



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:35 am BST

PDB ID : 1SX4
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

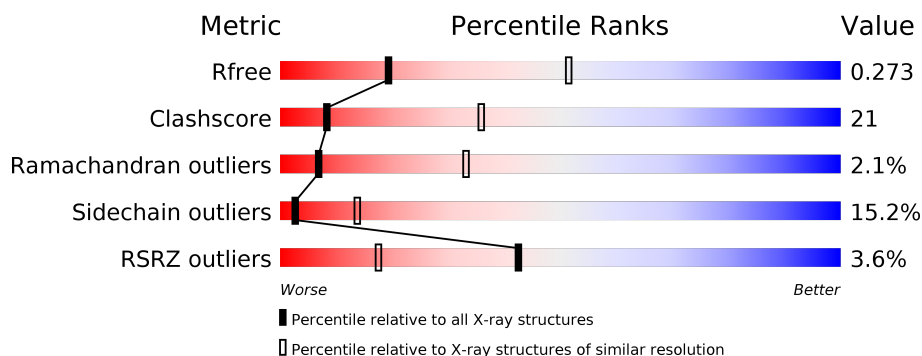
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>38%</div> <div>8%</div> </div> </div>
1	B	524	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>35%</div> <div>8%</div> </div> </div>
1	C	524	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>35%</div> <div>9%</div> </div> </div>
1	D	524	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>6%</div> </div> </div>
1	E	524	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>37%</div> <div>7%</div> </div> </div>
1	F	524	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>35%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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			

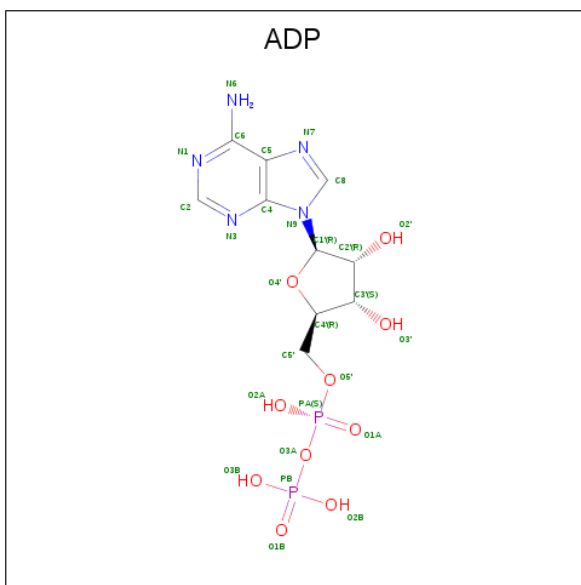
- Molecule 2 is a protein called groES protein.

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is water.

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

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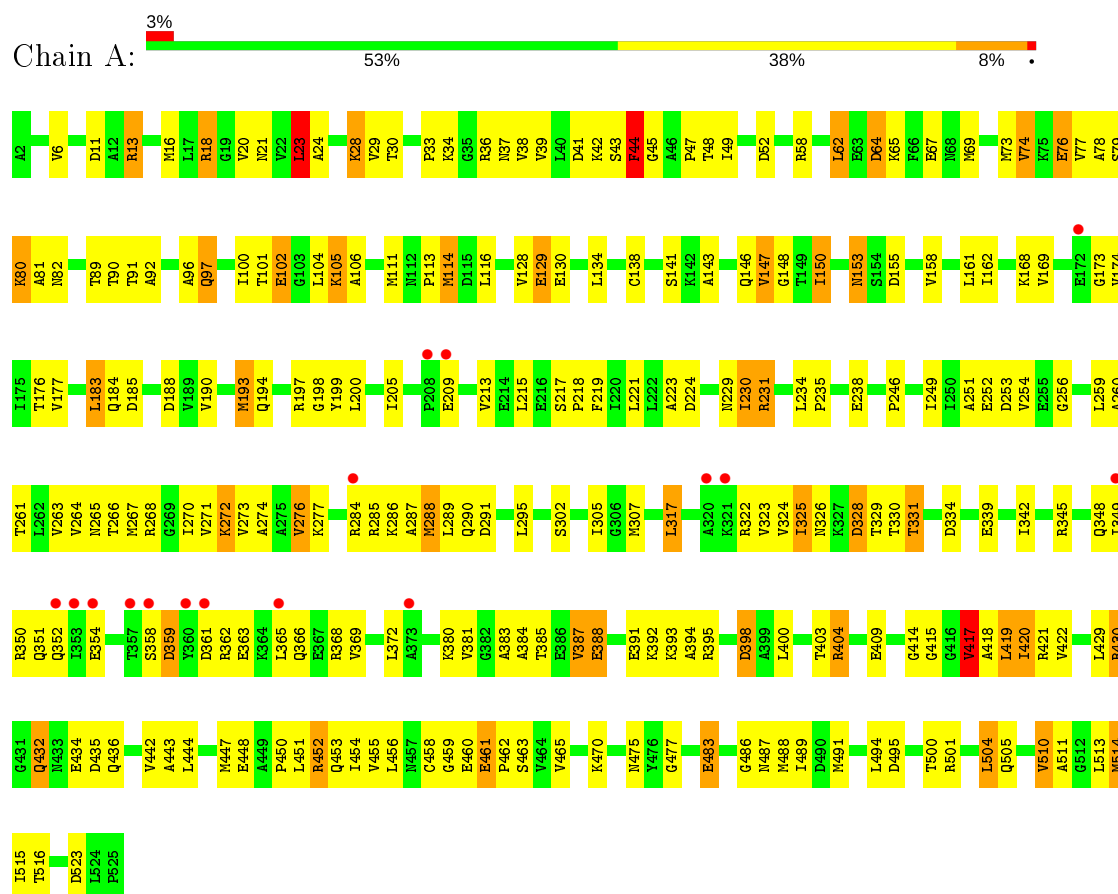
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	8	Total 8	O 8	0	0
5	G	13	Total 13	O 13	0	0
5	H	12	Total 12	O 12	0	0
5	I	19	Total 19	O 19	0	0
5	J	14	Total 14	O 14	0	0
5	K	14	Total 14	O 14	0	0
5	L	16	Total 16	O 16	0	0
5	M	10	Total 10	O 10	0	0
5	N	21	Total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

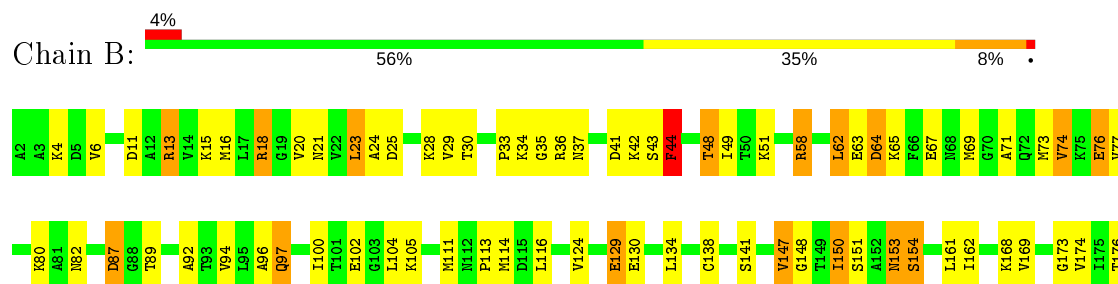
3 Residue-property plots

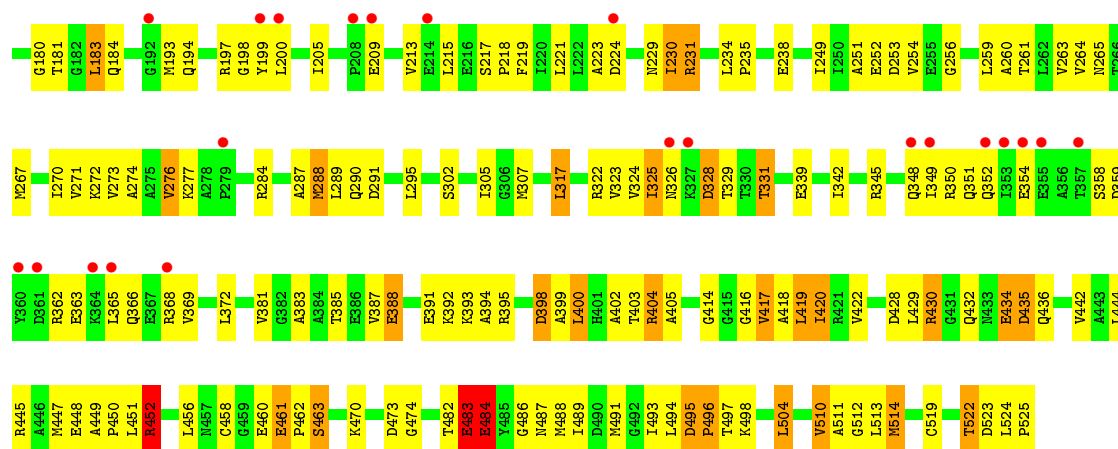
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

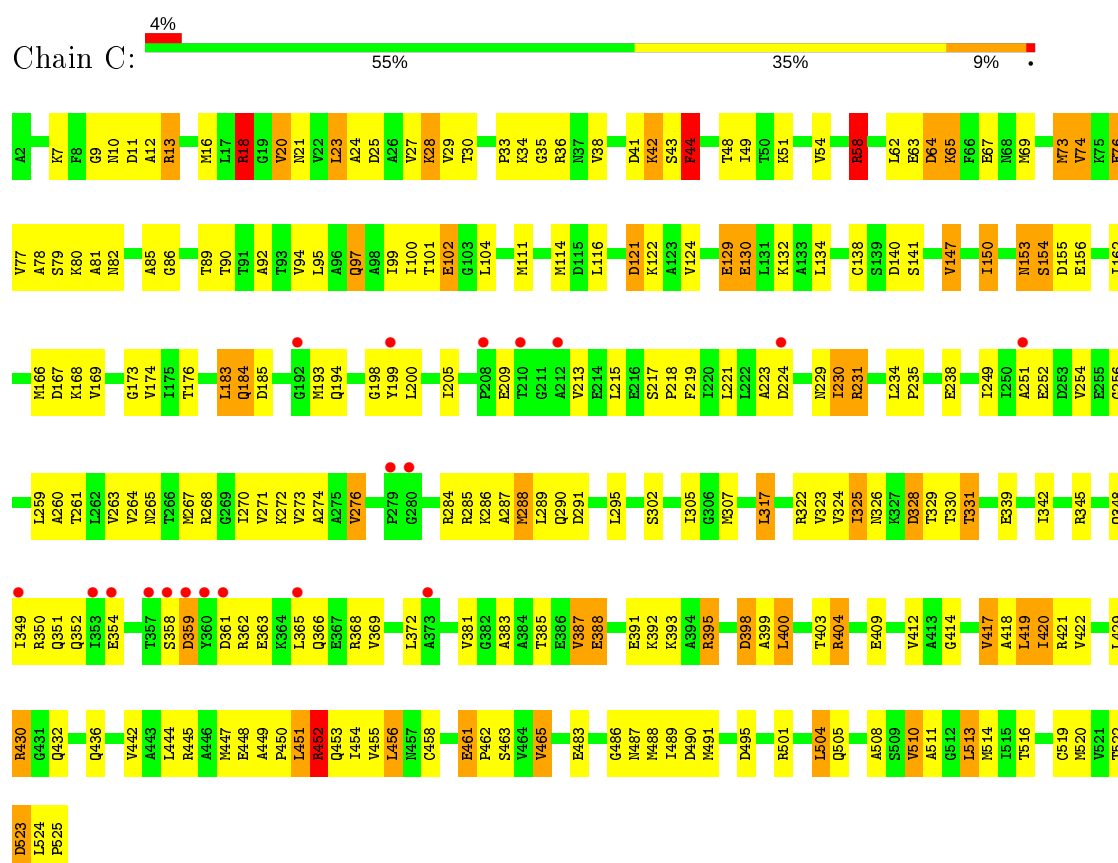


• Molecule 1: groEL protein

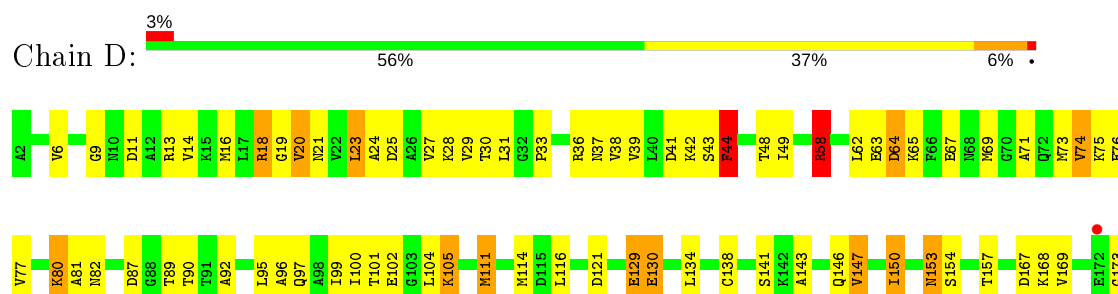


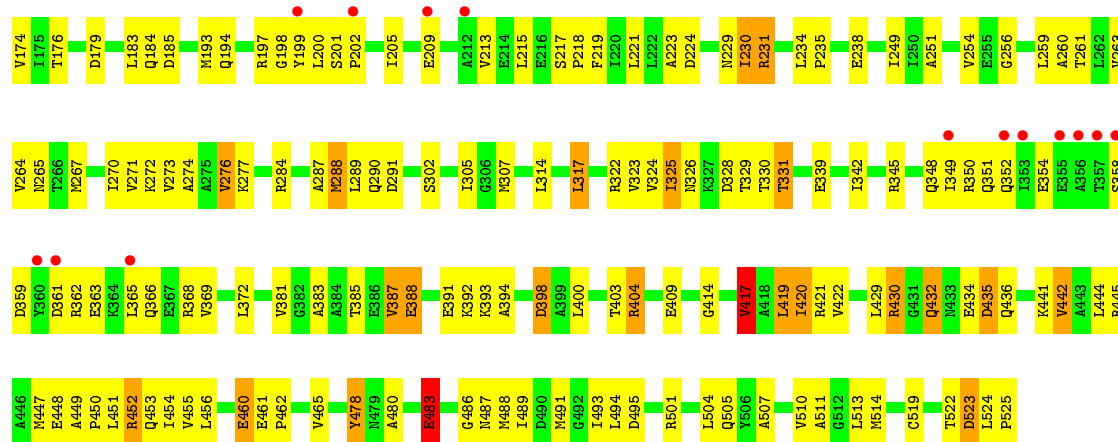


• Molecule 1: groEL protein

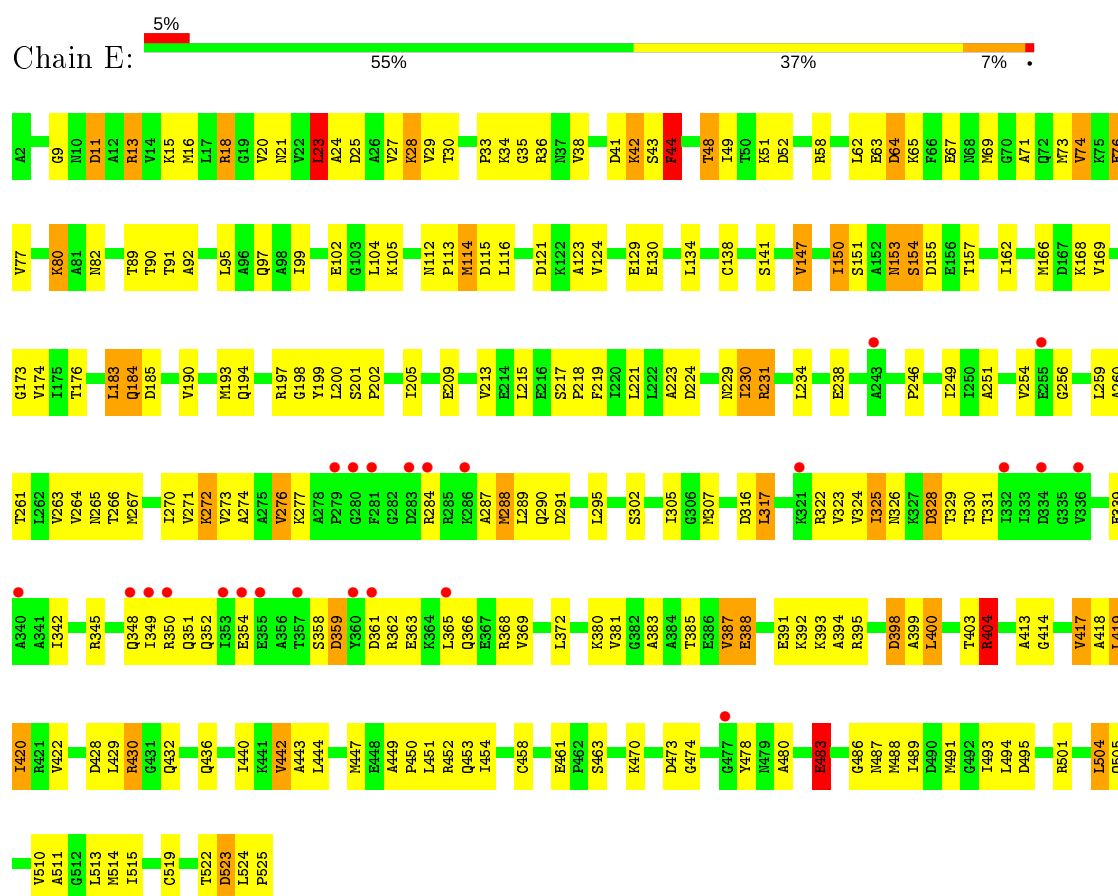


• Molecule 1: groEL protein

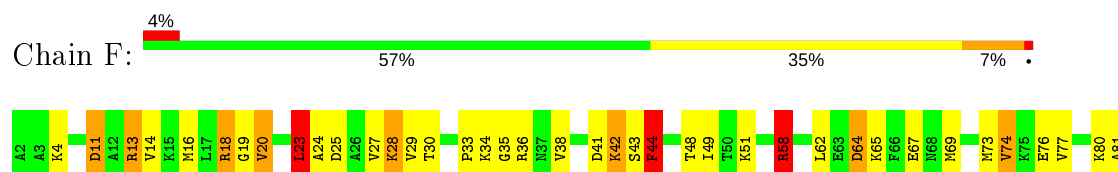


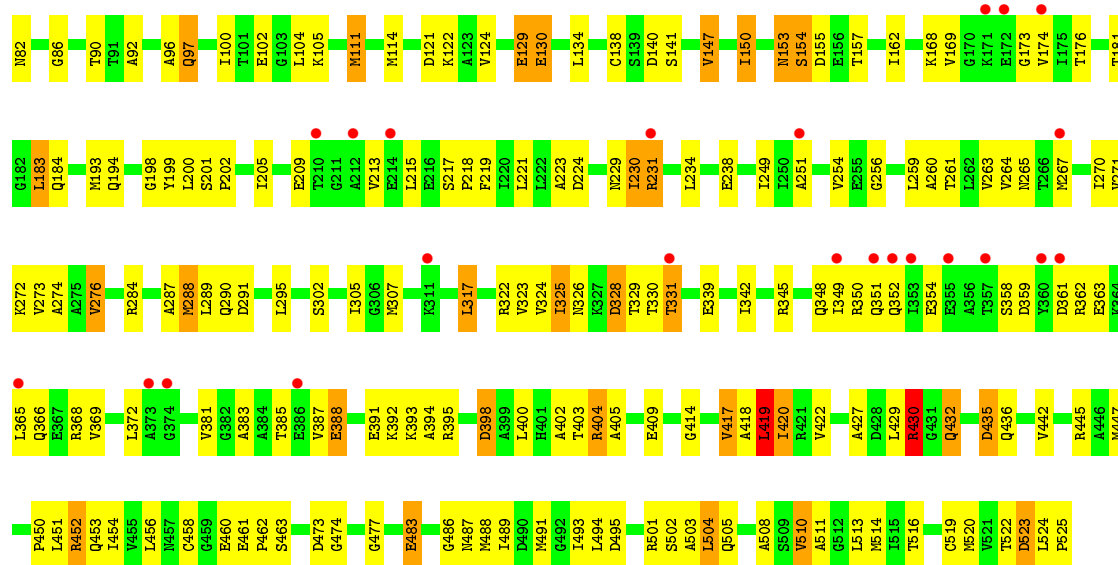


• Molecule 1: groEL protein

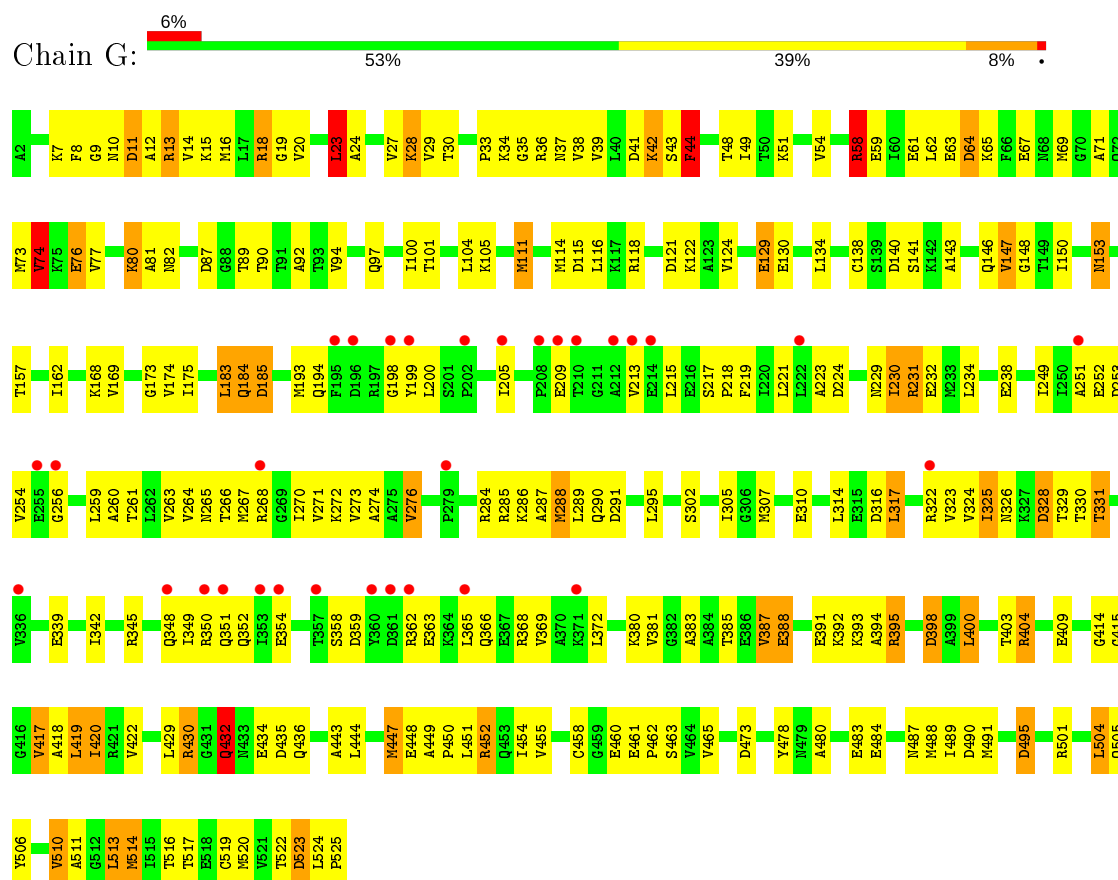


• Molecule 1: groEL protein

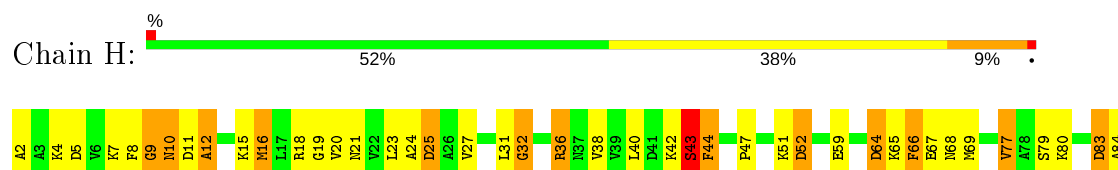


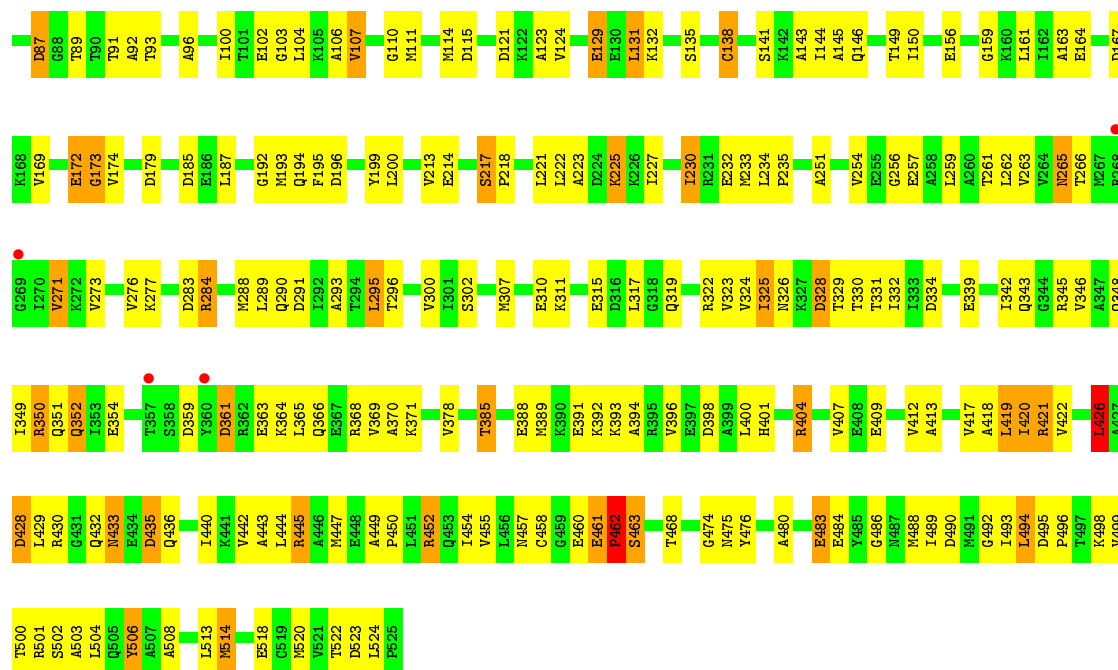


• Molecule 1: groEL protein



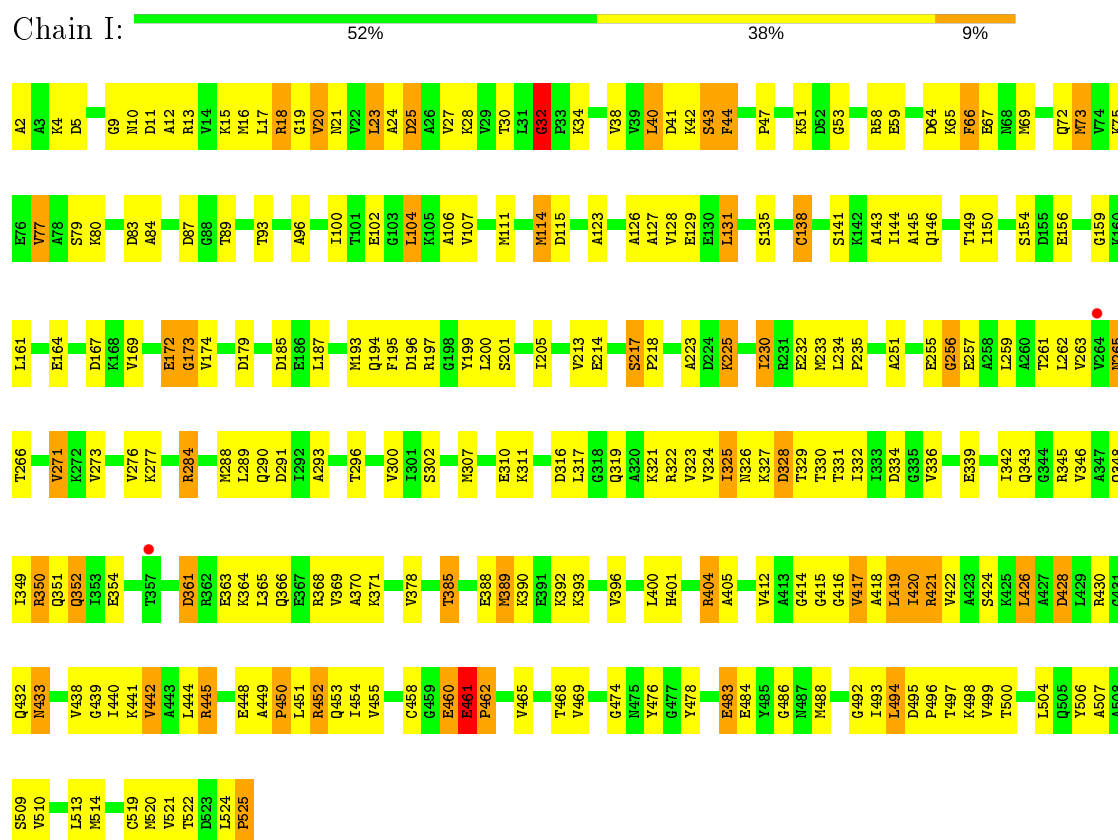
• Molecule 1: groEL protein





- Molecule 1: groEL protein

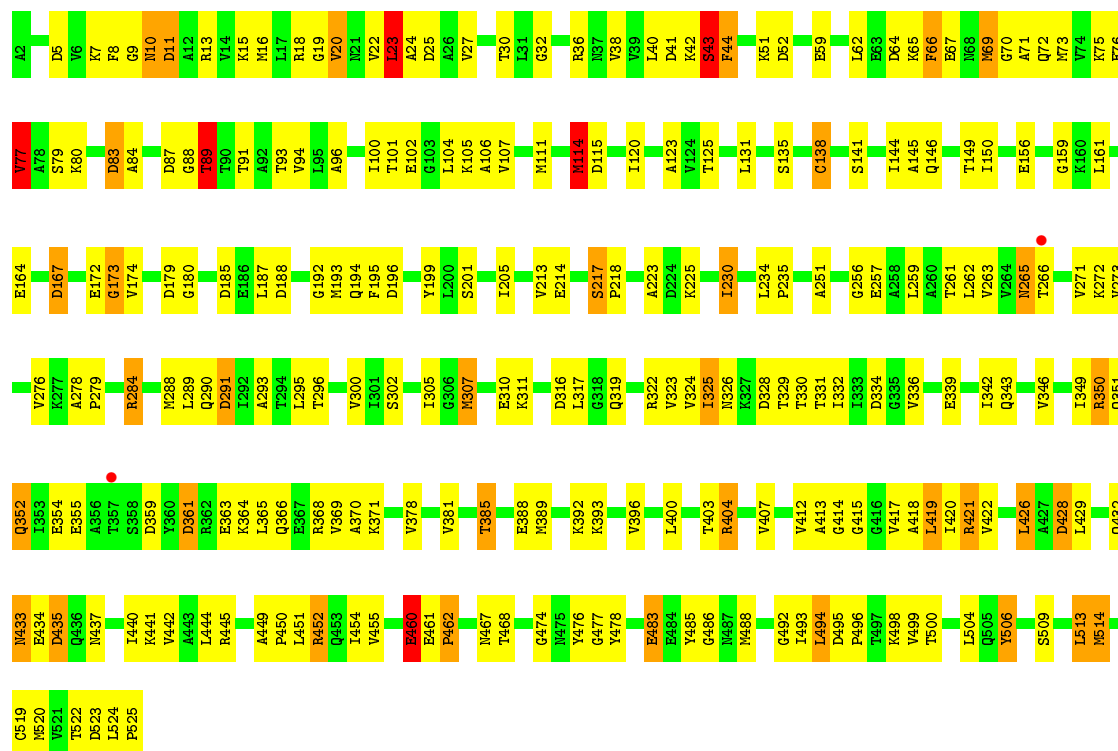
Chain I:



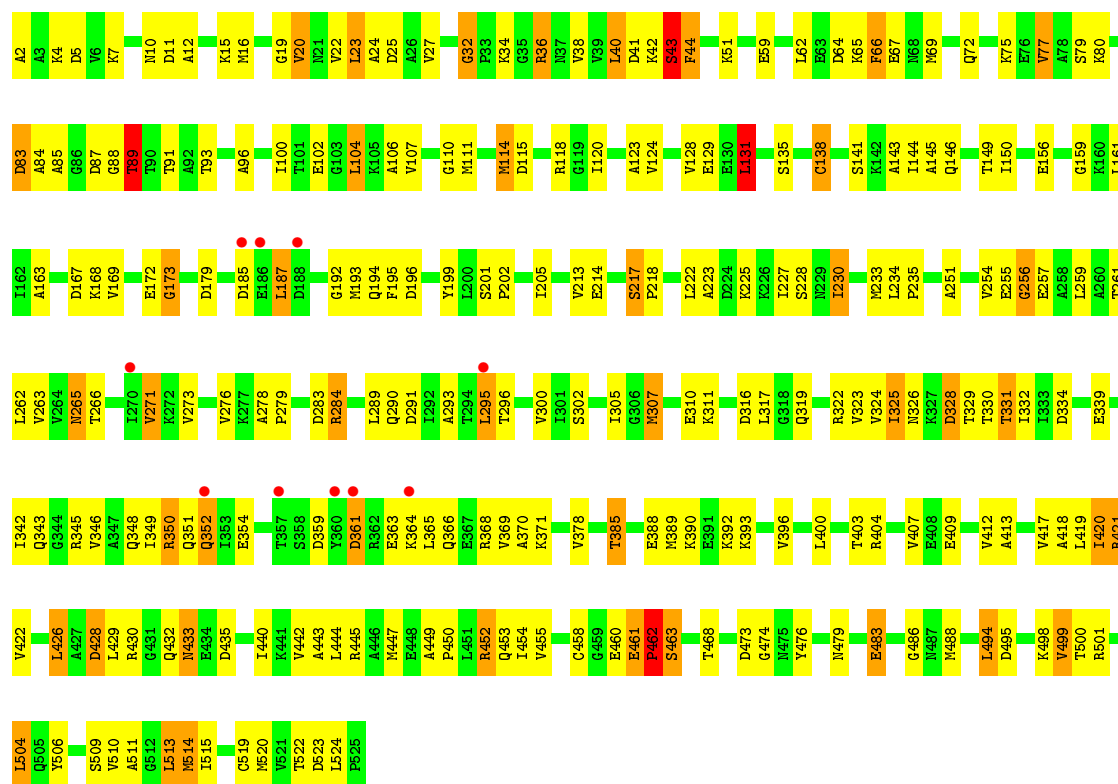
- Molecule 1: groEL protein

Chain J:

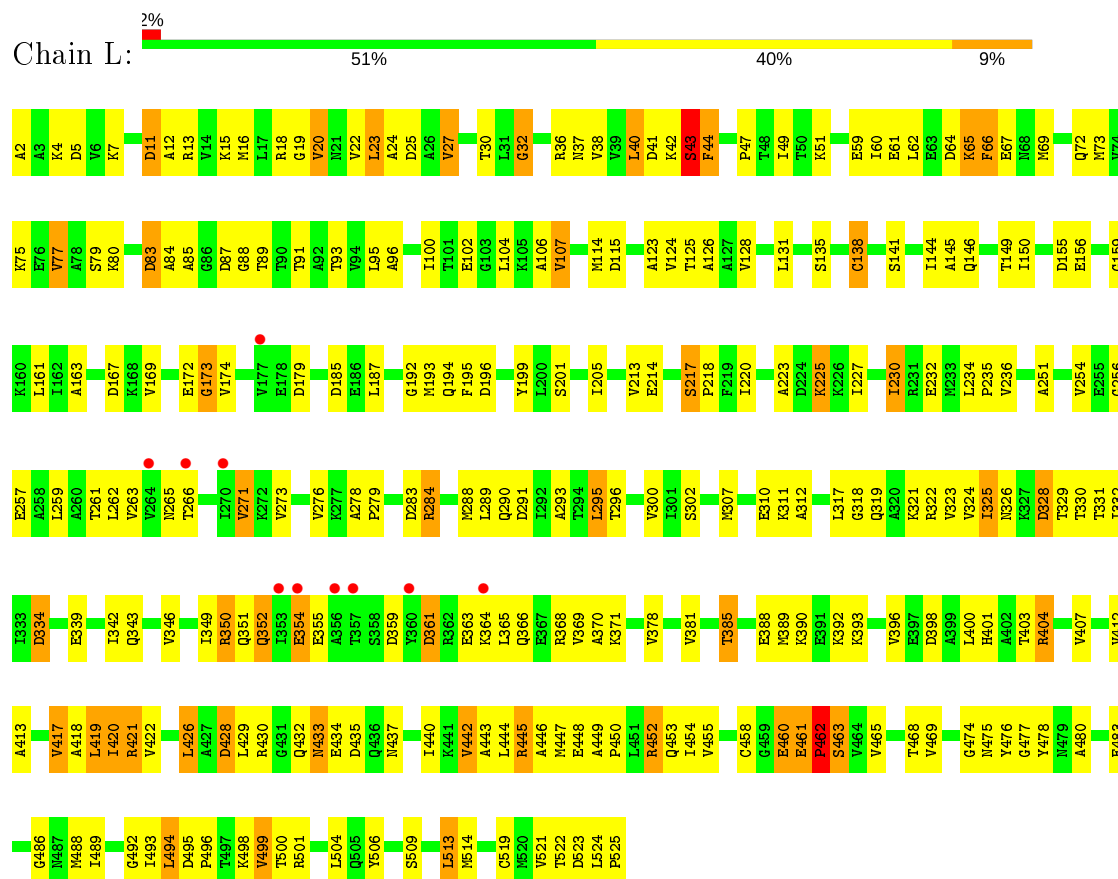




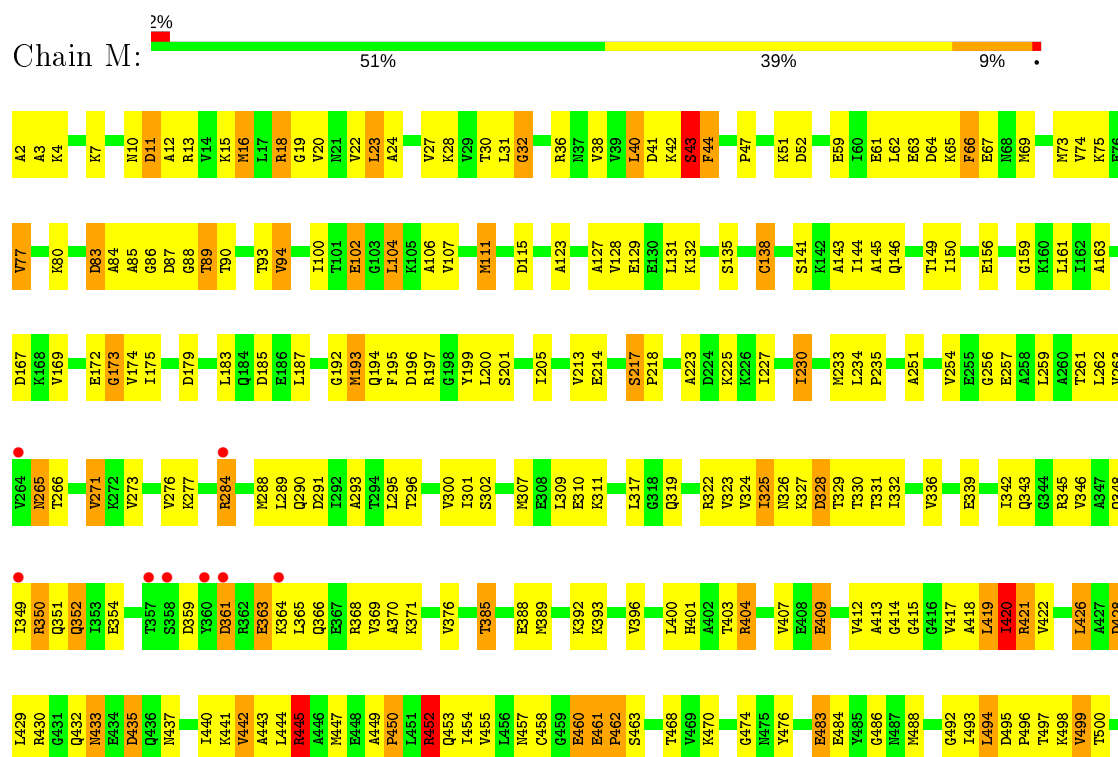
• Molecule 1: groEL protein



• Molecule 1: groEL protein

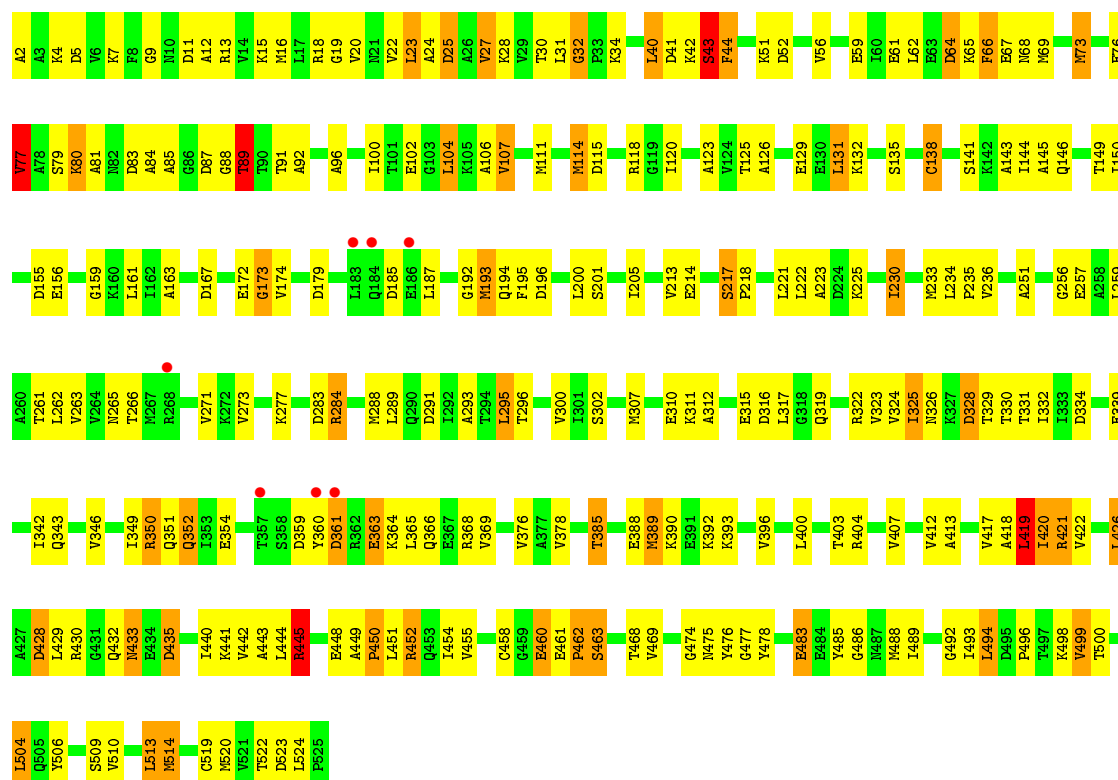


- Molecule 1: groEL protein

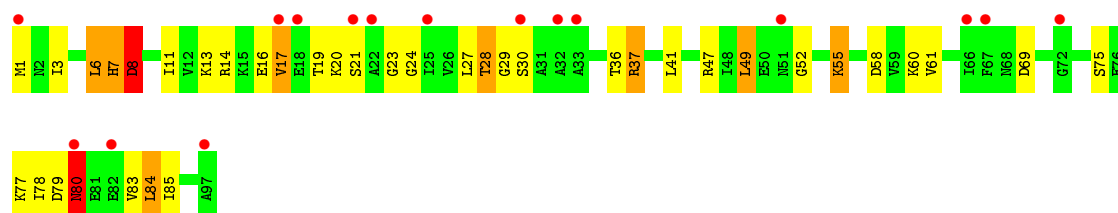




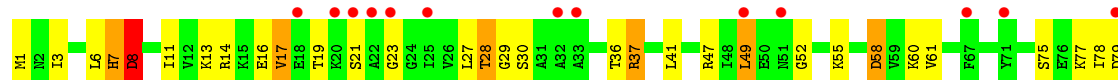
• Molecule 1: groEL protein

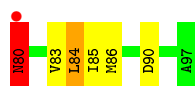


• Molecule 2: groES protein

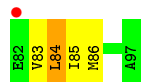
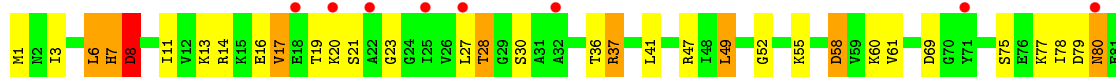


• Molecule 2: groES protein





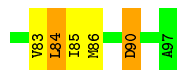
- Molecule 2: groES protein



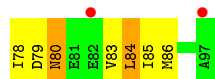
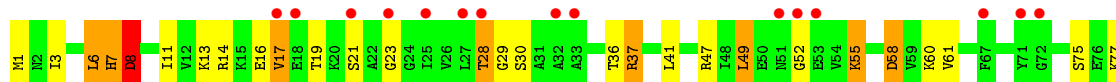
- Molecule 2: groES protein



- Molecule 2: groES protein

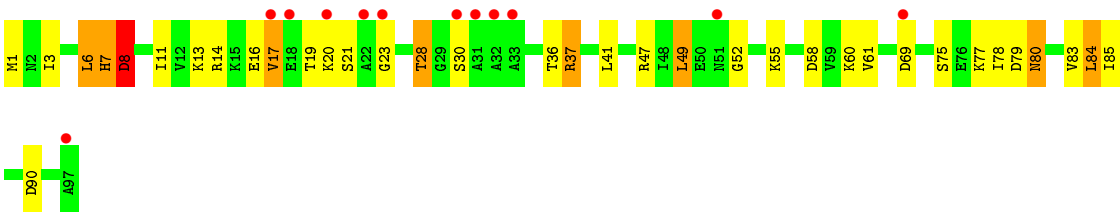


- Molecule 2: groES protein



- 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 40.07 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 96.7 (40.07-2.99)	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)	0.28 , 56.0	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	0.90	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: MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.26	27/3884 (0.7%)	1.17	27/5243 (0.5%)
1	B	1.09	12/3884 (0.3%)	1.10	20/5243 (0.4%)
1	C	1.20	17/3884 (0.4%)	1.20	31/5243 (0.6%)
1	D	1.22	19/3884 (0.5%)	1.14	15/5243 (0.3%)
1	E	1.01	11/3884 (0.3%)	1.07	22/5243 (0.4%)
1	F	0.98	12/3884 (0.3%)	1.06	21/5243 (0.4%)
1	G	1.16	18/3884 (0.5%)	1.16	28/5243 (0.5%)
1	H	1.06	7/3884 (0.2%)	1.11	25/5243 (0.5%)
1	I	1.18	10/3884 (0.3%)	1.16	17/5243 (0.3%)
1	J	1.07	9/3884 (0.2%)	1.15	26/5243 (0.5%)
1	K	0.95	4/3884 (0.1%)	1.06	21/5243 (0.4%)
1	L	0.87	1/3884 (0.0%)	1.03	20/5243 (0.4%)
1	M	1.08	16/3884 (0.4%)	1.13	19/5243 (0.4%)
1	N	1.09	13/3884 (0.3%)	1.13	26/5243 (0.5%)
2	O	0.65	0/732	0.91	3/983 (0.3%)
2	P	0.61	0/732	0.89	3/983 (0.3%)
2	Q	0.66	0/732	0.92	3/983 (0.3%)
2	R	0.73	0/732	0.92	3/983 (0.3%)
2	S	0.67	0/732	0.92	3/983 (0.3%)
2	T	0.65	0/732	0.91	2/983 (0.2%)
2	U	0.65	0/732	0.90	5/983 (0.5%)
All	All	1.06	176/59500 (0.3%)	1.10	340/80283 (0.4%)

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 (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	GLU	CD-OE1	9.80	1.36	1.25
1	I	461	GLU	CD-OE1	9.36	1.35	1.25
1	N	483	GLU	CD-OE2	8.57	1.35	1.25
1	I	484	GLU	CD-OE1	8.36	1.34	1.25
1	D	71	ALA	CA-CB	-8.26	1.35	1.52
1	D	483	GLU	CD-OE1	8.05	1.34	1.25
1	D	130	GLU	CD-OE2	8.00	1.34	1.25
1	C	73	MET	SD-CE	7.91	2.22	1.77
1	A	129	GLU	CD-OE2	7.86	1.34	1.25
1	I	73	MET	CG-SD	7.83	2.01	1.81
1	N	514	MET	SD-CE	7.75	2.21	1.77
1	A	44	PHE	CE2-CZ	7.67	1.51	1.37
1	J	114	MET	SD-CE	7.62	2.20	1.77
1	G	105	LYS	CD-CE	7.53	1.70	1.51
1	C	78	ALA	CA-CB	-7.50	1.36	1.52
1	A	434	GLU	CG-CD	7.27	1.62	1.51
1	I	483	GLU	CD-OE2	7.03	1.33	1.25
1	B	71	ALA	CA-CB	-7.00	1.37	1.52
1	A	114	MET	CG-SD	6.99	1.99	1.81
1	I	461	GLU	CD-OE2	6.98	1.33	1.25
1	D	417	VAL	CB-CG1	-6.97	1.38	1.52
1	A	417	VAL	CB-CG1	-6.92	1.38	1.52
1	A	483	GLU	CD-OE1	6.92	1.33	1.25
1	D	129	GLU	CD-OE2	6.89	1.33	1.25
1	D	111	MET	SD-CE	6.85	2.16	1.77
1	C	79	SER	CB-OG	6.81	1.51	1.42
1	C	129	GLU	CD-OE2	6.74	1.33	1.25
1	A	102	GLU	CD-OE1	6.71	1.33	1.25
1	E	44	PHE	CE1-CZ	6.69	1.50	1.37
1	F	111	MET	SD-CE	6.69	2.15	1.77
1	G	434	GLU	CD-OE1	6.66	1.32	1.25
1	E	105	LYS	CD-CE	6.64	1.67	1.51
1	C	130	GLU	CD-OE1	6.63	1.32	1.25
1	D	434	GLU	CD-OE1	6.62	1.32	1.25
1	E	114	MET	SD-CE	6.57	2.14	1.77
1	B	129	GLU	CD-OE2	6.53	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	483	GLU	CD-OE2	6.51	1.32	1.25
1	F	42	LYS	CD-CE	6.48	1.67	1.51
1	C	465	VAL	CB-CG1	-6.47	1.39	1.52
1	C	76	GLU	CD-OE1	6.47	1.32	1.25
1	J	76	GLU	CD-OE1	6.46	1.32	1.25
1	C	461	GLU	CD-OE2	6.45	1.32	1.25
1	G	76	GLU	C-O	6.41	1.35	1.23
1	A	44	PHE	CD1-CE1	6.38	1.52	1.39
1	I	484	GLU	CD-OE2	6.38	1.32	1.25
1	I	18	ARG	CZ-NH2	6.35	1.41	1.33
1	E	44	PHE	CD2-CE2	6.32	1.51	1.39
1	K	114	MET	SD-CE	6.31	2.13	1.77
1	A	44	PHE	CE1-CZ	6.31	1.49	1.37
1	C	508	ALA	CA-CB	-6.30	1.39	1.52
1	C	132	LYS	CD-CE	6.30	1.67	1.51
1	M	484	GLU	CD-OE1	6.29	1.32	1.25
1	H	518	GLU	CD-OE1	6.19	1.32	1.25
1	C	42	LYS	CD-CE	6.19	1.66	1.51
1	D	44	PHE	CD2-CE2	6.18	1.51	1.39
1	E	71	ALA	CA-CB	-6.18	1.39	1.52
1	D	460	GLU	CD-OE2	6.17	1.32	1.25
1	N	61	GLU	CD-OE2	6.12	1.32	1.25
1	F	111	MET	CG-SD	-6.11	1.65	1.81
1	G	129	GLU	CD-OE2	6.09	1.32	1.25
1	A	44	PHE	CD2-CE2	6.09	1.51	1.39
1	J	506	TYR	CB-CG	-6.08	1.42	1.51
1	F	14	VAL	CB-CG2	-6.05	1.40	1.52
1	D	14	VAL	CB-CG1	-6.04	1.40	1.52
1	G	129	GLU	CD-OE1	6.03	1.32	1.25
1	B	484	GLU	CD-OE2	6.02	1.32	1.25
1	M	461	GLU	CD-OE1	6.01	1.32	1.25
1	G	8	PHE	CE1-CZ	6.00	1.48	1.37
1	M	63	GLU	CD-OE2	6.00	1.32	1.25
1	A	105	LYS	CD-CE	5.99	1.66	1.51
1	F	20	VAL	CB-CG1	-5.99	1.40	1.52
1	M	483	GLU	CD-OE2	5.97	1.32	1.25
1	D	14	VAL	CB-CG2	-5.94	1.40	1.52
1	B	434	GLU	CD-OE1	5.93	1.32	1.25
1	B	44	PHE	CB-CG	5.92	1.61	1.51
1	M	409	GLU	CD-OE1	5.92	1.32	1.25
1	J	514	MET	SD-CE	5.88	2.10	1.77
1	M	88	GLY	C-O	-5.85	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	483	GLU	CD-OE2	5.85	1.32	1.25
1	M	484	GLU	CD-OE2	5.83	1.32	1.25
1	I	58	ARG	CZ-NH2	5.82	1.40	1.33
1	G	8	PHE	CB-CG	-5.78	1.41	1.51
1	A	465	VAL	CB-CG1	-5.77	1.40	1.52
1	G	8	PHE	CD2-CE2	5.76	1.50	1.39
1	C	44	PHE	CB-CG	5.76	1.61	1.51
1	F	44	PHE	CB-CG	5.75	1.61	1.51
1	D	105	LYS	C-O	5.74	1.34	1.23
1	F	130	GLU	CD-OE1	5.74	1.31	1.25
1	N	16	MET	CG-SD	-5.74	1.66	1.81
1	L	73	MET	CG-SD	5.73	1.96	1.81
1	H	12	ALA	CA-CB	-5.72	1.40	1.52
1	D	44	PHE	CD1-CE1	5.71	1.50	1.39
1	A	105	LYS	CE-NZ	5.71	1.63	1.49
1	A	483	GLU	CD-OE2	5.70	1.31	1.25
1	A	452	ARG	NE-CZ	5.68	1.40	1.33
1	A	455	VAL	CB-CG1	5.67	1.64	1.52
1	E	44	PHE	CE2-CZ	5.65	1.48	1.37
1	K	461	GLU	CD-OE2	5.64	1.31	1.25
1	I	448	GLU	CD-OE1	-5.62	1.19	1.25
1	B	483	GLU	CD-OE2	5.62	1.31	1.25
1	G	105	LYS	C-O	5.62	1.34	1.23
1	M	111	MET	SD-CE	5.62	2.09	1.77
1	J	94	VAL	C-O	5.60	1.33	1.23
1	G	74	VAL	CB-CG1	-5.60	1.41	1.52
1	G	111	MET	CG-SD	-5.60	1.66	1.81
1	G	42	LYS	CD-CE	5.59	1.65	1.51
1	G	71	ALA	CA-CB	-5.59	1.40	1.52
1	A	105	LYS	C-O	5.58	1.33	1.23
1	N	114	MET	SD-CE	5.56	2.08	1.77
1	J	483	GLU	CD-OE2	5.53	1.31	1.25
1	N	461	GLU	CD-OE1	5.53	1.31	1.25
1	A	76	GLU	CD-OE1	5.52	1.31	1.25
1	B	461	GLU	CD-OE2	5.50	1.31	1.25
1	C	20	VAL	CA-CB	-5.50	1.43	1.54
1	G	432	GLN	CG-CD	5.49	1.63	1.51
1	J	77	VAL	CB-CG2	-5.49	1.41	1.52
1	N	77	VAL	CB-CG2	-5.49	1.41	1.52
1	I	405	ALA	CA-CB	-5.49	1.41	1.52
1	J	460	GLU	CD-OE2	5.48	1.31	1.25
1	M	445	ARG	NE-CZ	5.44	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	94	VAL	C-O	5.43	1.33	1.23
1	A	90	THR	CB-CG2	5.41	1.70	1.52
1	M	102	GLU	CG-CD	5.40	1.60	1.51
1	B	94	VAL	CB-CG1	-5.40	1.41	1.52
1	D	44	PHE	CE1-CZ	5.39	1.47	1.37
1	E	76	GLU	CD-OE2	5.39	1.31	1.25
1	H	484	GLU	CD-OE1	5.38	1.31	1.25
1	N	76	GLU	CG-CD	5.38	1.60	1.51
1	A	129	GLU	CD-OE1	5.38	1.31	1.25
1	M	18	ARG	NE-CZ	5.37	1.40	1.33
1	M	508	ALA	CA-CB	-5.37	1.41	1.52
1	D	114	MET	CG-SD	5.37	1.95	1.81
1	G	61	GLU	CD-OE2	5.37	1.31	1.25
1	N	76	GLU	CD-OE2	5.37	1.31	1.25
1	A	78	ALA	CA-CB	-5.36	1.41	1.52
1	E	44	PHE	CD1-CE1	5.35	1.50	1.39
1	H	506	TYR	CB-CG	-5.35	1.43	1.51
1	M	61	GLU	CD-OE2	5.34	1.31	1.25
1	F	508	ALA	CA-CB	-5.29	1.41	1.52
1	B	483	GLU	CD-OE1	5.29	1.31	1.25
1	F	129	GLU	CD-OE2	5.29	1.31	1.25
1	D	20	VAL	CB-CG2	-5.29	1.41	1.52
1	E	483	GLU	CD-OE2	5.29	1.31	1.25
1	G	44	PHE	CB-CG	5.27	1.60	1.51
1	M	74	VAL	CB-CG2	-5.27	1.41	1.52
1	J	441	LYS	CD-CE	5.26	1.64	1.51
1	A	510	VAL	CB-CG2	-5.26	1.41	1.52
1	H	18	ARG	CZ-NH1	5.24	1.39	1.33
1	A	128	VAL	CB-CG2	-5.23	1.41	1.52
1	C	18	ARG	CG-CD	5.22	1.65	1.51
1	N	445	ARG	NE-CZ	5.21	1.39	1.33
1	A	459	GLY	C-O	-5.19	1.15	1.23
1	N	76	GLU	CD-OE1	5.18	1.31	1.25
1	F	129	GLU	CD-OE1	5.17	1.31	1.25
1	C	412	VAL	CB-CG2	-5.17	1.42	1.52
1	C	445	ARG	NE-CZ	5.16	1.39	1.33
1	N	56	VAL	CB-CG2	-5.16	1.42	1.52
1	K	514	MET	SD-CE	5.16	2.06	1.77
1	H	508	ALA	CA-CB	-5.15	1.41	1.52
1	B	44	PHE	CE2-CZ	5.14	1.47	1.37
1	D	478	TYR	CE2-CZ	5.13	1.45	1.38
1	C	156	GLU	CD-OE2	5.12	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	94	VAL	CB-CG2	-5.12	1.42	1.52
1	E	42	LYS	CD-CE	5.11	1.64	1.51
1	B	105	LYS	CE-NZ	5.09	1.61	1.49
1	E	63	GLU	CD-OE1	5.09	1.31	1.25
1	F	432	GLN	CG-CD	5.09	1.62	1.51
1	M	414	GLY	C-O	5.08	1.31	1.23
1	B	76	GLU	CD-OE1	5.06	1.31	1.25
1	F	105	LYS	CD-CE	5.03	1.63	1.51
1	A	44	PHE	CG-CD1	5.03	1.46	1.38
1	G	14	VAL	CB-CG1	-5.02	1.42	1.52
1	D	44	PHE	CE2-CZ	5.02	1.46	1.37
1	N	73	MET	CG-SD	5.02	1.94	1.81
1	A	106	ALA	CA-CB	-5.01	1.42	1.52
1	A	461	GLU	CD-OE2	5.01	1.31	1.25

All (340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	83	ASP	CB-CG-OD2	10.21	127.49	118.30
1	G	13	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	D	421	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	J	428	ASP	CB-CG-OD2	9.67	127.00	118.30
1	C	452	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	A	421	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	K	83	ASP	CB-CG-OD2	9.24	126.61	118.30
1	C	13	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	C	134	LEU	CB-CG-CD2	-9.12	95.50	111.00
1	G	513	LEU	CB-CG-CD2	-8.92	95.83	111.00
1	M	462	PRO	N-CD-CG	-8.60	90.29	103.20
1	D	64	ASP	CB-CG-OD2	8.57	126.01	118.30
1	C	421	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	E	41	ASP	CB-CG-OD2	8.36	125.82	118.30
1	H	462	PRO	N-CD-CG	-8.23	90.86	103.20
1	K	41	ASP	CB-CG-OD2	8.22	125.69	118.30
1	C	140	ASP	CB-CG-OD2	8.21	125.69	118.30
1	L	462	PRO	N-CD-CG	-8.21	90.88	103.20
1	A	13	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	F	445	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	B	65	LYS	CD-CE-NZ	-8.19	92.86	111.70
1	G	395	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	G	140	ASP	CB-CG-OD2	8.13	125.62	118.30
1	H	83	ASP	CB-CG-OD2	8.12	125.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	462	PRO	N-CD-CG	-8.12	91.03	103.20
1	F	11	ASP	CB-CG-OD1	-8.09	111.02	118.30
1	G	36	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	J	25	ASP	CB-CG-OD2	8.00	125.50	118.30
1	J	13	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	M	115	ASP	CB-CG-OD2	7.93	125.43	118.30
1	G	36	ARG	NE-CZ-NH1	-7.91	116.34	120.30
1	M	83	ASP	CB-CG-OD2	7.91	125.42	118.30
1	G	64	ASP	CB-CG-OD2	7.88	125.39	118.30
1	E	395	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	N	41	ASP	CB-CG-OD2	7.81	125.33	118.30
1	F	65	LYS	CD-CE-NZ	-7.77	93.83	111.70
1	I	41	ASP	CB-CG-OD2	7.72	125.25	118.30
1	M	41	ASP	CB-CG-OD2	7.71	125.24	118.30
1	B	435	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	421	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	E	155	ASP	CB-CG-OD2	7.65	125.18	118.30
1	B	134	LEU	CB-CG-CD2	-7.58	98.11	111.00
1	A	495	ASP	CB-CG-OD2	7.54	125.09	118.30
1	C	395	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	C	395	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	E	36	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	F	13	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	G	495	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	514	MET	CG-SD-CE	-7.33	88.48	100.20
1	E	134	LEU	CB-CG-CD2	-7.25	98.68	111.00
1	L	11	ASP	CB-CG-OD2	7.20	124.78	118.30
1	K	428	ASP	CB-CG-OD2	7.20	124.78	118.30
1	E	65	LYS	CD-CE-NZ	-7.15	95.25	111.70
1	M	328	ASP	CB-CG-OD2	7.13	124.72	118.30
1	E	64	ASP	CB-CG-OD2	7.10	124.69	118.30
2	Q	58	ASP	CB-CG-OD2	7.09	124.68	118.30
1	I	5	ASP	CB-CG-OD2	7.09	124.68	118.30
1	B	41	ASP	CB-CG-OD2	7.08	124.68	118.30
1	L	115	ASP	CB-CG-OD2	7.03	124.63	118.30
1	L	83	ASP	CB-CG-OD2	6.99	124.59	118.30
1	L	428	ASP	CB-CG-OD2	6.94	124.54	118.30
1	J	83	ASP	CB-CG-OD2	6.93	124.54	118.30
1	L	495	ASP	CB-CG-OD2	6.93	124.53	118.30
1	J	11	ASP	CB-CG-OD2	6.92	124.53	118.30
1	G	28	LYS	CD-CE-NZ	-6.89	95.84	111.70
1	N	462	PRO	N-CD-CG	-6.88	92.88	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	11	ASP	CB-CG-OD2	6.88	124.49	118.30
1	D	495	ASP	CB-CG-OD2	6.87	124.48	118.30
1	D	421	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	J	495	ASP	CB-CG-OD2	6.78	124.40	118.30
1	D	41	ASP	CB-CG-OD2	6.75	124.38	118.30
1	C	25	ASP	CB-CG-OD2	6.75	124.37	118.30
1	I	428	ASP	CB-CG-OD2	6.70	124.33	118.30
1	K	495	ASP	CB-CG-OD2	6.67	124.30	118.30
1	C	41	ASP	CB-CG-OD2	6.67	124.30	118.30
1	E	115	ASP	CB-CG-OD2	6.67	124.30	118.30
1	H	5	ASP	CB-CG-OD1	-6.66	112.31	118.30
1	N	428	ASP	CB-CG-OD2	6.63	124.27	118.30
1	N	435	ASP	CB-CG-OD2	6.62	124.25	118.30
1	J	115	ASP	CB-CG-OD2	6.61	124.25	118.30
1	E	13	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	H	64	ASP	CB-CG-OD1	6.59	124.23	118.30
1	N	25	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	183	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	523	ASP	CB-CG-OD2	6.57	124.21	118.30
1	M	16	MET	CG-SD-CE	-6.56	89.70	100.20
1	H	428	ASP	CB-CG-OD2	6.55	124.20	118.30
2	R	8	ASP	CB-CG-OD2	6.54	124.19	118.30
1	G	41	ASP	CB-CG-OD2	6.53	124.18	118.30
1	F	36	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	J	328	ASP	CB-CG-OD2	6.52	124.17	118.30
1	I	414	GLY	C-N-CA	-6.50	108.65	122.30
1	M	11	ASP	CB-CG-OD2	6.49	124.14	118.30
1	F	41	ASP	CB-CG-OD2	6.48	124.14	118.30
1	C	421	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	G	514	MET	CG-SD-CE	-6.46	89.87	100.20
1	I	450	PRO	N-CD-CG	-6.46	93.52	103.20
1	A	36	ARG	NE-CZ-NH2	6.44	123.52	120.30
2	O	58	ASP	CB-CG-OD2	6.44	124.09	118.30
1	H	495	ASP	CB-CG-OD2	6.41	124.07	118.30
1	E	523	ASP	CB-CG-OD2	6.40	124.06	118.30
1	F	155	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	36	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	C	155	ASP	CB-CG-OD2	6.37	124.03	118.30
1	J	435	ASP	CB-CG-OD2	6.36	124.02	118.30
1	J	334	ASP	CB-CG-OD2	6.34	124.00	118.30
1	I	495	ASP	CB-CG-OD2	6.33	124.00	118.30
1	F	419	LEU	CB-CG-CD2	-6.32	100.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	36	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	36	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	N	83	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	D	523	ASP	CB-CG-OD2	6.29	123.96	118.30
1	G	65	LYS	CD-CE-NZ	-6.25	97.32	111.70
1	J	41	ASP	CB-CG-OD2	6.25	123.93	118.30
1	J	462	PRO	N-CD-CG	-6.24	93.83	103.20
1	N	52	ASP	CB-CG-OD2	6.24	123.92	118.30
1	K	115	ASP	CB-CG-OD2	6.24	123.91	118.30
1	F	134	LEU	CB-CG-CD2	-6.23	100.41	111.00
1	G	118	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	28	LYS	CD-CE-NZ	-6.21	97.43	111.70
1	D	179	ASP	CB-CG-OD1	6.19	123.87	118.30
1	E	121	ASP	CB-CG-OD1	6.19	123.87	118.30
1	J	316	ASP	CB-CG-OD2	6.19	123.87	118.30
1	K	25	ASP	CB-CG-OD2	6.19	123.87	118.30
1	E	23	LEU	CA-CB-CG	6.17	129.50	115.30
1	E	11	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	D	87	ASP	CB-CG-OD1	6.16	123.85	118.30
1	J	5	ASP	CB-CG-OD2	6.16	123.85	118.30
1	J	5	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	H	36	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	N	334	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	328	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	328	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	185	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	513	LEU	CB-CG-CD2	-6.13	100.58	111.00
1	H	426	LEU	CB-CG-CD1	-6.12	100.59	111.00
1	M	428	ASP	CB-CG-OD2	6.11	123.80	118.30
1	I	25	ASP	CB-CG-OD1	6.11	123.80	118.30
2	P	8	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	36	ARG	NE-CZ-NH1	-6.09	117.26	120.30
2	P	58	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	65	LYS	CD-CE-NZ	-6.06	97.76	111.70
1	H	18	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	F	445	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	B	395	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	H	283	ASP	CB-CG-OD2	6.03	123.72	118.30
1	K	334	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	87	ASP	CB-CG-OD2	6.02	123.72	118.30
1	G	328	ASP	CB-CG-OD2	6.01	123.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	328	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	451	LEU	CB-CG-CD2	-5.98	100.83	111.00
1	M	52	ASP	CB-CG-OD1	5.97	123.67	118.30
1	G	490	ASP	CB-CG-OD2	5.97	123.67	118.30
1	N	64	ASP	CB-CG-OD2	5.95	123.66	118.30
1	M	361	ASP	CB-CG-OD2	5.95	123.65	118.30
1	N	450	PRO	N-CD-CG	-5.94	94.29	103.20
2	T	79	ASP	CB-CG-OD2	5.93	123.64	118.30
1	M	452	ARG	NE-CZ-NH1	-5.93	117.34	120.30
1	B	36	ARG	NE-CZ-NH1	-5.93	117.34	120.30
1	J	523	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	28	LYS	CD-CE-NZ	-5.92	98.08	111.70
1	I	316	ASP	CB-CG-OD2	5.91	123.62	118.30
1	G	395	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	G	118	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	M	414	GLY	C-N-CA	-5.90	109.92	122.30
2	P	79	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	513	LEU	CB-CG-CD1	5.88	121.00	111.00
1	N	328	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	41	ASP	CB-CG-OD2	5.86	123.58	118.30
1	I	115	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	134	LEU	CB-CG-CD2	-5.86	101.05	111.00
1	L	65	LYS	CD-CE-NZ	-5.85	98.24	111.70
1	E	428	ASP	CB-CG-OD2	5.85	123.56	118.30
1	H	196	ASP	CB-CG-OD2	5.83	123.55	118.30
2	U	58	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	62	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	E	183	LEU	CA-CB-CG	5.79	128.62	115.30
1	K	196	ASP	CB-CG-OD2	5.79	123.51	118.30
1	K	25	ASP	CB-CG-OD1	5.78	123.50	118.30
2	T	58	ASP	CB-CG-OD2	5.77	123.50	118.30
2	R	79	ASP	CB-CG-OD2	5.77	123.49	118.30
1	L	523	ASP	CB-CG-OD2	5.76	123.49	118.30
1	N	155	ASP	CB-CG-OD2	5.75	123.48	118.30
2	O	79	ASP	CB-CG-OD2	5.75	123.48	118.30
1	G	134	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	H	334	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	23	LEU	CA-CB-CG	5.74	128.50	115.30
1	G	185	ASP	CB-CG-OD2	5.74	123.46	118.30
1	D	361	ASP	CB-CG-OD2	5.74	123.46	118.30
1	C	490	ASP	CB-CG-OD1	5.73	123.46	118.30
1	F	183	LEU	CA-CB-CG	5.73	128.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	404	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	435	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	M	450	PRO	N-CD-CG	-5.72	94.62	103.20
1	K	462	PRO	N-CD-CG	-5.70	94.66	103.20
1	C	523	ASP	CB-CG-OD2	5.69	123.42	118.30
1	H	398	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	183	LEU	CA-CB-CG	5.68	128.36	115.30
1	F	64	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	188	ASP	CB-CG-OD2	5.67	123.41	118.30
1	M	196	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	64	ASP	CB-CG-OD2	5.66	123.39	118.30
1	I	328	ASP	CB-CG-OD2	5.65	123.38	118.30
1	L	361	ASP	CB-CG-OD2	5.65	123.38	118.30
1	N	5	ASP	CB-CG-OD2	5.64	123.38	118.30
1	L	334	ASP	CB-CG-OD2	5.64	123.37	118.30
1	K	25	ASP	OD1-CG-OD2	-5.63	112.60	123.30
1	B	428	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	185	ASP	CB-CG-OD2	5.62	123.36	118.30
1	L	5	ASP	CB-CG-OD2	5.62	123.36	118.30
1	I	17	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	A	435	ASP	CB-CG-OD2	5.61	123.35	118.30
1	J	359	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	445	ARG	NE-CZ-NH1	-5.59	117.51	120.30
2	U	90	ASP	CB-CG-OD2	5.58	123.33	118.30
1	K	5	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	435	ASP	CB-CG-OD2	5.58	123.32	118.30
1	M	420	ILE	CG1-CB-CG2	-5.57	99.14	111.40
1	M	495	ASP	CB-CG-OD2	5.55	123.29	118.30
2	Q	79	ASP	CB-CG-OD2	5.54	123.29	118.30
1	F	23	LEU	CA-CB-CG	5.54	128.04	115.30
1	L	25	ASP	CB-CG-OD2	5.54	123.28	118.30
1	H	361	ASP	CB-CG-OD2	5.53	123.28	118.30
1	G	523	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	58	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	D	134	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	A	183	LEU	CA-CB-CG	5.50	127.95	115.30
1	I	196	ASP	CB-CG-OD2	5.50	123.25	118.30
1	F	523	ASP	CB-CG-OD2	5.50	123.25	118.30
1	N	40	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	D	36	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	H	435	ASP	CB-CG-OD2	5.47	123.22	118.30
2	R	58	ASP	CB-CG-OD2	5.47	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ASP	CB-CG-OD2	5.46	123.21	118.30
1	N	115	ASP	CB-CG-OD2	5.46	123.21	118.30
1	H	115	ASP	CB-CG-OD2	5.46	123.21	118.30
1	G	316	ASP	CB-CG-OD2	5.45	123.20	118.30
1	L	398	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	445	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	S	69	ASP	CB-CG-OD2	5.44	123.19	118.30
1	H	359	ASP	CB-CG-OD2	5.43	123.19	118.30
1	K	328	ASP	CB-CG-OD2	5.43	123.19	118.30
1	N	52	ASP	OD1-CG-OD2	-5.42	113.00	123.30
1	H	52	ASP	CB-CG-OD2	5.42	123.18	118.30
2	S	90	ASP	CB-CG-OD2	5.42	123.18	118.30
1	H	25	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	514	MET	CG-SD-CE	-5.41	91.54	100.20
1	C	65	LYS	CD-CE-NZ	-5.41	99.25	111.70
1	D	167	ASP	CB-CG-OD2	5.41	123.17	118.30
1	K	316	ASP	CB-CG-OD2	5.41	123.16	118.30
1	H	87	ASP	CB-CG-OD2	5.40	123.16	118.30
1	H	16	MET	CG-SD-CE	-5.39	91.57	100.20
1	F	28	LYS	CD-CE-NZ	-5.39	99.31	111.70
1	A	448	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	C	111	MET	CA-CB-CG	-5.38	104.16	113.30
1	B	495	ASP	CB-CG-OD2	5.38	123.14	118.30
1	H	490	ASP	CB-CG-OD1	5.38	123.14	118.30
1	I	461	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	K	131	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	H	514	MET	CG-SD-CE	-5.37	91.61	100.20
1	A	415	GLY	N-CA-C	-5.37	99.68	113.10
1	J	23	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	I	525	PRO	CA-C-O	-5.37	107.32	120.20
1	E	316	ASP	CB-CG-OD2	5.37	123.13	118.30
2	U	79	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	395	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	N	283	ASP	CB-CG-OD2	5.35	123.12	118.30
1	M	435	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	28	LYS	CD-CE-NZ	-5.35	99.40	111.70
1	A	155	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	64	ASP	CB-CG-OD2	5.33	123.10	118.30
1	J	414	GLY	C-N-CA	-5.33	111.11	122.30
1	C	361	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	328	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	359	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	114	MET	CG-SD-CE	5.30	108.68	100.20
1	N	52	ASP	CB-CG-OD1	5.30	123.07	118.30
1	F	435	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	404	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	K	473	ASP	CB-CG-OD2	5.28	123.05	118.30
1	N	361	ASP	CB-CG-OD2	5.28	123.05	118.30
1	J	69	MET	CG-SD-CE	-5.27	91.76	100.20
1	C	64	ASP	CB-CG-OD2	5.27	123.04	118.30
1	L	41	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	111	MET	CA-CB-CG	-5.26	104.35	113.30
1	N	523	ASP	CB-CG-OD1	5.25	123.03	118.30
2	O	69	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	452	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	U	69	ASP	CB-CG-OD2	5.23	123.01	118.30
1	I	361	ASP	CB-CG-OD2	5.23	123.00	118.30
1	H	328	ASP	CB-CG-OD2	5.22	123.00	118.30
1	J	361	ASP	CB-CG-OD2	5.22	123.00	118.30
1	G	11	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	C	328	ASP	CB-CG-OD2	5.21	122.99	118.30
1	K	461	GLU	OE1-CD-OE2	5.21	129.55	123.30
1	G	183	LEU	CA-CB-CG	5.19	127.25	115.30
1	F	328	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	456	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	G	101	THR	OG1-CB-CG2	-5.19	98.06	110.00
1	F	361	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	167	ASP	CB-CG-OD2	5.18	122.96	118.30
1	L	283	ASP	CB-CG-OD2	5.18	122.96	118.30
1	N	196	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	121	ASP	N-CA-CB	5.17	119.91	110.60
1	A	500	THR	CA-CB-CG2	-5.17	105.16	112.40
1	N	419	LEU	CA-CB-CG	5.17	127.19	115.30
1	J	188	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	496	PRO	N-CD-CG	-5.16	95.46	103.20
1	F	430	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	N	316	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	359	ASP	CB-CG-OD2	5.14	122.93	118.30
1	J	52	ASP	CB-CG-OD1	5.14	122.93	118.30
1	K	359	ASP	CB-CG-OD2	5.14	122.93	118.30
2	S	79	ASP	CB-CG-OD2	5.14	122.92	118.30
1	J	167	ASP	CB-CG-OD2	5.14	122.92	118.30
1	L	196	ASP	CB-CG-OD2	5.13	122.92	118.30
1	K	36	ARG	NE-CZ-NH1	5.13	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	514	MET	CG-SD-CE	-5.13	91.99	100.20
1	F	140	ASP	CB-CG-OD2	5.13	122.91	118.30
1	E	361	ASP	CB-CG-OD2	5.12	122.91	118.30
1	N	359	ASP	CB-CG-OD2	5.10	122.89	118.30
1	G	23	LEU	CA-CB-CG	5.10	127.03	115.30
1	L	501	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	L	155	ASP	CB-CG-OD2	5.09	122.88	118.30
1	L	359	ASP	CB-CG-OD2	5.09	122.88	118.30
1	G	115	ASP	CB-CG-OD2	5.09	122.88	118.30
1	M	461	GLU	N-CA-CB	-5.07	101.47	110.60
2	Q	69	ASP	CB-CG-OD2	5.07	122.86	118.30
1	J	291	ASP	CB-CG-OD2	5.06	122.86	118.30
1	G	87	ASP	CB-CG-OD2	5.06	122.85	118.30
1	M	359	ASP	CB-CG-OD2	5.06	122.85	118.30
1	K	361	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	522	THR	OG1-CB-CG2	-5.04	98.41	110.00
1	G	473	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	359	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	15	LYS	CD-CE-NZ	-5.02	100.16	111.70
1	J	196	ASP	CB-CG-OD2	5.02	122.82	118.30
1	K	283	ASP	CB-CG-OD2	5.01	122.81	118.30
2	U	8	ASP	CB-CG-OD2	5.00	122.80	118.30

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 ⓘ

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	190	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3856	0	3976	188	0
1	C	3856	0	3976	191	0
1	D	3856	0	3976	180	0
1	E	3856	0	3976	172	0
1	F	3856	0	3976	168	0
1	G	3856	0	3976	185	0
1	H	3856	0	3976	168	0
1	I	3856	0	3976	175	0
1	J	3856	0	3976	162	0
1	K	3856	0	3976	171	0
1	L	3856	0	3976	184	1
1	M	3856	0	3976	190	0
1	N	3856	0	3976	173	0
2	O	728	0	762	24	0
2	P	728	0	762	19	0
2	Q	728	0	762	20	0
2	R	728	0	762	15	0
2	S	728	0	762	17	0
2	T	728	0	762	16	0
2	U	728	0	762	16	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
5	N	21	0	0	8	0
All	All	59457	0	61082	2532	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 21.

All (2532) 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:SD	1:I:73:MET:CG	2.01	1.48
1:A:73:MET:CE	1:A:73:MET:SD	2.01	1.46
1:J:288:MET:SD	1:J:288:MET:CE	2.02	1.46
1:I:114:MET:CE	1:I:114:MET:SD	2.02	1.46
1:A:16:MET:SD	1:A:16:MET:CE	2.02	1.45
1:B:114:MET:CE	1:B:114:MET:SD	2.05	1.45
1:H:114:MET:CE	1:H:114:MET:SD	2.04	1.45
1:K:514:MET:CE	1:K:514:MET:SD	2.06	1.42
1:M:111:MET:SD	1:M:111:MET:CE	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:CE	1:E:114:MET:SD	2.14	1.35
1:F:111:MET:CE	1:F:111:MET:SD	2.15	1.33
1:D:111:MET:SD	1:D:111:MET:CE	2.16	1.33
1:J:114:MET:SD	1:J:114:MET:CE	2.20	1.30
1:N:514:MET:CE	1:N:514:MET:SD	2.21	1.27
1:C:73:MET:SD	1:C:73:MET:CE	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:HH11	1:B:18:ARG:CG	1.62	1.11
1:F:18:ARG:CG	1:F:18:ARG:HH11	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:HG2	1:M:452:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:419:LEU:HD21	1:J:500:THR:CG2	1.86	1.05
1:D:430:ARG:HH11	1:D:430:ARG:HG2	1.22	1.04
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:HH11	1:N:452:ARG:HG2	1.25	1.01
1:D:414:GLY:O	1:D:417:VAL:HG12	1.61	1.00
1:D:18:ARG:CB	1:D:18:ARG:HH11	1.74	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
1:M:65:LYS:O	1:M:66:PHE:HB2	1.58	1.00
1:H:452:ARG:HH11	1:H:452:ARG:HG2	1.27	1.00
1:L:69:MET:HE1	1:L:522:THR:HB	1.44	0.99
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:CG	1:C:18:ARG:HH11	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:NH1	1:B:18:ARG:HG2	1.76	0.95
1:B:463:SER:HB3	5:H:537:HOH:O	1.66	0.95
1:C:18:ARG:CB	1:C:18:ARG:HH11	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:CB	1:B:18:ARG:HH11	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:NH1	1:F:18:ARG:HG2	1.76	0.94
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HB3	1:A:18:ARG:HH11	1.35	0.91
1:D:432:GLN:NE2	1:D:436:GLN:HE22	1.69	0.91
1:E:44:PHE:H	1:E:44:PHE:HD1	1.13	0.91
1:F:430:ARG:HH11	1:F:430:ARG:HG2	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:K:452:ARG:HH11	1:K:452:ARG:HG2	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:E:18:ARG:CG	1:E:18:ARG:HH11	1.86	0.88
1:D:44:PHE:HD1	1:D:44:PHE:H	1.14	0.88
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.52	0.88
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:HG3	1:A:404:ARG:HH11	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:G:44:PHE:H	1:G:44:PHE:HD1	1.20	0.86
1:D:18:ARG:CG	1:D:18:ARG:HH11	1.88	0.86
1:L:131:LEU:HD12	1:L:422:VAL:HG11	1.54	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:452:ARG:HH11	1:I:452:ARG:HG2	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
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:C:100:ILE:HD11	1:C:514:MET:HE1	1.57	0.85
1:F:44:PHE:HD1	1:F:44:PHE:H	1.22	0.85
1:A:18:ARG:CB	1:A:18:ARG:HH11	1.89	0.85
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.38	0.85
1:J:69:MET:HE1	1:J:522:THR:HB	1.55	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:H:69:MET:HE1	1:H:522:THR:HB	1.57	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:149:THR:HG23	1:J:159:GLY:HA3	1.57	0.84
1:J:65:LYS:HG3	5:J:536:HOH:O	1.76	0.84
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:HH11	1:J:404:ARG:HG2	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: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:B:18:ARG:NH1	1:B:18:ARG:CG	2.33	0.79
1:D:234:LEU:O	1:D:238:GLU:HG3	1.81	0.79
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.64	0.79
1:N:452:ARG:NH1	1:N:452:ARG:HG2	1.96	0.79
1:B:305:ILE:HG12	1:C:267:MET:HE3	1.64	0.79
1:D:100:ILE:HD11	1:D:514:MET:HE3	1.63	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:F:417:VAL:HG11	1:F:488:MET:HG3	1.65	0.78
1:H:69:MET:CE	1:H:522:THR:HB	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:404:ARG:HH11	1:I:404:ARG:HG2	1.47	0.78
1:N:69:MET:HE1	1:N:522:THR:HB	1.64	0.78
1:D:414:GLY:O	1:D:417:VAL:CG1	2.31	0.78
1:B:18:ARG:HB3	1:B:18:ARG:HH11	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:CG	1:A:18:ARG:HH11	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:HD23	1:I:494:LEU:O	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: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:G:510:VAL:HG23	1:G:514:MET:CE	2.14	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
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:NH1	1:H:452:ARG:HG2	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:I:69:MET:HE1	1:I:522:THR:HB	1.68	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:HG2	1:C:18:ARG:HH11	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: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: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:NH1	1:G:18:ARG:HG2	1.94	0.73
1:M:69:MET:CE	1:M:522:THR:HB	2.18	0.73
1:D:305:ILE:HG12	1:E:267:MET:HE3	1.71	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:G:510:VAL:HG23	1:G:514:MET:HE2	1.70	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:N:404:ARG:HH11	1:N:404:ARG:HG2	1.53	0.73
1:A:510:VAL:HG23	1:A:514:MET:HE3	1.70	0.73
1:C:74:VAL:O	1:C:77:VAL:HG13	1.89	0.73
1:I:131:LEU:HD13	1:I:422:VAL:HG11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASP:O	1:A:363:GLU:OE2	2.07	0.73
1:C:18:ARG:NH1	1:C:18:ARG:CG	2.46	0.72
1:G:452:ARG:HH11	1:G:452:ARG:HG2	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: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:265:ASN:HA	1:D:270:ILE:HD12	1.71	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:H:131:LEU:HD12	1:H:422:VAL:HG11	1.70	0.72
1:E:380:LYS:HD3	5:E:606:HOH:O	1.90	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:F:414:GLY:O	1:F:417:VAL:CG1	2.36	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:CB	1:G:18:ARG:HH11	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:NH1	1:C:18:ARG:HB3	2.05	0.71
1:I:419:LEU:HD21	1:I:500:THR:HG23	1.71	0.71
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.70	0.71
1:J:494:LEU:HD23	1:J:494:LEU:O	1.90	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:291:ASP:OD2	1:K:368:ARG:HD2	1.90	0.71
1:K:32:GLY:HA2	1:K:454:ILE:HD13	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:404:ARG:HH11	1:I:404:ARG:CG	2.03	0.70
1:I:64:ASP:HB3	1:I:67:GLU:HB2	1.73	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:CG	1:M:404:ARG:HH11	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:I:100:ILE:O	1:I:104:LEU:HB2	1.91	0.70
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:HG13	1:E:514:MET:HE1	1.74	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: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:NH1	1:F:18:ARG:CG	2.35	0.69
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.74	0.69
1:M:27:VAL:HG11	1:M:93:THR:HG21	1.74	0.69
1:D:417:VAL:O	1:D:420:ILE:HG22	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:A:430:ARG:HG2	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:487:ASN:O	1:G:491:MET:HG3	1.93	0.69
1:I:65:LYS:O	1:I:66:PHE:CB	2.40	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:N	1:E:44:PHE:CD1	2.59	0.69
1:J:100:ILE:O	1:J:104:LEU:HB2	1.92	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: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:D:510:VAL:HG23	1:D:514:MET:CE	2.23	0.68
1:J:174:VAL:HG21	1:J:194:GLN:HB3	1.75	0.68
1:L:494:LEU:HD23	1:L:494:LEU:O	1.93	0.68
2:S:7:HIS:O	2:S:8:ASP:HB3	1.92	0.68
1:L:404:ARG:CG	1:L:404:ARG:HH11	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:84:ALA:O	1:M:498:LYS:HE2	1.94	0.68
1:M:83:ASP:OD2	1:M:327:LYS:HE2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:O	1:A:369:VAL:HG13	1.93	0.68
1:E:18:ARG:NH1	1:E:18:ARG:HG2	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:HB3	1:F:18:ARG:HH11	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: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:A:38:VAL:HG13	1:G:519:CYS:HB3	1.74	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:K:452:ARG:HG2	1:K:452:ARG:NH1	2.10	0.67
1:N:11:ASP:O	1:N:12:ALA:C	2.31	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
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:B:16:MET:O	1:B:20:VAL:HG23	1.94	0.67
1:G:510:VAL:CG2	1:G:514:MET:HE2	2.24	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:G:23:LEU:CD1	1:G:23:LEU:C	2.63	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: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:B:147:VAL:HG22	1:B:403:THR:HG22	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:100:ILE:HD11	1:A:514:MET:HE1	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:C:305:ILE:HG12	1:D:267:MET:HE3	1.78	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
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:B:486:GLY:HA3	1:B:491:MET:HE2	1.78	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:HB3	1:B:18:ARG:NH1	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:NH1	1:D:430:ARG:HG2	1.99	0.65
1:J:193:MET:CE	1:J:195:PHE:HD1	2.09	0.65
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.55	0.65
1:C:510:VAL:HG12	1:D:385:THR:HG21	1.78	0.65
1:D:430:ARG:CG	1:D:430:ARG:HH11	2.02	0.65
1:I:179:ASP:OD1	1:I:393:LYS:HD2	1.96	0.65
1:C:381:VAL:HG12	1:C:392:LYS:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:ILE:HG21	1:G:403:THR:HG21	1.79	0.65
1:A:385:THR:HG21	1:G:510:VAL:HG12	1.79	0.65
1:C:229:ASN:HB3	1:C:231:ARG:HG3	1.78	0.65
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.77	0.65
1:E:288:MET:HG3	1:E:368:ARG:HD2	1.78	0.65
1:F:100:ILE:HD11	1:F:514:MET:HE3	1.79	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:L:452:ARG:HG2	1:L:452:ARG:NH1	2.09	0.65
1:N:69:MET:CE	1:N:522:THR:HB	2.27	0.65
1:C:451:LEU:HD23	1:C:451:LEU:C	2.17	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
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: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: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:M:64:ASP:HB3	1:M:67:GLU:HB2	1.78	0.64
1:M:47:PRO:HG2	1:N:73:MET:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:GLN:HE21	1:D:436:GLN:NE2	1.96	0.64
1:G:100:ILE:HD11	1:G:514:MET:HE1	1.80	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:NH1	1:I:452:ARG:HG2	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
1:I:69:MET:CE	1:I:522:THR:HB	2.28	0.63
1:I:72:GLN:HE22	1:I:75:LYS:HZ3	1.44	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:NH1	1:C:430:ARG:HG2	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:N:149:THR:CG2	1:N:156:GLU:HA	2.28	0.63
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.80	0.63
1:A:49:ILE:HD13	1:G:513:LEU:HB3	1.81	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:138:CYS:SG	1:J:144:ILE:HD13	2.39	0.63
1:J:43:SER:HB3	1:J:44:PHE:CD1	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:238:GLU:OE2	2:O:23:GLY:C	2.38	0.62
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:NH1	1:F:430:ARG:HG2	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:L:16:MET:O	1:L:20:VAL:HG12	2.00	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:NH1	1:E:430:ARG:HG2	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:522:THR:OG1	1:D:523:ASP:N	2.25	0.61
1:D:6:VAL:HG23	1:D:6:VAL:O	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:305:ILE:HD12	1:C:307:MET:HE2	1.82	0.61
1:E:417:VAL:O	1:E:420:ILE:HG22	1.99	0.61
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.82	0.61
1:C:23:LEU:CD1	1:C:23:LEU:C	2.68	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
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: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:K:69:MET:HE1	1:K:522:THR:HB	1.83	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: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:HD12	2:R:84:LEU:N	2.15	0.61
1:A:270:ILE:HG12	2:O:27:LEU:HD13	1.81	0.61
1:A:162:ILE:HG21	1:A:403:THR:HG21	1.83	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:F:486:GLY:HA3	1:F:491:MET:CE	2.31	0.61
1:G:288:MET:HG3	1:G:368:ARG:HD2	1.82	0.61
1:M:452:ARG:CG	1:M:452:ARG:NH1	2.58	0.61
1:A:504:LEU:HD22	1:A:504:LEU:O	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:E:305:ILE:HG12	1:F:267:MET:HE3	1.82	0.60
1:G:381:VAL:CG1	1:G:392:LYS:CG	2.79	0.60
1:B:34:LYS:HD2	1:B:458:CYS:SG	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:496:PRO:HB2	1:I:499:VAL:HG13	1.83	0.60
1:I:80:LYS:HA	1:I:83:ASP:HB2	1.82	0.60
1:H:193:MET:CE	1:H:195:PHE:HD1	2.14	0.60
1:I:493:ILE:N	1:I:493:ILE:HD13	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
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:HG2	1:A:18:ARG:NH1	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:I:492:GLY:C	1:I:493:ILE:HD13	2.22	0.60
1:B:162:ILE:HG21	1:B:403:THR:HG21	1.84	0.60
1:B:64:ASP:HB3	1:B:67:GLU:HB2	1.82	0.60
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.84	0.60
1:E:18:ARG:NH1	1:E:18:ARG:CG	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:259:LEU:O	1:J:263:VAL:HG23	2.02	0.60
1:J:87:ASP:HB3	1:J:499:VAL:HG21	1.84	0.60
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:E:229:ASN:HB3	1:E:231:ARG:HG3	1.84	0.59
1:E:162:ILE:HG21	1:E:403:THR:HG21	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:421:ARG:HD2	1:N:474:GLY:O	2.02	0.59
1:G:510:VAL:CG2	1:G:514:MET:CE	2.80	0.59
1:H:496:PRO:HB2	1:H:499:VAL:HG13	1.84	0.59
1:I:73:MET:CB	1:I:73:MET:SD	2.90	0.59
1:J:404:ARG:CG	1:J:404:ARG:HH11	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
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.42	0.59
1:C:288:MET:HG3	1:C:368:ARG:HD2	1.83	0.59
1:D:383:ALA:HB1	1:D:388:GLU:HB3	1.85	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:223:ALA:O	1:L:251:ALA:HA	2.03	0.59
1:L:72:GLN:NE2	1:L:72:GLN:HA	2.17	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:409:GLU:OE2	1:C:501:ARG:NH2	2.27	0.59
1:D:510:VAL:HG23	1:D:514:MET:HE2	1.83	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:I:284:ARG:HH11	1:I:364:LYS:HD2	1.67	0.59
1:A:451:LEU:HD23	1:A:451:LEU:C	2.22	0.59
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.83	0.59
1:E:18:ARG:NH1	1:E:18:ARG:HB3	2.15	0.59
1:F:345:ARG:HA	1:F:348:GLN:HE21	1.67	0.59
1:G:452:ARG:NH1	1:G:452:ARG:HG2	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: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

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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:B:510:VAL:HG23	1:B:514:MET:CE	2.34	0.58
1:F:76:GLU:OE1	1:G:387:VAL:HG22	2.02	0.58
1:G:451:LEU:C	1:G:451:LEU:HD23	2.22	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:I:138:CYS:SG	1:I:144:ILE:HD13	2.44	0.58
1:I:87:ASP:HB3	1:I:499:VAL:HG21	1.84	0.58
1:K:149:THR:CG2	1:K:156:GLU:HA	2.33	0.58
1:K:66:PHE:H	1:K:69:MET:HG3	1.67	0.58
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.68	0.58
1:C:114:MET:HE3	1:C:114:MET:O	2.03	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: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:B:261:THR:HG23	2:P:29:GLY:H	1.68	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:M:492:GLY:C	1:M:493:ILE:HD13	2.24	0.58
1:B:394:ALA:O	1:B:398:ASP:HB2	2.04	0.58
1:F:486:GLY:HA3	1:F:491:MET:HE2	1.85	0.58
1:G:28:LYS:O	1:G:29:VAL:C	2.40	0.58
1:I:193:MET:CE	1:I:195:PHE:HD1	2.17	0.58
1:K:325:ILE:HG22	1:K:330:THR:HA	1.85	0.58
1:K:102:GLU:HB3	1:K:442:VAL:HG22	1.86	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:I:494:LEU:HD23	1:I:494:LEU:C	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:47:ARG:HD2	2:T:49:LEU:HB2	1.86	0.58
1:G:429:LEU:O	1:G:430:ARG:HG2	2.04	0.57
1:H:11:ASP:O	1:H:12:ALA:C	2.38	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: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:G:510:VAL:HG23	1:G:514:MET:HE3	1.86	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: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: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:305:ILE:HG12	1:G:267:MET:HE3	1.85	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: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:L:43:SER:HB3	1:L:44:PHE:CD1	2.39	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:CG	1:A:16:MET:CE	2.82	0.57
1:B:63:GLU:HG3	1:B:63:GLU:O	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:510:VAL:HG23	1:B:514:MET:HE3	1.87	0.57
1:D:324:VAL:HB	1:D:331:THR:HG23	1.87	0.57
1:E:404:ARG:HG3	1:E:404:ARG:HH11	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: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:150:ILE:HD13	1:D:493:ILE:HA	1.87	0.56
1:D:18:ARG:HG2	1:D:18:ARG:NH1	2.20	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:L:11:ASP:O	1:L:12:ALA:C	2.41	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:419:LEU:HG	1:A:447:MET:HG2	1.88	0.56
1:B:74:VAL:HG13	1:B:514:MET:HE1	1.86	0.56
1:G:432:GLN:NE2	1:G:436:GLN:HE22	2.04	0.56
1:N:13:ARG:HD2	1:N:104:LEU:HD11	1.88	0.56
1:A:381:VAL:HG21	1:A:393:LYS:HA	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:G:28:LYS:O	1:G:30:THR:N	2.38	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: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:326:ASN:HD22	1:D:329:THR:HB	1.71	0.56
1:F:404:ARG:HG3	1:F:404:ARG:HH11	1.69	0.56
1:G:260:ALA:O	1:G:264:VAL:HG23	2.06	0.56
1:I:15:LYS:HB3	1:I:66:PHE:HB3	1.88	0.56
1:J:223:ALA:O	1:J:251:ALA:HA	2.05	0.56
1:J:43:SER:HB3	1:J:44:PHE:HD1	1.71	0.56
1:L:462:PRO:O	1:L:463:SER:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:510:VAL:HG23	1:E:514:MET:HE2	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: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: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:D:510:VAL:HG23	1:D:514:MET:HE1	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: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:E:305:ILE:HD12	1:E:307:MET:HE1	1.87	0.56
1:H:173:GLY:O	1:H:404:ARG:NH2	2.38	0.56
1:M:106:ALA:HA	1:M:111:MET:HE3	1.88	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:C:510:VAL:HG23	1:C:514:MET:CE	2.36	0.55
1:G:18:ARG:NH1	1:G:18:ARG:CG	2.50	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
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:105:LYS:HD3	1:K:110:GLY:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.89	0.55
1:I:66:PHE:H	1:I:69:MET:HG3	1.72	0.55
1:M:441:LYS:O	1:M:442:VAL:C	2.45	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:G:23:LEU:C	1:G:23:LEU:HD13	2.25	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:HH11	1:D:452:ARG:HG2	1.71	0.55
1:H:16:MET:HG3	1:H:520:MET:SD	2.46	0.55
1:L:392:LYS:O	1:L:396:VAL:HG23	2.07	0.55
1:L:131:LEU:HD13	1:L:422:VAL:HG11	1.87	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:N	2:P:84:LEU:HD12	2.22	0.55
1:C:510:VAL:CG2	1:C:514:MET:HE2	2.37	0.55
1:D:18:ARG:HG2	1:D:18:ARG:HH11	1.72	0.55
1:D:451:LEU:C	1:D:451:LEU:HD23	2.26	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:N	1:F:44:PHE:HD1	1.99	0.55
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:102:GLU:OE2	1:N:445:ARG:NH1	2.39	0.55
1:N:30:THR:HB	1:N:51:LYS:O	2.07	0.55
1:A:486:GLY:HA3	1:A:491:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:28:LYS:HD2	1:C:453:GLN:CD	2.28	0.54
1:J:149:THR:HG21	1:J:156:GLU:HA	1.88	0.54
1:B:100:ILE:HD11	1:B:514:MET:HE1	1.88	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:E:91:THR:O	1:E:92:ALA:C	2.44	0.54
1:H:428:ASP:O	1:H:429:LEU:C	2.45	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:C:409:GLU:CD	1:C:501:ARG:HH21	2.10	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:486:GLY:HA3	1:A:491:MET:HE2	1.89	0.54
1:B:223:ALA:O	1:B:251:ALA:HA	2.07	0.54
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.90	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:262:LEU:HD22	1:L:273:VAL:HG11	1.88	0.54
1:L:36:ARG:O	1:L:51:LYS:HG2	2.06	0.54
1:L:385:THR:HG23	1:L:388:GLU:HB2	1.88	0.54
1:G:130:GLU:HB3	1:G:422:VAL:HB	1.90	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:D:44:PHE:N	1:D:44:PHE:CD1	2.61	0.54
1:E:16:MET:O	1:E:20:VAL:HG23	2.07	0.54
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.90	0.54
1:A:6:VAL:HG23	1:A:6:VAL:O	2.07	0.54
1:C:305:ILE:O	1:C:305:ILE:HG22	2.08	0.54
1:C:194:GLN:HB2	1:C:331:THR:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:476:TYR:HA	1:H:486:GLY:O	2.07	0.54
1:L:64:ASP:C	1:L:65:LYS:O	2.39	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:D:23:LEU:C	1:D:23:LEU:CD1	2.76	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:M:145:ALA:O	1:M:149:THR:HG23	2.08	0.54
1:L:47:PRO:HG2	1:M:73:MET:CG	2.38	0.54
1:D:452:ARG:NH1	1:D:452:ARG:HG2	2.23	0.54
1:I:385:THR:HG23	1:I:388:GLU:HB2	1.88	0.54
1:J:8:PHE:O	1:J:9:GLY:C	2.45	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: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
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.90	0.53
1:N:19:GLY:HA3	1:N:67:GLU:O	2.08	0.53
1:D:217:SER:N	1:D:218:PRO:HD3	2.23	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:A:39:VAL:HB	1:G:520:MET:HG2	1.90	0.53
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.16	0.53
1:L:65:LYS:O	1:L:66:PHE:CB	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:194:GLN:HB2	1:G:331:THR:HB	1.91	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: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: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: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: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:199:TYR:HB3	1:C:325:ILE:HD11	1.91	0.53
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:CG	1:J:514:MET:CE	2.85	0.53
1:L:100:ILE:HD13	1:L:514:MET:SD	2.49	0.53
1:A:305:ILE:HD12	1:A:307:MET:HE1	1.91	0.53
1:B:6:VAL:O	1:B:6:VAL:HG23	2.08	0.53
1:E:217:SER:N	1:E:218:PRO:HD3	2.24	0.53
1:E:35:GLY:HA3	1:E:51:LYS:HE2	1.90	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: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:K:106:ALA:HA	1:K:111:MET:HE3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:510:VAL:O	1:G:511:ALA:C	2.47	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: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: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: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:76:GLU:O	1:A:80:LYS:HB2	2.09	0.52
1:B:150:ILE:CG2	1:B:151:SER:N	2.72	0.52
1:B:199:TYR:HB3	1:B:325:ILE:HD11	1.91	0.52
1:B:44:PHE:HD1	1:B:44:PHE:N	1.92	0.52
1:C:28:LYS:O	1:C:29:VAL:C	2.45	0.52
1:D:510:VAL:O	1:D:511:ALA:C	2.46	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
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.91	0.52
1:I:497:THR:O	1:I:498:LYS:C	2.47	0.52
1:I:75:LYS:NZ	5:I:537:HOH:O	2.10	0.52
1:N:451:LEU:O	1:N:452:ARG:C	2.47	0.52
1:A:324:VAL:HB	1:A:331:THR:HG23	1.90	0.52
1:A:16:MET:HE1	1:A:514:MET:HB3	1.91	0.52
1:D:394:ALA:O	1:D:398:ASP:HB2	2.09	0.52
1:G:28:LYS:C	1:G:30:THR:N	2.56	0.52
1:H:36:ARG:O	1:H:51:LYS:HG2	2.10	0.52
1:J:437:ASN:HA	1:J:440:ILE:HD12	1.90	0.52
1:J:16:MET:HG3	1:J:520:MET:SD	2.49	0.52
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.91	0.52
1:L:428:ASP:O	1:L:429:LEU:C	2.48	0.52
1:D:287:ALA:O	1:D:290:GLN:HB3	2.10	0.52
1:D:430:ARG:CG	1:D:430:ARG:NH1	2.64	0.52
1:E:444:LEU:O	1:E:447:MET:HB2	2.10	0.52
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.91	0.52
1:M:404:ARG:NH1	1:M:404:ARG:CG	2.66	0.52
1:C:510:VAL:HG23	1:C:514:MET:HE2	1.91	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:N:145:ALA:O	1:N:149:THR:HG23	2.10	0.52
1:B:114:MET:HB3	1:B:114:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ILE:HD12	1:D:307:MET:HE2	1.91	0.52
1:E:287:ALA:O	1:E:290:GLN:HB3	2.10	0.52
1:E:194:GLN:HB2	1:E:331:THR:HB	1.92	0.52
1:H:433:ASN:OD1	1:H:435:ASP:HB2	2.10	0.52
1:H:65:LYS:CA	5:H:528:HOH:O	2.55	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:11:ASP:O	1:M:12:ALA:C	2.46	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:288:MET:O	1:G:291:ASP:HB2	2.10	0.52
1:G:302:SER:H	1:G:307:MET:HE3	1.75	0.52
1:G:69:MET:O	1:G:73:MET:HG3	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
1:C:452:ARG:HG2	1:C:452:ARG:NH1	2.26	0.52
1:E:451:LEU:HD23	1:E:451:LEU:C	2.31	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:D:100:ILE:O	1:D:101:THR:C	2.44	0.51
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:K:522:THR:OG1	1:K:523:ASP:N	2.43	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:147:VAL:HG22	1:A:403:THR:HG22	1.92	0.51
1:E:511:ALA:O	1:E:515:ILE:HG23	2.11	0.51
1:F:302:SER:H	1:F:307:MET:HE3	1.74	0.51
1:F:194:GLN:HB2	1:F:331:THR:HB	1.92	0.51
1:F:417:VAL:O	1:F:418:ALA:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLU:HB3	1:D:442:VAL:HG22	1.91	0.51
1:E:44:PHE:N	1:E:44:PHE:HD1	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: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:23:LEU:CD1	1:B:23:LEU:C	2.79	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:M:326:ASN:ND2	1:M:329:THR:HB	2.25	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: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:M:13:ARG:HD2	1:M:104:LEU:HD11	1.92	0.51
1:M:428:ASP:O	1:M:429:LEU:C	2.48	0.51
1:E:261:THR:HG23	2:S:29:GLY:H	1.76	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:B:42:LYS:HG2	1:B:44:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:342:ILE:O	1:K:346:VAL:HG23	2.10	0.51
1:K:64:ASP:HB3	1:K:67:GLU:HB2	1.92	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:H:494:LEU:C	1:H:494:LEU:HD23	2.30	0.51
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.51	0.51
1:K:199:TYR:HA	1:K:276:VAL:HG12	1.93	0.51
1:L:24:ALA:HA	1:L:27:VAL:HG12	1.92	0.51
5:K:536:HOH:O	1:L:65:LYS:HB3	2.10	0.51
1:M:404:ARG:NH1	1:M:404:ARG:HG2	2.08	0.51
1:D:385:THR:OG1	1:D:388:GLU:HB2	2.11	0.51
1:F:452:ARG:NH1	1:F:452:ARG:HG2	2.25	0.51
1:H:417:VAL:HG21	1:H:488:MET:HG3	1.93	0.51
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.93	0.51
1:K:7:LYS:HD2	1:K:66:PHE:CE2	2.46	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:J:284:ARG:O	1:J:288:MET:HG3	2.11	0.50
1:J:77:VAL:HG22	1:J:506:TYR:CD1	2.46	0.50
1:L:293:ALA:HB2	1:L:300:VAL:HG23	1.93	0.50
1:N:106:ALA:HA	1:N:111:MET:HE3	1.93	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:F:473:ASP:O	1:F:474:GLY:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:326:ASN:HB2	1:M:329:THR:H	1.75	0.50
1:M:43:SER:HB3	1:M:44:PHE:CD1	2.47	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:D:455:VAL:HG21	1:D:465:VAL:HG11	1.92	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:I:197:ARG:HD2	1:I:277:LYS:HB2	1.92	0.50
1:K:428:ASP:O	1:K:429:LEU:C	2.49	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:B:302:SER:H	1:B:307:MET:HE3	1.76	0.50
1:F:124:VAL:HG13	1:F:504:LEU:HD13	1.93	0.50
1:G:385:THR:OG1	1:G:388:GLU:HB2	2.11	0.50
1:G:42:LYS:HG2	1:G:44:PHE:CD2	2.47	0.50
1:K:77:VAL:HG11	1:K:510:VAL:HB	1.93	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:C:121:ASP:O	1:C:122:LYS:C	2.44	0.50
1:D:80:LYS:O	1:D:81:ALA:C	2.49	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:A:28:LYS:O	1:A:29:VAL:C	2.48	0.50
1:C:452:ARG:HH12	1:C:463:SER:HB3	1.76	0.50
1:D:510:VAL:CG2	1:D:514:MET:HE1	2.42	0.50
1:E:339:GLU:HA	1:E:342:ILE:HB	1.93	0.50
1:I:426:LEU:CD1	1:I:444:LEU:HD21	2.41	0.50
1:K:361:ASP:O	1:K:365:LEU:HG	2.11	0.50
1:K:43:SER:HB3	1:K:44:PHE:CD1	2.46	0.50
1:L:475:ASN:ND2	1:L:489:ILE:HD12	2.27	0.50
1:M:217:SER:N	1:M:218:PRO:CD	2.74	0.50
1:M:47:PRO:CG	1:N:73:MET:HG3	2.41	0.50
1:C:270:ILE:HG12	2:Q:27:LEU:HD13	1.94	0.50
1:A:238:GLU:OE2	2:O:24:GLY:N	2.45	0.50
1:A:510:VAL:HG23	1:A:514:MET:HE2	1.91	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:C:524:LEU:CD2	1:C:525:PRO:HD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:456:LEU:HD13	1:F:462:PRO:CG	2.42	0.50
1:F:82:ASN:ND2	1:F:86:GLY:HA2	2.27	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:D:28:LYS:C	1:D:30:THR:N	2.64	0.50
1:E:200:LEU:HD13	1:E:254:VAL:HB	1.94	0.50
1:E:95:LEU:O	1:E:99:ILE:HG13	2.12	0.50
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: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:234:LEU:N	1:I:235:PRO:HD2	2.27	0.50
1:I:77:VAL:HG11	1:I:510:VAL:HB	1.94	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:A:199:TYR:HB3	1:A:325:ILE:HD11	1.94	0.49
1:B:305:ILE:HG12	1:C:267:MET:CE	2.40	0.49
1:C:130:GLU:HB3	1:C:422:VAL:HB	1.94	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: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
1:N:126:ALA:HB1	1:N:426:LEU:HD22	1.94	0.49
1:N:64:ASP:OD1	1:N:65:LYS:O	2.30	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:C:23:LEU:HD13	1:C:23:LEU:C	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:16:MET:CE	1:B:514:MET:HB3	2.42	0.49
1:C:102:GLU:OE1	1:C:102:GLU:HA	2.12	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:11:ASP:O	1:I:12:ALA:C	2.48	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:A:268:ARG:HH22	2:O:20:LYS:HZ2	1.60	0.49
2:T:37:ARG:HH11	2:T:37:ARG:HG2	1.76	0.49
1:F:305:ILE:HG22	1:F:305:ILE:O	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:106:ALA:HA	1:M:111:MET:CE	2.42	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
1:A:288:MET:O	1:A:291:ASP:HB2	2.12	0.49
1:A:510:VAL:O	1:A:511:ALA:C	2.50	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:305:ILE:HD12	1:G:307:MET:HE1	1.94	0.49
2:Q:7:HIS:ND1	2:Q:7:HIS:O	2.42	0.49
1:A:429:LEU:O	1:A:430:ARG:HG2	2.13	0.49
1:A:80:LYS:O	1:A:81:ALA:C	2.50	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:O	1:C:451:LEU:HD23	2.13	0.49
1:H:284:ARG:NH1	1:H:364:LYS:HD2	2.26	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:G:184:GLN:H	1:G:184:GLN:CD	2.15	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:J:288:MET:CG	1:J:288:MET:CE	2.90	0.49
1:K:443:ALA:O	1:K:447:MET:HG3	2.13	0.49
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.93	0.49
1:N:25:ASP:OD1	1:N:28:LYS:HE2	2.13	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: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:361:ASP:O	1:M:365:LEU:HG	2.12	0.49
1:M:135:SER:HA	1:M:412:VAL:HG12	1.94	0.49
1:N:433:ASN:CG	1:N:435:ASP:HB2	2.33	0.49
1:F:519:CYS:HB3	1:G:38:VAL:HG22	1.95	0.49
1:G:44:PHE:N	1:G:44:PHE:CD1	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:D:409:GLU:CD	1:D:501:ARG:HH21	2.13	0.48
1:F:305:ILE:HD12	1:F:307:MET:HE1	1.93	0.48
1:G:121:ASP:O	1:G:122:LYS:C	2.51	0.48
1:I:389:MET:HE2	1:I:390:LYS:HG3	1.94	0.48
1:K:392:LYS:O	1:K:396:VAL:HG23	2.13	0.48
1:K:444:LEU:HA	1:K:444:LEU:HD23	1.57	0.48
1:K:87:ASP:HB3	1:K:499:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:LYS:HA	1:L:83:ASP:HB2	1.94	0.48
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:CG	1:A:430:ARG:NH1	2.70	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:233:MET:C	1:H:235:PRO:HD2	2.34	0.48
1:H:16:MET:SD	1:H:514:MET:HG2	2.53	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:N	1:M:493:ILE:HD13	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:L:389:MET:HE2	1:L:390:LYS:HG3	1.95	0.48
1:N:135:SER:HA	1:N:412:VAL:HG12	1.96	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:113:PRO:O	1:A:114:MET:C	2.48	0.48
1:A:143:ALA:HA	1:A:146:GLN:NE2	2.28	0.48
1:C:349:ILE:HA	1:C:352:GLN:HG2	1.93	0.48
1:K:173:GLY:O	1:K:404:ARG:NH2	2.45	0.48
1:K:494:LEU:HD23	1:K:494:LEU:C	2.32	0.48
1:N:126:ALA:CB	1:N:426:LEU:HD22	2.43	0.48
1:N:22:VAL:HG11	1:N:62:LEU:HD21	1.96	0.48
1:B:270:ILE:HG12	2:P:27:LEU:HD13	1.96	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: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:N:106:ALA:HA	1:N:111:MET:CE	2.44	0.48
1:C:69:MET:CE	1:D:39:VAL:HG12	2.44	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:510:VAL:HG23	1:F:514:MET:CE	2.42	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:452:ARG:CG	1:I:452:ARG:NH1	2.75	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:J:342:ILE:O	1:J:346:VAL:HG23	2.13	0.48
1:K:106:ALA:HA	1:K:111:MET:CE	2.43	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:A:28:LYS:HD2	1:A:453:GLN:CD	2.34	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:F:199:TYR:HB3	1:F:325:ILE:HD11	1.95	0.48
1:F:162:ILE:HG21	1:F:403:THR:HG21	1.94	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: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:N:7:LYS:HD2	1:N:66:PHE:CE2	2.48	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: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:E:76:GLU:O	1:E:80:LYS: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:K:389:MET:HE2	1:K:390:LYS:HG3	1.96	0.48
1:M:346:VAL:O	1:M:350:ARG:HB2	2.13	0.48
1:M:28:LYS:HD2	1:M:453:GLN:OE1	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
1:F:35:GLY:HA3	1:F:51:LYS:HE2	1.95	0.48
1:I:366:GLN:HA	1:I:369:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:325:ILE:HG22	1:J:330:THR:HA	1.95	0.48
1:J:494:LEU:HD23	1:J:494:LEU:C	2.34	0.48
1:K:293:ALA:HB2	1:K:300:VAL:HG23	1.95	0.48
1:N:293:ALA:HB2	1:N:300:VAL:HG23	1.96	0.48
1:N:77:VAL:HG11	1:N:510:VAL:CG1	2.44	0.48
2:P:17:VAL:O	2:P:17:VAL:HG12	2.14	0.48
2:R:17:VAL:HG12	2:R:17:VAL:O	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:C:219:PHE:HB3	1:C:317:LEU:HD23	1.95	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:M:15:LYS:HB3	1:M:66:PHE:HB3	1.96	0.48
1:N:262:LEU:HD22	1:N:273:VAL:HG11	1.96	0.48
1:N:32:GLY:CA	1:N:454:ILE:HG23	2.44	0.48
1:A:270:ILE:HD11	2:O:27:LEU:HB2	1.96	0.48
1:A:96:ALA:O	1:A:97:GLN:C	2.52	0.47
1:E:486:GLY:HA3	1:E:491:MET:CE	2.44	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: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:429:LEU:HB3	1:M:440:ILE:HG21	1.96	0.47
1:M:494:LEU:HD23	1:M:494:LEU:C	2.35	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:A:23:LEU:C	1:A:23:LEU:CD1	2.83	0.47
1:B:28:LYS:C	1:B:30:THR:N	2.67	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: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:217:SER:N	1:I:218:PRO:HD3	2.28	0.47
1:J:102:GLU:HB3	1:J:442:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:PRO:HG2	1:J:73:MET:HG3	1.96	0.47
1:K:524:LEU:HD23	1:K:524:LEU:HA	1.76	0.47
1:K:72:GLN:HE22	1:K:75:LYS:NZ	2.12	0.47
1:N:234:LEU:N	1:N:235:PRO:HD2	2.29	0.47
1:A:259:LEU:O	1:A:263:VAL:HG23	2.14	0.47
1:A:82:ASN:HB2	1:A:89:THR:CG2	2.45	0.47
1:B:69:MET:O	1:B:73:MET:HG3	2.15	0.47
1:C:524:LEU:HA	1:C:524:LEU:HD23	1.62	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:235:PRO:HG3	1:N:310:GLU:HA	1.95	0.47
1:N:77:VAL:HG22	1:N:506:TYR:CD1	2.49	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:NH1	1:G:404:ARG:HG3	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:510:VAL:CG2	1:B:514:MET:HE2	2.45	0.47
1:H:413:ALA:HB1	1:H:417:VAL:HB	1.97	0.47
1:I:290:GLN:NE2	1:I:290:GLN:O	2.46	0.47
1:I:32:GLY:HA2	1:I:454:ILE:HD13	1.97	0.47
1:I:441:LYS:O	1:I:442:VAL:C	2.53	0.47
1:I:451:LEU:HD21	1:I:465:VAL:HG12	1.97	0.47
1:N:217:SER:N	1:N:218:PRO:HD3	2.28	0.47
1:N:44:PHE:N	1:N:44:PHE:CD1	2.83	0.47
2:Q:17:VAL:O	2:Q:17:VAL:HG12	2.14	0.47
1:A:504:LEU:C	1:A:504:LEU:HD22	2.34	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:F:96:ALA:O	1:F:97:GLN:C	2.51	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:I:149:THR:HG21	1:I:156:GLU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:351:GLN:HA	1:J:354:GLU:HG2	1.97	0.47
1:J:492:GLY:C	1:J:493:ILE:HD13	2.35	0.47
1:K:426:LEU:CD1	1:K:444:LEU:HD21	2.44	0.47
1:K:72:GLN:HA	1:K:72:GLN:NE2	2.29	0.47
1:M:80:LYS:HA	1:M:83:ASP:HB2	1.95	0.47
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.96	0.47
1:E:452:ARG:HG2	1:E:452:ARG:HH11	1.80	0.47
1:E:486:GLY:HA3	1:E:491:MET:HE2	1.96	0.47
1:F:432:GLN:NE2	1:F:436:GLN:HE22	2.12	0.47
1:G:185:ASP:HA	1:G:380:LYS:O	2.15	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: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:319:GLN:O	1:M:336:VAL:HG23	2.15	0.47
1:M:428:ASP:O	1:M:430:ARG:HG2	2.14	0.47
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:524:LEU:HD23	1:N:524:LEU:HA	1.59	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:E:221:LEU:HB3	1:E:249:ILE:HD13	1.97	0.47
1:J:10:ASN:O	1:J:11:ASP:C	2.52	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:M:366:GLN:HA	1:M:369:VAL:HG22	1.96	0.47
1:M:44:PHE:CD1	1:M:44:PHE:N	2.83	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:C:124:VAL:HG13	1:C:504:LEU:HD13	1.97	0.47
1:D:25:ASP:N	1:D:25:ASP:OD1	2.46	0.47
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.96	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:458:CYS:SG	1:L:480:ALA:HB1	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:192:GLY:O	1:M:193:MET:HB2	2.14	0.47
1:L:49:ILE:HD12	1:M:513:LEU:HD23	1.97	0.47
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.43	0.47
1:A:510:VAL:CG2	1:A:514:MET:HE2	2.45	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:180:GLY:HA3	1:J:381:VAL:O	2.14	0.47
1:J:135:SER:HA	1:J:412:VAL:HG12	1.97	0.47
1:J:44:PHE:N	1:J:44:PHE:CD1	2.83	0.47
1:M:77:VAL:HG11	1:M:510:VAL:HB	1.97	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:100:ILE:O	1:C:101:THR:C	2.51	0.47
1:C:34:LYS:HD2	1:C:458:CYS:SG	2.55	0.47
1:C:58:ARG:HH11	1:C:58:ARG:HG3	1.79	0.47
1:E:25:ASP:N	1:E:25:ASP:OD1	2.47	0.47
1:F:510:VAL:HG23	1:F:514:MET:HE2	1.96	0.47
1:G:199:TYR:HB3	1:G:325:ILE:HD11	1.96	0.47
1:G:54:VAL:O	1:G:58:ARG:CG	2.63	0.47
1:H:444:LEU:HA	1:H:444:LEU:HD23	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: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:D:147:VAL:O	1:D:150:ILE:HG22	2.15	0.46
1:E:489:ILE:HD13	1:E:494:LEU:HD22	1.95	0.46
1:E:150:ILE:HG21	1:E:494:LEU:O	2.15	0.46
1:F:339:GLU:HA	1:F:342:ILE:HB	1.97	0.46
1:G:305:ILE:HG22	1:G:305:ILE:O	2.15	0.46
1:I:161:LEU:HD21	1:I:185:ASP:HB3	1.96	0.46
1:K:453:GLN:O	1:K:454:ILE:C	2.52	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:C:270:ILE:CD1	2:Q:27:LEU:HB2	2.45	0.46
1:A:91:THR:O	1:A:92:ALA:C	2.52	0.46
1:G:324:VAL:O	1:G:331:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:MET:HE2	1:H:522:THR:HB	1.95	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:HG12	1:B:267:MET:HE3	1.98	0.46
1:A:510:VAL:CG2	1:A:514:MET:CE	2.90	0.46
1:C:169:VAL:HB	1:C:173:GLY:HA3	1.97	0.46
1:F:489:ILE:CD1	1:F:494:LEU:HD22	2.46	0.46
1:K:366:GLN:HA	1:K:369:VAL:HG22	1.96	0.46
1:K:88:GLY:O	1:K:91:THR:N	2.48	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:290:GLN:NE2	1:M:293:ALA:HB3	2.30	0.46
1:M:69:MET:HE2	1:M:522:THR:HB	1.95	0.46
1:A:150:ILE:HG21	1:A:494:LEU:O	2.16	0.46
1:A:443:ALA:O	1:A:444:LEU:C	2.52	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:NH1	1:C:404:ARG:HG3	2.27	0.46
1:I:44:PHE:N	1:I:44:PHE:CD1	2.84	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:351:GLN:HA	1:M:354:GLU:HG2	1.97	0.46
1:M:19:GLY:HA3	1:M:67:GLU:O	2.15	0.46
1:N:494:LEU:HD23	1:N:494:LEU:O	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:219:PHE:HB3	1:A:317:LEU:HD23	1.98	0.46
1:A:102:GLU:HB3	1:A:442:VAL:HG22	1.98	0.46
1:B:21:ASN:ND2	1:B:97:GLN:OE1	2.48	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:E:16:MET:HE1	1:E:514:MET:HB3	1.98	0.46
1:G:28:LYS:C	1:G:30:THR:H	2.18	0.46
1:I:135:SER:HA	1:I:412:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:111:MET:HG2	1:B:435:ASP:OD1	2.16	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:C:7:LYS:HB3	1:C:12:ALA:HB2	1.98	0.46
1:F:486:GLY:HA3	1:F:491:MET:HE1	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:87:ASP:HB3	1:H:499:VAL:HG21	1.98	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: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:B:16:MET:HE1	1:B:514:MET:HB3	1.98	0.46
1:C:224:ASP:OD1	1:C:286:LYS:HG2	2.16	0.46
1:D:259:LEU:O	1:D:263:VAL:HG23	2.15	0.46
1:D:6:VAL:CG2	1:D:6:VAL:O	2.64	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:J:18:ARG:O	1:J:19:GLY:C	2.52	0.46
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.96	0.46
1:K:40:LEU:HD12	1:L:521:VAL:HB	1.98	0.46
1:M:524:LEU:CD2	1:M:525:PRO:HD2	2.45	0.46
1:M:86:GLY:O	1:M:87:ASP:HB2	2.14	0.46
1:N:428:ASP:O	1:N:429:LEU:C	2.54	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:D:273:VAL:HG12	1:D:274:ALA:N	2.31	0.46
1:D:28:LYS:O	1:D:30:THR:N	2.48	0.46
1:D:288:MET:O	1:D:291:ASP:HB2	2.16	0.46
1:F:486:GLY:CA	1:F:491:MET:CE	2.94	0.46
1:F:510:VAL:O	1:F:511:ALA:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:284:ARG:NH1	1:L:364:LYS:HD2	2.27	0.46
1:N:106:ALA:O	1:N:107:VAL:C	2.54	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: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:F:114:MET:O	1:F:114:MET:HE3	2.16	0.46
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.98	0.46
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.97	0.46
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:B:96:ALA:O	1:B:97:GLN:C	2.54	0.46
1:C:510:VAL:O	1:C:511:ALA:C	2.51	0.46
1:D:349:ILE:HA	1:D:352:GLN:HG2	1.95	0.46
1:F:28:LYS:O	1:F:29:VAL:C	2.55	0.46
1:G:80:LYS:O	1:G:81:ALA:C	2.53	0.46
1:H:164:GLU:O	1:H:167:ASP:HB3	2.15	0.46
1:I:77:VAL:HG22	1:I:506:TYR:CD1	2.51	0.46
1:K:22:VAL:HG11	1:K:62:LEU:HD21	1.98	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:HD23	1:M:444:LEU:HA	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
1:C:100:ILE:CD1	1:C:514:MET:HE1	2.38	0.45
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: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:138:CYS:SG	1:K:144:ILE:HD13	2.56	0.45
1:K:462:PRO:O	1:K:463:SER:C	2.54	0.45
1:B:305:ILE:HD12	1:B:307:MET:HE1	1.99	0.45
1:C:200:LEU:HD13	1:C:254:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:LEU:C	1:G:23:LEU:HD12	2.37	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: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
2:P:7:HIS:O	2:P:7:HIS:ND1	2.48	0.45
2:R:37:ARG:HH11	2:R:37:ARG:HG2	1.82	0.45
1:B:28:LYS:O	1:B:29:VAL:C	2.53	0.45
1:B:324:VAL:O	1:B:331:THR:HG22	2.17	0.45
1:B:511:ALA:O	1:B:512:GLY:C	2.52	0.45
1:C:100:ILE:HD11	1:C:514:MET:CE	2.38	0.45
1:C:399:ALA:O	1:C:400:LEU:C	2.54	0.45
1:C:414:GLY:HA2	1:C:495:ASP:OD2	2.17	0.45
1:F:502:SER:O	1:F:503:ALA:C	2.55	0.45
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.99	0.45
1:K:370:ALA:O	1:K:371:LYS:C	2.54	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:O	2:S:17:VAL:HG12	2.15	0.45
1:A:221:LEU:HD13	1:A:317:LEU:HD11	1.99	0.45
1:A:6:VAL:CG2	1:A:6:VAL:O	2.63	0.45
1:B:451:LEU:HD23	1:B:451:LEU:C	2.37	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:F:486:GLY:CA	1:F:491:MET:HE2	2.46	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:J:214:GLU:HG3	1:J:324:VAL:HG22	1.97	0.45
1:J:444:LEU:HA	1:J:444:LEU:HD23	1.56	0.45
1:J:32:GLY:CA	1:J:454:ILE:HD13	2.44	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:120:ILE:HA	1:N:443:ALA:HB2	1.99	0.45
1:N:88:GLY:O	1:N:89:THR:C	2.54	0.45
2:P:23:GLY:H	2:Q:80:ASN:ND2	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:84:LEU:CD1	2:R:84:LEU:N	2.78	0.45
1:B:161:LEU:HA	1:B:161:LEU:HD12	1.84	0.45
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.99	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:A:461:GLU:OE1	1:N:463:SER:HB3	2.16	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:28:LYS:O	1:D:29:VAL:C	2.49	0.45
1:D:96:ALA:HB2	1:D:507:ALA:HB1	1.99	0.45
1:E:473:ASP:O	1:E:474:GLY:C	2.55	0.45
1:E:510:VAL:HG23	1:E:514:MET:HE3	1.98	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:HD12	1:K:420:ILE:HG23	1.64	0.45
1:L:44:PHE:N	1:L:44:PHE:CD1	2.84	0.45
1:M:513:LEU:HA	1:M:513:LEU:HD12	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:E:417:VAL:O	1:E:418:ALA:C	2.55	0.45
1:E:34:LYS:HD2	1:E:458:CYS:SG	2.57	0.45
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.98	0.45
1:I:126:ALA:HB1	1:I:426:LEU:CD2	2.47	0.45
1:J:104:LEU:HA	1:J:104:LEU:HD12	1.41	0.45
1:J:452:ARG:CG	1:J:452:ARG:NH1	2.76	0.45
1:K:452:ARG:CG	1:K:452:ARG:NH1	2.73	0.45
1:L:524:LEU:HD23	1:L:524:LEU:HA	1.59	0.45
1:M:104:LEU:HA	1:M:104:LEU:HD12	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:B:305:ILE:HG23	1:C:267:MET:HE2	1.98	0.45
1:C:273:VAL:HG12	1:C:274:ALA:N	2.32	0.45
1:C:487:ASN:OD1	1:C:487:ASN:C	2.55	0.45
1:E:162:ILE:O	1:E:166:MET:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:LEU:HB3	1:E:49:ILE:HD13	1.99	0.45
1:F:28:LYS:C	1:F:30:THR:N	2.68	0.45
1:G:23:LEU:HD12	1:G:24:ALA:N	2.31	0.45
1:H:10:ASN:O	1:H:11:ASP:C	2.55	0.45
1:I:370:ALA:O	1:I:371:LYS:C	2.54	0.45
1:M:193:MET:HE2	1:M:195:PHE:HD1	1.81	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:C:90:THR:O	1:C:94:VAL:HG23	2.17	0.45
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:I:72:GLN:HA	1:I:72:GLN:NE2	2.32	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:A:147:VAL:O	1:A:148:GLY:C	2.53	0.45
1:C:85:ALA:O	1:C:86:GLY:C	2.51	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: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:428:ASP:O	1:H:430:ARG:HG2	2.17	0.45
1:H:426:LEU:CD1	1:H:444:LEU:HD21	2.47	0.45
1:J:100:ILE:HG23	1:J:104:LEU:HD22	1.99	0.45
1:J:80:LYS:HA	1:J:83:ASP:HB2	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:HA	1:N:23:LEU:HD23	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:268:ARG:HH22	2:Q:20:LYS:HZ2	1.64	0.45
1:B:23:LEU:HD13	1:B:23:LEU:C	2.38	0.44
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:I:106:ALA:HA	1:I:111:MET:HE3	1.98	0.44
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:201:SER:HA	1:D:202:PRO:HD3	1.85	0.44
1:D:19:GLY:HA3	1:D:67:GLU:O	2.17	0.44
1:F:201:SER:HA	1:F:202:PRO:HD3	1.86	0.44
1:G:114:MET:O	1:G:114:MET:HE3	2.17	0.44
1:G:417:VAL:O	1:G:418:ALA:C	2.56	0.44
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.99	0.44
1:I:77:VAL:HG22	1:I:506:TYR:HD1	1.82	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:L:443:ALA:O	1:L:447:MET:HG3	2.17	0.44
1:N:492:GLY:C	1:N:493:ILE:HD13	2.37	0.44
1:N:68:ASN:HB3	5:N:532:HOH:O	2.16	0.44
1:B:349:ILE:HA	1:B:352:GLN:HG2	1.96	0.44
1:A:513:LEU:HB3	1:B:49:ILE:HD13	1.99	0.44
1:C:417:VAL:O	1:C:418:ALA:C	2.56	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:88:GLY:O	1:J:89:THR:C	2.55	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:HA	1:N:444:LEU:HD23	1.44	0.44
1:A:417:VAL:O	1:A:418:ALA:C	2.53	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:D:116:LEU:HA	1:D:116:LEU:HD23	1.66	0.44
1:C:519:CYS:CB	1:D:38:VAL:HG13	2.39	0.44
1:F:150:ILE:HD13	1:F:493:ILE:HA	1.98	0.44
1:F:451:LEU:C	1:F:451:LEU:HD23	2.37	0.44
1:H:8:PHE:O	1:H:9:GLY:C	2.56	0.44
1:I:169:VAL:HG13	1:I:173:GLY:HA3	1.99	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:106:ALA:CA	1:M:111:MET:HE3	2.47	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:HG12	2:T:17:VAL:O	2.18	0.44
1:A:234:LEU:N	1:A:235:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:A:494:LEU:N	2.32	0.44
1:B:150:ILE:HD13	1:B:493:ILE:HA	2.00	0.44
1:C:432:GLN:HG3	1:C:432:GLN:H	1.64	0.44
1:C:432:GLN:HE21	1:C:436:GLN:HE22	1.63	0.44
1:C:65:LYS:NZ	1:C:523:ASP:HB2	2.32	0.44
1:C:58:ARG:HG3	1:C:58:ARG:NH1	2.32	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:H:524:LEU:HA	1:H:524:LEU:HD23	1.64	0.44
1:I:325:ILE:HG22	1:I:330:THR:HA	1.99	0.44
1:K:120:ILE:HA	1:K:443:ALA:HB2	2.00	0.44
1:K:85:ALA:HB1	1:K:499:VAL:HB	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:NH1	2:T:37:ARG:HG2	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:106:ALA:HA	1:J:111:MET:HE3	1.98	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:HG23	1:N:420:ILE:HD12	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:N	1:K:44:PHE:CD1	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:L:494:LEU:C	1:L:494:LEU:HD23	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:LYS:HD2	1:M:66:PHE:CE2	2.53	0.44
1:N:475:ASN:ND2	1:N:489:ILE:HD12	2.33	0.44
1:C:162:ILE:O	1:C:166:MET:HG3	2.18	0.44
1:C:20:VAL:HG23	1:C:20:VAL:H	1.58	0.44
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: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:A:267:MET:HE3	1:G:305:ILE:HG12	1.99	0.44
1:H:104:LEU:HA	1:H:104:LEU:HD12	1.48	0.44
1:H:52:ASP:C	1:H:52:ASP:OD1	2.56	0.44
1:L:444:LEU:HD23	1:L:444:LEU:HA	1.53	0.44
1:N:519:CYS:SG	1:N:520:MET:N	2.91	0.44
2:P:78:ILE:HD13	2:P:83:VAL:HG21	1.98	0.44
1:B:219:PHE:HB3	1:B:317:LEU:HD23	2.00	0.44
1:G:44:PHE:N	1:G:44:PHE:HD1	2.01	0.44
1:G:524:LEU:HA	1:G:524:LEU:HD23	1.57	0.44
1:K:233:MET:C	1:K:235:PRO:HD2	2.38	0.44
1:N:236:VAL:HG22	1:N:312:ALA:O	2.17	0.44
1:N:441:LYS:O	1:N:442:VAL:C	2.55	0.44
1:B:24:ALA:O	1:B:28:LYS:HG3	2.18	0.43
1:B:510:VAL:CG2	1:B:514:MET:CE	2.95	0.43
1:E:478:TYR:CE2	1:E:480:ALA:HA	2.53	0.43
1:F:23:LEU:CD1	1:F:23:LEU:C	2.86	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:HA	1:H:433:ASN:HD22	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: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
1:I:172:GLU:O	1:I:173:GLY:O	2.36	0.43
1:I:19:GLY:HA3	1:I:67:GLU:O	2.18	0.43
1:J:7:LYS:HD2	1:J:66:PHE:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:LEU:HD21	1:M:277:LYS:HG3	2.00	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:E:201:SER:HA	1:E:202:PRO:HD3	1.83	0.43
1:E:69:MET:O	1:E:73:MET:HG3	2.18	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:513:LEU:HA	1:K:513:LEU:HD12	1.87	0.43
1:K:16:MET:SD	1:K:514:MET:HG2	2.59	0.43
1:L:361:ASP:O	1:L:365:LEU:HG	2.17	0.43
1:M:497:THR:O	1:M:498:LYS:C	2.57	0.43
2:O:37:ARG:NH1	2:O:37:ARG:HG2	2.33	0.43
1:B:486:GLY:CA	1:B:491:MET:HE2	2.46	0.43
1:D:288:MET:HG3	1:D:368:ARG:CD	2.45	0.43
1:E:489:ILE:HD13	1:E:494:LEU:CD2	2.48	0.43
1:E:510:VAL:CG2	1:E:514:MET:HE2	2.47	0.43
1:G:111:MET:HG2	1:G:435:ASP:OD1	2.18	0.43
1:I:104:LEU:HD12	1:I:104:LEU:HA	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:K:168:LYS:HD2	1:K:187:LEU:HD13	1.99	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
1:B:270:ILE:HD11	2:P:27:LEU:HB2	2.00	0.43
2:T:23:GLY:H	2:U:80:ASN:ND2	2.16	0.43
1:A:194:GLN:HB2	1:A:331:THR:CB	2.48	0.43
1:B:234:LEU:N	1:B:235:PRO:HD2	2.34	0.43
1:B:4:LYS:HD2	1:B:522:THR:O	2.19	0.43
1:D:65:LYS:NZ	1:D:523:ASP:HB2	2.33	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:HD3	1:H:15:LYS:HA	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:389:MET:HE2	1:N:390:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:100:ILE:O	1:A:101:THR:C	2.57	0.43
1:B:252:GLU:O	1:B:253:ASP:HB2	2.19	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:246:PRO:HB3	1:E:272:LYS:HB3	2.01	0.43
1:E:194:GLN:HG3	1:E:330:THR:O	2.19	0.43
1:F:44:PHE:N	1:F:44:PHE:CD1	2.60	0.43
1:F:513:LEU:HA	1:F:513:LEU:HD23	1.80	0.43
1:I:174:VAL:HG21	1:I:194:GLN:HB3	2.01	0.43
1:I:32:GLY:CA	1:I:454:ILE:HG23	2.48	0.43
1:K:169:VAL:HG13	1:K:173:GLY:HA3	2.01	0.43
1:L:60:ILE:HD13	1:L:60:ILE:HA	1.85	0.43
1:N:403:THR:O	1:N:407:VAL:HG23	2.18	0.43
2:Q:84:LEU:N	2:Q:84:LEU:HD12	2.34	0.43
1:B:25:ASP:OD1	1:B:25:ASP:N	2.46	0.43
1:C:238:GLU:OE2	2:Q:23:GLY:C	2.56	0.43
1:D:28:LYS:HD2	1:D:453:GLN:CD	2.38	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:325:ILE:HG22	1:H:330:THR:HA	2.00	0.43
1:H:32:GLY:CA	1:H:454:ILE:HG23	2.49	0.43
1:I:13:ARG:HE	1:I:107:VAL:HG21	1.83	0.43
1:J:451:LEU:O	1:J:452:ARG:C	2.54	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:B:147:VAL:O	1:B:148:GLY:C	2.55	0.43
1:B:434:GLU:O	1:B:435:ASP:C	2.57	0.43
1:G:478:TYR:CE2	1:G:480:ALA:HA	2.53	0.43
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.42	0.43
1:H:77:VAL:HG22	1:H:506:TYR:HD1	1.84	0.43
1:J:15:LYS:HD3	1:J:15:LYS:HA	1.74	0.43
1:J:205:ILE:HA	1:J:213:VAL:HG22	2.01	0.43
1:J:70:GLY:O	1:J:71:ALA:C	2.55	0.43
1:L:429:LEU:HB3	1:L:440:ILE:HG21	2.01	0.43
1:M:370:ALA:O	1:M:371:LYS:C	2.56	0.43
1:N:161:LEU:HD21	1:N:185:ASP:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:HA	1:C:116:LEU:HD23	1.52	0.43
1:D:221:LEU:HB3	1:D:249:ILE:HD13	2.01	0.43
1:D:28:LYS:C	1:D:30:THR:H	2.22	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:F:28:LYS:HD2	1:F:453:GLN:CD	2.39	0.43
1:G:54:VAL:O	1:G:58:ARG:HG2	2.19	0.43
1:H:265:ASN:HD22	1:H:265:ASN:HA	1.59	0.43
1:H:68:ASN:HB3	5:H:528:HOH:O	2.18	0.43
1:I:438:VAL:O	1:I:439:GLY:C	2.57	0.43
1:K:201:SER:HA	1:K:202:PRO:HD3	1.89	0.43
1:L:433:ASN:HA	1:L:433:ASN:HD22	1.50	0.43
2:S:37:ARG:HH11	2:S:37:ARG:HG2	1.83	0.43
1:G:268:ARG:HH22	2:U:20:LYS:HZ2	1.67	0.43
1:A:158:VAL:HG12	1:A:162:ILE:HD12	2.01	0.43
1:B:432:GLN:HE21	1:B:436:GLN:HE22	1.65	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
1:I:43:SER:HB3	1:I:44:PHE:CD1	2.54	0.43
1:J:72:GLN:HE22	1:J:75:LYS:NZ	2.16	0.43
1:L:433:ASN:CG	1:L:435:ASP:HB2	2.39	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
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:198:GLY:C	1:B:276:VAL:HG12	2.39	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:153:ASN:O	1:F:154:SER:HB2	2.18	0.42
1:F:58:ARG:HG2	1:F:58:ARG:H	1.67	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:L:7:LYS:HG2	1:L:11:ASP:HB2	2.01	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:430:ARG:NH1	1:B:430:ARG:CG	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ASP:O	1:B:474:GLY:C	2.57	0.42
1:B:486:GLY:CA	1:B:491:MET:CE	2.96	0.42
1:C:184:GLN:H	1:C:184:GLN:CD	2.23	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:G:443:ALA:O	1:G:444:LEU:C	2.57	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:N:102:GLU:HB3	1:N:442:VAL:HG22	2.01	0.42
1:A:384:ALA:O	1:G:506:TYR:HE1	2.02	0.42
1:A:452:ARG:HH11	1:A:452:ARG:HG2	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
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:H:492:GLY:C	1:H:493:ILE:HD13	2.39	0.42
1:I:433:ASN:HA	1:I:433:ASN:HD22	1.39	0.42
1:J:492:GLY:O	1:J:493:ILE:HD13	2.19	0.42
1:K:163:ALA:O	1:K:167:ASP:HB2	2.19	0.42
1:K:77:VAL:HG22	1:K:506:TYR:CD1	2.54	0.42
1:M:15:LYS:HD3	1:M:15:LYS:HA	1.70	0.42
1:B:35:GLY:HA3	1:B:51:LYS:HE2	2.00	0.42
1:B:416:GLY:HA2	5:B:607:HOH:O	2.18	0.42
1:B:42:LYS:HG2	1:B:44:PHE:CD2	2.54	0.42
1:C:42:LYS:HG2	1:C:44:PHE:CE2	2.54	0.42
1:D:444:LEU:O	1:D:447:MET:HB2	2.19	0.42
1:D:95:LEU:O	1:D:99:ILE:HG13	2.18	0.42
1:E:169:VAL:HB	1:E:173:GLY:HA3	2.00	0.42
1:E:324:VAL:O	1:E:331:THR:HG22	2.19	0.42
1:E:199:TYR:HB3	1:E:325:ILE:HD11	2.00	0.42
1:G:15:LYS:O	1:G:16:MET:C	2.55	0.42
1:H:420:ILE:HG23	1:H:420:ILE:HD12	1.65	0.42
1:H:44:PHE:CD1	1:H:44:PHE:N	2.87	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:409:GLU:OE2	1:K:501:ARG:NH2	2.52	0.42
1:K:66:PHE:HA	1:K:69:MET:HE3	2.01	0.42
1:K:66:PHE:N	1:K:69:MET:HE3	2.35	0.42
1:M:266:THR:HG21	1:M:273:VAL:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:84:LEU:CD1	2:S:84:LEU:N	2.82	0.42
2:U:41:LEU:O	2:U:61:VAL:HG13	2.19	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:A:44:PHE:HB2	1:A:45:GLY:H	1.66	0.42
1:C:270:ILE:HD11	2:Q:27:LEU:HB2	1.99	0.42
1:E:362:ARG:HG2	1:E:366:GLN:NE2	2.34	0.42
1:F:121:ASP:O	1:F:122:LYS:C	2.57	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
1:G:198:GLY:C	1:G:276:VAL:HG12	2.39	0.42
1:H:346:VAL:O	1:H:350:ARG:HB2	2.18	0.42
1:K:426:LEU:O	1:K:444:LEU:HD11	2.19	0.42
1:N:131:LEU:HD13	1:N:422:VAL:HG11	2.01	0.42
1:N:66:PHE:N	1:N:69:MET:HE3	2.34	0.42
1:B:102:GLU:HB3	1:B:442:VAL:HG22	2.01	0.42
1:C:487:ASN:OD1	1:C:489:ILE:N	2.52	0.42
1:C:16:MET:HE1	1:C:514:MET:HB3	2.01	0.42
1:C:82:ASN:HB2	1:C:89:THR:HG21	2.00	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:A:39:VAL:HG12	1:G:69:MET:CE	2.50	0.42
1:K:227:ILE:HB	1:K:254:VAL:HG22	2.01	0.42
1:L:290:GLN:O	1:L:290:GLN:NE2	2.50	0.42
1:L:452:ARG:CG	1:L:452:ARG:NH1	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:266:THR:CG2	1:A:273:VAL:HB	2.50	0.42
1:A:185:ASP:HA	1:A:380:LYS:O	2.19	0.42
1:D:153:ASN:O	1:D:153:ASN:ND2	2.53	0.42
1:D:16:MET:HE1	1:D:514:MET:HB3	2.01	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:F:74:VAL:HG13	1:F:514:MET:HE3	2.01	0.42
1:G:273:VAL:HG12	1:G:274:ALA:N	2.34	0.42
1:I:404:ARG:NH1	1:I:404:ARG:CG	2.73	0.42
1:J:265:ASN:HD22	1:J:265:ASN:HA	1.59	0.42
1:J:305:ILE:HD12	1:J:307:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:199:TYR:HA	1:M:276:VAL:HG12	2.02	0.42
1:M:419:LEU:O	1:M:420:ILE:C	2.58	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:CG2	1:B:6:VAL:O	2.67	0.42
1:C:362:ARG:HG2	1:C:366:GLN:NE2	2.33	0.42
1:D:486:GLY:HA3	1:D:491:MET:CE	2.49	0.42
1:E:153:ASN:O	1:E:154:SER:CB	2.67	0.42
1:D:519:CYS:HB3	1:E:38:VAL:HG22	2.01	0.42
1:G:232:GLU:HA	1:G:310:GLU:CD	2.40	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: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:HA	1:K:104:LEU:HD12	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:HG2	1:M:363:GLU:H	1.65	0.42
1:B:15:LYS:O	1:B:16:MET:C	2.58	0.42
1:B:221:LEU:HD23	1:B:249:ILE:HD12	2.02	0.42
1:D:146:GLN:HE21	1:D:146:GLN:HB2	1.58	0.42
1:E:28:LYS:HD2	1:E:453:GLN:CD	2.41	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:HG3	1:G:432:GLN:H	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:233:MET:C	1:M:235:PRO:HD2	2.40	0.42
1:M:419:LEU:CD2	1:M:500:THR:HG23	2.40	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:246:PRO:HB3	1:A:272:LYS:HB3	2.01	0.42
1:A:74:VAL:O	1:A:77:VAL:CG1	2.59	0.42
1:B:510:VAL:O	1:B:511:ALA:C	2.54	0.42
1:D:31:LEU:HD23	1:D:453:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:ALA:O	1:E:444:LEU:C	2.58	0.42
1:G:221:LEU:HD13	1:G:317:LEU:HD11	2.02	0.42
1:G:349:ILE:HA	1:G:352:GLN:HG2	1.92	0.42
1:H:370:ALA:O	1:H:371:LYS:C	2.57	0.42
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.29	0.42
1:I:64:ASP:C	1:I:65:LYS:O	2.57	0.42
1:K:124:VAL:HG13	1:K:504:LEU:HD13	2.01	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:417:VAL:HG21	1:M:488:MET:HG3	2.02	0.42
1:M:77:VAL:HG22	1:M:506:TYR:CD1	2.55	0.42
1:A:261:THR:HG23	2:O:29:GLY:H	1.85	0.42
2:O:84:LEU:N	2:O:84:LEU:CD1	2.83	0.42
1:A:197:ARG:HD2	1:A:277:LYS:HB2	2.02	0.41
1:A:34:LYS:HD2	1:A:458:CYS:SG	2.60	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:D:198:GLY:C	1:D:276:VAL:HG12	2.40	0.41
1:F:221:LEU:HD13	1:F:317:LEU:HD11	2.02	0.41
1:J:193:MET:HE2	1:J:195:PHE:HD1	1.84	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:M:127:ALA:O	1:M:128:VAL:C	2.57	0.41
1:A:33:PRO:HA	1:A:153:ASN:ND2	2.26	0.41
1:A:444:LEU:O	1:A:447:MET:HB2	2.19	0.41
1:A:486:GLY:CA	1:A:491:MET:CE	2.98	0.41
1:A:486:GLY:CA	1:A:491:MET:HE2	2.50	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:G:116:LEU:HD23	1:G:116:LEU:HA	1.67	0.41
1:I:127:ALA:O	1:I:128:VAL:C	2.57	0.41
1:I:96:ALA:O	1:I:100:ILE:HG13	2.20	0.41
1:J:101:THR:HG22	1:J:105:LYS:HE3	2.02	0.41
1:J:106:ALA:HA	1:J:111:MET:CE	2.50	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:409:GLU:HB2	1:M:497:THR:HB	2.01	0.41
1:A:193:MET:HG3	1:A:194:GLN:N	2.35	0.41
1:C:23:LEU:HD12	1:C:23:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:LEU:HA	1:E:116:LEU:HD23	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
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:HA	1:I:15:LYS:HD3	1.67	0.41
1:I:364:LYS:HA	1:I:364:LYS:HD3	1.84	0.41
1:J:64:ASP:C	1:J:65:LYS:O	2.58	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: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
2:U:6:LEU:O	2:U:7:HIS:C	2.58	0.41
1:A:200:LEU:HD13	1:A:254:VAL:HB	2.01	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:404:ARG:NH1	1:D:404:ARG:HG3	2.26	0.41
1:E:114:MET:HB3	1:E:114:MET:HE2	2.03	0.41
1:E:28:LYS:O	1:E:29:VAL:C	2.54	0.41
1:F:19:GLY:HA3	1:F:67:GLU:O	2.21	0.41
1:G:415:GLY:HA2	1:G:454:ILE:HD12	2.01	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:27:VAL:HG12	1:G:90:THR:HG23	2.03	0.41
1:H:7:LYS:HD2	1:H:66:PHE:CZ	2.55	0.41
1:I:233:MET:C	1:I:235:PRO:HD2	2.40	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
2:O:41:LEU:O	2:O:61:VAL:HG13	2.21	0.41
1:E:515:ILE:HG21	1:E:515:ILE:HD13	1.83	0.41
1:G:451:LEU:HD23	1:G:451:LEU:O	2.21	0.41
1:H:290:GLN:O	1:H:290:GLN:NE2	2.53	0.41
1:H:462:PRO:O	1:H:463:SER:C	2.59	0.41
1:J:478:TYR:HB2	1:J:485:TYR:CD2	2.55	0.41
1:K:418:ALA:O	1:K:422:VAL:HG13	2.20	0.41
1:K:511:ALA:O	1:K:515:ILE:HD12	2.20	0.41
1:K:16:MET:HG3	1:K:520:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:174:VAL:HG21	1:L:194:GLN:HB3	2.02	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: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:A:69:MET:O	1:A:73:MET:HG3	2.21	0.41
1:B:169:VAL:HB	1:B:173:GLY:HA3	2.02	0.41
1:C:114:MET:CE	1:C:114:MET:O	2.68	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:E:184:GLN:CD	1:E:184:GLN:H	2.23	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:346:VAL:O	1:J:350:ARG:HB2	2.21	0.41
1:K:345:ARG:HA	1:K:348:GLN:HE21	1.85	0.41
1:K:88:GLY:O	1:K:89:THR:C	2.59	0.41
1:L:437:ASN:HA	1:L:440:ILE:HD12	2.02	0.41
1:M:193:MET:CE	1:M:195:PHE:CD1	2.98	0.41
1:M:32:GLY:HA2	1:M:454:ILE:HG23	2.01	0.41
1:A:432:GLN:HE21	1:A:436:GLN:HE22	1.67	0.41
1:A:62:LEU:HD12	1:A:62:LEU:HA	1.80	0.41
1:B:153:ASN:O	1:B:153:ASN:ND2	2.54	0.41
1:B:20:VAL:HG13	1:B:74:VAL:HG21	2.01	0.41
1:B:399:ALA:O	1:B:400:LEU:C	2.57	0.41
1:B:489:ILE:HD13	1:B:494:LEU:HD22	2.03	0.41
1:B:402:ALA:HB1	1:B:496:PRO:HG2	2.01	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:432:GLN:HE21	1:E:436:GLN:NE2	2.17	0.41
1:F:430:ARG:CG	1:F:430:ARG:NH1	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
1:G:513:LEU:HD23	1:G:513:LEU:HA	1.67	0.41
1:H:129:GLU:O	1:H:132:LYS:N	2.54	0.41
1:H:172:GLU:O	1:H:173:GLY:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:370:ALA:O	1:L:371:LYS:C	2.59	0.41
1:M:284:ARG:O	1:M:288:MET:HG3	2.21	0.41
1:N:69:MET:HE1	1:N:522:THR:CB	2.45	0.41
1:B:510:VAL:HG23	1:B:514:MET:HE2	2.02	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:460:GLU:O	1:F:462:PRO:HD3	2.20	0.41
1:F:76:GLU:O	1:F:76:GLU:HG2	2.21	0.41
1:G:19:GLY:HA3	1:G:67:GLU:O	2.21	0.41
1:H:502:SER:O	1:H:503:ALA:C	2.59	0.41
1:I:460:GLU:HG2	1:I:460:GLU:H	1.70	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:L:417:VAL:O	1:L:418:ALA:C	2.59	0.41
1:L:61:GLU:HG2	1:M:3:ALA:HA	2.02	0.41
1:N:22:VAL:HG11	1:N:62:LEU:CD2	2.51	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:C:513:LEU:HA	1:C:513:LEU:HD23	1.76	0.41
1:C:73:MET:CG	1:C:73:MET:CE	2.98	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:F:4:LYS:HG3	1:G:59:GLU:O	2.21	0.41
1:G:224:ASP:OD1	1:G:286:LYS:HG2	2.20	0.41
1:G:54:VAL:O	1:G:58:ARG:HG3	2.21	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:H:91:THR:O	1:H:92:ALA:C	2.59	0.41
1:I:255:GLU:O	1:I:256:GLY:C	2.59	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:465:VAL:HG11	1:I:478:TYR:CD2	2.56	0.41
1:K:11:ASP:O	1:K:12:ALA:C	2.56	0.41
1:L:106:ALA:O	1:L:107:VAL:C	2.57	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:L:95:LEU:HD23	1:L:446:ALA:O	2.20	0.41
1:M:193:MET:H	1:M:376:VAL:HG21	1.86	0.41
2:O:6:LEU:O	2:O:7:HIS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:60:LYS:HG2	2:S:63:ASP:OD2	2.21	0.41
2:T:6:LEU:O	2:T:7:HIS:C	2.59	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:B:42:LYS:HE2	1:B:48:THR:OG1	2.20	0.41
1:C:486:GLY:HA3	1:C:491:MET:CE	2.51	0.41
1:E:524:LEU:HD22	1:E:525:PRO:HD2	2.01	0.41
1:F:429:LEU:HD12	1:F:429:LEU:HA	1.83	0.41
1:F:69:MET:CE	1:G:39:VAL:HG12	2.51	0.41
1:G:147:VAL:O	1:G:148:GLY:C	2.58	0.41
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:I:417:VAL:HG21	1:I:488:MET:HG3	2.03	0.41
1:J:290:GLN:NE2	1:J:293:ALA:HB3	2.35	0.41
1:M:290:GLN:O	1:M:293:ALA:HB3	2.21	0.41
1:M:77:VAL:HG22	1:M:506:TYR:HD1	1.85	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
1:A:28:LYS:C	1:A:30:THR:N	2.71	0.41
1:D:169:VAL:HB	1:D:173:GLY:HA3	2.03	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:I:66:PHE:HA	1:I:520:MET:HE1	2.03	0.41
1:K:255:GLU:O	1:K:256:GLY:C	2.60	0.41
1:K:265:ASN:HD22	1:K:265:ASN:HA	1.60	0.41
1:K:479:ASN:OD1	1:K:479:ASN:C	2.59	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: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:Q:6:LEU:O	2:Q:7:HIS:C	2.60	0.41
1:E:270:ILE:HG12	2:S:27:LEU:HD13	2.03	0.41
1:B:402:ALA:O	1:B:405:ALA:HB3	2.21	0.40
1:E:150:ILE:CG2	1:E:151:SER:N	2.84	0.40
1:E:399:ALA:O	1:E:400:LEU:C	2.59	0.40
1:F:524:LEU:HD23	1:F:525:PRO:HD2	2.03	0.40
1:H:364:LYS:HA	1:H:364:LYS:HD3	1.90	0.40
1:I:417:VAL:O	1:I:418:ALA:C	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:451:LEU:O	1:I:452:ARG:C	2.58	0.40
1:J:519:CYS:SG	1:J:520:MET:N	2.94	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:L:492:GLY:C	1:L:493:ILE:HD13	2.41	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
1:N:80:LYS:O	1:N:81:ALA:C	2.58	0.40
2:U:7:HIS:ND1	2:U:7:HIS:O	2.53	0.40
1:B:417:VAL:O	1:B:418:ALA:C	2.59	0.40
1:C:199:TYR:CZ	1:C:205:ILE:HD11	2.57	0.40
1:C:198:GLY:C	1:C:276:VAL:HG12	2.41	0.40
1:D:44:PHE:N	1:D:44:PHE:HD1	1.97	0.40
1:E:112:ASN:HA	1:E:113:PRO:HD3	1.86	0.40
1:H:106:ALA:HA	1:H:111:MET:CE	2.52	0.40
1:H:522:THR:OG1	1:H:523:ASP:N	2.55	0.40
1:H:77:VAL:HG22	1:H:506:TYR:CD1	2.56	0.40
1:I:416:GLY:O	1:I:419:LEU:N	2.51	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: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:M:111:MET:CG	1:M:111:MET:CE	2.97	0.40
1:M:47:PRO:HG2	1:N:73:MET:CG	2.47	0.40
1:N:31:LEU:O	1:N:32:GLY:O	2.40	0.40
1:A:362:ARG:HG2	1:A:366:GLN:NE2	2.37	0.40
1:C:23:LEU:O	1:C:24:ALA:C	2.60	0.40
1:D:314:LEU:O	1:D:317:LEU:HB2	2.21	0.40
1:D:58:ARG:HA	1:D:75:LYS:HE2	2.02	0.40
1:E:124:VAL:HG13	1:E:504:LEU:HD13	2.02	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:G:34:LYS:HD2	1:G:458:CYS:SG	2.61	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:370:ALA:O	1:J:371:LYS:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:365:LEU:O	1:K:369:VAL:HG13	2.20	0.40
1:J:38:VAL:HG22	1:K:519:CYS:HB3	2.02	0.40
1:L:225:LYS:HE3	1:L:232:GLU:OE2	2.22	0.40
1:N:233:MET:C	1:N:235:PRO:HD2	2.42	0.40
1:N:91:THR:O	1:N:92:ALA:C	2.58	0.40
1:A:475:ASN:N	1:A:475:ASN:HD22	2.16	0.40
1:B:20:VAL:H	1:B:20:VAL:HG23	1.62	0.40
1:E:197:ARG:HD2	1:E:277:LYS:HB2	2.03	0.40
1:E:23:LEU:CD1	1:E:23:LEU:C	2.89	0.40
1:E:28:LYS:C	1:E:30:THR:N	2.73	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:428:ASP:O	1:J:429:LEU:C	2.59	0.40
1:J:524:LEU:HD22	1:J:525:PRO:HD2	2.02	0.40
1:K:305:ILE:HD12	1:K:307:MET:HE2	2.02	0.40
1:K:80:LYS:HA	1:K:83:ASP:HB2	2.02	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: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:B:238:GLU:OE2	2:P:23:GLY:C	2.60	0.40
1:B:116:LEU:HA	1:B:116:LEU:HD23	1.54	0.40
1:B:28:LYS:C	1:B:30:THR:H	2.25	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:F:169:VAL:HB	1:F:173:GLY:HA3	2.03	0.40
1:F:198:GLY:C	1:F:276:VAL:HG12	2.42	0.40
1:F:489:ILE:HD13	1:F:494:LEU:HD22	2.03	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:HA	1:I:265:ASN:HD22	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:L:15:LYS:HE2	1:L:18:ARG:HH12	1.86	0.40
1:L:453:GLN:O	1:L:454:ILE:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:270:ILE:CD1	2:P:27:LEU:HB2	2.52	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/524 (100%)	478 (92%)	40 (8%)	4 (1%)	19	57
1	B	522/524 (100%)	477 (91%)	39 (8%)	6 (1%)	14	50
1	C	522/524 (100%)	475 (91%)	41 (8%)	6 (1%)	14	50
1	D	522/524 (100%)	475 (91%)	41 (8%)	6 (1%)	14	50
1	E	522/524 (100%)	477 (91%)	40 (8%)	5 (1%)	15	53
1	F	522/524 (100%)	478 (92%)	38 (7%)	6 (1%)	14	50
1	G	522/524 (100%)	473 (91%)	44 (8%)	5 (1%)	15	53
1	H	522/524 (100%)	473 (91%)	39 (8%)	10 (2%)	8	36
1	I	522/524 (100%)	474 (91%)	35 (7%)	13 (2%)	5	28
1	J	522/524 (100%)	473 (91%)	41 (8%)	8 (2%)	10	42
1	K	522/524 (100%)	471 (90%)	42 (8%)	9 (2%)	9	39
1	L	522/524 (100%)	476 (91%)	36 (7%)	10 (2%)	8	36
1	M	522/524 (100%)	469 (90%)	42 (8%)	11 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	522/524 (100%)	470 (90%)	40 (8%)	12 (2%)	6	30
2	O	95/97 (98%)	75 (79%)	12 (13%)	8 (8%)	1	4
2	P	95/97 (98%)	75 (79%)	12 (13%)	8 (8%)	1	4
2	Q	95/97 (98%)	75 (79%)	12 (13%)	8 (8%)	1	4
2	R	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	4
2	S	95/97 (98%)	75 (79%)	12 (13%)	8 (8%)	1	4
2	T	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	4
2	U	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	4
All	All	7973/8015 (100%)	7159 (90%)	647 (8%)	167 (2%)	7	33

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	345 (85%)	59 (15%)	3	15
1	B	404/404 (100%)	345 (85%)	59 (15%)	3	15
1	C	404/404 (100%)	345 (85%)	59 (15%)	3	15
1	D	404/404 (100%)	346 (86%)	58 (14%)	3	15
1	E	404/404 (100%)	346 (86%)	58 (14%)	3	15
1	F	404/404 (100%)	345 (85%)	59 (15%)	3	15
1	G	404/404 (100%)	344 (85%)	60 (15%)	3	14
1	H	404/404 (100%)	345 (85%)	59 (15%)	3	15
1	I	404/404 (100%)	342 (85%)	62 (15%)	2	13
1	J	404/404 (100%)	344 (85%)	60 (15%)	3	14
1	K	404/404 (100%)	345 (85%)	59 (15%)	3	15
1	L	404/404 (100%)	341 (84%)	63 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	404/404 (100%)	345 (85%)	59 (15%)	3	15
1	N	404/404 (100%)	342 (85%)	62 (15%)	2	13
2	O	80/80 (100%)	65 (81%)	15 (19%)	1	8
2	P	80/80 (100%)	64 (80%)	16 (20%)	1	7
2	Q	80/80 (100%)	64 (80%)	16 (20%)	1	7
2	R	80/80 (100%)	64 (80%)	16 (20%)	1	7
2	S	80/80 (100%)	65 (81%)	15 (19%)	1	8
2	T	80/80 (100%)	63 (79%)	17 (21%)	1	5
2	U	80/80 (100%)	66 (82%)	14 (18%)	2	10
All	All	6216/6216 (100%)	5271 (85%)	945 (15%)	3	14

All (945) 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
1	A	58	ARG
1	A	62	LEU
1	A	74	VAL
1	A	79	SER
1	A	80	LYS
1	A	97	GLN
1	A	129	GLU
1	A	138	CYS
1	A	141	SER
1	A	147	VAL
1	A	150	ILE
1	A	153	ASN
1	A	168	LYS
1	A	174	VAL
1	A	176	THR
1	A	177	VAL
1	A	183	LEU
1	A	184	GLN

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Mol	Chain	Res	Type
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	358	SER
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	430	ARG
1	A	432	GLN
1	A	463	SER
1	A	470	LYS
1	A	483	GLU
1	A	504	LEU
1	B	11	ASP
1	B	18	ARG
1	B	23	LEU
1	B	43	SER
1	B	44	PHE
1	B	48	THR
1	B	58	ARG
1	B	62	LEU

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Mol	Chain	Res	Type
1	B	74	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
1	B	150	ILE
1	B	153	ASN
1	B	168	LYS
1	B	174	VAL
1	B	176	THR
1	B	183	LEU
1	B	184	GLN
1	B	193	MET
1	B	209	GLU
1	B	215	LEU
1	B	230	ILE
1	B	231	ARG
1	B	272	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	358	SER
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

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Mol	Chain	Res	Type
1	B	430	ARG
1	B	452	ARG
1	B	461	GLU
1	B	463	SER
1	B	470	LYS
1	B	483	GLU
1	B	484	GLU
1	B	504	LEU
1	B	510	VAL
1	C	10	ASN
1	C	11	ASP
1	C	18	ARG
1	C	23	LEU
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	80	LYS
1	C	97	GLN
1	C	102	GLU
1	C	129	GLU
1	C	138	CYS
1	C	141	SER
1	C	147	VAL
1	C	150	ILE
1	C	153	ASN
1	C	168	LYS
1	C	174	VAL
1	C	176	THR
1	C	183	LEU
1	C	184	GLN
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

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Mol	Chain	Res	Type
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	358	SER
1	C	387	VAL
1	C	388	GLU
1	C	391	GLU
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	430	ARG
1	C	452	ARG
1	C	461	GLU
1	C	483	GLU
1	C	504	LEU
1	C	510	VAL
1	D	11	ASP
1	D	18	ARG
1	D	23	LEU
1	D	43	SER
1	D	44	PHE
1	D	48	THR
1	D	58	ARG
1	D	62	LEU
1	D	63	GLU
1	D	74	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

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Mol	Chain	Res	Type
1	D	150	ILE
1	D	153	ASN
1	D	157	THR
1	D	168	LYS
1	D	174	VAL
1	D	176	THR
1	D	183	LEU
1	D	184	GLN
1	D	193	MET
1	D	209	GLU
1	D	215	LEU
1	D	230	ILE
1	D	231	ARG
1	D	272	LYS
1	D	276	VAL
1	D	284	ARG
1	D	288	MET
1	D	289	LEU
1	D	317	LEU
1	D	322	ARG
1	D	323	VAL
1	D	325	ILE
1	D	328	ASP
1	D	331	THR
1	D	350	ARG
1	D	358	SER
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	430	ARG
1	D	432	GLN
1	D	442	VAL
1	D	452	ARG
1	D	461	GLU
1	D	483	GLU
1	D	504	LEU

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Mol	Chain	Res	Type
1	E	11	ASP
1	E	18	ARG
1	E	23	LEU
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	74	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	153	ASN
1	E	157	THR
1	E	168	LYS
1	E	174	VAL
1	E	176	THR
1	E	183	LEU
1	E	184	GLN
1	E	193	MET
1	E	209	GLU
1	E	215	LEU
1	E	230	ILE
1	E	231	ARG
1	E	272	LYS
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	358	SER

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Mol	Chain	Res	Type
1	E	387	VAL
1	E	388	GLU
1	E	391	GLU
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	430	ARG
1	E	442	VAL
1	E	461	GLU
1	E	463	SER
1	E	470	LYS
1	E	483	GLU
1	E	504	LEU
1	F	11	ASP
1	F	18	ARG
1	F	23	LEU
1	F	43	SER
1	F	44	PHE
1	F	48	THR
1	F	58	ARG
1	F	62	LEU
1	F	74	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
1	F	153	ASN
1	F	157	THR
1	F	168	LYS
1	F	174	VAL
1	F	176	THR
1	F	181	THR
1	F	183	LEU
1	F	184	GLN
1	F	193	MET
1	F	209	GLU

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Mol	Chain	Res	Type
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	358	SER
1	F	387	VAL
1	F	388	GLU
1	F	391	GLU
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	430	ARG
1	F	452	ARG
1	F	461	GLU
1	F	463	SER
1	F	483	GLU
1	F	504	LEU
1	F	510	VAL
1	G	11	ASP
1	G	18	ARG
1	G	23	LEU
1	G	43	SER
1	G	44	PHE
1	G	48	THR
1	G	58	ARG
1	G	62	LEU
1	G	63	GLU

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Mol	Chain	Res	Type
1	G	74	VAL
1	G	80	LYS
1	G	97	GLN
1	G	129	GLU
1	G	138	CYS
1	G	141	SER
1	G	147	VAL
1	G	150	ILE
1	G	153	ASN
1	G	157	THR
1	G	168	LYS
1	G	174	VAL
1	G	183	LEU
1	G	184	GLN
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	358	SER
1	G	387	VAL
1	G	388	GLU
1	G	391	GLU
1	G	398	ASP
1	G	400	LEU
1	G	404	ARG
1	G	417	VAL
1	G	419	LEU
1	G	420	ILE

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Mol	Chain	Res	Type
1	G	430	ARG
1	G	432	GLN
1	G	452	ARG
1	G	461	GLU
1	G	463	SER
1	G	483	GLU
1	G	484	GLU
1	G	504	LEU
1	G	510	VAL
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	59	GLU
1	H	77	VAL
1	H	79	SER
1	H	89	THR
1	H	107	VAL
1	H	129	GLU
1	H	131	LEU
1	H	138	CYS
1	H	141	SER
1	H	172	GLU
1	H	187	LEU
1	H	217	SER
1	H	225	LYS
1	H	230	ILE
1	H	265	ASN
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	322	ARG
1	H	325	ILE
1	H	328	ASP

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Mol	Chain	Res	Type
1	H	331	THR
1	H	339	GLU
1	H	343	GLN
1	H	350	ARG
1	H	352	GLN
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	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	460	GLU
1	H	461	GLU
1	H	468	THR
1	H	483	GLU
1	H	494	LEU
1	H	504	LEU
1	H	513	LEU
1	I	10	ASN
1	I	20	VAL
1	I	23	LEU
1	I	40	LEU
1	I	42	LYS
1	I	44	PHE
1	I	59	GLU
1	I	77	VAL
1	I	79	SER
1	I	89	THR
1	I	104	LEU
1	I	129	GLU
1	I	131	LEU
1	I	138	CYS
1	I	141	SER
1	I	172	GLU

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Mol	Chain	Res	Type
1	I	187	LEU
1	I	201	SER
1	I	217	SER
1	I	225	LYS
1	I	230	ILE
1	I	265	ASN
1	I	271	VAL
1	I	284	ARG
1	I	289	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	363	GLU
1	I	378	VAL
1	I	385	THR
1	I	389	MET
1	I	400	LEU
1	I	401	HIS
1	I	404	ARG
1	I	419	LEU
1	I	420	ILE
1	I	421	ARG
1	I	424	SER
1	I	426	LEU
1	I	432	GLN
1	I	433	ASN
1	I	445	ARG
1	I	452	ARG
1	I	460	GLU
1	I	461	GLU
1	I	468	THR
1	I	483	GLU

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Mol	Chain	Res	Type
1	I	494	LEU
1	I	504	LEU
1	I	509	SER
1	I	513	LEU
1	J	10	ASN
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	59	GLU
1	J	77	VAL
1	J	79	SER
1	J	89	THR
1	J	107	VAL
1	J	114	MET
1	J	138	CYS
1	J	141	SER
1	J	172	GLU
1	J	187	LEU
1	J	201	SER
1	J	217	SER
1	J	225	LYS
1	J	230	ILE
1	J	265	ASN
1	J	271	VAL
1	J	284	ARG
1	J	289	LEU
1	J	302	SER
1	J	307	MET
1	J	311	LYS
1	J	317	LEU
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	355	GLU
1	J	363	GLU

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Mol	Chain	Res	Type
1	J	378	VAL
1	J	385	THR
1	J	389	MET
1	J	400	LEU
1	J	404	ARG
1	J	419	LEU
1	J	420	ILE
1	J	421	ARG
1	J	426	LEU
1	J	432	GLN
1	J	433	ASN
1	J	445	ARG
1	J	452	ARG
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	504	LEU
1	J	509	SER
1	J	513	LEU
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	59	GLU
1	K	77	VAL
1	K	79	SER
1	K	89	THR
1	K	104	LEU
1	K	107	VAL
1	K	118	ARG
1	K	129	GLU
1	K	131	LEU
1	K	138	CYS
1	K	141	SER
1	K	172	GLU
1	K	187	LEU

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Mol	Chain	Res	Type
1	K	217	SER
1	K	225	LYS
1	K	230	ILE
1	K	265	ASN
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	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	363	GLU
1	K	378	VAL
1	K	385	THR
1	K	400	LEU
1	K	420	ILE
1	K	421	ARG
1	K	426	LEU
1	K	432	GLN
1	K	433	ASN
1	K	452	ARG
1	K	460	GLU
1	K	461	GLU
1	K	468	THR
1	K	483	GLU
1	K	494	LEU
1	K	499	VAL
1	K	504	LEU
1	K	509	SER
1	K	513	LEU
1	L	20	VAL
1	L	23	LEU
1	L	27	VAL

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Mol	Chain	Res	Type
1	L	40	LEU
1	L	42	LYS
1	L	43	SER
1	L	44	PHE
1	L	59	GLU
1	L	77	VAL
1	L	79	SER
1	L	89	THR
1	L	107	VAL
1	L	114	MET
1	L	138	CYS
1	L	141	SER
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	265	ASN
1	L	271	VAL
1	L	284	ARG
1	L	289	LEU
1	L	295	LEU
1	L	302	SER
1	L	307	MET
1	L	311	LYS
1	L	317	LEU
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	400	LEU
1	L	401	HIS

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Mol	Chain	Res	Type
1	L	404	ARG
1	L	419	LEU
1	L	420	ILE
1	L	421	ARG
1	L	426	LEU
1	L	432	GLN
1	L	433	ASN
1	L	445	ARG
1	L	452	ARG
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	10	ASN
1	M	20	VAL
1	M	23	LEU
1	M	40	LEU
1	M	42	LYS
1	M	43	SER
1	M	44	PHE
1	M	59	GLU
1	M	77	VAL
1	M	89	THR
1	M	104	LEU
1	M	107	VAL
1	M	138	CYS
1	M	141	SER
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	265	ASN
1	M	271	VAL
1	M	284	ARG
1	M	289	LEU

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Mol	Chain	Res	Type
1	M	302	SER
1	M	307	MET
1	M	311	LYS
1	M	317	LEU
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
1	M	352	GLN
1	M	363	GLU
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	426	LEU
1	M	432	GLN
1	M	433	ASN
1	M	445	ARG
1	M	452	ARG
1	M	460	GLU
1	M	461	GLU
1	M	468	THR
1	M	483	GLU
1	M	494	LEU
1	M	499	VAL
1	M	504	LEU
1	M	509	SER
1	M	513	LEU
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

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Mol	Chain	Res	Type
1	N	59	GLU
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	118	ARG
1	N	131	LEU
1	N	138	CYS
1	N	141	SER
1	N	172	GLU
1	N	187	LEU
1	N	201	SER
1	N	217	SER
1	N	225	LYS
1	N	230	ILE
1	N	265	ASN
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	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	363	GLU
1	N	378	VAL
1	N	385	THR
1	N	389	MET
1	N	400	LEU
1	N	419	LEU
1	N	420	ILE
1	N	421	ARG

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Mol	Chain	Res	Type
1	N	426	LEU
1	N	432	GLN
1	N	433	ASN
1	N	445	ARG
1	N	452	ARG
1	N	460	GLU
1	N	468	THR
1	N	483	GLU
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	37	ARG
2	O	55	LYS
2	O	60	LYS
2	O	75	SER
2	O	77	LYS
2	O	80	ASN
2	O	84	LEU
2	P	1	MET
2	P	3	ILE
2	P	6	LEU
2	P	8	ASP
2	P	14	ARG
2	P	28	THR
2	P	30	SER
2	P	36	THR
2	P	37	ARG
2	P	55	LYS
2	P	58	ASP
2	P	60	LYS
2	P	75	SER
2	P	77	LYS

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Mol	Chain	Res	Type
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	37	ARG
2	Q	55	LYS
2	Q	58	ASP
2	Q	60	LYS
2	Q	75	SER
2	Q	77	LYS
2	Q	84	LEU
2	Q	86	MET
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	37	ARG
2	R	55	LYS
2	R	60	LYS
2	R	75	SER
2	R	77	LYS
2	R	78	ILE
2	R	84	LEU
2	R	86	MET
2	S	1	MET
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

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Mol	Chain	Res	Type
2	S	37	ARG
2	S	55	LYS
2	S	60	LYS
2	S	75	SER
2	S	77	LYS
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	37	ARG
2	T	55	LYS
2	T	58	ASP
2	T	60	LYS
2	T	75	SER
2	T	77	LYS
2	T	80	ASN
2	T	84	LEU
2	T	86	MET
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	37	ARG
2	U	55	LYS
2	U	60	LYS
2	U	75	SER
2	U	77	LYS
2	U	84	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) 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	265	ASN
1	A	326	ASN
1	A	348	GLN
1	A	351	GLN
1	A	432	GLN
1	A	453	GLN
1	A	457	ASN
1	A	475	ASN
1	B	21	ASN
1	B	82	ASN
1	B	97	GLN
1	B	146	GLN
1	B	153	ASN
1	B	326	ASN
1	B	348	GLN
1	B	351	GLN
1	B	432	GLN
1	B	453	GLN
1	B	457	ASN
1	B	475	ASN
1	C	21	ASN
1	C	82	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
1	C	351	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

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Mol	Chain	Res	Type
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	432	GLN
1	D	453	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	432	GLN
1	E	453	GLN
1	E	457	ASN
1	E	475	ASN
1	F	21	ASN
1	F	82	ASN
1	F	97	GLN
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	432	GLN
1	F	453	GLN
1	F	457	ASN
1	F	475	ASN
1	G	21	ASN
1	G	37	ASN
1	G	97	GLN
1	G	146	GLN
1	G	153	ASN
1	G	265	ASN
1	G	319	GLN
1	G	326	ASN
1	G	348	GLN
1	G	351	GLN
1	G	432	GLN

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Mol	Chain	Res	Type
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	265	ASN
1	H	348	GLN
1	H	351	GLN
1	H	366	GLN
1	H	433	ASN
1	H	436	GLN
1	I	21	ASN
1	I	72	GLN
1	I	97	GLN
1	I	146	GLN
1	I	265	ASN
1	I	348	GLN
1	I	351	GLN
1	I	366	GLN
1	I	433	ASN
1	I	436	GLN
1	J	21	ASN
1	J	72	GLN
1	J	97	GLN
1	J	146	GLN
1	J	265	ASN
1	J	348	GLN
1	J	351	GLN
1	J	433	ASN
1	J	436	GLN
1	K	21	ASN
1	K	72	GLN
1	K	97	GLN
1	K	146	GLN
1	K	265	ASN
1	K	290	GLN
1	K	348	GLN
1	K	351	GLN
1	K	366	GLN
1	K	433	ASN

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Mol	Chain	Res	Type
1	K	436	GLN
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	348	GLN
1	L	351	GLN
1	L	366	GLN
1	L	433	ASN
1	L	436	GLN
1	M	21	ASN
1	M	37	ASN
1	M	72	GLN
1	M	97	GLN
1	M	146	GLN
1	M	265	ASN
1	M	326	ASN
1	M	348	GLN
1	M	351	GLN
1	M	366	GLN
1	M	433	ASN
1	M	436	GLN
1	N	21	ASN
1	N	72	GLN
1	N	97	GLN
1	N	146	GLN
1	N	265	ASN
1	N	348	GLN
1	N	351	GLN
1	N	433	ASN
1	N	436	GLN
2	O	68	ASN
2	O	80	ASN
2	P	68	ASN
2	P	80	ASN
2	Q	68	ASN
2	Q	80	ASN
2	R	68	ASN
2	R	80	ASN
2	S	68	ASN

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Mol	Chain	Res	Type
2	S	80	ASN
2	T	68	ASN
2	T	80	ASN
2	U	68	ASN
2	U	80	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	B	600	3	24,29,29	1.70	6 (25%)	29,45,45	2.70	11 (37%)
4	ADP	C	600	3	24,29,29	1.40	5 (20%)	29,45,45	2.95	14 (48%)
4	ADP	F	600	3	24,29,29	1.12	2 (8%)	29,45,45	2.29	11 (37%)
4	ADP	A	600	3	24,29,29	1.56	6 (25%)	29,45,45	2.91	12 (41%)
4	ADP	D	600	3	24,29,29	1.78	5 (20%)	29,45,45	2.82	12 (41%)
4	ADP	G	600	3	24,29,29	1.47	3 (12%)	29,45,45	2.82	14 (48%)
4	ADP	E	600	3	24,29,29	1.38	5 (20%)	29,45,45	2.43	11 (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	B	600	3	-	6/12/32/32	0/3/3/3
4	ADP	C	600	3	-	7/12/32/32	0/3/3/3
4	ADP	F	600	3	-	7/12/32/32	0/3/3/3
4	ADP	A	600	3	-	7/12/32/32	0/3/3/3
4	ADP	D	600	3	-	7/12/32/32	0/3/3/3
4	ADP	G	600	3	-	7/12/32/32	0/3/3/3
4	ADP	E	600	3	-	7/12/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	600	ADP	C2-N3	4.86	1.39	1.32
4	B	600	ADP	C2'-C1'	-4.04	1.47	1.53
4	D	600	ADP	C2'-C1'	-3.89	1.47	1.53
4	D	600	ADP	O4'-C1'	-3.80	1.35	1.41
4	B	600	ADP	C2-N3	3.74	1.38	1.32
4	D	600	ADP	C2-N3	3.50	1.37	1.32
4	E	600	ADP	C2-N3	3.28	1.37	1.32
4	A	600	ADP	O4'-C4'	-3.26	1.37	1.45
4	D	600	ADP	O4'-C4'	-3.22	1.37	1.45
4	A	600	ADP	C2-N3	3.20	1.37	1.32
4	C	600	ADP	C2-N3	3.17	1.37	1.32
4	G	600	ADP	O4'-C4'	-3.12	1.38	1.45
4	C	600	ADP	O4'-C4'	-3.08	1.38	1.45
4	D	600	ADP	C2-N1	3.01	1.39	1.33
4	B	600	ADP	C2-N1	2.95	1.39	1.33
4	A	600	ADP	C2'-C1'	-2.85	1.49	1.53
4	F	600	ADP	C2-N3	2.76	1.36	1.32
4	C	600	ADP	C2'-C1'	-2.70	1.49	1.53
4	E	600	ADP	O4'-C1'	-2.68	1.37	1.41
4	E	600	ADP	C2'-C1'	-2.57	1.49	1.53
4	E	600	ADP	C2-N1	2.40	1.38	1.33
4	B	600	ADP	O4'-C1'	-2.39	1.37	1.41
4	G	600	ADP	C4-N3	-2.37	1.32	1.35
4	B	600	ADP	O4'-C4'	-2.37	1.39	1.45
4	F	600	ADP	C2-N1	2.30	1.38	1.33
4	E	600	ADP	O4'-C4'	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	600	ADP	C2-N1	2.22	1.38	1.33
4	A	600	ADP	PA-O1A	-2.17	1.43	1.50
4	A	600	ADP	O3'-C3'	-2.14	1.37	1.43
4	B	600	ADP	C4-N3	2.14	1.38	1.35
4	A	600	ADP	O4'-C1'	-2.12	1.38	1.41
4	C	600	ADP	O4'-C1'	-2.09	1.38	1.41

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	600	ADP	N3-C2-N1	-7.05	117.66	128.68
4	D	600	ADP	O4'-C1'-C2'	-7.04	96.64	106.93
4	G	600	ADP	O4'-C1'-C2'	-6.57	97.32	106.93
4	G	600	ADP	C4-C5-N7	-6.18	102.96	109.40
4	A	600	ADP	N3-C2-N1	-5.99	119.32	128.68
4	A	600	ADP	C5-C6-N6	5.87	129.27	120.35
4	C	600	ADP	C5-C6-N6	5.46	128.65	120.35
4	F	600	ADP	N3-C2-N1	-5.45	120.16	128.68
4	C	600	ADP	C4-C5-N7	-5.42	103.75	109.40
4	B	600	ADP	C4-C5-N7	-5.35	103.83	109.40
4	C	600	ADP	PA-O3A-PB	-5.34	114.50	132.83
4	C	600	ADP	N3-C2-N1	-5.32	120.36	128.68
4	B	600	ADP	O4'-C1'-C2'	-5.24	99.26	106.93
4	B	600	ADP	N3-C2-N1	-5.24	120.49	128.68
4	E	600	ADP	PA-O3A-PB	-5.15	115.16	132.83
4	F	600	ADP	PA-O3A-PB	-5.12	115.25	132.83
4	E	600	ADP	N3-C2-N1	-5.05	120.78	128.68
4	D	600	ADP	PA-O3A-PB	-4.99	115.72	132.83
4	G	600	ADP	PA-O3A-PB	-4.93	115.90	132.83
4	E	600	ADP	C4-C5-N7	-4.89	104.30	109.40
4	B	600	ADP	PA-O3A-PB	-4.89	116.05	132.83
4	G	600	ADP	C5-C6-N6	4.88	127.77	120.35
4	A	600	ADP	PA-O3A-PB	-4.87	116.11	132.83
4	C	600	ADP	O4'-C1'-C2'	-4.84	99.86	106.93
4	A	600	ADP	O4'-C1'-C2'	-4.59	100.22	106.93
4	C	600	ADP	O3B-PB-O3A	4.46	119.60	104.64
4	A	600	ADP	C4-C5-N7	-4.35	104.86	109.40
4	F	600	ADP	C4-C5-N7	-4.20	105.02	109.40
4	A	600	ADP	O2B-PB-O1B	4.20	127.12	110.68
4	D	600	ADP	O2B-PB-O3A	-4.15	90.71	104.64
4	B	600	ADP	C1'-N9-C4	-4.08	119.48	126.64
4	A	600	ADP	C1'-N9-C4	-3.98	119.64	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	600	ADP	O2B-PB-O1B	3.95	126.16	110.68
4	C	600	ADP	O2B-PB-O1B	3.95	126.14	110.68
4	E	600	ADP	C1'-N9-C4	-3.85	119.88	126.64
4	G	600	ADP	O5'-C5'-C4'	3.79	122.05	108.99
4	B	600	ADP	C5-C6-N6	3.73	126.02	120.35
4	A	600	ADP	N6-C6-N1	-3.70	110.89	118.57
4	C	600	ADP	O2B-PB-O3A	-3.69	92.25	104.64
4	A	600	ADP	O3B-PB-O1B	-3.62	96.50	110.68
4	F	600	ADP	O4'-C1'-C2'	-3.61	101.65	106.93
4	B	600	ADP	O3'-C3'-C4'	-3.58	100.70	111.05
4	B	600	ADP	O2B-PB-O3A	-3.51	92.87	104.64
4	G	600	ADP	N3-C2-N1	-3.48	123.23	128.68
4	C	600	ADP	C1'-N9-C4	-3.41	120.64	126.64
4	C	600	ADP	O5'-C5'-C4'	3.37	120.60	108.99
4	E	600	ADP	O3'-C3'-C4'	-3.30	101.51	111.05
4	A	600	ADP	O2B-PB-O3A	-3.30	93.58	104.64
4	D	600	ADP	O5'-C5'-C4'	3.22	120.07	108.99
4	F	600	ADP	C5-C6-N6	3.18	125.18	120.35
4	E	600	ADP	O2B-PB-O3A	-3.17	94.01	104.64
4	D	600	ADP	C1'-N9-C4	-3.15	121.10	126.64
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	E	600	ADP	O4'-C1'-C2'	-3.08	102.43	106.93
4	E	600	ADP	O5'-C5'-C4'	3.05	119.49	108.99
4	A	600	ADP	O3B-PB-O3A	3.03	114.79	104.64
4	D	600	ADP	C4-C5-N7	-3.02	106.25	109.40
4	A	600	ADP	O5'-C5'-C4'	3.01	119.36	108.99
4	G	600	ADP	N6-C6-N1	-2.99	112.37	118.57
4	D	600	ADP	O3B-PB-O1B	-2.87	99.43	110.68
4	E	600	ADP	O2B-PB-O1B	2.83	121.77	110.68
4	G	600	ADP	O2B-PB-O1B	2.79	121.61	110.68
4	C	600	ADP	N6-C6-N1	-2.77	112.81	118.57
4	B	600	ADP	O2B-PB-O1B	2.77	121.52	110.68
4	G	600	ADP	C3'-C2'-C1'	-2.69	96.92	100.98
4	F	600	ADP	O2B-PB-O1B	2.69	121.22	110.68
4	C	600	ADP	O3B-PB-O1B	-2.65	100.30	110.68
4	G	600	ADP	O2B-PB-O3A	-2.64	95.78	104.64
4	D	600	ADP	O3B-PB-O3A	2.51	113.06	104.64
4	E	600	ADP	C5-C6-N6	2.47	124.11	120.35
4	G	600	ADP	O5'-PA-O1A	-2.45	99.49	109.07
4	F	600	ADP	O3'-C3'-C4'	-2.42	104.04	111.05
4	F	600	ADP	C1'-N9-C4	-2.41	122.41	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	600	ADP	O2A-PA-O5'	2.39	118.86	107.75
4	B	600	ADP	O5'-C5'-C4'	2.39	117.21	108.99
4	G	600	ADP	O2A-PA-O1A	2.34	123.80	112.24
4	F	600	ADP	O2B-PB-O3A	-2.25	97.08	104.64
4	F	600	ADP	O5'-C5'-C4'	2.23	116.68	108.99
4	E	600	ADP	O3B-PB-O3A	2.20	112.02	104.64
4	G	600	ADP	O2A-PA-O5'	2.20	117.96	107.75
4	D	600	ADP	O2A-PA-O1A	2.19	123.05	112.24
4	C	600	ADP	O3'-C3'-C4'	-2.18	104.75	111.05
4	G	600	ADP	O4'-C4'-C3'	-2.17	100.82	105.11
4	D	600	ADP	O4'-C4'-C3'	-2.12	100.93	105.11

There are no chirality outliers.

All (48) torsion outliers are listed below:

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

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

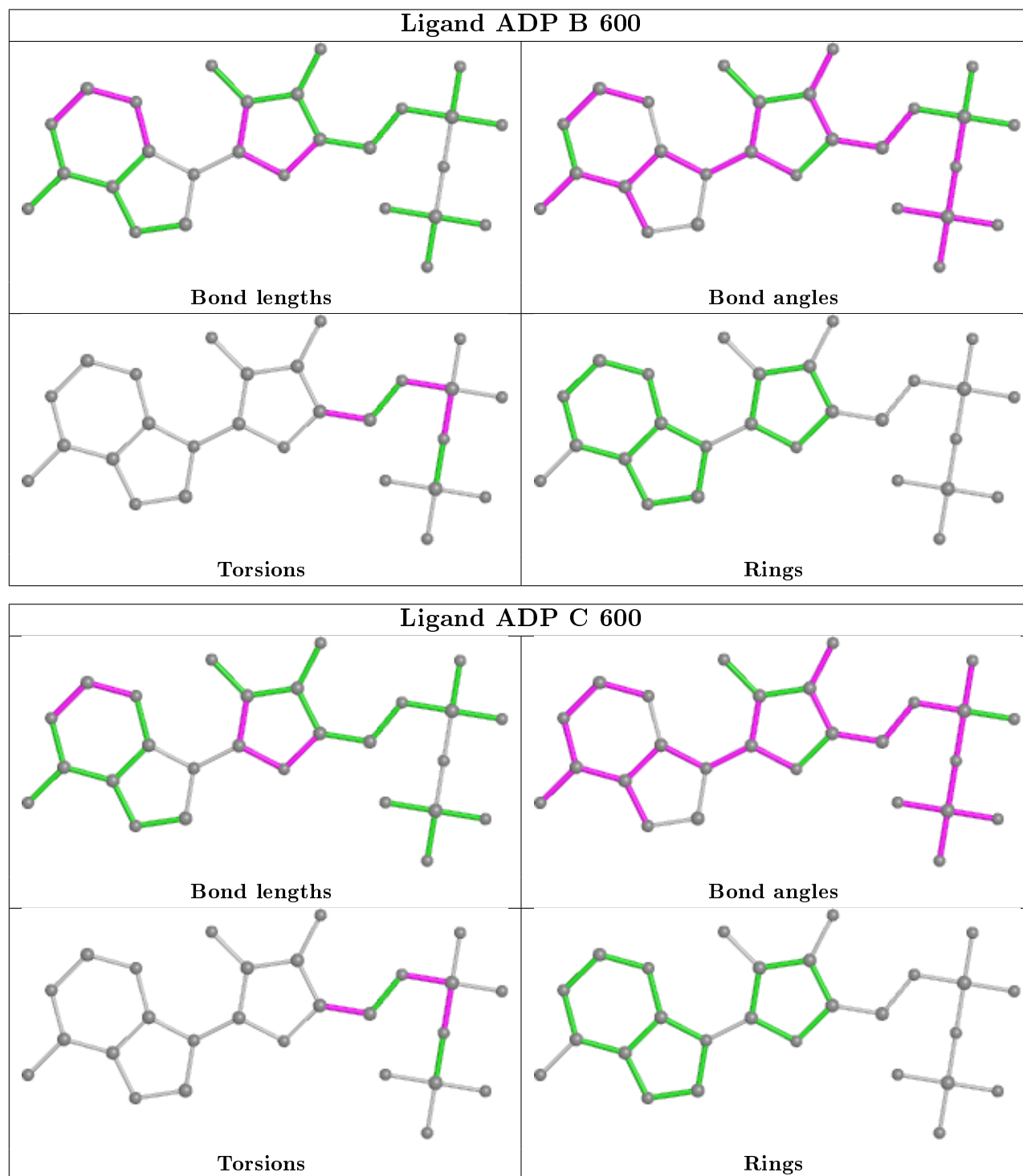
There are no ring outliers.

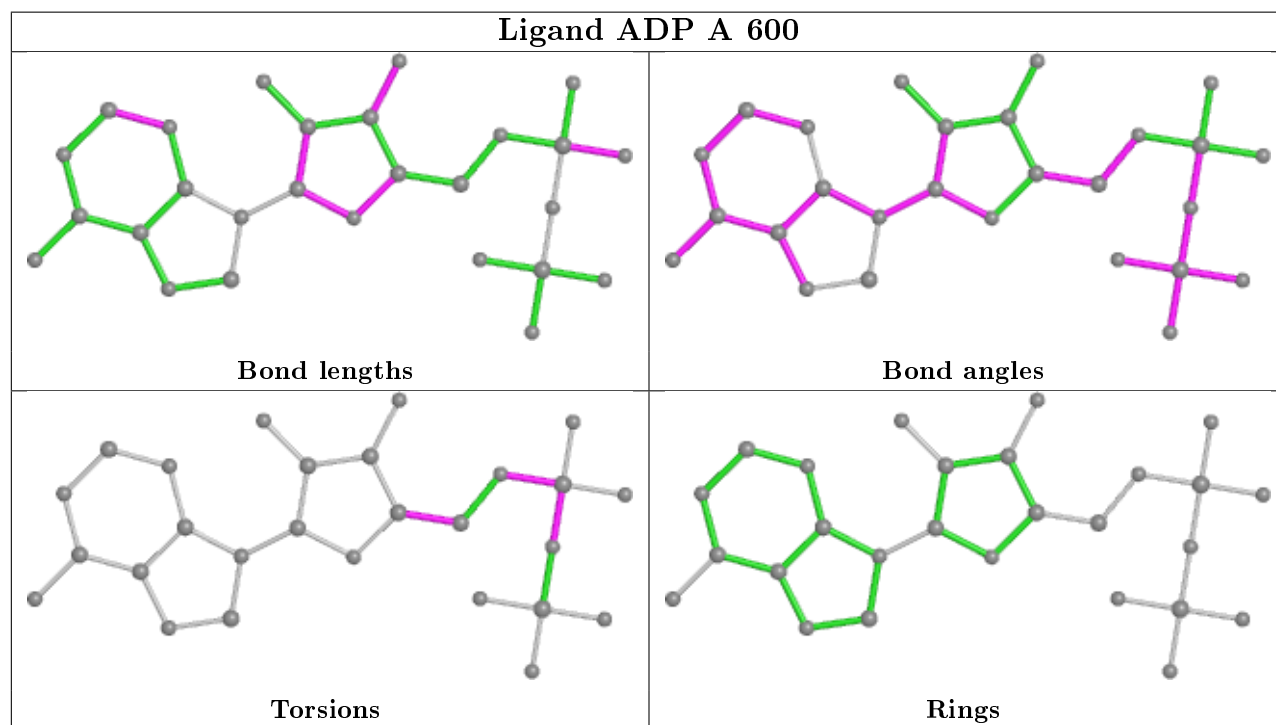
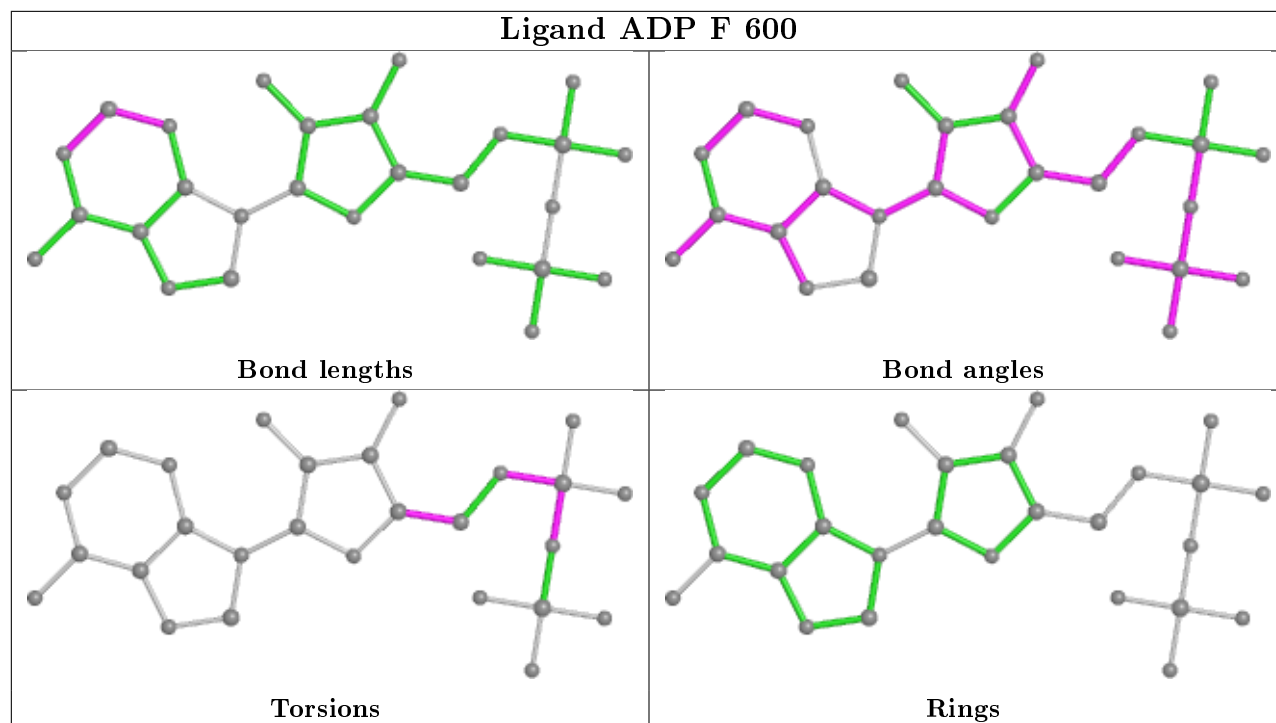
6 monomers are involved in 7 short contacts:

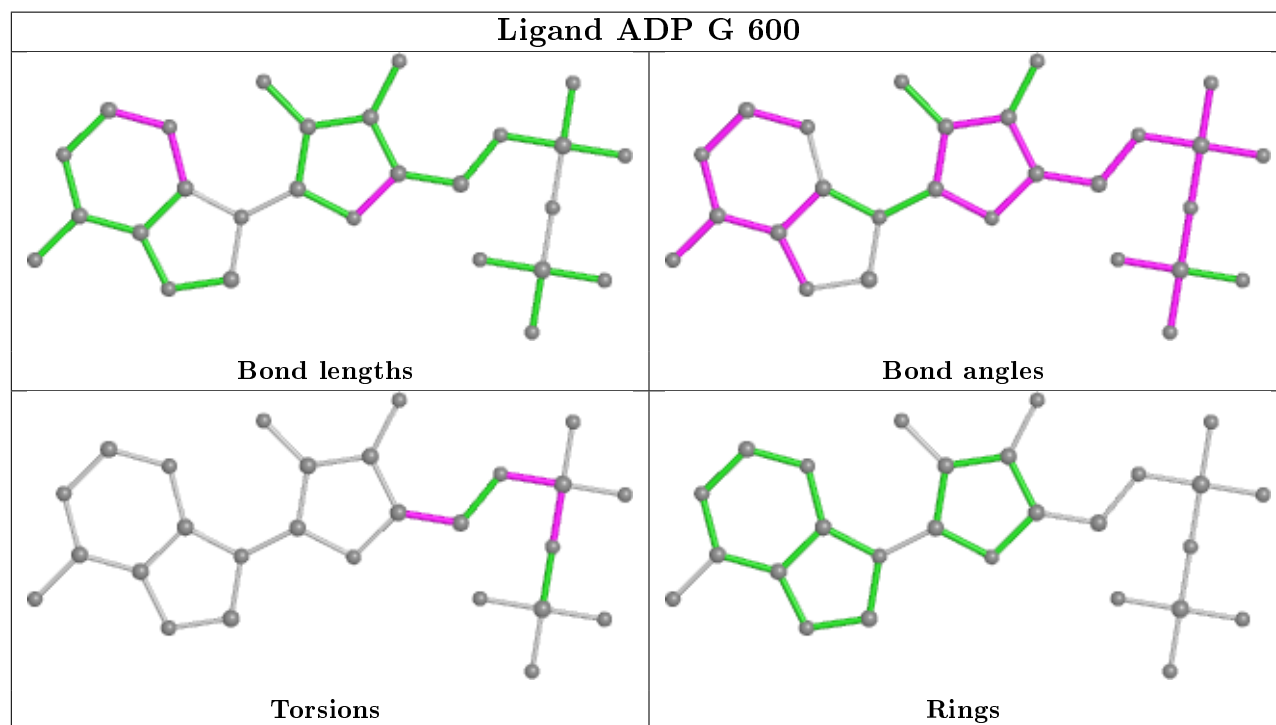
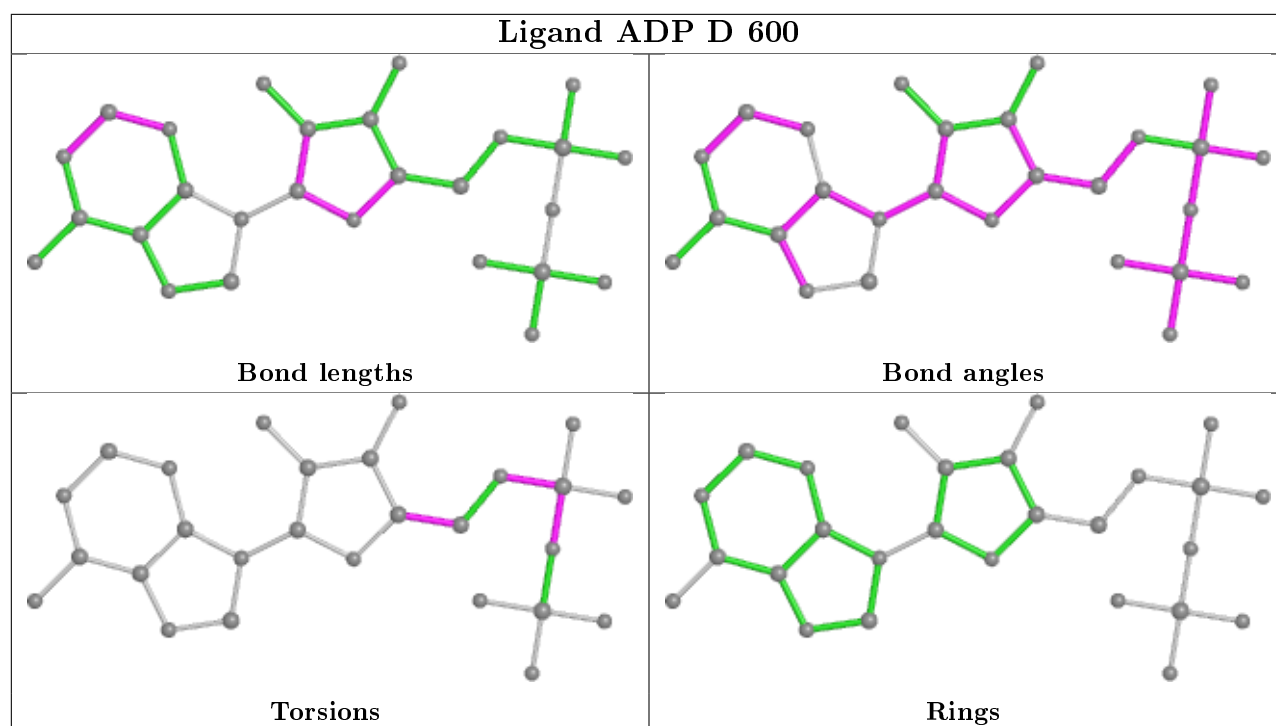
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	ADP	2	0
4	C	600	ADP	1	0
4	A	600	ADP	1	0
4	D	600	ADP	1	0
4	G	600	ADP	1	0
4	E	600	ADP	1	0

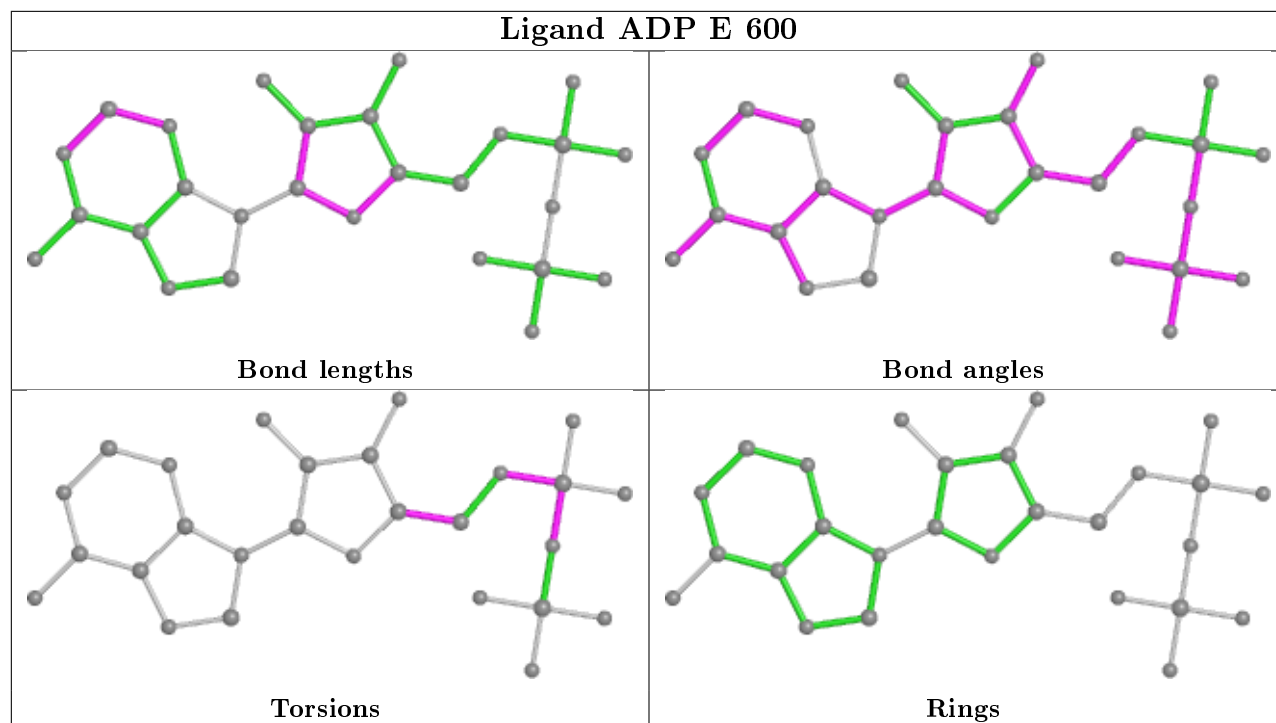
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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%)	-0.04	16 (3%)	49	21	2, 2, 3, 5	0
1	B	524/524 (100%)	0.09	22 (4%)	36	14	2, 2, 3, 5	0
1	C	524/524 (100%)	-0.07	19 (3%)	42	17	2, 2, 3, 5	0
1	D	524/524 (100%)	-0.11	15 (2%)	51	23	2, 2, 3, 5	0
1	E	524/524 (100%)	0.14	24 (4%)	32	12	2, 2, 3, 5	0
1	F	524/524 (100%)	0.15	23 (4%)	34	13	2, 2, 3, 5	0
1	G	524/524 (100%)	0.09	31 (5%)	22	7	2, 2, 3, 5	0
1	H	524/524 (100%)	-0.19	4 (0%)	86	65	2, 2, 3, 5	0
1	I	524/524 (100%)	-0.26	2 (0%)	92	79	2, 2, 3, 5	0
1	J	524/524 (100%)	-0.19	2 (0%)	92	79	2, 2, 3, 5	0
1	K	524/524 (100%)	-0.01	10 (1%)	66	37	2, 2, 3, 5	0
1	L	524/524 (100%)	0.00	10 (1%)	66	37	2, 2, 3, 5	0
1	M	524/524 (100%)	-0.11	8 (1%)	73	46	2, 2, 3, 5	0
1	N	524/524 (100%)	-0.08	7 (1%)	77	51	2, 2, 3, 5	0
2	O	97/97 (100%)	0.86	16 (16%)	1	0	2, 2, 2, 3	0
2	P	97/97 (100%)	0.75	14 (14%)	2	1	2, 2, 2, 3	0
2	Q	97/97 (100%)	0.57	9 (9%)	8	3	2, 2, 2, 3	0
2	R	97/97 (100%)	0.72	13 (13%)	3	1	2, 2, 2, 3	0
2	S	97/97 (100%)	0.73	15 (15%)	2	1	2, 2, 2, 3	0
2	T	97/97 (100%)	0.73	17 (17%)	1	0	2, 2, 2, 3	0
2	U	97/97 (100%)	0.71	12 (12%)	4	1	2, 2, 2, 3	0
All	All	8015/8015 (100%)	0.02	289 (3%)	42	17	2, 2, 3, 5	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	208	PRO	10.5
1	C	361	ASP	10.2
1	A	361	ASP	9.9
1	E	361	ASP	7.8
1	B	361	ASP	6.9
1	F	361	ASP	6.6
1	D	357	THR	6.6
1	A	357	THR	6.2
2	U	30	SER	6.1
2	R	30	SER	6.1
1	G	199	TYR	5.7
1	D	212	ALA	5.7
2	U	32	ALA	5.6
1	D	361	ASP	5.6
1	C	357	THR	5.6
1	E	353	ILE	5.6
1	G	361	ASP	5.5
1	K	360	TYR	5.4
2	R	80	ASN	4.9
2	O	80	ASN	4.9
2	P	32	ALA	4.9
1	E	280	GLY	4.8
1	C	212	ALA	4.8
1	B	355	GLU	4.8
1	F	349	ILE	4.7
1	G	209	GLU	4.6
1	A	349	ILE	4.6
2	S	32	ALA	4.6
1	F	355	GLU	4.6
1	F	357	THR	4.5
1	L	354	GLU	4.5
2	O	22	ALA	4.4
2	R	18	GLU	4.4
2	U	31	ALA	4.4
2	O	25	ILE	4.3
1	B	353	ILE	4.3
1	B	224	ASP	4.3
1	G	354	GLU	4.3
1	A	353	ILE	4.2
1	C	208	PRO	4.2
1	G	212	ALA	4.1
1	B	357	THR	4.1
1	L	357	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	T	97	ALA	4.0
1	B	365	LEU	4.0
1	F	210	THR	3.9
2	U	17	VAL	3.9
2	R	22	ALA	3.9
1	C	360	TYR	3.8
1	L	264	VAL	3.8
1	G	353	ILE	3.8
2	R	51	ASN	3.8
1	H	360	TYR	3.8
1	B	354	GLU	3.7
1	M	360	TYR	3.7
2	S	36	THR	3.7
2	S	30	SER	3.7
2	T	25	ILE	3.7
1	C	279	PRO	3.7
1	N	183	LEU	3.7
2	T	52	GLY	3.7
1	A	208	PRO	3.6
1	G	279	PRO	3.6
1	F	353	ILE	3.6
2	U	33	ALA	3.6
1	B	360	TYR	3.6
1	D	365	LEU	3.5
1	I	264	VAL	3.5
1	K	186	GLU	3.5
1	G	268	ARG	3.5
1	E	281	PHE	3.5
1	C	353	ILE	3.5
2	U	18	GLU	3.5
1	K	188	ASP	3.5
1	C	199	TYR	3.5
1	G	205	ILE	3.5
1	G	251	ALA	3.4
1	A	358	SER	3.4
2	P	25	ILE	3.4
2	T	17	VAL	3.4
1	F	365	LEU	3.4
1	F	214	GLU	3.4
2	O	82	GLU	3.4
1	G	210	THR	3.4
1	M	358	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	365	LEU	3.3
2	U	23	GLY	3.3
2	Q	18	GLU	3.3
1	B	349	ILE	3.3
2	S	18	GLU	3.3
2	S	80	ASN	3.3
1	C	280	GLY	3.3
1	E	354	GLU	3.2
1	D	349	ILE	3.2
2	P	67	PHE	3.2
2	Q	71	TYR	3.2
1	G	198	GLY	3.2
1	E	279	PRO	3.2
2	S	31	ALA	3.1
2	R	79	ASP	3.1
1	F	352	GLN	3.1
1	L	266	THR	3.1
1	E	355	GLU	3.1
1	M	357	THR	3.1
1	F	373	ALA	3.1
2	S	51	ASN	3.1
2	Q	32	ALA	3.1
2	P	49	LEU	3.1
1	G	256	GLY	3.1
1	N	361	ASP	3.0
2	U	51	ASN	3.0
2	P	18	GLU	3.0
1	E	243	ALA	3.0
2	O	17	VAL	3.0
1	A	360	TYR	3.0
2	O	32	ALA	3.0
1	M	364	LYS	3.0
2	S	17	VAL	3.0
2	O	72	GLY	2.9
1	D	358	SER	2.9
1	F	360	TYR	2.9
2	T	53	GLU	2.9
2	Q	25	ILE	2.9
2	R	17	VAL	2.9
2	R	20	LYS	2.9
2	S	33	ALA	2.9
2	Q	20	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	354	GLU	2.9
2	O	18	GLU	2.9
2	P	80	ASN	2.9
1	H	357	THR	2.9
1	A	284	ARG	2.9
1	D	199	TYR	2.9
1	A	365	LEU	2.9
1	C	365	LEU	2.9
2	S	21	SER	2.8
1	G	255	GLU	2.8
1	F	212	ALA	2.8
1	E	284	ARG	2.8
2	O	21	SER	2.8
1	L	364	LYS	2.8
2	O	97	ALA	2.8
2	R	33	ALA	2.8
1	N	360	TYR	2.8
2	T	18	GLU	2.8
1	E	334	ASP	2.8
1	E	336	VAL	2.8
2	R	21	SER	2.8
1	G	195	PHE	2.8
1	H	268	ARG	2.8
1	M	264	VAL	2.7
1	E	340	ALA	2.7
1	E	283	ASP	2.7
1	N	268	ARG	2.7
1	G	214	GLU	2.7
1	D	360	TYR	2.7
1	B	208	PRO	2.7
1	M	284	ARG	2.7
1	F	331	THR	2.7
1	F	172	GLU	2.7
1	G	360	TYR	2.7
2	U	22	ALA	2.7
2	T	51	ASN	2.7
1	C	358	SER	2.6
2	U	97	ALA	2.6
1	D	353	ILE	2.6
2	O	30	SER	2.6
1	A	320	ALA	2.6
2	T	27	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	224	ASP	2.6
2	O	51	ASN	2.6
2	P	51	ASN	2.6
1	G	357	THR	2.6
1	G	350	ARG	2.6
1	G	202	PRO	2.6
1	C	349	ILE	2.6
1	A	373	ALA	2.6
1	C	210	THR	2.6
2	T	72	GLY	2.6
2	O	1	MET	2.6
1	D	209	GLU	2.6
2	P	21	SER	2.6
1	B	352	GLN	2.6
2	Q	82	GLU	2.6
1	B	348	GLN	2.5
2	R	25	ILE	2.5
1	K	185	ASP	2.5
1	L	353	ILE	2.5
1	G	348	GLN	2.5
1	A	209	GLU	2.5
2	Q	80	ASN	2.5
1	L	360	TYR	2.5
1	E	321	LYS	2.5
1	D	356	ALA	2.5
1	M	361	ASP	2.5
1	B	279	PRO	2.5
2	P	71	TYR	2.5
1	C	359	ASP	2.5
2	S	1	MET	2.5
1	E	360	TYR	2.5
1	G	351	GLN	2.5
2	Q	22	ALA	2.4
1	B	364	LYS	2.4
2	S	72	GLY	2.4
2	O	67	PHE	2.4
1	K	361	ASP	2.4
2	P	33	ALA	2.4
1	E	332	ILE	2.4
1	F	311	LYS	2.4
1	L	356	ALA	2.4
1	N	186	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	251	ALA	2.4
1	F	231	ARG	2.4
1	G	365	LEU	2.4
1	F	171	LYS	2.4
1	B	368	ARG	2.4
1	K	295	LEU	2.4
1	N	357	THR	2.4
2	P	20	LYS	2.4
1	A	352	GLN	2.4
1	L	177	VAL	2.4
1	J	357	THR	2.4
2	T	21	SER	2.4
2	S	67	PHE	2.3
2	T	71	TYR	2.3
1	F	374	GLY	2.3
1	G	322	ARG	2.3
1	G	362	ARG	2.3
1	E	286	LYS	2.3
1	C	192	GLY	2.3
1	B	327	LYS	2.3
2	R	28	THR	2.3
1	C	354	GLU	2.3
1	B	209	GLU	2.3
1	H	269	GLY	2.3
1	B	199	TYR	2.3
1	F	174	VAL	2.3
2	T	33	ALA	2.3
2	R	82	GLU	2.2
1	A	172	GLU	2.2
1	C	373	ALA	2.2
2	O	66	ILE	2.2
1	F	386	GLU	2.2
1	E	350	ARG	2.2
1	G	371	LYS	2.2
1	F	351	GLN	2.2
1	K	357	THR	2.2
1	B	200	LEU	2.2
1	E	357	THR	2.2
1	B	192	GLY	2.2
2	P	79	ASP	2.2
2	T	67	PHE	2.2
1	L	270	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	T	32	ALA	2.2
1	K	352	GLN	2.2
2	P	23	GLY	2.2
2	P	22	ALA	2.2
1	D	355	GLU	2.2
1	A	321	LYS	2.2
1	E	255	GLU	2.2
1	G	196	ASP	2.2
2	T	23	GLY	2.2
1	E	348	GLN	2.1
1	N	184	GLN	2.1
1	G	222	LEU	2.1
1	G	213	VAL	2.1
1	D	172	GLU	2.1
1	E	349	ILE	2.1
1	M	349	ILE	2.1
2	T	82	GLU	2.1
1	F	251	ALA	2.1
2	S	37	ARG	2.1
2	Q	27	LEU	2.1
1	I	357	THR	2.1
1	B	214	GLU	2.1
1	K	364	LYS	2.1
2	U	20	LYS	2.1
1	E	477	GLY	2.1
1	G	336	VAL	2.0
1	J	266	THR	2.0
2	S	66	ILE	2.0
2	T	28	THR	2.0
1	D	352	GLN	2.0
1	K	270	ILE	2.0
1	B	326	ASN	2.0
2	U	69	ASP	2.0
2	O	33	ALA	2.0
1	F	267	MET	2.0
1	D	202	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

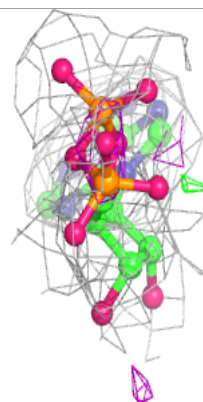
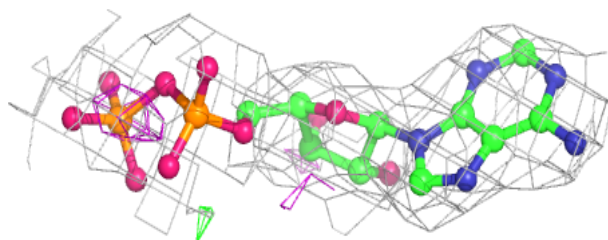
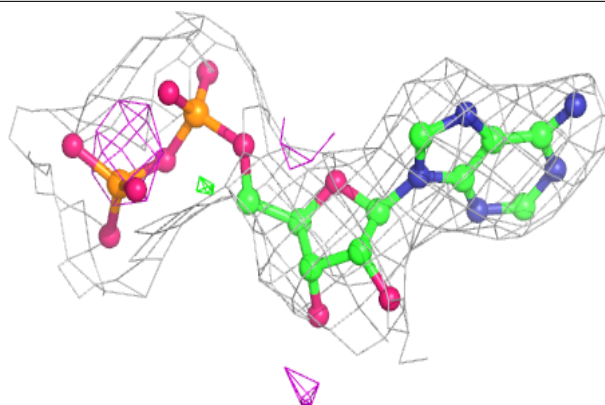
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	C	601	1/1	0.90	0.27	2,2,2,2	0
3	MG	B	601	1/1	0.92	0.30	2,2,2,2	0
3	MG	A	601	1/1	0.93	0.34	2,2,2,2	0
4	ADP	F	600	27/27	0.93	0.21	2,2,3,5	0
4	ADP	E	600	27/27	0.93	0.20	2,2,3,5	0
4	ADP	B	600	27/27	0.94	0.20	2,2,4,5	0
4	ADP	A	600	27/27	0.95	0.18	2,2,3,6	0
4	ADP	D	600	27/27	0.96	0.18	2,2,4,5	0
4	ADP	G	600	27/27	0.96	0.17	2,2,4,5	0
3	MG	E	601	1/1	0.96	0.27	2,2,2,2	0
4	ADP	C	600	27/27	0.97	0.17	2,2,4,5	0
3	MG	D	601	1/1	0.97	0.38	2,2,2,2	0
3	MG	G	601	1/1	0.97	0.29	2,2,2,2	0
3	MG	F	601	1/1	0.97	0.37	2,2,2,2	0

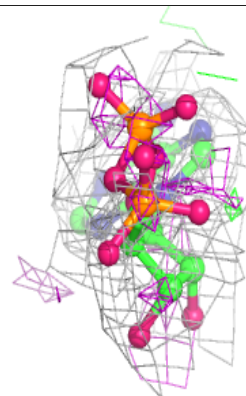
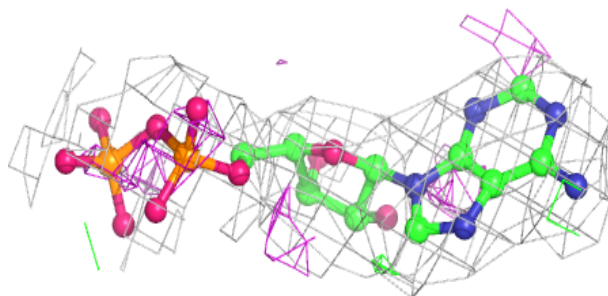
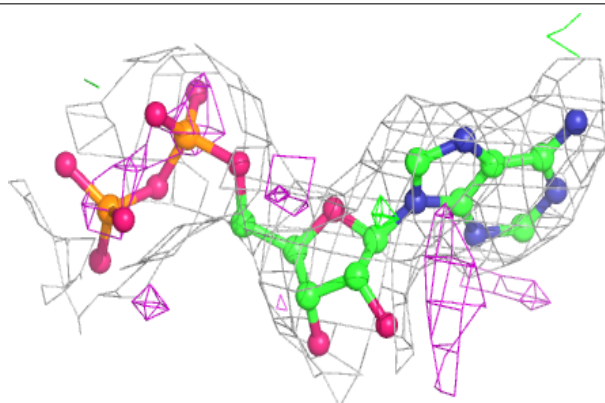
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

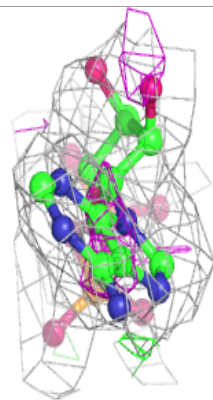
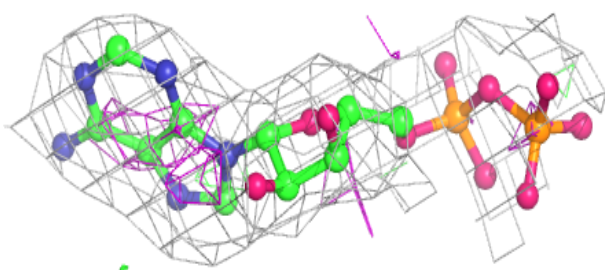
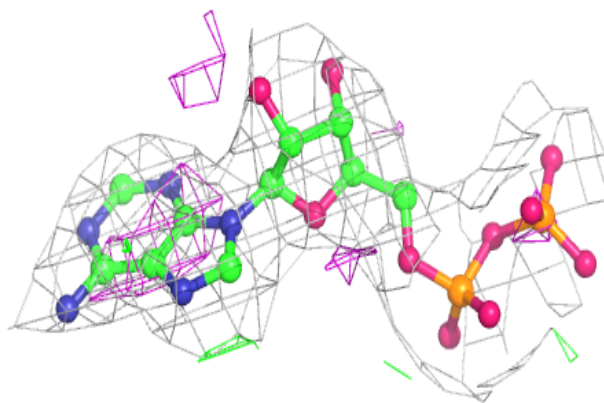
**Electron density around ADP E 600:**

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

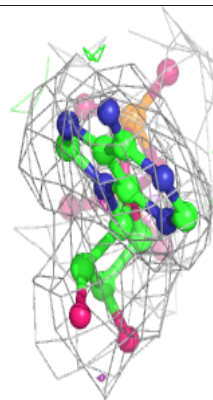
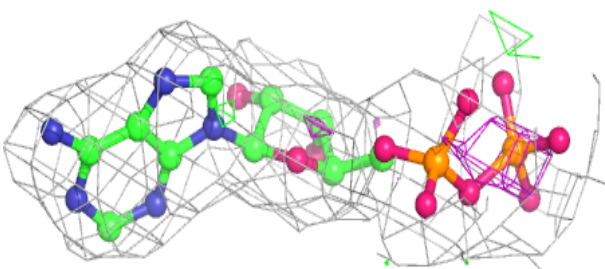
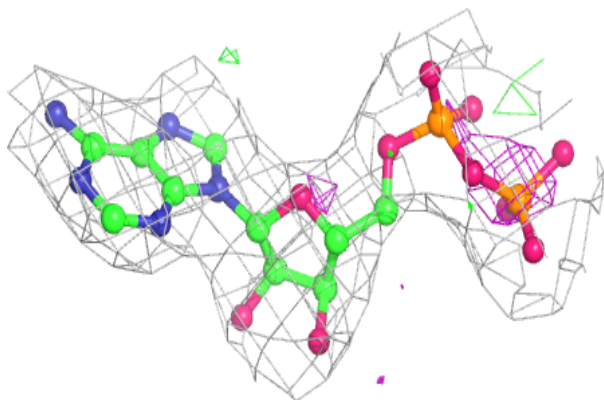


Electron density around ADP B 600:

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

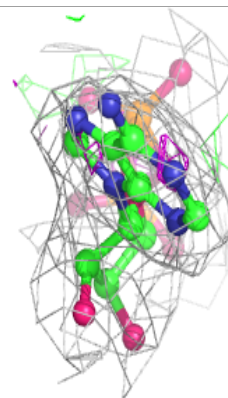
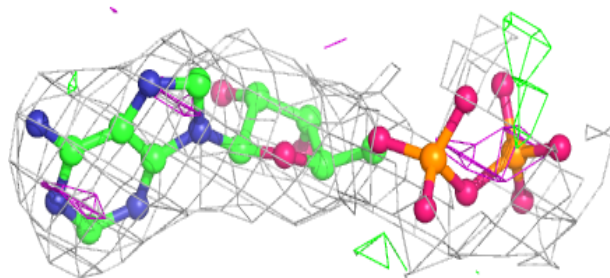
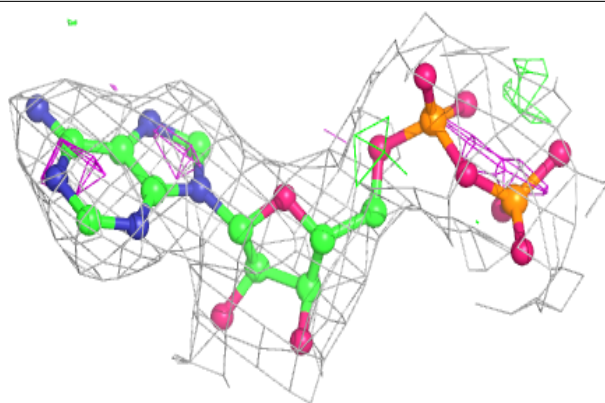
**Electron density around ADP A 600:**

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

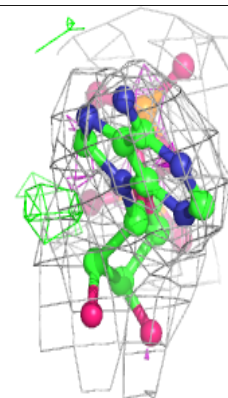
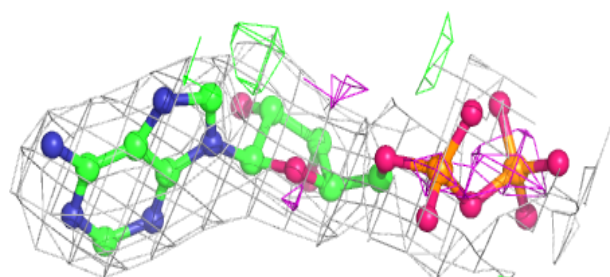
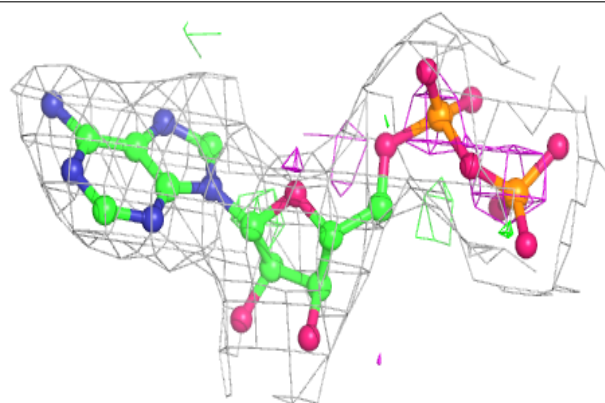


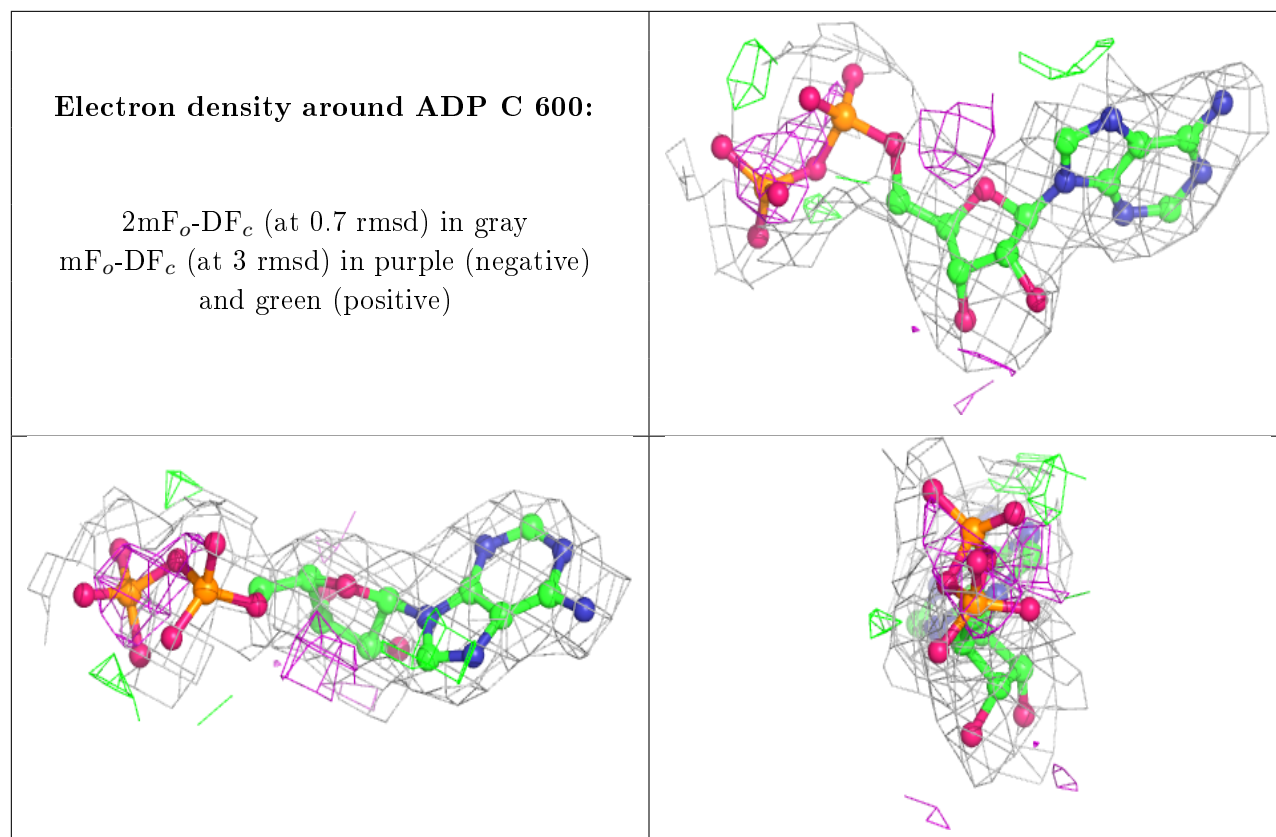
Electron density around ADP D 600:

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

**Electron density around ADP 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.