PRO:O	1:A:114:MET:C	2.48	0.53
1:E:305:ILE:HG12	1:F:267:MET:HE3	1.90	0.53
1:G:287:ALA:O	1:G:290:GLN:HB3	2.08	0.53
1:H:223:ALA:O	1:H:251:ALA:HA	2.08	0.53
1:I:24:ALA:HA	1:I:27:VAL:HG12	1.91	0.53
1:M:426:LEU:CD1	1:M:444:LEU:HD21	2.39	0.53
2:O:47:ARG:HD2	2:O:49:LEU:HB2	1.89	0.53
1:D:42:LYS:HG2	1:D:44:PHE:CE2	2.44	0.52
1:G:124:VAL:HG13	1:G:504:LEU:HD13	1.91	0.52
1:I:126:ALA:CB	1:I:426:LEU:HD22	2.39	0.52
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.90	0.52
1:J:494:LEU:HD23	1:J:494:LEU:C	2.34	0.52
1:K:433:ASN:OD1	1:K:435:ASP:HB2	2.08	0.52
1:B:444:LEU:O	1:B:447:MET:HB2	2.09	0.52
1:D:74:VAL:HG13	1:D:514:MET:HE1	1.92	0.52
1:F:18:ARG:NH1	1:F:18:ARG:HB3	2.23	0.52
1:F:324:VAL:HB	1:F:331:THR:HG23	1.91	0.52
1:I:28:LYS:HD2	1:I:453:GLN:OE1	2.09	0.52
1:I:66:PHE:HD1	1:I:520:MET:HE2	1.74	0.52
1:M:494:LEU:HD23	1:M:494:LEU:C	2.35	0.52
1:N:284:ARG:NH1	1:N:364:LYS:HD2	2.22	0.52
2:R:11:ILE:HG12	2:R:85:ILE:HG12	1.91	0.52
1:A:23:LEU:C	1:A:23:LEU:CD1	2.83	0.52
1:A:76:GLU:O	1:A:80:LYS:HB2	2.09	0.52
1:A:96:ALA:O	1:A:97:GLN:C	2.52	0.52
1:B:44:PHE:HD1	1:B:44:PHE:N	1.92	0.52
1:B:199:TYR:HB3	1:B:325:ILE:HD11	1.91	0.52
1:D:76:GLU:OE1	1:E:387:VAL:HG22	2.10	0.52
1:F:28:LYS:O	1:F:30:THR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.91	0.52
1:A:324:VAL:HB	1:A:331:THR:HG23	1.90	0.52
1:B:28:LYS:C	1:B:30:THR:N	2.67	0.52
1:D:394:ALA:O	1:D:398:ASP:HB2	2.09	0.52
1:H:36:ARG:O	1:H:51:LYS:HG2	2.10	0.52
1:J:16:MET:HG3	1:J:520:MET:SD	2.49	0.52
1:J:437:ASN:HA	1:J:440:ILE:HD12	1.90	0.52
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.91	0.52
1:D:287:ALA:O	1:D:290:GLN:HB3	2.10	0.52
1:D:430:ARG:NH1	1:D:430:ARG:CG	2.64	0.52
1:E:444:LEU:O	1:E:447:MET:HB2	2.10	0.52
1:G:302:SER:H	1:G:307:MET:HE3	1.75	0.52
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.91	0.52
1:K:302:SER:H	1:K:307:MET:HE3	1.75	0.52
1:M:404:ARG:CG	1:M:404:ARG:NH1	2.66	0.52
1:D:302:SER:H	1:D:307:MET:HE3	1.75	0.52
1:F:42:LYS:HG2	1:F:44:PHE:CD2	2.45	0.52
1:J:164:GLU:O	1:J:167:ASP:HB3	2.10	0.52
1:K:106:ALA:CA	1:K:111:MET:HE3	2.38	0.52
1:N:145:ALA:O	1:N:149:THR:HG23	2.10	0.52
1:E:194:GLN:HB2	1:E:331:THR:HB	1.92	0.52
1:E:287:ALA:O	1:E:290:GLN:HB3	2.10	0.52
1:F:96:ALA:O	1:F:97:GLN:C	2.51	0.52
1:H:65:LYS:CA	5:H:528:HOH:O	2.55	0.52
1:H:433:ASN:OD1	1:H:435:ASP:HB2	2.10	0.52
1:I:441:LYS:O	1:I:442:VAL:C	2.53	0.52
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.92	0.52
1:J:413:ALA:HB1	1:J:417:VAL:HB	1.91	0.52
1:M:437:ASN:HA	1:M:440:ILE:HD12	1.91	0.52
1:M:449:ALA:N	1:M:450:PRO:CD	2.73	0.52
1:N:149:THR:HG21	1:N:156:GLU:HA	1.90	0.52
1:B:217:SER:N	1:B:218:PRO:HD3	2.25	0.52
1:B:419:LEU:HG	1:B:447:MET:HG2	1.92	0.52
1:G:69:MET:O	1:G:73:MET:HG3	2.10	0.52
1:G:288:MET:O	1:G:291:ASP:HB2	2.10	0.52
1:H:455:VAL:HG11	1:H:461:GLU:O	2.09	0.52
1:J:217:SER:N	1:J:218:PRO:HD3	2.25	0.52
1:M:262:LEU:HD22	1:M:273:VAL:HG11	1.91	0.52
2:Q:37:ARG:HG2	2:Q:37:ARG:HH11	1.74	0.52
1:J:77:VAL:HG22	1:J:506:TYR:HD1	1.74	0.52
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:ARG:HG2	1:C:452:ARG:NH1	2.26	0.52
1:H:342:ILE:O	1:H:346:VAL:HG23	2.10	0.52
1:H:452:ARG:NH1	1:H:452:ARG:CG	2.69	0.52
1:I:143:ALA:O	1:I:146:GLN:HB3	2.10	0.52
1:J:10:ASN:O	1:J:11:ASP:C	2.52	0.52
1:D:199:TYR:HB3	1:D:325:ILE:HD11	1.92	0.51
1:F:487:ASN:O	1:F:491:MET:HG3	2.10	0.51
1:J:323:VAL:HG12	1:J:332:ILE:HA	1.92	0.51
1:J:492:GLY:C	1:J:493:ILE:HD13	2.35	0.51
1:L:16:MET:SD	1:L:514:MET:HG2	2.50	0.51
1:L:366:GLN:HA	1:L:369:VAL:HG22	1.92	0.51
1:A:28:LYS:O	1:A:29:VAL:C	2.48	0.51
1:A:147:VAL:HG22	1:A:403:THR:HG22	1.92	0.51
1:A:504:LEU:HD22	1:A:504:LEU:C	2.34	0.51
1:E:511:ALA:O	1:E:515:ILE:HG23	2.11	0.51
1:F:194:GLN:HB2	1:F:331:THR:HB	1.92	0.51
1:L:123:ALA:HB2	1:L:440:ILE:HG23	1.92	0.51
1:L:419:LEU:CD2	1:L:500:THR:HG21	2.38	0.51
1:C:100:ILE:O	1:C:101:THR:C	2.51	0.51
1:D:102:GLU:HB3	1:D:442:VAL:HG22	1.91	0.51
1:E:44:PHE:HD1	1:E:44:PHE:N	1.96	0.51
1:H:234:LEU:N	1:H:235:PRO:HD2	2.25	0.51
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.92	0.51
1:K:16:MET:O	1:K:20:VAL:HG12	2.10	0.51
1:K:522:THR:OG1	1:K:523:ASP:N	2.43	0.51
1:L:323:VAL:HG12	1:L:332:ILE:HA	1.91	0.51
1:M:214:GLU:HG3	1:M:324:VAL:HG22	1.93	0.51
1:M:296:THR:HB	1:M:319:GLN:H	1.75	0.51
1:M:418:ALA:O	1:M:422:VAL:HG13	2.09	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.10	0.51
1:B:181:THR:N	5:B:604:HOH:O	2.29	0.51
1:B:305:ILE:O	1:B:305:ILE:HG22	2.11	0.51
1:B:429:LEU:O	1:B:430:ARG:HG2	2.11	0.51
1:C:217:SER:N	1:C:218:PRO:HD3	2.25	0.51
1:C:326:ASN:HD22	1:C:329:THR:HB	1.76	0.51
1:G:217:SER:N	1:G:218:PRO:HD3	2.26	0.51
1:H:149:THR:HG21	1:H:156:GLU:HA	1.91	0.51
1:H:262:LEU:HD22	1:H:273:VAL:HG11	1.92	0.51
1:I:524:LEU:HD23	1:I:525:PRO:HD2	1.91	0.51
1:K:351:GLN:HA	1:K:354:GLU:HG2	1.93	0.51
1:K:453:GLN:O	1:K:454:ILE:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:326:ASN:ND2	1:M:329:THR:HB	2.25	0.51
1:A:91:THR:O	1:A:92:ALA:C	2.52	0.51
1:A:198:GLY:O	1:A:276:VAL:HG12	2.11	0.51
1:C:82:ASN:HB2	1:C:89:THR:CG2	2.40	0.51
1:E:259:LEU:O	1:E:263:VAL:HG23	2.11	0.51
1:E:305:ILE:HG22	1:E:305:ILE:O	2.10	0.51
1:H:412:VAL:CG2	1:H:418:ALA:HB2	2.41	0.51
1:J:36:ARG:O	1:J:51:LYS:HG2	2.11	0.51
1:L:145:ALA:O	1:L:149:THR:HG23	2.09	0.51
1:N:218:PRO:HG3	1:N:323:VAL:HG22	1.92	0.51
2:O:78:ILE:HD13	2:O:83:VAL:HG21	1.91	0.51
1:D:487:ASN:O	1:D:491:MET:HG3	2.10	0.51
1:E:261:THR:HG23	2:S:29:GLY:H	1.76	0.51
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.93	0.51
1:H:138:CYS:SG	1:H:144:ILE:HD13	2.51	0.51
1:J:16:MET:O	1:J:20:VAL:CG1	2.57	0.51
1:K:66:PHE:N	1:K:69:MET:HE3	2.26	0.51
1:M:13:ARG:HD2	1:M:104:LEU:HD11	1.92	0.51
1:A:223:ALA:O	1:A:251:ALA:HA	2.11	0.51
1:A:387:VAL:HG22	1:G:76:GLU:OE1	2.10	0.51
1:A:443:ALA:O	1:A:444:LEU:C	2.52	0.51
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.46	0.51
1:E:326:ASN:HD22	1:E:329:THR:HB	1.75	0.51
1:G:326:ASN:HD22	1:G:329:THR:HB	1.74	0.51
1:H:361:ASP:O	1:H:365:LEU:HG	2.10	0.51
1:J:262:LEU:HD22	1:J:273:VAL:HG11	1.91	0.51
1:K:64:ASP:HB3	1:K:67:GLU:HB2	1.92	0.51
1:K:342:ILE:O	1:K:346:VAL:HG23	2.10	0.51
2:R:47:ARG:HD2	2:R:49:LEU:HB2	1.92	0.51
2:U:11:ILE:HG12	2:U:85:ILE:HG12	1.92	0.51
1:B:381:VAL:HG11	1:B:392:LYS:CG	2.31	0.51
1:C:522:THR:OG1	1:C:523:ASP:N	2.44	0.51
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.93	0.51
1:E:288:MET:HG3	1:E:368:ARG:CD	2.41	0.51
1:H:351:GLN:HA	1:H:354:GLU:HG2	1.93	0.51
1:J:433:ASN:OD1	1:J:435:ASP:HB2	2.10	0.51
1:E:18:ARG:HB2	1:E:67:GLU:HG2	1.91	0.51
1:E:42:LYS:HG2	1:E:44:PHE:CE2	2.45	0.51
1:G:28:LYS:C	1:G:30:THR:H	2.18	0.51
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.51	0.51
1:K:66:PHE:HD1	1:K:520:MET:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:TYR:HA	1:K:276:VAL:HG12	1.93	0.51
5:K:536:HOH:O	1:L:65:LYS:HB3	2.10	0.51
1:L:24:ALA:HA	1:L:27:VAL:HG12	1.92	0.51
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.08	0.51
1:D:385:THR:OG1	1:D:388:GLU:HB2	2.11	0.51
1:F:452:ARG:HG2	1:F:452:ARG:NH1	2.25	0.51
1:H:417:VAL:HG21	1:H:488:MET:HG3	1.93	0.51
1:J:18:ARG:O	1:J:19:GLY:C	2.52	0.51
1:K:7:LYS:HD2	1:K:66:PHE:CE2	2.46	0.51
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.93	0.51
1:N:428:ASP:O	1:N:429:LEU:C	2.54	0.51
1:A:270:ILE:CD1	2:O:27:LEU:HB2	2.40	0.50
1:B:82:ASN:HB2	1:B:89:THR:CG2	2.41	0.50
1:C:430:ARG:NH1	1:C:430:ARG:CG	2.74	0.50
1:D:510:VAL:HG12	1:E:385:THR:HG21	1.93	0.50
1:E:130:GLU:HB3	1:E:422:VAL:HB	1.94	0.50
1:F:510:VAL:O	1:F:511:ALA:C	2.52	0.50
1:J:77:VAL:HG22	1:J:506:TYR:CD1	2.46	0.50
1:J:284:ARG:O	1:J:288:MET:HG3	2.11	0.50
1:L:293:ALA:HB2	1:L:300:VAL:HG23	1.93	0.50
1:N:106:ALA:O	1:N:107:VAL:C	2.54	0.50
1:E:150:ILE:CD1	1:E:493:ILE:HA	2.41	0.50
1:F:259:LEU:O	1:F:263:VAL:HG23	2.10	0.50
1:G:522:THR:OG1	1:G:523:ASP:N	2.39	0.50
1:J:218:PRO:HG3	1:J:323:VAL:HG22	1.92	0.50
1:M:43:SER:HB3	1:M:44:PHE:CD1	2.47	0.50
1:M:326:ASN:HB2	1:M:329:THR:H	1.75	0.50
2:T:7:HIS:O	2:T:7:HIS:ND1	2.42	0.50
1:C:223:ALA:O	1:C:251:ALA:HA	2.11	0.50
1:C:510:VAL:O	1:C:511:ALA:C	2.51	0.50
1:D:455:VAL:HG21	1:D:465:VAL:HG11	1.92	0.50
1:F:28:LYS:O	1:F:29:VAL:C	2.55	0.50
1:F:198:GLY:O	1:F:276:VAL:HG12	2.12	0.50
1:F:287:ALA:O	1:F:290:GLN:HB3	2.10	0.50
1:G:80:LYS:O	1:G:81:ALA:C	2.53	0.50
1:I:197:ARG:HD2	1:I:277:LYS:HB2	1.92	0.50
1:L:213:VAL:HB	1:L:325:ILE:CG1	2.38	0.50
1:M:412:VAL:HG23	1:M:418:ALA:HB2	1.93	0.50
2:T:84:LEU:N	2:T:84:LEU:HD12	2.25	0.50
1:A:486:GLY:HA3	1:A:491:MET:CE	2.37	0.50
1:F:124:VAL:HG13	1:F:504:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:LYS:HG2	1:G:44:PHE:CD2	2.47	0.50
1:G:385:THR:OG1	1:G:388:GLU:HB2	2.11	0.50
1:K:77:VAL:HG11	1:K:510:VAL:HB	1.93	0.50
1:K:462:PRO:O	1:K:463:SER:C	2.54	0.50
1:L:217:SER:N	1:L:218:PRO:CD	2.74	0.50
2:O:16:GLU:HB2	2:O:19:THR:OG1	2.12	0.50
1:B:511:ALA:O	1:B:512:GLY:C	2.52	0.50
1:G:23:LEU:C	1:G:23:LEU:HD12	2.37	0.50
1:L:192:GLY:HA2	1:L:295:LEU:HD11	1.94	0.50
1:M:433:ASN:OD1	1:M:435:ASP:HB2	2.12	0.50
1:N:43:SER:HB3	1:N:44:PHE:CD1	2.46	0.50
1:A:260:ALA:O	1:A:264:VAL:HG23	2.11	0.50
1:B:28:LYS:O	1:B:29:VAL:C	2.53	0.50
1:C:270:ILE:HG12	2:Q:27:LEU:HD13	1.94	0.50
1:C:399:ALA:O	1:C:400:LEU:C	2.54	0.50
1:C:452:ARG:HH12	1:C:463:SER:HB3	1.76	0.50
1:E:339:GLU:HA	1:E:342:ILE:HB	1.93	0.50
1:F:502:SER:O	1:F:503:ALA:C	2.55	0.50
1:I:426:LEU:CD1	1:I:444:LEU:HD21	2.41	0.50
1:K:43:SER:HB3	1:K:44:PHE:CD1	2.46	0.50
1:K:361:ASP:O	1:K:365:LEU:HG	2.11	0.50
1:L:475:ASN:ND2	1:L:489:ILE:HD12	2.27	0.50
1:M:47:PRO:CG	1:N:73:MET:HG3	2.41	0.50
1:M:217:SER:N	1:M:218:PRO:CD	2.74	0.50
1:A:238:GLU:OE2	2:O:24:GLY:N	2.45	0.50
1:B:153:ASN:O	1:B:154:SER:HB2	2.11	0.50
1:B:414:GLY:HA2	1:B:495:ASP:OD2	2.11	0.50
1:B:451:LEU:HD23	1:B:451:LEU:C	2.37	0.50
1:C:524:LEU:CD2	1:C:525:PRO:HD2	2.42	0.50
1:F:82:ASN:ND2	1:F:86:GLY:HA2	2.27	0.50
1:F:456:LEU:HD13	1:F:462:PRO:CG	2.42	0.50
1:H:21:ASN:O	1:H:25:ASP:N	2.36	0.50
1:H:32:GLY:HA2	1:H:454:ILE:HG23	1.92	0.50
1:I:16:MET:O	1:I:20:VAL:HG12	2.11	0.50
1:K:234:LEU:N	1:K:235:PRO:HD2	2.27	0.50
1:L:217:SER:N	1:L:218:PRO:HD3	2.27	0.50
1:N:88:GLY:O	1:N:89:THR:C	2.54	0.50
1:D:28:LYS:O	1:D:29:VAL:C	2.49	0.50
1:E:95:LEU:O	1:E:99:ILE:HG13	2.12	0.50
1:E:200:LEU:HD13	1:E:254:VAL:HB	1.94	0.50
1:E:473:ASP:O	1:E:474:GLY:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:455:VAL:HG21	1:G:465:VAL:HG11	1.92	0.50
1:I:524:LEU:CD2	1:I:525:PRO:HD2	2.42	0.50
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.18	0.50
1:L:77:VAL:HG22	1:L:506:TYR:CD1	2.47	0.50
1:M:234:LEU:N	1:M:235:PRO:HD2	2.26	0.50
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.93	0.50
1:M:290:GLN:NE2	1:M:290:GLN:O	2.43	0.50
1:N:192:GLY:HA2	1:N:295:LEU:HD11	1.94	0.50
1:D:28:LYS:C	1:D:30:THR:N	2.64	0.50
1:F:402:ALA:O	1:F:405:ALA:HB3	2.12	0.50
1:H:15:LYS:HB3	1:H:66:PHE:HB3	1.94	0.50
1:I:77:VAL:HG11	1:I:510:VAL:HB	1.94	0.50
1:I:234:LEU:N	1:I:235:PRO:HD2	2.27	0.50
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.18	0.50
1:M:419:LEU:HD21	1:M:500:THR:HG22	1.90	0.50
1:N:426:LEU:CD1	1:N:444:LEU:HD21	2.42	0.50
1:D:130:GLU:HB3	1:D:422:VAL:HB	1.94	0.49
1:H:7:LYS:HD2	1:H:66:PHE:CE2	2.47	0.49
1:H:19:GLY:HA3	1:H:67:GLU:O	2.12	0.49
1:K:370:ALA:O	1:K:371:LYS:C	2.54	0.49
1:A:199:TYR:HB3	1:A:325:ILE:HD11	1.94	0.49
1:B:150:ILE:CG2	1:B:151:SER:N	2.72	0.49
1:C:130:GLU:HB3	1:C:422:VAL:HB	1.94	0.49
1:C:487:ASN:C	1:C:487:ASN:OD1	2.55	0.49
1:H:10:ASN:O	1:H:11:ASP:C	2.55	0.49
1:H:217:SER:N	1:H:218:PRO:HD3	2.26	0.49
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.94	0.49
1:I:38:VAL:HG12	1:I:40:LEU:HD13	1.92	0.49
1:I:370:ALA:O	1:I:371:LYS:C	2.54	0.49
1:L:302:SER:H	1:L:307:MET:HE3	1.77	0.49
1:N:64:ASP:OD1	1:N:65:LYS:O	2.30	0.49
1:N:126:ALA:HB1	1:N:426:LEU:HD22	1.94	0.49
1:N:143:ALA:O	1:N:146:GLN:HB3	2.13	0.49
1:N:325:ILE:HG22	1:N:330:THR:HA	1.94	0.49
2:O:37:ARG:HG2	2:O:37:ARG:HH11	1.76	0.49
2:T:11:ILE:HG12	2:T:85:ILE:HG12	1.94	0.49
1:E:305:ILE:HG23	1:F:267:MET:HE3	1.94	0.49
1:F:28:LYS:C	1:F:30:THR:N	2.68	0.49
1:F:100:ILE:HD11	1:F:514:MET:HE3	1.94	0.49
1:F:223:ALA:O	1:F:251:ALA:HA	2.12	0.49
1:F:520:MET:HG2	1:G:39:VAL:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:VAL:HG21	1:H:194:GLN:HB3	1.95	0.49
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.93	0.49
1:J:418:ALA:O	1:J:422:VAL:HG13	2.12	0.49
1:K:69:MET:HE1	1:K:522:THR:HB	1.94	0.49
1:K:135:SER:HA	1:K:412:VAL:HG12	1.94	0.49
1:M:174:VAL:HG12	1:M:376:VAL:HG13	1.94	0.49
1:A:147:VAL:O	1:A:148:GLY:C	2.53	0.49
1:C:85:ALA:O	1:C:86:GLY:C	2.51	0.49
1:C:449:ALA:N	1:C:450:PRO:CD	2.75	0.49
1:F:288:MET:HG3	1:F:368:ARG:CD	2.42	0.49
1:F:516:THR:OG1	1:G:37:ASN:ND2	2.45	0.49
1:I:217:SER:N	1:I:218:PRO:CD	2.76	0.49
1:J:361:ASP:O	1:J:365:LEU:HG	2.12	0.49
1:K:20:VAL:HG21	1:K:100:ILE:HD12	1.94	0.49
1:K:385:THR:HG23	1:K:388:GLU:HB2	1.94	0.49
1:L:455:VAL:HG11	1:L:461:GLU:O	2.11	0.49
1:N:492:GLY:C	1:N:493:ILE:HD13	2.37	0.49
2:T:37:ARG:HG2	2:T:37:ARG:HH11	1.76	0.49
1:B:23:LEU:C	1:B:23:LEU:HD13	2.38	0.49
1:F:305:ILE:O	1:F:305:ILE:HG22	2.12	0.49
1:G:223:ALA:O	1:G:251:ALA:HA	2.13	0.49
1:H:169:VAL:HG22	1:H:173:GLY:HA3	1.95	0.49
1:M:183:LEU:HD22	1:N:360:TYR:CG	2.47	0.49
2:P:11:ILE:HG12	2:P:85:ILE:HG12	1.93	0.49
2:R:67:PHE:CG	2:R:86:MET:HE2	2.48	0.49
1:A:288:MET:O	1:A:291:ASP:HB2	2.12	0.49
1:B:273:VAL:HG12	1:B:274:ALA:N	2.27	0.49
1:B:513:LEU:HB3	1:C:49:ILE:HD13	1.94	0.49
1:G:417:VAL:O	1:G:418:ALA:C	2.56	0.49
2:Q:7:HIS:O	2:Q:7:HIS:ND1	2.42	0.49
1:A:429:LEU:O	1:A:430:ARG:HG2	2.13	0.49
1:B:96:ALA:O	1:B:97:GLN:C	2.54	0.49
1:C:153:ASN:O	1:C:154:SER:CB	2.60	0.49
1:C:450:PRO:O	1:C:454:ILE:HG13	2.12	0.49
1:C:451:LEU:HD23	1:C:451:LEU:O	2.13	0.49
1:E:417:VAL:O	1:E:418:ALA:C	2.55	0.49
1:H:284:ARG:NH1	1:H:364:LYS:HD2	2.26	0.49
1:J:88:GLY:O	1:J:89:THR:C	2.55	0.49
1:J:284:ARG:NH1	1:J:364:LYS:HD2	2.25	0.49
1:K:161:LEU:HD21	1:K:185:ASP:HB3	1.95	0.49
1:K:476:TYR:HA	1:K:486:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:VAL:HG12	1:L:40:LEU:HD13	1.94	0.49
1:N:346:VAL:O	1:N:350:ARG:HB2	2.12	0.49
1:A:194:GLN:HG3	1:A:330:THR:O	2.13	0.49
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.93	0.49
1:C:147:VAL:O	1:C:150:ILE:HG22	2.12	0.49
1:F:381:VAL:HG11	1:F:392:LYS:CG	2.38	0.49
1:F:451:LEU:HD23	1:F:451:LEU:C	2.37	0.49
1:G:288:MET:HG3	1:G:368:ARG:CD	2.43	0.49
1:G:448:GLU:O	1:G:452:ARG:HD2	2.12	0.49
1:H:8:PHE:O	1:H:9:GLY:C	2.56	0.49
1:J:288:MET:CE	1:J:288:MET:CG	2.90	0.49
1:K:443:ALA:O	1:K:447:MET:HG3	2.13	0.49
1:N:25:ASP:OD1	1:N:28:LYS:HE2	2.13	0.49
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.93	0.49
2:O:23:GLY:H	2:P:80:ASN:ND2	2.09	0.49
2:S:7:HIS:O	2:S:7:HIS:ND1	2.45	0.49
2:U:84:LEU:HD12	2:U:84:LEU:N	2.27	0.49
1:A:489:ILE:CD1	1:A:494:LEU:HD22	2.43	0.49
1:G:259:LEU:O	1:G:263:VAL:HG23	2.12	0.49
1:G:305:ILE:HB	1:G:307:MET:HE2	1.95	0.49
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.95	0.49
1:L:290:GLN:NE2	1:L:293:ALA:HB3	2.28	0.49
1:M:135:SER:HA	1:M:412:VAL:HG12	1.94	0.49
1:M:361:ASP:O	1:M:365:LEU:HG	2.12	0.49
1:F:519:CYS:HB3	1:G:38:VAL:HG22	1.95	0.49
1:G:44:PHE:CD1	1:G:44:PHE:N	2.63	0.49
1:G:77:VAL:HG23	1:G:92:ALA:HB1	1.95	0.49
1:J:385:THR:HG23	1:J:388:GLU:HB2	1.94	0.49
1:K:217:SER:N	1:K:218:PRO:HD3	2.28	0.49
1:M:496:PRO:HB2	1:M:499:VAL:HG13	1.94	0.49
1:N:77:VAL:HG22	1:N:506:TYR:HD1	1.78	0.49
1:A:339:GLU:HA	1:A:342:ILE:HB	1.95	0.48
1:A:489:ILE:HD13	1:A:494:LEU:CD2	2.43	0.48
1:B:28:LYS:O	1:B:30:THR:N	2.46	0.48
1:C:288:MET:HG3	1:C:368:ARG:CD	2.43	0.48
1:K:87:ASP:HB3	1:K:499:VAL:HG21	1.95	0.48
1:K:392:LYS:O	1:K:396:VAL:HG23	2.13	0.48
1:K:444:LEU:HD23	1:K:444:LEU:HA	1.57	0.48
1:L:80:LYS:HA	1:L:83:ASP:HB2	1.94	0.48
1:L:494:LEU:HD23	1:L:494:LEU:C	2.38	0.48
1:M:75:LYS:NZ	5:M:535:HOH:O	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:161:LEU:HD21	1:M:185:ASP:HB3	1.94	0.48
1:N:412:VAL:HG23	1:N:418:ALA:HB2	1.94	0.48
1:N:496:PRO:HB2	1:N:499:VAL:HG13	1.95	0.48
2:O:7:HIS:O	2:O:7:HIS:ND1	2.46	0.48
2:U:37:ARG:HG2	2:U:37:ARG:HH11	1.78	0.48
1:A:430:ARG:NH1	1:A:430:ARG:CG	2.70	0.48
1:C:443:ALA:O	1:C:447:MET:HE3	2.13	0.48
1:D:381:VAL:HG11	1:D:392:LYS:CG	2.37	0.48
1:D:456:LEU:HD13	1:D:462:PRO:CG	2.43	0.48
1:E:513:LEU:HB3	1:F:49:ILE:HD13	1.95	0.48
1:G:194:GLN:HG3	1:G:330:THR:O	2.13	0.48
1:H:16:MET:SD	1:H:514:MET:HG2	2.53	0.48
1:H:52:ASP:C	1:H:52:ASP:OD1	2.56	0.48
1:K:36:ARG:O	1:K:51:LYS:HG2	2.13	0.48
1:L:87:ASP:HB3	1:L:499:VAL:HG21	1.95	0.48
1:M:403:THR:O	1:M:407:VAL:HG23	2.13	0.48
1:M:493:ILE:HD13	1:M:493:ILE:N	2.29	0.48
1:A:82:ASN:HB2	1:A:89:THR:HG21	1.95	0.48
1:F:28:LYS:HE3	1:F:453:GLN:NE2	2.28	0.48
1:K:233:MET:C	1:K:235:PRO:HD2	2.38	0.48
1:N:135:SER:HA	1:N:412:VAL:HG12	1.96	0.48
1:N:441:LYS:O	1:N:442:VAL:C	2.55	0.48
1:N:448:GLU:HB3	1:N:452:ARG:HD2	1.95	0.48
1:N:514:MET:CE	1:N:514:MET:CG	2.92	0.48
1:A:143:ALA:HA	1:A:146:GLN:NE2	2.28	0.48
1:B:270:ILE:HG12	2:P:27:LEU:HD13	1.96	0.48
1:C:349:ILE:HA	1:C:352:GLN:HG2	1.93	0.48
1:F:23:LEU:C	1:F:23:LEU:CD1	2.86	0.48
1:K:173:GLY:O	1:K:404:ARG:NH2	2.45	0.48
1:N:22:VAL:HG11	1:N:62:LEU:HD21	1.96	0.48
1:N:126:ALA:CB	1:N:426:LEU:HD22	2.43	0.48
1:A:302:SER:H	1:A:307:MET:HE3	1.78	0.48
1:A:404:ARG:HG3	1:A:404:ARG:NH1	2.18	0.48
1:B:82:ASN:HB2	1:B:89:THR:HG21	1.96	0.48
1:C:221:LEU:HB3	1:C:249:ILE:HD13	1.94	0.48
1:C:417:VAL:O	1:C:418:ALA:C	2.56	0.48
1:I:476:TYR:HA	1:I:486:GLY:O	2.13	0.48
1:K:143:ALA:O	1:K:146:GLN:HB3	2.13	0.48
1:L:161:LEU:HD21	1:L:185:ASP:HB3	1.94	0.48
1:M:497:THR:O	1:M:498:LYS:C	2.57	0.48
1:C:69:MET:CE	1:D:39:VAL:HG12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:ALA:O	1:E:28:LYS:HG3	2.14	0.48
1:E:430:ARG:NH1	1:E:430:ARG:CG	2.77	0.48
1:F:305:ILE:HB	1:F:307:MET:HE2	1.95	0.48
1:G:430:ARG:NH1	1:G:430:ARG:CG	2.72	0.48
1:H:80:LYS:HA	1:H:83:ASP:HB2	1.96	0.48
1:I:4:LYS:HB3	1:I:522:THR:O	2.13	0.48
1:I:83:ASP:OD2	1:I:327:LYS:HE2	2.14	0.48
1:I:452:ARG:NH1	1:I:452:ARG:CG	2.75	0.48
1:J:342:ILE:O	1:J:346:VAL:HG23	2.13	0.48
1:K:214:GLU:HG3	1:K:324:VAL:HG22	1.94	0.48
1:K:218:PRO:HG3	1:K:323:VAL:HG22	1.95	0.48
2:S:16:GLU:HB2	2:S:19:THR:OG1	2.13	0.48
1:B:221:LEU:HB3	1:B:249:ILE:HD13	1.94	0.48
1:B:288:MET:O	1:B:291:ASP:HB2	2.13	0.48
1:B:482:THR:O	1:B:484:GLU:HG2	2.13	0.48
1:C:16:MET:HE1	1:C:514:MET:HB3	1.95	0.48
1:F:162:ILE:HG21	1:F:403:THR:HG21	1.94	0.48
1:F:199:TYR:HB3	1:F:325:ILE:HD11	1.95	0.48
1:F:524:LEU:CD2	1:F:525:PRO:HD2	2.43	0.48
1:I:428:ASP:O	1:I:430:ARG:HG2	2.13	0.48
1:J:161:LEU:HD21	1:J:185:ASP:HB3	1.96	0.48
1:J:234:LEU:N	1:J:235:PRO:HD2	2.29	0.48
1:J:429:LEU:HB3	1:J:440:ILE:HG21	1.96	0.48
1:M:476:TYR:HA	1:M:486:GLY:O	2.13	0.48
1:M:524:LEU:HA	1:M:524:LEU:HD23	1.61	0.48
1:N:7:LYS:HD2	1:N:66:PHE:CE2	2.48	0.48
1:N:428:ASP:O	1:N:430:ARG:HG2	2.13	0.48
1:N:478:TYR:HB2	1:N:485:TYR:CE2	2.49	0.48
1:A:100:ILE:O	1:A:101:THR:C	2.57	0.48
1:B:194:GLN:HB2	1:B:331:THR:HB	1.95	0.48
1:D:339:GLU:HA	1:D:342:ILE:HB	1.96	0.48
1:E:76:GLU:O	1:E:80:LYS:HB2	2.14	0.48
1:E:198:GLY:O	1:E:276:VAL:HG12	2.13	0.48
1:E:288:MET:O	1:E:291:ASP:HB2	2.14	0.48
1:F:419:LEU:HG	1:F:447:MET:HG2	1.96	0.48
1:J:366:GLN:HA	1:J:369:VAL:HG22	1.95	0.48
1:M:28:LYS:HD2	1:M:453:GLN:OE1	2.13	0.48
1:M:106:ALA:HA	1:M:111:MET:CE	2.42	0.48
1:M:346:VAL:O	1:M:350:ARG:HB2	2.13	0.48
2:S:11:ILE:HG12	2:S:85:ILE:HG12	1.95	0.48
1:C:162:ILE:HG21	1:C:403:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:GLY:HA3	1:F:51:LYS:HE2	1.95	0.48
1:I:106:ALA:CA	1:I:111:MET:HE3	2.44	0.48
1:I:366:GLN:HA	1:I:369:VAL:HG22	1.95	0.48
1:J:325:ILE:HG22	1:J:330:THR:HA	1.95	0.48
1:K:293:ALA:HB2	1:K:300:VAL:HG23	1.95	0.48
1:N:77:VAL:HG11	1:N:510:VAL:CG1	2.44	0.48
1:N:293:ALA:HB2	1:N:300:VAL:HG23	1.96	0.48
2:P:17:VAL:O	2:P:17:VAL:HG12	2.14	0.48
2:R:17:VAL:O	2:R:17:VAL:HG12	2.14	0.48
1:A:39:VAL:HG23	1:G:517:THR:HG23	1.96	0.48
1:A:64:ASP:HB3	1:A:67:GLU:HB2	1.95	0.48
1:A:270:ILE:HD11	2:O:27:LEU:HB2	1.96	0.48
1:B:147:VAL:O	1:B:148:GLY:C	2.55	0.48
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.95	0.48
1:D:28:LYS:HD2	1:D:453:GLN:CD	2.38	0.48
1:H:163:ALA:O	1:H:167:ASP:HB2	2.14	0.48
1:I:342:ILE:O	1:I:346:VAL:HG23	2.14	0.48
1:J:451:LEU:O	1:J:452:ARG:C	2.54	0.48
1:M:15:LYS:HB3	1:M:66:PHE:HB3	1.96	0.48
1:N:32:GLY:CA	1:N:454:ILE:HG23	2.44	0.48
1:N:262:LEU:HD22	1:N:273:VAL:HG11	1.96	0.48
2:Q:67:PHE:CG	2:Q:86:MET:HE2	2.48	0.48
1:B:434:GLU:O	1:B:435:ASP:C	2.57	0.47
1:C:238:GLU:OE2	2:Q:23:GLY:C	2.56	0.47
1:F:102:GLU:HB3	1:F:442:VAL:HG22	1.95	0.47
1:G:394:ALA:O	1:G:398:ASP:HB2	2.13	0.47
1:H:102:GLU:HB3	1:H:442:VAL:HG22	1.96	0.47
1:I:293:ALA:HB2	1:I:300:VAL:HG23	1.96	0.47
1:J:106:ALA:CA	1:J:111:MET:HE3	2.43	0.47
1:J:131:LEU:HD12	1:J:422:VAL:CG1	2.37	0.47
1:K:192:GLY:HA2	1:K:295:LEU:HD11	1.96	0.47
1:L:365:LEU:O	1:L:369:VAL:HG13	2.14	0.47
1:M:370:ALA:O	1:M:371:LYS:C	2.56	0.47
1:M:429:LEU:HB3	1:M:440:ILE:HG21	1.96	0.47
1:M:524:LEU:HD23	1:M:525:PRO:HD2	1.95	0.47
2:O:80:ASN:ND2	2:U:23:GLY:H	2.12	0.47
1:B:288:MET:HG3	1:B:368:ARG:CD	2.43	0.47
1:E:223:ALA:O	1:E:251:ALA:HA	2.13	0.47
1:E:273:VAL:HG12	1:E:274:ALA:N	2.29	0.47
1:E:519:CYS:HB3	1:F:38:VAL:HG22	1.95	0.47
1:F:28:LYS:HD2	1:F:453:GLN:CD	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:MET:O	1:F:291:ASP:HB2	2.14	0.47
1:F:513:LEU:HB3	1:G:49:ILE:HD13	1.96	0.47
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.95	0.47
1:H:391:GLU:O	1:H:394:ALA:HB3	2.14	0.47
1:I:47:PRO:HG2	1:J:73:MET:HG3	1.96	0.47
1:I:217:SER:N	1:I:218:PRO:HD3	2.28	0.47
1:I:438:VAL:O	1:I:439:GLY:C	2.57	0.47
1:J:70:GLY:O	1:J:71:ALA:C	2.55	0.47
1:J:102:GLU:HB3	1:J:442:VAL:HG22	1.95	0.47
1:K:72:GLN:HE22	1:K:75:LYS:NZ	2.12	0.47
1:K:524:LEU:HA	1:K:524:LEU:HD23	1.76	0.47
1:L:433:ASN:CG	1:L:435:ASP:HB2	2.39	0.47
1:N:234:LEU:N	1:N:235:PRO:HD2	2.29	0.47
1:A:82:ASN:HB2	1:A:89:THR:CG2	2.45	0.47
1:A:259:LEU:O	1:A:263:VAL:HG23	2.14	0.47
1:B:69:MET:O	1:B:73:MET:HG3	2.15	0.47
1:C:524:LEU:HD23	1:C:524:LEU:HA	1.62	0.47
1:D:28:LYS:C	1:D:30:THR:H	2.22	0.47
1:E:16:MET:HE1	1:E:514:MET:HB3	1.96	0.47
1:F:64:ASP:HB3	1:F:67:GLU:HB2	1.95	0.47
1:H:135:SER:HA	1:H:412:VAL:HG12	1.97	0.47
1:J:478:TYR:HB2	1:J:485:TYR:CE2	2.49	0.47
1:K:413:ALA:HB1	1:K:417:VAL:HB	1.95	0.47
1:L:218:PRO:HG3	1:L:323:VAL:HG22	1.96	0.47
1:M:24:ALA:HA	1:M:27:VAL:HG12	1.96	0.47
1:M:420:ILE:CD1	1:M:470:LYS:HE3	2.44	0.47
1:N:77:VAL:HG22	1:N:506:TYR:CD1	2.49	0.47
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.95	0.47
1:A:287:ALA:O	1:A:290:GLN:HB3	2.15	0.47
1:D:223:ALA:O	1:D:251:ALA:HA	2.14	0.47
1:G:18:ARG:HB2	1:G:67:GLU:HG2	1.95	0.47
1:G:362:ARG:HG2	1:G:366:GLN:NE2	2.30	0.47
1:G:404:ARG:HG3	1:G:404:ARG:NH1	2.28	0.47
1:J:319:GLN:O	1:J:336:VAL:HG23	2.13	0.47
1:K:290:GLN:O	1:K:293:ALA:HB3	2.15	0.47
1:B:326:ASN:HD22	1:B:329:THR:HB	1.79	0.47
1:B:473:ASP:O	1:B:474:GLY:C	2.57	0.47
1:C:114:MET:HE3	1:C:114:MET:CA	2.43	0.47
1:C:184:GLN:H	1:C:184:GLN:CD	2.23	0.47
1:G:443:ALA:O	1:G:444:LEU:C	2.57	0.47
1:H:413:ALA:HB1	1:H:417:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:GLY:HA2	1:I:454:ILE:HD13	1.97	0.47
1:I:290:GLN:NE2	1:I:290:GLN:O	2.46	0.47
1:I:451:LEU:HD21	1:I:465:VAL:HG12	1.97	0.47
1:N:44:PHE:CD1	1:N:44:PHE:N	2.83	0.47
1:N:73:MET:SD	1:N:514:MET:HE2	2.54	0.47
1:N:217:SER:N	1:N:218:PRO:HD3	2.28	0.47
2:Q:17:VAL:O	2:Q:17:VAL:HG12	2.14	0.47
1:B:524:LEU:CD2	1:B:525:PRO:HD2	2.44	0.47
1:E:524:LEU:HD23	1:E:525:PRO:HD2	1.97	0.47
1:G:169:VAL:HB	1:G:173:GLY:HA3	1.96	0.47
1:G:460:GLU:O	1:G:462:PRO:HD3	2.14	0.47
1:H:492:GLY:C	1:H:493:ILE:HD13	2.39	0.47
1:I:149:THR:HG21	1:I:156:GLU:HA	1.96	0.47
1:J:351:GLN:HA	1:J:354:GLU:HG2	1.97	0.47
1:K:72:GLN:NE2	1:K:72:GLN:HA	2.29	0.47
1:K:426:LEU:CD1	1:K:444:LEU:HD21	2.44	0.47
1:M:80:LYS:HA	1:M:83:ASP:HB2	1.95	0.47
1:N:302:SER:H	1:N:307:MET:HE3	1.79	0.47
1:B:197:ARG:HD2	1:B:277:LYS:HB2	1.97	0.47
1:B:287:ALA:O	1:B:290:GLN:HB3	2.14	0.47
1:B:522:THR:OG1	1:B:523:ASP:N	2.48	0.47
1:D:111:MET:HG2	1:D:435:ASP:OD1	2.15	0.47
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.96	0.47
1:E:221:LEU:HB3	1:E:249:ILE:HD13	1.97	0.47
1:E:452:ARG:HH11	1:E:452:ARG:HG2	1.80	0.47
1:F:121:ASP:O	1:F:122:LYS:C	2.57	0.47
1:F:432:GLN:NE2	1:F:436:GLN:HE22	2.12	0.47
1:G:15:LYS:O	1:G:16:MET:C	2.55	0.47
1:G:185:ASP:HA	1:G:380:LYS:O	2.15	0.47
1:G:198:GLY:C	1:G:276:VAL:HG12	2.39	0.47
1:G:524:LEU:CD2	1:G:525:PRO:HD2	2.44	0.47
1:H:296:THR:HB	1:H:319:GLN:H	1.80	0.47
1:J:32:GLY:HA3	1:J:454:ILE:HG23	1.97	0.47
1:K:23:LEU:HD11	1:K:75:LYS:HG3	1.96	0.47
1:L:234:LEU:N	1:L:235:PRO:HD2	2.30	0.47
1:L:351:GLN:HA	1:L:354:GLU:HG2	1.97	0.47
1:L:404:ARG:CG	1:L:404:ARG:NH1	2.70	0.47
1:M:44:PHE:CD1	1:M:44:PHE:N	2.83	0.47
1:M:319:GLN:O	1:M:336:VAL:HG23	2.15	0.47
1:M:366:GLN:HA	1:M:369:VAL:HG22	1.96	0.47
1:M:428:ASP:O	1:M:430:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:470:LYS:O	5:M:526:HOH:O	2.20	0.47
1:N:24:ALA:HA	1:N:27:VAL:HG12	1.95	0.47
1:N:389:MET:C	1:N:389:MET:HE2	2.40	0.47
1:N:524:LEU:HD23	1:N:524:LEU:HA	1.59	0.47
2:P:37:ARG:HG2	2:P:37:ARG:HH11	1.80	0.47
2:P:41:LEU:O	2:P:61:VAL:HG13	2.14	0.47
2:Q:23:GLY:H	2:R:80:ASN:ND2	2.13	0.47
1:A:221:LEU:HB3	1:A:249:ILE:HD13	1.96	0.47
1:B:16:MET:CE	1:B:514:MET:HB3	2.42	0.47
1:B:198:GLY:C	1:B:276:VAL:HG12	2.39	0.47
1:C:124:VAL:HG13	1:C:504:LEU:HD13	1.97	0.47
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.96	0.47
1:D:25:ASP:N	1:D:25:ASP:OD1	2.46	0.47
1:H:161:LEU:HD21	1:H:185:ASP:HB3	1.97	0.47
1:H:455:VAL:HG11	1:H:462:PRO:HA	1.97	0.47
1:J:192:GLY:HA2	1:J:295:LEU:HD11	1.97	0.47
1:L:49:ILE:HD12	1:M:513:LEU:HD23	1.97	0.47
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.55	0.47
1:M:192:GLY:O	1:M:193:MET:HB2	2.14	0.47
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.43	0.47
1:B:339:GLU:HA	1:B:342:ILE:HB	1.97	0.47
1:C:291:ASP:HB3	1:C:372:LEU:HD21	1.97	0.47
1:F:194:GLN:HG3	1:F:330:THR:O	2.14	0.47
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.97	0.47
1:H:409:GLU:OE2	1:H:501:ARG:NH2	2.45	0.47
1:J:44:PHE:CD1	1:J:44:PHE:N	2.83	0.47
1:J:135:SER:HA	1:J:412:VAL:HG12	1.97	0.47
1:J:180:GLY:HA3	1:J:381:VAL:O	2.14	0.47
1:M:77:VAL:HG11	1:M:510:VAL:HB	1.97	0.47
1:M:419:LEU:O	1:M:420:ILE:C	2.58	0.47
1:N:65:LYS:CA	5:N:532:HOH:O	2.62	0.47
1:A:77:VAL:HG23	1:A:92:ALA:HB1	1.96	0.47
1:C:34:LYS:HD2	1:C:458:CYS:SG	2.55	0.47
1:C:58:ARG:HG3	1:C:58:ARG:HH11	1.79	0.47
1:E:25:ASP:OD1	1:E:25:ASP:N	2.47	0.47
1:G:54:VAL:O	1:G:58:ARG:CG	2.63	0.47
1:G:199:TYR:HB3	1:G:325:ILE:HD11	1.96	0.47
1:H:444:LEU:HD23	1:H:444:LEU:HA	1.59	0.47
1:K:403:THR:O	1:K:407:VAL:HG23	2.14	0.47
1:L:325:ILE:HG22	1:L:330:THR:HA	1.96	0.47
1:M:233:MET:C	1:M:235:PRO:HD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:HG13	1:A:74:VAL:CG1	2.39	0.46
1:C:35:GLY:HA3	1:C:51:LYS:HE2	1.97	0.46
1:C:270:ILE:CD1	2:Q:27:LEU:HB2	2.45	0.46
1:D:147:VAL:O	1:D:150:ILE:HG22	2.15	0.46
1:E:28:LYS:HD2	1:E:453:GLN:CD	2.41	0.46
1:E:150:ILE:HG21	1:E:494:LEU:O	2.15	0.46
1:E:489:ILE:HD13	1:E:494:LEU:HD22	1.95	0.46
1:F:339:GLU:HA	1:F:342:ILE:HB	1.97	0.46
1:G:232:GLU:HA	1:G:310:GLU:CD	2.40	0.46
1:G:305:ILE:O	1:G:305:ILE:HG22	2.15	0.46
1:I:161:LEU:HD21	1:I:185:ASP:HB3	1.96	0.46
1:L:22:VAL:HG11	1:L:62:LEU:HD21	1.97	0.46
1:M:143:ALA:O	1:M:146:GLN:HB3	2.15	0.46
1:M:197:ARG:HD2	1:M:277:LYS:HB2	1.97	0.46
1:M:443:ALA:O	1:M:447:MET:HG3	2.15	0.46
1:N:106:ALA:CA	1:N:111:MET:HE3	2.41	0.46
1:B:510:VAL:O	1:B:511:ALA:C	2.54	0.46
1:E:443:ALA:O	1:E:444:LEU:C	2.58	0.46
1:G:324:VAL:O	1:G:331:THR:HG22	2.16	0.46
1:H:221:LEU:HD12	1:H:222:LEU:N	2.31	0.46
1:H:225:LYS:HE3	1:H:232:GLU:OE2	2.15	0.46
1:H:366:GLN:HA	1:H:369:VAL:HG22	1.97	0.46
1:H:370:ALA:O	1:H:371:LYS:C	2.57	0.46
1:I:323:VAL:HG12	1:I:332:ILE:HA	1.96	0.46
1:M:38:VAL:HG12	1:M:40:LEU:HD13	1.97	0.46
1:A:305:ILE:HB	1:A:307:MET:HE2	1.98	0.46
1:C:169:VAL:HB	1:C:173:GLY:HA3	1.97	0.46
1:C:305:ILE:HB	1:C:307:MET:HE2	1.96	0.46
1:D:198:GLY:C	1:D:276:VAL:HG12	2.40	0.46
1:F:489:ILE:CD1	1:F:494:LEU:HD22	2.46	0.46
1:K:88:GLY:O	1:K:91:THR:N	2.48	0.46
1:K:366:GLN:HA	1:K:369:VAL:HG22	1.96	0.46
1:L:15:LYS:HB3	1:L:66:PHE:HB3	1.98	0.46
1:L:126:ALA:HB1	1:L:426:LEU:HD22	1.96	0.46
1:M:69:MET:HE2	1:M:522:THR:HB	1.95	0.46
1:M:290:GLN:NE2	1:M:293:ALA:HB3	2.30	0.46
1:A:150:ILE:HG21	1:A:494:LEU:O	2.16	0.46
1:B:429:LEU:O	1:B:430:ARG:NH1	2.46	0.46
1:C:252:GLU:OE1	1:C:285:ARG:NH1	2.48	0.46
1:C:404:ARG:HG3	1:C:404:ARG:NH1	2.27	0.46
1:I:44:PHE:N	1:I:44:PHE:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:ALA:O	1:I:128:VAL:C	2.57	0.46
1:J:293:ALA:HB2	1:J:300:VAL:HG23	1.97	0.46
1:K:38:VAL:HG12	1:K:40:LEU:HD13	1.96	0.46
1:L:15:LYS:HA	1:L:15:LYS:HD3	1.72	0.46
1:L:163:ALA:O	1:L:167:ASP:HB2	2.15	0.46
1:L:403:THR:O	1:L:407:VAL:HG23	2.16	0.46
1:L:496:PRO:HB2	1:L:499:VAL:HG13	1.97	0.46
1:M:19:GLY:HA3	1:M:67:GLU:O	2.15	0.46
1:M:302:SER:H	1:M:307:MET:HE3	1.81	0.46
1:M:351:GLN:HA	1:M:354:GLU:HG2	1.97	0.46
1:N:494:LEU:O	1:N:494:LEU:HD23	2.16	0.46
2:Q:41:LEU:O	2:Q:61:VAL:HG13	2.16	0.46
2:U:17:VAL:O	2:U:17:VAL:HG12	2.15	0.46
1:A:102:GLU:HB3	1:A:442:VAL:HG22	1.98	0.46
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.98	0.46
1:B:21:ASN:ND2	1:B:97:GLN:OE1	2.48	0.46
1:B:305:ILE:HB	1:B:307:MET:HE2	1.98	0.46
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.97	0.46
1:D:197:ARG:HD2	1:D:277:LYS:HB2	1.98	0.46
1:I:135:SER:HA	1:I:412:VAL:HG12	1.97	0.46
1:J:417:VAL:HG21	1:J:488:MET:HG3	1.97	0.46
1:L:428:ASP:O	1:L:430:ARG:HG2	2.15	0.46
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.98	0.46
1:M:127:ALA:O	1:M:128:VAL:C	2.57	0.46
1:M:412:VAL:CG2	1:M:418:ALA:HB2	2.46	0.46
1:N:213:VAL:HB	1:N:325:ILE:CG1	2.39	0.46
2:U:6:LEU:O	2:U:7:HIS:C	2.58	0.46
1:B:111:MET:HG2	1:B:435:ASP:OD1	2.16	0.46
1:C:7:LYS:HB3	1:C:12:ALA:HB2	1.98	0.46
1:C:23:LEU:C	1:C:23:LEU:HD12	2.40	0.46
1:C:339:GLU:HA	1:C:342:ILE:HB	1.98	0.46
1:C:385:THR:OG1	1:C:388:GLU:HB2	2.15	0.46
1:H:87:ASP:HB3	1:H:499:VAL:HG21	1.98	0.46
1:H:266:THR:HG22	1:H:271:VAL:O	2.16	0.46
1:H:436:GLN:O	1:H:440:ILE:HG13	2.15	0.46
1:H:462:PRO:O	1:H:463:SER:C	2.59	0.46
1:I:199:TYR:HA	1:I:276:VAL:HG12	1.97	0.46
1:I:419:LEU:CD2	1:I:500:THR:HG23	2.35	0.46
1:J:278:ALA:HB1	1:J:279:PRO:HD2	1.97	0.46
1:K:69:MET:HE2	1:K:522:THR:HB	1.96	0.46
1:L:492:GLY:C	1:L:493:ILE:HD13	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:342:ILE:O	1:M:346:VAL:HG23	2.16	0.46
1:N:104:LEU:HD12	1:N:104:LEU:HA	1.45	0.46
1:N:266:THR:HG21	1:N:273:VAL:H	1.81	0.46
2:R:7:HIS:O	2:R:7:HIS:ND1	2.48	0.46
2:T:41:LEU:O	2:T:61:VAL:HG13	2.15	0.46
1:C:224:ASP:OD1	1:C:286:LYS:HG2	2.16	0.46
1:C:510:VAL:HG23	1:C:514:MET:CE	2.36	0.46
1:D:6:VAL:O	1:D:6:VAL:CG2	2.64	0.46
1:D:259:LEU:O	1:D:263:VAL:HG23	2.15	0.46
1:E:349:ILE:HA	1:E:352:GLN:HG2	1.93	0.46
1:F:221:LEU:HB3	1:F:249:ILE:HD13	1.98	0.46
1:H:218:PRO:HG3	1:H:323:VAL:HG22	1.97	0.46
1:I:233:MET:C	1:I:235:PRO:HD2	2.40	0.46
1:K:40:LEU:HD12	1:L:521:VAL:HB	1.98	0.46
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.96	0.46
1:M:86:GLY:O	1:M:87:ASP:HB2	2.14	0.46
1:M:524:LEU:CD2	1:M:525:PRO:HD2	2.45	0.46
2:T:78:ILE:HD13	2:T:83:VAL:HG21	1.97	0.46
1:A:44:PHE:HD1	1:A:44:PHE:N	1.93	0.46
1:C:100:ILE:HD11	1:C:514:MET:HE3	1.98	0.46
1:D:28:LYS:O	1:D:30:THR:N	2.48	0.46
1:D:273:VAL:HG12	1:D:274:ALA:N	2.31	0.46
1:D:288:MET:O	1:D:291:ASP:HB2	2.16	0.46
1:E:184:GLN:H	1:E:184:GLN:CD	2.23	0.46
1:G:501:ARG:HD3	1:G:505:GLN:OE1	2.15	0.46
1:H:412:VAL:CG2	1:H:418:ALA:CB	2.94	0.46
1:H:475:ASN:ND2	1:H:489:ILE:HD12	2.30	0.46
1:K:88:GLY:O	1:K:89:THR:C	2.59	0.46
1:L:284:ARG:NH1	1:L:364:LYS:HD2	2.27	0.46
1:L:370:ALA:O	1:L:371:LYS:C	2.59	0.46
2:O:11:ILE:HG12	2:O:85:ILE:HG12	1.97	0.46
1:A:105:LYS:HD3	1:H:110:GLY:O	2.15	0.46
1:A:429:LEU:HD12	1:A:429:LEU:HA	1.63	0.46
1:B:15:LYS:O	1:B:16:MET:C	2.58	0.46
1:B:399:ALA:O	1:B:400:LEU:C	2.57	0.46
1:C:259:LEU:O	1:C:263:VAL:HG23	2.15	0.46
1:C:288:MET:O	1:C:291:ASP:HB2	2.16	0.46
1:E:305:ILE:HB	1:E:307:MET:HE2	1.97	0.46
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.98	0.46
1:H:172:GLU:O	1:H:173:GLY:C	2.59	0.46
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:96:ALA:O	1:J:100:ILE:HG13	2.16	0.46
1:K:7:LYS:HD2	1:K:66:PHE:CZ	2.50	0.46
1:L:419:LEU:CD2	1:L:500:THR:HG23	2.44	0.46
1:M:36:ARG:O	1:M:51:LYS:HG2	2.16	0.46
1:N:404:ARG:HG2	1:N:404:ARG:NH1	2.27	0.46
1:A:417:VAL:O	1:A:418:ALA:C	2.53	0.46
1:D:349:ILE:HA	1:D:352:GLN:HG2	1.95	0.46
1:E:486:GLY:CA	1:E:491:MET:HE2	2.41	0.46
1:H:164:GLU:O	1:H:167:ASP:HB3	2.15	0.46
1:H:502:SER:O	1:H:503:ALA:C	2.59	0.46
1:I:77:VAL:HG22	1:I:506:TYR:CD1	2.51	0.46
1:I:255:GLU:O	1:I:256:GLY:C	2.59	0.46
1:K:22:VAL:HG11	1:K:62:LEU:HD21	1.98	0.46
1:K:106:ALA:HA	1:K:111:MET:CE	2.43	0.46
1:K:284:ARG:NH1	1:K:364:LYS:HD2	2.27	0.46
1:M:323:VAL:HG12	1:M:332:ILE:HA	1.97	0.46
1:M:444:LEU:HA	1:M:444:LEU:HD23	1.60	0.46
1:N:193:MET:N	1:N:376:VAL:CG2	2.79	0.46
2:O:17:VAL:O	2:O:17:VAL:HG12	2.15	0.46
2:T:6:LEU:O	2:T:7:HIS:C	2.59	0.46
1:C:69:MET:O	1:C:73:MET:HG3	2.16	0.45
1:D:441:LYS:O	1:D:445:ARG:HB2	2.16	0.45
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.16	0.45
1:G:147:VAL:O	1:G:148:GLY:C	2.58	0.45
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.98	0.45
1:J:266:THR:HG21	1:J:273:VAL:H	1.81	0.45
1:K:11:ASP:O	1:K:12:ALA:C	2.56	0.45
1:K:138:CYS:SG	1:K:144:ILE:HD13	2.56	0.45
1:L:106:ALA:O	1:L:107:VAL:C	2.57	0.45
1:L:417:VAL:O	1:L:418:ALA:C	2.59	0.45
2:O:6:LEU:O	2:O:7:HIS:C	2.58	0.45
1:C:200:LEU:HD13	1:C:254:VAL:HB	1.98	0.45
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.98	0.45
1:I:214:GLU:HG3	1:I:324:VAL:HG22	1.99	0.45
1:I:361:ASP:O	1:I:365:LEU:HG	2.16	0.45
1:I:365:LEU:O	1:I:369:VAL:HG13	2.15	0.45
1:K:479:ASN:C	1:K:479:ASN:OD1	2.59	0.45
1:L:124:VAL:O	1:L:128:VAL:HG23	2.16	0.45
1:L:455:VAL:HG13	1:L:460:GLU:HB2	1.99	0.45
1:L:524:LEU:CD2	1:L:525:PRO:HD2	2.46	0.45
1:N:2:ALA:O	1:N:4:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:7:HIS:O	2:P:7:HIS:ND1	2.48	0.45
2:R:37:ARG:HG2	2:R:37:ARG:HH11	1.82	0.45
1:A:28:LYS:C	1:A:30:THR:N	2.71	0.45
1:B:324:VAL:O	1:B:331:THR:HG22	2.17	0.45
1:C:414:GLY:HA2	1:C:495:ASP:OD2	2.17	0.45
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.99	0.45
1:K:255:GLU:O	1:K:256:GLY:C	2.60	0.45
1:M:217:SER:N	1:M:218:PRO:HD3	2.31	0.45
1:M:392:LYS:O	1:M:396:VAL:HG23	2.16	0.45
1:N:351:GLN:HA	1:N:354:GLU:HG2	1.98	0.45
2:S:17:VAL:HG12	2:S:17:VAL:O	2.15	0.45
1:A:6:VAL:O	1:A:6:VAL:CG2	2.63	0.45
1:A:221:LEU:HD13	1:A:317:LEU:HD11	1.99	0.45
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.97	0.45
1:E:429:LEU:O	1:E:430:ARG:HG2	2.16	0.45
1:E:450:PRO:O	1:E:454:ILE:HG13	2.16	0.45
1:H:429:LEU:HB3	1:H:440:ILE:HG21	1.99	0.45
1:I:412:VAL:HG23	1:I:418:ALA:HB2	1.98	0.45
1:I:417:VAL:O	1:I:418:ALA:C	2.55	0.45
1:I:451:LEU:O	1:I:452:ARG:C	2.58	0.45
1:J:32:GLY:CA	1:J:454:ILE:HD13	2.44	0.45
1:J:214:GLU:HG3	1:J:324:VAL:HG22	1.97	0.45
1:J:444:LEU:HD23	1:J:444:LEU:HA	1.56	0.45
1:L:149:THR:HG21	1:L:156:GLU:HA	1.97	0.45
1:M:22:VAL:HG11	1:M:62:LEU:CD2	2.46	0.45
1:N:80:LYS:O	1:N:81:ALA:C	2.58	0.45
1:N:120:ILE:HA	1:N:443:ALA:HB2	1.99	0.45
2:P:23:GLY:H	2:Q:80:ASN:ND2	2.13	0.45
2:R:84:LEU:N	2:R:84:LEU:CD1	2.78	0.45
1:A:461:GLU:OE1	1:N:463:SER:HB3	2.16	0.45
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.84	0.45
1:B:417:VAL:O	1:B:418:ALA:C	2.59	0.45
1:B:510:VAL:HG23	1:B:514:MET:CE	2.34	0.45
1:C:198:GLY:C	1:C:276:VAL:HG12	2.41	0.45
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.99	0.45
1:F:486:GLY:CA	1:F:491:MET:CE	2.94	0.45
1:G:252:GLU:OE1	1:G:285:ARG:NH1	2.50	0.45
1:J:419:LEU:CD2	1:J:500:THR:HG23	2.37	0.45
1:J:496:PRO:HB2	1:J:499:VAL:HG13	1.98	0.45
1:K:64:ASP:OD1	1:K:65:LYS:O	2.33	0.45
1:N:233:MET:C	1:N:235:PRO:HD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ALA:O	1:A:447:MET:HE3	2.16	0.45
1:C:23:LEU:O	1:C:24:ALA:C	2.60	0.45
1:C:28:LYS:O	1:C:30:THR:N	2.50	0.45
1:C:221:LEU:HD13	1:C:317:LEU:HD11	1.98	0.45
1:C:513:LEU:HB3	1:D:49:ILE:HD13	1.99	0.45
1:D:96:ALA:HB2	1:D:507:ALA:HB1	1.99	0.45
1:E:28:LYS:O	1:E:29:VAL:C	2.54	0.45
1:G:175:ILE:HG21	1:G:400:LEU:HD21	1.99	0.45
1:I:16:MET:HG3	1:I:520:MET:SD	2.57	0.45
1:J:272:LYS:NZ	1:K:228:SER:HB3	2.31	0.45
1:K:205:ILE:HA	1:K:213:VAL:HG22	1.99	0.45
1:K:420:ILE:HG23	1:K:420:ILE:HD12	1.64	0.45
1:L:44:PHE:CD1	1:L:44:PHE:N	2.84	0.45
1:M:513:LEU:HD12	1:M:513:LEU:HA	1.86	0.45
1:N:513:LEU:HD12	1:N:513:LEU:HA	1.79	0.45
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.77	0.45
1:A:288:MET:HG3	1:A:368:ARG:CD	2.46	0.45
1:B:238:GLU:OE2	2:P:23:GLY:C	2.60	0.45
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.98	0.45
1:E:34:LYS:HD2	1:E:458:CYS:SG	2.57	0.45
1:I:126:ALA:HB1	1:I:426:LEU:CD2	2.47	0.45
1:J:104:LEU:HD12	1:J:104:LEU:HA	1.41	0.45
1:J:370:ALA:O	1:J:371:LYS:C	2.58	0.45
1:J:452:ARG:NH1	1:J:452:ARG:CG	2.76	0.45
1:K:452:ARG:NH1	1:K:452:ARG:CG	2.73	0.45
1:L:524:LEU:HA	1:L:524:LEU:HD23	1.59	0.45
1:M:104:LEU:HD12	1:M:104:LEU:HA	1.44	0.45
2:Q:78:ILE:HD13	2:Q:83:VAL:HG21	1.97	0.45
1:A:273:VAL:HG12	1:A:274:ALA:N	2.31	0.45
1:B:291:ASP:HB3	1:B:372:LEU:HD21	1.99	0.45
1:C:273:VAL:HG12	1:C:274:ALA:N	2.32	0.45
1:D:305:ILE:HB	1:D:307:MET:HE2	1.98	0.45
1:D:513:LEU:HB3	1:E:49:ILE:HD13	1.99	0.45
1:E:23:LEU:CD1	1:E:23:LEU:C	2.89	0.45
1:E:162:ILE:O	1:E:166:MET:HG3	2.15	0.45
1:F:198:GLY:C	1:F:276:VAL:HG12	2.42	0.45
1:G:23:LEU:HD12	1:G:24:ALA:N	2.31	0.45
1:N:284:ARG:O	1:N:288:MET:HG3	2.17	0.45
1:A:326:ASN:HD22	1:A:329:THR:HB	1.82	0.45
1:B:91:THR:O	1:B:92:ALA:C	2.59	0.45
1:C:90:THR:O	1:C:94:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ARG:HG3	1:D:58:ARG:NH1	2.31	0.45
1:F:130:GLU:HB3	1:F:422:VAL:HB	1.99	0.45
1:F:427:ALA:HB3	5:F:606:HOH:O	2.15	0.45
1:H:389:MET:C	1:H:389:MET:HE2	2.42	0.45
1:I:72:GLN:HA	1:I:72:GLN:NE2	2.32	0.45
1:J:66:PHE:HD1	1:J:520:MET:HE2	1.81	0.45
1:J:290:GLN:O	1:J:293:ALA:HB3	2.16	0.45
1:K:34:LYS:HB2	1:K:458:CYS:SG	2.57	0.45
1:L:88:GLY:O	1:L:91:THR:N	2.50	0.45
1:N:77:VAL:HG11	1:N:510:VAL:HB	1.99	0.45
1:N:255:GLU:O	1:N:256:GLY:C	2.60	0.45
1:A:198:GLY:C	1:A:276:VAL:HG12	2.42	0.45
1:D:291:ASP:HB3	1:D:372:LEU:HD21	1.99	0.45
1:D:429:LEU:HD12	1:D:429:LEU:HA	1.70	0.45
1:E:114:MET:O	1:E:114:MET:HE3	2.17	0.45
1:F:200:LEU:HD13	1:F:254:VAL:HB	1.99	0.45
1:H:266:THR:HG21	1:H:273:VAL:H	1.82	0.45
1:H:426:LEU:CD1	1:H:444:LEU:HD21	2.47	0.45
1:H:428:ASP:O	1:H:430:ARG:HG2	2.17	0.45
1:J:80:LYS:HA	1:J:83:ASP:HB2	1.99	0.45
1:J:100:ILE:HG23	1:J:104:LEU:HD22	1.99	0.45
1:L:266:THR:HG21	1:L:273:VAL:H	1.82	0.45
1:M:293:ALA:HB2	1:M:300:VAL:HG23	1.97	0.45
1:N:23:LEU:HD23	1:N:23:LEU:HA	1.85	0.45
1:N:326:ASN:ND2	1:N:329:THR:HB	2.32	0.45
1:N:419:LEU:HD22	1:N:500:THR:CG2	2.42	0.45
1:C:448:GLU:O	1:C:452:ARG:HD2	2.18	0.44
1:D:324:VAL:O	1:D:331:THR:HG22	2.18	0.44
1:F:429:LEU:O	1:F:430:ARG:HG2	2.18	0.44
1:J:11:ASP:O	1:J:12:ALA:C	2.59	0.44
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.99	0.44
1:K:417:VAL:O	1:K:418:ALA:C	2.60	0.44
1:L:40:LEU:HD12	1:M:521:VAL:HB	1.98	0.44
1:N:392:LYS:O	1:N:396:VAL:HG23	2.18	0.44
1:B:20:VAL:HG13	1:B:74:VAL:HG11	1.99	0.44
1:C:194:GLN:HG3	1:C:330:THR:O	2.16	0.44
1:C:444:LEU:O	1:C:447:MET:HB2	2.17	0.44
1:D:19:GLY:HA3	1:D:67:GLU:O	2.17	0.44
1:D:201:SER:HA	1:D:202:PRO:HD3	1.85	0.44
1:F:201:SER:HA	1:F:202:PRO:HD3	1.86	0.44
1:H:479:ASN:OD1	1:H:479:ASN:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:VAL:HG22	1:I:506:TYR:HD1	1.82	0.44
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.99	0.44
1:K:149:THR:HG21	1:K:156:GLU:HA	1.98	0.44
1:K:290:GLN:NE2	1:K:293:ALA:HB3	2.32	0.44
1:K:389:MET:C	1:K:389:MET:HE2	2.43	0.44
1:L:443:ALA:O	1:L:447:MET:HG3	2.17	0.44
1:N:68:ASN:HB3	5:N:532:HOH:O	2.16	0.44
1:A:16:MET:HE3	1:A:514:MET:SD	2.58	0.44
1:A:184:GLN:H	1:A:184:GLN:CD	2.26	0.44
1:A:513:LEU:HB3	1:B:49:ILE:HD13	1.99	0.44
1:B:349:ILE:HA	1:B:352:GLN:HG2	1.96	0.44
1:F:96:ALA:C	1:F:98:ALA:N	2.75	0.44
1:F:456:LEU:HD13	1:F:462:PRO:HG3	2.00	0.44
1:H:392:LYS:O	1:H:396:VAL:HG23	2.18	0.44
1:J:64:ASP:OD1	1:J:65:LYS:O	2.36	0.44
1:J:428:ASP:O	1:J:429:LEU:C	2.59	0.44
1:K:15:LYS:HB3	1:K:66:PHE:HB3	1.99	0.44
1:L:43:SER:HB3	1:L:44:PHE:HD1	1.82	0.44
1:N:444:LEU:HD23	1:N:444:LEU:HA	1.44	0.44
2:U:67:PHE:CG	2:U:86:MET:HE2	2.52	0.44
1:A:477:GLY:HA3	1:A:488:MET:SD	2.57	0.44
1:C:456:LEU:HD13	1:C:462:PRO:HG3	2.00	0.44
1:C:519:CYS:CB	1:D:38:VAL:HG13	2.39	0.44
1:D:116:LEU:HA	1:D:116:LEU:HD23	1.66	0.44
1:D:121:ASP:O	1:D:122:LYS:C	2.60	0.44
1:E:414:GLY:O	1:E:488:MET:HE2	2.17	0.44
1:F:150:ILE:HD13	1:F:493:ILE:HA	1.98	0.44
1:F:399:ALA:O	1:F:400:LEU:C	2.60	0.44
1:I:169:VAL:HG13	1:I:173:GLY:HA3	1.99	0.44
1:J:305:ILE:HD12	1:J:307:MET:HE2	2.00	0.44
1:K:412:VAL:HG23	1:K:418:ALA:HB2	2.00	0.44
1:K:428:ASP:O	1:K:430:ARG:HG2	2.17	0.44
1:M:64:ASP:C	1:M:65:LYS:O	2.56	0.44
1:N:193:MET:H	1:N:376:VAL:HG21	1.81	0.44
2:Q:37:ARG:HG2	2:Q:37:ARG:NH1	2.32	0.44
2:T:17:VAL:O	2:T:17:VAL:HG12	2.18	0.44
1:A:234:LEU:N	1:A:235:PRO:HD2	2.33	0.44
1:A:324:VAL:O	1:A:331:THR:HG22	2.17	0.44
1:A:451:LEU:HD23	1:A:451:LEU:O	2.18	0.44
1:A:494:LEU:N	1:A:494:LEU:HD23	2.32	0.44
1:B:150:ILE:HD13	1:B:493:ILE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:O	1:B:260:ALA:C	2.61	0.44
1:C:58:ARG:HG3	1:C:58:ARG:NH1	2.32	0.44
1:C:65:LYS:NZ	1:C:523:ASP:HB2	2.32	0.44
1:C:432:GLN:H	1:C:432:GLN:HG3	1.64	0.44
1:C:432:GLN:HE21	1:C:436:GLN:HE22	1.63	0.44
1:G:54:VAL:O	1:G:54:VAL:HG22	2.17	0.44
1:G:76:GLU:O	1:G:80:LYS:HB2	2.18	0.44
1:G:399:ALA:O	1:G:400:LEU:C	2.60	0.44
1:H:524:LEU:HD23	1:H:524:LEU:HA	1.64	0.44
1:I:325:ILE:HG22	1:I:330:THR:HA	1.99	0.44
1:K:85:ALA:HB1	1:K:499:VAL:HB	2.00	0.44
1:K:120:ILE:HA	1:K:443:ALA:HB2	2.00	0.44
1:L:32:GLY:HA2	1:L:454:ILE:HG23	2.00	0.44
1:N:200:LEU:HD21	1:N:277:LYS:HG3	2.00	0.44
2:T:37:ARG:HG2	2:T:37:ARG:NH1	2.33	0.44
1:B:460:GLU:O	1:B:462:PRO:HD3	2.18	0.44
1:C:455:VAL:O	1:C:458:CYS:HB2	2.18	0.44
1:E:291:ASP:HB3	1:E:372:LEU:HD21	2.00	0.44
1:I:18:ARG:HB2	1:I:67:GLU:HG2	1.99	0.44
1:J:199:TYR:HA	1:J:276:VAL:HG12	2.00	0.44
1:K:213:VAL:HB	1:K:325:ILE:CG1	2.42	0.44
1:L:30:THR:HB	1:L:51:LYS:O	2.17	0.44
1:N:420:ILE:HD12	1:N:420:ILE:HG23	1.67	0.44
1:B:259:LEU:O	1:B:263:VAL:HG23	2.18	0.44
1:B:362:ARG:HG2	1:B:366:GLN:NE2	2.33	0.44
1:D:58:ARG:HG3	1:D:58:ARG:HH11	1.82	0.44
1:F:25:ASP:N	1:F:25:ASP:OD1	2.49	0.44
1:I:205:ILE:HA	1:I:213:VAL:HG22	2.00	0.44
1:I:418:ALA:O	1:I:422:VAL:HG13	2.18	0.44
1:K:44:PHE:CD1	1:K:44:PHE:N	2.86	0.44
1:L:278:ALA:HB1	1:L:279:PRO:HD2	1.98	0.44
1:L:346:VAL:O	1:L:350:ARG:HB2	2.16	0.44
1:L:412:VAL:HG23	1:L:418:ALA:HB2	1.98	0.44
1:M:7:LYS:HD2	1:M:66:PHE:CE2	2.53	0.44
1:M:18:ARG:HB2	1:M:67:GLU:HG2	1.98	0.44
1:M:205:ILE:HA	1:M:213:VAL:HG22	2.00	0.44
1:M:265:ASN:HD22	1:M:265:ASN:HA	1.60	0.44
1:M:455:VAL:O	1:M:458:CYS:HB2	2.17	0.44
1:N:475:ASN:ND2	1:N:489:ILE:HD12	2.33	0.44
1:C:20:VAL:HG23	1:C:20:VAL:H	1.58	0.44
1:C:162:ILE:O	1:C:166:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ASN:HD22	1:D:21:ASN:HA	1.64	0.44
1:D:460:GLU:O	1:D:462:PRO:HD3	2.18	0.44
1:D:487:ASN:C	1:D:487:ASN:OD1	2.60	0.44
1:E:185:ASP:HA	1:E:380:LYS:O	2.18	0.44
1:E:381:VAL:HG11	1:E:392:LYS:CG	2.43	0.44
1:F:511:ALA:O	1:F:512:GLY:C	2.61	0.44
1:H:91:THR:O	1:H:92:ALA:C	2.59	0.44
1:H:104:LEU:HA	1:H:104:LEU:HD12	1.48	0.44
1:I:428:ASP:O	1:I:429:LEU:C	2.59	0.44
1:J:441:LYS:O	1:J:442:VAL:C	2.61	0.44
1:K:502:SER:O	1:K:503:ALA:C	2.61	0.44
1:L:444:LEU:HD23	1:L:444:LEU:HA	1.53	0.44
1:N:91:THR:O	1:N:92:ALA:C	2.58	0.44
2:P:78:ILE:HD13	2:P:83:VAL:HG21	1.98	0.44
1:A:434:GLU:O	1:A:435:ASP:C	2.60	0.44
1:B:219:PHE:HB3	1:B:317:LEU:HD23	2.00	0.44
1:G:44:PHE:HD1	1:G:44:PHE:N	2.01	0.44
1:G:524:LEU:HD23	1:G:524:LEU:HA	1.57	0.44
1:K:399:ALA:O	1:K:400:LEU:C	2.60	0.44
1:N:236:VAL:HG22	1:N:312:ALA:O	2.17	0.44
2:Q:6:LEU:O	2:Q:7:HIS:C	2.60	0.44
1:B:24:ALA:O	1:B:28:LYS:HG3	2.18	0.43
1:B:28:LYS:C	1:B:30:THR:H	2.25	0.43
1:D:16:MET:HE1	1:D:514:MET:O	2.17	0.43
1:D:443:ALA:O	1:D:444:LEU:C	2.61	0.43
1:E:478:TYR:CE2	1:E:480:ALA:HA	2.53	0.43
1:F:362:ARG:HG2	1:F:366:GLN:NE2	2.33	0.43
1:H:199:TYR:HA	1:H:276:VAL:HG12	2.00	0.43
1:H:433:ASN:HD22	1:H:433:ASN:HA	1.47	0.43
1:I:225:LYS:HE3	1:I:232:GLU:OE2	2.17	0.43
1:L:85:ALA:HB1	1:L:499:VAL:HB	1.98	0.43
1:M:31:LEU:H	1:M:457:ASN:ND2	2.16	0.43
2:R:41:LEU:O	2:R:61:VAL:HG13	2.17	0.43
1:A:28:LYS:HD2	1:A:453:GLN:NE2	2.33	0.43
1:C:42:LYS:HG2	1:C:44:PHE:CD2	2.52	0.43
1:D:77:VAL:HG23	1:D:92:ALA:HB1	2.00	0.43
1:E:102:GLU:HB3	1:E:442:VAL:HG22	2.00	0.43
1:E:399:ALA:O	1:E:400:LEU:C	2.59	0.43
1:G:266:THR:CG2	1:G:273:VAL:HB	2.49	0.43
1:G:487:ASN:OD1	1:G:489:ILE:N	2.50	0.43
1:H:293:ALA:HB2	1:H:300:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:GLY:HA3	1:I:67:GLU:O	2.18	0.43
1:I:172:GLU:O	1:I:173:GLY:O	2.36	0.43
1:J:7:LYS:HD2	1:J:66:PHE:CE2	2.52	0.43
1:L:13:ARG:HD2	1:L:104:LEU:HD11	2.00	0.43
1:L:126:ALA:CB	1:L:426:LEU:HD22	2.48	0.43
1:M:8:PHE:O	1:M:9:GLY:C	2.59	0.43
1:M:200:LEU:HD21	1:M:277:LYS:HG3	2.00	0.43
1:N:519:CYS:SG	1:N:520:MET:N	2.91	0.43
1:A:516:THR:OG1	1:B:37:ASN:ND2	2.48	0.43
1:C:395:ARG:O	1:C:398:ASP:CB	2.66	0.43
1:C:473:ASP:O	1:C:474:GLY:C	2.60	0.43
1:D:96:ALA:C	1:D:98:ALA:N	2.74	0.43
1:E:69:MET:O	1:E:73:MET:HG3	2.18	0.43
1:E:201:SER:HA	1:E:202:PRO:HD3	1.83	0.43
1:F:524:LEU:HA	1:F:524:LEU:HD23	1.61	0.43
1:I:164:GLU:O	1:I:167:ASP:HB3	2.18	0.43
1:J:524:LEU:CD2	1:J:525:PRO:HD2	2.47	0.43
1:K:16:MET:SD	1:K:514:MET:HG2	2.59	0.43
1:K:513:LEU:HD12	1:K:513:LEU:HA	1.87	0.43
1:L:361:ASP:O	1:L:365:LEU:HG	2.17	0.43
1:L:453:GLN:O	1:L:454:ILE:C	2.60	0.43
1:N:66:PHE:N	1:N:69:MET:HE3	2.33	0.43
2:O:37:ARG:HG2	2:O:37:ARG:NH1	2.33	0.43
1:A:23:LEU:C	1:A:23:LEU:HD13	2.43	0.43
1:B:270:ILE:HD11	2:P:27:LEU:HB2	2.00	0.43
1:C:96:ALA:O	1:C:97:GLN:C	2.59	0.43
1:D:288:MET:HG3	1:D:368:ARG:CD	2.45	0.43
1:E:100:ILE:O	1:E:101:THR:C	2.56	0.43
1:E:489:ILE:HD13	1:E:494:LEU:CD2	2.48	0.43
1:G:111:MET:HG2	1:G:435:ASP:OD1	2.18	0.43
1:H:69:MET:HE2	1:H:522:THR:HB	1.98	0.43
1:H:451:LEU:O	1:H:452:ARG:C	2.59	0.43
1:I:104:LEU:HA	1:I:104:LEU:HD12	1.48	0.43
1:I:351:GLN:HA	1:I:354:GLU:HG2	2.01	0.43
1:J:403:THR:O	1:J:407:VAL:HG23	2.18	0.43
1:J:497:THR:O	1:J:498:LYS:C	2.61	0.43
1:K:168:LYS:HD2	1:K:187:LEU:HD13	1.99	0.43
1:L:475:ASN:CG	1:L:489:ILE:HD12	2.44	0.43
1:M:88:GLY:O	1:M:89:THR:C	2.60	0.43
1:M:149:THR:HG21	1:M:156:GLU:HA	1.99	0.43
1:M:163:ALA:O	1:M:167:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:23:GLY:H	2:U:80:ASN:ND2	2.16	0.43
1:A:15:LYS:O	1:A:16:MET:C	2.60	0.43
1:A:73:MET:O	1:A:74:VAL:C	2.60	0.43
1:A:194:GLN:HB2	1:A:331:THR:CB	2.48	0.43
1:A:510:VAL:CG2	1:A:514:MET:CE	2.90	0.43
1:B:4:LYS:HD2	1:B:522:THR:O	2.19	0.43
1:B:234:LEU:N	1:B:235:PRO:HD2	2.34	0.43
1:C:28:LYS:C	1:C:30:THR:N	2.73	0.43
1:D:65:LYS:NZ	1:D:523:ASP:HB2	2.33	0.43
1:E:28:LYS:C	1:E:30:THR:N	2.73	0.43
1:F:291:ASP:HB3	1:F:372:LEU:HD21	2.00	0.43
1:G:221:LEU:HB3	1:G:249:ILE:HD13	2.00	0.43
1:H:15:LYS:HA	1:H:15:LYS:HD3	1.69	0.43
1:K:15:LYS:HD3	1:K:15:LYS:HA	1.71	0.43
1:L:326:ASN:ND2	1:L:329:THR:HB	2.33	0.43
1:L:449:ALA:N	1:L:450:PRO:CD	2.81	0.43
1:N:205:ILE:HA	1:N:213:VAL:HG22	2.00	0.43
1:N:361:ASP:O	1:N:365:LEU:HG	2.17	0.43
1:N:413:ALA:HB1	1:N:417:VAL:HB	2.00	0.43
2:S:86:MET:HG3	2:S:90:ASP:HB2	1.99	0.43
1:C:21:ASN:ND2	1:C:97:GLN:OE1	2.49	0.43
1:D:200:LEU:HD13	1:D:254:VAL:HB	2.01	0.43
1:E:194:GLN:HG3	1:E:330:THR:O	2.19	0.43
1:E:246:PRO:HB3	1:E:272:LYS:HB3	2.01	0.43
1:F:44:PHE:N	1:F:44:PHE:CD1	2.60	0.43
1:F:513:LEU:HD23	1:F:513:LEU:HA	1.80	0.43
1:G:473:ASP:O	1:G:474:GLY:C	2.61	0.43
1:I:32:GLY:CA	1:I:454:ILE:HG23	2.48	0.43
1:I:174:VAL:HG21	1:I:194:GLN:HB3	2.01	0.43
1:K:169:VAL:HG13	1:K:173:GLY:HA3	2.01	0.43
1:L:60:ILE:HA	1:L:60:ILE:HD13	1.85	0.43
1:N:403:THR:O	1:N:407:VAL:HG23	2.18	0.43
1:N:462:PRO:O	1:N:463:SER:C	2.61	0.43
2:Q:84:LEU:HD12	2:Q:84:LEU:N	2.34	0.43
1:A:121:ASP:O	1:A:122:LYS:C	2.60	0.43
1:B:25:ASP:OD1	1:B:25:ASP:N	2.46	0.43
1:D:456:LEU:HD13	1:D:462:PRO:HG3	2.00	0.43
1:E:451:LEU:HD23	1:E:451:LEU:O	2.19	0.43
1:G:82:ASN:HB2	1:G:89:THR:CG2	2.48	0.43
1:H:32:GLY:CA	1:H:454:ILE:HG23	2.49	0.43
1:H:325:ILE:HG22	1:H:330:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:13:ARG:HE	1:I:107:VAL:HG21	1.83	0.43
1:J:56:VAL:O	1:J:57:ALA:C	2.62	0.43
1:N:163:ALA:O	1:N:167:ASP:HB2	2.18	0.43
1:A:252:GLU:O	1:A:253:ASP:HB2	2.19	0.43
1:E:96:ALA:O	1:E:97:GLN:C	2.60	0.43
1:G:478:TYR:CE2	1:G:480:ALA:HA	2.53	0.43
1:H:77:VAL:HG22	1:H:506:TYR:HD1	1.84	0.43
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.42	0.43
1:J:15:LYS:HA	1:J:15:LYS:HD3	1.74	0.43
1:J:205:ILE:HA	1:J:213:VAL:HG22	2.01	0.43
1:L:429:LEU:HB3	1:L:440:ILE:HG21	2.01	0.43
1:N:161:LEU:HD21	1:N:185:ASP:HB3	2.00	0.43
1:A:96:ALA:C	1:A:98:ALA:N	2.74	0.43
1:A:420:ILE:HD13	1:A:451:LEU:HD13	2.00	0.43
1:B:150:ILE:HG22	1:B:151:SER:N	2.34	0.43
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.52	0.43
1:D:221:LEU:HB3	1:D:249:ILE:HD13	2.01	0.43
1:D:232:GLU:HA	1:D:310:GLU:CD	2.44	0.43
1:D:426:LEU:C	1:D:428:ASP:N	2.76	0.43
1:E:147:VAL:O	1:E:150:ILE:HG22	2.19	0.43
1:E:501:ARG:HD3	1:E:505:GLN:OE1	2.19	0.43
1:F:273:VAL:HG12	1:F:274:ALA:N	2.33	0.43
1:F:324:VAL:O	1:F:331:THR:HG22	2.19	0.43
1:G:54:VAL:O	1:G:58:ARG:HG2	2.19	0.43
1:G:268:ARG:HH22	2:U:20:LYS:HZ2	1.67	0.43
1:H:68:ASN:HB3	5:H:528:HOH:O	2.18	0.43
1:H:265:ASN:HD22	1:H:265:ASN:HA	1.59	0.43
1:K:20:VAL:O	1:K:21:ASN:C	2.61	0.43
1:K:201:SER:HA	1:K:202:PRO:HD3	1.89	0.43
1:L:433:ASN:HD22	1:L:433:ASN:HA	1.50	0.43
1:M:119:GLY:O	1:M:120:ILE:C	2.59	0.43
2:S:37:ARG:HH11	2:S:37:ARG:HG2	1.83	0.43
1:A:158:VAL:HG12	1:A:162:ILE:HD12	2.01	0.43
1:B:184:GLN:H	1:B:184:GLN:CD	2.26	0.43
1:B:432:GLN:HE21	1:B:436:GLN:HE22	1.65	0.43
1:F:479:ASN:OD1	1:F:479:ASN:C	2.62	0.43
1:H:255:GLU:O	1:H:256:GLY:C	2.62	0.43
1:I:43:SER:HB3	1:I:44:PHE:CD1	2.54	0.43
1:I:64:ASP:C	1:I:65:LYS:O	2.57	0.43
1:I:213:VAL:HB	1:I:325:ILE:CG1	2.42	0.43
1:I:346:VAL:O	1:I:350:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:GLN:HE22	1:J:75:LYS:NZ	2.16	0.43
1:J:255:GLU:O	1:J:256:GLY:C	2.62	0.43
1:K:8:PHE:O	1:K:9:GLY:C	2.60	0.43
1:L:420:ILE:HD11	1:L:448:GLU:HB3	2.01	0.43
1:M:266:THR:HG22	1:M:271:VAL:O	2.19	0.43
1:M:420:ILE:HG23	1:M:420:ILE:HD12	1.61	0.43
1:N:8:PHE:O	1:N:9:GLY:C	2.62	0.43
2:P:44:GLY:O	2:P:45:ASN:C	2.62	0.43
2:S:78:ILE:HD13	2:S:83:VAL:HG21	2.01	0.43
1:A:42:LYS:HG2	1:A:44:PHE:CD2	2.54	0.42
1:B:429:LEU:HD12	1:B:429:LEU:HA	1.72	0.42
1:D:362:ARG:HG2	1:D:366:GLN:NE2	2.33	0.42
1:F:58:ARG:H	1:F:58:ARG:HG2	1.67	0.42
1:F:153:ASN:O	1:F:154:SER:HB2	2.18	0.42
1:F:414:GLY:C	1:F:416:GLY:N	2.74	0.42
1:G:7:LYS:HB3	1:G:12:ALA:HB2	2.00	0.42
1:K:100:ILE:CG2	1:K:104:LEU:HD22	2.49	0.42
1:K:497:THR:O	1:K:498:LYS:C	2.60	0.42
1:L:7:LYS:HG2	1:L:11:ASP:HB2	2.01	0.42
1:L:502:SER:O	1:L:503:ALA:C	2.62	0.42
1:M:131:LEU:HD12	1:M:422:VAL:CG1	2.38	0.42
1:M:284:ARG:NH1	1:M:364:LYS:HD2	2.31	0.42
1:M:433:ASN:HD22	1:M:433:ASN:HA	1.55	0.42
1:N:342:ILE:O	1:N:346:VAL:HG23	2.19	0.42
1:B:252:GLU:O	1:B:253:ASP:HB2	2.19	0.42
1:B:430:ARG:NH1	1:B:430:ARG:CG	2.71	0.42
1:C:102:GLU:OE1	1:C:102:GLU:HA	2.12	0.42
1:D:234:LEU:N	1:D:235:PRO:HD2	2.34	0.42
1:G:339:GLU:HA	1:G:342:ILE:HB	2.01	0.42
1:J:233:MET:C	1:J:235:PRO:HD2	2.45	0.42
1:K:32:GLY:HA2	1:K:454:ILE:HG23	1.99	0.42
1:K:346:VAL:O	1:K:350:ARG:HB2	2.19	0.42
1:L:64:ASP:O	1:L:65:LYS:C	2.57	0.42
1:L:255:GLU:O	1:L:256:GLY:C	2.62	0.42
1:N:102:GLU:HB3	1:N:442:VAL:HG22	2.01	0.42
1:N:106:ALA:HA	1:N:111:MET:CE	2.44	0.42
1:N:429:LEU:C	1:N:430:ARG:HG2	2.43	0.42
1:A:384:ALA:O	1:G:506:TYR:HE1	2.02	0.42
1:A:452:ARG:HG2	1:A:452:ARG:HH11	1.83	0.42
1:B:200:LEU:HD13	1:B:254:VAL:HB	1.99	0.42
1:F:28:LYS:HE3	1:F:453:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:ILE:HG21	1:H:163:ALA:HA	2.01	0.42
1:H:172:GLU:O	1:H:173:GLY:O	2.37	0.42
1:I:433:ASN:HD22	1:I:433:ASN:HA	1.39	0.42
1:J:492:GLY:O	1:J:493:ILE:HD13	2.19	0.42
1:K:77:VAL:HG22	1:K:506:TYR:CD1	2.54	0.42
1:K:163:ALA:O	1:K:167:ASP:HB2	2.19	0.42
1:M:15:LYS:HD3	1:M:15:LYS:HA	1.70	0.42
1:N:501:ARG:O	1:N:502:SER:C	2.59	0.42
1:N:512:GLY:O	1:N:513:LEU:C	2.62	0.42
2:P:67:PHE:CG	2:P:86:MET:HE2	2.54	0.42
1:B:35:GLY:HA3	1:B:51:LYS:HE2	2.00	0.42
1:B:42:LYS:HG2	1:B:44:PHE:CD2	2.54	0.42
1:B:416:GLY:HA2	5:B:607:HOH:O	2.18	0.42
1:C:42:LYS:HG2	1:C:44:PHE:CE2	2.54	0.42
1:D:95:LEU:O	1:D:99:ILE:HG13	2.18	0.42
1:D:444:LEU:O	1:D:447:MET:HB2	2.19	0.42
1:E:169:VAL:HB	1:E:173:GLY:HA3	2.00	0.42
1:E:199:TYR:HB3	1:E:325:ILE:HD11	2.00	0.42
1:E:324:VAL:O	1:E:331:THR:HG22	2.19	0.42
1:E:510:VAL:O	1:E:511:ALA:C	2.62	0.42
1:H:44:PHE:CD1	1:H:44:PHE:N	2.87	0.42
1:H:420:ILE:HD12	1:H:420:ILE:HG23	1.65	0.42
1:I:131:LEU:HD12	1:I:422:VAL:CG1	2.40	0.42
1:I:266:THR:HG22	1:I:271:VAL:O	2.20	0.42
1:I:521:VAL:HG12	1:I:522:THR:N	2.33	0.42
1:I:524:LEU:HD23	1:I:524:LEU:HA	1.67	0.42
1:K:99:ILE:O	1:K:100:ILE:C	2.62	0.42
1:K:409:GLU:OE2	1:K:501:ARG:NH2	2.52	0.42
1:M:266:THR:HG21	1:M:273:VAL:H	1.84	0.42
1:N:172:GLU:O	1:N:173:GLY:C	2.62	0.42
2:S:84:LEU:N	2:S:84:LEU:CD1	2.82	0.42
2:U:41:LEU:O	2:U:61:VAL:HG13	2.19	0.42
1:A:44:PHE:HB2	1:A:45:GLY:H	1.66	0.42
1:A:169:VAL:HB	1:A:173:GLY:HA3	2.02	0.42
1:A:291:ASP:HB3	1:A:372:LEU:HD21	2.02	0.42
1:C:270:ILE:HD11	2:Q:27:LEU:HB2	1.99	0.42
1:D:23:LEU:C	1:D:23:LEU:HD13	2.45	0.42
1:E:113:PRO:O	1:E:114:MET:C	2.62	0.42
1:E:362:ARG:HG2	1:E:366:GLN:NE2	2.34	0.42
1:F:395:ARG:O	1:F:398:ASP:HB3	2.20	0.42
1:F:501:ARG:HD3	1:F:505:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:GLY:C	1:H:34:LYS:H	2.26	0.42
1:H:346:VAL:O	1:H:350:ARG:HB2	2.18	0.42
1:J:64:ASP:C	1:J:65:LYS:O	2.58	0.42
1:K:426:LEU:O	1:K:444:LEU:HD11	2.19	0.42
1:L:70:GLY:O	1:L:71:ALA:C	2.62	0.42
1:N:131:LEU:HD13	1:N:422:VAL:HG11	2.01	0.42
1:A:21:ASN:O	1:A:22:VAL:C	2.62	0.42
1:A:39:VAL:HG12	1:G:69:MET:CE	2.50	0.42
1:B:80:LYS:O	1:B:81:ALA:C	2.62	0.42
1:B:96:ALA:C	1:B:98:ALA:N	2.77	0.42
1:B:102:GLU:HB3	1:B:442:VAL:HG22	2.01	0.42
1:B:121:ASP:O	1:B:122:LYS:C	2.62	0.42
1:C:82:ASN:HB2	1:C:89:THR:HG21	2.00	0.42
1:C:487:ASN:OD1	1:C:489:ILE:N	2.52	0.42
1:D:85:ALA:O	1:D:86:GLY:C	2.62	0.42
1:E:123:ALA:HB2	1:E:440:ILE:HG23	2.00	0.42
1:E:266:THR:CG2	1:E:273:VAL:HB	2.49	0.42
1:F:477:GLY:HA3	1:F:488:MET:SD	2.59	0.42
1:K:227:ILE:HB	1:K:254:VAL:HG22	2.01	0.42
1:L:290:GLN:NE2	1:L:290:GLN:O	2.50	0.42
1:L:452:ARG:NH1	1:L:452:ARG:CG	2.75	0.42
1:L:513:LEU:HD12	1:L:513:LEU:HA	1.81	0.42
1:M:413:ALA:CB	1:M:417:VAL:HB	2.50	0.42
2:U:37:ARG:HG2	2:U:37:ARG:NH1	2.34	0.42
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.57	0.42
1:A:185:ASP:HA	1:A:380:LYS:O	2.19	0.42
1:A:266:THR:CG2	1:A:273:VAL:HB	2.50	0.42
1:D:153:ASN:ND2	1:D:153:ASN:O	2.53	0.42
1:F:24:ALA:O	1:F:28:LYS:HG3	2.19	0.42
1:F:349:ILE:HA	1:F:352:GLN:HG2	1.95	0.42
1:G:273:VAL:HG12	1:G:274:ALA:N	2.34	0.42
1:H:80:LYS:O	1:H:81:ALA:C	2.63	0.42
1:I:233:MET:HE1	1:I:249:ILE:HD12	2.02	0.42
1:I:404:ARG:CG	1:I:404:ARG:NH1	2.73	0.42
1:J:265:ASN:HD22	1:J:265:ASN:HA	1.59	0.42
1:K:77:VAL:HG22	1:K:506:TYR:HD1	1.85	0.42
1:L:205:ILE:HA	1:L:213:VAL:HG22	2.02	0.42
1:L:220:ILE:O	1:L:318:GLY:N	2.49	0.42
1:L:469:VAL:HG22	1:L:477:GLY:HA2	2.01	0.42
1:L:479:ASN:OD1	1:L:479:ASN:C	2.60	0.42
1:M:199:TYR:HA	1:M:276:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:448:GLU:O	1:M:449:ALA:C	2.62	0.42
1:N:419:LEU:HD11	1:N:504:LEU:HG	2.02	0.42
1:A:224:ASP:OD1	1:A:286:LYS:HG2	2.19	0.42
1:B:6:VAL:O	1:B:6:VAL:CG2	2.67	0.42
1:C:147:VAL:O	1:C:148:GLY:C	2.63	0.42
1:C:362:ARG:HG2	1:C:366:GLN:NE2	2.33	0.42
1:D:519:CYS:HB3	1:E:38:VAL:HG22	2.01	0.42
1:E:153:ASN:O	1:E:154:SER:CB	2.67	0.42
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.60	0.42
1:I:290:GLN:NE2	1:I:293:ALA:HB3	2.35	0.42
1:J:66:PHE:O	1:J:67:GLU:C	2.61	0.42
1:J:84:ALA:O	1:J:498:LYS:HE2	2.19	0.42
1:J:419:LEU:HD23	1:J:500:THR:CG2	2.46	0.42
1:J:524:LEU:HA	1:J:524:LEU:HD23	1.63	0.42
1:K:104:LEU:HD12	1:K:104:LEU:HA	1.63	0.42
1:K:418:ALA:HB3	5:K:531:HOH:O	2.19	0.42
1:M:174:VAL:HG21	1:M:194:GLN:HB3	2.02	0.42
1:M:363:GLU:H	1:M:363:GLU:HG2	1.65	0.42
1:B:221:LEU:HD23	1:B:249:ILE:HD12	2.02	0.42
1:B:409:GLU:CD	1:B:501:ARG:HH21	2.27	0.42
1:C:441:LYS:O	1:C:442:VAL:C	2.62	0.42
1:D:146:GLN:HE21	1:D:146:GLN:HB2	1.58	0.42
1:E:42:LYS:HE2	1:E:48:THR:CB	2.49	0.42
1:E:489:ILE:CD1	1:E:494:LEU:HD22	2.49	0.42
1:G:200:LEU:HD13	1:G:254:VAL:HB	2.02	0.42
1:G:432:GLN:H	1:G:432:GLN:HG3	1.74	0.42
1:I:200:LEU:HD21	1:I:277:LYS:HG3	2.02	0.42
1:L:284:ARG:O	1:L:288:MET:HG3	2.20	0.42
1:M:419:LEU:CD2	1:M:500:THR:HG23	2.40	0.42
1:M:433:ASN:CG	1:M:435:ASP:HB2	2.45	0.42
1:N:18:ARG:HB2	1:N:67:GLU:HG2	2.00	0.42
1:N:85:ALA:HB1	1:N:499:VAL:HB	2.02	0.42
1:A:74:VAL:O	1:A:77:VAL:CG1	2.59	0.42
1:A:246:PRO:HB3	1:A:272:LYS:HB3	2.01	0.42
1:A:261:THR:HG23	2:O:29:GLY:H	1.85	0.42
1:C:453:GLN:O	1:C:454:ILE:C	2.63	0.42
1:D:31:LEU:HD23	1:D:453:GLN:HB3	2.02	0.42
1:G:221:LEU:HD13	1:G:317:LEU:HD11	2.02	0.42
1:G:238:GLU:OE2	2:U:23:GLY:C	2.63	0.42
1:G:349:ILE:HA	1:G:352:GLN:HG2	1.92	0.42
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:ILE:O	1:I:100:ILE:C	2.61	0.42
1:K:124:VAL:HG13	1:K:504:LEU:HD13	2.01	0.42
1:L:10:ASN:O	1:L:11:ASP:C	2.61	0.42
1:L:227:ILE:HB	1:L:254:VAL:HG22	2.01	0.42
1:L:455:VAL:HG11	1:L:462:PRO:HA	2.01	0.42
1:M:77:VAL:HG22	1:M:506:TYR:CD1	2.55	0.42
1:M:417:VAL:HG21	1:M:488:MET:HG3	2.02	0.42
2:O:84:LEU:N	2:O:84:LEU:CD1	2.83	0.42
2:R:6:LEU:O	2:R:7:HIS:C	2.63	0.42
1:A:34:LYS:HD2	1:A:458:CYS:SG	2.60	0.41
1:A:197:ARG:HD2	1:A:277:LYS:HB2	2.02	0.41
1:B:87:ASP:OD1	4:B:600:ADP:O1B	2.37	0.41
1:C:455:VAL:HG21	1:C:465:VAL:HG11	2.02	0.41
1:F:221:LEU:HD13	1:F:317:LEU:HD11	2.02	0.41
1:F:443:ALA:C	1:F:447:MET:HE3	2.45	0.41
1:K:266:THR:HG21	1:K:273:VAL:H	1.85	0.41
1:L:7:LYS:HD2	1:L:66:PHE:CE2	2.55	0.41
1:L:56:VAL:O	1:L:57:ALA:C	2.63	0.41
1:A:33:PRO:HA	1:A:153:ASN:ND2	2.26	0.41
1:A:259:LEU:O	1:A:260:ALA:C	2.63	0.41
1:A:444:LEU:O	1:A:447:MET:HB2	2.19	0.41
1:D:478:TYR:CE2	1:D:480:ALA:HA	2.55	0.41
1:E:265:ASN:CA	1:E:270:ILE:HD12	2.44	0.41
1:F:449:ALA:O	1:F:450:PRO:C	2.62	0.41
1:G:74:VAL:HG13	1:G:514:MET:HE1	2.02	0.41
1:G:96:ALA:C	1:G:98:ALA:N	2.77	0.41
1:G:116:LEU:HD23	1:G:116:LEU:HA	1.67	0.41
1:I:96:ALA:O	1:I:100:ILE:HG13	2.20	0.41
1:I:210:THR:O	1:I:211:GLY:C	2.62	0.41
1:J:101:THR:HG22	1:J:105:LYS:HE3	2.02	0.41
1:J:477:GLY:O	1:J:485:TYR:HA	2.20	0.41
1:K:144:ILE:HG21	1:K:163:ALA:HA	2.02	0.41
1:L:104:LEU:HA	1:L:104:LEU:HD12	1.50	0.41
1:L:381:VAL:HG21	1:L:393:LYS:HA	2.02	0.41
1:M:255:GLU:O	1:M:256:GLY:C	2.62	0.41
1:M:409:GLU:HB2	1:M:497:THR:HB	2.01	0.41
1:N:99:ILE:O	1:N:100:ILE:C	2.63	0.41
1:E:116:LEU:HD23	1:E:116:LEU:HA	1.61	0.41
1:E:429:LEU:HD12	1:E:429:LEU:HA	1.74	0.41
1:G:10:ASN:HB2	5:G:612:HOH:O	2.18	0.41
1:G:143:ALA:HA	1:G:146:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:GLY:O	1:H:107:VAL:HG13	2.20	0.41
1:H:404:ARG:HH11	1:H:404:ARG:CG	2.29	0.41
1:I:15:LYS:HD3	1:I:15:LYS:HA	1.67	0.41
1:I:364:LYS:HD3	1:I:364:LYS:HA	1.84	0.41
1:J:23:LEU:HD11	1:J:75:LYS:HG3	2.01	0.41
1:J:88:GLY:O	1:J:91:THR:N	2.54	0.41
1:K:492:GLY:C	1:K:493:ILE:HD13	2.45	0.41
1:M:213:VAL:HB	1:M:325:ILE:CG1	2.45	0.41
1:N:34:LYS:HB2	1:N:458:CYS:SG	2.60	0.41
1:A:200:LEU:HD13	1:A:254:VAL:HB	2.01	0.41
1:A:305:ILE:HG12	1:B:267:MET:HE3	2.02	0.41
1:A:456:LEU:HD13	1:A:462:PRO:HG3	2.00	0.41
1:A:515:ILE:HG21	1:A:515:ILE:HD13	1.71	0.41
1:B:448:GLU:O	1:B:452:ARG:HD2	2.20	0.41
1:D:100:ILE:HD11	1:D:514:MET:CE	2.51	0.41
1:D:404:ARG:HG3	1:D:404:ARG:NH1	2.26	0.41
1:F:19:GLY:HA3	1:F:67:GLU:O	2.21	0.41
1:G:27:VAL:HG12	1:G:90:THR:HG23	2.03	0.41
1:G:35:GLY:HA3	1:G:51:LYS:HE2	2.02	0.41
1:G:82:ASN:HB2	1:G:89:THR:HG21	2.02	0.41
1:G:415:GLY:HA2	1:G:454:ILE:HD12	2.01	0.41
1:H:7:LYS:HD2	1:H:66:PHE:CZ	2.55	0.41
1:I:194:GLN:O	1:I:371:LYS:HE3	2.20	0.41
1:I:507:ALA:O	1:I:510:VAL:HG12	2.20	0.41
1:K:449:ALA:HB3	1:K:450:PRO:HD3	2.02	0.41
1:L:131:LEU:HD12	1:L:422:VAL:CG1	2.37	0.41
1:N:370:ALA:O	1:N:371:LYS:C	2.62	0.41
2:O:41:LEU:O	2:O:61:VAL:HG13	2.21	0.41
1:A:409:GLU:CD	1:A:498:LYS:HB2	2.45	0.41
1:E:198:GLY:C	1:E:276:VAL:HG12	2.46	0.41
1:E:515:ILE:HD13	1:E:515:ILE:HG21	1.83	0.41
1:G:451:LEU:HD23	1:G:451:LEU:O	2.21	0.41
1:G:486:GLY:CA	1:G:491:MET:HE2	2.50	0.41
1:H:290:GLN:O	1:H:290:GLN:NE2	2.53	0.41
1:I:8:PHE:O	1:I:9:GLY:C	2.63	0.41
1:J:478:TYR:HB2	1:J:485:TYR:CD2	2.55	0.41
1:K:16:MET:HG3	1:K:520:MET:SD	2.60	0.41
1:K:418:ALA:O	1:K:422:VAL:HG13	2.20	0.41
1:K:441:LYS:O	1:K:442:VAL:C	2.63	0.41
1:K:511:ALA:O	1:K:515:ILE:HD12	2.20	0.41
1:L:174:VAL:HG21	1:L:194:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:MET:C	1:L:235:PRO:HD2	2.45	0.41
1:L:412:VAL:CG2	1:L:418:ALA:HB2	2.50	0.41
1:M:173:GLY:O	1:M:175:ILE:HG13	2.21	0.41
1:M:301:ILE:HG21	1:M:309:LEU:HD23	2.01	0.41
2:R:78:ILE:HD13	2:R:83:VAL:HG21	2.02	0.41
1:A:69:MET:O	1:A:73:MET:HG3	2.21	0.41
1:A:190:VAL:HG11	1:A:194:GLN:NE2	2.36	0.41
1:A:460:GLU:O	1:A:462:PRO:HD3	2.21	0.41
1:B:169:VAL:HB	1:B:173:GLY:HA3	2.02	0.41
1:C:234:LEU:N	1:C:235:PRO:HD2	2.35	0.41
1:D:221:LEU:HD13	1:D:317:LEU:HD11	2.02	0.41
1:D:305:ILE:HG23	1:E:267:MET:HE3	2.03	0.41
1:G:194:GLN:CG	1:G:331:THR:HB	2.51	0.41
1:G:395:ARG:O	1:G:398:ASP:CB	2.69	0.41
1:J:172:GLU:O	1:J:173:GLY:C	2.63	0.41
1:J:346:VAL:O	1:J:350:ARG:HB2	2.21	0.41
1:J:502:SER:O	1:J:503:ALA:C	2.64	0.41
1:K:345:ARG:HA	1:K:348:GLN:HE21	1.85	0.41
1:L:91:THR:O	1:L:92:ALA:C	2.63	0.41
1:L:437:ASN:HA	1:L:440:ILE:HD12	2.02	0.41
1:M:32:GLY:HA2	1:M:454:ILE:HG23	2.01	0.41
1:M:193:MET:CE	1:M:195:PHE:CD1	2.98	0.41
1:M:479:ASN:OD1	1:M:479:ASN:C	2.63	0.41
1:N:66:PHE:O	1:N:67:GLU:C	2.62	0.41
1:A:62:LEU:HD12	1:A:62:LEU:HA	1.80	0.41
1:A:66:PHE:O	1:A:67:GLU:C	2.63	0.41
1:A:432:GLN:HE21	1:A:436:GLN:HE22	1.67	0.41
1:A:487:ASN:OD1	1:A:487:ASN:C	2.64	0.41
1:B:20:VAL:HG13	1:B:74:VAL:HG21	2.01	0.41
1:B:153:ASN:ND2	1:B:153:ASN:O	2.54	0.41
1:B:402:ALA:HB1	1:B:496:PRO:HG2	2.01	0.41
1:B:489:ILE:HD13	1:B:494:LEU:HD22	2.03	0.41
1:D:150:ILE:HG21	1:D:494:LEU:O	2.20	0.41
1:D:270:ILE:CD1	2:R:27:LEU:HB2	2.51	0.41
1:D:420:ILE:HD13	1:D:451:LEU:HD13	2.02	0.41
1:E:414:GLY:C	1:E:416:GLY:N	2.73	0.41
1:E:432:GLN:HE21	1:E:436:GLN:NE2	2.17	0.41
1:F:430:ARG:NH1	1:F:430:ARG:CG	2.77	0.41
1:G:20:VAL:HG13	1:G:74:VAL:HG21	2.02	0.41
1:G:291:ASP:HB3	1:G:372:LEU:HD21	2.03	0.41
1:G:314:LEU:O	1:G:317:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:513:LEU:HA	1:G:513:LEU:HD23	1.67	0.41
1:H:129:GLU:O	1:H:132:LYS:N	2.54	0.41
1:H:227:ILE:HB	1:H:254:VAL:HG22	2.03	0.41
1:K:194:GLN:HG3	1:K:331:THR:HB	2.03	0.41
1:L:66:PHE:N	1:L:69:MET:HE3	2.35	0.41
1:M:284:ARG:O	1:M:288:MET:HG3	2.21	0.41
1:B:519:CYS:HB3	1:C:38:VAL:HG22	2.03	0.41
1:C:419:LEU:HG	1:C:447:MET:HG2	2.02	0.41
1:D:524:LEU:HD23	1:D:525:PRO:HD2	2.02	0.41
1:F:76:GLU:O	1:F:76:GLU:HG2	2.21	0.41
1:F:184:GLN:H	1:F:184:GLN:CD	2.29	0.41
1:F:460:GLU:O	1:F:462:PRO:HD3	2.20	0.41
1:G:19:GLY:HA3	1:G:67:GLU:O	2.21	0.41
1:I:460:GLU:H	1:I:460:GLU:HG2	1.70	0.41
1:J:389:MET:C	1:J:389:MET:HE2	2.46	0.41
1:J:513:LEU:HD12	1:J:513:LEU:HA	1.61	0.41
1:K:266:THR:HG22	1:K:271:VAL:O	2.21	0.41
1:K:278:ALA:HB1	1:K:279:PRO:HD2	2.01	0.41
1:K:433:ASN:CG	1:K:435:ASP:HB2	2.45	0.41
1:L:61:GLU:HG2	1:M:3:ALA:HA	2.02	0.41
1:L:389:MET:HE2	1:L:389:MET:C	2.46	0.41
1:N:22:VAL:HG11	1:N:62:LEU:CD2	2.51	0.41
1:A:61:GLU:C	1:A:62:LEU:HD13	2.46	0.41
1:A:276:VAL:CG1	1:A:325:ILE:HD12	2.51	0.41
1:A:501:ARG:HD3	1:A:505:GLN:OE1	2.21	0.41
1:B:42:LYS:HE2	1:B:48:THR:OG1	2.20	0.41
1:B:111:MET:O	1:B:113:PRO:HD3	2.21	0.41
1:B:456:LEU:HD13	1:B:462:PRO:CG	2.50	0.41
1:C:73:MET:CE	1:C:73:MET:CG	2.98	0.41
1:C:513:LEU:HA	1:C:513:LEU:HD23	1.76	0.41
1:D:91:THR:O	1:D:92:ALA:C	2.63	0.41
1:D:96:ALA:C	1:D:98:ALA:H	2.28	0.41
1:D:147:VAL:O	1:D:148:GLY:C	2.63	0.41
1:D:448:GLU:HB3	1:D:452:ARG:HD2	2.03	0.41
1:E:21:ASN:HD22	1:E:21:ASN:HA	1.60	0.41
1:E:524:LEU:HD22	1:E:525:PRO:HD2	2.01	0.41
1:F:4:LYS:HG3	1:G:59:GLU:O	2.21	0.41
1:F:69:MET:CE	1:G:39:VAL:HG12	2.51	0.41
1:F:429:LEU:HD12	1:F:429:LEU:HA	1.83	0.41
1:G:54:VAL:O	1:G:58:ARG:HG3	2.21	0.41
1:G:224:ASP:OD1	1:G:286:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:455:VAL:HG21	1:G:465:VAL:CG1	2.51	0.41
1:G:524:LEU:HD23	1:G:525:PRO:HD2	2.03	0.41
1:H:144:ILE:HD11	1:H:407:VAL:HG22	2.02	0.41
1:H:290:GLN:O	1:H:293:ALA:HB3	2.21	0.41
1:H:419:LEU:HD23	1:H:500:THR:CG2	2.42	0.41
1:I:284:ARG:O	1:I:288:MET:HG3	2.21	0.41
1:I:412:VAL:CG2	1:I:418:ALA:HB2	2.51	0.41
1:I:417:VAL:HG21	1:I:488:MET:HG3	2.03	0.41
1:I:465:VAL:HG11	1:I:478:TYR:CD2	2.56	0.41
1:J:290:GLN:NE2	1:J:293:ALA:HB3	2.35	0.41
1:L:95:LEU:HD23	1:L:446:ALA:O	2.20	0.41
1:L:172:GLU:O	1:L:173:GLY:C	2.64	0.41
1:L:236:VAL:HG22	1:L:312:ALA:O	2.20	0.41
1:L:325:ILE:HA	1:L:329:THR:O	2.21	0.41
1:M:77:VAL:HG22	1:M:506:TYR:HD1	1.85	0.41
1:M:193:MET:H	1:M:376:VAL:HG21	1.86	0.41
1:M:290:GLN:O	1:M:293:ALA:HB3	2.21	0.41
1:N:174:VAL:CG2	1:N:194:GLN:HB3	2.48	0.41
2:P:86:MET:HG3	2:P:90:ASP:HB2	2.03	0.41
2:Q:11:ILE:HG12	2:Q:85:ILE:HG12	2.01	0.41
2:S:60:LYS:HG2	2:S:63:ASP:OD2	2.21	0.41
1:B:443:ALA:O	1:B:444:LEU:C	2.64	0.41
1:C:69:MET:O	1:C:70:GLY:C	2.63	0.41
1:D:169:VAL:HB	1:D:173:GLY:HA3	2.03	0.41
1:E:270:ILE:HG12	2:S:27:LEU:HD13	2.03	0.41
1:G:403:THR:O	1:G:404:ARG:C	2.64	0.41
1:I:266:THR:HG21	1:I:273:VAL:H	1.85	0.41
1:I:345:ARG:HA	1:I:348:GLN:HE21	1.86	0.41
1:J:99:ILE:O	1:J:100:ILE:C	2.64	0.41
1:K:265:ASN:HD22	1:K:265:ASN:HA	1.60	0.41
1:M:345:ARG:HA	1:M:348:GLN:HE21	1.86	0.41
1:M:365:LEU:O	1:M:369:VAL:HG13	2.21	0.41
1:M:453:GLN:O	1:M:454:ILE:C	2.63	0.41
1:N:174:VAL:HG11	1:N:194:GLN:HB2	2.03	0.41
1:N:363:GLU:H	1:N:363:GLU:HG2	1.63	0.41
2:O:55:LYS:HE2	2:O:55:LYS:H	1.86	0.41
2:T:67:PHE:CG	2:T:86:MET:HE2	2.56	0.41
1:A:426:LEU:C	1:A:428:ASP:N	2.78	0.40
1:A:473:ASP:O	1:A:474:GLY:C	2.63	0.40
1:B:402:ALA:O	1:B:405:ALA:HB3	2.21	0.40
1:C:443:ALA:O	1:C:444:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ILE:CG2	1:E:151:SER:N	2.84	0.40
1:F:91:THR:O	1:F:92:ALA:C	2.63	0.40
1:F:524:LEU:HD23	1:F:525:PRO:HD2	2.03	0.40
1:G:259:LEU:O	1:G:260:ALA:C	2.64	0.40
1:H:364:LYS:HA	1:H:364:LYS:HD3	1.90	0.40
1:L:135:SER:HA	1:L:412:VAL:HG12	2.03	0.40
1:L:465:VAL:HG11	1:L:478:TYR:CD2	2.57	0.40
1:M:227:ILE:HB	1:M:254:VAL:HG22	2.03	0.40
1:N:469:VAL:HG22	1:N:477:GLY:HA2	2.02	0.40
1:N:504:LEU:HD23	1:N:504:LEU:HA	1.77	0.40
2:U:7:HIS:O	2:U:7:HIS:ND1	2.53	0.40
1:C:165:ALA:C	1:C:167:ASP:N	2.78	0.40
1:C:199:TYR:CZ	1:C:205:ILE:HD11	2.57	0.40
1:D:44:PHE:HD1	1:D:44:PHE:N	1.97	0.40
1:E:96:ALA:C	1:E:98:ALA:N	2.76	0.40
1:E:112:ASN:HA	1:E:113:PRO:HD3	1.86	0.40
1:F:23:LEU:C	1:F:23:LEU:HD13	2.46	0.40
1:H:77:VAL:HG22	1:H:506:TYR:CD1	2.56	0.40
1:H:522:THR:OG1	1:H:523:ASP:N	2.55	0.40
1:I:416:GLY:O	1:I:419:LEU:N	2.51	0.40
1:I:475:ASN:CG	1:I:489:ILE:HD12	2.46	0.40
1:J:519:CYS:SG	1:J:520:MET:N	2.94	0.40
1:L:32:GLY:HA2	1:L:454:ILE:CD1	2.49	0.40
1:L:72:GLN:HE22	1:L:75:LYS:NZ	2.20	0.40
1:L:169:VAL:HG13	1:L:173:GLY:HA3	2.03	0.40
1:L:199:TYR:HA	1:L:276:VAL:HG12	2.02	0.40
1:L:266:THR:HG22	1:L:271:VAL:O	2.21	0.40
1:M:47:PRO:HG2	1:N:73:MET:CG	2.47	0.40
1:M:111:MET:CE	1:M:111:MET:CG	2.97	0.40
1:M:162:ILE:O	1:M:163:ALA:C	2.64	0.40
1:N:31:LEU:O	1:N:32:GLY:O	2.40	0.40
2:P:6:LEU:O	2:P:7:HIS:C	2.63	0.40
1:A:362:ARG:HG2	1:A:366:GLN:NE2	2.37	0.40
1:B:486:GLY:CA	1:B:491:MET:CE	2.96	0.40
1:C:232:GLU:HA	1:C:310:GLU:CD	2.46	0.40
1:D:58:ARG:HA	1:D:75:LYS:HE2	2.02	0.40
1:D:314:LEU:O	1:D:317:LEU:HB2	2.21	0.40
1:D:399:ALA:O	1:D:400:LEU:C	2.65	0.40
1:D:479:ASN:OD1	1:D:479:ASN:C	2.64	0.40
1:E:124:VAL:HG13	1:E:504:LEU:HD13	2.02	0.40
1:F:100:ILE:O	1:F:101:THR:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:GLU:O	1:F:435:ASP:C	2.62	0.40
1:G:34:LYS:HD2	1:G:458:CYS:SG	2.61	0.40
1:G:252:GLU:O	1:G:253:ASP:HB2	2.22	0.40
1:G:381:VAL:CG1	1:G:392:LYS:HG2	2.46	0.40
1:H:31:LEU:H	1:H:457:ASN:ND2	2.20	0.40
1:H:345:ARG:HA	1:H:348:GLN:HE21	1.87	0.40
1:J:38:VAL:HG22	1:K:519:CYS:HB3	2.02	0.40
1:J:501:ARG:O	1:J:502:SER:C	2.63	0.40
1:K:10:ASN:O	1:K:11:ASP:C	2.65	0.40
1:K:124:VAL:O	1:K:128:VAL:HG23	2.22	0.40
1:K:222:LEU:CD1	1:K:293:ALA:HA	2.52	0.40
1:K:325:ILE:CG2	1:K:330:THR:HG23	2.52	0.40
1:K:365:LEU:O	1:K:369:VAL:HG13	2.20	0.40
1:L:225:LYS:HE3	1:L:232:GLU:OE2	2.22	0.40
2:R:44:GLY:O	2:R:45:ASN:C	2.62	0.40
1:A:475:ASN:N	1:A:475:ASN:HD22	2.16	0.40
1:B:20:VAL:HG23	1:B:20:VAL:H	1.62	0.40
1:E:197:ARG:HD2	1:E:277:LYS:HB2	2.03	0.40
1:E:413:ALA:HB1	1:E:417:VAL:HG13	2.03	0.40
1:G:417:VAL:HA	1:G:420:ILE:HG22	2.01	0.40
1:I:420:ILE:HG21	1:I:469:VAL:HG12	2.04	0.40
1:J:524:LEU:HD22	1:J:525:PRO:HD2	2.02	0.40
1:K:80:LYS:HA	1:K:83:ASP:HB2	2.02	0.40
1:K:106:ALA:O	1:K:107:VAL:C	2.62	0.40
1:K:127:ALA:O	1:K:128:VAL:C	2.63	0.40
1:L:321:LYS:HB2	1:L:334:ASP:HB3	2.02	0.40
1:L:524:LEU:HD23	1:L:525:PRO:HD2	2.02	0.40
1:M:451:LEU:O	1:M:452:ARG:C	2.63	0.40
1:N:18:ARG:HB2	1:N:67:GLU:CG	2.52	0.40
1:N:221:LEU:HD12	1:N:222:LEU:N	2.37	0.40
1:N:478:TYR:HB2	1:N:485:TYR:CD2	2.56	0.40
1:A:193:MET:HG3	1:A:194:GLN:N	2.35	0.40
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.54	0.40
1:B:270:ILE:CD1	2:P:27:LEU:HB2	2.52	0.40
1:C:28:LYS:HD2	1:C:453:GLN:NE2	2.36	0.40
1:C:77:VAL:CG2	1:C:92:ALA:HB1	2.50	0.40
1:D:194:GLN:HG3	1:D:330:THR:O	2.22	0.40
1:E:64:ASP:HB3	1:E:67:GLU:HB2	2.02	0.40
1:E:165:ALA:O	1:E:166:MET:C	2.64	0.40
1:E:434:GLU:O	1:E:435:ASP:C	2.64	0.40
1:F:73:MET:O	1:F:74:VAL:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:VAL:HB	1:F:173:GLY:HA3	2.03	0.40
1:F:489:ILE:HD13	1:F:494:LEU:HD22	2.03	0.40
1:G:13:ARG:O	1:G:14:VAL:C	2.60	0.40
1:G:14:VAL:O	1:G:15:LYS:C	2.61	0.40
1:H:42:LYS:O	1:H:43:SER:C	2.65	0.40
1:H:365:LEU:O	1:H:369:VAL:HG13	2.21	0.40
1:I:102:GLU:OE2	1:I:445:ARG:NH1	2.54	0.40
1:I:265:ASN:HD22	1:I:265:ASN:HA	1.59	0.40
1:I:290:GLN:O	1:I:293:ALA:HB3	2.22	0.40
1:I:392:LYS:O	1:I:396:VAL:HG23	2.22	0.40
1:J:119:GLY:O	1:J:120:ILE:C	2.65	0.40
1:J:419:LEU:O	1:J:420:ILE:C	2.63	0.40
1:K:506:TYR:O	1:K:507:ALA:C	2.62	0.40
1:L:15:LYS:HE2	1:L:18:ARG:HH12	1.86	0.40
1:L:23:LEU:HD11	1:L:75:LYS:HG3	2.03	0.40
1:M:129:GLU:O	1:M:132:LYS:N	2.54	0.40
1:M:288:MET:HG2	1:M:368:ARG:HD3	2.03	0.40
1:N:129:GLU:O	1:N:132:LYS:N	2.54	0.40
2:T:55:LYS:H	2:T:55:LYS:HE2	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:354:GLU:OE1	1:L:354:GLU:OE1[2_655]	1.71	0.49

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	522/524 (100%)	478 (92%)	40 (8%)	4 (1%)	16 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	522/524 (100%)	477 (91%)	39 (8%)	6 (1%)	11	43
1	C	522/524 (100%)	475 (91%)	41 (8%)	6 (1%)	11	43
1	D	522/524 (100%)	475 (91%)	41 (8%)	6 (1%)	11	43
1	E	522/524 (100%)	477 (91%)	40 (8%)	5 (1%)	12	45
1	F	522/524 (100%)	478 (92%)	38 (7%)	6 (1%)	11	43
1	G	522/524 (100%)	473 (91%)	44 (8%)	5 (1%)	12	45
1	H	522/524 (100%)	473 (91%)	39 (8%)	10 (2%)	6	30
1	I	522/524 (100%)	474 (91%)	35 (7%)	13 (2%)	4	23
1	J	522/524 (100%)	473 (91%)	41 (8%)	8 (2%)	8	35
1	K	522/524 (100%)	471 (90%)	42 (8%)	9 (2%)	7	32
1	L	522/524 (100%)	476 (91%)	36 (7%)	10 (2%)	6	30
1	M	522/524 (100%)	469 (90%)	42 (8%)	11 (2%)	5	27
1	N	522/524 (100%)	470 (90%)	40 (8%)	12 (2%)	5	25
2	O	95/97 (98%)	75 (79%)	12 (13%)	8 (8%)	0	3
2	P	95/97 (98%)	75 (79%)	12 (13%)	8 (8%)	0	3
2	Q	95/97 (98%)	75 (79%)	12 (13%)	8 (8%)	0	3
2	R	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	0	3
2	S	95/97 (98%)	75 (79%)	12 (13%)	8 (8%)	0	3
2	T	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	0	3
2	U	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	0	3
All	All	7973/8015 (100%)	7159 (90%)	647 (8%)	167 (2%)	5	27

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	B	44	PHE
1	B	483	GLU
1	C	9	GLY
1	C	44	PHE
1	D	44	PHE
1	E	44	PHE
1	F	44	PHE
1	G	44	PHE
1	I	173	GLY

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Mol	Chain	Res	Type
1	M	173	GLY
1	M	463	SER
2	O	7	HIS
2	O	17	VAL
2	P	7	HIS
2	P	17	VAL
2	Q	7	HIS
2	Q	17	VAL
2	R	7	HIS
2	R	17	VAL
2	S	7	HIS
2	S	17	VAL
2	T	7	HIS
2	T	17	VAL
2	U	7	HIS
2	U	17	VAL
1	A	256	GLY
1	B	58	ARG
1	B	498	LYS
1	C	58	ARG
1	C	256	GLY
1	D	58	ARG
1	D	256	GLY
1	D	483	GLU
1	E	154	SER
1	E	256	GLY
1	F	58	ARG
1	G	9	GLY
1	G	256	GLY
1	H	32	GLY
1	H	173	GLY
1	H	256	GLY
1	H	462	PRO
1	I	53	GLY
1	I	66	PHE
1	I	256	GLY
1	I	417	VAL
1	J	43	SER
1	J	173	GLY
1	J	256	GLY
1	K	32	GLY
1	K	173	GLY

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Mol	Chain	Res	Type
1	K	256	GLY
1	L	32	GLY
1	L	173	GLY
1	L	256	GLY
1	L	417	VAL
1	L	462	PRO
1	L	463	SER
1	M	32	GLY
1	M	66	PHE
1	M	193	MET
1	M	256	GLY
1	M	462	PRO
1	N	32	GLY
1	N	43	SER
1	N	66	PHE
1	N	173	GLY
1	N	256	GLY
1	N	462	PRO
1	N	463	SER
2	O	52	GLY
2	P	52	GLY
2	Q	49	LEU
2	Q	52	GLY
2	R	52	GLY
2	S	49	LEU
2	S	52	GLY
2	T	52	GLY
2	T	80	ASN
2	U	49	LEU
2	U	80	ASN
1	B	154	SER
1	B	256	GLY
1	C	154	SER
1	E	483	GLU
1	F	256	GLY
1	G	58	ARG
1	H	43	SER
1	H	66	PHE
1	H	257	GLU
1	H	315	GLU
1	I	43	SER
1	I	442	VAL

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Mol	Chain	Res	Type
1	I	462	PRO
1	J	66	PHE
1	J	89	THR
1	J	257	GLU
1	J	462	PRO
1	K	43	SER
1	K	66	PHE
1	K	89	THR
1	K	257	GLU
1	K	462	PRO
1	K	463	SER
1	L	257	GLU
1	M	43	SER
1	N	89	THR
2	O	49	LEU
2	O	80	ASN
2	P	8	ASP
2	P	49	LEU
2	P	80	ASN
2	Q	8	ASP
2	Q	80	ASN
2	R	28	THR
2	R	49	LEU
2	R	80	ASN
2	S	8	ASP
2	S	80	ASN
2	T	8	ASP
2	T	49	LEU
2	U	8	ASP
2	U	52	GLY
1	C	81	ALA
1	D	154	SER
1	G	447	MET
1	I	9	GLY
1	I	257	GLU
1	L	43	SER
1	L	66	PHE
1	M	257	GLU
1	N	9	GLY
1	N	257	GLU
1	N	315	GLU
2	O	28	THR

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Mol	Chain	Res	Type
2	P	21	SER
2	R	21	SER
2	S	21	SER
2	S	28	THR
2	T	28	THR
2	U	28	THR
1	A	334	ASP
1	F	81	ALA
1	F	154	SER
1	H	463	SER
1	I	334	ASP
1	M	89	THR
1	N	193	MET
2	O	8	ASP
2	O	21	SER
2	P	28	THR
2	Q	21	SER
2	Q	28	THR
2	R	8	ASP
2	T	21	SER
2	U	21	SER
1	F	483	GLU
1	I	154	SER
1	J	120	ILE
1	H	9	GLY
1	I	32	GLY
1	L	442	VAL
1	A	47	PRO
1	E	9	GLY
1	M	442	VAL
1	D	9	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	331 (82%)	73 (18%)	2	9
1	B	404/404 (100%)	333 (82%)	71 (18%)	2	10
1	C	404/404 (100%)	330 (82%)	74 (18%)	2	9
1	D	404/404 (100%)	333 (82%)	71 (18%)	2	10
1	E	404/404 (100%)	329 (81%)	75 (19%)	1	9
1	F	404/404 (100%)	330 (82%)	74 (18%)	2	9
1	G	404/404 (100%)	331 (82%)	73 (18%)	2	9
1	H	404/404 (100%)	331 (82%)	73 (18%)	2	9
1	I	404/404 (100%)	328 (81%)	76 (19%)	1	9
1	J	404/404 (100%)	327 (81%)	77 (19%)	1	8
1	K	404/404 (100%)	330 (82%)	74 (18%)	2	9
1	L	404/404 (100%)	329 (81%)	75 (19%)	1	9
1	M	404/404 (100%)	328 (81%)	76 (19%)	1	9
1	N	404/404 (100%)	328 (81%)	76 (19%)	1	9
2	O	80/80 (100%)	65 (81%)	15 (19%)	1	9
2	P	80/80 (100%)	65 (81%)	15 (19%)	1	9
2	Q	80/80 (100%)	65 (81%)	15 (19%)	1	9
2	R	80/80 (100%)	65 (81%)	15 (19%)	1	9
2	S	80/80 (100%)	65 (81%)	15 (19%)	1	9
2	T	80/80 (100%)	65 (81%)	15 (19%)	1	9
2	U	80/80 (100%)	65 (81%)	15 (19%)	1	9
All	All	6216/6216 (100%)	5073 (82%)	1143 (18%)	1	9

All (1143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	18	ARG
1	A	23	LEU
1	A	43	SER
1	A	44	PHE
1	A	48	THR
1	A	52	ASP

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Mol	Chain	Res	Type
1	A	58	ARG
1	A	62	LEU
1	A	63	GLU
1	A	74	VAL
1	A	77	VAL
1	A	79	SER
1	A	80	LYS
1	A	97	GLN
1	A	129	GLU
1	A	141	SER
1	A	147	VAL
1	A	150	ILE
1	A	168	LYS
1	A	174	VAL
1	A	176	THR
1	A	177	VAL
1	A	181	THR
1	A	183	LEU
1	A	184	GLN
1	A	190	VAL
1	A	193	MET
1	A	209	GLU
1	A	215	LEU
1	A	230	ILE
1	A	231	ARG
1	A	272	LYS
1	A	276	VAL
1	A	284	ARG
1	A	288	MET
1	A	289	LEU
1	A	295	LEU
1	A	317	LEU
1	A	322	ARG
1	A	323	VAL
1	A	325	ILE
1	A	328	ASP
1	A	331	THR
1	A	350	ARG
1	A	355	GLU
1	A	358	SER
1	A	368	ARG
1	A	379	ILE

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Mol	Chain	Res	Type
1	A	381	VAL
1	A	387	VAL
1	A	388	GLU
1	A	391	GLU
1	A	398	ASP
1	A	400	LEU
1	A	404	ARG
1	A	417	VAL
1	A	419	LEU
1	A	420	ILE
1	A	422	VAL
1	A	430	ARG
1	A	432	GLN
1	A	442	VAL
1	A	447	MET
1	A	454	ILE
1	A	461	GLU
1	A	463	SER
1	A	470	LYS
1	A	483	GLU
1	A	494	LEU
1	A	499	VAL
1	A	504	LEU
1	A	510	VAL
1	B	11	ASP
1	B	18	ARG
1	B	23	LEU
1	B	42	LYS
1	B	43	SER
1	B	44	PHE
1	B	48	THR
1	B	58	ARG
1	B	62	LEU
1	B	63	GLU
1	B	74	VAL
1	B	77	VAL
1	B	80	LYS
1	B	97	GLN
1	B	129	GLU
1	B	138	CYS
1	B	141	SER
1	B	147	VAL

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Mol	Chain	Res	Type
1	B	150	ILE
1	B	157	THR
1	B	168	LYS
1	B	174	VAL
1	B	176	THR
1	B	177	VAL
1	B	183	LEU
1	B	184	GLN
1	B	190	VAL
1	B	193	MET
1	B	209	GLU
1	B	215	LEU
1	B	230	ILE
1	B	231	ARG
1	B	242	LYS
1	B	276	VAL
1	B	284	ARG
1	B	288	MET
1	B	289	LEU
1	B	295	LEU
1	B	317	LEU
1	B	322	ARG
1	B	323	VAL
1	B	325	ILE
1	B	328	ASP
1	B	331	THR
1	B	350	ARG
1	B	355	GLU
1	B	358	SER
1	B	381	VAL
1	B	387	VAL
1	B	388	GLU
1	B	391	GLU
1	B	398	ASP
1	B	400	LEU
1	B	404	ARG
1	B	417	VAL
1	B	419	LEU
1	B	420	ILE
1	B	422	VAL
1	B	430	ARG
1	B	442	VAL

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Mol	Chain	Res	Type
1	B	447	MET
1	B	452	ARG
1	B	461	GLU
1	B	463	SER
1	B	464	VAL
1	B	470	LYS
1	B	483	GLU
1	B	484	GLU
1	B	499	VAL
1	B	504	LEU
1	B	510	VAL
1	C	6	VAL
1	C	7	LYS
1	C	10	ASN
1	C	11	ASP
1	C	18	ARG
1	C	23	LEU
1	C	42	LYS
1	C	43	SER
1	C	44	PHE
1	C	48	THR
1	C	58	ARG
1	C	62	LEU
1	C	63	GLU
1	C	74	VAL
1	C	77	VAL
1	C	80	LYS
1	C	97	GLN
1	C	102	GLU
1	C	129	GLU
1	C	138	CYS
1	C	141	SER
1	C	144	ILE
1	C	147	VAL
1	C	150	ILE
1	C	157	THR
1	C	164	GLU
1	C	168	LYS
1	C	174	VAL
1	C	176	THR
1	C	177	VAL
1	C	183	LEU

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Mol	Chain	Res	Type
1	C	184	GLN
1	C	190	VAL
1	C	193	MET
1	C	209	GLU
1	C	215	LEU
1	C	230	ILE
1	C	231	ARG
1	C	272	LYS
1	C	276	VAL
1	C	284	ARG
1	C	288	MET
1	C	289	LEU
1	C	295	LEU
1	C	317	LEU
1	C	322	ARG
1	C	323	VAL
1	C	325	ILE
1	C	328	ASP
1	C	331	THR
1	C	350	ARG
1	C	355	GLU
1	C	358	SER
1	C	381	VAL
1	C	387	VAL
1	C	388	GLU
1	C	391	GLU
1	C	392	LYS
1	C	398	ASP
1	C	400	LEU
1	C	404	ARG
1	C	417	VAL
1	C	419	LEU
1	C	420	ILE
1	C	422	VAL
1	C	430	ARG
1	C	442	VAL
1	C	447	MET
1	C	452	ARG
1	C	461	GLU
1	C	483	GLU
1	C	499	VAL
1	C	504	LEU

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Mol	Chain	Res	Type
1	C	510	VAL
1	D	11	ASP
1	D	18	ARG
1	D	23	LEU
1	D	42	LYS
1	D	43	SER
1	D	44	PHE
1	D	48	THR
1	D	54	VAL
1	D	58	ARG
1	D	62	LEU
1	D	63	GLU
1	D	74	VAL
1	D	77	VAL
1	D	80	LYS
1	D	97	GLN
1	D	129	GLU
1	D	138	CYS
1	D	141	SER
1	D	147	VAL
1	D	150	ILE
1	D	157	THR
1	D	168	LYS
1	D	174	VAL
1	D	176	THR
1	D	177	VAL
1	D	183	LEU
1	D	184	GLN
1	D	190	VAL
1	D	193	MET
1	D	209	GLU
1	D	215	LEU
1	D	230	ILE
1	D	231	ARG
1	D	276	VAL
1	D	284	ARG
1	D	288	MET
1	D	289	LEU
1	D	295	LEU
1	D	317	LEU
1	D	322	ARG
1	D	323	VAL

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Mol	Chain	Res	Type
1	D	325	ILE
1	D	328	ASP
1	D	331	THR
1	D	350	ARG
1	D	355	GLU
1	D	358	SER
1	D	379	ILE
1	D	381	VAL
1	D	387	VAL
1	D	388	GLU
1	D	391	GLU
1	D	398	ASP
1	D	400	LEU
1	D	404	ARG
1	D	417	VAL
1	D	419	LEU
1	D	420	ILE
1	D	422	VAL
1	D	430	ARG
1	D	432	GLN
1	D	442	VAL
1	D	447	MET
1	D	454	ILE
1	D	461	GLU
1	D	463	SER
1	D	483	GLU
1	D	484	GLU
1	D	499	VAL
1	D	504	LEU
1	D	510	VAL
1	E	11	ASP
1	E	18	ARG
1	E	23	LEU
1	E	42	LYS
1	E	43	SER
1	E	44	PHE
1	E	48	THR
1	E	52	ASP
1	E	58	ARG
1	E	62	LEU
1	E	63	GLU
1	E	74	VAL

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Mol	Chain	Res	Type
1	E	77	VAL
1	E	80	LYS
1	E	97	GLN
1	E	129	GLU
1	E	138	CYS
1	E	141	SER
1	E	147	VAL
1	E	150	ILE
1	E	157	THR
1	E	168	LYS
1	E	172	GLU
1	E	174	VAL
1	E	176	THR
1	E	177	VAL
1	E	181	THR
1	E	183	LEU
1	E	184	GLN
1	E	190	VAL
1	E	193	MET
1	E	209	GLU
1	E	215	LEU
1	E	230	ILE
1	E	231	ARG
1	E	276	VAL
1	E	284	ARG
1	E	288	MET
1	E	289	LEU
1	E	295	LEU
1	E	317	LEU
1	E	322	ARG
1	E	323	VAL
1	E	325	ILE
1	E	328	ASP
1	E	350	ARG
1	E	355	GLU
1	E	358	SER
1	E	379	ILE
1	E	381	VAL
1	E	387	VAL
1	E	388	GLU
1	E	391	GLU
1	E	392	LYS

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Mol	Chain	Res	Type
1	E	398	ASP
1	E	400	LEU
1	E	404	ARG
1	E	417	VAL
1	E	419	LEU
1	E	420	ILE
1	E	422	VAL
1	E	430	ARG
1	E	432	GLN
1	E	442	VAL
1	E	447	MET
1	E	452	ARG
1	E	461	GLU
1	E	463	SER
1	E	464	VAL
1	E	470	LYS
1	E	483	GLU
1	E	484	GLU
1	E	499	VAL
1	E	504	LEU
1	E	510	VAL
1	F	6	VAL
1	F	7	LYS
1	F	11	ASP
1	F	18	ARG
1	F	23	LEU
1	F	42	LYS
1	F	43	SER
1	F	44	PHE
1	F	48	THR
1	F	58	ARG
1	F	62	LEU
1	F	63	GLU
1	F	74	VAL
1	F	77	VAL
1	F	80	LYS
1	F	97	GLN
1	F	129	GLU
1	F	138	CYS
1	F	141	SER
1	F	147	VAL
1	F	150	ILE

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Mol	Chain	Res	Type
1	F	157	THR
1	F	168	LYS
1	F	174	VAL
1	F	176	THR
1	F	177	VAL
1	F	181	THR
1	F	183	LEU
1	F	184	GLN
1	F	190	VAL
1	F	193	MET
1	F	209	GLU
1	F	215	LEU
1	F	230	ILE
1	F	231	ARG
1	F	272	LYS
1	F	276	VAL
1	F	284	ARG
1	F	288	MET
1	F	289	LEU
1	F	295	LEU
1	F	317	LEU
1	F	322	ARG
1	F	323	VAL
1	F	325	ILE
1	F	328	ASP
1	F	331	THR
1	F	350	ARG
1	F	355	GLU
1	F	358	SER
1	F	381	VAL
1	F	387	VAL
1	F	388	GLU
1	F	391	GLU
1	F	392	LYS
1	F	398	ASP
1	F	400	LEU
1	F	404	ARG
1	F	417	VAL
1	F	419	LEU
1	F	420	ILE
1	F	422	VAL
1	F	430	ARG

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Mol	Chain	Res	Type
1	F	432	GLN
1	F	442	VAL
1	F	447	MET
1	F	452	ARG
1	F	461	GLU
1	F	463	SER
1	F	483	GLU
1	F	484	GLU
1	F	499	VAL
1	F	504	LEU
1	F	510	VAL
1	G	11	ASP
1	G	15	LYS
1	G	18	ARG
1	G	23	LEU
1	G	42	LYS
1	G	43	SER
1	G	44	PHE
1	G	48	THR
1	G	51	LYS
1	G	58	ARG
1	G	62	LEU
1	G	63	GLU
1	G	74	VAL
1	G	77	VAL
1	G	80	LYS
1	G	97	GLN
1	G	105	LYS
1	G	129	GLU
1	G	141	SER
1	G	147	VAL
1	G	150	ILE
1	G	157	THR
1	G	164	GLU
1	G	168	LYS
1	G	172	GLU
1	G	174	VAL
1	G	176	THR
1	G	177	VAL
1	G	183	LEU
1	G	184	GLN
1	G	190	VAL

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Mol	Chain	Res	Type
1	G	193	MET
1	G	209	GLU
1	G	215	LEU
1	G	230	ILE
1	G	231	ARG
1	G	272	LYS
1	G	276	VAL
1	G	284	ARG
1	G	288	MET
1	G	289	LEU
1	G	295	LEU
1	G	317	LEU
1	G	322	ARG
1	G	323	VAL
1	G	325	ILE
1	G	328	ASP
1	G	331	THR
1	G	350	ARG
1	G	355	GLU
1	G	358	SER
1	G	368	ARG
1	G	381	VAL
1	G	387	VAL
1	G	388	GLU
1	G	391	GLU
1	G	400	LEU
1	G	404	ARG
1	G	417	VAL
1	G	419	LEU
1	G	420	ILE
1	G	422	VAL
1	G	430	ARG
1	G	432	GLN
1	G	442	VAL
1	G	452	ARG
1	G	461	GLU
1	G	463	SER
1	G	483	GLU
1	G	484	GLU
1	G	499	VAL
1	G	504	LEU
1	G	510	VAL

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Mol	Chain	Res	Type
1	H	7	LYS
1	H	10	ASN
1	H	20	VAL
1	H	23	LEU
1	H	40	LEU
1	H	42	LYS
1	H	43	SER
1	H	44	PHE
1	H	48	THR
1	H	59	GLU
1	H	65	LYS
1	H	77	VAL
1	H	79	SER
1	H	89	THR
1	H	104	LEU
1	H	107	VAL
1	H	129	GLU
1	H	131	LEU
1	H	138	CYS
1	H	141	SER
1	H	147	VAL
1	H	172	GLU
1	H	187	LEU
1	H	217	SER
1	H	225	LYS
1	H	230	ILE
1	H	238	GLU
1	H	265	ASN
1	H	267	MET
1	H	271	VAL
1	H	284	ARG
1	H	289	LEU
1	H	295	LEU
1	H	302	SER
1	H	307	MET
1	H	311	LYS
1	H	317	LEU
1	H	321	LYS
1	H	322	ARG
1	H	325	ILE
1	H	328	ASP
1	H	331	THR

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Mol	Chain	Res	Type
1	H	339	GLU
1	H	343	GLN
1	H	350	ARG
1	H	352	GLN
1	H	355	GLU
1	H	363	GLU
1	H	378	VAL
1	H	385	THR
1	H	389	MET
1	H	400	LEU
1	H	401	HIS
1	H	404	ARG
1	H	419	LEU
1	H	420	ILE
1	H	421	ARG
1	H	426	LEU
1	H	432	GLN
1	H	433	ASN
1	H	445	ARG
1	H	452	ARG
1	H	454	ILE
1	H	460	GLU
1	H	461	GLU
1	H	468	THR
1	H	483	GLU
1	H	489	ILE
1	H	493	ILE
1	H	494	LEU
1	H	499	VAL
1	H	504	LEU
1	H	513	LEU
1	I	7	LYS
1	I	10	ASN
1	I	14	VAL
1	I	20	VAL
1	I	23	LEU
1	I	40	LEU
1	I	42	LYS
1	I	44	PHE
1	I	48	THR
1	I	59	GLU
1	I	77	VAL

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Mol	Chain	Res	Type
1	I	79	SER
1	I	89	THR
1	I	104	LEU
1	I	107	VAL
1	I	129	GLU
1	I	131	LEU
1	I	138	CYS
1	I	141	SER
1	I	147	VAL
1	I	172	GLU
1	I	187	LEU
1	I	217	SER
1	I	225	LYS
1	I	230	ILE
1	I	238	GLU
1	I	265	ASN
1	I	267	MET
1	I	271	VAL
1	I	284	ARG
1	I	289	LEU
1	I	295	LEU
1	I	302	SER
1	I	307	MET
1	I	311	LYS
1	I	317	LEU
1	I	321	LYS
1	I	322	ARG
1	I	325	ILE
1	I	328	ASP
1	I	331	THR
1	I	339	GLU
1	I	343	GLN
1	I	350	ARG
1	I	352	GLN
1	I	354	GLU
1	I	355	GLU
1	I	363	GLU
1	I	378	VAL
1	I	385	THR
1	I	389	MET
1	I	400	LEU
1	I	401	HIS

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Mol	Chain	Res	Type
1	I	404	ARG
1	I	419	LEU
1	I	420	ILE
1	I	421	ARG
1	I	424	SER
1	I	425	LYS
1	I	426	LEU
1	I	432	GLN
1	I	433	ASN
1	I	441	LYS
1	I	445	ARG
1	I	452	ARG
1	I	454	ILE
1	I	460	GLU
1	I	461	GLU
1	I	468	THR
1	I	483	GLU
1	I	493	ILE
1	I	494	LEU
1	I	499	VAL
1	I	504	LEU
1	I	509	SER
1	I	513	LEU
1	J	7	LYS
1	J	10	ASN
1	J	11	ASP
1	J	20	VAL
1	J	23	LEU
1	J	40	LEU
1	J	42	LYS
1	J	43	SER
1	J	44	PHE
1	J	48	THR
1	J	59	GLU
1	J	77	VAL
1	J	89	THR
1	J	104	LEU
1	J	107	VAL
1	J	131	LEU
1	J	138	CYS
1	J	141	SER
1	J	147	VAL

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Mol	Chain	Res	Type
1	J	172	GLU
1	J	187	LEU
1	J	201	SER
1	J	210	THR
1	J	217	SER
1	J	225	LYS
1	J	230	ILE
1	J	238	GLU
1	J	265	ASN
1	J	267	MET
1	J	271	VAL
1	J	284	ARG
1	J	289	LEU
1	J	290	GLN
1	J	295	LEU
1	J	302	SER
1	J	307	MET
1	J	311	LYS
1	J	317	LEU
1	J	321	LYS
1	J	322	ARG
1	J	325	ILE
1	J	331	THR
1	J	339	GLU
1	J	343	GLN
1	J	350	ARG
1	J	352	GLN
1	J	354	GLU
1	J	355	GLU
1	J	363	GLU
1	J	378	VAL
1	J	385	THR
1	J	389	MET
1	J	400	LEU
1	J	401	HIS
1	J	404	ARG
1	J	419	LEU
1	J	420	ILE
1	J	421	ARG
1	J	425	LYS
1	J	426	LEU
1	J	429	LEU

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Mol	Chain	Res	Type
1	J	432	GLN
1	J	433	ASN
1	J	441	LYS
1	J	445	ARG
1	J	452	ARG
1	J	454	ILE
1	J	460	GLU
1	J	461	GLU
1	J	467	ASN
1	J	468	THR
1	J	483	GLU
1	J	494	LEU
1	J	499	VAL
1	J	504	LEU
1	J	509	SER
1	J	513	LEU
1	K	7	LYS
1	K	10	ASN
1	K	20	VAL
1	K	23	LEU
1	K	40	LEU
1	K	42	LYS
1	K	43	SER
1	K	44	PHE
1	K	48	THR
1	K	59	GLU
1	K	65	LYS
1	K	77	VAL
1	K	79	SER
1	K	89	THR
1	K	104	LEU
1	K	107	VAL
1	K	129	GLU
1	K	131	LEU
1	K	138	CYS
1	K	141	SER
1	K	147	VAL
1	K	172	GLU
1	K	187	LEU
1	K	217	SER
1	K	225	LYS
1	K	230	ILE

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Mol	Chain	Res	Type
1	K	238	GLU
1	K	265	ASN
1	K	267	MET
1	K	271	VAL
1	K	284	ARG
1	K	289	LEU
1	K	295	LEU
1	K	302	SER
1	K	307	MET
1	K	311	LYS
1	K	317	LEU
1	K	321	LYS
1	K	322	ARG
1	K	325	ILE
1	K	328	ASP
1	K	331	THR
1	K	339	GLU
1	K	343	GLN
1	K	350	ARG
1	K	352	GLN
1	K	354	GLU
1	K	355	GLU
1	K	363	GLU
1	K	378	VAL
1	K	385	THR
1	K	389	MET
1	K	400	LEU
1	K	404	ARG
1	K	420	ILE
1	K	421	ARG
1	K	425	LYS
1	K	426	LEU
1	K	429	LEU
1	K	432	GLN
1	K	433	ASN
1	K	441	LYS
1	K	452	ARG
1	K	454	ILE
1	K	460	GLU
1	K	461	GLU
1	K	468	THR
1	K	483	GLU

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Mol	Chain	Res	Type
1	K	489	ILE
1	K	494	LEU
1	K	499	VAL
1	K	504	LEU
1	K	509	SER
1	K	513	LEU
1	L	7	LYS
1	L	10	ASN
1	L	20	VAL
1	L	23	LEU
1	L	27	VAL
1	L	40	LEU
1	L	42	LYS
1	L	43	SER
1	L	44	PHE
1	L	48	THR
1	L	59	GLU
1	L	77	VAL
1	L	79	SER
1	L	89	THR
1	L	104	LEU
1	L	107	VAL
1	L	129	GLU
1	L	131	LEU
1	L	138	CYS
1	L	141	SER
1	L	147	VAL
1	L	172	GLU
1	L	187	LEU
1	L	201	SER
1	L	217	SER
1	L	225	LYS
1	L	230	ILE
1	L	238	GLU
1	L	265	ASN
1	L	267	MET
1	L	271	VAL
1	L	284	ARG
1	L	289	LEU
1	L	295	LEU
1	L	302	SER
1	L	307	MET

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Mol	Chain	Res	Type
1	L	311	LYS
1	L	317	LEU
1	L	321	LYS
1	L	322	ARG
1	L	325	ILE
1	L	328	ASP
1	L	331	THR
1	L	339	GLU
1	L	343	GLN
1	L	350	ARG
1	L	352	GLN
1	L	354	GLU
1	L	355	GLU
1	L	363	GLU
1	L	378	VAL
1	L	385	THR
1	L	389	MET
1	L	400	LEU
1	L	401	HIS
1	L	404	ARG
1	L	412	VAL
1	L	419	LEU
1	L	420	ILE
1	L	421	ARG
1	L	425	LYS
1	L	426	LEU
1	L	432	GLN
1	L	433	ASN
1	L	452	ARG
1	L	454	ILE
1	L	460	GLU
1	L	461	GLU
1	L	468	THR
1	L	483	GLU
1	L	494	LEU
1	L	499	VAL
1	L	504	LEU
1	L	509	SER
1	L	513	LEU
1	M	7	LYS
1	M	10	ASN
1	M	20	VAL

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Mol	Chain	Res	Type
1	M	23	LEU
1	M	40	LEU
1	M	42	LYS
1	M	43	SER
1	M	44	PHE
1	M	48	THR
1	M	59	GLU
1	M	62	LEU
1	M	77	VAL
1	M	89	THR
1	M	104	LEU
1	M	107	VAL
1	M	129	GLU
1	M	131	LEU
1	M	138	CYS
1	M	141	SER
1	M	147	VAL
1	M	172	GLU
1	M	187	LEU
1	M	201	SER
1	M	217	SER
1	M	225	LYS
1	M	230	ILE
1	M	238	GLU
1	M	265	ASN
1	M	267	MET
1	M	271	VAL
1	M	284	ARG
1	M	289	LEU
1	M	295	LEU
1	M	302	SER
1	M	307	MET
1	M	311	LYS
1	M	317	LEU
1	M	321	LYS
1	M	322	ARG
1	M	325	ILE
1	M	328	ASP
1	M	331	THR
1	M	339	GLU
1	M	343	GLN
1	M	350	ARG

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Mol	Chain	Res	Type
1	M	352	GLN
1	M	354	GLU
1	M	355	GLU
1	M	363	GLU
1	M	378	VAL
1	M	385	THR
1	M	389	MET
1	M	400	LEU
1	M	401	HIS
1	M	404	ARG
1	M	419	LEU
1	M	420	ILE
1	M	421	ARG
1	M	425	LYS
1	M	426	LEU
1	M	429	LEU
1	M	432	GLN
1	M	433	ASN
1	M	445	ARG
1	M	452	ARG
1	M	454	ILE
1	M	460	GLU
1	M	461	GLU
1	M	468	THR
1	M	483	GLU
1	M	489	ILE
1	M	494	LEU
1	M	499	VAL
1	M	504	LEU
1	M	509	SER
1	M	513	LEU
1	N	7	LYS
1	N	10	ASN
1	N	20	VAL
1	N	23	LEU
1	N	27	VAL
1	N	40	LEU
1	N	42	LYS
1	N	43	SER
1	N	44	PHE
1	N	48	THR
1	N	59	GLU

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Mol	Chain	Res	Type
1	N	65	LYS
1	N	77	VAL
1	N	79	SER
1	N	80	LYS
1	N	89	THR
1	N	104	LEU
1	N	107	VAL
1	N	129	GLU
1	N	131	LEU
1	N	138	CYS
1	N	141	SER
1	N	147	VAL
1	N	172	GLU
1	N	187	LEU
1	N	217	SER
1	N	225	LYS
1	N	230	ILE
1	N	238	GLU
1	N	265	ASN
1	N	267	MET
1	N	271	VAL
1	N	284	ARG
1	N	289	LEU
1	N	295	LEU
1	N	302	SER
1	N	307	MET
1	N	311	LYS
1	N	317	LEU
1	N	321	LYS
1	N	322	ARG
1	N	325	ILE
1	N	328	ASP
1	N	331	THR
1	N	339	GLU
1	N	343	GLN
1	N	350	ARG
1	N	352	GLN
1	N	355	GLU
1	N	363	GLU
1	N	378	VAL
1	N	385	THR
1	N	389	MET

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Mol	Chain	Res	Type
1	N	400	LEU
1	N	404	ARG
1	N	419	LEU
1	N	420	ILE
1	N	421	ARG
1	N	425	LYS
1	N	426	LEU
1	N	432	GLN
1	N	433	ASN
1	N	441	LYS
1	N	445	ARG
1	N	452	ARG
1	N	454	ILE
1	N	460	GLU
1	N	461	GLU
1	N	468	THR
1	N	483	GLU
1	N	493	ILE
1	N	494	LEU
1	N	499	VAL
1	N	504	LEU
1	N	509	SER
1	N	513	LEU
2	O	1	MET
2	O	3	ILE
2	O	6	LEU
2	O	8	ASP
2	O	14	ARG
2	O	28	THR
2	O	30	SER
2	O	36	THR
2	O	48	ILE
2	O	55	LYS
2	O	75	SER
2	O	77	LYS
2	O	78	ILE
2	O	80	ASN
2	O	84	LEU
2	P	1	MET
2	P	3	ILE
2	P	6	LEU
2	P	8	ASP

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Mol	Chain	Res	Type
2	P	14	ARG
2	P	28	THR
2	P	30	SER
2	P	36	THR
2	P	48	ILE
2	P	55	LYS
2	P	75	SER
2	P	77	LYS
2	P	78	ILE
2	P	80	ASN
2	P	84	LEU
2	Q	1	MET
2	Q	3	ILE
2	Q	6	LEU
2	Q	8	ASP
2	Q	14	ARG
2	Q	28	THR
2	Q	30	SER
2	Q	36	THR
2	Q	48	ILE
2	Q	55	LYS
2	Q	64	ILE
2	Q	77	LYS
2	Q	78	ILE
2	Q	80	ASN
2	Q	84	LEU
2	R	1	MET
2	R	3	ILE
2	R	6	LEU
2	R	8	ASP
2	R	14	ARG
2	R	28	THR
2	R	30	SER
2	R	36	THR
2	R	48	ILE
2	R	55	LYS
2	R	75	SER
2	R	77	LYS
2	R	78	ILE
2	R	80	ASN
2	R	84	LEU
2	S	1	MET

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Mol	Chain	Res	Type
2	S	3	ILE
2	S	6	LEU
2	S	8	ASP
2	S	14	ARG
2	S	28	THR
2	S	30	SER
2	S	36	THR
2	S	48	ILE
2	S	55	LYS
2	S	75	SER
2	S	77	LYS
2	S	78	ILE
2	S	80	ASN
2	S	84	LEU
2	T	1	MET
2	T	3	ILE
2	T	6	LEU
2	T	8	ASP
2	T	14	ARG
2	T	28	THR
2	T	30	SER
2	T	36	THR
2	T	48	ILE
2	T	55	LYS
2	T	75	SER
2	T	77	LYS
2	T	78	ILE
2	T	80	ASN
2	T	84	LEU
2	U	1	MET
2	U	3	ILE
2	U	6	LEU
2	U	8	ASP
2	U	14	ARG
2	U	28	THR
2	U	30	SER
2	U	36	THR
2	U	48	ILE
2	U	55	LYS
2	U	64	ILE
2	U	77	LYS
2	U	78	ILE

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Mol	Chain	Res	Type
2	U	80	ASN
2	U	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	37	ASN
1	A	82	ASN
1	A	97	GLN
1	A	146	GLN
1	A	153	ASN
1	A	326	ASN
1	A	348	GLN
1	A	351	GLN
1	A	352	GLN
1	A	366	GLN
1	A	432	GLN
1	A	453	GLN
1	A	457	ASN
1	A	475	ASN
1	A	505	GLN
1	B	21	ASN
1	B	72	GLN
1	B	82	ASN
1	B	146	GLN
1	B	153	ASN
1	B	326	ASN
1	B	348	GLN
1	B	352	GLN
1	B	366	GLN
1	B	432	GLN
1	B	453	GLN
1	B	457	ASN
1	B	475	ASN
1	C	21	ASN
1	C	97	GLN
1	C	146	GLN
1	C	153	ASN
1	C	265	ASN
1	C	326	ASN
1	C	348	GLN

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Mol	Chain	Res	Type
1	C	351	GLN
1	C	352	GLN
1	C	366	GLN
1	C	432	GLN
1	C	457	ASN
1	C	475	ASN
1	D	21	ASN
1	D	37	ASN
1	D	146	GLN
1	D	153	ASN
1	D	265	ASN
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	352	GLN
1	D	366	GLN
1	D	432	GLN
1	D	457	ASN
1	D	475	ASN
1	E	21	ASN
1	E	82	ASN
1	E	146	GLN
1	E	153	ASN
1	E	326	ASN
1	E	348	GLN
1	E	351	GLN
1	E	352	GLN
1	E	366	GLN
1	E	432	GLN
1	E	453	GLN
1	E	457	ASN
1	E	475	ASN
1	F	21	ASN
1	F	82	ASN
1	F	146	GLN
1	F	153	ASN
1	F	265	ASN
1	F	326	ASN
1	F	348	GLN
1	F	351	GLN
1	F	352	GLN
1	F	366	GLN

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Mol	Chain	Res	Type
1	F	432	GLN
1	F	453	GLN
1	F	457	ASN
1	F	475	ASN
1	G	21	ASN
1	G	37	ASN
1	G	72	GLN
1	G	97	GLN
1	G	146	GLN
1	G	153	ASN
1	G	265	ASN
1	G	326	ASN
1	G	348	GLN
1	G	351	GLN
1	G	352	GLN
1	G	432	GLN
1	G	453	GLN
1	G	457	ASN
1	G	475	ASN
1	H	21	ASN
1	H	72	GLN
1	H	97	GLN
1	H	146	GLN
1	H	153	ASN
1	H	265	ASN
1	H	326	ASN
1	H	348	GLN
1	H	351	GLN
1	H	433	ASN
1	H	436	GLN
1	H	475	ASN
1	I	21	ASN
1	I	72	GLN
1	I	97	GLN
1	I	146	GLN
1	I	153	ASN
1	I	265	ASN
1	I	326	ASN
1	I	348	GLN
1	I	351	GLN
1	I	433	ASN
1	I	436	GLN

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Mol	Chain	Res	Type
1	I	475	ASN
1	J	21	ASN
1	J	72	GLN
1	J	97	GLN
1	J	146	GLN
1	J	194	GLN
1	J	265	ASN
1	J	290	GLN
1	J	348	GLN
1	J	351	GLN
1	J	433	ASN
1	J	436	GLN
1	J	475	ASN
1	K	21	ASN
1	K	72	GLN
1	K	97	GLN
1	K	146	GLN
1	K	265	ASN
1	K	348	GLN
1	K	351	GLN
1	K	366	GLN
1	K	433	ASN
1	K	436	GLN
1	K	475	ASN
1	L	21	ASN
1	L	37	ASN
1	L	72	GLN
1	L	97	GLN
1	L	146	GLN
1	L	265	ASN
1	L	326	ASN
1	L	348	GLN
1	L	351	GLN
1	L	433	ASN
1	L	436	GLN
1	L	475	ASN
1	M	21	ASN
1	M	72	GLN
1	M	82	ASN
1	M	97	GLN
1	M	146	GLN
1	M	265	ASN

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Mol	Chain	Res	Type
1	M	326	ASN
1	M	348	GLN
1	M	351	GLN
1	M	433	ASN
1	M	436	GLN
1	M	475	ASN
1	N	10	ASN
1	N	21	ASN
1	N	72	GLN
1	N	82	ASN
1	N	97	GLN
1	N	146	GLN
1	N	153	ASN
1	N	265	ASN
1	N	326	ASN
1	N	348	GLN
1	N	351	GLN
1	N	433	ASN
1	N	436	GLN
1	N	475	ASN
2	O	2	ASN
2	O	45	ASN
2	O	80	ASN
2	P	45	ASN
2	P	68	ASN
2	P	80	ASN
2	Q	2	ASN
2	Q	45	ASN
2	Q	51	ASN
2	Q	80	ASN
2	R	2	ASN
2	R	45	ASN
2	R	68	ASN
2	R	80	ASN
2	S	45	ASN
2	S	68	ASN
2	S	80	ASN
2	T	2	ASN
2	T	45	ASN
2	T	80	ASN
2	U	45	ASN
2	U	51	ASN

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Mol	Chain	Res	Type
2	U	68	ASN
2	U	80	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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ADP	G	600	3	28,29,29	1.24	3 (10%)	43,45,45	2.80	22 (51%)
4	ADP	C	600	3	28,29,29	1.30	3 (10%)	43,45,45	2.77	21 (48%)
4	ADP	B	600	3	28,29,29	1.48	5 (17%)	43,45,45	2.76	18 (41%)
4	ADP	A	600	3	28,29,29	1.35	3 (10%)	43,45,45	2.67	21 (48%)
4	ADP	E	600	3	28,29,29	1.21	4 (14%)	43,45,45	2.63	16 (37%)
4	ADP	D	600	3	28,29,29	1.58	6 (21%)	43,45,45	2.62	19 (44%)
4	ADP	F	600	3	28,29,29	1.01	1 (3%)	43,45,45	2.38	16 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	G	600	3	-	7/16/32/32	0/3/3/3
4	ADP	C	600	3	-	7/16/32/32	0/3/3/3
4	ADP	B	600	3	-	7/16/32/32	0/3/3/3
4	ADP	A	600	3	-	7/16/32/32	0/3/3/3
4	ADP	E	600	3	-	7/16/32/32	0/3/3/3
4	ADP	D	600	3	-	7/16/32/32	0/3/3/3
4	ADP	F	600	3	-	7/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	600	ADP	C2-N3	3.38	1.39	1.33
4	A	600	ADP	O4'-C4'	-3.27	1.37	1.45
4	D	600	ADP	O4'-C4'	-3.24	1.37	1.45
4	D	600	ADP	PA-O3A	3.17	1.62	1.59
4	D	600	ADP	C2-N1	3.14	1.39	1.33
4	G	600	ADP	O4'-C4'	-3.13	1.38	1.45
4	C	600	ADP	O4'-C4'	-3.10	1.38	1.45
4	B	600	ADP	C2-N1	3.08	1.39	1.33
4	D	600	ADP	C8-N7	3.02	1.37	1.31
4	G	600	ADP	C8-N7	2.92	1.37	1.31
4	B	600	ADP	C8-N7	2.91	1.37	1.31
4	D	600	ADP	O4'-C1'	-2.69	1.35	1.42
4	E	600	ADP	C8-N7	2.67	1.36	1.31
4	C	600	ADP	PA-O3A	2.67	1.62	1.59
4	E	600	ADP	C2-N1	2.50	1.38	1.33
4	F	600	ADP	C2-N1	2.40	1.38	1.33
4	B	600	ADP	O4'-C4'	-2.38	1.39	1.45
4	B	600	ADP	C2-N3	2.36	1.38	1.33
4	C	600	ADP	C2-N1	2.31	1.38	1.33
4	B	600	ADP	C4-N3	2.24	1.38	1.34
4	E	600	ADP	O4'-C4'	-2.23	1.40	1.45
4	A	600	ADP	PA-O1A	-2.20	1.43	1.50
4	D	600	ADP	C2-N3	2.14	1.37	1.33
4	A	600	ADP	O3'-C3'	-2.03	1.37	1.43
4	E	600	ADP	O4'-C1'	-2.02	1.37	1.42

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	600	ADP	N3-C2-N1	-7.22	117.66	128.58
4	E	600	ADP	N9-C8-N7	-7.05	103.94	113.94
4	G	600	ADP	N9-C8-N7	-6.75	104.36	113.94
4	G	600	ADP	C4-C5-N7	-6.67	102.96	110.58
4	B	600	ADP	N9-C8-N7	-6.41	104.84	113.94
4	E	600	ADP	C5-N7-C8	6.31	113.37	103.45
4	A	600	ADP	N3-C2-N1	-6.12	119.32	128.58
4	G	600	ADP	C5-N7-C8	6.11	113.05	103.45
4	B	600	ADP	C5-N7-C8	6.05	112.96	103.45
4	C	600	ADP	C4-C5-N7	-5.98	103.75	110.58
4	B	600	ADP	C4-C5-N7	-5.91	103.83	110.58
4	C	600	ADP	N9-C8-N7	-5.86	105.62	113.94
4	D	600	ADP	N9-C8-N7	-5.60	106.00	113.94
4	F	600	ADP	N3-C2-N1	-5.56	120.16	128.58
4	C	600	ADP	C5-N7-C8	5.51	112.11	103.45
4	E	600	ADP	C4-C5-N7	-5.50	104.30	110.58
4	F	600	ADP	N9-C8-N7	-5.49	106.14	113.94
4	C	600	ADP	N3-C2-N1	-5.43	120.36	128.58
4	B	600	ADP	N3-C2-N1	-5.35	120.49	128.58
4	E	600	ADP	N3-C2-N1	-5.15	120.78	128.58
4	F	600	ADP	C5-N7-C8	5.12	111.50	103.45
4	A	600	ADP	C4-C5-N7	-5.00	104.86	110.58
4	A	600	ADP	N9-C8-N7	-4.93	106.94	113.94
4	G	600	ADP	C5-C4-N3	-4.88	120.00	126.72
4	F	600	ADP	C4-C5-N7	-4.86	105.02	110.58
4	B	600	ADP	C4-N9-C8	4.69	110.66	105.74
4	E	600	ADP	C4-N9-C8	4.68	110.65	105.74
4	D	600	ADP	O4'-C1'-C2'	-4.66	96.64	106.62
4	B	600	ADP	C5-C4-N3	-4.61	120.36	126.72
4	C	600	ADP	O3B-PB-O3A	4.46	119.60	104.64
4	D	600	ADP	C5-N7-C8	4.46	110.46	103.45
4	A	600	ADP	C5-N7-C8	4.45	110.44	103.45
4	G	600	ADP	O4'-C1'-C2'	-4.34	97.32	106.62
4	C	600	ADP	C5-C4-N3	-4.33	120.75	126.72
4	F	600	ADP	C5-C4-N3	-4.31	120.79	126.72
4	A	600	ADP	O2B-PB-O1B	4.18	127.12	110.83
4	D	600	ADP	O2B-PB-O3A	-4.15	90.71	104.64
4	A	600	ADP	C5-C4-N3	-3.98	121.23	126.72
4	G	600	ADP	C5-C4-N9	3.97	110.14	105.81
4	D	600	ADP	O2B-PB-O1B	3.93	126.16	110.83
4	C	600	ADP	O2B-PB-O1B	3.93	126.14	110.83
4	E	600	ADP	C5-C4-N3	-3.88	121.38	126.72
4	D	600	ADP	C2-N3-C4	3.84	121.21	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ADP	C2-N3-C4	3.84	121.21	111.83
4	G	600	ADP	O5'-C5'-C4'	3.83	122.05	108.99
4	D	600	ADP	C4-C5-N7	-3.79	106.25	110.58
4	A	600	ADP	C2-N3-C4	3.73	120.93	111.83
4	C	600	ADP	O2B-PB-O3A	-3.69	92.25	104.64
4	A	600	ADP	O3B-PB-O1B	-3.68	96.50	110.83
4	F	600	ADP	C2-N3-C4	3.64	120.72	111.83
4	B	600	ADP	O3'-C3'-C4'	-3.61	100.70	111.08
4	G	600	ADP	N3-C2-N1	-3.53	123.23	128.58
4	B	600	ADP	O2B-PB-O3A	-3.51	92.87	104.64
4	G	600	ADP	C4-N9-C8	3.51	109.42	105.74
4	C	600	ADP	C2-N3-C4	3.50	120.38	111.83
4	C	600	ADP	C4-N9-C8	3.50	109.41	105.74
4	D	600	ADP	C5-C4-N3	-3.44	121.98	126.72
4	B	600	ADP	O4'-C1'-C2'	-3.44	99.26	106.62
4	C	600	ADP	O5'-C5'-C4'	3.41	120.60	108.99
4	A	600	ADP	N6-C6-N1	-3.36	110.89	118.38
4	E	600	ADP	O3'-C3'-C4'	-3.33	101.51	111.08
4	A	600	ADP	O2B-PB-O3A	-3.30	93.58	104.64
4	E	600	ADP	C2-N3-C4	3.27	119.83	111.83
4	D	600	ADP	O5'-C5'-C4'	3.25	120.07	108.99
4	A	600	ADP	O4'-C1'-N9	3.23	114.30	108.09
4	E	600	ADP	O2B-PB-O3A	-3.17	94.01	104.64
4	C	600	ADP	O4'-C1'-C2'	-3.16	99.86	106.62
4	F	600	ADP	O3B-PB-O3A	3.15	115.21	104.64
4	B	600	ADP	O3B-PB-O3A	3.13	115.14	104.64
4	D	600	ADP	C4-N9-C8	3.11	109.00	105.74
4	E	600	ADP	O5'-C5'-C4'	3.08	119.49	108.99
4	B	600	ADP	C4-N9-C1'	-3.06	119.48	126.63
4	A	600	ADP	O5'-C5'-C4'	3.04	119.36	108.99
4	A	600	ADP	O3B-PB-O3A	3.03	114.79	104.64
4	B	600	ADP	O4'-C1'-N9	3.00	113.85	108.09
4	A	600	ADP	C4-N9-C1'	-2.99	119.64	126.63
4	A	600	ADP	O4'-C1'-C2'	-2.99	100.22	106.62
4	A	600	ADP	C4-N9-C8	2.94	108.83	105.74
4	D	600	ADP	O3A-PA-O1A	-2.94	101.86	110.70
4	D	600	ADP	O3B-PB-O1B	-2.93	99.43	110.83
4	C	600	ADP	C5-C4-N9	2.92	108.99	105.81
4	E	600	ADP	C4-N9-C1'	-2.89	119.88	126.63
4	C	600	ADP	O4'-C1'-N9	2.88	113.62	108.09
4	F	600	ADP	O4'-C1'-N9	2.87	113.60	108.09
4	B	600	ADP	C6-C5-N7	2.84	137.57	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ADP	C5-C4-N9	2.83	108.89	105.81
4	B	600	ADP	N3-C4-N9	2.81	131.95	127.17
4	A	600	ADP	O2A-PA-O3A	-2.81	99.69	107.27
4	E	600	ADP	O2B-PB-O1B	2.81	121.77	110.83
4	F	600	ADP	C5-C4-N9	2.80	108.87	105.81
4	A	600	ADP	C6-C5-N7	2.80	137.49	132.09
4	G	600	ADP	O2B-PB-O1B	2.77	121.61	110.83
4	B	600	ADP	O2B-PB-O1B	2.74	121.52	110.83
4	C	600	ADP	O3B-PB-O1B	-2.70	100.30	110.83
4	G	600	ADP	N6-C6-N1	-2.70	112.37	118.38
4	F	600	ADP	O2B-PB-O1B	2.66	121.22	110.83
4	G	600	ADP	C2-N3-C4	2.66	118.32	111.83
4	G	600	ADP	O2B-PB-O3A	-2.64	95.78	104.64
4	C	600	ADP	C6-C5-N7	2.59	137.08	132.09
4	G	600	ADP	C6-C5-C4	2.58	120.70	117.18
4	G	600	ADP	O3A-PA-O1A	-2.58	102.95	110.70
4	F	600	ADP	C4-N9-C8	2.57	108.43	105.74
4	C	600	ADP	C4-N9-C1'	-2.56	120.64	126.63
4	D	600	ADP	O3B-PB-O3A	2.51	113.06	104.64
4	C	600	ADP	N6-C6-N1	-2.50	112.81	118.38
4	C	600	ADP	O2A-PA-O5'	2.49	118.86	107.57
4	F	600	ADP	O3'-C3'-C4'	-2.45	104.04	111.08
4	G	600	ADP	O2A-PA-O1A	2.44	123.80	112.44
4	A	600	ADP	C5-C6-N6	2.42	129.27	123.29
4	B	600	ADP	O5'-C5'-C4'	2.41	117.21	108.99
4	E	600	ADP	O4'-C1'-N9	2.41	112.72	108.09
4	G	600	ADP	C3'-C2'-C1'	-2.40	96.92	101.46
4	G	600	ADP	O5'-PA-O1A	-2.38	99.49	108.94
4	D	600	ADP	C4-N9-C1'	-2.36	121.10	126.63
4	F	600	ADP	O4'-C1'-C2'	-2.32	101.65	106.62
4	G	600	ADP	O2A-PA-O5'	2.29	117.96	107.57
4	D	600	ADP	O2A-PA-O1A	2.28	123.05	112.44
4	F	600	ADP	O5'-C5'-C4'	2.26	116.68	108.99
4	F	600	ADP	O2B-PB-O3A	-2.25	97.08	104.64
4	D	600	ADP	C5-C4-N9	2.24	108.26	105.81
4	F	600	ADP	O3A-PA-O1A	-2.22	104.03	110.70
4	G	600	ADP	O4'-C1'-N9	2.22	112.35	108.09
4	C	600	ADP	O3'-C3'-C4'	-2.21	104.75	111.08
4	E	600	ADP	O3B-PB-O3A	2.20	112.02	104.64
4	E	600	ADP	N3-C4-N9	2.19	130.90	127.17
4	G	600	ADP	C6-C5-N7	2.19	136.30	132.09
4	G	600	ADP	O4'-C4'-C3'	-2.18	100.82	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	600	ADP	C5-C6-N6	2.16	128.65	123.29
4	D	600	ADP	O4'-C4'-C3'	-2.13	100.93	105.15
4	E	600	ADP	C6-C5-N7	2.12	136.18	132.09
4	A	600	ADP	O2A-PA-O1A	2.04	121.95	112.44
4	D	600	ADP	C2-N1-C6	2.03	122.07	118.73
4	B	600	ADP	O3B-PB-O1B	-2.03	102.93	110.83

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ADP	C5'-O5'-PA-O1A
4	A	600	ADP	C5'-O5'-PA-O2A
4	A	600	ADP	O4'-C4'-C5'-O5'
4	A	600	ADP	C3'-C4'-C5'-O5'
4	B	600	ADP	C5'-O5'-PA-O1A
4	B	600	ADP	C5'-O5'-PA-O2A
4	B	600	ADP	C5'-O5'-PA-O3A
4	B	600	ADP	O4'-C4'-C5'-O5'
4	C	600	ADP	C5'-O5'-PA-O1A
4	C	600	ADP	C5'-O5'-PA-O2A
4	C	600	ADP	C5'-O5'-PA-O3A
4	C	600	ADP	O4'-C4'-C5'-O5'
4	D	600	ADP	C5'-O5'-PA-O1A
4	D	600	ADP	C5'-O5'-PA-O2A
4	D	600	ADP	C5'-O5'-PA-O3A
4	D	600	ADP	O4'-C4'-C5'-O5'
4	D	600	ADP	C3'-C4'-C5'-O5'
4	E	600	ADP	C5'-O5'-PA-O2A
4	E	600	ADP	C5'-O5'-PA-O3A
4	E	600	ADP	O4'-C4'-C5'-O5'
4	F	600	ADP	C5'-O5'-PA-O2A
4	F	600	ADP	C5'-O5'-PA-O3A
4	F	600	ADP	O4'-C4'-C5'-O5'
4	G	600	ADP	C5'-O5'-PA-O1A
4	G	600	ADP	C5'-O5'-PA-O2A
4	G	600	ADP	C5'-O5'-PA-O3A
4	G	600	ADP	O4'-C4'-C5'-O5'
4	B	600	ADP	C3'-C4'-C5'-O5'
4	C	600	ADP	C3'-C4'-C5'-O5'
4	E	600	ADP	C3'-C4'-C5'-O5'
4	F	600	ADP	C3'-C4'-C5'-O5'

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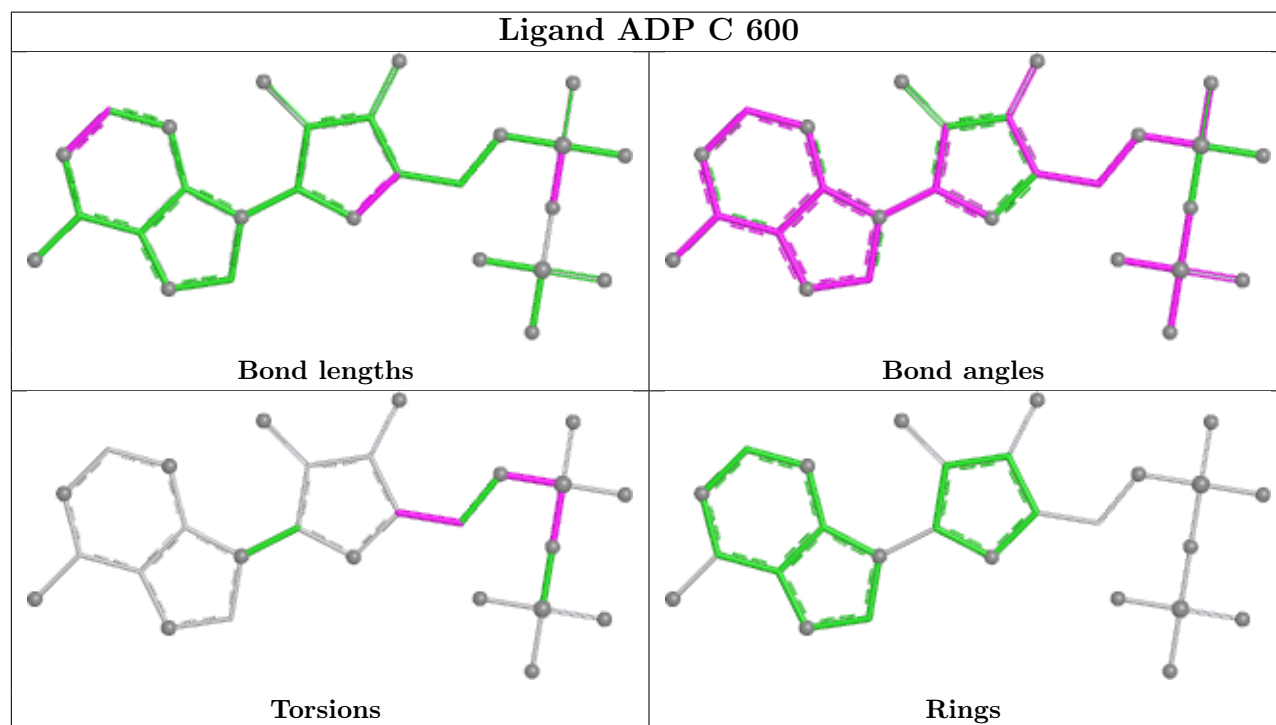
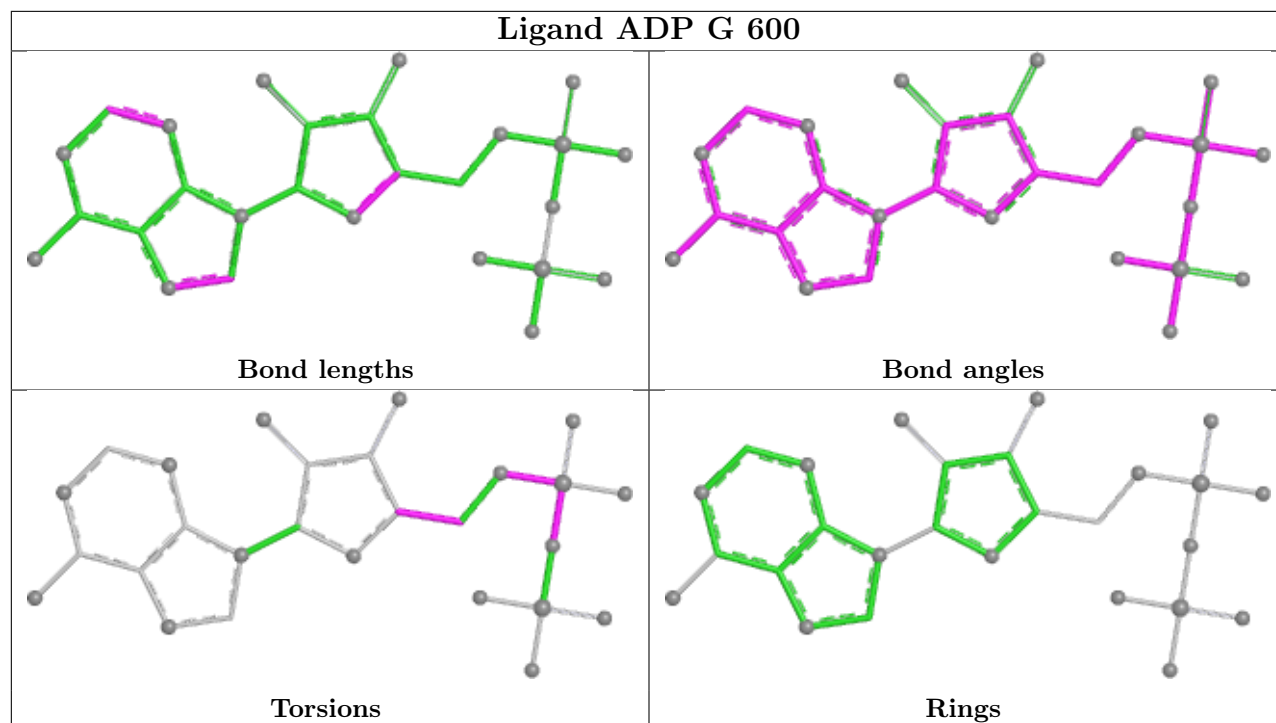
Mol	Chain	Res	Type	Atoms
4	G	600	ADP	C3'-C4'-C5'-O5'
4	F	600	ADP	PB-O3A-PA-O1A
4	G	600	ADP	PB-O3A-PA-O1A
4	B	600	ADP	PB-O3A-PA-O2A
4	A	600	ADP	C5'-O5'-PA-O3A
4	E	600	ADP	C5'-O5'-PA-O1A
4	F	600	ADP	C5'-O5'-PA-O1A
4	A	600	ADP	PB-O3A-PA-O1A
4	A	600	ADP	PB-O3A-PA-O2A
4	C	600	ADP	PB-O3A-PA-O2A
4	D	600	ADP	PB-O3A-PA-O1A
4	D	600	ADP	PB-O3A-PA-O2A
4	E	600	ADP	PB-O3A-PA-O1A
4	E	600	ADP	PB-O3A-PA-O2A
4	F	600	ADP	PB-O3A-PA-O2A
4	G	600	ADP	PB-O3A-PA-O2A
4	C	600	ADP	PB-O3A-PA-O1A
4	B	600	ADP	PB-O3A-PA-O1A

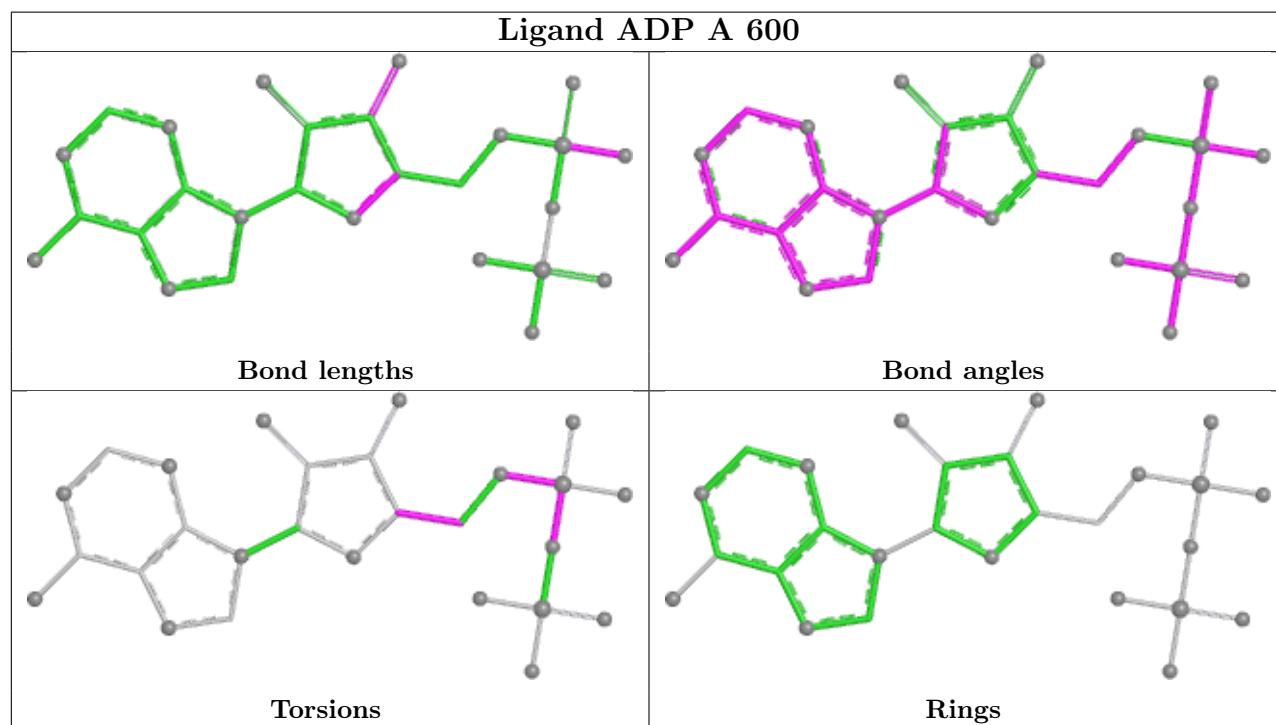
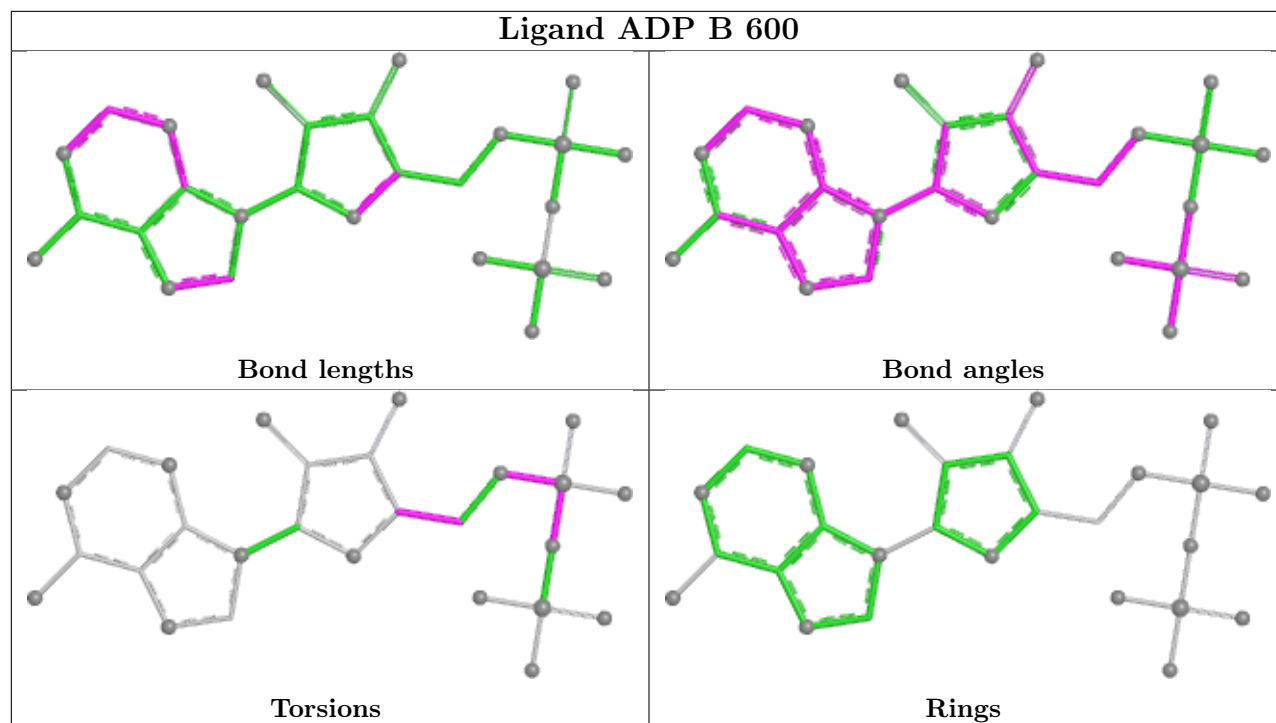
There are no ring outliers.

6 monomers are involved in 7 short contacts:

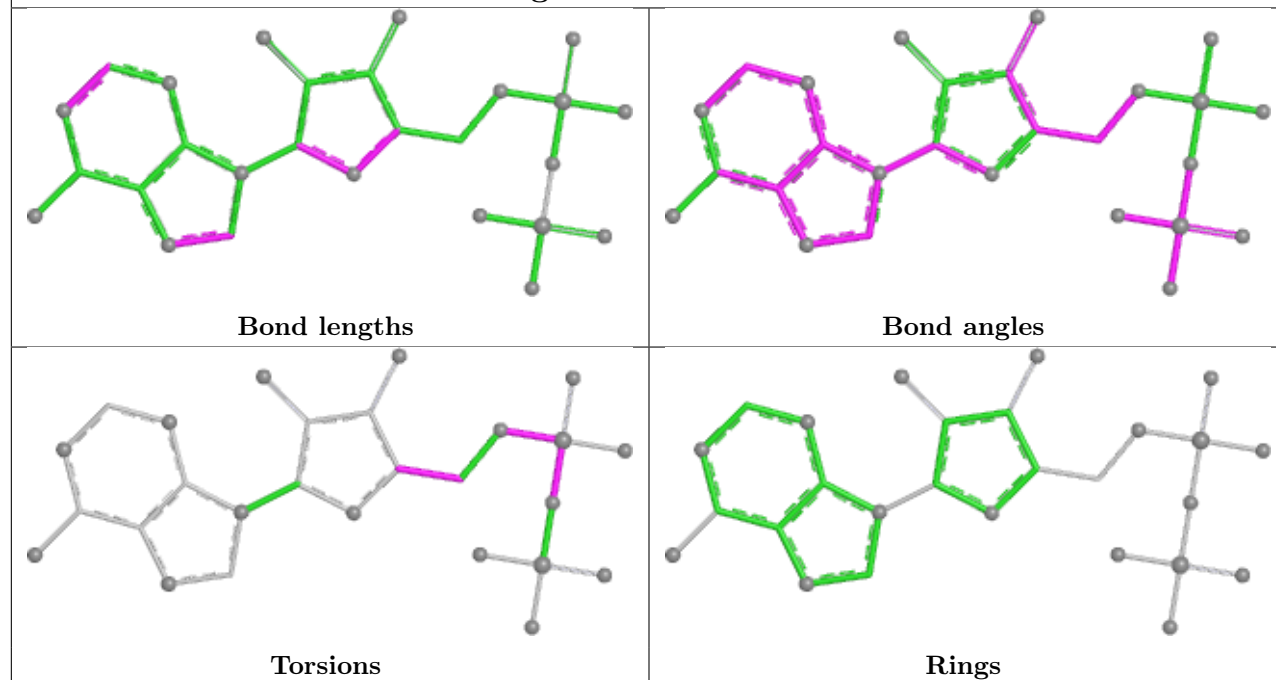
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	600	ADP	1	0
4	C	600	ADP	1	0
4	B	600	ADP	2	0
4	A	600	ADP	1	0
4	E	600	ADP	1	0
4	D	600	ADP	1	0

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

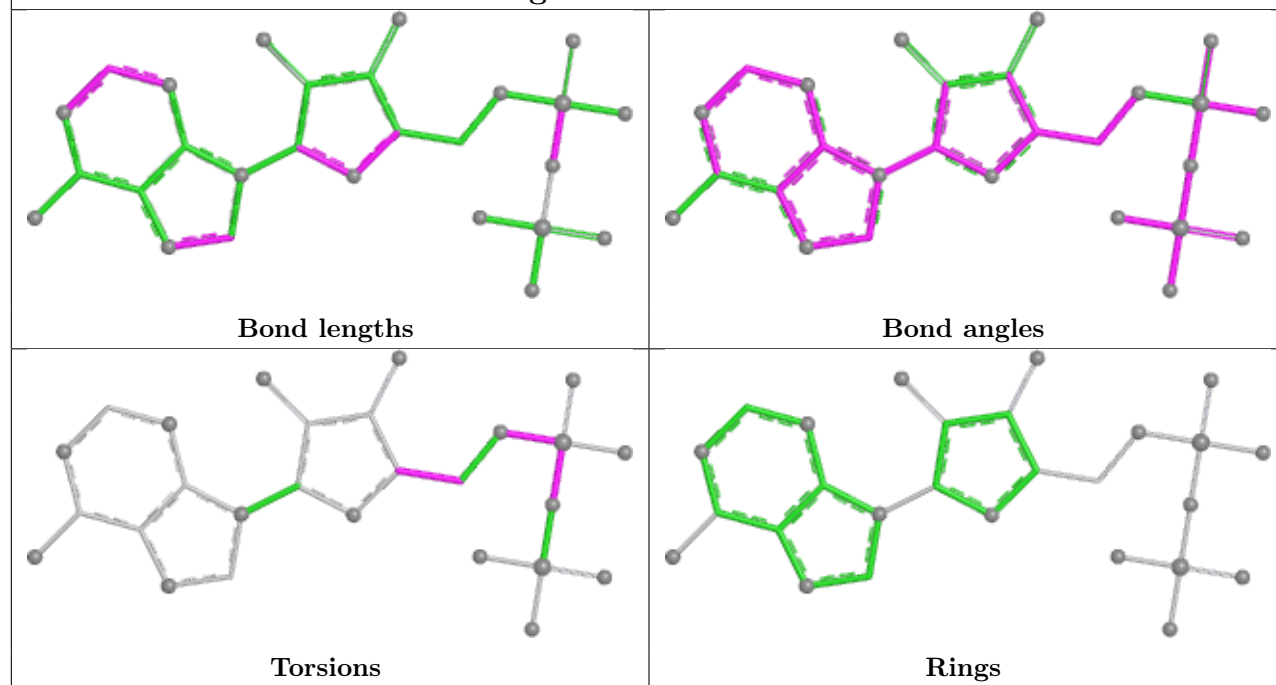


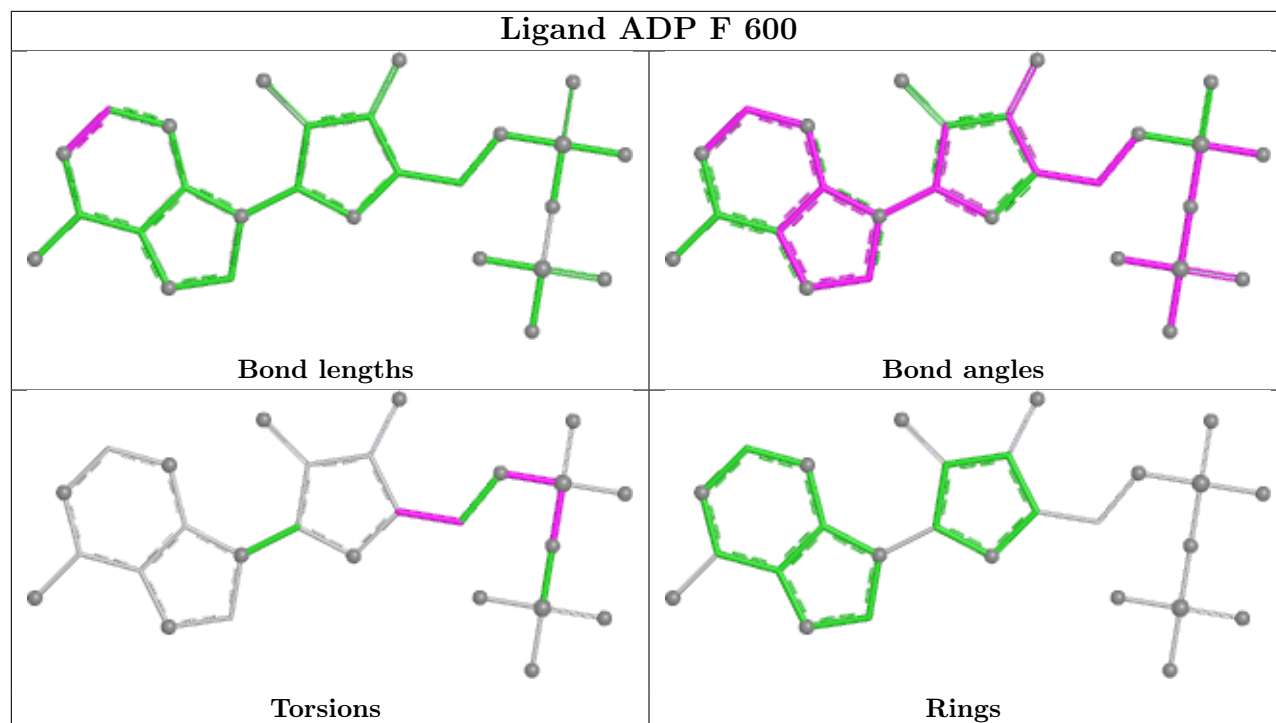


Ligand ADP E 600



Ligand ADP D 600





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	524/524 (100%)	0.13	18 (3%)	48	27	2, 2, 3, 5	0
1	B	524/524 (100%)	0.28	22 (4%)	40	22	2, 2, 3, 5	0
1	C	524/524 (100%)	0.13	23 (4%)	39	21	2, 2, 3, 5	0
1	D	524/524 (100%)	0.11	21 (4%)	42	23	2, 2, 3, 5	0
1	E	524/524 (100%)	0.42	36 (6%)	23	12	2, 2, 3, 5	0
1	F	524/524 (100%)	0.50	54 (10%)	12	6	2, 2, 3, 5	0
1	G	524/524 (100%)	0.25	43 (8%)	17	9	2, 2, 3, 5	0
1	H	524/524 (100%)	0.36	24 (4%)	37	20	2, 2, 3, 5	0
1	I	524/524 (100%)	-0.14	2 (0%)	88	76	2, 2, 3, 5	0
1	J	524/524 (100%)	-0.14	4 (0%)	82	64	2, 2, 3, 5	0
1	K	524/524 (100%)	0.35	27 (5%)	33	17	2, 2, 3, 5	0
1	L	524/524 (100%)	0.50	33 (6%)	26	13	2, 2, 3, 5	0
1	M	524/524 (100%)	-0.09	7 (1%)	75	53	2, 2, 3, 5	0
1	N	524/524 (100%)	-0.01	4 (0%)	82	64	2, 2, 3, 5	0
2	O	97/97 (100%)	0.54	10 (10%)	12	6	2, 2, 2, 3	0
2	P	97/97 (100%)	0.33	6 (6%)	26	14	2, 2, 2, 3	0
2	Q	97/97 (100%)	0.33	4 (4%)	41	23	2, 2, 2, 3	0
2	R	97/97 (100%)	0.38	7 (7%)	21	11	2, 2, 2, 3	0
2	S	97/97 (100%)	0.40	3 (3%)	51	30	2, 2, 2, 3	0
2	T	97/97 (100%)	0.58	8 (8%)	17	9	2, 2, 2, 3	0
2	U	97/97 (100%)	0.54	5 (5%)	33	17	2, 2, 2, 3	0
All	All	8015/8015 (100%)	0.21	361 (4%)	38	20	2, 2, 3, 5	0

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	208	PRO	6.4
1	L	354	GLU	6.3
1	C	361	ASP	5.9
1	G	283	ASP	5.9
1	H	231	ARG	5.7
1	A	361	ASP	5.6
1	F	305	ILE	5.5
1	E	271	VAL	5.4
1	F	268	ARG	5.3
1	F	283	ASP	4.9
1	K	231	ARG	4.8
1	H	268	ARG	4.7
1	D	228	SER	4.6
2	Q	25	ILE	4.6
1	F	387	VAL	4.5
2	S	32	ALA	4.5
1	F	281	PHE	4.3
1	C	311	LYS	4.3
1	G	305	ILE	4.3
2	T	18	GLU	4.3
1	F	242	LYS	4.2
1	E	477	GLY	4.2
1	D	242	LYS	4.2
2	T	52	GLY	4.2
1	E	334	ASP	4.1
2	O	30	SER	4.1
2	R	25	ILE	4.1
1	G	361	ASP	4.0
1	F	349	ILE	4.0
1	D	361	ASP	4.0
1	F	313	THR	4.0
1	D	268	ARG	4.0
1	F	271	VAL	3.9
1	F	361	ASP	3.9
1	E	268	ARG	3.9
1	B	153	ASN	3.8
2	P	49	LEU	3.8
1	K	200	LEU	3.7
1	A	387	VAL	3.7
1	L	242	LYS	3.6
1	B	271	VAL	3.6
1	F	257	GLU	3.6
1	L	366	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	243	ALA	3.6
1	K	186	GLU	3.6
1	G	355	GLU	3.6
1	E	227	ILE	3.6
1	C	305	ILE	3.5
2	U	25	ILE	3.5
1	B	387	VAL	3.5
1	F	203	TYR	3.5
1	L	262	LEU	3.5
1	F	277	LYS	3.4
1	F	300	VAL	3.4
1	F	299	THR	3.4
1	L	200	LEU	3.4
1	L	231	ARG	3.4
1	E	254	VAL	3.4
1	H	428	ASP	3.4
1	E	203	TYR	3.4
1	L	236	VAL	3.4
1	F	231	ARG	3.4
1	E	208	PRO	3.4
1	E	231	ARG	3.4
1	F	253	ASP	3.4
1	E	353	ILE	3.4
1	H	238	GLU	3.3
1	F	226	LYS	3.3
1	F	282	GLY	3.3
2	P	72	GLY	3.3
1	A	305	ILE	3.3
1	D	271	VAL	3.3
1	G	302	SER	3.3
1	L	203	TYR	3.3
1	L	268	ARG	3.3
2	O	72	GLY	3.3
1	G	314	LEU	3.3
2	R	17	VAL	3.3
1	F	308	GLU	3.3
1	L	250	ILE	3.3
2	T	49	LEU	3.3
1	E	253	ASP	3.2
1	A	383	ALA	3.2
1	L	195	PHE	3.2
1	F	301	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	Q	26	VAL	3.1
1	D	254	VAL	3.1
1	F	241	ALA	3.1
1	E	361	ASP	3.1
1	G	304	GLU	3.1
1	A	271	VAL	3.1
2	U	30	SER	3.1
1	L	484	GLU	3.1
1	A	384	ALA	3.1
1	A	183	LEU	3.1
1	F	374	GLY	3.1
1	G	357	THR	3.1
1	D	357	THR	3.0
1	H	301	ILE	3.0
1	A	283	ASP	3.0
1	C	355	GLU	3.0
1	F	252	GLU	3.0
1	B	244	GLY	3.0
1	C	257	GLU	3.0
1	D	365	LEU	3.0
1	C	212	ALA	3.0
1	C	360	TYR	3.0
2	U	31	ALA	3.0
1	E	305	ILE	3.0
1	H	250	ILE	3.0
2	O	32	ALA	3.0
1	K	281	PHE	3.0
1	F	372	LEU	2.9
1	N	231	ARG	2.9
1	B	484	GLU	2.9
1	G	209	GLU	2.9
1	A	353	ILE	2.9
1	L	357	THR	2.9
1	D	317	LEU	2.9
2	T	25	ILE	2.9
1	B	361	ASP	2.9
2	P	31	ALA	2.9
1	G	281	PHE	2.9
1	K	283	ASP	2.8
1	F	303	GLU	2.8
1	G	308	GLU	2.8
1	B	254	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	244	GLY	2.8
1	L	271	VAL	2.8
1	E	206	ASN	2.8
1	E	314	LEU	2.8
1	K	262	LEU	2.8
1	F	307	MET	2.8
1	E	372	LEU	2.8
1	F	298	GLY	2.8
1	C	203	TYR	2.8
1	B	231	ARG	2.8
1	F	279	PRO	2.8
1	G	364	LYS	2.8
1	N	242	LYS	2.8
1	H	309	LEU	2.8
2	U	18	GLU	2.8
2	Q	27	LEU	2.8
1	G	299	THR	2.8
1	L	255	GLU	2.8
1	E	269	GLY	2.7
1	G	282	GLY	2.7
1	K	182	GLY	2.7
1	L	382	GLY	2.7
1	N	284	ARG	2.7
2	O	22	ALA	2.7
1	H	272	LYS	2.7
1	C	384	ALA	2.7
1	G	227	ILE	2.7
1	F	357	THR	2.7
1	L	495	ASP	2.7
1	L	238	GLU	2.7
1	H	242	LYS	2.7
1	L	272	LYS	2.7
1	K	203	TYR	2.7
1	M	110	GLY	2.7
2	R	80	ASN	2.7
1	K	268	ARG	2.6
2	O	80	ASN	2.6
2	T	50	GLU	2.6
1	E	387	VAL	2.6
1	M	236	VAL	2.6
1	K	360	TYR	2.6
1	C	307	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	188	ASP	2.6
1	G	298	GLY	2.6
2	O	17	VAL	2.6
1	C	306	GLY	2.6
1	F	248	LEU	2.6
2	O	49	LEU	2.6
1	H	221	LEU	2.5
1	F	264	VAL	2.5
1	G	303	GLU	2.5
2	T	97	ALA	2.5
1	B	208	PRO	2.5
1	F	306	GLY	2.5
1	H	249	ILE	2.5
1	G	307	MET	2.5
1	G	300	VAL	2.5
2	T	51	ASN	2.5
1	E	202	PRO	2.5
1	G	231	ARG	2.5
1	F	240	VAL	2.5
2	U	17	VAL	2.5
1	C	231	ARG	2.5
1	D	231	ARG	2.5
1	D	306	GLY	2.5
1	K	303	GLU	2.4
2	T	53	GLU	2.4
1	E	245	LYS	2.4
1	G	261	THR	2.4
1	B	384	ALA	2.4
2	Q	32	ALA	2.4
2	R	30	SER	2.4
1	B	326	ASN	2.4
1	F	192	GLY	2.4
1	G	240	VAL	2.4
1	L	240	VAL	2.4
1	L	387	VAL	2.4
1	K	227	ILE	2.4
1	A	389	MET	2.4
1	H	277	LYS	2.4
1	H	172	GLU	2.4
1	M	231	ARG	2.4
2	R	18	GLU	2.4
1	E	313	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	313	THR	2.4
1	C	271	VAL	2.4
1	F	174	VAL	2.4
1	G	360	TYR	2.4
1	E	243	ALA	2.4
2	P	25	ILE	2.4
1	G	284	ARG	2.4
2	S	30	SER	2.4
1	K	264	VAL	2.4
1	F	256	GLY	2.4
1	G	306	GLY	2.4
1	A	360	TYR	2.4
1	D	227	ILE	2.4
1	H	243	ALA	2.4
1	K	480	ALA	2.4
2	O	82	GLU	2.4
1	G	210	THR	2.3
1	D	241	ALA	2.3
1	E	321	LYS	2.3
1	M	243	ALA	2.3
1	M	272	LYS	2.3
2	R	51	ASN	2.3
1	C	281	PHE	2.3
1	G	387	VAL	2.3
1	A	390	LYS	2.3
1	B	170	GLY	2.3
1	C	286	LYS	2.3
1	G	280	GLY	2.3
1	H	270	ILE	2.3
1	L	210	THR	2.3
1	E	46	ALA	2.3
1	F	222	LEU	2.3
1	G	309	LEU	2.3
1	H	484	GLU	2.3
1	K	236	VAL	2.3
1	F	286	LYS	2.3
1	F	297	GLY	2.3
1	G	257	GLU	2.3
1	F	235	PRO	2.3
1	D	374	GLY	2.3
2	O	25	ILE	2.3
1	B	152	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	372	LEU	2.3
1	H	203	TYR	2.3
1	E	153	ASN	2.3
1	E	207	LYS	2.3
1	E	257	GLU	2.3
1	G	254	VAL	2.3
1	G	354	GLU	2.3
1	K	381	VAL	2.3
1	G	244	GLY	2.3
2	P	32	ALA	2.3
1	D	284	ARG	2.3
1	F	351	GLN	2.3
1	K	327	LYS	2.3
1	L	307	MET	2.2
2	O	31	ALA	2.2
1	E	210	THR	2.2
1	C	304	GLU	2.2
1	N	238	GLU	2.2
1	C	342	ILE	2.2
1	B	210	THR	2.2
1	B	242	LYS	2.2
1	K	226	LYS	2.2
1	B	269	GLY	2.2
1	E	282	GLY	2.2
1	F	244	GLY	2.2
1	A	242	LYS	2.2
1	A	385	THR	2.2
1	B	203	TYR	2.2
1	B	302	SER	2.2
1	F	302	SER	2.2
1	H	227	ILE	2.2
1	K	301	ILE	2.2
1	L	270	ILE	2.2
1	F	386	GLU	2.2
1	G	255	GLU	2.2
1	C	243	ALA	2.2
1	I	243	ALA	2.2
1	F	327	LYS	2.2
1	G	311	LYS	2.2
1	J	281	PHE	2.2
1	A	299	THR	2.2
1	J	247	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	214	GLU	2.2
1	F	206	ASN	2.2
2	R	53	GLU	2.2
1	D	263	VAL	2.1
1	D	199	TYR	2.1
1	G	199	TYR	2.1
1	B	200	LEU	2.1
1	F	432	GLN	2.1
1	G	222	LEU	2.1
1	C	302	SER	2.1
1	D	327	LYS	2.1
1	K	286	LYS	2.1
1	L	327	LYS	2.1
1	H	109	ALA	2.1
1	C	299	THR	2.1
1	E	272	LYS	2.1
1	F	309	LEU	2.1
1	A	252	GLU	2.1
1	F	170	GLY	2.1
1	F	238	GLU	2.1
1	M	238	GLU	2.1
1	E	281	PHE	2.1
1	C	240	VAL	2.1
1	L	254	VAL	2.1
1	K	272	LYS	2.1
1	L	277	LYS	2.1
1	L	313	THR	2.1
1	E	341	ALA	2.1
1	E	306	GLY	2.1
2	P	18	GLU	2.1
1	A	228	SER	2.1
1	K	206	ASN	2.1
1	H	236	VAL	2.1
1	L	39	VAL	2.1
1	F	196	ASP	2.1
1	M	242	LYS	2.1
1	J	234	LEU	2.1
1	K	357	THR	2.1
1	L	360	TYR	2.1
1	I	343	GLN	2.1
1	E	228	SER	2.1
1	H	433	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	207	LYS	2.1
1	E	301	ILE	2.1
1	G	183	LEU	2.1
1	G	250	ILE	2.1
1	D	316	ASP	2.1
1	A	184	GLN	2.1
1	D	338	GLU	2.1
1	B	305	ILE	2.0
1	G	312	ALA	2.0
1	L	239	ALA	2.0
1	L	428	ASP	2.0
1	D	244	GLY	2.0
1	G	366	GLN	2.0
1	F	304	GLU	2.0
1	J	303	GLU	2.0
1	L	226	LYS	2.0
1	B	183	LEU	2.0
1	K	358	SER	2.0
1	H	423	ALA	2.0
1	K	241	ALA	2.0
2	S	22	ALA	2.0
1	E	283	ASP	2.0
1	G	334	ASP	2.0
1	H	271	VAL	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](#)

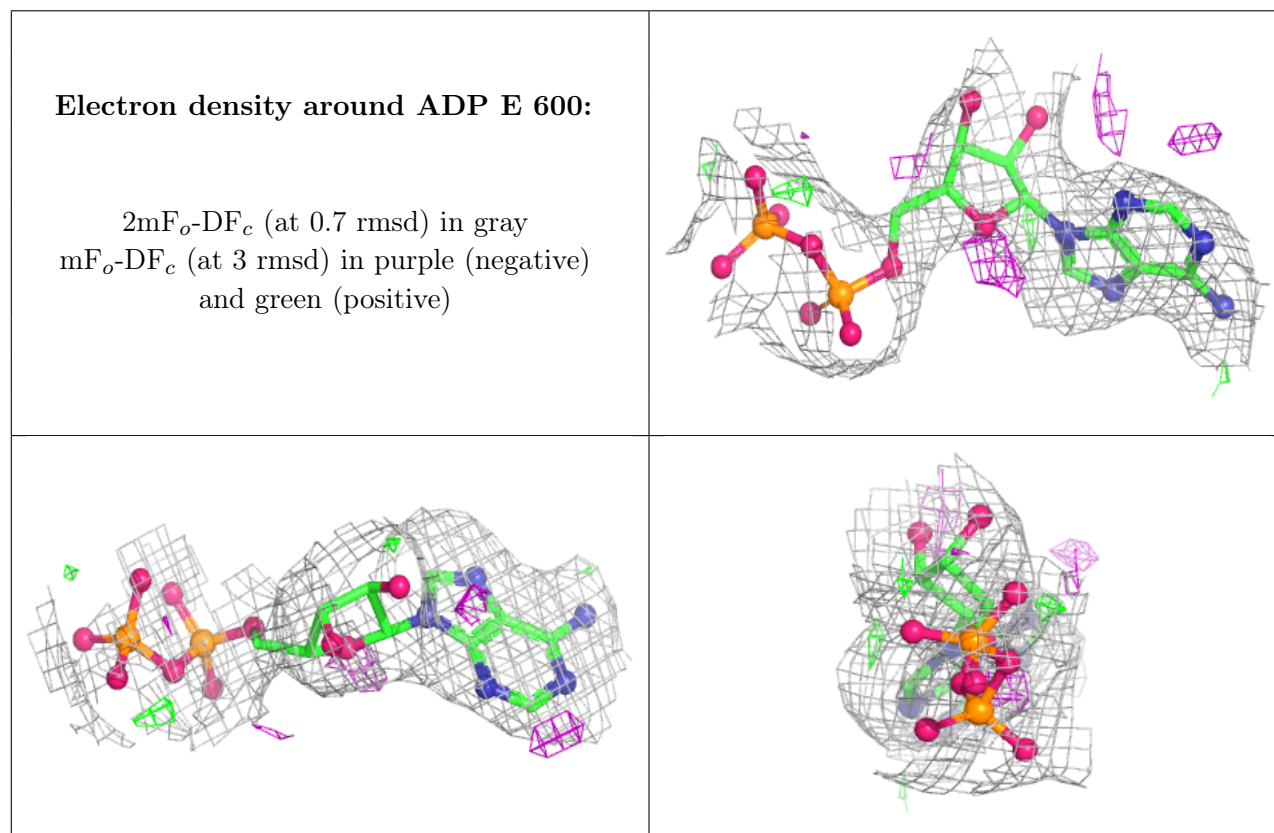
There are no oligosaccharides in this entry.

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.

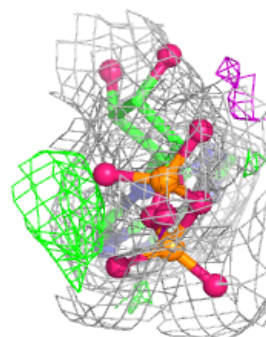
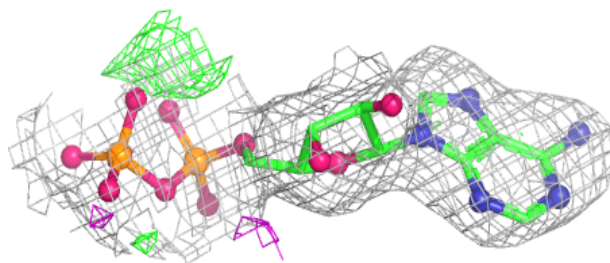
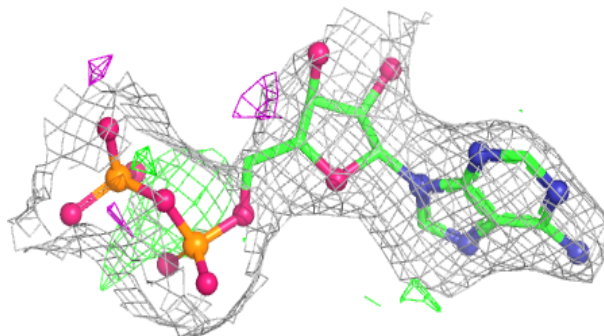
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	601	1/1	0.88	0.13	2,2,2,2	0
3	MG	B	601	1/1	0.93	0.16	2,2,2,2	0
4	ADP	E	600	27/27	0.95	0.08	2,2,3,5	0
4	ADP	F	600	27/27	0.95	0.08	2,2,3,5	0
4	ADP	B	600	27/27	0.96	0.07	2,2,4,5	0
3	MG	A	601	1/1	0.96	0.21	2,2,2,2	0
3	MG	G	601	1/1	0.96	0.15	2,2,2,2	0
4	ADP	C	600	27/27	0.97	0.06	2,2,4,5	0
4	ADP	D	600	27/27	0.97	0.06	2,2,4,5	0
4	ADP	A	600	27/27	0.97	0.06	2,2,3,6	0
3	MG	D	601	1/1	0.97	0.18	2,2,2,2	0
4	ADP	G	600	27/27	0.97	0.07	2,2,4,5	0
3	MG	E	601	1/1	0.98	0.13	2,2,2,2	0
3	MG	F	601	1/1	0.98	0.18	2,2,2,2	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.

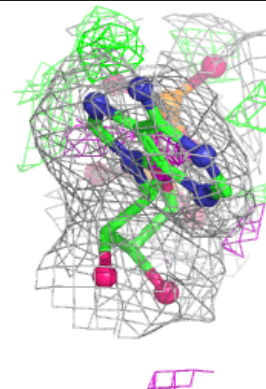
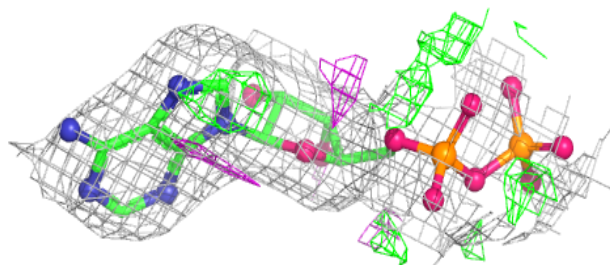
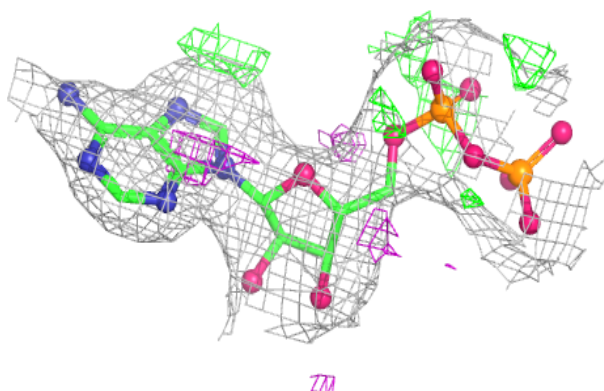


Electron density around ADP F 600:

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

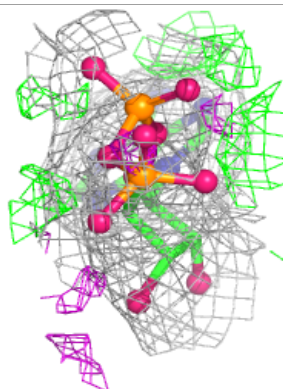
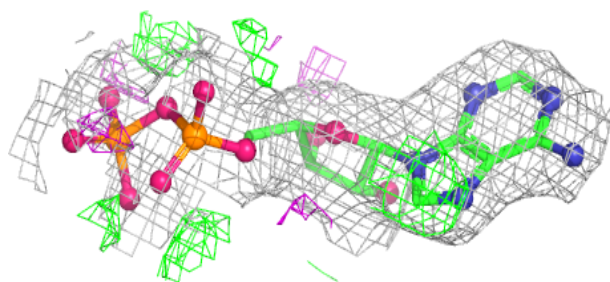
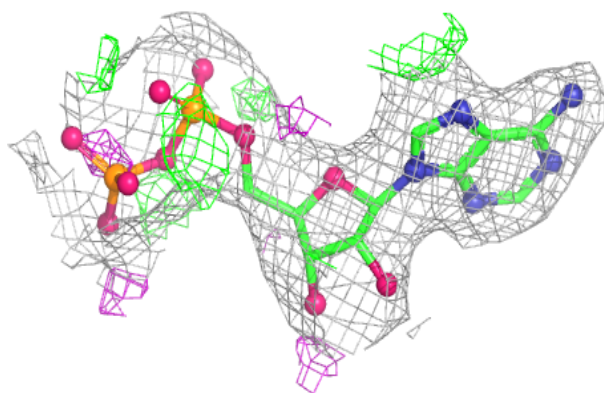
**Electron density around ADP B 600:**

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

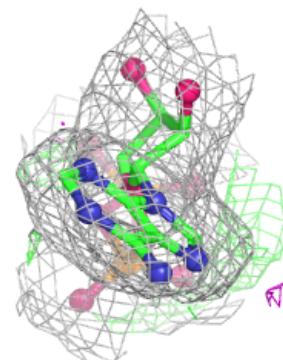
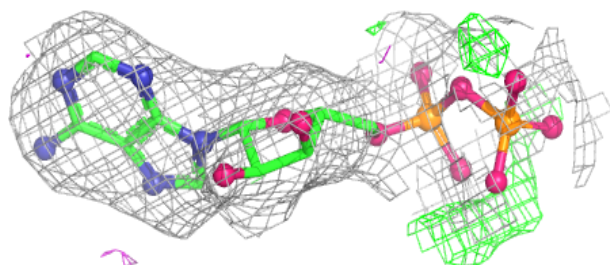
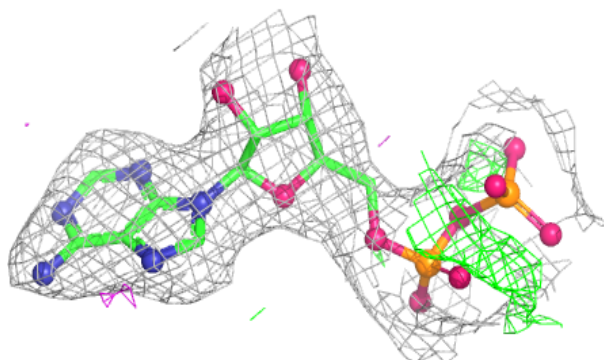


Electron density around ADP C 600:

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

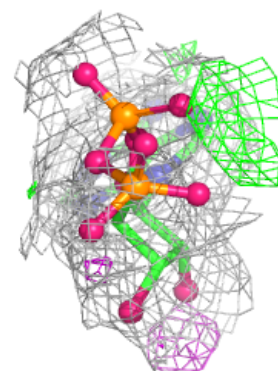
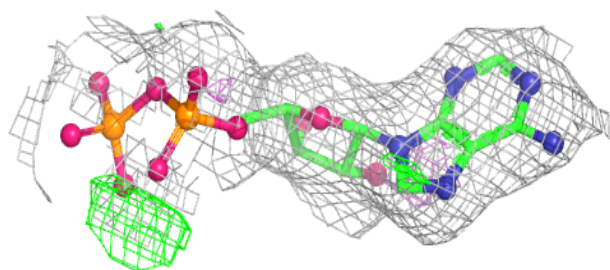
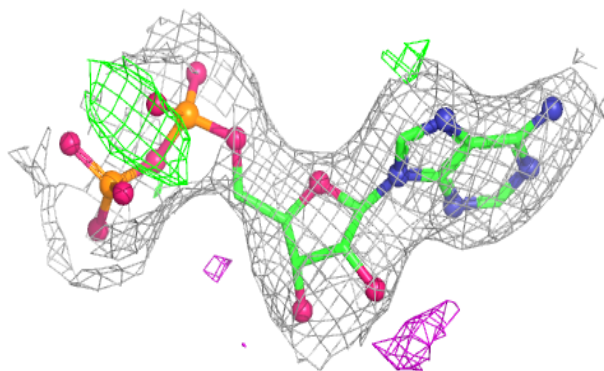
**Electron density around ADP D 600:**

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

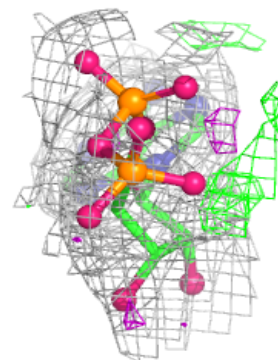
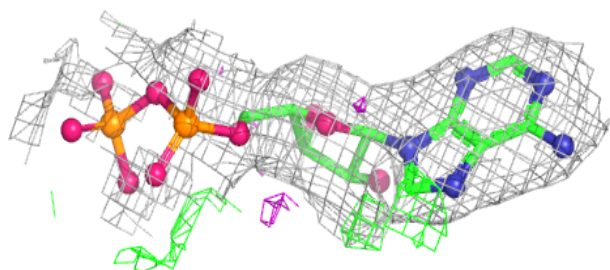
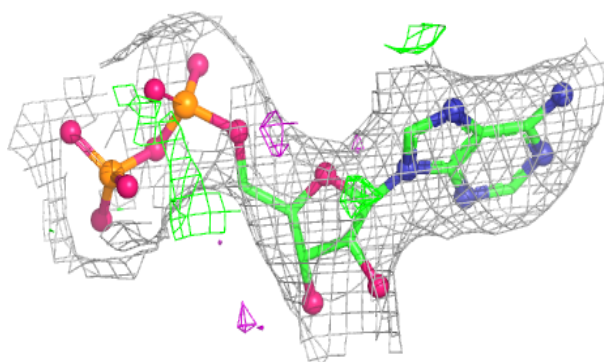


Electron density around ADP A 600:

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

**Electron density around ADP G 600:**

$2mF_o-DF_c$ (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.