



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:27 AM EDT

PDB ID : 1SVT / pdb_00001svt
Title : Crystal structure of GroEL14-GroES7-(ADP-AlFx)7
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.
Deposited on : 2004-03-29
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

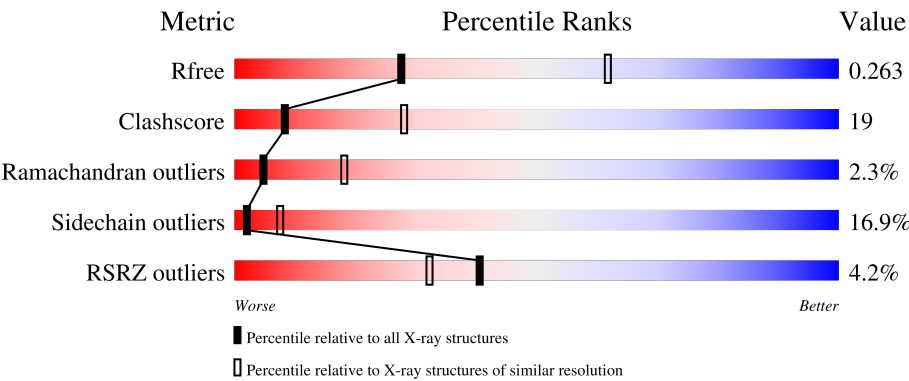
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	524	5% 52%37%9%
1	B	524	5% 57%34%8%
1	C	524	5% 53%36%9%
1	D	524	7% 53%37%9%
1	E	524	8% 58%34%6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AF3	A	602	-	-	X	-
6	AF3	C	602	-	-	X	-
6	AF3	D	602	-	-	X	-
6	AF3	F	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 59498 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
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	I	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	J	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	K	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	L	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	M	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	N	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			

- Molecule 2 is a protein called groES protein.

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

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

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

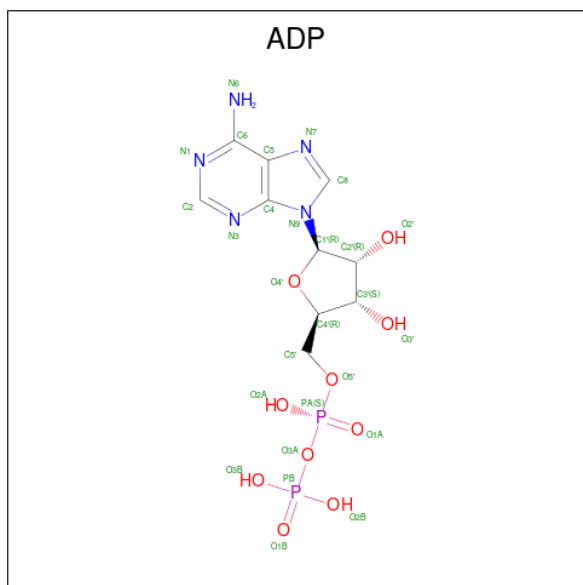
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

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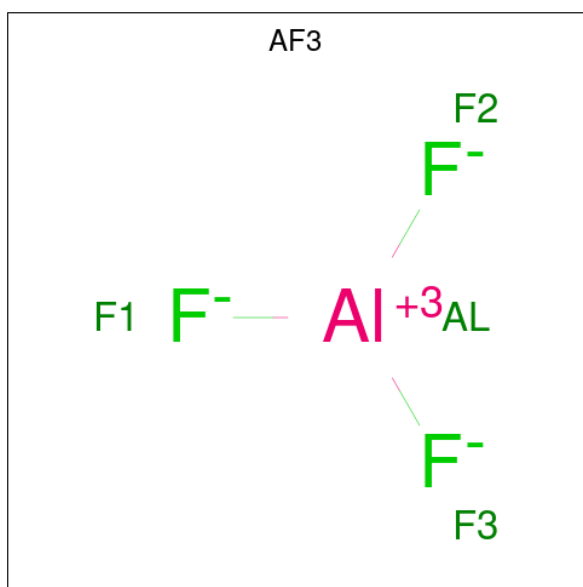
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		
4	G	1	Total	K	0	0
			1	1		

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



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

- Molecule 6 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Al	F	0	0
			4	1	3		
6	B	1	Total	Al	F	0	0
			4	1	3		
6	C	1	Total	Al	F	0	0
			4	1	3		
6	D	1	Total	Al	F	0	0
			4	1	3		
6	E	1	Total	Al	F	0	0
			4	1	3		
6	F	1	Total	Al	F	0	0
			4	1	3		
6	G	1	Total	Al	F	0	0
			4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	19	Total	O	0	0
			19	19		
7	B	10	Total	O	0	0
			10	10		
7	C	21	Total	O	0	0
			21	21		
7	D	14	Total	O	0	0
			14	14		
7	E	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	11	Total 11	O 11	0	0
7	G	20	Total 20	O 20	0	0
7	H	11	Total 11	O 11	0	0
7	I	17	Total 17	O 17	0	0
7	J	12	Total 12	O 12	0	0
7	K	14	Total 14	O 14	0	0
7	L	13	Total 13	O 13	0	0
7	M	10	Total 10	O 10	0	0
7	N	10	Total 10	O 10	0	0

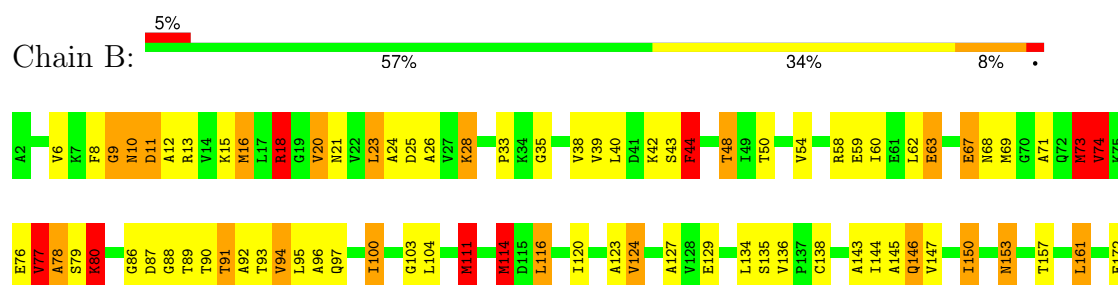
3 Residue-property plots [i](#)

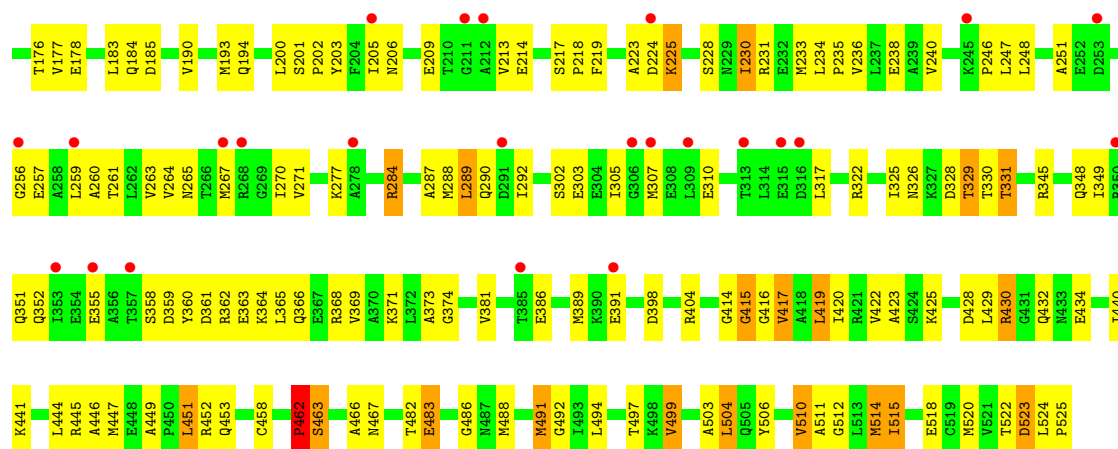
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: groEL protein

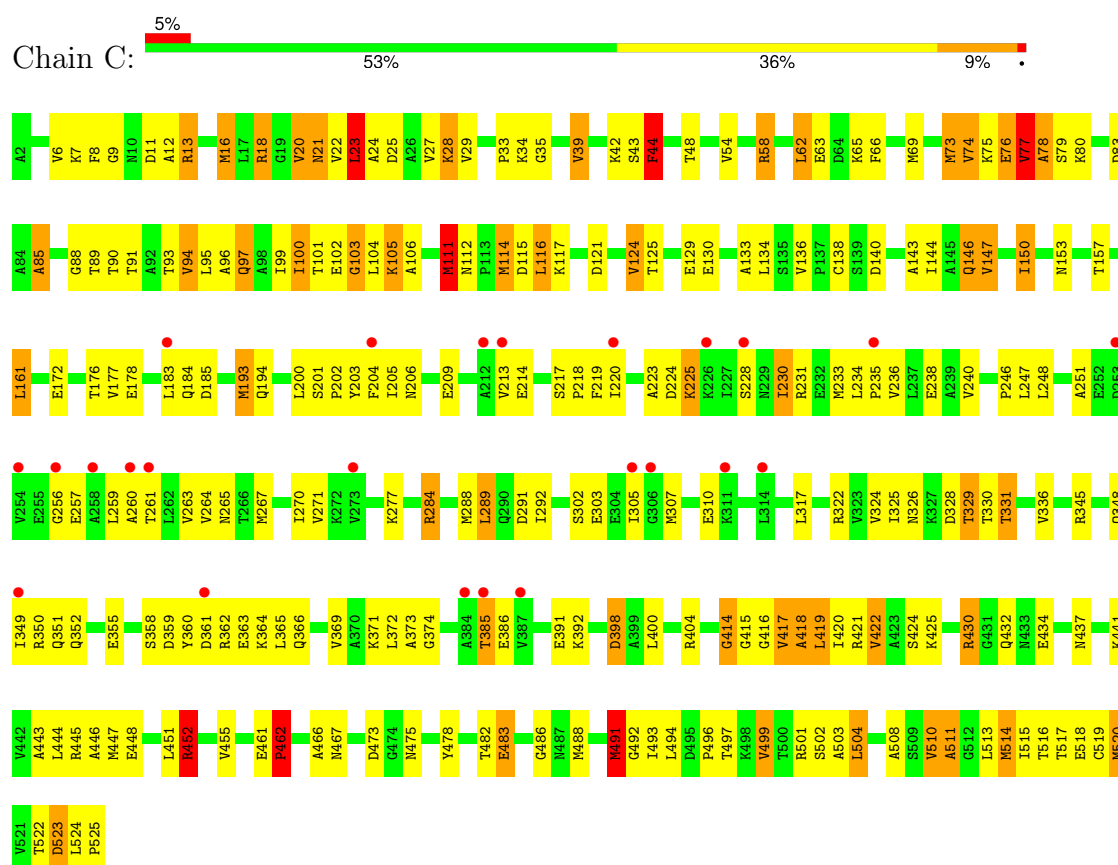


• Molecule 1: groEL protein

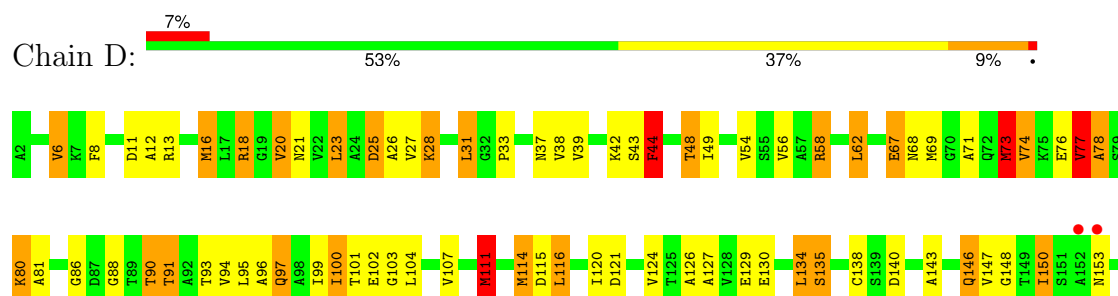


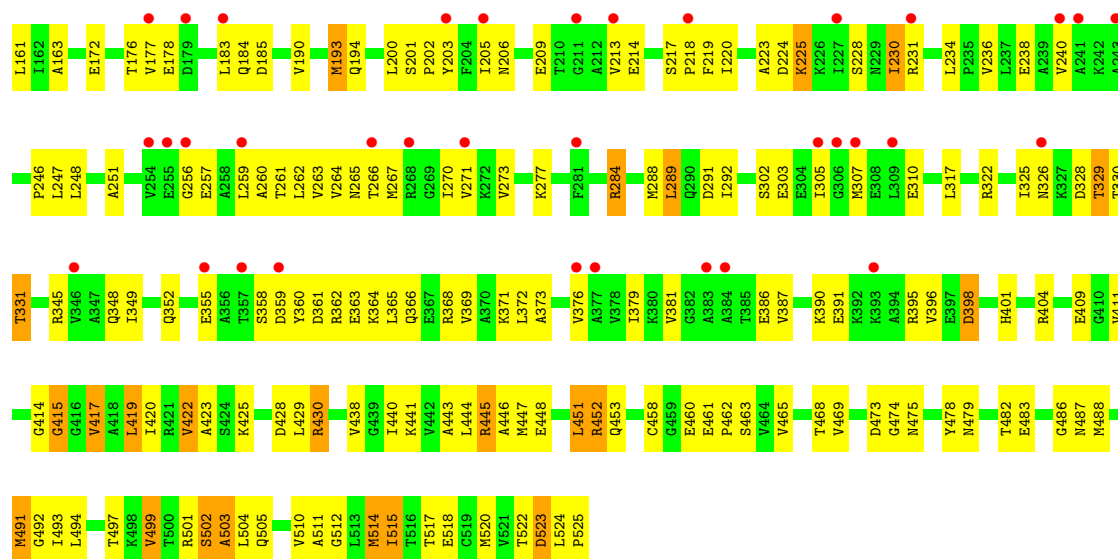


• Molecule 1: groEL protein

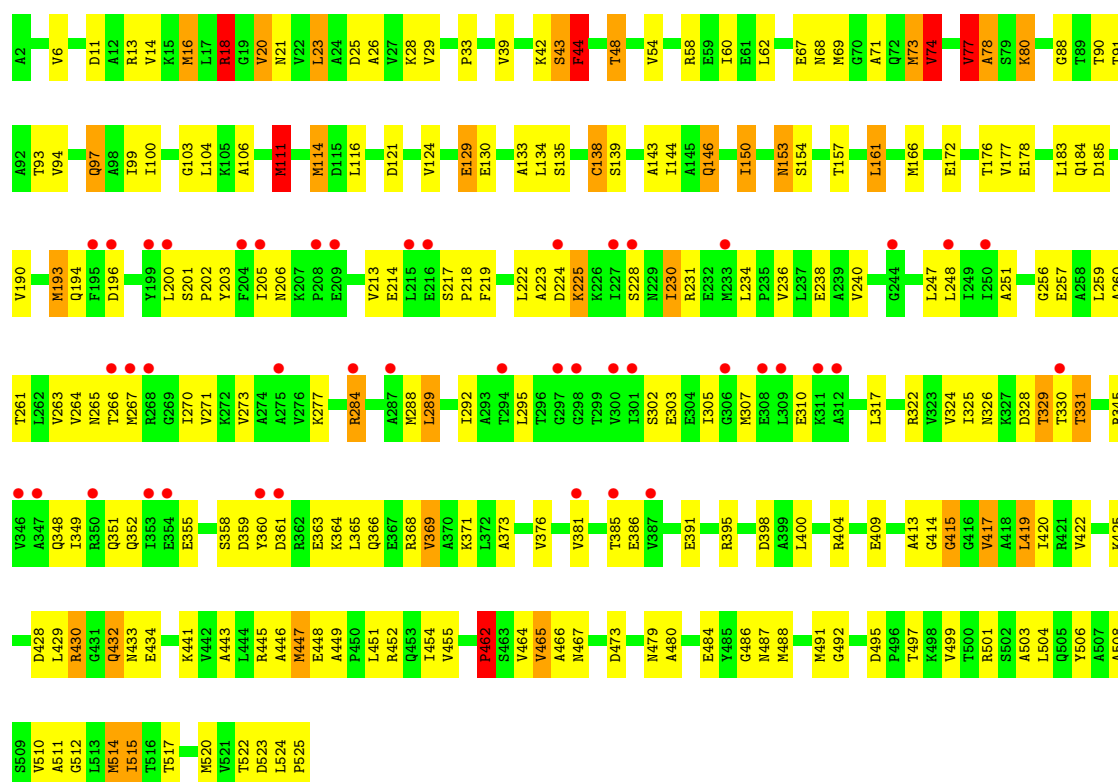


• Molecule 1: groEL protein



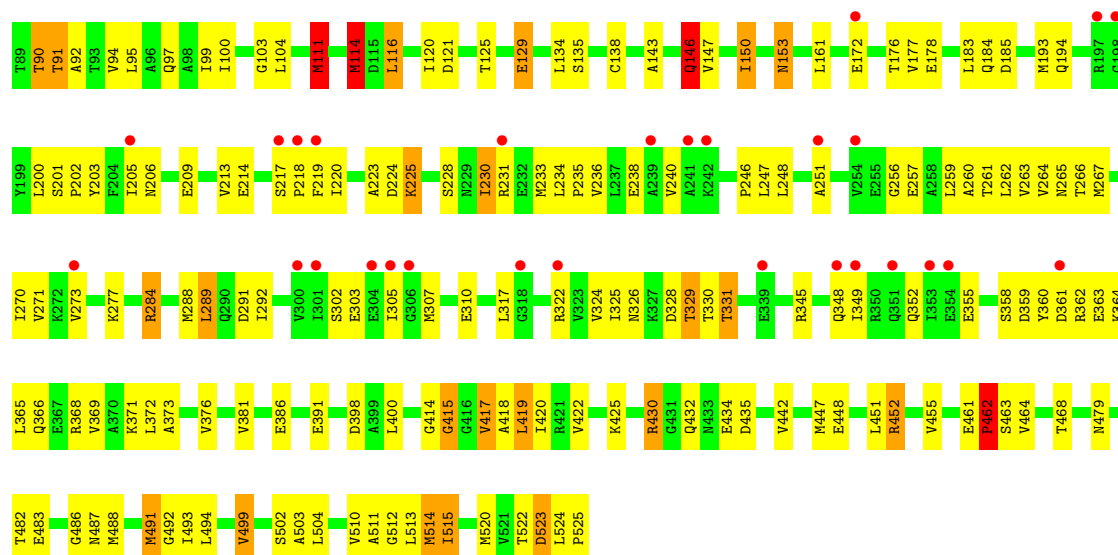


• Molecule 1: groEL protein

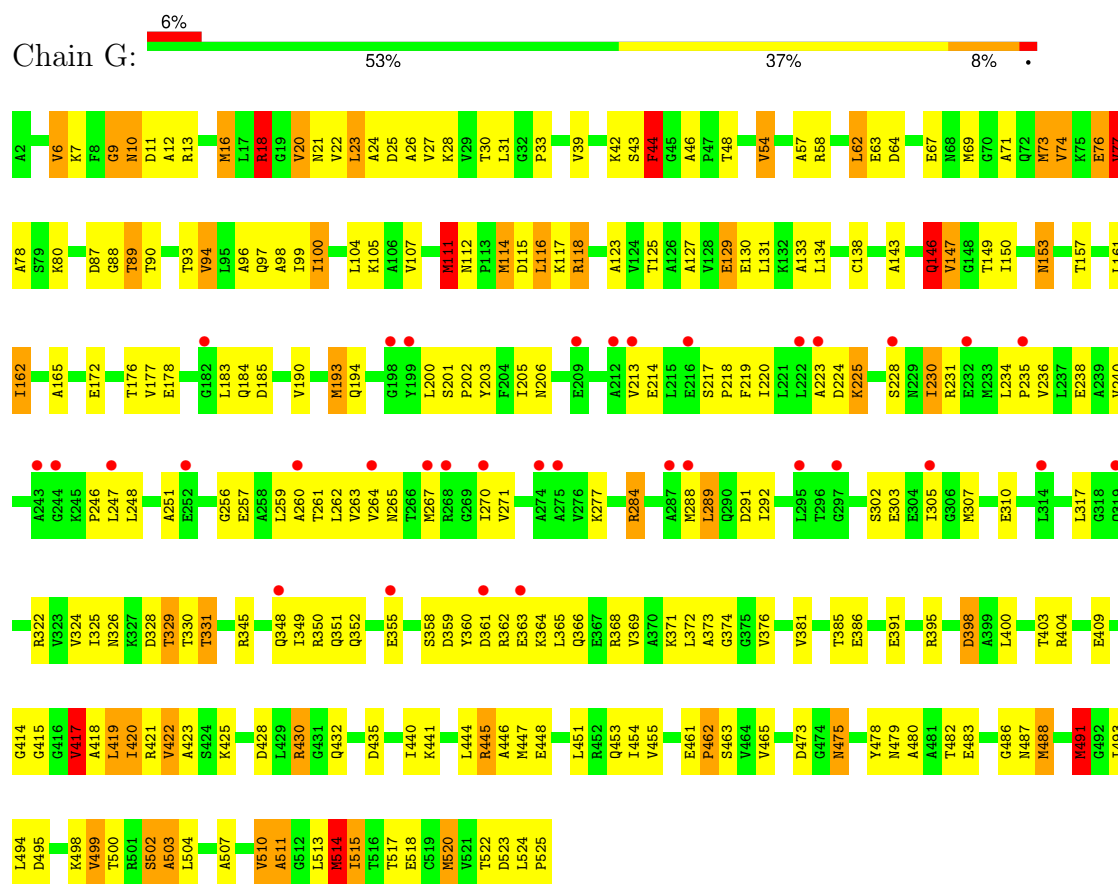


• Molecule 1: groEL protein

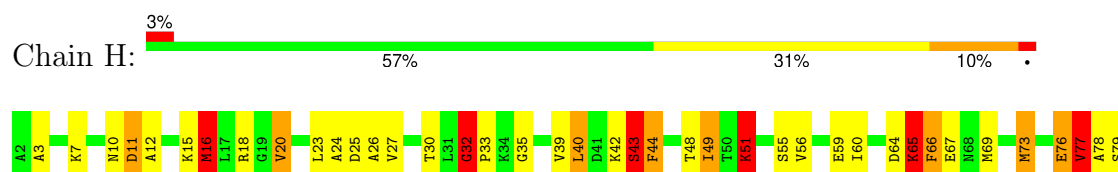


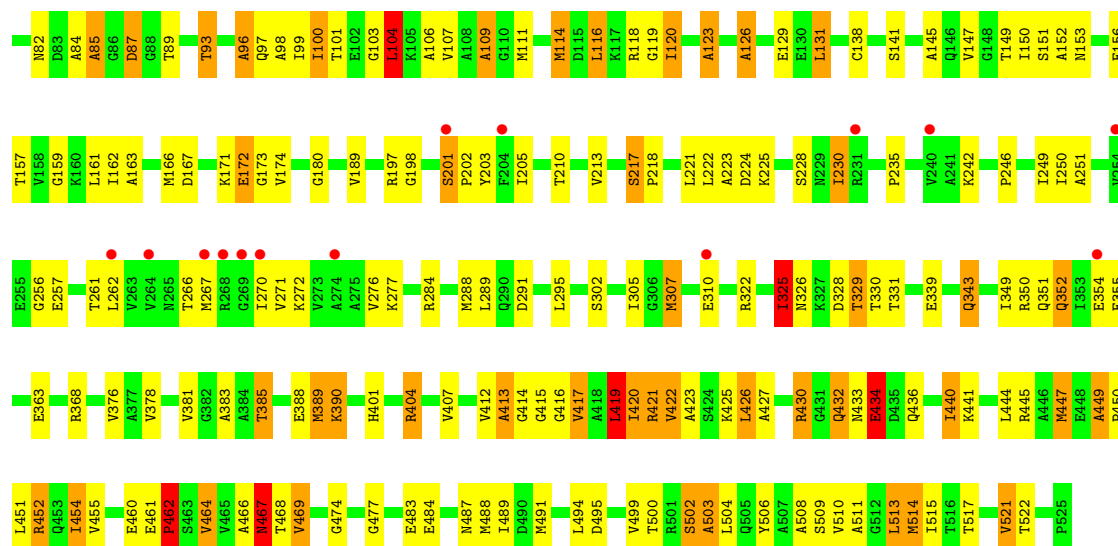


• Molecule 1: groEL protein



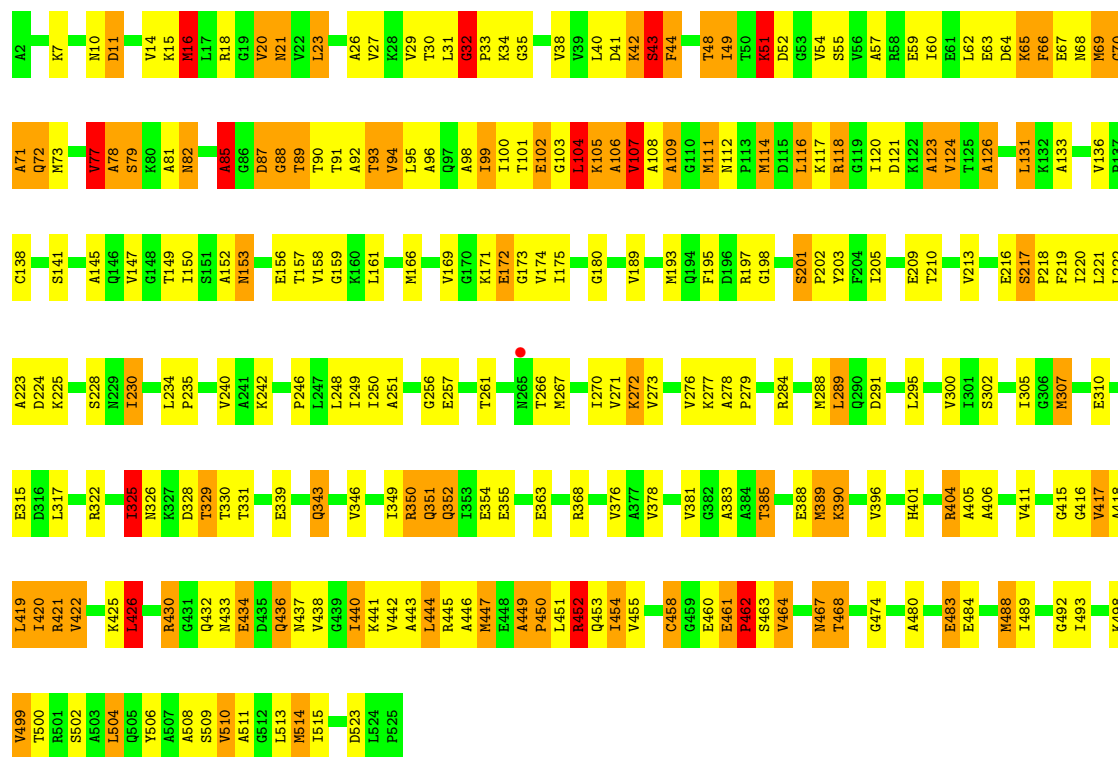
• Molecule 1: groEL protein





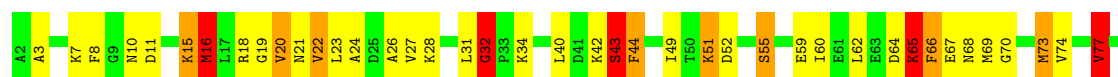
• Molecule 1: groEL protein

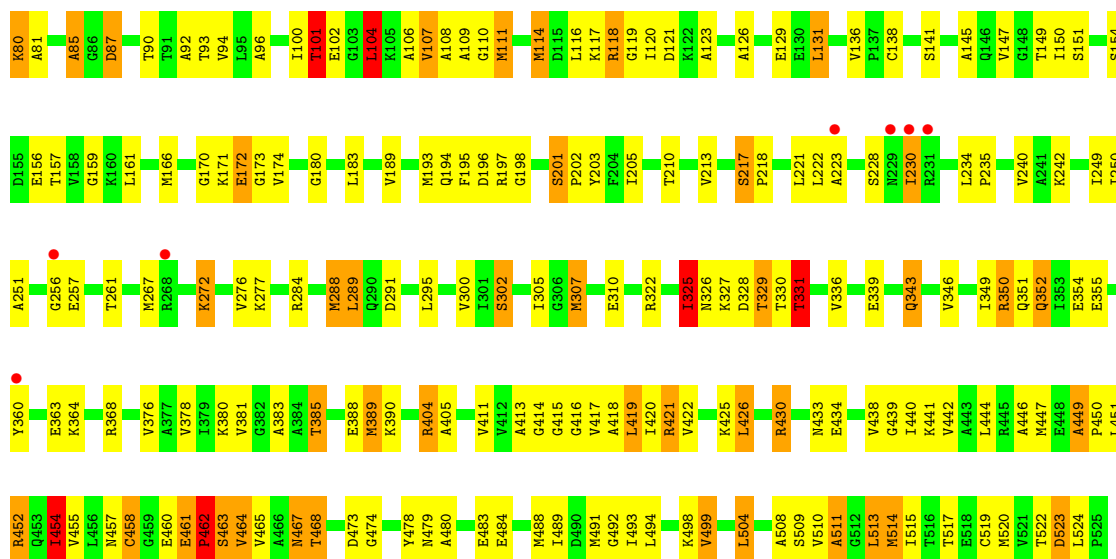
Chain I: 50% 33% 15%



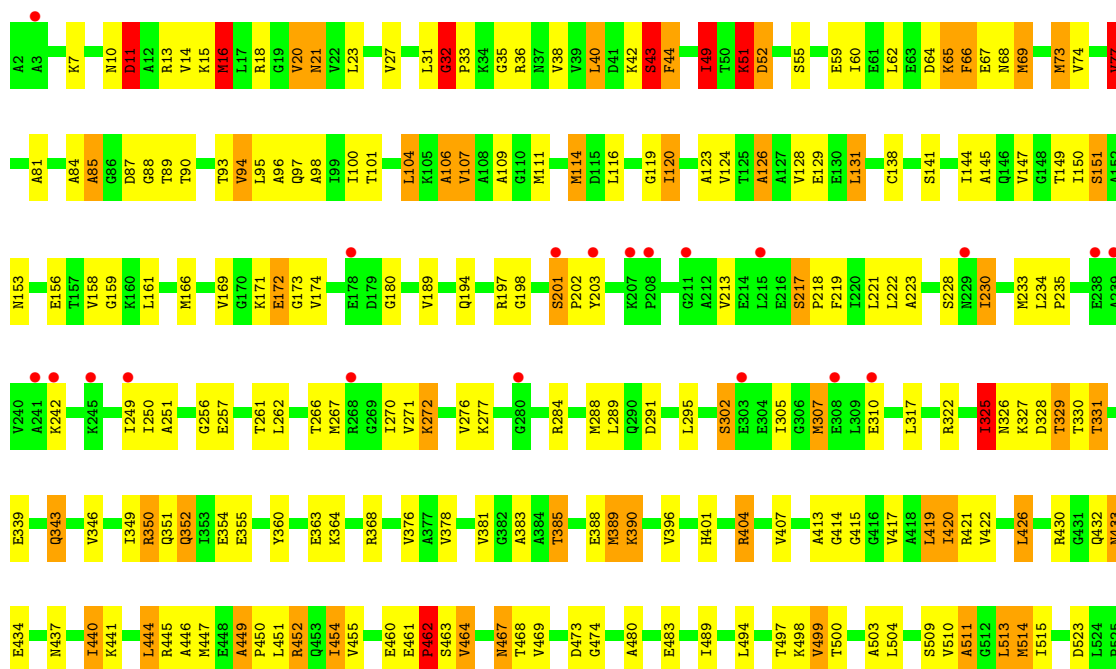
• Molecule 1: groEL protein

Chain J: 55% 34% 10%

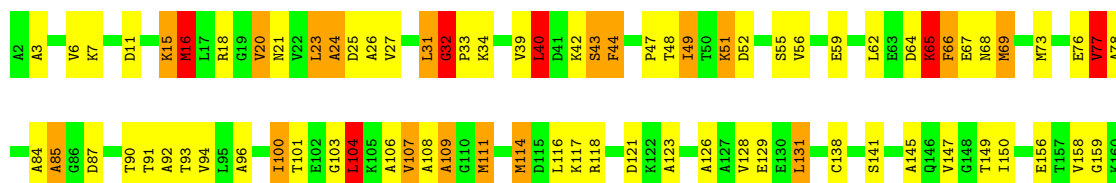


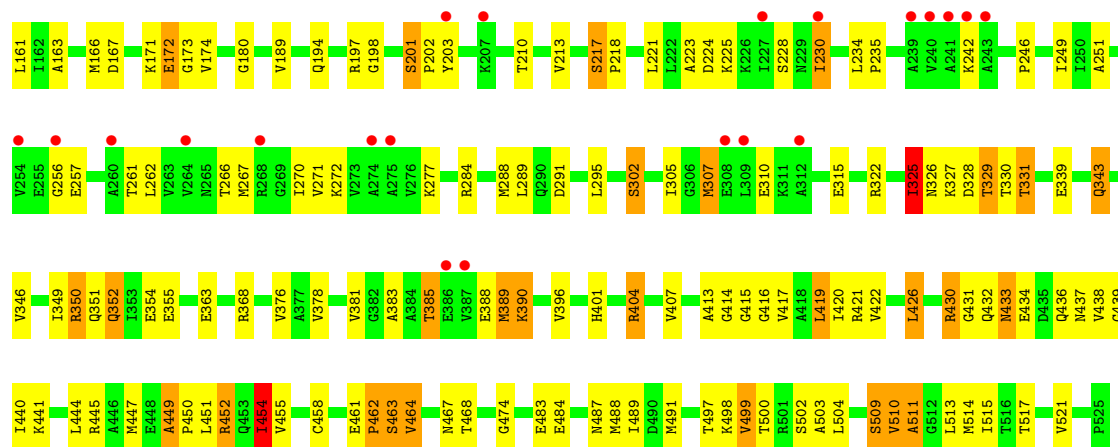


• Molecule 1: groEL protein

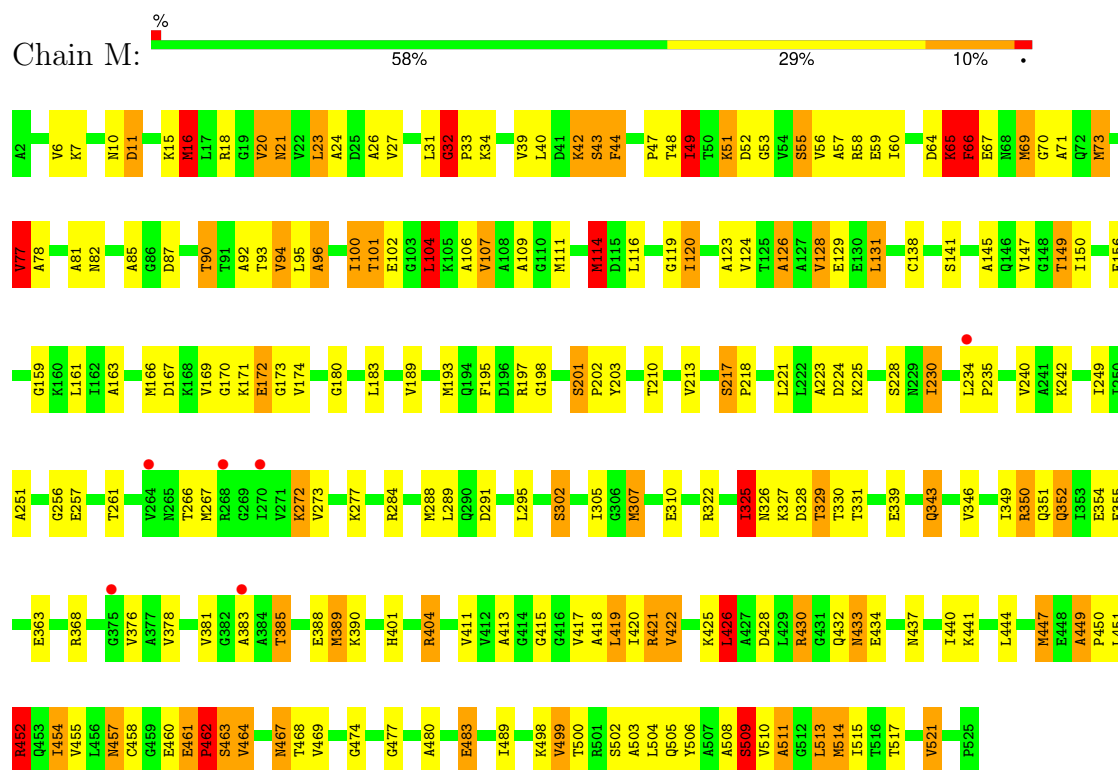


• Molecule 1: groEL protein

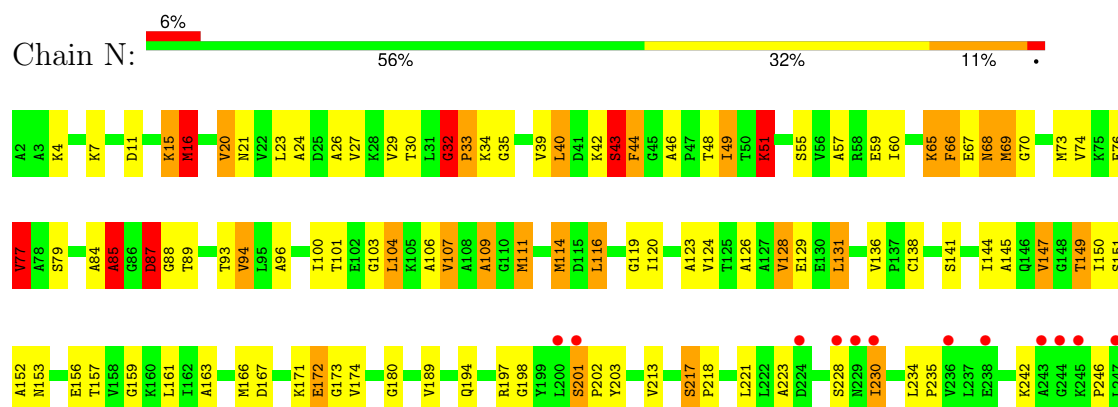


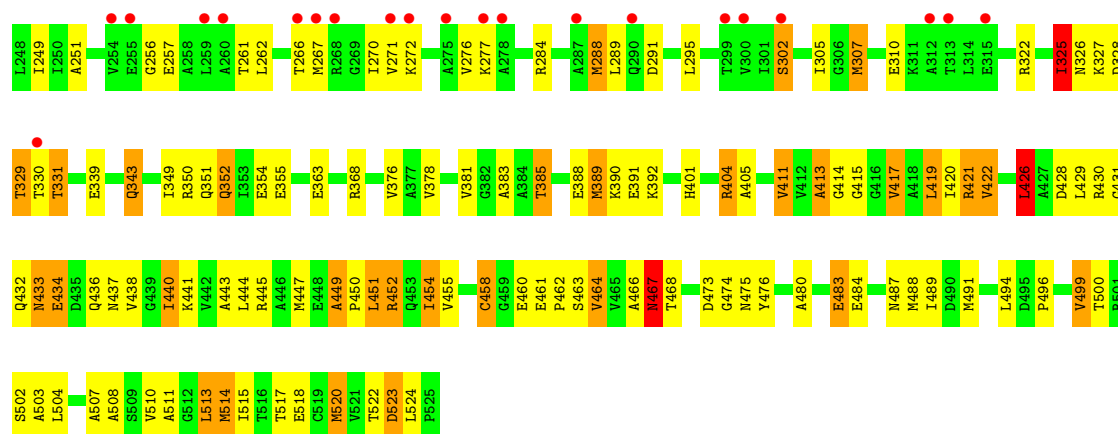


• Molecule 1: groEL protein



• Molecule 1: groEL protein





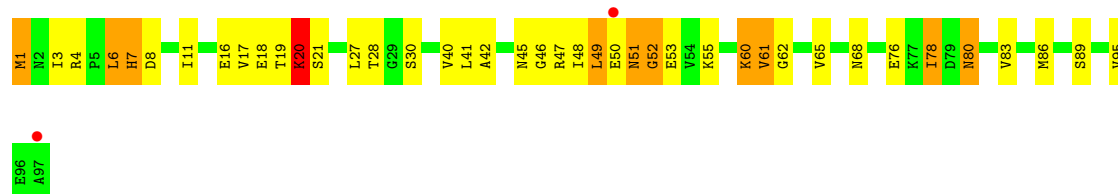
• Molecule 2: groES protein



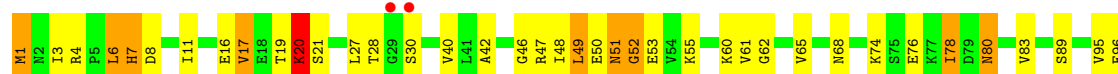
• Molecule 2: groES protein



• Molecule 2: groES protein



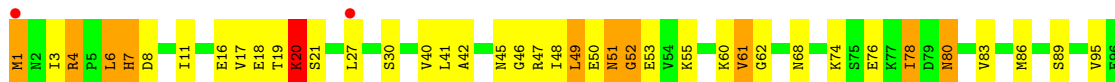
• Molecule 2: groES protein



A97

- Molecule 2: groES protein

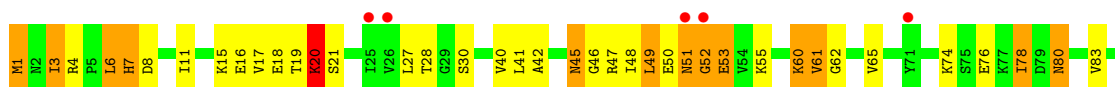
Chain S:  2% 59% 30% 10%



A97

- Molecule 2: groES protein

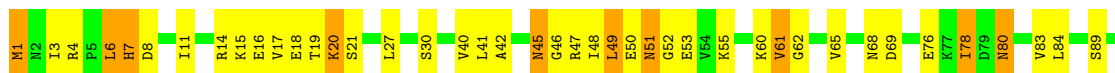
Chain T:  6% 57% 29% 13%



M86
S89
V95
E96
A97

- Molecule 2: groES protein

Chain U:  56% 34% 10%



V95
E96
A97

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	255.55Å 266.86Å 187.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.81 49.39 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.39-2.81) 78.9 (49.39-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.32Å)	Xtriage
Refinement program	REFMAC refmac_5.1.19	Depositor
R, R_{free}	0.247 , 0.274 0.244 , 0.263	Depositor DCC
R_{free} test set	6710 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.958	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 94.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	59498	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 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.65	42/3883 (1.1%)	1.48	32/5243 (0.6%)
1	B	1.57	35/3883 (0.9%)	1.41	37/5243 (0.7%)
1	C	1.74	64/3883 (1.6%)	1.49	33/5243 (0.6%)
1	D	1.64	45/3883 (1.2%)	1.46	35/5243 (0.7%)
1	E	1.38	27/3883 (0.7%)	1.34	27/5243 (0.5%)
1	F	1.37	18/3883 (0.5%)	1.31	19/5243 (0.4%)
1	G	1.58	52/3883 (1.3%)	1.44	27/5243 (0.5%)
1	H	1.56	49/3884 (1.3%)	1.41	25/5243 (0.5%)
1	I	1.78	82/3884 (2.1%)	1.54	45/5243 (0.9%)
1	J	1.55	31/3884 (0.8%)	1.41	30/5243 (0.6%)
1	K	1.36	23/3884 (0.6%)	1.34	19/5243 (0.4%)
1	L	1.29	21/3884 (0.5%)	1.31	17/5243 (0.3%)
1	M	1.55	39/3884 (1.0%)	1.42	25/5243 (0.5%)
1	N	1.56	41/3884 (1.1%)	1.42	31/5243 (0.6%)
2	O	0.88	2/732 (0.3%)	0.97	2/983 (0.2%)
2	P	0.86	1/732 (0.1%)	0.97	2/983 (0.2%)
2	Q	0.85	0/732	0.98	2/983 (0.2%)
2	R	0.83	1/732 (0.1%)	0.99	2/983 (0.2%)
2	S	0.80	0/732	0.96	1/983 (0.1%)
2	T	0.79	0/732	0.98	2/983 (0.2%)
2	U	0.83	0/732	0.99	2/983 (0.2%)
All	All	1.50	573/59493 (1.0%)	1.38	415/80283 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	8

All (573) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	MET	SD-CE	21.22	2.32	1.79
1	A	73	MET	SD-CE	19.05	2.27	1.79
1	F	73	MET	SD-CE	19.03	2.27	1.79
1	N	514	MET	SD-CE	18.04	2.24	1.79
1	H	114	MET	SD-CE	17.42	2.23	1.79
1	G	73	MET	SD-CE	16.80	2.21	1.79
1	B	514	MET	SD-CE	16.64	2.21	1.79
1	N	16	MET	SD-CE	16.46	2.20	1.79
1	J	114	MET	SD-CE	16.11	2.19	1.79
1	E	73	MET	SD-CE	15.96	2.19	1.79
1	E	111	MET	SD-CE	15.55	2.18	1.79
1	D	73	MET	SD-CE	15.06	2.17	1.79
1	H	514	MET	SD-CE	14.46	2.15	1.79
1	B	111	MET	SD-CE	14.04	2.14	1.79
1	F	111	MET	SD-CE	13.70	2.13	1.79
1	D	111	MET	SD-CE	13.61	2.13	1.79
1	C	514	MET	SD-CE	13.56	2.13	1.79
1	A	111	MET	SD-CE	13.52	2.13	1.79
1	J	514	MET	SD-CE	13.51	2.13	1.79
1	M	114	MET	SD-CE	13.47	2.13	1.79
1	N	114	MET	SD-CE	12.73	2.11	1.79
1	B	73	MET	SD-CE	12.41	2.10	1.79
1	I	417	VAL	CA-CB	-12.25	1.40	1.54
1	I	78	ALA	CA-C	12.19	1.69	1.52
1	J	16	MET	SD-CE	12.03	2.09	1.79
1	I	114	MET	SD-CE	11.99	2.09	1.79
1	C	94	VAL	C-O	11.99	1.39	1.24
1	I	102	GLU	C-O	11.72	1.39	1.24
1	C	83	ASP	C-O	11.52	1.39	1.24
1	I	510	VAL	CA-C	-11.27	1.38	1.52
1	K	114	MET	SD-CE	11.16	2.07	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	111	MET	SD-CE	11.06	2.07	1.79
1	F	16	MET	SD-CE	11.04	2.07	1.79
1	K	69	MET	SD-CE	-11.01	1.52	1.79
1	K	449	ALA	CA-CB	-10.76	1.39	1.53
1	C	111	MET	SD-CE	10.71	2.06	1.79
1	I	16	MET	SD-CE	10.46	2.05	1.79
1	B	16	MET	SD-CE	10.44	2.05	1.79
1	I	447	MET	SD-CE	10.34	2.05	1.79
1	I	85	ALA	CA-CB	10.33	1.71	1.53
1	K	16	MET	SD-CE	10.18	2.05	1.79
1	M	514	MET	SD-CE	10.12	2.04	1.79
1	M	69	MET	SD-CE	-9.96	1.54	1.79
1	B	114	MET	SD-CE	9.96	2.04	1.79
1	J	288	MET	SD-CE	9.93	2.04	1.79
1	M	94	VAL	C-O	9.91	1.36	1.24
1	M	16	MET	SD-CE	9.86	2.04	1.79
1	L	114	MET	SD-CE	9.79	2.04	1.79
1	D	465	VAL	CA-CB	-9.55	1.44	1.54
1	J	92	ALA	CA-CB	-9.35	1.38	1.53
1	F	114	MET	SD-CE	9.29	2.02	1.79
1	A	114	MET	SD-CE	9.28	2.02	1.79
1	I	104	LEU	CA-C	-9.14	1.40	1.52
1	C	105	LYS	C-O	9.10	1.34	1.24
1	N	69	MET	SD-CE	-8.96	1.57	1.79
1	N	288	MET	SD-CE	8.89	2.01	1.79
1	I	480	ALA	CA-CB	-8.86	1.38	1.53
1	M	449	ALA	CA-CB	-8.75	1.42	1.53
1	B	35	GLY	C-O	8.71	1.32	1.23
1	C	502	SER	CA-C	-8.67	1.41	1.52
1	E	114	MET	SD-CE	8.67	2.01	1.79
1	I	449	ALA	CA-CB	-8.60	1.42	1.53
1	M	60	ILE	CA-CB	-8.59	1.44	1.54
1	I	99	ILE	CA-CB	-8.51	1.44	1.54
1	D	16	MET	SD-CE	8.48	2.00	1.79
1	K	514	MET	SD-CE	8.47	2.00	1.79
1	C	452	ARG	C-O	8.40	1.33	1.24
1	K	18	ARG	NE-CZ	8.39	1.42	1.33
1	I	442	VAL	CA-C	-8.36	1.43	1.52
1	H	288	MET	SD-CE	8.31	2.00	1.79
1	H	16	MET	SD-CE	8.30	2.00	1.79
1	C	11	ASP	CA-C	-8.24	1.42	1.52
1	I	78	ALA	C-O	-8.20	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	111	MET	SD-CE	8.11	1.99	1.79
1	N	85	ALA	CA-CB	8.04	1.67	1.53
1	D	114	MET	SD-CE	8.02	1.99	1.79
1	I	99	ILE	C-O	8.00	1.32	1.24
1	C	511	ALA	CA-CB	7.95	1.66	1.53
1	A	145	ALA	CA-CB	-7.91	1.41	1.53
1	I	54	VAL	CA-CB	-7.87	1.43	1.54
1	I	452	ARG	NE-CZ	7.84	1.41	1.33
1	I	288	MET	SD-CE	7.81	1.99	1.79
1	B	87	ASP	C-O	-7.81	1.15	1.23
1	C	503	ALA	CA-CB	-7.80	1.41	1.53
1	G	503	ALA	C-O	-7.78	1.15	1.24
1	I	446	ALA	C-O	-7.71	1.14	1.24
1	D	71	ALA	CA-CB	-7.67	1.40	1.53
1	I	77	VAL	CA-CB	7.64	1.62	1.54
1	H	449	ALA	CA-CB	-7.62	1.43	1.53
1	D	121	ASP	CG-OD1	7.62	1.39	1.25
1	E	14	VAL	CA-CB	-7.62	1.45	1.54
1	B	60	ILE	CA-CB	-7.59	1.45	1.54
1	A	71	ALA	CA-CB	-7.58	1.40	1.53
1	C	443	ALA	CA-CB	-7.56	1.41	1.53
1	I	69	MET	SD-CE	-7.56	1.60	1.79
1	L	104	LEU	CA-C	-7.56	1.43	1.52
1	A	449	ALA	C-O	-7.55	1.17	1.24
1	G	491	MET	SD-CE	-7.50	1.60	1.79
1	J	480	ALA	CA-CB	-7.49	1.40	1.53
1	A	100	ILE	CA-C	-7.47	1.43	1.52
1	L	16	MET	SD-CE	7.47	1.98	1.79
1	H	98	ALA	C-O	7.46	1.33	1.24
1	C	475	ASN	N-CA	-7.42	1.38	1.46
1	D	90	THR	C-O	-7.40	1.15	1.24
1	G	395	ARG	NE-CZ	7.37	1.41	1.33
1	I	461	GLU	CD-OE2	7.34	1.39	1.25
1	I	109	ALA	N-CA	-7.34	1.36	1.46
1	C	144	ILE	CA-CB	-7.30	1.45	1.54
1	A	97	GLN	C-O	-7.28	1.14	1.24
1	C	77	VAL	CA-CB	7.28	1.62	1.54
1	C	398	ASP	CG-OD1	7.27	1.39	1.25
1	E	16	MET	SD-CE	7.27	1.97	1.79
1	H	26	ALA	CA-CB	-7.25	1.41	1.53
1	L	111	MET	SD-CE	7.22	1.97	1.79
1	A	478	TYR	CA-C	-7.21	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	ASP	N-CA	-7.18	1.36	1.46
1	B	71	ALA	CA-CB	-7.16	1.42	1.53
1	N	24	ALA	CA-CB	-7.16	1.41	1.53
1	F	26	ALA	CA-C	-7.15	1.43	1.52
1	M	100	ILE	CA-CB	-7.12	1.46	1.54
1	H	18	ARG	NE-CZ	7.11	1.40	1.33
1	J	449	ALA	CA-CB	-7.11	1.44	1.53
1	M	73	MET	CG-SD	7.06	1.98	1.80
1	M	509	SER	C-O	7.05	1.32	1.24
1	C	78	ALA	CA-C	-7.04	1.43	1.52
1	C	76	GLU	CD-OE1	7.03	1.38	1.25
1	A	165	ALA	CA-CB	-7.02	1.42	1.53
1	A	443	ALA	CA-CB	-6.99	1.42	1.53
1	G	11	ASP	CA-C	-6.99	1.44	1.52
1	I	111	MET	SD-CE	6.98	1.97	1.79
1	A	121	ASP	CG-OD1	6.97	1.38	1.25
1	D	26	ALA	CA-CB	-6.95	1.42	1.53
1	F	26	ALA	C-O	-6.95	1.15	1.24
1	I	77	VAL	C-O	6.95	1.31	1.24
1	H	24	ALA	CA-CB	-6.94	1.41	1.53
1	B	440	ILE	CA-CB	-6.93	1.46	1.54
1	G	446	ALA	CA-CB	-6.92	1.41	1.53
1	C	112	ASN	C-O	-6.92	1.15	1.24
1	N	128	VAL	CA-CB	-6.91	1.45	1.54
1	C	503	ALA	C-O	-6.91	1.16	1.24
1	L	69	MET	SD-CE	-6.88	1.62	1.79
1	N	26	ALA	CA-CB	-6.87	1.42	1.53
1	J	418	ALA	CA-CB	-6.85	1.42	1.53
1	I	510	VAL	C-O	-6.84	1.16	1.24
1	D	440	ILE	CA-CB	-6.84	1.46	1.54
1	H	12	ALA	CA-CB	-6.81	1.42	1.53
1	L	449	ALA	CA-CB	-6.79	1.44	1.53
1	C	398	ASP	CB-CG	6.77	1.69	1.52
1	N	480	ALA	CA-CB	-6.77	1.41	1.53
1	H	447	MET	SD-CE	6.76	1.96	1.79
1	C	117	LYS	CB-CG	-6.75	1.32	1.52
1	I	72	GLN	N-CA	-6.74	1.37	1.46
1	C	116	LEU	CA-C	-6.74	1.43	1.52
1	C	452	ARG	NE-CZ	6.74	1.40	1.33
1	C	502	SER	C-O	-6.73	1.16	1.24
1	E	166	MET	SD-CE	6.71	1.96	1.79
1	F	99	ILE	CA-CB	-6.69	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	483	GLU	CD-OE2	6.69	1.38	1.25
1	D	116	LEU	CA-C	-6.67	1.44	1.52
1	E	514	MET	SD-CE	6.67	1.96	1.79
1	H	49	ILE	CA-CB	-6.67	1.46	1.54
1	C	508	ALA	CA-CB	-6.66	1.43	1.53
1	M	461	GLU	CD-OE2	6.65	1.38	1.25
1	A	96	ALA	CA-C	-6.65	1.44	1.52
1	B	11	ASP	CA-C	-6.64	1.44	1.52
1	I	405	ALA	CA-CB	-6.63	1.41	1.53
1	B	100	ILE	CA-C	-6.62	1.44	1.52
1	D	502	SER	C-O	-6.62	1.16	1.24
1	F	78	ALA	CA-CB	-6.61	1.43	1.53
1	A	18	ARG	NE-CZ	6.60	1.40	1.33
1	C	117	LYS	CA-C	-6.60	1.44	1.52
1	D	20	VAL	CA-CB	-6.59	1.45	1.54
1	J	439	GLY	C-O	-6.57	1.16	1.23
1	B	144	ILE	CA-CB	-6.56	1.47	1.54
1	C	121	ASP	CG-OD1	6.56	1.37	1.25
1	M	447	MET	SD-CE	6.54	1.96	1.79
1	C	97	GLN	CB-CG	-6.53	1.32	1.52
1	D	96	ALA	C-O	-6.52	1.16	1.24
1	K	469	VAL	CA-CB	-6.51	1.47	1.54
1	N	79	SER	C-O	-6.51	1.16	1.24
1	N	445	ARG	NE-CZ	6.51	1.40	1.33
1	I	41	ASP	C-O	-6.48	1.14	1.23
1	G	500	THR	CA-CB	-6.48	1.43	1.53
1	H	3	ALA	CA-CB	-6.48	1.42	1.53
1	J	491	MET	SD-CE	6.45	1.95	1.79
1	M	452	ARG	NE-CZ	6.43	1.40	1.33
1	J	442	VAL	C-O	-6.42	1.16	1.24
1	I	406	ALA	CA-CB	-6.42	1.43	1.53
1	H	73	MET	CG-SD	6.41	1.96	1.80
1	G	12	ALA	CA-CB	-6.40	1.43	1.53
1	M	18	ARG	NE-CZ	6.39	1.40	1.33
1	B	116	LEU	CA-C	-6.37	1.44	1.52
1	N	449	ALA	CA-CB	-6.37	1.45	1.53
1	G	146	GLN	C-O	-6.36	1.16	1.24
1	A	35	GLY	C-O	6.36	1.30	1.23
1	H	118	ARG	NE-CZ	6.36	1.40	1.33
1	C	78	ALA	C-O	-6.34	1.16	1.24
1	M	96	ALA	CA-CB	-6.34	1.43	1.53
1	I	107	VAL	CA-C	-6.33	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	114	MET	SD-CE	6.32	1.95	1.79
1	I	82	ASN	C-O	-6.30	1.16	1.24
1	I	18	ARG	CZ-NH2	6.30	1.41	1.33
1	J	92	ALA	CA-C	6.30	1.61	1.52
1	G	520	MET	SD-CE	-6.30	1.63	1.79
1	E	449	ALA	CA-CB	-6.29	1.45	1.53
1	G	76	GLU	CD-OE2	6.27	1.37	1.25
1	B	136	VAL	CA-CB	-6.26	1.46	1.54
1	G	99	ILE	N-CA	-6.26	1.39	1.46
1	E	18	ARG	NE-CZ	6.26	1.40	1.33
1	L	18	ARG	NE-CZ	6.26	1.40	1.33
1	A	502	SER	C-O	-6.25	1.17	1.24
1	A	407	VAL	CA-CB	-6.25	1.46	1.54
1	G	511	ALA	C-O	6.24	1.31	1.24
1	I	118	ARG	NE-CZ	6.24	1.40	1.33
1	M	480	ALA	CA-CB	-6.22	1.43	1.53
1	C	85	ALA	C-O	6.21	1.31	1.24
1	D	396	VAL	CA-CB	-6.21	1.46	1.54
1	H	423	ALA	CA-CB	-6.21	1.43	1.53
1	J	87	ASP	C-O	6.20	1.30	1.23
1	M	26	ALA	CA-CB	-6.20	1.43	1.53
1	H	449	ALA	CA-C	-6.20	1.45	1.52
1	L	288	MET	SD-CE	6.19	1.95	1.79
1	D	503	ALA	CA-CB	-6.19	1.43	1.53
1	A	76	GLU	CD-OE1	6.18	1.37	1.25
1	F	493	ILE	CA-CB	-6.18	1.46	1.54
1	I	514	MET	SD-CE	6.16	1.95	1.79
1	N	483	GLU	CD-OE2	6.16	1.37	1.25
1	G	514	MET	SD-CE	6.15	1.95	1.79
1	D	130	GLU	CD-OE1	6.15	1.37	1.25
1	I	488	MET	SD-CE	-6.15	1.64	1.79
1	A	76	GLU	CD-OE2	6.14	1.37	1.25
1	D	446	ALA	CA-C	-6.14	1.44	1.52
1	K	445	ARG	NE-CZ	6.13	1.39	1.33
1	A	517	THR	CA-CB	-6.12	1.44	1.53
1	F	73	MET	CG-SD	6.11	1.96	1.80
1	B	20	VAL	CA-CB	-6.09	1.47	1.54
1	N	508	ALA	CA-CB	-6.08	1.43	1.53
1	N	109	ALA	N-CA	-6.08	1.38	1.46
1	A	39	VAL	CA-CB	-6.06	1.47	1.54
1	E	413	ALA	CA-CB	-6.05	1.43	1.53
1	F	12	ALA	CA-CB	-6.05	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	440	ILE	CA-CB	-6.05	1.47	1.54
1	I	458	CYS	C-O	-6.05	1.15	1.24
1	J	18	ARG	NE-CZ	6.05	1.39	1.33
1	I	508	ALA	CA-CB	-6.04	1.43	1.53
1	B	18	ARG	NE-CZ	6.03	1.39	1.33
1	G	20	VAL	CA-CB	-6.02	1.47	1.54
1	K	288	MET	SD-CE	6.02	1.94	1.79
1	D	127	ALA	C-O	-6.02	1.17	1.24
1	H	432	GLN	CA-C	-6.02	1.46	1.53
1	F	84	ALA	CA-C	-6.00	1.47	1.52
1	M	49	ILE	CA-CB	-5.98	1.47	1.54
1	E	20	VAL	CA-CB	-5.97	1.47	1.54
1	G	404	ARG	NE-CZ	5.97	1.39	1.33
1	M	511	ALA	CA-CB	-5.97	1.44	1.53
1	N	476	TYR	CA-C	-5.96	1.45	1.52
1	I	94	VAL	C-O	5.94	1.31	1.24
1	L	24	ALA	C-O	-5.94	1.17	1.24
1	G	480	ALA	CA-CB	-5.94	1.43	1.53
1	D	193	MET	SD-CE	5.93	1.94	1.79
1	C	493	ILE	CA-CB	-5.93	1.46	1.54
1	A	157	THR	CA-C	-5.93	1.45	1.52
1	I	81	ALA	CA-C	5.93	1.60	1.52
1	C	475	ASN	CA-C	-5.91	1.44	1.52
1	H	25	ASP	CA-C	-5.91	1.44	1.52
1	D	12	ALA	CA-CB	-5.91	1.44	1.53
1	K	73	MET	CG-SD	5.91	1.95	1.80
1	G	502	SER	C-O	-5.89	1.17	1.24
1	C	16	MET	SD-CE	5.89	1.94	1.79
1	C	446	ALA	CA-CB	-5.87	1.43	1.53
1	M	128	VAL	CA-CB	-5.87	1.47	1.54
1	C	336	VAL	CA-CB	5.86	1.61	1.54
1	G	57	ALA	CA-CB	-5.86	1.44	1.53
1	N	451	LEU	C-O	-5.86	1.17	1.24
1	N	520	MET	SD-CE	-5.85	1.65	1.79
1	E	503	ALA	CA-CB	-5.85	1.44	1.53
1	H	116	LEU	C-O	-5.83	1.17	1.24
1	G	105	LYS	C-O	5.82	1.30	1.24
1	G	16	MET	SD-CE	5.82	1.94	1.79
1	C	79	SER	C-O	-5.81	1.17	1.24
1	J	511	ALA	CA-CB	-5.81	1.44	1.53
1	M	31	LEU	CG-CD1	5.80	1.71	1.52
1	H	3	ALA	C-O	-5.80	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	106	ALA	CA-CB	-5.79	1.44	1.53
1	D	404	ARG	NE-CZ	5.79	1.39	1.33
1	I	434	GLU	CD-OE1	5.79	1.36	1.25
1	F	61	GLU	C-O	-5.78	1.17	1.23
1	C	478	TYR	CA-C	-5.78	1.45	1.52
1	G	94	VAL	C-O	5.78	1.31	1.24
1	H	99	ILE	CA-CB	-5.78	1.47	1.54
1	M	104	LEU	CA-C	-5.77	1.45	1.52
1	M	32	GLY	CA-C	5.77	1.60	1.51
1	J	68	ASN	C-O	-5.77	1.17	1.24
1	E	78	ALA	CA-C	-5.76	1.45	1.52
1	N	507	ALA	CA-C	-5.76	1.45	1.52
1	D	451	LEU	CA-C	-5.76	1.45	1.52
1	G	18	ARG	NE-CZ	5.76	1.39	1.33
1	G	46	ALA	CA-CB	-5.75	1.44	1.53
1	C	102	GLU	CG-CD	5.75	1.66	1.52
2	O	86	MET	SD-CE	-5.75	1.65	1.79
1	I	123	ALA	C-O	-5.75	1.17	1.24
1	J	405	ALA	CA-CB	-5.74	1.43	1.53
1	H	76	GLU	CD-OE1	5.74	1.36	1.25
1	G	157	THR	CA-C	-5.73	1.45	1.52
1	N	405	ALA	CA-CB	-5.73	1.43	1.53
1	J	104	LEU	C-O	-5.73	1.17	1.24
1	G	502	SER	CA-C	-5.72	1.45	1.52
1	C	99	ILE	N-CA	-5.72	1.39	1.46
1	E	71	ALA	CA-CB	-5.71	1.44	1.53
1	G	30	THR	CA-CB	-5.71	1.43	1.53
1	N	443	ALA	CA-CB	-5.71	1.43	1.53
1	H	24	ALA	CA-C	-5.71	1.45	1.52
1	A	465	VAL	CA-CB	-5.70	1.48	1.54
1	A	493	ILE	CA-CB	-5.70	1.46	1.54
1	I	23	LEU	CA-CB	-5.70	1.44	1.53
1	D	474	GLY	C-O	-5.70	1.16	1.23
1	C	496	PRO	C-O	-5.69	1.17	1.23
1	B	145	ALA	CA-CB	-5.69	1.44	1.53
1	C	446	ALA	C-O	-5.69	1.16	1.24
1	D	446	ALA	CA-CB	-5.69	1.44	1.53
1	I	89	THR	C-O	-5.68	1.17	1.24
1	D	62	LEU	CG-CD2	-5.68	1.33	1.52
1	J	26	ALA	C-O	-5.68	1.17	1.23
1	D	493	ILE	CA-CB	-5.67	1.46	1.54
1	I	112	ASN	C-O	-5.66	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	461	GLU	CD-OE1	5.66	1.36	1.25
1	M	521	VAL	CA-CB	-5.65	1.47	1.54
1	I	461	GLU	CD-OE1	5.64	1.36	1.25
1	H	30	THR	CA-CB	-5.64	1.44	1.53
1	A	107	VAL	CA-CB	-5.64	1.47	1.54
1	H	506	TYR	CA-C	-5.64	1.45	1.52
1	H	123	ALA	C-O	-5.63	1.17	1.24
1	H	503	ALA	C-O	-5.62	1.17	1.24
1	L	25	ASP	CA-C	-5.62	1.44	1.52
1	A	446	ALA	C-O	-5.62	1.16	1.24
1	L	118	ARG	NE-CZ	5.62	1.39	1.33
1	B	74	VAL	CA-CB	-5.62	1.46	1.54
1	D	478	TYR	CA-C	-5.62	1.46	1.52
1	I	88	GLY	C-O	5.61	1.32	1.24
1	K	128	VAL	CA-CB	-5.61	1.46	1.54
1	D	398	ASP	CB-CG	5.61	1.66	1.52
1	H	78	ALA	CA-CB	5.60	1.62	1.53
1	B	111	MET	CG-SD	5.60	1.94	1.80
1	C	420	ILE	C-O	5.60	1.31	1.24
1	C	418	ALA	CA-CB	-5.59	1.44	1.53
1	I	89	THR	CA-CB	-5.59	1.44	1.53
1	I	468	THR	C-O	-5.59	1.17	1.24
1	M	71	ALA	CA-CB	-5.58	1.44	1.53
1	B	503	ALA	CA-CB	-5.58	1.44	1.53
1	D	422	VAL	CA-CB	5.57	1.61	1.54
1	C	114	MET	SD-CE	5.57	1.93	1.79
1	D	458	CYS	C-O	-5.57	1.16	1.24
1	C	422	VAL	CA-CB	5.57	1.62	1.54
1	L	100	ILE	CA-CB	-5.56	1.48	1.54
1	C	520	MET	SD-CE	-5.55	1.65	1.79
1	J	28	LYS	CA-C	-5.55	1.45	1.52
1	I	18	ARG	NE-CZ	5.53	1.39	1.33
1	G	99	ILE	CA-CB	-5.53	1.47	1.54
1	G	493	ILE	CA-CB	-5.53	1.45	1.53
1	H	39	VAL	C-O	-5.52	1.17	1.24
1	I	108	ALA	CA-C	5.52	1.60	1.52
1	G	475	ASN	CA-C	-5.51	1.45	1.52
1	I	440	ILE	CA-CB	-5.51	1.48	1.54
1	G	112	ASN	C-O	-5.51	1.17	1.24
1	I	506	TYR	CA-C	-5.50	1.45	1.52
1	I	436	GLN	C-O	5.50	1.31	1.24
1	C	147	VAL	CA-CB	-5.50	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	125	THR	C-O	5.49	1.31	1.24
1	J	446	ALA	C-O	-5.49	1.16	1.24
1	I	104	LEU	C-O	-5.49	1.17	1.24
1	M	56	VAL	CA-CB	-5.49	1.48	1.54
1	N	518	GLU	CA-C	-5.49	1.45	1.52
1	D	469	VAL	CA-CB	-5.49	1.47	1.54
1	M	66	PHE	N-CA	5.49	1.53	1.46
1	I	32	GLY	CA-C	5.48	1.59	1.51
1	A	80	LYS	C-O	5.48	1.30	1.24
1	K	503	ALA	C-O	-5.48	1.17	1.24
1	G	488	MET	SD-CE	-5.47	1.65	1.79
1	G	445	ARG	NE-CZ	5.47	1.39	1.33
1	K	106	ALA	CA-CB	-5.47	1.44	1.53
1	L	445	ARG	NE-CZ	5.47	1.39	1.33
1	G	116	LEU	CA-C	-5.46	1.45	1.52
1	N	116	LEU	C-O	-5.46	1.17	1.24
1	H	419	LEU	CA-C	5.46	1.60	1.52
1	C	97	GLN	C-O	-5.46	1.17	1.24
1	J	118	ARG	NE-CZ	5.45	1.39	1.33
1	C	446	ALA	CA-C	-5.45	1.45	1.52
1	H	440	ILE	CA-CB	-5.45	1.48	1.54
1	N	76	GLU	CD-OE1	5.45	1.35	1.25
1	J	111	MET	SD-CE	5.44	1.93	1.79
1	K	114	MET	CG-SD	5.44	1.94	1.80
1	D	451	LEU	C-O	-5.44	1.17	1.24
1	D	126	ALA	CA-CB	-5.43	1.44	1.53
1	I	109	ALA	CA-CB	-5.43	1.45	1.53
1	M	464	VAL	CA-CB	-5.43	1.48	1.54
2	P	17	VAL	CA-CB	5.43	1.61	1.54
1	B	63	GLU	CA-C	-5.42	1.45	1.52
1	A	510	VAL	CA-CB	-5.42	1.48	1.54
1	C	96	ALA	CA-CB	-5.42	1.44	1.53
1	G	39	VAL	CA-CB	-5.42	1.47	1.54
2	R	17	VAL	CA-CB	5.41	1.61	1.54
1	C	12	ALA	CA-CB	-5.41	1.45	1.53
1	B	10	ASN	C-O	5.41	1.30	1.24
1	G	71	ALA	CA-CB	-5.41	1.44	1.53
1	H	100	ILE	C-O	-5.41	1.17	1.24
1	H	104	LEU	C-O	-5.41	1.17	1.24
1	I	57	ALA	CA-CB	-5.41	1.45	1.53
1	J	458	CYS	C-O	-5.40	1.16	1.24
1	E	506	TYR	C-O	-5.39	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	491	MET	CG-SD	-5.39	1.67	1.80
1	H	445	ARG	CZ-NH1	5.39	1.40	1.32
1	I	82	ASN	N-CA	-5.39	1.39	1.46
1	I	93	THR	CA-C	-5.39	1.45	1.52
1	E	26	ALA	CA-CB	-5.39	1.44	1.53
1	I	29	VAL	C-O	-5.39	1.18	1.24
1	N	87	ASP	CG-OD1	5.39	1.35	1.25
1	H	508	ALA	CA-CB	-5.39	1.45	1.53
1	G	498	LYS	C-O	-5.38	1.17	1.24
1	M	452	ARG	CB-CG	-5.38	1.36	1.52
1	C	503	ALA	CA-C	-5.38	1.46	1.52
1	I	509	SER	CA-C	5.38	1.59	1.52
1	D	379	ILE	CA-CB	-5.37	1.47	1.54
1	J	468	THR	C-O	-5.37	1.17	1.24
1	N	49	ILE	CA-CB	-5.37	1.48	1.54
1	E	144	ILE	CA-CB	-5.37	1.48	1.54
1	I	79	SER	CA-C	5.37	1.59	1.52
1	E	121	ASP	CG-OD1	5.37	1.35	1.25
1	N	74	VAL	CA-CB	-5.37	1.47	1.54
1	I	153	ASN	CA-C	5.36	1.59	1.52
1	H	514	MET	C-O	-5.35	1.17	1.24
1	I	14	VAL	CA-CB	-5.34	1.48	1.54
1	I	445	ARG	CA-C	-5.34	1.45	1.52
1	G	54	VAL	CA-CB	-5.33	1.46	1.54
1	H	40	LEU	CA-C	-5.33	1.46	1.52
1	E	99	ILE	CA-CB	-5.33	1.48	1.54
1	K	511	ALA	C-O	-5.33	1.17	1.24
1	B	483	GLU	CD-OE1	5.32	1.35	1.25
1	L	454	ILE	CA-CB	-5.32	1.48	1.54
1	A	60	ILE	CA-CB	-5.32	1.48	1.54
1	M	483	GLU	CD-OE2	5.32	1.35	1.25
1	K	74	VAL	CA-CB	-5.32	1.47	1.54
1	K	414	GLY	C-O	5.31	1.30	1.24
1	N	116	LEU	CA-C	-5.31	1.45	1.52
1	A	123	ALA	C-O	-5.31	1.18	1.24
1	I	105	LYS	C-O	-5.31	1.17	1.24
1	N	4	LYS	CA-C	-5.31	1.46	1.52
1	J	31	LEU	C-O	5.30	1.30	1.24
1	L	3	ALA	CA-CB	-5.30	1.44	1.53
1	F	74	VAL	CA-C	-5.30	1.45	1.52
1	G	478	TYR	CA-C	-5.30	1.46	1.52
1	J	461	GLU	CD-OE2	5.29	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	VAL	CA-C	-5.29	1.46	1.52
1	H	434	GLU	CD-OE1	5.29	1.35	1.25
1	E	454	ILE	CA-CB	-5.28	1.48	1.54
1	D	443	ALA	CA-CB	-5.27	1.45	1.53
1	F	90	THR	CA-C	-5.27	1.46	1.52
1	M	505	GLN	N-CA	-5.27	1.39	1.46
1	I	102	GLU	CG-CD	5.26	1.65	1.52
1	N	57	ALA	CA-CB	-5.26	1.45	1.53
1	N	431	GLY	N-CA	5.26	1.49	1.44
1	H	521	VAL	C-O	-5.26	1.18	1.24
2	O	17	VAL	CA-CB	5.25	1.61	1.54
1	G	13	ARG	C-O	-5.25	1.17	1.24
1	D	438	VAL	CA-CB	-5.24	1.48	1.54
1	C	432	GLN	CG-CD	5.24	1.65	1.52
1	A	418	ALA	CA-CB	-5.24	1.45	1.53
1	D	115	ASP	CG-OD2	5.24	1.35	1.25
1	D	140	ASP	CA-C	5.24	1.59	1.52
1	F	57	ALA	CA-CB	-5.23	1.45	1.53
1	J	508	ALA	CA-CB	-5.23	1.45	1.53
1	I	71	ALA	CA-CB	-5.23	1.45	1.53
1	B	446	ALA	C-O	-5.22	1.17	1.24
1	N	46	ALA	CA-CB	-5.22	1.44	1.52
1	G	10	ASN	CA-C	5.22	1.59	1.52
1	L	26	ALA	CA-CB	-5.22	1.45	1.53
1	I	502	SER	C-O	-5.21	1.18	1.24
1	C	8	PHE	C-O	5.21	1.30	1.23
1	M	506	TYR	CA-C	-5.21	1.46	1.52
1	C	510	VAL	C-O	-5.20	1.18	1.24
1	E	404	ARG	NE-CZ	5.20	1.38	1.33
1	K	11	ASP	CA-C	-5.20	1.46	1.52
1	B	449	ALA	CA-CB	-5.20	1.45	1.53
1	I	26	ALA	CA-CB	-5.20	1.45	1.53
1	A	43	SER	N-CA	5.20	1.52	1.46
1	C	404	ARG	NE-CZ	5.20	1.38	1.33
1	F	121	ASP	CG-OD1	5.20	1.35	1.25
1	G	107	VAL	CA-CB	-5.20	1.48	1.54
1	I	422	VAL	CB-CG2	-5.20	1.35	1.52
1	C	475	ASN	CA-CB	-5.19	1.46	1.53
1	E	480	ALA	CA-CB	-5.19	1.45	1.53
1	N	149	THR	CA-CB	5.19	1.61	1.53
1	H	467	ASN	C-O	-5.19	1.18	1.24
1	G	118	ARG	C-O	-5.18	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	90	THR	CA-CB	-5.18	1.45	1.53
1	K	116	LEU	C-O	-5.18	1.18	1.24
1	I	87	ASP	C-O	5.18	1.29	1.23
1	G	454	ILE	CA-CB	-5.17	1.48	1.54
1	H	93	THR	CA-C	-5.17	1.46	1.52
1	I	449	ALA	CA-C	-5.17	1.46	1.52
1	M	95	LEU	CA-C	-5.17	1.46	1.52
1	M	288	MET	SD-CE	5.17	1.92	1.79
1	B	38	VAL	CA-CB	-5.17	1.48	1.54
1	L	40	LEU	CA-C	-5.17	1.46	1.52
1	B	389	MET	SD-CE	5.16	1.92	1.79
1	A	63	GLU	CA-CB	-5.16	1.45	1.53
1	H	502	SER	C-O	-5.16	1.18	1.24
1	N	94	VAL	C-O	5.16	1.30	1.24
1	D	401	HIS	CA-C	-5.16	1.46	1.52
1	H	162	ILE	CA-CB	-5.16	1.48	1.54
1	L	414	GLY	C-O	5.16	1.29	1.24
1	M	6	VAL	CA-CB	-5.15	1.48	1.54
1	A	44	PHE	N-CA	5.15	1.52	1.46
1	H	469	VAL	CA-CB	-5.15	1.48	1.54
1	N	68	ASN	C-O	-5.14	1.18	1.24
1	E	508	ALA	CA-CB	-5.14	1.45	1.53
1	I	99	ILE	CB-CG1	5.14	1.63	1.53
1	B	11	ASP	C-O	-5.14	1.18	1.24
1	G	76	GLU	CD-OE1	5.13	1.35	1.25
1	B	127	ALA	C-O	-5.13	1.18	1.24
1	G	134	LEU	CA-C	-5.13	1.45	1.52
1	I	81	ALA	N-CA	5.13	1.52	1.46
1	L	511	ALA	CA-CB	-5.13	1.45	1.53
1	G	26	ALA	C-O	-5.13	1.17	1.24
1	J	478	TYR	CA-C	-5.12	1.46	1.52
1	L	6	VAL	CA-CB	-5.11	1.48	1.54
1	J	73	MET	SD-CE	-5.11	1.66	1.79
1	M	23	LEU	CA-CB	-5.11	1.45	1.53
1	H	93	THR	C-O	-5.11	1.18	1.24
1	A	427	ALA	CA-CB	-5.10	1.44	1.53
1	B	404	ARG	NE-CZ	5.10	1.38	1.33
1	B	506	TYR	CA-C	-5.10	1.46	1.52
1	I	30	THR	CA-CB	-5.09	1.45	1.53
1	D	514	MET	SD-CE	5.09	1.92	1.79
1	J	85	ALA	CA-CB	5.09	1.62	1.53
1	A	405	ALA	CA-CB	-5.08	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	ARG	CB-CG	-5.08	1.37	1.52
1	K	432	GLN	CA-C	-5.08	1.47	1.53
1	K	38	VAL	C-O	-5.08	1.18	1.24
1	N	467	ASN	N-CA	-5.08	1.40	1.46
1	A	79	SER	N-CA	-5.08	1.40	1.46
1	E	60	ILE	CA-CB	-5.08	1.48	1.54
1	H	87	ASP	CG-OD1	5.08	1.34	1.25
1	H	495	ASP	CG-OD2	5.07	1.34	1.25
1	E	26	ALA	CA-C	-5.07	1.46	1.52
1	C	105	LYS	CD-CE	5.07	1.67	1.52
1	L	510	VAL	C-O	-5.07	1.18	1.24
1	N	74	VAL	C-O	-5.06	1.18	1.24
1	B	123	ALA	C-O	-5.06	1.18	1.24
1	F	67	GLU	C-O	-5.06	1.17	1.24
1	M	92	ALA	CA-CB	-5.06	1.45	1.53
1	I	87	ASP	CG-OD1	5.05	1.34	1.25
1	B	458	CYS	CA-C	-5.05	1.45	1.52
1	G	398	ASP	CG-OD1	5.05	1.34	1.25
1	I	449	ALA	C-O	-5.05	1.19	1.24
1	A	144	ILE	CA-CB	-5.05	1.48	1.54
1	G	510	VAL	C-O	-5.05	1.18	1.24
1	N	488	MET	C-O	-5.05	1.17	1.24
1	D	99	ILE	C-O	-5.04	1.18	1.24
1	D	107	VAL	C-O	-5.04	1.18	1.24
1	E	465	VAL	CA-CB	-5.03	1.48	1.54
1	I	94	VAL	CA-CB	-5.03	1.48	1.54
1	A	96	ALA	C-O	-5.03	1.18	1.24
1	A	129	GLU	CD-OE2	5.03	1.34	1.25
1	C	11	ASP	C-O	-5.03	1.18	1.24
1	N	440	ILE	CA-CB	-5.02	1.48	1.54
1	B	12	ALA	CA-CB	-5.02	1.45	1.53
1	A	26	ALA	CA-CB	-5.02	1.45	1.53
1	D	468	THR	C-O	-5.02	1.17	1.24
1	C	462	PRO	C-O	-5.01	1.17	1.24
1	E	484	GLU	CD-OE2	5.01	1.34	1.25
1	D	163	ALA	CA-CB	-5.00	1.45	1.53
1	H	414	GLY	C-O	5.00	1.30	1.23
1	K	49	ILE	CA-CB	-5.00	1.48	1.54

All (415) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	116	LEU	N-CA-C	-10.56	99.77	111.28
1	B	116	LEU	N-CA-C	-10.04	100.33	111.28
1	J	414	GLY	N-CA-C	9.67	125.14	114.40
1	D	116	LEU	N-CA-C	-9.42	101.01	111.28
1	A	21	ASN	N-CA-C	9.41	122.40	111.11
1	I	77	VAL	N-CA-C	-9.39	101.19	110.30
1	I	116	LEU	N-CA-C	-9.08	101.27	111.71
1	B	415	GLY	N-CA-C	-9.04	100.98	114.90
1	G	77	VAL	N-CA-C	-8.97	102.10	110.53
1	A	415	GLY	N-CA-C	-8.88	102.96	115.30
1	A	100	ILE	N-CA-C	-8.78	102.28	110.53
1	I	136	VAL	N-CA-C	8.73	116.57	107.76
1	I	81	ALA	N-CA-C	-8.56	100.83	111.11
1	H	56	VAL	N-CA-C	-8.38	102.55	110.42
1	G	462	PRO	N-CD-CG	-8.30	90.74	103.20
1	J	416	GLY	N-CA-C	-8.23	103.45	115.30
1	B	100	ILE	N-CA-C	-8.17	102.85	110.53
1	H	77	VAL	N-CA-C	-8.14	102.12	111.00
1	D	446	ALA	N-CA-C	-8.04	103.49	113.38
1	N	414	GLY	N-CA-C	8.01	123.48	114.67
1	G	21	ASN	N-CA-C	7.95	119.58	111.07
1	A	78	ALA	N-CA-C	-7.93	102.72	111.36
1	A	116	LEU	N-CA-C	-7.90	102.62	111.07
1	A	67	GLU	N-CA-C	-7.87	102.70	111.28
1	A	77	VAL	N-CA-C	-7.81	102.49	111.00
1	B	78	ALA	N-CA-C	-7.77	102.81	111.82
1	H	416	GLY	N-CA-C	-7.69	104.22	115.30
1	D	523	ASP	N-CA-C	7.65	120.62	110.53
1	M	53	GLY	N-CA-C	7.60	122.10	112.83
1	L	416	GLY	N-CA-C	-7.54	104.44	115.30
1	J	51	LYS	N-CA-C	-7.52	102.64	112.41
1	K	523	ASP	N-CA-C	7.47	120.50	110.35
1	B	523	ASP	N-CA-C	7.38	120.10	110.43
1	K	51	LYS	N-CA-C	-7.33	102.88	112.41
1	E	21	ASN	N-CA-C	7.31	119.88	111.11
1	L	414	GLY	N-CA-C	7.30	122.70	114.67
1	M	81	ALA	N-CA-C	-7.30	103.01	110.97
1	I	109	ALA	N-CA-C	-7.28	104.55	113.50
1	M	82	ASN	N-CA-C	7.26	120.11	111.33
1	D	97	GLN	N-CA-C	-7.25	104.41	113.18
1	D	21	ASN	N-CA-C	7.24	119.17	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	81	ALA	N-CA-C	-7.19	103.38	111.07
1	D	77	VAL	N-CA-C	-7.18	103.78	110.53
1	G	329	THR	N-CA-C	7.16	119.18	107.23
1	C	124	VAL	N-CA-C	7.14	118.76	110.62
1	D	423	ALA	N-CA-C	7.14	123.15	111.37
1	N	523	ASP	N-CA-C	7.11	120.03	110.35
1	E	415	GLY	N-CA-C	-7.08	103.99	114.90
1	K	31	LEU	N-CA-C	7.08	118.64	111.07
1	I	325	ILE	N-CA-C	7.00	117.92	108.11
1	A	423	ALA	N-CA-C	7.00	118.91	111.28
1	J	55	SER	N-CA-C	6.99	118.97	111.36
1	L	31	LEU	N-CA-C	6.98	118.58	110.97
1	C	421	ARG	N-CA-C	-6.98	102.75	112.45
1	I	417	VAL	CB-CA-C	-6.95	103.12	111.81
1	D	95	LEU	N-CA-C	-6.95	103.47	112.23
1	I	510	VAL	CA-C-O	-6.93	113.74	120.95
1	B	86	GLY	N-CA-C	-6.93	105.50	114.85
1	D	48	THR	CA-C-N	-6.92	114.61	123.19
1	D	48	THR	C-N-CA	-6.92	114.61	123.19
1	G	499	VAL	N-CA-CB	6.89	118.61	110.55
1	B	451	LEU	N-CA-C	-6.86	103.80	111.28
1	K	77	VAL	N-CA-C	-6.86	104.08	110.53
1	J	523	ASP	N-CA-C	6.85	119.67	110.35
1	A	329	THR	N-CA-C	6.81	118.60	107.23
1	J	499	VAL	N-CA-CB	6.75	118.45	110.55
1	D	86	GLY	N-CA-C	-6.75	105.74	114.85
1	E	77	VAL	N-CA-C	-6.74	103.91	110.72
1	C	116	LEU	N-CA-C	-6.72	103.20	111.33
1	I	401	HIS	N-CA-C	6.70	119.20	111.02
1	D	124	VAL	N-CA-C	6.69	118.24	110.62
1	A	523	ASP	N-CA-C	6.68	119.35	110.53
1	N	77	VAL	N-CA-C	-6.67	104.02	110.42
1	I	452	ARG	NE-CZ-NH2	6.64	125.18	119.20
1	I	48	THR	OG1-CB-CG2	-6.63	96.05	109.30
1	A	95	LEU	N-CA-C	-6.62	104.14	111.82
1	M	126	ALA	N-CA-C	-6.58	104.03	111.14
1	N	116	LEU	N-CA-C	-6.57	104.12	111.28
1	A	473	ASP	N-CA-C	6.56	118.91	109.14
1	I	124	VAL	N-CA-C	6.55	116.71	110.42
1	I	523	ASP	N-CA-C	6.54	119.25	110.35
1	D	67	GLU	N-CA-C	-6.54	104.15	111.28
1	H	462	PRO	N-CD-CG	-6.53	93.41	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	325	ILE	N-CA-C	6.51	117.23	108.11
1	M	32	GLY	N-CA-C	6.50	125.61	112.34
1	I	133	ALA	N-CA-C	-6.47	103.74	111.69
1	F	67	GLU	N-CA-C	-6.46	104.28	111.71
1	H	514	MET	N-CA-C	6.43	118.29	111.28
1	D	25	ASP	N-CA-C	6.40	119.06	111.71
1	K	60	ILE	N-CA-C	6.38	117.28	109.30
1	C	146	GLN	CA-C-N	-6.37	112.54	120.56
1	C	146	GLN	C-N-CA	-6.37	112.54	120.56
1	G	446	ALA	N-CA-C	-6.34	105.54	113.28
1	A	26	ALA	N-CA-C	-6.34	105.03	112.89
2	T	65	VAL	N-CA-C	6.33	117.60	108.48
1	G	417	VAL	N-CA-C	-6.30	104.14	111.00
1	B	77	VAL	N-CA-C	-6.30	104.36	110.72
2	U	65	VAL	N-CA-C	6.29	117.55	108.48
1	I	60	ILE	N-CA-C	6.29	117.16	109.30
1	J	77	VAL	N-CA-C	-6.29	104.37	110.72
1	K	499	VAL	N-CA-CB	6.29	117.91	110.55
2	Q	65	VAL	N-CA-C	6.29	117.53	108.48
1	G	100	ILE	N-CA-C	-6.28	104.63	110.53
1	D	78	ALA	N-CA-C	-6.26	104.53	111.36
1	N	417	VAL	CB-CA-C	-6.26	103.96	111.97
1	F	26	ALA	N-CA-C	-6.22	104.04	111.69
1	J	462	PRO	N-CD-CG	-6.21	93.88	103.20
1	B	67	GLU	N-CA-C	-6.21	104.51	111.28
1	N	48	THR	OG1-CB-CG2	-6.20	96.91	109.30
1	H	26	ALA	N-CA-C	-6.19	103.12	112.04
1	L	51	LYS	N-CA-C	-6.18	104.37	112.41
1	H	96	ALA	N-CA-C	-6.16	104.64	111.36
1	A	385	THR	CB-CA-C	-6.16	106.70	114.40
1	F	77	VAL	N-CA-C	-6.15	104.75	110.53
2	O	65	VAL	N-CA-C	6.13	117.31	108.48
1	F	523	ASP	N-CA-C	6.13	117.95	110.41
1	K	462	PRO	N-CD-CG	-6.12	94.02	103.20
1	B	21	ASN	N-CA-C	6.11	118.45	111.11
1	K	124	VAL	N-CA-C	6.09	116.27	110.42
1	J	60	ILE	N-CA-C	6.09	116.92	109.30
1	L	33	PRO	N-CA-C	-6.09	106.05	114.27
1	D	31	LEU	N-CA-C	6.08	119.08	109.96
1	H	427	ALA	N-CA-C	6.08	119.96	112.54
1	M	42	LYS	N-CA-C	-6.07	99.50	108.79
1	M	94	VAL	O-C-N	6.07	128.00	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	422	VAL	N-CA-CB	6.06	119.67	110.58
1	L	325	ILE	N-CA-C	6.06	116.60	108.11
1	B	39	VAL	CB-CA-C	-6.05	102.12	110.96
1	M	60	ILE	N-CA-C	6.05	117.39	109.58
1	M	462	PRO	N-CD-CG	-6.05	94.13	103.20
1	D	428	ASP	N-CA-C	6.05	120.36	112.92
1	B	499	VAL	N-CA-C	6.04	116.81	110.72
1	H	517	THR	OG1-CB-CG2	-6.03	97.23	109.30
1	I	10	ASN	N-CA-C	6.02	118.37	111.02
1	M	499	VAL	N-CA-CB	6.01	118.27	110.57
1	A	146	GLN	CA-C-N	-6.01	112.99	120.56
1	A	146	GLN	C-N-CA	-6.01	112.99	120.56
1	I	42	LYS	N-CA-C	-6.00	99.94	109.07
1	A	48	THR	CA-C-N	-6.00	114.32	122.91
1	A	48	THR	C-N-CA	-6.00	114.32	122.91
2	R	65	VAL	N-CA-C	6.00	117.13	108.48
1	B	423	ALA	N-CA-C	6.00	118.59	111.33
1	C	21	ASN	N-CA-C	5.99	117.48	111.07
1	J	325	ILE	N-CA-C	5.98	116.48	108.11
1	M	55	SER	N-CA-C	5.97	117.46	111.07
1	N	144	ILE	N-CA-C	-5.97	104.51	110.30
1	I	51	LYS	N-CA-C	-5.94	104.69	112.41
1	A	499	VAL	N-CA-CB	5.94	117.50	110.55
1	G	488	MET	N-CA-C	5.94	117.75	111.28
1	C	329	THR	N-CA-C	5.94	118.90	107.44
1	G	500	THR	OG1-CB-CG2	-5.92	97.45	109.30
1	J	8	PHE	N-CA-C	5.92	119.18	109.72
1	C	35	GLY	CA-C-O	-5.91	116.26	121.58
1	K	473	ASP	N-CA-C	5.90	118.67	109.52
1	H	522	THR	OG1-CB-CG2	-5.90	97.49	109.30
1	K	325	ILE	N-CA-C	5.89	116.97	108.48
1	B	127	ALA	N-CA-C	-5.89	104.86	111.28
1	F	499	VAL	N-CA-CB	5.89	118.11	110.57
1	F	146	GLN	CA-C-N	-5.89	112.39	120.46
1	F	146	GLN	C-N-CA	-5.89	112.39	120.46
1	M	325	ILE	N-CA-C	5.88	116.35	108.11
1	N	475	ASN	N-CA-C	5.88	120.71	112.72
1	F	434	GLU	N-CA-C	5.87	117.67	111.28
1	I	20	VAL	CA-C-O	-5.87	115.17	121.27
1	B	146	GLN	CA-C-N	-5.86	113.18	120.56
1	B	146	GLN	C-N-CA	-5.86	113.18	120.56
1	C	499	VAL	N-CA-CB	5.86	117.40	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	496	PRO	CA-C-O	-5.85	114.64	121.95
1	N	473	ASP	N-CA-C	5.83	118.05	109.24
2	Q	76	GLU	N-CA-C	5.83	117.83	109.14
1	B	434	GLU	N-CA-C	5.83	117.63	111.28
1	N	94	VAL	CB-CA-C	-5.82	104.28	112.14
1	D	91	THR	OG1-CB-CG2	-5.79	97.71	109.30
1	J	438	VAL	N-CA-C	-5.79	104.71	110.62
1	I	126	ALA	N-CA-C	-5.79	104.89	111.14
1	B	462	PRO	N-CD-CG	-5.77	94.54	103.20
1	A	31	LEU	N-CA-C	5.77	118.93	109.76
1	B	50	THR	N-CA-C	5.77	118.04	108.99
1	H	109	ALA	N-CA-C	-5.76	106.42	113.50
1	A	449	ALA	N-CA-C	5.76	121.34	113.16
1	K	126	ALA	N-CA-C	-5.75	104.92	111.14
1	E	196	ASP	N-CA-C	5.75	118.68	110.68
1	I	445	ARG	N-CA-C	-5.73	105.78	112.89
1	M	183	LEU	N-CA-C	-5.73	106.13	113.23
1	N	29	VAL	N-CA-C	-5.73	105.82	112.98
1	I	510	VAL	N-CA-CB	5.72	118.33	110.54
1	D	329	THR	N-CA-C	5.72	118.48	107.44
1	L	109	ALA	N-CA-C	-5.72	106.14	113.23
1	C	514	MET	CG-SD-CE	-5.72	88.32	100.90
1	E	124	VAL	N-CA-C	5.72	116.45	110.62
1	I	21	ASN	N-CA-C	5.71	117.97	111.11
1	A	124	VAL	N-CA-C	5.70	116.44	110.62
1	C	94	VAL	O-C-N	5.70	128.24	121.80
1	B	428	ASP	N-CA-C	5.70	119.92	112.92
1	B	8	PHE	N-CA-C	5.69	119.00	109.95
1	C	385	THR	CB-CA-C	-5.69	107.29	114.40
1	I	510	VAL	N-CA-C	-5.69	104.82	110.62
1	E	385	THR	CB-CA-C	-5.68	107.30	114.40
1	F	415	GLY	N-CA-C	-5.67	106.16	114.90
1	M	240	VAL	N-CA-C	5.67	116.31	110.82
1	B	499	VAL	N-CA-CB	5.66	119.08	110.58
1	D	411	VAL	CB-CA-C	-5.66	101.95	110.55
1	E	91	THR	OG1-CB-CG2	-5.66	97.99	109.30
1	E	116	LEU	N-CA-C	-5.65	105.12	111.28
1	H	33	PRO	N-CA-C	-5.65	106.65	114.27
1	N	39	VAL	N-CA-C	-5.63	100.30	108.36
1	C	79	SER	CA-CB-OG	-5.63	99.83	111.10
1	G	385	THR	CB-CA-C	-5.63	107.37	114.40
1	K	21	ASN	N-CA-C	5.63	118.14	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	LEU	N-CA-C	-5.62	105.14	112.23
1	N	458	CYS	CA-CB-SG	-5.62	101.46	114.40
1	H	414	GLY	N-CA-C	5.62	124.66	115.73
1	J	22	VAL	N-CA-C	5.61	115.81	110.42
1	G	39	VAL	CB-CA-C	-5.61	103.21	110.84
1	B	94	VAL	N-CA-C	5.61	118.06	111.05
1	B	95	LEU	N-CA-C	-5.59	104.81	111.69
1	G	428	ASP	N-CA-C	5.59	119.80	112.92
1	D	146	GLN	CA-C-N	-5.59	113.52	120.56
1	D	146	GLN	C-N-CA	-5.59	113.52	120.56
1	I	108	ALA	CA-C-O	5.58	126.31	119.05
1	N	60	ILE	N-CA-C	5.58	116.25	108.89
1	M	69	MET	CA-C-N	5.56	126.28	119.99
1	M	69	MET	C-N-CA	5.56	126.28	119.99
1	J	10	ASN	N-CA-C	5.56	117.02	111.07
1	E	78	ALA	N-CA-C	-5.56	105.30	111.36
1	I	104	LEU	N-CA-C	-5.55	105.38	111.82
1	H	412	VAL	N-CA-C	5.55	116.16	108.23
1	N	484	GLU	N-CA-C	5.54	118.58	109.72
1	J	331	THR	CB-CA-C	5.53	118.66	110.14
1	N	422	VAL	N-CA-C	-5.53	105.14	110.72
1	N	517	THR	OG1-CB-CG2	-5.52	98.25	109.30
1	B	510	VAL	N-CA-C	5.52	115.72	110.42
1	C	13	ARG	N-CA-C	5.52	117.10	111.14
1	H	60	ILE	N-CA-C	5.51	116.19	109.30
1	F	462	PRO	N-CD-CG	-5.51	94.93	103.20
1	A	104	LEU	N-CA-C	-5.51	105.66	112.38
1	J	517	THR	OG1-CB-CG2	-5.51	98.28	109.30
1	M	51	LYS	N-CA-C	-5.51	105.87	112.59
1	L	499	VAL	N-CA-CB	5.50	116.99	110.55
1	L	517	THR	OG1-CB-CG2	-5.50	98.30	109.30
1	H	126	ALA	N-CA-C	-5.49	105.21	111.14
1	K	33	PRO	N-CA-C	-5.49	106.86	114.27
1	A	409	GLU	N-CA-C	5.49	121.20	113.02
1	D	473	ASP	N-CA-C	5.49	117.53	109.24
1	I	88	GLY	CA-C-O	5.49	125.29	119.03
1	I	462	PRO	N-CD-CG	-5.49	94.97	103.20
1	L	108	ALA	N-CA-C	-5.49	106.43	113.01
1	J	170	GLY	N-CA-C	-5.48	105.77	112.68
1	E	74	VAL	N-CA-C	-5.48	104.24	111.09
1	G	507	ALA	N-CA-C	-5.47	105.22	111.07
1	D	100	ILE	N-CA-C	-5.46	105.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	451	LEU	CA-C-N	-5.45	112.91	120.38
1	N	451	LEU	C-N-CA	-5.45	112.91	120.38
1	D	134	LEU	CB-CA-C	-5.44	100.56	110.63
1	J	183	LEU	N-CA-C	-5.44	106.48	113.23
1	M	48	THR	OG1-CB-CG2	-5.44	98.42	109.30
1	N	32	GLY	N-CA-C	5.43	123.42	112.34
1	C	75	LYS	CA-C-O	5.43	125.94	119.10
1	H	51	LYS	N-CA-C	-5.42	105.97	112.59
1	N	426	LEU	N-CA-C	5.42	119.62	111.81
1	C	29	VAL	CA-C-N	-5.42	112.56	122.38
1	C	29	VAL	C-N-CA	-5.42	112.56	122.38
1	N	33	PRO	N-CA-C	-5.42	106.95	114.27
1	D	415	GLY	N-CA-C	-5.42	106.56	114.90
1	E	434	GLU	N-CA-C	5.42	117.18	111.28
1	E	462	PRO	N-CD-CG	-5.42	95.08	103.20
1	G	9	GLY	CA-C-N	-5.42	113.02	120.28
1	G	9	GLY	C-N-CA	-5.42	113.02	120.28
1	M	33	PRO	N-CA-C	-5.42	106.96	114.27
1	K	444	LEU	N-CA-C	-5.41	105.28	111.07
1	A	510	VAL	CA-C-O	-5.41	115.50	121.29
1	L	438	VAL	N-CA-C	-5.41	103.71	111.17
1	E	48	THR	CA-C-N	-5.40	115.18	122.91
1	E	48	THR	C-N-CA	-5.40	115.18	122.91
1	B	96	ALA	N-CA-C	-5.40	105.42	112.23
1	E	428	ASP	N-CA-C	5.40	119.56	112.92
1	N	94	VAL	N-CA-C	5.40	116.12	110.62
1	F	329	THR	N-CA-C	5.39	117.84	107.44
1	C	9	GLY	CA-C-N	-5.39	113.06	120.28
1	C	9	GLY	C-N-CA	-5.39	113.06	120.28
1	I	175	ILE	N-CA-C	5.37	115.59	107.75
1	J	154	SER	N-CA-C	5.36	118.59	111.30
1	B	79	SER	CA-CB-OG	-5.36	100.39	111.10
1	F	49	ILE	CG1-CB-CG2	-5.36	94.62	110.70
1	H	10	ASN	N-CA-C	5.36	116.81	110.97
1	C	101	THR	OG1-CB-CG2	-5.35	98.59	109.30
1	J	101	THR	OG1-CB-CG2	-5.35	98.60	109.30
2	P	76	GLU	N-CA-C	5.35	117.11	109.14
2	T	76	GLU	N-CA-C	5.35	117.11	109.14
1	E	29	VAL	N-CA-C	-5.34	106.06	113.00
1	E	464	VAL	N-CA-C	5.34	115.54	110.42
1	I	69	MET	CA-C-N	5.34	126.02	119.99
1	I	69	MET	C-N-CA	5.34	126.02	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	80	LYS	N-CA-C	5.33	117.53	111.02
1	I	18	ARG	N-CA-CB	5.33	117.95	110.12
2	O	76	GLU	N-CA-C	5.32	117.07	109.14
1	E	106	ALA	N-CA-C	-5.32	105.15	111.69
1	I	453	GLN	CA-C-O	-5.32	114.86	120.55
1	C	414	GLY	O-C-N	-5.31	118.57	122.71
1	G	149	THR	N-CA-C	5.30	117.47	111.11
1	N	499	VAL	N-CA-CB	5.30	116.76	110.55
1	B	91	THR	OG1-CB-CG2	-5.30	98.70	109.30
1	L	77	VAL	N-CA-CB	-5.30	104.84	110.62
1	B	26	ALA	N-CA-C	-5.29	105.56	112.23
1	B	329	THR	N-CA-C	5.29	116.95	107.80
1	M	426	LEU	N-CA-C	5.29	119.42	111.81
1	C	20	VAL	CA-C-N	-5.29	113.57	120.44
1	C	20	VAL	C-N-CA	-5.29	113.57	120.44
1	I	79	SER	CA-C-N	5.29	127.62	120.38
1	I	79	SER	C-N-CA	5.29	127.62	120.38
1	C	523	ASP	N-CA-C	5.28	117.49	110.53
2	R	76	GLU	N-CA-C	5.28	117.00	109.14
1	D	395	ARG	N-CA-C	-5.27	105.12	112.45
1	C	34	LYS	CA-C-N	5.26	125.68	120.31
1	C	34	LYS	C-N-CA	5.26	125.68	120.31
1	F	116	LEU	N-CA-C	-5.26	104.96	111.33
1	H	417	VAL	CB-CA-C	-5.26	105.08	111.87
1	N	109	ALA	N-CA-C	-5.26	106.71	113.23
1	A	460	GLU	N-CA-C	5.25	118.15	109.85
1	F	13	ARG	N-CA-C	5.25	116.81	111.14
1	I	450	PRO	N-CD-CG	-5.25	95.32	103.20
1	J	26	ALA	N-CA-C	-5.25	104.47	112.04
1	I	468	THR	N-CA-CB	5.25	118.02	110.20
1	A	452	ARG	N-CA-C	5.25	117.00	111.28
1	G	89	THR	OG1-CB-CG2	-5.25	98.81	109.30
1	M	517	THR	CA-C-N	-5.25	113.99	122.23
1	M	517	THR	C-N-CA	-5.25	113.99	122.23
1	J	108	ALA	N-CA-C	-5.24	106.84	113.18
1	G	67	GLU	N-CA-C	-5.24	105.57	111.28
1	I	70	GLY	N-CA-C	-5.24	106.30	112.64
1	A	39	VAL	CB-CA-C	-5.24	103.81	110.98
1	M	149	THR	N-CA-C	5.24	116.99	111.28
1	K	52	ASP	N-CA-C	5.23	118.21	107.69
1	N	51	LYS	N-CA-C	-5.22	106.23	112.59
1	A	29	VAL	CA-C-N	-5.21	112.94	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	VAL	C-N-CA	-5.21	112.94	122.38
1	I	444	LEU	O-C-N	5.21	127.44	122.07
1	L	48	THR	OG1-CB-CG2	-5.20	98.90	109.30
1	I	32	GLY	N-CA-C	5.19	122.94	112.34
1	B	9	GLY	CA-C-N	-5.19	113.32	120.28
1	B	9	GLY	C-N-CA	-5.19	113.32	120.28
2	U	76	GLU	N-CA-C	5.19	116.87	109.14
1	E	26	ALA	N-CA-C	-5.18	105.71	111.36
1	G	87	ASP	N-CA-C	-5.17	101.40	108.38
1	I	33	PRO	N-CA-C	-5.17	107.29	114.27
1	L	39	VAL	N-CA-C	-5.17	100.97	108.36
1	A	149	THR	N-CA-C	5.16	116.59	111.07
1	D	56	VAL	N-CA-C	-5.16	105.47	110.42
1	E	146	GLN	CA-C-N	-5.16	113.39	120.46
1	E	146	GLN	C-N-CA	-5.16	113.39	120.46
1	I	426	LEU	N-CA-C	5.16	119.73	112.72
1	H	116	LEU	N-CA-C	-5.16	105.09	111.33
1	J	454	ILE	CB-CA-C	-5.16	105.28	111.88
1	B	458	CYS	N-CA-C	-5.15	106.69	113.17
1	F	74	VAL	CB-CA-C	-5.14	104.19	112.16
1	N	136	VAL	N-CA-C	5.14	113.53	107.77
1	A	428	ASP	N-CA-C	5.14	119.51	112.88
1	H	425	LYS	CA-C-N	-5.14	114.42	122.95
1	H	425	LYS	C-N-CA	-5.14	114.42	122.95
1	B	80	LYS	N-CA-C	5.14	116.57	111.07
1	D	460	GLU	N-CA-C	5.13	117.67	109.81
1	J	473	ASP	N-CA-C	5.13	117.61	109.50
1	I	23	LEU	CB-CA-C	-5.13	102.27	110.79
1	M	170	GLY	N-CA-C	-5.13	106.54	112.29
1	D	90	THR	CB-CA-C	-5.13	102.83	110.88
1	H	413	ALA	N-CA-C	5.12	118.22	110.64
1	I	240	VAL	N-CA-C	5.12	115.79	110.82
2	P	65	VAL	N-CA-C	5.12	116.73	108.85
1	L	76	GLU	N-CA-C	5.12	116.94	111.36
1	N	93	THR	OG1-CB-CG2	-5.12	99.07	109.30
1	L	56	VAL	N-CA-C	-5.11	105.34	110.30
1	G	26	ALA	N-CA-C	-5.11	105.79	112.23
1	B	48	THR	CA-C-N	-5.11	115.61	122.91
1	B	48	THR	C-N-CA	-5.11	115.61	122.91
1	J	32	GLY	N-CA-C	5.11	122.76	112.34
1	D	499	VAL	N-CA-CB	5.10	118.23	110.58
1	N	431	GLY	CA-C-O	-5.10	116.82	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	ASP	N-CA-C	5.10	117.16	109.41
1	J	136	VAL	N-CA-C	5.10	113.48	107.77
1	F	95	LEU	N-CA-C	-5.10	105.42	111.69
2	S	76	GLU	N-CA-C	5.10	116.73	109.14
1	I	443	ALA	N-CA-C	-5.10	105.81	112.23
1	G	71	ALA	N-CA-C	-5.09	105.91	111.82
1	E	97	GLN	N-CA-C	-5.09	106.33	112.54
1	C	100	ILE	N-CA-C	-5.09	105.75	110.53
1	J	74	VAL	CB-CA-C	-5.09	104.27	112.16
1	J	108	ALA	CA-C-O	5.09	125.62	119.11
1	C	140	ASP	N-CA-C	5.09	117.81	110.28
1	B	124	VAL	N-CA-C	5.08	116.42	110.62
1	C	91	THR	O-C-N	5.08	127.31	122.03
1	H	325	ILE	N-CA-C	5.08	115.22	108.11
1	K	480	ALA	N-CA-C	5.07	118.57	112.38
1	F	499	VAL	N-CA-C	5.07	115.30	110.53
1	J	196	ASP	N-CA-C	5.07	118.56	110.70
1	G	499	VAL	N-CA-C	5.06	115.28	110.42
1	H	508	ALA	N-CA-C	5.06	116.49	111.07
1	D	401	HIS	CB-CA-C	-5.06	101.44	110.70
1	F	50	THR	N-CA-C	5.06	116.75	108.76
1	C	483	GLU	CB-CA-C	-5.06	104.75	111.63
1	E	395	ARG	N-CA-C	-5.05	105.23	111.40
1	L	431	GLY	CA-C-O	-5.05	116.87	121.72
1	D	90	THR	CA-C-O	-5.05	115.52	120.82
1	K	36	ARG	N-CA-C	-5.05	102.99	110.46
1	K	94	VAL	CB-CA-C	-5.05	105.33	112.14
1	M	77	VAL	N-CA-C	-5.04	105.41	110.30
1	F	464	VAL	N-CA-C	5.04	115.65	110.36
1	E	473	ASP	N-CA-C	5.03	117.05	109.41
1	G	473	ASP	N-CA-C	5.02	117.05	109.41
1	D	8	PHE	N-CA-C	5.02	117.75	109.72
1	E	446	ALA	N-CA-C	-5.01	107.16	113.28
1	C	39	VAL	CB-CA-C	-5.01	103.36	110.83
1	E	329	THR	N-CA-C	5.01	117.10	107.44
1	G	421	ARG	CA-C-N	-5.00	112.54	120.55
1	G	421	ARG	C-N-CA	-5.00	112.54	120.55
1	J	465	VAL	N-CA-C	-5.00	105.83	110.53

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	SER	Peptide
1	H	32	GLY	Peptide
1	I	32	GLY	Peptide
1	J	32	GLY	Peptide
1	K	32	GLY	Peptide
1	L	32	GLY	Peptide
1	M	32	GLY	Peptide
1	N	32	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3974	170	0
1	B	3855	0	3976	163	0
1	C	3855	0	3975	168	0
1	D	3855	0	3976	156	0
1	E	3855	0	3975	137	0
1	F	3855	0	3976	147	0
1	G	3855	0	3974	169	0
1	H	3856	0	3976	135	0
1	I	3856	0	3976	189	0
1	J	3856	0	3976	159	0
1	K	3856	0	3976	146	0
1	L	3856	0	3976	155	0
1	M	3856	0	3976	163	0
1	N	3856	0	3976	165	0
2	O	728	0	762	30	0
2	P	728	0	762	26	0
2	Q	728	0	762	28	0
2	R	728	0	762	24	0
2	S	728	0	762	26	0
2	T	728	0	762	31	0
2	U	728	0	762	28	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	27	0	12	2	0
5	B	27	0	12	1	0
5	C	27	0	12	3	0
5	D	27	0	12	3	0
5	E	27	0	12	1	0
5	F	27	0	12	2	0
5	G	27	0	12	1	0
6	A	4	0	0	3	0
6	B	4	0	0	0	0
6	C	4	0	0	2	0
6	D	4	0	0	2	0
6	E	4	0	0	1	0
6	F	4	0	0	2	0
6	G	4	0	0	1	0
7	A	19	0	0	2	0
7	B	10	0	0	1	0
7	C	21	0	0	5	0
7	D	14	0	0	4	0
7	E	12	0	0	3	0
7	F	11	0	0	3	0
7	G	20	0	0	2	0
7	H	11	0	0	2	0
7	I	17	0	0	4	0
7	J	12	0	0	1	0
7	K	14	0	0	2	0
7	L	13	0	0	3	0
7	M	10	0	0	6	0
7	N	10	0	0	5	0
All	All	59498	0	61076	2309	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (2309) 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:N:288:MET:CE	1:N:288:MET:SD	2.01	1.46
1:F:114:MET:CE	1:F:114:MET:SD	2.02	1.46
1:I:447:MET:CE	1:I:447:MET:SD	2.05	1.45
1:K:16:MET:CE	1:K:16:MET:SD	2.05	1.45
1:B:114:MET:CE	1:B:114:MET:SD	2.04	1.45
1:J:288:MET:CE	1:J:288:MET:SD	2.04	1.45
1:B:16:MET:CE	1:B:16:MET:SD	2.05	1.44
1:M:514:MET:SD	1:M:514:MET:CE	2.04	1.44
1:I:16:MET:CE	1:I:16:MET:SD	2.05	1.44
1:L:114:MET:CE	1:L:114:MET:SD	2.04	1.44
1:M:16:MET:CE	1:M:16:MET:SD	2.04	1.44
1:A:114:MET:CE	1:A:114:MET:SD	2.02	1.44
1:C:111:MET:CE	1:C:111:MET:SD	2.06	1.43
1:G:111:MET:CE	1:G:111:MET:SD	2.07	1.43
1:F:16:MET:CE	1:F:16:MET:SD	2.07	1.42
1:K:114:MET:CE	1:K:114:MET:SD	2.07	1.41
1:I:114:MET:CE	1:I:114:MET:SD	2.09	1.39
1:J:16:MET:CE	1:J:16:MET:SD	2.09	1.39
1:B:73:MET:SD	1:B:73:MET:CE	2.10	1.39
1:N:114:MET:CE	1:N:114:MET:SD	2.11	1.39
1:A:111:MET:CE	1:A:111:MET:SD	2.13	1.37
1:F:111:MET:CE	1:F:111:MET:SD	2.13	1.36
1:J:514:MET:SD	1:J:514:MET:CE	2.13	1.36
1:B:111:MET:SD	1:B:111:MET:CE	2.14	1.35
1:C:514:MET:CE	1:C:514:MET:SD	2.13	1.35
1:D:111:MET:CE	1:D:111:MET:SD	2.13	1.35
1:H:514:MET:CE	1:H:514:MET:SD	2.15	1.34
1:M:114:MET:CE	1:M:114:MET:SD	2.13	1.34
1:D:73:MET:CE	1:D:73:MET:SD	2.17	1.33
1:E:111:MET:CE	1:E:111:MET:SD	2.18	1.31
1:E:73:MET:CE	1:E:73:MET:SD	2.19	1.30
1:J:114:MET:CE	1:J:114:MET:SD	2.19	1.30
1:N:16:MET:CE	1:N:16:MET:SD	2.20	1.29
1:G:73:MET:CE	1:G:73:MET:SD	2.21	1.28
1:B:514:MET:SD	1:B:514:MET:CE	2.21	1.28
1:H:114:MET:SD	1:H:114:MET:CE	2.23	1.26
1:N:514:MET:CE	1:N:514:MET:SD	2.24	1.26
1:C:18:ARG:CB	1:C:18:ARG:HH11	1.52	1.23
1:A:73:MET:CE	1:A:73:MET:SD	2.27	1.23
1:F:73:MET:CE	1:F:73:MET:SD	2.27	1.22
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.06	1.17
1:C:73:MET:CE	1:C:73:MET:SD	2.32	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.10	1.16
1:C:18:ARG:HB3	1:C:18:ARG:NH1	1.60	1.15
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.22	1.14
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.05	1.14
1:B:18:ARG:CB	1:B:18:ARG:HH11	1.61	1.13
1:F:430:ARG:HG2	1:F:430:ARG:HH11	1.04	1.13
1:B:18:ARG:NH1	1:B:18:ARG:HB3	1.64	1.11
1:G:90:THR:O	1:G:94:VAL:HG23	1.47	1.11
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.00	1.10
1:J:404:ARG:HG2	1:J:404:ARG:HH11	1.11	1.10
1:C:18:ARG:HH11	1:C:18:ARG:CG	1.65	1.10
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.11	1.09
1:D:430:ARG:HG2	1:D:430:ARG:HH11	1.16	1.09
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.05	1.07
1:F:18:ARG:CB	1:F:18:ARG:HH11	1.68	1.06
1:H:326:ASN:HD22	1:H:329:THR:HB	1.20	1.06
1:I:404:ARG:HG2	1:I:404:ARG:HH11	1.11	1.05
1:E:430:ARG:HH11	1:E:430:ARG:HG2	0.89	1.05
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.19	1.05
1:A:452:ARG:NH1	7:A:614:HOH:O	1.88	1.04
1:N:404:ARG:HG2	1:N:404:ARG:HH11	1.21	1.04
1:I:444:LEU:HD23	1:I:447:MET:CE	1.87	1.04
1:C:90:THR:O	1:C:94:VAL:HG23	1.56	1.03
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.40	1.03
1:L:444:LEU:HA	1:L:447:MET:HE3	1.32	1.03
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.41	1.02
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.42	1.01
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.42	1.00
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.43	1.00
1:D:18:ARG:HH11	1:D:18:ARG:CG	1.73	1.00
1:I:326:ASN:HD22	1:I:329:THR:HB	1.25	1.00
1:E:18:ARG:CB	1:E:18:ARG:HH11	1.74	1.00
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.26	1.00
1:A:18:ARG:HH11	1:A:18:ARG:CG	1.74	0.99
1:B:305:ILE:HG12	1:C:267:MET:HE3	1.45	0.99
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.41	0.99
1:J:326:ASN:HD22	1:J:329:THR:HB	1.26	0.98
1:E:18:ARG:HH11	1:E:18:ARG:CG	1.76	0.98
1:A:18:ARG:HH11	1:A:18:ARG:CB	1.76	0.98
1:N:444:LEU:HA	1:N:447:MET:HE3	1.45	0.98
1:N:326:ASN:HD22	1:N:329:THR:HB	1.23	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:444:LEU:HA	1:J:447:MET:HE3	1.45	0.98
1:L:326:ASN:HD22	1:L:329:THR:HB	1.26	0.98
1:E:430:ARG:HG2	1:E:430:ARG:NH1	1.65	0.97
1:G:18:ARG:CB	1:G:18:ARG:HH11	1.76	0.97
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.44	0.97
1:C:510:VAL:CG1	1:C:514:MET:HE1	1.94	0.97
1:F:305:ILE:HG12	1:G:267:MET:HE3	1.47	0.97
1:F:18:ARG:HB3	1:F:18:ARG:NH1	1.79	0.97
2:T:50:GLU:HG2	2:U:51:ASN:HB2	1.47	0.97
1:A:430:ARG:HG2	1:A:430:ARG:NH1	1.72	0.97
1:E:138:CYS:HA	7:E:611:HOH:O	1.63	0.96
1:M:326:ASN:HD22	1:M:329:THR:HB	1.27	0.96
1:I:425:LYS:NZ	7:I:540:HOH:O	1.90	0.96
1:K:326:ASN:HD22	1:K:329:THR:HB	1.29	0.96
2:P:50:GLU:HG2	2:Q:51:ASN:HB2	1.47	0.95
1:E:430:ARG:HH11	1:E:430:ARG:CG	1.79	0.95
1:G:18:ARG:NH1	1:G:18:ARG:HB3	1.82	0.95
1:J:73:MET:HE2	1:J:514:MET:HE2	1.46	0.94
1:B:430:ARG:HG2	1:B:430:ARG:NH1	1.76	0.94
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.50	0.93
1:D:18:ARG:HH11	1:D:18:ARG:CB	1.81	0.93
1:C:305:ILE:HG12	1:D:267:MET:HE3	1.51	0.93
1:F:18:ARG:HH11	1:F:18:ARG:CG	1.83	0.92
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.51	0.92
2:S:95:VAL:HG11	2:T:1:MET:HE2	1.52	0.92
1:F:18:ARG:HH11	1:F:18:ARG:HB3	1.35	0.91
1:F:430:ARG:HG2	1:F:430:ARG:NH1	1.76	0.91
1:B:18:ARG:HH11	1:B:18:ARG:CG	1.83	0.91
1:C:430:ARG:HG2	1:C:430:ARG:NH1	1.77	0.91
2:S:50:GLU:HG2	2:T:51:ASN:HB2	1.53	0.91
1:C:514:MET:HB2	1:C:514:MET:HE3	1.53	0.90
1:K:65:LYS:O	1:K:66:PHE:HB2	1.68	0.90
1:D:18:ARG:HH11	1:D:18:ARG:HG2	1.34	0.90
1:M:444:LEU:HA	1:M:447:MET:HE3	1.52	0.89
1:N:65:LYS:O	1:N:66:PHE:HB2	1.71	0.89
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.54	0.89
1:I:444:LEU:HD23	1:I:447:MET:HE1	1.52	0.89
1:A:18:ARG:NH1	1:A:18:ARG:HB3	1.87	0.89
1:D:18:ARG:NH1	1:D:18:ARG:HB3	1.88	0.89
1:A:267:MET:HE3	1:G:305:ILE:HG12	1.54	0.89
1:M:404:ARG:HG2	1:M:404:ARG:NH1	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:425:LYS:NZ	7:M:532:HOH:O	2.06	0.88
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.56	0.88
1:G:430:ARG:HG2	1:G:430:ARG:NH1	1.81	0.88
1:A:510:VAL:CG1	1:A:514:MET:HE1	2.04	0.87
2:Q:50:GLU:HG2	2:R:51:ASN:HB2	1.55	0.87
1:B:69:MET:HE2	1:B:520:MET:HE2	1.56	0.87
1:B:90:THR:O	1:B:94:VAL:HG23	1.73	0.87
1:C:18:ARG:CB	1:C:18:ARG:NH1	2.23	0.86
1:C:349:ILE:HA	1:C:352:GLN:CG	2.05	0.86
1:C:414:GLY:O	1:C:417:VAL:HG12	1.75	0.86
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.57	0.86
1:B:349:ILE:HA	1:B:352:GLN:CG	2.05	0.86
1:I:106:ALA:O	1:I:109:ALA:HB3	1.76	0.86
1:E:18:ARG:HB3	1:E:18:ARG:NH1	1.90	0.86
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.56	0.86
1:A:414:GLY:O	1:A:417:VAL:HG12	1.76	0.85
1:F:486:GLY:HA3	1:F:491:MET:HE2	1.58	0.85
1:G:349:ILE:HA	1:G:352:GLN:CG	2.05	0.85
1:F:90:THR:O	1:F:94:VAL:HG23	1.76	0.84
1:G:409:GLU:OE1	7:G:619:HOH:O	1.95	0.84
1:D:349:ILE:HA	1:D:352:GLN:CG	2.07	0.84
1:A:486:GLY:HA3	1:A:491:MET:HE2	1.57	0.84
1:H:326:ASN:HD22	1:H:329:THR:CB	1.89	0.84
1:H:444:LEU:HD23	1:H:447:MET:CE	2.07	0.84
1:C:18:ARG:NH1	1:C:18:ARG:CG	2.38	0.84
1:K:444:LEU:HD23	1:K:447:MET:CE	2.08	0.84
1:A:69:MET:HE2	1:A:520:MET:HE2	1.59	0.84
1:B:18:ARG:HH11	1:B:18:ARG:HB3	1.23	0.84
1:I:404:ARG:HG2	1:I:404:ARG:NH1	1.92	0.83
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.39	0.83
1:N:73:MET:HE2	1:N:514:MET:HE2	1.59	0.83
1:B:351:GLN:HE22	1:C:209:GLU:HB3	1.43	0.83
1:G:18:ARG:HH11	1:G:18:ARG:HB3	1.39	0.83
1:J:404:ARG:HG2	1:J:404:ARG:NH1	1.90	0.83
1:L:444:LEU:HD23	1:L:447:MET:CE	2.08	0.83
1:D:305:ILE:HG12	1:E:267:MET:HE3	1.60	0.83
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.61	0.83
1:N:106:ALA:O	1:N:109:ALA:HB3	1.78	0.83
1:H:65:LYS:O	1:H:66:PHE:HB2	1.77	0.83
1:E:18:ARG:HH11	1:E:18:ARG:HG2	1.40	0.83
1:I:444:LEU:HA	1:I:447:MET:HE3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.60	0.83
1:E:349:ILE:HA	1:E:352:GLN:CG	2.08	0.83
1:J:73:MET:CE	1:J:514:MET:HE2	2.09	0.82
1:K:444:LEU:HA	1:K:447:MET:HE3	1.60	0.82
1:A:18:ARG:CB	1:A:18:ARG:NH1	2.41	0.82
1:A:349:ILE:HA	1:A:352:GLN:CG	2.09	0.82
1:I:65:LYS:O	1:I:66:PHE:HB2	1.76	0.82
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.62	0.82
1:G:414:GLY:O	1:G:417:VAL:HG12	1.80	0.82
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.60	0.82
1:M:404:ARG:HH11	1:M:404:ARG:CG	1.90	0.82
1:K:131:LEU:HD12	1:K:422:VAL:HG11	1.62	0.82
1:H:444:LEU:HA	1:H:447:MET:HE3	1.62	0.81
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.62	0.81
1:D:462:PRO:HD2	7:D:608:HOH:O	1.81	0.81
1:E:486:GLY:HA3	1:E:491:MET:HE2	1.61	0.81
1:J:65:LYS:O	1:J:66:PHE:HB2	1.79	0.81
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.61	0.81
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.62	0.81
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.63	0.81
2:O:50:GLU:HG2	2:P:51:ASN:HB2	1.61	0.81
1:C:206:ASN:HD21	1:C:214:GLU:H	1.29	0.81
1:E:18:ARG:CB	1:E:18:ARG:NH1	2.43	0.81
1:F:510:VAL:CG1	1:F:514:MET:HE1	2.11	0.80
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.61	0.80
1:D:18:ARG:CB	1:D:18:ARG:NH1	2.43	0.80
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.61	0.80
1:B:486:GLY:HA3	1:B:491:MET:HE2	1.63	0.80
2:Q:95:VAL:HG11	2:R:1:MET:HE2	1.62	0.80
1:C:510:VAL:CG1	1:C:514:MET:CE	2.60	0.80
2:O:95:VAL:HG11	2:P:1:MET:HE2	1.64	0.80
1:I:326:ASN:HD22	1:I:329:THR:CB	1.94	0.80
1:J:291:ASP:OD2	1:J:368:ARG:HD2	1.81	0.80
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.63	0.79
1:A:90:THR:O	1:A:94:VAL:HG23	1.82	0.79
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.64	0.79
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.62	0.79
1:F:414:GLY:O	1:F:417:VAL:HG12	1.82	0.79
1:B:514:MET:CE	1:B:514:MET:HB2	2.12	0.79
1:C:18:ARG:HH11	1:C:18:ARG:HG2	1.47	0.79
5:C:600:ADP:O3B	6:C:602:AF3:F2	1.90	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:MET:CE	1:C:514:MET:HB2	2.12	0.79
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.64	0.79
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.65	0.79
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.63	0.79
1:L:131:LEU:HD12	1:L:422:VAL:HG11	1.64	0.79
1:M:131:LEU:HD12	1:M:422:VAL:HG11	1.64	0.79
1:F:305:ILE:HG23	1:G:267:MET:HG2	1.64	0.78
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.65	0.78
1:A:234:LEU:O	1:A:238:GLU:HG3	1.83	0.78
1:D:430:ARG:HG2	1:D:430:ARG:NH1	1.84	0.78
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.64	0.78
1:F:349:ILE:HA	1:F:352:GLN:CG	2.13	0.78
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.66	0.78
1:I:444:LEU:HA	1:I:447:MET:CE	2.13	0.78
1:N:444:LEU:HD23	1:N:447:MET:CE	2.13	0.78
1:B:206:ASN:HD21	1:B:214:GLU:H	1.32	0.78
1:J:415:GLY:H	1:J:417:VAL:HG23	1.49	0.78
1:J:326:ASN:HD22	1:J:329:THR:CB	1.97	0.78
1:C:510:VAL:HG13	1:C:514:MET:HE1	1.64	0.78
2:O:1:MET:HE2	2:U:95:VAL:HG11	1.65	0.78
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.66	0.77
1:D:234:LEU:O	1:D:238:GLU:HG3	1.83	0.77
1:G:18:ARG:HH11	1:G:18:ARG:CG	1.97	0.77
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.64	0.77
1:L:326:ASN:HD22	1:L:329:THR:CB	1.97	0.77
1:H:404:ARG:HH11	1:H:404:ARG:CG	1.94	0.77
1:L:455:VAL:HG11	1:L:462:PRO:HA	1.63	0.77
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.65	0.77
1:N:326:ASN:HD22	1:N:329:THR:CB	1.96	0.77
1:B:18:ARG:CB	1:B:18:ARG:NH1	2.33	0.77
1:I:131:LEU:HD12	1:I:422:VAL:HG11	1.66	0.77
1:A:305:ILE:HG12	1:B:267:MET:HE3	1.67	0.77
1:B:259:LEU:O	1:B:263:VAL:HG23	1.85	0.77
1:C:325:ILE:HG22	1:C:330:THR:HG23	1.65	0.77
1:G:234:LEU:O	1:G:238:GLU:HG3	1.85	0.77
1:N:415:GLY:H	1:N:417:VAL:HG23	1.47	0.77
1:B:414:GLY:O	1:B:417:VAL:HG12	1.85	0.77
1:I:404:ARG:HH11	1:I:404:ARG:CG	1.92	0.77
1:E:414:GLY:O	1:E:417:VAL:HG12	1.85	0.76
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.67	0.76
1:K:444:LEU:HD23	1:K:447:MET:HE3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:PRO:HD2	7:A:613:HOH:O	1.86	0.76
1:L:32:GLY:HA2	1:L:454:ILE:HG23	1.68	0.76
1:A:430:ARG:HH11	1:A:430:ARG:CG	1.90	0.76
1:B:510:VAL:CG1	1:B:514:MET:CE	2.63	0.76
1:M:32:GLY:HA2	1:M:454:ILE:HG23	1.68	0.76
1:I:32:GLY:HA2	1:I:454:ILE:HG23	1.67	0.76
1:N:73:MET:CE	1:N:514:MET:HE2	2.15	0.76
2:O:51:ASN:HB2	2:U:50:GLU:HG2	1.68	0.76
1:D:452:ARG:NH1	7:D:609:HOH:O	2.18	0.76
1:E:430:ARG:NH1	1:E:430:ARG:CG	2.42	0.76
1:I:455:VAL:HG11	1:I:462:PRO:HA	1.67	0.76
1:E:305:ILE:HG12	1:F:267:MET:HE3	1.68	0.76
1:H:415:GLY:H	1:H:417:VAL:HG23	1.49	0.76
1:A:510:VAL:HG12	1:A:514:MET:CE	2.16	0.75
1:E:206:ASN:HD21	1:E:214:GLU:H	1.35	0.75
1:N:131:LEU:HD12	1:N:422:VAL:HG11	1.68	0.75
1:G:510:VAL:CG1	1:G:514:MET:HE1	2.17	0.75
1:A:325:ILE:HG22	1:A:330:THR:HG23	1.69	0.75
1:B:325:ILE:HG22	1:B:330:THR:HG23	1.68	0.75
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.69	0.75
1:H:444:LEU:HD23	1:H:447:MET:HE3	1.66	0.75
1:A:206:ASN:HD21	1:A:214:GLU:H	1.33	0.75
1:B:510:VAL:CG1	1:B:514:MET:HE1	2.17	0.75
1:E:259:LEU:O	1:E:263:VAL:HG23	1.86	0.75
1:A:419:LEU:HG	1:A:447:MET:HG2	1.67	0.75
1:F:69:MET:HE2	1:F:520:MET:HE2	1.68	0.75
1:J:404:ARG:HH11	1:J:404:ARG:CG	1.95	0.74
1:M:326:ASN:HD22	1:M:329:THR:CB	1.99	0.74
1:E:260:ALA:O	1:E:264:VAL:HG23	1.86	0.74
1:J:425:LYS:NZ	7:J:537:HOH:O	2.21	0.74
1:A:209:GLU:HB3	1:G:351:GLN:HE22	1.52	0.74
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.70	0.74
1:E:325:ILE:HG22	1:E:330:THR:HG23	1.69	0.74
1:N:96:ALA:O	1:N:100:ILE:HG13	1.88	0.74
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.70	0.74
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.70	0.74
1:I:16:MET:CE	1:I:16:MET:HB2	2.18	0.74
1:I:415:GLY:H	1:I:417:VAL:HG23	1.53	0.74
1:J:444:LEU:HD23	1:J:447:MET:HE3	1.70	0.74
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.69	0.74
1:J:444:LEU:HD23	1:J:447:MET:CE	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:THR:O	1:D:94:VAL:HG23	1.89	0.73
1:B:514:MET:HB2	1:B:514:MET:HE3	1.70	0.73
1:F:325:ILE:HG22	1:F:330:THR:HG23	1.69	0.73
1:N:65:LYS:O	1:N:66:PHE:CB	2.34	0.73
1:A:486:GLY:CA	1:A:491:MET:HE2	2.16	0.73
1:A:510:VAL:HG12	1:A:514:MET:HE1	1.70	0.73
1:D:259:LEU:O	1:D:263:VAL:HG23	1.88	0.73
1:H:123:ALA:HB2	1:H:440:ILE:HG23	1.69	0.73
1:K:455:VAL:HG11	1:K:462:PRO:HA	1.68	0.73
1:C:100:ILE:HG13	1:C:511:ALA:HB1	1.70	0.73
1:G:260:ALA:O	1:G:264:VAL:HG23	1.88	0.73
1:L:123:ALA:HB2	1:L:440:ILE:HG23	1.71	0.73
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.71	0.73
1:K:326:ASN:HD22	1:K:329:THR:CB	2.02	0.73
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.70	0.73
1:I:166:MET:CE	1:I:171:LYS:HA	2.19	0.72
1:L:65:LYS:O	1:L:66:PHE:HB2	1.86	0.72
1:F:260:ALA:O	1:F:264:VAL:HG23	1.89	0.72
1:L:511:ALA:O	1:L:515:ILE:HD12	1.88	0.72
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.69	0.72
1:L:444:LEU:HD23	1:L:447:MET:HE1	1.71	0.72
1:M:444:LEU:HD23	1:M:447:MET:CE	2.20	0.72
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.72	0.72
1:H:32:GLY:HA2	1:H:454:ILE:HG23	1.72	0.72
1:C:510:VAL:HG13	1:C:514:MET:CE	2.20	0.72
1:K:32:GLY:HA2	1:K:454:ILE:HG23	1.72	0.72
1:F:366:GLN:O	1:F:369:VAL:HG22	1.90	0.72
1:K:96:ALA:O	1:K:100:ILE:HG13	1.89	0.72
1:M:428:ASP:HB2	7:M:534:HOH:O	1.90	0.72
1:D:69:MET:HE2	1:D:520:MET:HE2	1.71	0.71
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.71	0.71
1:H:455:VAL:HG11	1:H:462:PRO:HA	1.72	0.71
1:E:69:MET:HE2	1:E:520:MET:HE2	1.72	0.71
1:G:325:ILE:HG22	1:G:330:THR:HG23	1.70	0.71
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.71	0.71
1:J:131:LEU:HD12	1:J:422:VAL:HG11	1.70	0.71
1:G:206:ASN:HD21	1:G:214:GLU:H	1.37	0.71
1:J:149:THR:HG21	1:J:156:GLU:HA	1.73	0.71
1:K:213:VAL:HB	1:K:325:ILE:HG12	1.70	0.71
1:L:415:GLY:H	1:L:417:VAL:HG23	1.54	0.71
2:R:50:GLU:HG2	2:S:51:ASN:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:MET:HE2	1:C:520:MET:HE2	1.72	0.71
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.70	0.71
1:M:65:LYS:O	1:M:66:PHE:HB2	1.90	0.71
1:N:166:MET:CE	1:N:171:LYS:HA	2.21	0.71
1:D:486:GLY:HA3	1:D:491:MET:HE2	1.73	0.71
1:D:366:GLN:O	1:D:369:VAL:HG22	1.90	0.71
1:G:486:GLY:HA3	1:G:491:MET:HE2	1.72	0.71
1:I:149:THR:HG21	1:I:156:GLU:HA	1.73	0.71
1:L:126:ALA:HB1	1:L:426:LEU:HD22	1.71	0.71
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.70	0.71
1:E:234:LEU:O	1:E:238:GLU:HG3	1.91	0.71
1:I:444:LEU:HD23	1:I:447:MET:HE3	1.71	0.71
1:D:206:ASN:HD21	1:D:214:GLU:H	1.36	0.71
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.72	0.71
1:C:260:ALA:O	1:C:264:VAL:HG23	1.91	0.71
1:D:18:ARG:HG2	1:D:18:ARG:NH1	2.06	0.71
1:D:510:VAL:CG1	1:D:514:MET:HE1	2.20	0.71
1:H:404:ARG:HG2	1:H:404:ARG:NH1	1.91	0.71
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.73	0.71
1:N:444:LEU:HD23	1:N:447:MET:HE3	1.72	0.71
1:D:44:PHE:H	1:D:44:PHE:HD1	1.38	0.70
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.71	0.70
1:M:49:ILE:CD1	1:N:73:MET:HE3	2.21	0.70
1:B:44:PHE:HD1	1:B:44:PHE:H	1.39	0.70
1:E:90:THR:O	1:E:94:VAL:HG23	1.90	0.70
1:B:260:ALA:O	1:B:264:VAL:HG23	1.92	0.70
1:F:234:LEU:O	1:F:238:GLU:HG3	1.91	0.70
1:G:270:ILE:HD13	2:U:27:LEU:HB3	1.74	0.70
1:M:149:THR:HG21	1:M:156:GLU:HA	1.73	0.70
1:N:291:ASP:OD2	1:N:368:ARG:HD2	1.92	0.70
1:J:106:ALA:CA	1:J:111:MET:HE3	2.22	0.70
1:A:260:ALA:O	1:A:264:VAL:HG23	1.91	0.70
1:B:234:LEU:O	1:B:238:GLU:HG3	1.91	0.70
1:C:270:ILE:HD13	2:Q:27:LEU:HB3	1.72	0.70
1:N:404:ARG:HH11	1:N:404:ARG:CG	2.01	0.70
1:F:486:GLY:CA	1:F:491:MET:HE2	2.21	0.69
1:C:366:GLN:O	1:C:369:VAL:HG22	1.92	0.69
1:C:524:LEU:CD2	1:C:525:PRO:HD2	2.23	0.69
1:F:259:LEU:O	1:F:263:VAL:HG23	1.91	0.69
1:G:42:LYS:HG2	1:G:44:PHE:CE2	2.26	0.69
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:GLY:HA2	1:J:454:ILE:HG23	1.74	0.69
1:K:404:ARG:HG2	1:K:404:ARG:NH1	1.96	0.69
5:A:600:ADP:O3B	6:A:602:AF3:F2	2.01	0.69
1:A:259:LEU:O	1:A:263:VAL:HG23	1.93	0.69
1:B:366:GLN:O	1:B:369:VAL:HG22	1.92	0.69
1:C:44:PHE:HD1	1:C:44:PHE:H	1.37	0.69
1:I:16:MET:CE	1:I:16:MET:CB	2.70	0.69
1:I:385:THR:HG23	1:I:388:GLU:HB2	1.74	0.69
1:C:430:ARG:NH1	1:C:430:ARG:CG	2.56	0.69
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.75	0.69
1:D:260:ALA:O	1:D:264:VAL:HG23	1.92	0.69
1:D:325:ILE:HG22	1:D:330:THR:HG23	1.74	0.69
1:F:18:ARG:HH11	1:F:18:ARG:HG2	1.57	0.69
1:J:96:ALA:O	1:J:100:ILE:HG13	1.93	0.69
1:J:123:ALA:HB2	1:J:440:ILE:HG23	1.75	0.69
1:M:172:GLU:OE1	1:M:172:GLU:HA	1.93	0.69
1:L:106:ALA:CA	1:L:111:MET:HE3	2.22	0.69
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.75	0.69
1:A:74:VAL:O	1:A:77:VAL:HG13	1.93	0.68
1:C:234:LEU:O	1:C:238:GLU:HG3	1.92	0.68
1:I:65:LYS:O	1:I:66:PHE:CB	2.41	0.68
1:C:486:GLY:HA3	1:C:491:MET:HE2	1.75	0.68
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.74	0.68
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.76	0.68
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.75	0.68
1:L:444:LEU:HD23	1:L:447:MET:HE3	1.74	0.68
1:F:486:GLY:HA3	1:F:491:MET:CE	2.23	0.68
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.74	0.68
1:C:16:MET:O	1:C:20:VAL:HG23	1.94	0.68
1:G:430:ARG:NH1	1:G:430:ARG:CG	2.57	0.68
1:K:65:LYS:O	1:K:66:PHE:CB	2.38	0.68
1:N:326:ASN:ND2	1:N:329:THR:HB	2.05	0.68
1:A:430:ARG:NH1	1:A:430:ARG:CG	2.50	0.68
1:C:259:LEU:O	1:C:263:VAL:HG23	1.94	0.68
1:C:414:GLY:O	1:C:417:VAL:CG1	2.42	0.68
1:L:149:THR:HG21	1:L:156:GLU:HA	1.76	0.68
1:H:421:ARG:HD2	1:H:474:GLY:O	1.94	0.67
1:B:419:LEU:HG	1:B:447:MET:HG2	1.75	0.67
1:C:65:LYS:HG2	7:C:606:HOH:O	1.94	0.67
1:D:414:GLY:O	1:D:417:VAL:HG12	1.94	0.67
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:LEU:CD2	1:B:525:PRO:HD2	2.24	0.67
1:E:510:VAL:CG1	1:E:514:MET:HE1	2.24	0.67
1:E:129:GLU:OE2	1:E:129:GLU:HA	1.93	0.67
1:M:96:ALA:O	1:M:100:ILE:HG13	1.95	0.67
1:C:125:THR:O	7:C:609:HOH:O	2.12	0.67
1:E:88:GLY:HA2	5:E:600:ADP:O2B	1.95	0.67
1:N:126:ALA:HB1	1:N:426:LEU:HD22	1.77	0.67
1:N:452:ARG:HG2	1:N:452:ARG:HH11	1.58	0.67
2:U:7:HIS:O	2:U:8:ASP:HB3	1.94	0.67
1:F:510:VAL:CG1	1:F:514:MET:CE	2.72	0.67
1:J:106:ALA:O	1:J:109:ALA:HB3	1.94	0.67
1:M:385:THR:HG23	1:M:388:GLU:HB2	1.76	0.67
1:A:365:LEU:O	1:A:369:VAL:HG13	1.95	0.66
1:E:18:ARG:NH1	1:E:18:ARG:HG2	2.05	0.66
1:F:44:PHE:HD1	1:F:44:PHE:H	1.41	0.66
1:F:430:ARG:NH1	1:F:430:ARG:CG	2.53	0.66
1:K:149:THR:HG21	1:K:156:GLU:HA	1.77	0.66
1:N:404:ARG:HG2	1:N:404:ARG:NH1	2.02	0.66
1:I:173:GLY:O	1:I:404:ARG:NH2	2.27	0.66
1:M:272:LYS:NZ	1:N:228:SER:HB3	2.10	0.66
1:C:44:PHE:N	1:C:44:PHE:CD1	2.62	0.66
1:H:434:GLU:N	7:H:536:HOH:O	1.93	0.66
1:A:510:VAL:CG1	1:A:514:MET:CE	2.71	0.66
2:R:7:HIS:O	2:R:8:ASP:HB3	1.95	0.66
1:C:417:VAL:HG11	1:C:488:MET:HG3	1.76	0.66
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.77	0.66
1:E:486:GLY:HA3	1:E:491:MET:CE	2.25	0.66
1:G:270:ILE:CD1	2:U:27:LEU:HB3	2.26	0.66
1:C:365:LEU:O	1:C:369:VAL:HG13	1.96	0.66
1:B:510:VAL:HG12	1:B:514:MET:HE3	1.78	0.66
1:H:131:LEU:HD12	1:H:422:VAL:HG11	1.78	0.66
1:I:77:VAL:HG12	1:I:78:ALA:N	2.09	0.66
1:I:106:ALA:CA	1:I:111:MET:HE3	2.26	0.66
1:J:166:MET:CE	1:J:171:LYS:HA	2.26	0.66
1:L:291:ASP:OD2	1:L:368:ARG:HD2	1.96	0.66
2:T:50:GLU:HG2	2:U:51:ASN:CB	2.23	0.66
1:J:415:GLY:N	1:J:417:VAL:HG23	2.11	0.66
1:M:419:LEU:HD12	1:M:447:MET:HB3	1.76	0.66
1:M:428:ASP:N	7:M:534:HOH:O	2.20	0.66
1:N:166:MET:HE2	1:N:171:LYS:HA	1.78	0.66
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:MET:HE2	1:J:171:LYS:HA	1.77	0.65
1:K:16:MET:O	1:K:20:VAL:HG12	1.96	0.65
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.78	0.65
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.78	0.65
1:F:419:LEU:HG	1:F:447:MET:HG2	1.78	0.65
1:N:106:ALA:CA	1:N:111:MET:HE3	2.27	0.65
1:B:486:GLY:CA	1:B:491:MET:HE2	2.26	0.65
1:H:66:PHE:HA	1:H:69:MET:HE3	1.78	0.65
1:M:421:ARG:HD2	1:M:474:GLY:O	1.95	0.65
1:N:173:GLY:O	1:N:404:ARG:NH2	2.29	0.65
1:E:366:GLN:O	1:E:369:VAL:HG22	1.96	0.65
1:F:69:MET:HE1	1:F:520:MET:HB3	1.79	0.65
1:I:149:THR:CG2	1:I:156:GLU:HA	2.26	0.65
1:J:172:GLU:HA	1:J:172:GLU:OE1	1.94	0.65
1:J:217:SER:N	1:J:218:PRO:HD3	2.12	0.65
2:P:7:HIS:NE2	2:P:48:ILE:HD11	2.12	0.65
1:C:448:GLU:O	1:C:452:ARG:HG3	1.95	0.65
1:C:524:LEU:HD23	1:C:525:PRO:HD2	1.77	0.65
1:D:44:PHE:CD1	1:D:44:PHE:N	2.65	0.65
1:G:44:PHE:HD1	1:G:44:PHE:H	1.41	0.65
1:G:415:GLY:O	1:G:451:LEU:HD23	1.96	0.65
1:B:44:PHE:N	1:B:44:PHE:CD1	2.65	0.65
1:B:74:VAL:O	1:B:77:VAL:HG13	1.95	0.65
1:B:360:TYR:HA	1:B:363:GLU:HG2	1.78	0.65
1:E:54:VAL:O	1:E:58:ARG:HG3	1.96	0.65
1:F:206:ASN:HD21	1:F:214:GLU:H	1.43	0.65
1:F:524:LEU:CD2	1:F:525:PRO:HD2	2.27	0.65
1:G:18:ARG:CB	1:G:18:ARG:NH1	2.46	0.65
1:A:415:GLY:O	1:A:451:LEU:HD23	1.97	0.65
1:J:73:MET:HE2	1:J:514:MET:CE	2.24	0.65
1:L:452:ARG:HG2	1:L:452:ARG:HH11	1.60	0.65
2:S:7:HIS:O	2:S:8:ASP:HB3	1.97	0.65
1:G:366:GLN:O	1:G:369:VAL:HG22	1.95	0.65
1:A:345:ARG:HA	1:A:348:GLN:HE21	1.60	0.65
1:B:88:GLY:HA2	5:B:600:ADP:O2B	1.95	0.65
1:C:351:GLN:HE22	1:D:209:GLU:HB3	1.61	0.65
1:I:106:ALA:HA	1:I:111:MET:HE3	1.79	0.65
2:P:50:GLU:HG2	2:Q:51:ASN:CB	2.23	0.65
1:C:73:MET:SD	1:D:49:ILE:HD11	2.38	0.64
1:G:259:LEU:O	1:G:263:VAL:HG23	1.96	0.64
2:T:50:GLU:CG	2:U:51:ASN:HB2	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:LYS:HB3	1:D:445:ARG:HH21	1.62	0.64
1:K:421:ARG:HD2	1:K:474:GLY:O	1.96	0.64
1:M:415:GLY:H	1:M:417:VAL:HG23	1.63	0.64
2:T:7:HIS:O	2:T:8:ASP:HB3	1.97	0.64
1:F:111:MET:HG2	1:F:116:LEU:HD21	1.78	0.64
1:I:16:MET:O	1:I:20:VAL:HG12	1.97	0.64
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.80	0.64
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.79	0.64
1:I:416:GLY:HA2	7:I:538:HOH:O	1.97	0.64
1:I:461:GLU:OE1	1:I:461:GLU:HA	1.96	0.64
1:J:455:VAL:HG11	1:J:462:PRO:HA	1.79	0.64
1:N:415:GLY:N	1:N:417:VAL:HG23	2.12	0.64
1:B:190:VAL:HG11	1:B:194:GLN:NE2	2.12	0.64
1:D:111:MET:HG2	1:D:116:LEU:HD21	1.80	0.64
1:E:360:TYR:HA	1:E:363:GLU:HG2	1.78	0.64
1:M:73:MET:HE2	1:M:514:MET:HE2	1.79	0.64
1:B:16:MET:HG3	1:B:520:MET:HE1	1.80	0.64
2:P:7:HIS:O	2:P:8:ASP:HB3	1.96	0.64
1:J:173:GLY:O	1:J:404:ARG:NH2	2.31	0.64
1:L:126:ALA:CB	1:L:426:LEU:HD22	2.28	0.64
1:B:18:ARG:HH11	1:B:18:ARG:HG2	1.62	0.64
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.46	0.64
1:F:125:THR:HG22	7:F:607:HOH:O	1.98	0.64
2:T:7:HIS:HB2	2:T:46:GLY:O	1.98	0.64
1:B:430:ARG:NH1	1:B:430:ARG:CG	2.55	0.64
1:E:365:LEU:O	1:E:369:VAL:HG13	1.97	0.64
1:H:174:VAL:HB	1:H:376:VAL:HG22	1.80	0.64
1:I:172:GLU:OE1	1:I:172:GLU:HA	1.98	0.64
1:I:217:SER:N	1:I:218:PRO:HD3	2.12	0.64
1:M:511:ALA:O	1:M:515:ILE:HD12	1.98	0.64
1:N:16:MET:CE	1:N:16:MET:HB2	2.28	0.64
1:H:415:GLY:N	1:H:417:VAL:HG23	2.13	0.63
1:J:106:ALA:HA	1:J:111:MET:HE3	1.79	0.63
1:J:149:THR:CG2	1:J:156:GLU:HA	2.28	0.63
1:D:74:VAL:O	1:D:77:VAL:HG13	1.98	0.63
1:I:272:LYS:NZ	1:J:228:SER:HB3	2.13	0.63
1:J:421:ARG:HD2	1:J:474:GLY:O	1.98	0.63
1:N:223:ALA:O	1:N:251:ALA:HA	1.98	0.63
1:D:302:SER:H	1:D:307:MET:HE3	1.64	0.63
1:A:486:GLY:HA3	1:A:491:MET:CE	2.29	0.63
1:H:106:ALA:O	1:H:109:ALA:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:THR:HG21	1:H:156:GLU:HA	1.81	0.63
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.79	0.63
1:J:16:MET:O	1:J:20:VAL:HG12	1.98	0.63
1:L:421:ARG:NH2	7:L:537:HOH:O	2.10	0.63
2:S:95:VAL:CG1	2:T:1:MET:HE2	2.27	0.63
2:U:7:HIS:HB2	2:U:46:GLY:O	1.98	0.63
1:D:518:GLU:HG3	1:D:518:GLU:O	1.99	0.63
1:H:65:LYS:O	1:H:66:PHE:CB	2.44	0.63
1:G:365:LEU:O	1:G:369:VAL:HG13	1.98	0.63
1:H:326:ASN:ND2	1:H:329:THR:HB	2.02	0.63
1:A:366:GLN:O	1:A:369:VAL:HG22	1.97	0.63
1:E:486:GLY:CA	1:E:491:MET:HE2	2.28	0.63
1:M:173:GLY:O	1:M:404:ARG:NH2	2.32	0.63
1:E:16:MET:O	1:E:20:VAL:HG23	1.99	0.62
1:G:345:ARG:HA	1:G:348:GLN:HE21	1.63	0.62
1:I:421:ARG:HD2	1:I:474:GLY:O	1.98	0.62
1:M:27:VAL:HG11	1:M:93:THR:HG21	1.81	0.62
1:F:360:TYR:HA	1:F:363:GLU:HG2	1.80	0.62
1:I:415:GLY:N	1:I:417:VAL:HG23	2.14	0.62
1:L:106:ALA:HA	1:L:111:MET:HE3	1.81	0.62
1:F:365:LEU:O	1:F:369:VAL:HG13	1.99	0.62
1:I:174:VAL:HB	1:I:376:VAL:HG22	1.80	0.62
1:I:221:LEU:HD23	1:I:249:ILE:HG23	1.82	0.62
1:B:486:GLY:HA3	1:B:491:MET:CE	2.28	0.62
1:C:206:ASN:ND2	1:C:214:GLU:H	1.95	0.62
1:E:419:LEU:HG	1:E:447:MET:HG2	1.81	0.62
1:G:33:PRO:HA	1:G:153:ASN:HD21	1.64	0.62
1:J:126:ALA:HB1	1:J:426:LEU:HD22	1.80	0.62
1:K:149:THR:CG2	1:K:156:GLU:HA	2.29	0.62
1:M:73:MET:CE	1:M:514:MET:HE2	2.29	0.62
2:P:95:VAL:HG11	2:Q:1:MET:HE2	1.82	0.62
1:C:416:GLY:HA2	7:C:623:HOH:O	1.98	0.62
1:E:150:ILE:CD1	1:E:492:GLY:O	2.47	0.62
1:G:360:TYR:HA	1:G:363:GLU:HG2	1.82	0.62
1:H:217:SER:N	1:H:218:PRO:HD3	2.14	0.62
1:L:217:SER:N	1:L:218:PRO:HD3	2.14	0.62
1:L:415:GLY:N	1:L:417:VAL:HG23	2.13	0.62
1:N:174:VAL:HB	1:N:376:VAL:HG22	1.82	0.62
1:H:16:MET:O	1:H:20:VAL:HG12	2.00	0.62
1:M:455:VAL:HG11	1:M:462:PRO:HA	1.80	0.62
1:D:448:GLU:HB3	1:D:452:ARG:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ASP:O	1:E:363:GLU:OE2	2.18	0.62
2:Q:50:GLU:O	2:Q:50:GLU:HG3	2.00	0.62
2:U:7:HIS:NE2	2:U:48:ILE:HD11	2.15	0.62
1:F:44:PHE:N	1:F:44:PHE:CD1	2.67	0.62
1:N:389:MET:HE2	1:N:390:LYS:HA	1.80	0.62
1:C:18:ARG:NH1	1:C:18:ARG:HG2	2.11	0.62
1:C:270:ILE:CD1	2:Q:27:LEU:HB3	2.29	0.62
1:C:284:ARG:HH11	1:C:364:LYS:HD2	1.64	0.62
1:C:518:GLU:HG3	1:C:518:GLU:O	2.00	0.62
1:N:444:LEU:HD23	1:N:447:MET:HE1	1.81	0.62
2:O:74:LYS:HD2	2:U:68:ASN:ND2	2.15	0.62
1:A:414:GLY:O	1:A:417:VAL:CG1	2.46	0.61
1:L:201:SER:C	1:L:203:TYR:H	2.08	0.61
1:M:201:SER:C	1:M:203:TYR:H	2.08	0.61
2:T:95:VAL:HG11	2:U:1:MET:HE2	1.81	0.61
1:A:206:ASN:ND2	1:A:214:GLU:H	1.98	0.61
1:E:150:ILE:HD11	1:E:492:GLY:O	2.00	0.61
1:F:74:VAL:O	1:F:77:VAL:HG13	2.00	0.61
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.66	0.61
2:O:50:GLU:HG3	2:O:50:GLU:O	1.99	0.61
2:P:50:GLU:HG3	2:P:50:GLU:O	2.00	0.61
1:C:444:LEU:O	1:C:447:MET:HB2	1.99	0.61
1:K:16:MET:CE	1:K:16:MET:HB2	2.30	0.61
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.80	0.61
1:M:49:ILE:HD13	1:N:73:MET:HE3	1.82	0.61
1:M:426:LEU:CD1	1:M:444:LEU:HD21	2.30	0.61
1:A:270:ILE:HD13	2:O:27:LEU:HB3	1.82	0.61
1:B:359:ASP:O	1:B:363:GLU:OE2	2.18	0.61
1:C:111:MET:HG2	1:C:116:LEU:HD21	1.82	0.61
2:T:7:HIS:NE2	2:T:48:ILE:HD11	2.15	0.61
1:B:28:LYS:HD2	1:B:453:GLN:NE2	2.16	0.61
1:L:77:VAL:HG12	1:L:78:ALA:N	2.14	0.61
2:Q:7:HIS:HB2	2:Q:46:GLY:O	2.00	0.61
1:A:103:GLY:HA3	1:A:515:ILE:HG21	1.83	0.61
1:A:302:SER:H	1:A:307:MET:HE3	1.66	0.61
1:G:44:PHE:CD1	1:G:44:PHE:N	2.67	0.61
1:I:149:THR:CG2	1:I:159:GLY:HA3	2.30	0.61
1:N:32:GLY:HA2	1:N:454:ILE:HG23	1.82	0.61
2:Q:7:HIS:O	2:Q:8:ASP:HB3	1.99	0.61
1:C:360:TYR:HA	1:C:363:GLU:HG2	1.82	0.61
2:U:50:GLU:HG3	2:U:50:GLU:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:ARG:CB	1:F:18:ARG:NH1	2.41	0.61
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.01	0.61
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.01	0.61
1:A:18:ARG:NH1	1:A:18:ARG:HG2	2.07	0.61
1:A:44:PHE:CD1	1:A:44:PHE:N	2.68	0.61
1:C:441:LYS:HB3	1:C:445:ARG:HH21	1.65	0.61
1:C:514:MET:CE	1:C:514:MET:CG	2.79	0.61
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.83	0.61
1:I:426:LEU:CD1	1:I:444:LEU:HD21	2.31	0.61
1:J:326:ASN:ND2	1:J:329:THR:HB	2.08	0.61
1:K:201:SER:C	1:K:203:TYR:H	2.09	0.61
1:L:326:ASN:ND2	1:L:329:THR:HB	2.08	0.61
1:M:444:LEU:HD23	1:M:447:MET:HE3	1.82	0.61
1:D:510:VAL:CG1	1:D:514:MET:CE	2.78	0.60
1:K:106:ALA:O	1:K:109:ALA:HB3	2.01	0.60
1:L:149:THR:CG2	1:L:156:GLU:HA	2.31	0.60
1:C:415:GLY:O	1:C:451:LEU:HD23	2.01	0.60
1:G:420:ILE:HD13	1:G:448:GLU:HG2	1.83	0.60
1:H:413:ALA:HB1	1:H:417:VAL:HB	1.83	0.60
2:O:7:HIS:NE2	2:O:48:ILE:HD11	2.16	0.60
1:B:510:VAL:CG1	1:B:514:MET:HE3	2.29	0.60
1:H:106:ALA:CA	1:H:111:MET:HE3	2.31	0.60
1:J:145:ALA:O	1:J:149:THR:HG23	2.02	0.60
1:H:385:THR:HG23	1:H:388:GLU:HB2	1.83	0.60
1:M:145:ALA:O	1:M:149:THR:HG23	2.01	0.60
1:M:149:THR:CG2	1:M:156:GLU:HA	2.31	0.60
2:S:50:GLU:HG3	2:S:50:GLU:O	2.01	0.60
1:C:54:VAL:O	1:C:58:ARG:HG3	2.02	0.60
1:D:16:MET:O	1:D:20:VAL:HG23	2.01	0.60
1:D:486:GLY:CA	1:D:491:MET:HE2	2.30	0.60
1:N:106:ALA:HA	1:N:111:MET:HE3	1.83	0.60
1:A:39:VAL:HG12	1:G:69:MET:HE3	1.84	0.60
1:N:172:GLU:OE1	1:N:172:GLU:HA	2.00	0.60
1:B:69:MET:HE3	1:C:39:VAL:CG1	2.32	0.60
1:D:365:LEU:O	1:D:369:VAL:HG13	2.00	0.60
1:F:359:ASP:O	1:F:363:GLU:OE2	2.20	0.60
1:I:107:VAL:HG11	1:I:515:ILE:HG23	1.84	0.60
1:M:326:ASN:ND2	1:M:329:THR:HB	2.09	0.60
1:N:413:ALA:HB1	1:N:417:VAL:HB	1.83	0.60
1:B:217:SER:N	1:B:218:PRO:HD3	2.17	0.60
1:G:284:ARG:HH11	1:G:364:LYS:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:149:THR:HG21	1:N:156:GLU:HA	1.84	0.60
1:A:486:GLY:C	1:A:491:MET:HE2	2.27	0.60
1:D:360:TYR:HA	1:D:363:GLU:HG2	1.83	0.60
2:O:6:LEU:O	2:O:7:HIS:O	2.19	0.60
1:N:217:SER:N	1:N:218:PRO:HD3	2.17	0.60
1:N:451:LEU:O	1:N:452:ARG:C	2.39	0.60
1:A:236:VAL:O	1:A:240:VAL:HG23	2.02	0.59
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.84	0.59
1:G:90:THR:O	1:G:94:VAL:CG2	2.38	0.59
1:H:444:LEU:HD23	1:H:447:MET:HE1	1.83	0.59
1:I:326:ASN:ND2	1:I:329:THR:HB	2.07	0.59
1:L:107:VAL:HG11	1:L:515:ILE:HG23	1.83	0.59
1:N:201:SER:C	1:N:203:TYR:H	2.10	0.59
2:T:50:GLU:HG3	2:T:50:GLU:O	2.00	0.59
1:A:44:PHE:H	1:A:44:PHE:HD1	1.47	0.59
1:A:441:LYS:HB3	1:A:445:ARG:HH21	1.67	0.59
1:C:359:ASP:O	1:C:363:GLU:OE2	2.20	0.59
1:I:166:MET:HE2	1:I:171:LYS:HA	1.84	0.59
1:M:47:PRO:HG2	1:N:73:MET:HG3	1.83	0.59
1:N:426:LEU:CD1	1:N:444:LEU:HD21	2.32	0.59
1:B:16:MET:CE	1:B:16:MET:CG	2.80	0.59
1:B:510:VAL:HG13	1:B:514:MET:CE	2.32	0.59
1:D:345:ARG:HA	1:D:348:GLN:HE21	1.67	0.59
1:H:201:SER:C	1:H:203:TYR:H	2.10	0.59
2:S:6:LEU:O	2:S:7:HIS:O	2.20	0.59
1:E:522:THR:OG1	1:E:523:ASP:N	2.35	0.59
1:E:524:LEU:CD2	1:E:525:PRO:HD2	2.33	0.59
1:I:417:VAL:HG21	1:I:488:MET:HE2	1.85	0.59
1:M:444:LEU:HA	1:M:447:MET:CE	2.30	0.59
1:A:217:SER:N	1:A:218:PRO:HD3	2.18	0.59
1:B:18:ARG:NH1	1:B:18:ARG:CG	2.55	0.59
1:L:65:LYS:O	1:L:66:PHE:CB	2.49	0.59
1:M:217:SER:N	1:M:218:PRO:HD3	2.17	0.59
1:M:461:GLU:OE1	1:M:461:GLU:HA	2.01	0.59
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.83	0.59
1:B:305:ILE:HG23	1:C:267:MET:HG2	1.83	0.59
1:I:149:THR:HG23	1:I:159:GLY:HA3	1.84	0.59
1:N:421:ARG:HD2	1:N:474:GLY:O	2.03	0.59
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.83	0.59
2:P:50:GLU:CG	2:Q:51:ASN:HB2	2.28	0.59
2:R:95:VAL:HG11	2:S:1:MET:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TYR:HA	1:A:363:GLU:HG2	1.85	0.59
1:C:466:ALA:O	1:C:467:ASN:C	2.44	0.59
1:D:6:VAL:O	1:D:6:VAL:CG2	2.50	0.59
1:D:284:ARG:HH11	1:D:364:LYS:HD2	1.68	0.59
1:D:512:GLY:O	1:D:515:ILE:HG13	2.02	0.59
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.82	0.59
1:J:201:SER:C	1:J:203:TYR:H	2.09	0.59
1:A:267:MET:HG2	1:G:305:ILE:HG23	1.85	0.59
1:D:135:SER:HB2	1:D:497:THR:OG1	2.02	0.59
1:E:345:ARG:HA	1:E:348:GLN:HE21	1.68	0.59
1:E:510:VAL:CG1	1:E:514:MET:CE	2.81	0.59
1:M:166:MET:CE	1:M:171:LYS:HA	2.33	0.59
1:N:126:ALA:CB	1:N:426:LEU:HD22	2.33	0.59
1:B:206:ASN:ND2	1:B:214:GLU:H	1.98	0.59
1:E:217:SER:N	1:E:218:PRO:HD3	2.17	0.59
1:G:510:VAL:HG12	1:G:514:MET:CE	2.33	0.59
1:K:16:MET:CE	1:K:16:MET:CB	2.81	0.59
1:K:217:SER:N	1:K:218:PRO:HD3	2.17	0.59
2:O:7:HIS:O	2:O:8:ASP:HB3	2.02	0.59
1:B:345:ARG:HA	1:B:348:GLN:HE21	1.68	0.59
1:G:511:ALA:O	1:G:515:ILE:HG12	2.02	0.59
1:M:65:LYS:O	1:M:66:PHE:CB	2.51	0.59
1:M:149:THR:HG22	1:M:159:GLY:HA3	1.85	0.59
2:P:7:HIS:HB2	2:P:46:GLY:O	2.01	0.59
1:G:510:VAL:CG1	1:G:514:MET:CE	2.81	0.58
2:R:50:GLU:HG3	2:R:50:GLU:O	2.03	0.58
1:D:461:GLU:OE2	1:J:452:ARG:NH2	2.35	0.58
1:L:145:ALA:O	1:L:149:THR:HG23	2.04	0.58
1:M:339:GLU:O	1:M:343:GLN:HB2	2.03	0.58
1:N:455:VAL:HG11	1:N:462:PRO:HA	1.84	0.58
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.85	0.58
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.86	0.58
1:M:49:ILE:HD11	1:N:73:MET:HE3	1.84	0.58
2:T:6:LEU:O	2:T:7:HIS:O	2.22	0.58
1:H:173:GLY:O	1:H:404:ARG:NH2	2.36	0.58
1:C:100:ILE:HG13	1:C:511:ALA:CB	2.33	0.58
1:E:44:PHE:HD1	1:E:44:PHE:H	1.50	0.58
1:D:88:GLY:N	6:D:602:AF3:F2	2.26	0.58
1:I:166:MET:HE3	1:I:171:LYS:HA	1.86	0.58
1:K:65:LYS:HA	7:K:528:HOH:O	2.02	0.58
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:HH11	1:A:364:LYS:HD2	1.69	0.58
1:B:265:ASN:HA	1:B:270:ILE:HD12	1.84	0.58
1:I:11:ASP:N	1:I:11:ASP:OD1	2.35	0.58
1:J:404:ARG:NH1	1:J:404:ARG:CG	2.60	0.58
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.86	0.58
1:L:49:ILE:CD1	1:M:73:MET:HE3	2.33	0.58
1:L:66:PHE:O	1:L:67:GLU:C	2.47	0.58
1:L:172:GLU:OE1	1:L:172:GLU:HA	2.03	0.58
1:N:73:MET:HE2	1:N:514:MET:CE	2.33	0.58
1:B:69:MET:HE1	1:B:520:MET:HB3	1.86	0.58
1:M:101:THR:HG22	1:M:102:GLU:OE1	2.03	0.58
1:C:520:MET:HG2	1:D:39:VAL:HB	1.86	0.58
1:E:206:ASN:ND2	1:E:214:GLU:H	2.00	0.58
1:F:88:GLY:HA2	5:F:600:ADP:O2B	2.04	0.58
1:H:106:ALA:HA	1:H:111:MET:HE3	1.84	0.58
1:L:62:LEU:N	1:L:68:ASN:OD1	2.33	0.58
1:M:404:ARG:NH1	1:M:404:ARG:CG	2.57	0.58
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.39	0.58
1:B:365:LEU:O	1:B:369:VAL:HG13	2.04	0.57
1:B:414:GLY:O	1:B:417:VAL:CG1	2.52	0.57
1:C:486:GLY:CA	1:C:491:MET:HE2	2.34	0.57
1:D:444:LEU:O	1:D:447:MET:HB2	2.04	0.57
1:E:415:GLY:O	1:E:451:LEU:HD23	2.04	0.57
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.86	0.57
1:L:166:MET:CE	1:L:171:LYS:HA	2.34	0.57
1:N:385:THR:HG23	1:N:388:GLU:HB2	1.85	0.57
1:E:351:GLN:HE22	1:F:209:GLU:HB3	1.68	0.57
1:F:217:SER:N	1:F:218:PRO:HD3	2.20	0.57
1:I:201:SER:C	1:I:203:TYR:H	2.12	0.57
1:M:223:ALA:O	1:M:251:ALA:HA	2.03	0.57
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.67	0.57
1:D:415:GLY:O	1:D:451:LEU:HD23	2.04	0.57
1:G:359:ASP:O	1:G:363:GLU:OE2	2.21	0.57
1:G:417:VAL:HG11	1:G:488:MET:HG3	1.86	0.57
2:S:7:HIS:NE2	2:S:48:ILE:HD11	2.19	0.57
1:B:33:PRO:HA	1:B:153:ASN:HD21	1.69	0.57
1:H:172:GLU:OE1	1:H:172:GLU:HA	2.04	0.57
1:L:149:THR:CG2	1:L:159:GLY:HA3	2.33	0.57
1:B:284:ARG:HH11	1:B:364:LYS:HD2	1.69	0.57
1:D:419:LEU:HG	1:D:447:MET:HG2	1.87	0.57
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:486:GLY:CA	1:G:491:MET:HE2	2.34	0.57
1:H:326:ASN:HB2	1:H:329:THR:H	1.70	0.57
1:K:444:LEU:HD23	1:K:447:MET:HE1	1.85	0.57
1:N:87:ASP:OD2	7:N:530:HOH:O	2.17	0.57
1:B:351:GLN:NE2	1:C:209:GLU:HB3	2.17	0.57
1:D:417:VAL:HG11	1:D:488:MET:HG3	1.85	0.57
1:H:145:ALA:O	1:H:149:THR:HG23	2.04	0.57
1:H:166:MET:CE	1:H:171:LYS:HA	2.35	0.57
1:I:339:GLU:O	1:I:343:GLN:HB2	2.05	0.57
2:O:7:HIS:HB2	2:O:46:GLY:O	2.03	0.57
2:R:7:HIS:NE2	2:R:48:ILE:HD11	2.20	0.57
1:A:143:ALA:HA	1:A:146:GLN:HE21	1.70	0.57
1:D:206:ASN:ND2	1:D:214:GLU:H	2.02	0.57
1:E:190:VAL:HG11	1:E:194:GLN:NE2	2.19	0.57
1:F:345:ARG:HA	1:F:348:GLN:HE21	1.69	0.57
1:H:149:THR:CG2	1:H:156:GLU:HA	2.35	0.57
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.85	0.57
1:K:339:GLU:O	1:K:343:GLN:HB2	2.05	0.57
1:L:173:GLY:O	1:L:404:ARG:NH2	2.36	0.57
1:F:486:GLY:C	1:F:491:MET:HE2	2.28	0.57
1:M:149:THR:CG2	1:M:159:GLY:HA3	2.34	0.57
1:N:145:ALA:O	1:N:149:THR:HG23	2.05	0.57
1:A:143:ALA:HA	1:A:146:GLN:NE2	2.20	0.57
1:C:74:VAL:O	1:C:77:VAL:HG13	2.05	0.57
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.04	0.57
1:N:66:PHE:H	1:N:69:MET:HG3	1.69	0.57
2:Q:6:LEU:O	2:Q:7:HIS:O	2.22	0.57
2:S:7:HIS:HB2	2:S:46:GLY:O	2.05	0.57
1:B:524:LEU:HD22	1:B:525:PRO:HD2	1.86	0.57
1:E:466:ALA:O	1:E:467:ASN:C	2.47	0.57
1:K:173:GLY:O	1:K:404:ARG:NH2	2.36	0.57
2:Q:7:HIS:NE2	2:Q:48:ILE:HD11	2.19	0.57
1:E:289:LEU:HA	1:E:292:ILE:HD12	1.87	0.56
1:J:66:PHE:O	1:J:67:GLU:C	2.48	0.56
1:L:90:THR:O	1:L:94:VAL:HG23	2.05	0.56
2:R:6:LEU:O	2:R:7:HIS:O	2.23	0.56
1:D:217:SER:N	1:D:218:PRO:HD3	2.19	0.56
1:E:284:ARG:HH11	1:E:364:LYS:HD2	1.70	0.56
1:H:451:LEU:O	1:H:452:ARG:C	2.46	0.56
1:A:54:VAL:O	1:A:58:ARG:HG3	2.05	0.56
1:E:305:ILE:HB	1:E:307:MET:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ILE:HD11	1:F:492:GLY:O	2.04	0.56
1:F:522:THR:OG1	1:F:523:ASP:N	2.37	0.56
1:G:143:ALA:HA	1:G:146:GLN:NE2	2.20	0.56
1:G:486:GLY:HA3	1:G:491:MET:CE	2.34	0.56
1:H:444:LEU:HA	1:H:447:MET:CE	2.35	0.56
1:I:444:LEU:CD2	1:I:447:MET:CE	2.75	0.56
1:I:447:MET:CE	1:I:447:MET:CG	2.83	0.56
1:J:493:ILE:HG22	1:J:493:ILE:O	2.04	0.56
1:N:149:THR:CG2	1:N:156:GLU:HA	2.35	0.56
2:P:6:LEU:O	2:P:7:HIS:O	2.22	0.56
1:B:194:GLN:HG3	1:B:331:THR:HB	1.87	0.56
1:K:166:MET:CE	1:K:171:LYS:HA	2.35	0.56
2:U:6:LEU:O	2:U:7:HIS:O	2.23	0.56
1:E:33:PRO:HA	1:E:153:ASN:HD21	1.70	0.56
1:H:426:LEU:CD1	1:H:444:LEU:HD21	2.36	0.56
1:L:213:VAL:HB	1:L:325:ILE:CG1	2.36	0.56
1:B:417:VAL:HG11	1:B:488:MET:HG3	1.88	0.56
1:G:302:SER:H	1:G:307:MET:HE3	1.70	0.56
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.86	0.56
1:F:236:VAL:O	1:F:240:VAL:HG23	2.05	0.56
1:I:325:ILE:HG22	1:I:330:THR:HG23	1.88	0.56
1:L:16:MET:O	1:L:20:VAL:HG12	2.05	0.56
1:M:11:ASP:OD1	1:M:11:ASP:N	2.37	0.56
1:M:16:MET:O	1:M:20:VAL:HG12	2.06	0.56
1:M:100:ILE:HG22	1:M:104:LEU:HD22	1.88	0.56
1:M:197:ARG:HD2	1:M:277:LYS:HB2	1.88	0.56
1:N:16:MET:O	1:N:20:VAL:HG12	2.05	0.56
1:B:466:ALA:O	1:B:467:ASN:C	2.48	0.56
1:I:65:LYS:HA	7:I:529:HOH:O	2.06	0.56
1:L:106:ALA:O	1:L:109:ALA:HB3	2.06	0.56
1:N:107:VAL:HG11	1:N:515:ILE:HG23	1.87	0.56
1:C:217:SER:N	1:C:218:PRO:HD3	2.20	0.56
1:F:23:LEU:O	1:F:24:ALA:C	2.49	0.56
1:I:96:ALA:O	1:I:100:ILE:HG13	2.06	0.56
1:C:305:ILE:HB	1:C:307:MET:HE2	1.88	0.55
1:E:302:SER:H	1:E:307:MET:HE3	1.70	0.55
1:F:63:GLU:O	1:F:63:GLU:HG2	2.06	0.55
1:H:426:LEU:HD12	1:H:444:LEU:HD21	1.88	0.55
1:J:34:LYS:HB2	1:J:458:CYS:SG	2.46	0.55
1:K:73:MET:HE2	1:K:514:MET:HE2	1.88	0.55
1:N:16:MET:CE	1:N:16:MET:CB	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:40:VAL:HB	2:U:62:GLY:H	1.71	0.55
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.86	0.55
1:I:426:LEU:HD12	1:I:444:LEU:HD21	1.86	0.55
1:K:351:GLN:HA	1:K:354:GLU:HG2	1.88	0.55
1:N:434:GLU:CB	7:N:529:HOH:O	2.54	0.55
1:A:42:LYS:HG2	1:A:44:PHE:CE2	2.41	0.55
1:B:430:ARG:NH2	7:B:609:HOH:O	2.24	0.55
1:D:524:LEU:CD2	1:D:525:PRO:HD2	2.37	0.55
1:F:417:VAL:HG11	1:F:488:MET:HG3	1.88	0.55
1:G:265:ASN:HA	1:G:270:ILE:HD12	1.88	0.55
1:J:223:ALA:O	1:J:251:ALA:HA	2.07	0.55
1:K:223:ALA:O	1:K:251:ALA:HA	2.06	0.55
1:N:433:ASN:HB3	1:N:436:GLN:H	1.71	0.55
1:E:44:PHE:N	1:E:44:PHE:CD1	2.74	0.55
1:F:510:VAL:HG13	1:F:514:MET:HE1	1.87	0.55
1:G:54:VAL:O	1:G:58:ARG:HG3	2.07	0.55
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.87	0.55
1:L:389:MET:HE2	1:L:390:LYS:HA	1.89	0.55
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.07	0.55
2:R:96:GLU:OE1	2:S:4:ARG:HD3	2.07	0.55
1:C:25:ASP:HA	1:C:28:LYS:HE2	1.87	0.55
1:C:419:LEU:HG	1:C:447:MET:HG2	1.88	0.55
1:C:510:VAL:HG12	1:C:514:MET:CE	2.35	0.55
1:F:305:ILE:HB	1:F:307:MET:HE2	1.89	0.55
1:I:451:LEU:O	1:I:452:ARG:C	2.46	0.55
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.89	0.55
1:J:339:GLU:O	1:J:343:GLN:HB2	2.07	0.55
1:H:511:ALA:O	1:H:515:ILE:HD12	2.07	0.55
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.47	0.55
1:M:444:LEU:HD23	1:M:447:MET:HE1	1.87	0.55
1:B:510:VAL:HG12	1:B:514:MET:CE	2.34	0.55
1:G:18:ARG:HH11	1:G:18:ARG:HG2	1.71	0.55
1:G:441:LYS:HB3	1:G:445:ARG:HH21	1.71	0.55
1:M:106:ALA:O	1:M:109:ALA:HB3	2.06	0.55
1:A:477:GLY:HA3	1:A:488:MET:SD	2.46	0.55
1:C:147:VAL:HG12	1:C:494:LEU:HB2	1.88	0.55
1:D:430:ARG:NH1	1:D:430:ARG:CG	2.61	0.55
1:E:74:VAL:O	1:E:77:VAL:HG13	2.06	0.55
1:H:351:GLN:HA	1:H:354:GLU:HG2	1.89	0.55
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.89	0.55
1:C:514:MET:CE	1:C:514:MET:CB	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:GLU:HA	1:G:129:GLU:OE2	2.05	0.55
1:K:426:LEU:CD1	1:K:444:LEU:HD21	2.37	0.55
1:A:305:ILE:HB	1:A:307:MET:HE2	1.89	0.55
1:B:524:LEU:HD23	1:B:525:PRO:HD2	1.89	0.55
1:G:69:MET:HE2	1:G:520:MET:HE2	1.87	0.55
1:M:426:LEU:HD12	1:M:444:LEU:HD21	1.88	0.55
1:M:449:ALA:HB3	1:M:450:PRO:CD	2.36	0.55
1:N:66:PHE:O	1:N:67:GLU:C	2.49	0.55
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.88	0.54
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.88	0.54
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.87	0.54
1:H:96:ALA:O	1:H:100:ILE:HG13	2.07	0.54
1:I:444:LEU:CD2	1:I:447:MET:HE1	2.32	0.54
1:K:213:VAL:HB	1:K:325:ILE:CG1	2.37	0.54
1:M:413:ALA:HB1	1:M:417:VAL:HB	1.89	0.54
1:N:221:LEU:HD23	1:N:249:ILE:HG23	1.87	0.54
1:D:236:VAL:O	1:D:240:VAL:HG23	2.07	0.54
1:D:326:ASN:HD22	1:D:329:THR:HB	1.71	0.54
1:I:197:ARG:HD2	1:I:277:LYS:HB2	1.88	0.54
1:K:172:GLU:OE1	1:K:172:GLU:HA	2.06	0.54
1:K:404:ARG:NH1	1:K:404:ARG:CG	2.67	0.54
1:M:272:LYS:HZ1	1:N:228:SER:HB3	1.72	0.54
2:P:47:ARG:HD3	2:P:49:LEU:HD12	1.88	0.54
1:F:18:ARG:NH1	1:F:18:ARG:CG	2.54	0.54
1:F:486:GLY:CA	1:F:491:MET:CE	2.85	0.54
1:I:100:ILE:HG22	1:I:104:LEU:HD22	1.89	0.54
1:L:415:GLY:CA	1:L:417:VAL:HG23	2.37	0.54
1:D:143:ALA:HA	1:D:146:GLN:NE2	2.23	0.54
1:K:326:ASN:ND2	1:K:329:THR:HB	2.11	0.54
1:K:413:ALA:HB1	1:K:417:VAL:HB	1.90	0.54
1:L:163:ALA:O	1:L:167:ASP:HB2	2.08	0.54
1:M:16:MET:HG2	1:M:70:GLY:HA2	1.87	0.54
1:N:33:PRO:CA	7:N:535:HOH:O	2.55	0.54
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.89	0.54
1:C:65:LYS:CG	7:C:606:HOH:O	2.53	0.54
1:E:69:MET:HE3	1:F:39:VAL:CG1	2.38	0.54
1:G:217:SER:N	1:G:218:PRO:HD3	2.23	0.54
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.88	0.54
1:K:325:ILE:HG22	1:K:330:THR:HG23	1.90	0.54
1:A:510:VAL:HG12	1:A:514:MET:HE3	1.88	0.54
1:H:149:THR:CG2	1:H:159:GLY:HA3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:85:ALA:HB1	1:I:499:VAL:HB	1.88	0.54
1:J:514:MET:CE	1:J:514:MET:CG	2.85	0.54
1:N:325:ILE:HG22	1:N:330:THR:HG23	1.88	0.54
1:B:326:ASN:HD22	1:B:329:THR:HB	1.71	0.54
1:G:289:LEU:HA	1:G:292:ILE:HD12	1.89	0.54
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.89	0.54
1:A:39:VAL:CG1	1:G:69:MET:HE3	2.37	0.54
1:B:305:ILE:O	1:B:305:ILE:HG22	2.07	0.54
1:E:228:SER:O	1:E:257:GLU:HB3	2.07	0.54
1:L:47:PRO:HG2	1:M:73:MET:HG3	1.90	0.54
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.90	0.54
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.89	0.54
1:G:414:GLY:O	1:G:417:VAL:CG1	2.52	0.54
1:I:389:MET:HE2	1:I:390:LYS:HA	1.89	0.54
2:T:40:VAL:HB	2:T:62:GLY:H	1.73	0.54
1:A:22:VAL:HG11	1:A:62:LEU:HD11	1.90	0.54
1:G:206:ASN:ND2	1:G:214:GLU:H	2.04	0.54
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.89	0.54
1:H:432:GLN:H	1:H:436:GLN:NE2	2.06	0.54
1:K:106:ALA:CA	1:K:111:MET:HE3	2.37	0.54
1:L:421:ARG:HD2	1:L:474:GLY:O	2.07	0.54
1:M:514:MET:CE	1:M:514:MET:CG	2.84	0.54
1:E:236:VAL:O	1:E:240:VAL:HG23	2.07	0.53
1:F:147:VAL:HG12	1:F:494:LEU:HB2	1.90	0.53
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.89	0.53
1:B:16:MET:HB3	1:B:16:MET:HE2	1.91	0.53
1:D:486:GLY:C	1:D:491:MET:HE2	2.32	0.53
1:A:261:THR:O	1:A:262:LEU:C	2.51	0.53
1:A:448:GLU:HB3	1:A:452:ARG:HD2	1.90	0.53
1:D:78:ALA:HB2	1:D:93:THR:OG1	2.09	0.53
1:D:305:ILE:HB	1:D:307:MET:HE2	1.89	0.53
1:F:16:MET:O	1:F:20:VAL:HG23	2.08	0.53
1:J:90:THR:O	1:J:94:VAL:HG23	2.08	0.53
1:K:62:LEU:N	1:K:68:ASN:OD1	2.33	0.53
1:K:145:ALA:O	1:K:149:THR:HG23	2.08	0.53
1:K:511:ALA:O	1:K:515:ILE:HD12	2.07	0.53
1:L:305:ILE:HB	1:L:307:MET:HE2	1.89	0.53
2:Q:40:VAL:HB	2:Q:62:GLY:H	1.74	0.53
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.08	0.53
1:B:54:VAL:O	1:B:58:ARG:HG3	2.08	0.53
1:H:73:MET:CE	1:H:514:MET:HE2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:305:ILE:HB	1:J:307:MET:HE2	1.90	0.53
1:K:451:LEU:O	1:K:452:ARG:C	2.51	0.53
1:J:325:ILE:HG22	1:J:330:THR:HG23	1.91	0.53
1:L:223:ALA:O	1:L:251:ALA:HA	2.09	0.53
1:F:18:ARG:NH1	1:F:18:ARG:HG2	2.23	0.53
2:R:7:HIS:HB2	2:R:46:GLY:O	2.08	0.53
1:C:482:THR:O	1:C:483:GLU:HB2	2.08	0.53
1:I:272:LYS:HZ1	1:J:228:SER:HB3	1.72	0.53
1:K:198:GLY:HA3	1:K:327:LYS:O	2.08	0.53
1:M:467:ASN:C	1:M:467:ASN:ND2	2.67	0.53
1:B:522:THR:OG1	1:B:523:ASP:N	2.40	0.53
1:G:444:LEU:O	1:G:447:MET:HB2	2.08	0.53
1:J:149:THR:HG23	1:J:159:GLY:HA3	1.91	0.53
1:K:27:VAL:HG11	1:K:93:THR:HG21	1.91	0.53
1:N:197:ARG:HD2	1:N:277:LYS:HB2	1.91	0.53
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.90	0.53
1:G:22:VAL:HG11	1:G:62:LEU:HD11	1.91	0.53
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.91	0.53
1:K:149:THR:CG2	1:K:159:GLY:HA3	2.39	0.53
1:M:16:MET:CE	1:M:16:MET:HB2	2.39	0.53
2:O:50:GLU:CG	2:P:51:ASN:HB2	2.34	0.53
2:U:78:ILE:HD13	2:U:83:VAL:HG21	1.91	0.53
1:C:265:ASN:HA	1:C:270:ILE:HD12	1.90	0.53
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.90	0.53
1:F:289:LEU:HA	1:F:292:ILE:HD12	1.92	0.53
1:K:221:LEU:HD23	1:K:249:ILE:HG23	1.90	0.53
1:M:437:ASN:HA	1:M:440:ILE:HD12	1.92	0.53
1:N:339:GLU:O	1:N:343:GLN:HB2	2.08	0.53
1:B:16:MET:CE	1:B:16:MET:HB3	2.38	0.52
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.89	0.52
1:F:510:VAL:HG13	1:F:514:MET:CE	2.40	0.52
1:H:213:VAL:HB	1:H:325:ILE:CG1	2.39	0.52
1:E:265:ASN:HA	1:E:270:ILE:HD12	1.90	0.52
1:I:223:ALA:O	1:I:251:ALA:HA	2.09	0.52
1:J:16:MET:CE	1:J:16:MET:HB2	2.39	0.52
1:J:351:GLN:HA	1:J:354:GLU:HG2	1.92	0.52
1:M:461:GLU:HB3	1:M:464:VAL:HB	1.91	0.52
1:A:359:ASP:O	1:A:363:GLU:OE2	2.26	0.52
1:E:230:ILE:CD1	1:E:261:THR:HG21	2.38	0.52
1:F:482:THR:O	1:F:483:GLU:HB2	2.09	0.52
1:G:172:GLU:HA	1:G:172:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:494:LEU:HD12	1:H:494:LEU:O	2.09	0.52
1:L:201:SER:O	1:L:203:TYR:N	2.43	0.52
1:H:149:THR:HG23	1:H:159:GLY:HA3	1.92	0.52
1:K:305:ILE:HB	1:K:307:MET:HE2	1.90	0.52
1:B:150:ILE:CD1	1:B:492:GLY:O	2.58	0.52
1:B:486:GLY:C	1:B:491:MET:HE2	2.34	0.52
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.45	0.52
1:I:91:THR:O	1:I:92:ALA:C	2.52	0.52
1:L:339:GLU:O	1:L:343:GLN:HB2	2.10	0.52
1:M:106:ALA:CA	1:M:111:MET:HE3	2.39	0.52
1:A:153:ASN:O	1:A:154:SER:HB2	2.09	0.52
1:F:54:VAL:O	1:F:58:ARG:HG3	2.09	0.52
1:K:97:GLN:O	1:K:97:GLN:HG2	2.09	0.52
1:K:389:MET:HE2	1:K:390:LYS:HA	1.90	0.52
1:L:351:GLN:HA	1:L:354:GLU:HG2	1.91	0.52
1:N:203:TYR:CD1	1:N:267:MET:HE1	2.45	0.52
1:A:228:SER:O	1:A:257:GLU:HB3	2.09	0.52
1:G:28:LYS:HD2	1:G:453:GLN:NE2	2.25	0.52
1:H:180:GLY:HA3	1:H:381:VAL:O	2.09	0.52
1:L:49:ILE:HD11	1:M:73:MET:HE3	1.90	0.52
1:L:73:MET:CE	1:L:514:MET:HE2	2.39	0.52
1:A:76:GLU:O	1:A:76:GLU:HG2	2.09	0.52
1:I:73:MET:HE2	1:I:514:MET:HE2	1.91	0.52
1:I:120:ILE:O	1:I:124:VAL:HG23	2.10	0.52
1:J:419:LEU:HD12	1:J:447:MET:HB3	1.90	0.52
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.92	0.52
1:L:49:ILE:HD12	1:M:513:LEU:HD23	1.92	0.52
1:M:305:ILE:HB	1:M:307:MET:HE2	1.90	0.52
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.92	0.52
5:A:600:ADP:PB	6:A:602:AF3:F2	2.58	0.52
1:C:345:ARG:HA	1:C:348:GLN:HE21	1.73	0.52
1:D:54:VAL:O	1:D:58:ARG:HG3	2.09	0.52
1:D:265:ASN:HA	1:D:270:ILE:HD12	1.92	0.52
1:D:359:ASP:O	1:D:363:GLU:OE2	2.28	0.52
1:G:100:ILE:HG13	1:G:511:ALA:HB1	1.91	0.52
1:G:417:VAL:O	1:G:418:ALA:C	2.52	0.52
1:H:452:ARG:HG2	1:H:452:ARG:HH11	1.74	0.52
1:M:107:VAL:HG11	1:M:515:ILE:HG23	1.92	0.52
1:B:150:ILE:HD11	1:B:492:GLY:O	2.10	0.52
1:C:42:LYS:HG2	1:C:44:PHE:CE2	2.45	0.52
1:G:486:GLY:C	1:G:491:MET:HE2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:419:LEU:HD12	1:I:447:MET:HB3	1.92	0.52
1:J:197:ARG:HD2	1:J:277:LYS:HB2	1.91	0.52
1:J:415:GLY:CA	1:J:417:VAL:HG23	2.40	0.52
1:N:33:PRO:HA	7:N:535:HOH:O	2.08	0.52
1:A:524:LEU:CD2	1:A:525:PRO:HD2	2.40	0.51
1:H:467:ASN:ND2	1:H:467:ASN:C	2.68	0.51
1:H:514:MET:CE	1:H:514:MET:CG	2.87	0.51
1:J:426:LEU:CD1	1:J:444:LEU:HD21	2.40	0.51
1:J:511:ALA:O	1:J:515:ILE:HD12	2.09	0.51
2:U:16:GLU:HB2	2:U:19:THR:OG1	2.11	0.51
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.75	0.51
1:B:289:LEU:HA	1:B:292:ILE:HD12	1.92	0.51
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.91	0.51
1:G:228:SER:O	1:G:257:GLU:HB3	2.10	0.51
1:I:44:PHE:H	1:I:44:PHE:HD1	1.58	0.51
2:T:16:GLU:HB2	2:T:19:THR:OG1	2.10	0.51
1:B:69:MET:HE3	1:C:39:VAL:HG11	1.91	0.51
1:C:194:GLN:HG3	1:C:331:THR:HB	1.92	0.51
1:D:6:VAL:O	1:D:6:VAL:HG23	2.09	0.51
1:D:510:VAL:HG12	1:D:514:MET:CE	2.40	0.51
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.93	0.51
1:E:512:GLY:O	1:E:515:ILE:HG13	2.10	0.51
1:J:413:ALA:HB1	1:J:417:VAL:HB	1.92	0.51
1:K:44:PHE:HD1	1:K:44:PHE:H	1.59	0.51
1:L:103:GLY:O	1:L:106:ALA:HB3	2.11	0.51
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.91	0.51
1:M:106:ALA:HA	1:M:111:MET:HE3	1.92	0.51
1:M:120:ILE:O	1:M:124:VAL:HG23	2.10	0.51
1:N:149:THR:HG23	1:N:159:GLY:HA3	1.92	0.51
1:A:194:GLN:HG3	1:A:331:THR:HB	1.92	0.51
1:A:479:ASN:C	1:A:479:ASN:OD1	2.53	0.51
1:C:305:ILE:HG23	1:D:267:MET:HG2	1.92	0.51
1:H:221:LEU:HD23	1:H:249:ILE:HG23	1.92	0.51
1:H:461:GLU:HB3	1:H:464:VAL:HB	1.93	0.51
1:K:73:MET:CE	1:K:514:MET:HE2	2.41	0.51
1:K:106:ALA:HB1	1:K:111:MET:HE3	1.93	0.51
1:M:66:PHE:H	1:M:69:MET:HG3	1.75	0.51
1:M:421:ARG:CD	1:M:474:GLY:O	2.58	0.51
1:N:44:PHE:HD1	1:N:44:PHE:H	1.58	0.51
2:O:50:GLU:O	2:O:51:ASN:HB3	2.10	0.51
2:R:50:GLU:O	2:R:51:ASN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:HA	1:A:28:LYS:HE2	1.93	0.51
1:C:230:ILE:CD1	1:C:261:THR:HG21	2.34	0.51
1:H:11:ASP:OD1	1:H:11:ASP:N	2.44	0.51
1:H:326:ASN:HD22	1:H:329:THR:CG2	2.24	0.51
1:I:198:GLY:O	1:I:276:VAL:HG12	2.10	0.51
1:I:452:ARG:HG2	1:I:452:ARG:HH11	1.75	0.51
1:K:180:GLY:HA3	1:K:381:VAL:O	2.11	0.51
1:L:64:ASP:C	1:L:65:LYS:O	2.52	0.51
1:A:326:ASN:HD22	1:A:329:THR:HB	1.75	0.51
1:B:15:LYS:O	1:B:16:MET:C	2.53	0.51
1:B:76:GLU:HG2	1:B:76:GLU:O	2.11	0.51
1:B:228:SER:O	1:B:257:GLU:HB3	2.11	0.51
1:C:522:THR:OG1	1:C:523:ASP:N	2.41	0.51
1:E:130:GLU:O	1:E:133:ALA:HB3	2.11	0.51
1:I:62:LEU:N	1:I:68:ASN:OD1	2.33	0.51
1:J:197:ARG:HG3	1:J:277:LYS:O	2.11	0.51
1:J:444:LEU:HD23	1:J:447:MET:HE1	1.91	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.10	0.51
1:C:302:SER:H	1:C:307:MET:HE3	1.75	0.51
1:D:284:ARG:NH1	1:D:364:LYS:HD2	2.26	0.51
1:E:288:MET:HE1	1:E:371:LYS:HE2	1.92	0.51
1:F:33:PRO:HA	1:F:153:ASN:HD21	1.75	0.51
1:F:510:VAL:HG12	1:F:514:MET:CE	2.41	0.51
1:I:415:GLY:CA	1:I:417:VAL:HG23	2.41	0.51
1:A:16:MET:O	1:A:20:VAL:HG23	2.11	0.51
1:C:103:GLY:O	1:C:106:ALA:N	2.41	0.51
1:G:172:GLU:OE2	1:G:350:ARG:CZ	2.59	0.51
1:K:228:SER:O	1:K:257:GLU:HB3	2.10	0.51
1:M:419:LEU:HD22	1:M:500:THR:CG2	2.41	0.51
2:T:47:ARG:HD3	2:T:49:LEU:HD12	1.93	0.51
1:F:302:SER:H	1:F:307:MET:HE3	1.76	0.51
1:I:82:ASN:HB2	1:I:89:THR:OG1	2.11	0.51
1:J:203:TYR:CD1	1:J:267:MET:HE1	2.46	0.51
1:K:166:MET:HE3	1:K:171:LYS:HA	1.91	0.51
1:L:65:LYS:HA	7:L:529:HOH:O	2.11	0.51
2:Q:47:ARG:HD3	2:Q:49:LEU:HD12	1.91	0.51
5:C:600:ADP:PB	6:C:602:AF3:F2	2.59	0.51
1:D:150:ILE:HD11	1:D:492:GLY:O	2.11	0.51
1:F:512:GLY:O	1:F:515:ILE:HG13	2.10	0.51
1:I:73:MET:CE	1:I:514:MET:HE2	2.40	0.51
1:J:172:GLU:OE1	1:J:172:GLU:CA	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:VAL:HB	1:J:376:VAL:HG22	1.93	0.51
1:K:415:GLY:H	1:K:417:VAL:HG23	1.76	0.51
1:K:467:ASN:ND2	1:K:467:ASN:C	2.68	0.51
1:L:64:ASP:O	1:L:65:LYS:O	2.29	0.51
1:M:39:VAL:HB	1:N:520:MET:HG2	1.92	0.51
1:M:90:THR:O	1:M:94:VAL:HG23	2.11	0.51
1:N:149:THR:CG2	1:N:159:GLY:HA3	2.40	0.51
2:U:47:ARG:HD3	2:U:49:LEU:HD12	1.93	0.51
1:B:25:ASP:HA	1:B:28:LYS:HE2	1.93	0.50
1:C:486:GLY:C	1:C:491:MET:HE2	2.36	0.50
1:D:461:GLU:OE1	1:J:463:SER:HB3	2.12	0.50
1:G:25:ASP:HA	1:G:28:LYS:HE2	1.92	0.50
1:H:197:ARG:HD2	1:H:277:LYS:HB2	1.92	0.50
1:J:65:LYS:O	1:J:66:PHE:CB	2.44	0.50
1:M:302:SER:H	1:M:307:MET:HE3	1.76	0.50
1:N:351:GLN:HA	1:N:354:GLU:HG2	1.93	0.50
1:A:417:VAL:HG11	1:A:488:MET:HG3	1.92	0.50
1:B:16:MET:O	1:B:20:VAL:HG23	2.11	0.50
1:B:415:GLY:O	1:B:451:LEU:HD23	2.12	0.50
1:D:100:ILE:HG13	1:D:511:ALA:HB1	1.92	0.50
1:D:194:GLN:HG3	1:D:331:THR:HB	1.93	0.50
1:H:201:SER:O	1:H:203:TYR:N	2.44	0.50
1:L:106:ALA:HA	1:L:111:MET:CE	2.41	0.50
1:M:100:ILE:CG2	1:M:104:LEU:HD22	2.40	0.50
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.92	0.50
1:C:88:GLY:HA2	5:C:600:ADP:O2B	2.12	0.50
1:E:225:LYS:HD3	1:E:303:GLU:CD	2.36	0.50
1:F:111:MET:HG3	1:F:435:ASP:OD1	2.11	0.50
1:F:206:ASN:ND2	1:F:214:GLU:H	2.08	0.50
1:G:305:ILE:HB	1:G:307:MET:HE2	1.94	0.50
1:I:106:ALA:HA	1:I:111:MET:CE	2.41	0.50
1:K:203:TYR:CD1	1:K:267:MET:HE1	2.46	0.50
1:K:444:LEU:HA	1:K:447:MET:CE	2.36	0.50
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.93	0.50
1:A:365:LEU:CD2	1:A:368:ARG:HH21	2.25	0.50
1:C:69:MET:HE3	1:D:39:VAL:CG1	2.41	0.50
1:D:228:SER:O	1:D:257:GLU:HB3	2.11	0.50
1:F:524:LEU:HD23	1:F:525:PRO:HD2	1.92	0.50
1:A:345:ARG:O	1:A:348:GLN:HB2	2.12	0.50
1:F:414:GLY:O	1:F:417:VAL:CG1	2.58	0.50
1:G:414:GLY:HA2	1:G:495:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:GLY:O	1:J:120:ILE:C	2.54	0.50
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.11	0.50
1:K:385:THR:HG23	1:K:388:GLU:HB2	1.93	0.50
1:L:404:ARG:NH1	1:L:404:ARG:CG	2.72	0.50
1:N:228:SER:O	1:N:257:GLU:HB3	2.11	0.50
1:N:466:ALA:O	1:N:467:ASN:C	2.52	0.50
2:P:78:ILE:HD13	2:P:83:VAL:HG21	1.93	0.50
1:D:270:ILE:HD13	2:R:27:LEU:HB3	1.94	0.50
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.12	0.50
1:E:417:VAL:HG11	1:E:488:MET:HG3	1.94	0.50
1:F:265:ASN:HA	1:F:270:ILE:HD12	1.92	0.50
1:H:325:ILE:HG22	1:H:330:THR:HG23	1.93	0.50
1:I:158:VAL:HG13	1:I:396:VAL:HG22	1.93	0.50
1:J:66:PHE:H	1:J:69:MET:HG3	1.76	0.50
1:M:44:PHE:HD1	1:M:44:PHE:H	1.59	0.50
1:M:213:VAL:HB	1:M:325:ILE:CG1	2.39	0.50
2:P:50:GLU:O	2:P:51:ASN:HB3	2.12	0.50
1:D:67:GLU:O	1:D:68:ASN:C	2.53	0.50
1:D:511:ALA:O	1:D:515:ILE:HG12	2.11	0.50
1:M:64:ASP:C	1:M:65:LYS:O	2.53	0.50
1:C:326:ASN:HD22	1:C:329:THR:HB	1.77	0.50
1:E:524:LEU:HD22	1:E:525:PRO:HD2	1.93	0.50
1:F:11:ASP:O	1:F:12:ALA:C	2.55	0.50
1:I:16:MET:CE	1:I:16:MET:CG	2.90	0.50
1:I:461:GLU:HB3	1:I:464:VAL:HB	1.94	0.50
1:J:117:LYS:O	1:J:118:ARG:C	2.54	0.50
2:R:40:VAL:HB	2:R:62:GLY:H	1.76	0.50
2:S:11:ILE:HD12	2:S:42:ALA:HB3	1.94	0.50
1:A:482:THR:O	1:A:483:GLU:HB2	2.11	0.50
1:C:236:VAL:O	1:C:240:VAL:HG23	2.12	0.50
1:E:23:LEU:CD1	1:E:23:LEU:C	2.84	0.50
1:E:486:GLY:C	1:E:491:MET:HE2	2.36	0.50
1:F:524:LEU:HD22	1:F:525:PRO:HD2	1.92	0.50
1:G:284:ARG:NH1	1:G:364:LYS:HD2	2.27	0.50
1:G:502:SER:O	1:G:503:ALA:C	2.53	0.50
1:H:326:ASN:HB2	1:H:329:THR:HB	1.93	0.50
1:K:149:THR:HG23	1:K:159:GLY:HA3	1.93	0.50
1:L:426:LEU:CD1	1:L:444:LEU:HD21	2.42	0.50
1:N:305:ILE:HB	1:N:307:MET:HE2	1.93	0.50
1:E:326:ASN:HD22	1:E:329:THR:HB	1.76	0.49
1:I:305:ILE:HB	1:I:307:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:106:ALA:HA	1:J:111:MET:CE	2.42	0.49
1:J:385:THR:HG23	1:J:388:GLU:HB2	1.94	0.49
1:L:502:SER:O	1:L:503:ALA:C	2.54	0.49
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.94	0.49
1:A:39:VAL:HB	1:G:520:MET:HG2	1.93	0.49
1:A:91:THR:O	1:A:92:ALA:C	2.54	0.49
1:B:302:SER:H	1:B:307:MET:HE3	1.77	0.49
1:C:284:ARG:NH1	1:C:364:LYS:HD2	2.25	0.49
1:G:6:VAL:O	1:G:6:VAL:CG2	2.57	0.49
1:G:305:ILE:O	1:G:305:ILE:HG22	2.12	0.49
1:H:389:MET:HE2	1:H:390:LYS:HA	1.92	0.49
1:I:217:SER:N	1:I:218:PRO:CD	2.75	0.49
1:K:64:ASP:OD1	1:K:65:LYS:O	2.29	0.49
1:K:66:PHE:H	1:K:69:MET:HG3	1.78	0.49
1:M:66:PHE:HA	1:M:69:MET:HE3	1.94	0.49
1:M:351:GLN:HA	1:M:354:GLU:HG2	1.93	0.49
1:B:225:LYS:HD3	1:B:303:GLU:CD	2.38	0.49
1:C:22:VAL:HG11	1:C:62:LEU:HD11	1.93	0.49
5:D:600:ADP:O1B	6:D:602:AF3:F2	2.19	0.49
1:E:487:ASN:O	1:E:491:MET:HG3	2.12	0.49
1:J:44:PHE:HD1	1:J:44:PHE:H	1.59	0.49
1:L:385:THR:HG23	1:L:388:GLU:HB2	1.94	0.49
1:M:201:SER:O	1:M:203:TYR:N	2.44	0.49
1:M:452:ARG:HH11	1:M:452:ARG:HG2	1.77	0.49
1:B:111:MET:HG2	1:B:116:LEU:HD21	1.93	0.49
1:F:143:ALA:HA	1:F:146:GLN:NE2	2.28	0.49
1:G:147:VAL:HG12	1:G:494:LEU:HB2	1.94	0.49
1:H:339:GLU:O	1:H:343:GLN:HB2	2.12	0.49
1:J:467:ASN:C	1:J:467:ASN:ND2	2.69	0.49
1:M:221:LEU:HD23	1:M:249:ILE:HG23	1.93	0.49
2:U:7:HIS:HB3	2:U:45:ASN:HD22	1.77	0.49
1:B:23:LEU:CD1	1:B:23:LEU:C	2.85	0.49
1:H:82:ASN:ND2	1:H:89:THR:OG1	2.45	0.49
1:I:16:MET:CB	1:I:16:MET:HE3	2.42	0.49
1:K:426:LEU:HD12	1:K:444:LEU:HD21	1.94	0.49
1:L:44:PHE:H	1:L:44:PHE:HD1	1.60	0.49
1:N:326:ASN:HB2	1:N:329:THR:HB	1.94	0.49
1:D:305:ILE:HG23	1:E:267:MET:HG2	1.94	0.49
1:K:119:GLY:O	1:K:120:ILE:C	2.54	0.49
1:K:461:GLU:OE1	1:K:461:GLU:HA	2.13	0.49
1:N:461:GLU:HB3	1:N:464:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:ARG:HD3	1:D:505:GLN:OE1	2.13	0.49
1:E:443:ALA:O	1:E:447:MET:HE3	2.13	0.49
1:I:455:VAL:CG1	1:I:462:PRO:HA	2.41	0.49
1:K:201:SER:O	1:K:203:TYR:N	2.44	0.49
1:L:444:LEU:HA	1:L:447:MET:CE	2.23	0.49
1:M:15:LYS:NZ	1:M:64:ASP:OD2	2.46	0.49
2:P:16:GLU:HB2	2:P:19:THR:OG1	2.13	0.49
2:Q:16:GLU:HB2	2:Q:19:THR:OG1	2.12	0.49
2:S:40:VAL:HB	2:S:62:GLY:H	1.77	0.49
1:B:147:VAL:HG12	1:B:494:LEU:HB2	1.94	0.49
1:B:365:LEU:CD2	1:B:368:ARG:HH21	2.25	0.49
1:D:524:LEU:HD23	1:D:525:PRO:HD2	1.93	0.49
1:E:486:GLY:CA	1:E:491:MET:CE	2.90	0.49
1:F:326:ASN:HD22	1:F:329:THR:HB	1.76	0.49
1:I:213:VAL:HB	1:I:325:ILE:CG1	2.41	0.49
1:J:149:THR:CG2	1:J:159:GLY:HA3	2.43	0.49
1:K:197:ARG:HD2	1:K:277:LYS:HB2	1.94	0.49
1:L:64:ASP:OD1	1:L:65:LYS:O	2.31	0.49
1:M:502:SER:O	1:M:503:ALA:C	2.55	0.49
1:N:302:SER:H	1:N:307:MET:HE3	1.78	0.49
2:U:50:GLU:O	2:U:51:ASN:HB3	2.13	0.49
1:B:11:ASP:OD1	1:B:11:ASP:N	2.45	0.49
1:B:224:ASP:O	1:B:225:LYS:HB3	2.13	0.49
1:B:236:VAL:O	1:B:240:VAL:HG23	2.13	0.49
1:G:236:VAL:O	1:G:240:VAL:HG23	2.13	0.49
1:H:223:ALA:O	1:H:251:ALA:HA	2.13	0.49
1:I:203:TYR:CD1	1:I:267:MET:HE1	2.48	0.49
1:K:107:VAL:HG11	1:K:515:ILE:HG23	1.94	0.49
1:N:35:GLY:O	1:N:51:LYS:HE3	2.12	0.49
1:B:305:ILE:HB	1:B:307:MET:HE2	1.95	0.49
1:C:63:GLU:O	1:C:63:GLU:HG2	2.13	0.49
1:C:305:ILE:HG22	1:C:305:ILE:O	2.13	0.49
1:E:455:VAL:HG21	1:E:465:VAL:HG11	1.95	0.49
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.94	0.49
1:G:16:MET:HG3	1:G:520:MET:HE1	1.94	0.49
1:G:172:GLU:OE2	1:G:350:ARG:NH2	2.45	0.49
1:J:451:LEU:O	1:J:452:ARG:C	2.54	0.49
1:L:228:SER:O	1:L:257:GLU:HB3	2.12	0.49
1:B:482:THR:O	1:B:483:GLU:HB2	2.12	0.48
1:B:486:GLY:CA	1:B:491:MET:CE	2.89	0.48
1:C:228:SER:O	1:C:257:GLU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:LYS:HE2	7:D:615:HOH:O	2.13	0.48
1:G:16:MET:SD	1:G:514:MET:HG3	2.53	0.48
1:H:420:ILE:HD13	1:H:420:ILE:HG23	1.64	0.48
1:J:213:VAL:HB	1:J:325:ILE:CG1	2.40	0.48
1:M:224:ASP:O	1:M:225:LYS:HB3	2.13	0.48
1:N:194:GLN:HB2	1:N:331:THR:HB	1.95	0.48
2:O:16:GLU:HB2	2:O:19:THR:OG1	2.13	0.48
2:O:50:GLU:HG2	2:P:51:ASN:CB	2.38	0.48
2:T:50:GLU:O	2:T:51:ASN:HB3	2.12	0.48
1:A:16:MET:HG3	1:A:520:MET:HE1	1.95	0.48
1:A:111:MET:HG3	1:A:435:ASP:OD1	2.13	0.48
1:E:441:LYS:HB3	1:E:445:ARG:HH21	1.79	0.48
1:G:23:LEU:O	1:G:24:ALA:C	2.56	0.48
1:J:16:MET:CE	1:J:16:MET:CB	2.91	0.48
1:J:488:MET:CE	1:J:493:ILE:HG21	2.43	0.48
1:M:415:GLY:N	1:M:417:VAL:HG23	2.27	0.48
1:M:461:GLU:OE1	1:M:461:GLU:CA	2.60	0.48
2:O:7:HIS:HB3	2:O:45:ASN:HD22	1.78	0.48
1:A:265:ASN:HA	1:A:270:ILE:HD12	1.95	0.48
1:B:288:MET:HE1	1:B:371:LYS:HE2	1.95	0.48
1:C:524:LEU:HD22	1:C:525:PRO:HD2	1.95	0.48
1:D:23:LEU:C	1:D:23:LEU:CD1	2.86	0.48
1:D:247:LEU:HD12	1:D:248:LEU:N	2.28	0.48
1:F:16:MET:CE	1:F:16:MET:CG	2.91	0.48
1:I:145:ALA:O	1:I:149:THR:HG23	2.13	0.48
1:K:100:ILE:CG2	1:K:104:LEU:HD22	2.43	0.48
1:K:174:VAL:HB	1:K:376:VAL:HG22	1.95	0.48
1:G:111:MET:HG3	1:G:435:ASP:OD1	2.13	0.48
1:G:510:VAL:HG12	1:G:514:MET:HE3	1.94	0.48
1:H:404:ARG:CG	1:H:404:ARG:NH1	2.60	0.48
1:I:66:PHE:O	1:I:67:GLU:C	2.56	0.48
1:J:389:MET:HE2	1:J:390:LYS:HA	1.95	0.48
2:O:40:VAL:HB	2:O:62:GLY:H	1.78	0.48
2:O:47:ARG:HD3	2:O:49:LEU:HD12	1.95	0.48
2:P:40:VAL:HB	2:P:62:GLY:H	1.77	0.48
2:U:7:HIS:CE1	2:U:48:ILE:HD11	2.48	0.48
1:B:16:MET:CE	1:B:16:MET:CB	2.90	0.48
1:B:444:LEU:O	1:B:447:MET:HB2	2.14	0.48
1:C:486:GLY:HA3	1:C:491:MET:CE	2.41	0.48
1:F:479:ASN:C	1:F:479:ASN:OD1	2.56	0.48
1:I:100:ILE:CG2	1:I:104:LEU:HD22	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:326:ASN:HB2	1:I:329:THR:HB	1.95	0.48
1:L:203:TYR:CD1	1:L:267:MET:HE1	2.49	0.48
2:S:50:GLU:O	2:S:51:ASN:HB3	2.12	0.48
2:T:7:HIS:HB3	2:T:45:ASN:HD22	1.78	0.48
1:B:100:ILE:HG13	1:B:511:ALA:HB1	1.96	0.48
1:C:289:LEU:HA	1:C:292:ILE:HD12	1.96	0.48
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.22	0.48
1:E:365:LEU:CD2	1:E:368:ARG:HH21	2.26	0.48
1:F:104:LEU:HD23	1:F:515:ILE:HG22	1.94	0.48
1:F:150:ILE:CD1	1:F:492:GLY:O	2.61	0.48
1:F:305:ILE:O	1:F:305:ILE:HG22	2.13	0.48
1:H:44:PHE:HD1	1:H:44:PHE:H	1.61	0.48
1:H:66:PHE:O	1:H:67:GLU:C	2.55	0.48
1:H:73:MET:HE2	1:H:514:MET:HE2	1.94	0.48
1:H:218:PRO:HB3	1:H:246:PRO:HG2	1.96	0.48
1:I:444:LEU:CD2	1:I:447:MET:HE3	2.41	0.48
1:K:126:ALA:HB1	1:K:426:LEU:HD22	1.95	0.48
1:M:24:ALA:HA	1:M:27:VAL:HG12	1.95	0.48
1:A:511:ALA:O	1:A:515:ILE:HG12	2.14	0.48
1:C:16:MET:HG3	1:C:520:MET:HE1	1.96	0.48
1:F:448:GLU:O	1:F:452:ARG:HG3	2.13	0.48
1:H:126:ALA:HB1	1:H:426:LEU:HD22	1.96	0.48
1:H:469:VAL:HG13	1:H:477:GLY:HA2	1.95	0.48
1:J:180:GLY:HA3	1:J:381:VAL:O	2.14	0.48
1:K:66:PHE:O	1:K:67:GLU:C	2.56	0.48
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.95	0.48
1:N:326:ASN:HB2	1:N:329:THR:H	1.78	0.48
2:Q:78:ILE:HD13	2:Q:83:VAL:HG21	1.95	0.48
2:R:47:ARG:HD3	2:R:49:LEU:HD12	1.94	0.48
2:R:78:ILE:HD13	2:R:83:VAL:HG21	1.96	0.48
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.94	0.48
1:K:461:GLU:HB3	1:K:464:VAL:HB	1.96	0.48
2:O:95:VAL:CG1	2:P:1:MET:HE2	2.40	0.48
2:R:11:ILE:HD12	2:R:42:ALA:HB3	1.96	0.48
1:A:358:SER:HB3	1:A:361:ASP:OD1	2.14	0.48
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.95	0.48
1:D:305:ILE:O	1:D:305:ILE:HG22	2.14	0.48
1:D:510:VAL:HG12	1:D:514:MET:HE3	1.96	0.48
1:I:16:MET:HB2	1:I:16:MET:HE2	1.94	0.48
1:I:180:GLY:HA3	1:I:381:VAL:O	2.13	0.48
1:L:73:MET:HE2	1:L:514:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:452:ARG:HG2	1:L:452:ARG:NH1	2.29	0.48
2:R:16:GLU:HB2	2:R:19:THR:OG1	2.14	0.48
1:E:143:ALA:HA	1:E:146:GLN:NE2	2.29	0.48
1:F:362:ARG:HG2	1:F:366:GLN:NE2	2.29	0.48
1:I:461:GLU:OE1	1:I:461:GLU:CA	2.58	0.48
1:J:194:GLN:HB2	1:J:331:THR:HB	1.96	0.48
1:J:221:LEU:HD23	1:J:249:ILE:HG23	1.96	0.48
1:K:88:GLY:O	1:K:89:THR:C	2.57	0.48
1:L:218:PRO:HB3	1:L:246:PRO:HG2	1.96	0.48
1:M:172:GLU:OE1	1:M:172:GLU:CA	2.61	0.48
1:M:451:LEU:O	1:M:452:ARG:C	2.57	0.48
2:S:16:GLU:HB2	2:S:19:THR:OG1	2.14	0.48
2:S:47:ARG:HD3	2:S:49:LEU:HD12	1.95	0.48
2:S:78:ILE:HD13	2:S:83:VAL:HG21	1.96	0.48
1:A:230:ILE:CD1	1:A:261:THR:HG21	2.39	0.47
1:E:524:LEU:HD23	1:E:525:PRO:HD2	1.96	0.47
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.96	0.47
1:F:365:LEU:CD2	1:F:368:ARG:HH21	2.27	0.47
1:G:94:VAL:O	1:G:98:ALA:HB2	2.14	0.47
1:H:521:VAL:HB	1:N:40:LEU:HD12	1.95	0.47
1:I:116:LEU:HD23	1:I:116:LEU:HA	1.80	0.47
1:M:34:LYS:HB2	1:M:458:CYS:SG	2.54	0.47
2:Q:7:HIS:HB3	2:Q:45:ASN:HD22	1.79	0.47
1:B:284:ARG:NH1	1:B:364:LYS:HD2	2.28	0.47
1:B:518:GLU:O	1:B:518:GLU:HG3	2.14	0.47
1:C:223:ALA:O	1:C:251:ALA:HA	2.15	0.47
1:G:143:ALA:HA	1:G:146:GLN:HE21	1.77	0.47
1:I:126:ALA:CB	1:I:426:LEU:HD22	2.44	0.47
1:I:234:LEU:N	1:I:235:PRO:HD2	2.29	0.47
1:I:326:ASN:HD22	1:I:329:THR:CG2	2.26	0.47
1:J:201:SER:O	1:J:203:TYR:N	2.47	0.47
2:S:68:ASN:ND2	2:T:74:LYS:HD2	2.29	0.47
1:D:289:LEU:HA	1:D:292:ILE:HD12	1.96	0.47
1:F:415:GLY:O	1:F:451:LEU:HD23	2.13	0.47
1:G:74:VAL:O	1:G:77:VAL:HG13	2.14	0.47
1:L:100:ILE:CG2	1:L:104:LEU:HD22	2.45	0.47
1:M:57:ALA:O	1:M:58:ARG:C	2.57	0.47
1:M:428:ASP:CA	7:M:534:HOH:O	2.58	0.47
2:P:7:HIS:CE1	2:P:48:ILE:HD11	2.50	0.47
1:A:514:MET:HE3	1:A:514:MET:HB2	1.43	0.47
1:D:100:ILE:O	1:D:101:THR:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:SER:O	1:F:257:GLU:HB3	2.13	0.47
1:G:514:MET:HE3	1:G:514:MET:HB2	1.35	0.47
1:H:198:GLY:O	1:H:276:VAL:HG12	2.15	0.47
1:I:71:ALA:O	1:I:72:GLN:C	2.56	0.47
1:I:152:ALA:O	1:I:153:ASN:HB3	2.13	0.47
1:K:452:ARG:HG2	1:K:452:ARG:HH11	1.80	0.47
1:L:66:PHE:HA	1:L:69:MET:HE3	1.95	0.47
1:L:174:VAL:HB	1:L:376:VAL:HG22	1.95	0.47
1:L:221:LEU:HD23	1:L:249:ILE:HG23	1.95	0.47
1:C:76:GLU:OE1	1:D:387:VAL:HG13	2.15	0.47
1:G:419:LEU:HG	1:G:447:MET:HG2	1.95	0.47
1:I:103:GLY:O	1:I:106:ALA:HB3	2.13	0.47
1:I:351:GLN:HA	1:I:354:GLU:HG2	1.97	0.47
1:I:419:LEU:CD2	1:I:500:THR:CG2	2.93	0.47
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.96	0.47
1:J:198:GLY:O	1:J:276:VAL:HG12	2.14	0.47
1:J:419:LEU:HA	1:J:419:LEU:HD13	1.61	0.47
1:J:461:GLU:HB3	1:J:464:VAL:HB	1.96	0.47
1:J:488:MET:HE3	1:J:493:ILE:CG2	2.44	0.47
1:K:198:GLY:O	1:K:276:VAL:HG12	2.14	0.47
1:L:166:MET:HE3	1:L:171:LYS:HA	1.97	0.47
1:M:64:ASP:OD1	1:M:65:LYS:O	2.33	0.47
2:P:7:HIS:HB3	2:P:45:ASN:HD22	1.79	0.47
1:A:224:ASP:O	1:A:225:LYS:HB3	2.15	0.47
1:A:486:GLY:CA	1:A:491:MET:CE	2.89	0.47
1:C:247:LEU:HD12	1:C:248:LEU:N	2.29	0.47
1:I:64:ASP:C	1:I:65:LYS:O	2.54	0.47
1:I:66:PHE:H	1:I:69:MET:HG3	1.79	0.47
1:I:220:ILE:HG12	1:I:248:LEU:HD23	1.97	0.47
1:K:13:ARG:O	1:K:14:VAL:C	2.55	0.47
1:M:126:ALA:HB1	1:M:426:LEU:HD22	1.97	0.47
1:M:326:ASN:HB2	1:M:329:THR:H	1.79	0.47
1:N:426:LEU:HD12	1:N:444:LEU:HD21	1.96	0.47
2:Q:41:LEU:O	2:Q:61:VAL:HG13	2.14	0.47
1:A:11:ASP:O	1:A:12:ALA:C	2.57	0.47
1:A:28:LYS:HD2	1:A:453:GLN:NE2	2.29	0.47
1:A:78:ALA:HB2	1:A:93:THR:OG1	2.14	0.47
1:C:193:MET:HE3	1:C:371:LYS:HD3	1.97	0.47
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.96	0.47
1:F:284:ARG:HH11	1:F:364:LYS:HD2	1.80	0.47
1:F:358:SER:HB3	1:F:361:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:455:VAL:HG11	1:F:462:PRO:HA	1.96	0.47
1:H:76:GLU:HG2	1:H:76:GLU:O	2.13	0.47
1:H:166:MET:HE3	1:H:171:LYS:HA	1.96	0.47
1:H:419:LEU:HD22	1:H:500:THR:CG2	2.45	0.47
1:J:66:PHE:HA	1:J:69:MET:HE3	1.95	0.47
1:J:106:ALA:CB	1:J:111:MET:HE3	2.44	0.47
1:K:66:PHE:HA	1:K:69:MET:HE3	1.96	0.47
1:L:34:LYS:HB2	1:L:458:CYS:SG	2.55	0.47
1:L:126:ALA:HB1	1:L:426:LEU:CD2	2.43	0.47
1:N:66:PHE:HA	1:N:69:MET:HE3	1.95	0.47
1:N:201:SER:O	1:N:203:TYR:N	2.47	0.47
1:B:462:PRO:O	1:B:463:SER:C	2.58	0.47
1:C:143:ALA:HA	1:C:146:GLN:HE21	1.80	0.47
1:D:310:GLU:OE1	1:D:310:GLU:N	2.47	0.47
1:D:486:GLY:HA3	1:D:491:MET:CE	2.44	0.47
1:F:487:ASN:O	1:F:491:MET:HG3	2.15	0.47
1:G:365:LEU:CD2	1:G:368:ARG:HH21	2.27	0.47
1:J:126:ALA:CB	1:J:426:LEU:HD22	2.43	0.47
1:J:326:ASN:HB2	1:J:329:THR:HB	1.97	0.47
1:K:35:GLY:O	1:K:51:LYS:HE3	2.14	0.47
1:L:326:ASN:HB2	1:L:329:THR:HB	1.96	0.47
1:M:428:ASP:CB	7:M:534:HOH:O	2.58	0.47
1:N:15:LYS:HB3	1:N:66:PHE:HB3	1.96	0.47
1:N:103:GLY:O	1:N:106:ALA:HB3	2.15	0.47
1:N:234:LEU:N	1:N:235:PRO:HD2	2.30	0.47
1:B:270:ILE:HD13	2:P:27:LEU:HB3	1.97	0.47
1:C:23:LEU:CD1	1:C:23:LEU:C	2.87	0.47
1:C:23:LEU:O	1:C:24:ALA:C	2.55	0.47
1:C:455:VAL:HG11	1:C:462:PRO:HA	1.97	0.47
1:D:143:ALA:HA	1:D:146:GLN:HE21	1.79	0.47
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.97	0.47
1:E:103:GLY:HA3	1:E:515:ILE:HG21	1.97	0.47
1:E:305:ILE:HG23	1:F:267:MET:HG2	1.95	0.47
1:G:77:VAL:HG22	1:G:78:ALA:N	2.30	0.47
1:I:224:ASP:O	1:I:225:LYS:HB3	2.14	0.47
1:K:419:LEU:HD13	1:K:419:LEU:HA	1.72	0.47
1:M:66:PHE:O	1:M:67:GLU:C	2.56	0.47
1:N:106:ALA:HA	1:N:111:MET:CE	2.44	0.47
1:A:129:GLU:OE2	1:A:129:GLU:HA	2.15	0.47
1:A:223:ALA:O	1:A:251:ALA:HA	2.14	0.47
1:E:201:SER:C	1:E:203:TYR:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:ARG:NH1	1:E:364:LYS:HD2	2.30	0.47
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.96	0.47
1:G:349:ILE:HA	1:G:352:GLN:HG2	1.95	0.47
1:J:228:SER:O	1:J:257:GLU:HB3	2.14	0.47
1:K:100:ILE:O	1:K:104:LEU:HB2	2.14	0.47
1:L:23:LEU:O	1:L:23:LEU:HD22	2.15	0.47
1:L:197:ARG:HD2	1:L:277:LYS:HB2	1.97	0.47
2:Q:50:GLU:O	2:Q:51:ASN:HB3	2.15	0.47
1:A:358:SER:HB3	1:A:361:ASP:HB2	1.98	0.46
1:A:502:SER:O	1:A:503:ALA:C	2.54	0.46
1:C:105:LYS:HD3	1:J:110:GLY:O	2.15	0.46
1:D:429:LEU:HD12	1:D:429:LEU:HA	1.71	0.46
1:K:90:THR:O	1:K:94:VAL:HG23	2.15	0.46
2:R:68:ASN:HD22	2:S:74:LYS:HD2	1.80	0.46
1:D:365:LEU:CD2	1:D:368:ARG:HH21	2.27	0.46
1:E:247:LEU:HD12	1:E:248:LEU:N	2.29	0.46
1:I:419:LEU:HA	1:I:419:LEU:HD13	1.65	0.46
1:K:16:MET:CE	1:K:16:MET:CG	2.93	0.46
1:L:262:LEU:O	1:L:266:THR:HG23	2.15	0.46
1:M:166:MET:HE2	1:M:171:LYS:HA	1.98	0.46
1:N:16:MET:HG2	1:N:70:GLY:HA2	1.96	0.46
2:S:7:HIS:HB3	2:S:45:ASN:HD22	1.80	0.46
1:A:310:GLU:OE1	1:A:310:GLU:N	2.48	0.46
1:B:201:SER:C	1:B:203:TYR:H	2.24	0.46
1:B:247:LEU:HD12	1:B:248:LEU:N	2.31	0.46
1:C:172:GLU:OE1	1:C:172:GLU:HA	2.15	0.46
1:D:33:PRO:HA	1:D:153:ASN:HD21	1.81	0.46
1:G:162:ILE:O	1:G:165:ALA:HB3	2.15	0.46
1:G:326:ASN:HD22	1:G:329:THR:HB	1.79	0.46
1:M:389:MET:HE2	1:M:390:LYS:HA	1.98	0.46
1:A:417:VAL:O	1:A:418:ALA:C	2.58	0.46
1:C:150:ILE:HD11	1:C:492:GLY:O	2.15	0.46
1:E:194:GLN:HG3	1:E:331:THR:HB	1.97	0.46
1:F:223:ALA:O	1:F:251:ALA:HA	2.16	0.46
1:F:288:MET:HE1	1:F:371:LYS:HE2	1.97	0.46
1:G:225:LYS:HD3	1:G:303:GLU:CD	2.41	0.46
1:K:126:ALA:CB	1:K:426:LEU:HD22	2.45	0.46
1:M:198:GLY:HA3	1:M:327:LYS:O	2.16	0.46
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.97	0.46
1:D:190:VAL:HG11	1:D:194:GLN:NE2	2.30	0.46
1:F:172:GLU:OE1	1:F:172:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:GLN:HG3	1:F:331:THR:HB	1.97	0.46
1:I:437:ASN:O	1:I:438:VAL:C	2.57	0.46
1:K:201:SER:C	1:K:203:TYR:N	2.74	0.46
1:L:106:ALA:C	1:L:111:MET:HE3	2.40	0.46
1:N:413:ALA:CB	1:N:417:VAL:HB	2.44	0.46
1:A:270:ILE:CD1	2:O:27:LEU:HB3	2.46	0.46
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.98	0.46
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.97	0.46
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.51	0.46
1:G:310:GLU:OE1	1:G:310:GLU:N	2.49	0.46
1:N:94:VAL:O	1:N:94:VAL:HG12	2.16	0.46
1:N:419:LEU:HD22	1:N:500:THR:CG2	2.45	0.46
1:D:201:SER:C	1:D:203:TYR:H	2.24	0.46
1:G:230:ILE:CD1	1:G:261:THR:HG21	2.38	0.46
1:H:449:ALA:N	1:H:450:PRO:CD	2.79	0.46
1:J:80:LYS:O	1:J:81:ALA:C	2.58	0.46
1:M:116:LEU:HD23	1:M:116:LEU:HA	1.84	0.46
1:N:452:ARG:HG2	1:N:452:ARG:NH1	2.27	0.46
1:N:514:MET:CE	1:N:514:MET:CG	2.93	0.46
1:A:130:GLU:O	1:A:133:ALA:HB3	2.15	0.46
1:A:291:ASP:HB3	1:A:372:LEU:HD11	1.98	0.46
1:A:451:LEU:HD13	1:A:451:LEU:C	2.41	0.46
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.71	0.46
1:B:429:LEU:O	1:B:430:ARG:NH1	2.49	0.46
1:E:153:ASN:O	1:E:154:SER:HB2	2.16	0.46
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.97	0.46
1:F:514:MET:HB2	1:F:514:MET:HE3	1.60	0.46
1:G:96:ALA:C	1:G:98:ALA:H	2.24	0.46
1:G:194:GLN:HG3	1:G:331:THR:HB	1.98	0.46
1:H:444:LEU:HD23	1:H:444:LEU:HA	1.69	0.46
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.97	0.46
1:N:43:SER:HB2	1:N:44:PHE:H	1.67	0.46
1:A:6:VAL:O	1:A:6:VAL:CG2	2.61	0.46
1:A:284:ARG:NH1	1:A:364:LYS:HD2	2.29	0.46
1:A:289:LEU:HA	1:A:292:ILE:HD12	1.98	0.46
1:B:414:GLY:C	1:B:416:GLY:N	2.69	0.46
1:C:172:GLU:OE2	1:C:350:ARG:NH2	2.48	0.46
1:F:224:ASP:O	1:F:225:LYS:HB3	2.15	0.46
1:G:224:ASP:O	1:G:225:LYS:HB3	2.16	0.46
1:H:166:MET:HE1	1:H:407:VAL:HG21	1.97	0.46
1:K:106:ALA:HA	1:K:111:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:197:ARG:HG3	1:N:277:LYS:O	2.16	0.46
1:N:444:LEU:HA	1:N:444:LEU:HD23	1.75	0.46
1:B:230:ILE:CD1	1:B:261:THR:HG21	2.41	0.46
1:D:479:ASN:C	1:D:479:ASN:OD1	2.58	0.46
1:F:230:ILE:CD1	1:F:261:THR:HG21	2.41	0.46
1:G:455:VAL:HG11	1:G:462:PRO:HA	1.97	0.46
1:H:224:ASP:O	1:H:225:LYS:HB3	2.15	0.46
1:H:415:GLY:CA	1:H:417:VAL:HG23	2.46	0.46
1:I:346:VAL:O	1:I:350:ARG:HB2	2.14	0.46
1:M:21:ASN:HD22	1:M:21:ASN:HA	1.46	0.46
1:M:166:MET:HE3	1:M:171:LYS:HA	1.97	0.46
1:N:511:ALA:O	1:N:515:ILE:HD12	2.16	0.46
2:O:78:ILE:HD13	2:O:83:VAL:HG21	1.98	0.46
1:A:201:SER:C	1:A:203:TYR:H	2.24	0.45
1:A:452:ARG:NH2	1:A:463:SER:HA	2.31	0.45
1:C:219:PHE:C	1:C:220:ILE:HG13	2.41	0.45
1:F:201:SER:C	1:F:203:TYR:H	2.24	0.45
1:H:100:ILE:O	1:H:104:LEU:HB2	2.16	0.45
1:I:49:ILE:HD12	1:I:513:LEU:HD23	1.97	0.45
1:I:326:ASN:HB2	1:I:329:THR:H	1.80	0.45
1:I:436:GLN:O	1:I:440:ILE:HG13	2.16	0.45
1:J:193:MET:HE2	1:J:195:PHE:HD1	1.81	0.45
1:L:326:ASN:HB2	1:L:329:THR:H	1.81	0.45
1:L:426:LEU:HD12	1:L:444:LEU:HD21	1.96	0.45
1:N:147:VAL:HG21	1:N:411:VAL:HG11	1.98	0.45
2:Q:68:ASN:ND2	2:R:74:LYS:HD2	2.31	0.45
1:D:224:ASP:O	1:D:225:LYS:HB3	2.16	0.45
1:G:240:VAL:HG21	1:G:247:LEU:HD22	1.98	0.45
1:G:345:ARG:O	1:G:348:GLN:HB2	2.16	0.45
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.99	0.45
1:I:209:GLU:OE1	1:I:209:GLU:N	2.49	0.45
1:I:404:ARG:NH1	1:I:404:ARG:CG	2.60	0.45
1:J:106:ALA:HB1	1:J:111:MET:HE3	1.96	0.45
1:N:180:GLY:HA3	1:N:381:VAL:O	2.15	0.45
1:A:205:ILE:CA	1:A:213:VAL:HG22	2.43	0.45
1:C:143:ALA:HA	1:C:146:GLN:NE2	2.31	0.45
1:C:310:GLU:N	1:C:310:GLU:OE1	2.48	0.45
1:D:225:LYS:HD3	1:D:303:GLU:CD	2.41	0.45
1:F:310:GLU:OE1	1:F:310:GLU:N	2.50	0.45
1:G:358:SER:HB3	1:G:361:ASP:HB2	1.98	0.45
1:L:201:SER:C	1:L:203:TYR:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:LYS:H	1:N:65:LYS:HG3	1.27	0.45
1:N:116:LEU:HD23	1:N:116:LEU:HA	1.87	0.45
1:A:305:ILE:O	1:A:305:ILE:HG22	2.17	0.45
1:B:441:LYS:HB3	1:B:445:ARG:HH21	1.82	0.45
1:H:35:GLY:O	1:H:51:LYS:HE3	2.17	0.45
1:I:63:GLU:HA	1:J:3:ALA:CB	2.47	0.45
1:I:511:ALA:O	1:I:515:ILE:HD12	2.16	0.45
1:K:234:LEU:N	1:K:235:PRO:HD2	2.32	0.45
1:N:419:LEU:HD13	1:N:419:LEU:HA	1.60	0.45
1:B:218:PRO:HB3	1:B:246:PRO:HG2	1.99	0.45
1:C:225:LYS:HD3	1:C:303:GLU:CD	2.42	0.45
1:D:482:THR:O	1:D:483:GLU:HB2	2.16	0.45
1:E:310:GLU:OE1	1:E:310:GLU:N	2.50	0.45
1:E:345:ARG:O	1:E:348:GLN:HB2	2.16	0.45
1:G:479:ASN:C	1:G:479:ASN:OD1	2.59	0.45
1:G:482:THR:O	1:G:483:GLU:HB2	2.16	0.45
1:I:149:THR:HG22	1:I:159:GLY:HA3	1.99	0.45
1:K:419:LEU:CD2	1:K:500:THR:HG23	2.47	0.45
1:L:430:ARG:HA	1:L:430:ARG:HD3	1.76	0.45
1:L:461:GLU:HB3	1:L:464:VAL:HB	1.99	0.45
1:M:100:ILE:O	1:M:104:LEU:HB2	2.16	0.45
1:M:326:ASN:HB2	1:M:329:THR:HB	1.97	0.45
7:M:529:HOH:O	1:N:68:ASN:HB3	2.16	0.45
2:O:20:LYS:HB3	2:O:27:LEU:HG	1.98	0.45
1:B:514:MET:CE	1:B:514:MET:CB	2.92	0.45
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.16	0.45
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.98	0.45
1:F:349:ILE:HA	1:F:352:GLN:HG2	1.97	0.45
1:G:88:GLY:N	6:G:602:AF3:F2	2.40	0.45
1:N:201:SER:C	1:N:203:TYR:N	2.74	0.45
2:T:3:ILE:H	2:T:3:ILE:HD12	1.82	0.45
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.98	0.45
1:G:201:SER:C	1:G:203:TYR:H	2.25	0.45
1:H:228:SER:O	1:H:257:GLU:HB3	2.16	0.45
1:J:16:MET:HG3	1:J:520:MET:HE1	1.98	0.45
1:J:24:ALA:HA	1:J:27:VAL:HG12	1.97	0.45
1:J:217:SER:N	1:J:218:PRO:CD	2.76	0.45
1:J:492:GLY:O	1:J:493:ILE:HD13	2.17	0.45
1:K:104:LEU:HD12	1:K:104:LEU:HA	1.46	0.45
1:K:326:ASN:HB2	1:K:329:THR:HB	1.99	0.45
1:M:417:VAL:O	1:M:418:ALA:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:78:ILE:HD13	2:T:83:VAL:HG21	1.99	0.45
1:A:329:THR:O	1:A:329:THR:HG22	2.16	0.45
1:C:78:ALA:HB2	1:C:93:THR:OG1	2.17	0.45
1:D:261:THR:O	1:D:262:LEU:C	2.58	0.45
1:F:129:GLU:OE2	1:F:129:GLU:HA	2.17	0.45
1:G:76:GLU:O	1:G:76:GLU:HG2	2.16	0.45
1:G:223:ALA:O	1:G:251:ALA:HA	2.17	0.45
1:G:487:ASN:O	1:G:491:MET:HG3	2.17	0.45
1:J:524:LEU:HD23	1:J:524:LEU:HA	1.78	0.45
1:L:270:ILE:HG22	1:L:271:VAL:HG23	1.98	0.45
1:M:203:TYR:CD1	1:M:267:MET:HE1	2.52	0.45
1:N:106:ALA:CB	1:N:111:MET:HE3	2.47	0.45
1:N:166:MET:HE3	1:N:171:LYS:HA	1.94	0.45
1:A:225:LYS:HD3	1:A:303:GLU:CD	2.42	0.45
1:A:452:ARG:HH22	1:A:463:SER:HB3	1.82	0.45
1:B:78:ALA:HB2	1:B:93:THR:OG1	2.16	0.45
1:B:233:MET:O	1:B:234:LEU:C	2.59	0.45
1:C:448:GLU:HB3	1:C:452:ARG:HD2	1.99	0.45
1:G:74:VAL:C	1:G:76:GLU:N	2.73	0.45
1:I:228:SER:O	1:I:257:GLU:HB3	2.17	0.45
1:K:222:LEU:HD23	1:K:250:ILE:HB	1.99	0.45
1:M:325:ILE:HG22	1:M:330:THR:HG23	1.98	0.45
1:A:461:GLU:OE1	1:N:463:SER:HB3	2.17	0.45
1:B:349:ILE:HA	1:B:352:GLN:HG2	1.92	0.45
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.98	0.45
1:C:358:SER:HB3	1:C:361:ASP:OD1	2.17	0.45
1:D:69:MET:HE1	1:D:520:MET:HB3	1.99	0.45
1:E:305:ILE:HG22	1:E:305:ILE:O	2.17	0.45
1:G:190:VAL:HG11	1:G:194:GLN:NE2	2.32	0.45
1:G:218:PRO:HB3	1:G:246:PRO:HG2	1.99	0.45
1:H:119:GLY:O	1:H:120:ILE:C	2.59	0.45
1:H:203:TYR:CD1	1:H:267:MET:HE1	2.51	0.45
1:H:262:LEU:O	1:H:266:THR:HG23	2.17	0.45
1:I:467:ASN:ND2	1:I:467:ASN:C	2.70	0.45
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.99	0.45
1:M:47:PRO:CG	1:N:73:MET:HG3	2.46	0.45
1:N:34:LYS:HB2	1:N:458:CYS:SG	2.57	0.45
1:C:224:ASP:O	1:C:225:LYS:HB3	2.17	0.44
1:D:76:GLU:O	1:D:80:LYS:HB2	2.17	0.44
1:F:247:LEU:HD12	1:F:248:LEU:N	2.31	0.44
1:G:518:GLU:O	1:G:518:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:THR:O	1:I:94:VAL:HG23	2.17	0.44
1:I:99:ILE:O	1:I:102:GLU:N	2.46	0.44
1:J:100:ILE:O	1:J:104:LEU:HB2	2.16	0.44
1:N:84:ALA:O	1:N:85:ALA:HB2	2.17	0.44
1:N:522:THR:OG1	1:N:523:ASP:N	2.50	0.44
1:C:362:ARG:HG2	1:C:366:GLN:NE2	2.32	0.44
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.98	0.44
1:E:224:ASP:O	1:E:225:LYS:HB3	2.17	0.44
1:E:510:VAL:HG13	1:E:514:MET:CE	2.47	0.44
1:H:163:ALA:O	1:H:167:ASP:HB2	2.17	0.44
1:J:198:GLY:HA3	1:J:327:LYS:O	2.16	0.44
1:K:430:ARG:HA	1:K:430:ARG:HD3	1.63	0.44
1:L:106:ALA:O	1:L:111:MET:HE3	2.17	0.44
1:L:198:GLY:HA3	1:L:327:LYS:O	2.17	0.44
1:M:169:VAL:HG13	1:M:173:GLY:HA3	2.00	0.44
1:D:291:ASP:HB3	1:D:372:LEU:HD11	1.99	0.44
1:G:247:LEU:HD12	1:G:248:LEU:N	2.32	0.44
1:I:415:GLY:C	1:I:417:VAL:H	2.25	0.44
1:K:326:ASN:HB2	1:K:329:THR:H	1.81	0.44
1:L:302:SER:H	1:L:307:MET:HE3	1.83	0.44
1:N:106:ALA:HB1	1:N:111:MET:HE3	1.98	0.44
2:U:14:ARG:NH2	2:U:84:LEU:HD21	2.33	0.44
1:C:291:ASP:HB3	1:C:372:LEU:HD11	1.99	0.44
1:F:234:LEU:HB2	1:F:235:PRO:CD	2.47	0.44
1:F:510:VAL:HG12	1:F:514:MET:HE3	1.98	0.44
1:H:65:LYS:H	1:H:65:LYS:HG3	1.35	0.44
1:H:152:ALA:O	1:H:153:ASN:HB3	2.17	0.44
1:I:430:ARG:HD3	1:I:430:ARG:HA	1.59	0.44
1:K:13:ARG:HA	1:K:16:MET:CE	2.47	0.44
1:K:144:ILE:CD1	1:K:407:VAL:HG22	2.48	0.44
1:K:262:LEU:O	1:K:266:THR:HG23	2.17	0.44
1:L:77:VAL:CG1	1:L:78:ALA:N	2.81	0.44
1:L:166:MET:HE2	1:L:171:LYS:HA	1.99	0.44
1:A:409:GLU:CD	1:A:501:ARG:HH21	2.24	0.44
1:C:66:PHE:O	1:C:69:MET:HB2	2.17	0.44
1:C:206:ASN:HD21	1:C:214:GLU:N	2.06	0.44
1:C:358:SER:HB3	1:C:361:ASP:HB2	1.99	0.44
1:C:516:THR:OG1	1:D:37:ASN:ND2	2.50	0.44
1:F:88:GLY:N	6:F:602:AF3:F2	2.40	0.44
1:F:225:LYS:HD3	1:F:303:GLU:CD	2.42	0.44
1:F:420:ILE:HD13	1:F:448:GLU:HG2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:MET:O	1:G:20:VAL:HG23	2.17	0.44
1:G:362:ARG:HG2	1:G:366:GLN:NE2	2.33	0.44
1:J:101:THR:HG22	1:J:102:GLU:OE1	2.17	0.44
1:L:437:ASN:HA	1:L:440:ILE:HD12	2.00	0.44
1:M:119:GLY:O	1:M:120:ILE:C	2.60	0.44
1:N:288:MET:CE	1:N:288:MET:CG	2.90	0.44
1:N:487:ASN:O	1:N:491:MET:HG3	2.17	0.44
1:B:345:ARG:O	1:B:348:GLN:HB2	2.17	0.44
1:C:288:MET:HE1	1:C:371:LYS:HE2	1.99	0.44
1:E:139:SER:N	7:E:611:HOH:O	2.37	0.44
1:E:324:VAL:HB	1:E:331:THR:HG23	2.00	0.44
1:E:479:ASN:OD1	1:E:479:ASN:C	2.60	0.44
1:H:217:SER:N	1:H:218:PRO:CD	2.80	0.44
1:H:466:ALA:O	1:H:467:ASN:C	2.58	0.44
1:J:16:MET:HG2	1:J:70:GLY:HA2	1.98	0.44
1:K:346:VAL:O	1:K:350:ARG:HB2	2.18	0.44
1:N:100:ILE:O	1:N:104:LEU:HB2	2.18	0.44
1:A:88:GLY:N	6:A:602:AF3:F2	2.40	0.44
1:B:20:VAL:HG23	1:B:20:VAL:H	1.62	0.44
1:E:409:GLU:CD	1:E:501:ARG:HH21	2.26	0.44
1:F:16:MET:HE2	1:F:16:MET:HB3	2.00	0.44
1:F:146:GLN:HE21	1:F:146:GLN:HB2	1.64	0.44
1:G:261:THR:O	1:G:262:LEU:C	2.61	0.44
1:I:73:MET:SD	1:I:514:MET:HE2	2.58	0.44
1:J:201:SER:C	1:J:203:TYR:N	2.75	0.44
1:M:10:ASN:O	1:M:11:ASP:C	2.61	0.44
2:S:68:ASN:HD22	2:T:74:LYS:HD2	1.82	0.44
2:T:60:LYS:H	2:T:60:LYS:HG2	1.66	0.44
1:A:147:VAL:CG2	1:A:403:THR:HG22	2.48	0.44
1:B:172:GLU:OE1	1:B:172:GLU:HA	2.17	0.44
1:C:201:SER:C	1:C:203:TYR:H	2.26	0.44
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.99	0.44
1:G:423:ALA:O	7:G:607:HOH:O	2.21	0.44
1:H:166:MET:HE2	1:H:171:LYS:HA	2.00	0.44
1:H:413:ALA:CB	1:H:417:VAL:HB	2.46	0.44
1:I:21:ASN:HD22	1:I:21:ASN:HA	1.44	0.44
1:L:40:LEU:HD12	1:M:521:VAL:HB	1.98	0.44
1:L:104:LEU:HD12	1:L:104:LEU:HA	1.64	0.44
1:L:487:ASN:O	1:L:491:MET:HG3	2.18	0.44
1:M:430:ARG:HD3	1:M:430:ARG:HA	1.69	0.44
1:A:103:GLY:O	1:A:106:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PRO:HB3	1:A:246:PRO:HG2	2.00	0.44
1:B:9:GLY:O	1:B:10:ASN:C	2.60	0.44
1:B:157:THR:O	1:B:161:LEU:HB2	2.18	0.44
1:D:345:ARG:O	1:D:348:GLN:HB2	2.18	0.44
1:G:130:GLU:O	1:G:133:ALA:HB3	2.18	0.44
1:G:193:MET:HE3	1:G:371:LYS:HD3	1.99	0.44
1:I:16:MET:HG2	1:I:70:GLY:HA2	2.00	0.44
1:I:222:LEU:HD23	1:I:250:ILE:HB	2.00	0.44
1:J:234:LEU:N	1:J:235:PRO:HD2	2.33	0.44
1:K:95:LEU:HD23	1:K:446:ALA:O	2.18	0.44
1:M:228:SER:O	1:M:257:GLU:HB3	2.18	0.44
1:M:234:LEU:N	1:M:235:PRO:HD2	2.32	0.44
2:O:11:ILE:HD12	2:O:42:ALA:HB3	1.98	0.44
2:Q:51:ASN:O	2:Q:52:GLY:C	2.61	0.44
2:R:68:ASN:ND2	2:S:74:LYS:HD2	2.32	0.44
2:U:18:GLU:O	2:U:19:THR:C	2.61	0.44
1:A:270:ILE:HD11	2:O:27:LEU:HD13	2.00	0.43
1:A:466:ALA:O	1:A:467:ASN:C	2.60	0.43
1:B:124:VAL:HG22	1:B:504:LEU:HD11	2.00	0.43
1:B:512:GLY:O	1:B:515:ILE:HG13	2.17	0.43
1:C:324:VAL:HB	1:C:331:THR:HG23	2.00	0.43
1:D:223:ALA:O	1:D:251:ALA:HA	2.18	0.43
1:D:522:THR:OG1	1:D:523:ASP:N	2.52	0.43
1:F:91:THR:O	1:F:92:ALA:C	2.60	0.43
1:H:270:ILE:HG22	1:H:271:VAL:HG23	1.99	0.43
1:I:43:SER:HB2	1:I:44:PHE:H	1.72	0.43
1:A:76:GLU:O	1:A:80:LYS:HB2	2.18	0.43
1:A:349:ILE:HA	1:A:352:GLN:HG2	1.97	0.43
1:A:524:LEU:HD23	1:A:525:PRO:HD2	2.00	0.43
1:C:513:LEU:HA	1:C:513:LEU:HD23	1.78	0.43
1:D:18:ARG:HB3	1:D:18:ARG:CZ	2.48	0.43
1:E:510:VAL:HG13	1:E:514:MET:HE1	2.00	0.43
1:F:513:LEU:HA	1:F:513:LEU:HD23	1.79	0.43
1:G:358:SER:HB3	1:G:361:ASP:OD1	2.18	0.43
1:H:126:ALA:CB	1:H:426:LEU:HD22	2.47	0.43
1:I:219:PHE:HB3	1:I:317:LEU:HD23	2.00	0.43
1:J:64:ASP:C	1:J:65:LYS:O	2.60	0.43
1:K:100:ILE:HG22	1:K:104:LEU:HD22	1.99	0.43
1:K:437:ASN:HA	1:K:440:ILE:HD12	2.00	0.43
1:B:16:MET:HG3	1:B:520:MET:CE	2.48	0.43
1:E:11:ASP:N	1:E:11:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ALA:O	1:E:251:ALA:HA	2.17	0.43
1:H:417:VAL:HG21	1:H:488:MET:HE2	1.99	0.43
1:I:218:PRO:HB3	1:I:246:PRO:HG2	2.00	0.43
1:K:444:LEU:HD23	1:K:444:LEU:HA	1.71	0.43
1:N:15:LYS:HD2	1:N:15:LYS:HA	1.82	0.43
1:A:82:ASN:HB2	1:A:89:THR:CG2	2.49	0.43
1:E:143:ALA:HA	1:E:146:GLN:HE21	1.82	0.43
1:E:514:MET:HE3	1:E:514:MET:HB2	1.62	0.43
1:G:104:LEU:HD23	1:G:515:ILE:HG22	1.99	0.43
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.99	0.43
1:I:88:GLY:O	1:I:91:THR:N	2.52	0.43
1:I:172:GLU:OE1	1:I:172:GLU:CA	2.64	0.43
1:J:117:LYS:HG2	1:J:121:ASP:OD2	2.19	0.43
2:O:3:ILE:CD1	2:O:3:ILE:H	2.31	0.43
2:U:11:ILE:HD12	2:U:42:ALA:HB3	2.00	0.43
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.99	0.43
1:B:240:VAL:HG21	1:B:247:LEU:HD22	2.00	0.43
1:F:103:GLY:HA3	1:F:515:ILE:HG21	1.99	0.43
1:G:219:PHE:C	1:G:220:ILE:HG13	2.43	0.43
1:G:475:ASN:HD22	1:G:475:ASN:HA	1.56	0.43
1:H:65:LYS:HA	7:H:528:HOH:O	2.19	0.43
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.99	0.43
1:H:487:ASN:O	1:H:491:MET:HG3	2.18	0.43
1:H:502:SER:O	1:H:503:ALA:C	2.61	0.43
1:I:35:GLY:O	1:I:51:LYS:HE3	2.18	0.43
1:I:65:LYS:HB3	7:I:529:HOH:O	2.17	0.43
1:J:15:LYS:NZ	1:J:64:ASP:OD2	2.52	0.43
1:L:49:ILE:HD13	1:M:73:MET:HE3	2.00	0.43
1:L:65:LYS:H	1:L:65:LYS:HG3	1.27	0.43
1:M:201:SER:C	1:M:203:TYR:N	2.74	0.43
2:S:18:GLU:O	2:S:19:THR:C	2.61	0.43
2:T:7:HIS:CE1	2:T:48:ILE:HD11	2.54	0.43
2:U:15:LYS:HB3	2:U:16:GLU:H	1.65	0.43
1:A:67:GLU:O	1:A:68:ASN:C	2.59	0.43
1:A:247:LEU:HD12	1:A:248:LEU:N	2.33	0.43
1:A:305:ILE:HG23	1:B:267:MET:HG2	2.00	0.43
1:B:91:THR:O	1:B:92:ALA:C	2.60	0.43
1:B:143:ALA:HA	1:B:146:GLN:HE21	1.84	0.43
1:D:11:ASP:N	1:D:11:ASP:OD1	2.51	0.43
1:E:213:VAL:HB	1:E:325:ILE:HG12	2.00	0.43
1:F:324:VAL:HB	1:F:331:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:LYS:HG2	1:G:44:PHE:CD2	2.53	0.43
1:G:288:MET:HE1	1:G:371:LYS:HE2	2.00	0.43
1:J:346:VAL:O	1:J:350:ARG:HB2	2.19	0.43
1:L:217:SER:N	1:L:218:PRO:CD	2.80	0.43
1:M:65:LYS:H	1:M:65:LYS:HG3	1.25	0.43
1:M:163:ALA:O	1:M:167:ASP:HB2	2.18	0.43
1:M:385:THR:O	1:M:388:GLU:HB3	2.18	0.43
1:N:218:PRO:HB3	1:N:246:PRO:HG2	2.00	0.43
2:O:3:ILE:H	2:O:3:ILE:HD12	1.83	0.43
1:C:130:GLU:O	1:C:133:ALA:HB3	2.18	0.43
1:C:434:GLU:O	1:C:437:ASN:HB2	2.18	0.43
1:D:362:ARG:HG2	1:D:366:GLN:NE2	2.33	0.43
1:H:103:GLY:O	1:H:106:ALA:HB3	2.18	0.43
1:H:461:GLU:OE1	1:H:461:GLU:HA	2.18	0.43
1:I:169:VAL:O	1:I:169:VAL:HG22	2.19	0.43
1:K:65:LYS:H	1:K:65:LYS:HG3	1.30	0.43
1:L:21:ASN:HD22	1:L:21:ASN:HA	1.55	0.43
1:L:158:VAL:HG13	1:L:396:VAL:HG22	2.01	0.43
1:L:234:LEU:N	1:L:235:PRO:HD2	2.34	0.43
1:L:451:LEU:O	1:L:452:ARG:C	2.62	0.43
1:M:104:LEU:HD12	1:M:104:LEU:HA	1.82	0.43
1:D:103:GLY:HA3	1:D:515:ILE:HG21	2.00	0.43
1:F:448:GLU:HB3	1:F:452:ARG:HD2	2.00	0.43
1:F:502:SER:O	1:F:503:ALA:C	2.56	0.43
1:G:147:VAL:HG23	1:G:403:THR:HG22	2.01	0.43
1:I:504:LEU:HA	1:I:504:LEU:HD23	1.79	0.43
1:K:272:LYS:NZ	1:L:228:SER:HB3	2.34	0.43
1:K:272:LYS:HZ1	1:L:228:SER:HB3	1.84	0.43
1:L:462:PRO:O	1:L:463:SER:C	2.62	0.43
1:M:16:MET:CE	1:M:16:MET:CB	2.96	0.43
1:M:217:SER:N	1:M:218:PRO:CD	2.82	0.43
1:N:166:MET:HE2	1:N:166:MET:HB3	1.85	0.43
1:A:150:ILE:HD11	1:A:492:GLY:O	2.19	0.43
1:B:524:LEU:HD23	1:B:524:LEU:HA	1.69	0.43
1:C:172:GLU:OE2	1:C:350:ARG:CZ	2.66	0.43
1:E:42:LYS:O	1:E:43:SER:C	2.62	0.43
1:G:234:LEU:HB2	1:G:235:PRO:CD	2.49	0.43
1:G:486:GLY:CA	1:G:491:MET:CE	2.97	0.43
1:I:31:LEU:O	1:I:32:GLY:O	2.37	0.43
1:I:104:LEU:HD12	1:I:104:LEU:HA	1.76	0.43
1:I:105:LYS:HB2	1:I:105:LYS:HE3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:415:GLY:C	1:I:417:VAL:N	2.77	0.43
1:K:151:SER:C	1:K:153:ASN:H	2.27	0.43
1:M:180:GLY:HA3	1:M:381:VAL:O	2.18	0.43
1:N:524:LEU:HD23	1:N:524:LEU:HA	1.81	0.43
1:A:193:MET:HE3	1:A:371:LYS:HD3	2.00	0.43
1:C:349:ILE:HA	1:C:352:GLN:HG2	1.94	0.43
1:D:147:VAL:HG12	1:D:494:LEU:HB2	2.01	0.43
1:E:150:ILE:HD13	1:E:492:GLY:O	2.19	0.43
1:I:117:LYS:HG2	1:I:121:ASP:OD2	2.19	0.43
1:I:201:SER:O	1:I:203:TYR:N	2.52	0.43
1:J:193:MET:HE2	1:J:195:PHE:CD1	2.54	0.43
1:K:233:MET:HE1	1:K:249:ILE:HD12	2.01	0.43
1:L:166:MET:HE1	1:L:407:VAL:HG21	2.01	0.43
1:L:194:GLN:HB2	1:L:331:THR:HB	2.01	0.43
1:L:509:SER:O	1:L:510:VAL:C	2.61	0.43
1:B:23:LEU:O	1:B:24:ALA:C	2.60	0.42
1:C:417:VAL:O	1:C:418:ALA:C	2.62	0.42
1:D:218:PRO:HB3	1:D:246:PRO:HG2	2.01	0.42
1:H:305:ILE:HB	1:H:307:MET:HE2	2.01	0.42
1:I:106:ALA:C	1:I:111:MET:HE3	2.44	0.42
1:I:117:LYS:O	1:I:118:ARG:C	2.62	0.42
1:J:488:MET:HE3	1:J:493:ILE:HG21	2.00	0.42
1:J:522:THR:OG1	1:J:523:ASP:N	2.51	0.42
1:K:419:LEU:HD22	1:K:500:THR:CG2	2.48	0.42
1:N:455:VAL:CG1	1:N:462:PRO:HA	2.49	0.42
1:N:502:SER:O	1:N:503:ALA:C	2.60	0.42
1:A:78:ALA:HB2	1:A:93:THR:HG1	1.84	0.42
1:E:100:ILE:HG13	1:E:511:ALA:HB1	2.00	0.42
1:F:103:GLY:O	1:F:104:LEU:C	2.58	0.42
1:F:240:VAL:HG21	1:F:247:LEU:HD22	2.01	0.42
1:F:345:ARG:O	1:F:348:GLN:HB2	2.18	0.42
1:I:385:THR:O	1:I:388:GLU:HB3	2.19	0.42
1:M:433:ASN:HD22	1:M:433:ASN:HA	1.54	0.42
1:N:16:MET:HG3	1:N:520:MET:HE1	2.01	0.42
2:T:18:GLU:O	2:T:19:THR:C	2.62	0.42
1:B:358:SER:HB3	1:B:361:ASP:HB2	2.02	0.42
1:C:510:VAL:CG1	1:C:514:MET:HE3	2.46	0.42
1:D:510:VAL:HG13	1:D:514:MET:CE	2.48	0.42
1:D:524:LEU:HD23	1:D:524:LEU:HA	1.93	0.42
1:E:103:GLY:O	1:E:104:LEU:C	2.62	0.42
1:E:266:THR:CG2	1:E:273:VAL:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:ALA:HB2	1:G:93:THR:OG1	2.19	0.42
1:J:289:LEU:HD22	1:J:300:VAL:HG13	2.01	0.42
2:O:41:LEU:O	2:O:61:VAL:HG13	2.20	0.42
2:O:74:LYS:HD2	2:U:68:ASN:HD22	1.82	0.42
1:A:234:LEU:HB2	1:A:235:PRO:CD	2.49	0.42
1:B:13:ARG:HD2	1:B:104:LEU:HD22	2.01	0.42
1:B:362:ARG:HG2	1:B:366:GLN:NE2	2.34	0.42
1:C:511:ALA:O	1:C:515:ILE:HG12	2.19	0.42
1:E:172:GLU:OE1	1:E:172:GLU:HA	2.18	0.42
1:E:222:LEU:HB3	1:E:289:LEU:CD2	2.49	0.42
1:J:455:VAL:CG1	1:J:462:PRO:HA	2.47	0.42
1:K:270:ILE:HG22	1:K:271:VAL:HG23	2.00	0.42
1:K:513:LEU:HD12	1:K:513:LEU:HA	1.80	0.42
1:N:428:ASP:O	1:N:429:LEU:C	2.61	0.42
1:N:434:GLU:HB2	7:N:529:HOH:O	2.18	0.42
2:T:11:ILE:HD12	2:T:42:ALA:HB3	2.00	0.42
1:A:146:GLN:HE21	1:A:146:GLN:HB2	1.61	0.42
1:C:33:PRO:HA	1:C:153:ASN:ND2	2.32	0.42
1:E:78:ALA:HB2	1:E:93:THR:OG1	2.20	0.42
1:F:68:ASN:HB3	7:F:612:HOH:O	2.19	0.42
1:F:233:MET:O	1:F:234:LEU:C	2.62	0.42
1:I:66:PHE:HA	1:I:69:MET:HE3	2.00	0.42
1:I:169:VAL:HG13	1:I:173:GLY:HA3	2.02	0.42
1:I:201:SER:C	1:I:203:TYR:N	2.77	0.42
1:I:421:ARG:CD	1:I:474:GLY:O	2.66	0.42
1:L:117:LYS:HG2	1:L:121:ASP:OD2	2.19	0.42
1:M:124:VAL:O	1:M:128:VAL:HG23	2.20	0.42
1:N:124:VAL:O	1:N:128:VAL:HG23	2.20	0.42
2:T:51:ASN:O	2:T:52:GLY:C	2.62	0.42
1:A:324:VAL:HB	1:A:331:THR:HG23	2.02	0.42
1:F:25:ASP:HA	1:F:28:LYS:HE2	2.00	0.42
1:H:64:ASP:C	1:H:65:LYS:O	2.59	0.42
1:I:62:LEU:HA	1:I:62:LEU:HD23	1.78	0.42
1:I:106:ALA:O	1:I:109:ALA:CB	2.57	0.42
1:I:417:VAL:HG23	1:I:417:VAL:H	1.48	0.42
1:L:224:ASP:O	1:L:225:LYS:HB3	2.20	0.42
1:L:433:ASN:HB3	1:L:436:GLN:H	1.83	0.42
1:L:444:LEU:HA	1:L:444:LEU:HD23	1.76	0.42
1:N:217:SER:N	1:N:218:PRO:CD	2.82	0.42
1:N:433:ASN:HD22	1:N:433:ASN:HA	1.57	0.42
2:T:15:LYS:HB3	2:T:16:GLU:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:20:LYS:HB3	2:T:27:LEU:HG	2.01	0.42
1:B:103:GLY:HA3	1:B:515:ILE:HG21	2.00	0.42
1:B:124:VAL:HG22	1:B:504:LEU:CD1	2.50	0.42
1:B:310:GLU:OE1	1:B:310:GLU:N	2.52	0.42
1:C:124:VAL:HG22	1:C:504:LEU:CD1	2.49	0.42
1:D:42:LYS:HG2	1:D:44:PHE:CE2	2.55	0.42
1:D:502:SER:O	1:D:503:ALA:C	2.55	0.42
1:E:146:GLN:HE21	1:E:146:GLN:HB2	1.66	0.42
1:E:510:VAL:HG12	1:E:514:MET:CE	2.50	0.42
1:G:147:VAL:CG2	1:G:403:THR:HG22	2.49	0.42
1:G:455:VAL:HG21	1:G:465:VAL:HG11	2.02	0.42
1:H:104:LEU:HA	1:H:104:LEU:HD12	1.45	0.42
1:I:44:PHE:CD1	1:I:44:PHE:N	2.88	0.42
1:I:270:ILE:HG22	1:I:271:VAL:HG23	2.01	0.42
1:I:444:LEU:HD23	1:I:444:LEU:HA	1.73	0.42
1:J:116:LEU:HD23	1:J:116:LEU:HA	1.92	0.42
1:J:166:MET:HE2	1:J:166:MET:HB3	1.96	0.42
1:K:158:VAL:HG13	1:K:396:VAL:HG22	2.00	0.42
1:K:360:TYR:CZ	1:K:364:LYS:HE3	2.55	0.42
1:K:497:THR:O	1:K:498:LYS:C	2.62	0.42
1:B:223:ALA:O	1:B:251:ALA:HA	2.19	0.42
1:C:21:ASN:O	1:C:22:VAL:C	2.63	0.42
1:D:80:LYS:O	1:D:81:ALA:C	2.63	0.42
1:E:157:THR:O	1:E:161:LEU:HB2	2.20	0.42
1:F:417:VAL:O	1:F:418:ALA:C	2.63	0.42
1:J:73:MET:SD	1:J:514:MET:HE2	2.59	0.42
1:N:16:MET:HB2	1:N:16:MET:HE3	2.01	0.42
1:D:219:PHE:C	1:D:220:ILE:HG13	2.44	0.42
1:D:288:MET:HE1	1:D:371:LYS:HE2	2.02	0.42
1:E:497:THR:N	7:E:604:HOH:O	2.52	0.42
1:G:400:LEU:O	1:G:400:LEU:HD13	2.19	0.42
1:I:289:LEU:HD22	1:I:300:VAL:HG13	2.01	0.42
1:J:104:LEU:HD12	1:J:104:LEU:HA	1.51	0.42
1:J:426:LEU:HD12	1:J:444:LEU:HD21	2.02	0.42
1:L:417:VAL:HG21	1:L:488:MET:HG3	2.02	0.42
1:M:346:VAL:O	1:M:350:ARG:HB2	2.20	0.42
1:N:391:GLU:O	1:N:392:LYS:C	2.63	0.42
2:Q:11:ILE:HD12	2:Q:42:ALA:HB3	2.02	0.42
2:U:41:LEU:O	2:U:61:VAL:HG13	2.20	0.42
1:A:267:MET:HG2	1:G:305:ILE:CG2	2.49	0.42
1:A:284:ARG:O	1:A:285:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ARG:HD3	1:A:505:GLN:OE1	2.20	0.42
1:B:143:ALA:HA	1:B:146:GLN:NE2	2.34	0.42
1:C:65:LYS:CB	7:C:606:HOH:O	2.68	0.42
1:C:157:THR:O	1:C:161:LEU:HB2	2.20	0.42
1:D:69:MET:HE3	1:E:39:VAL:CG1	2.50	0.42
1:D:510:VAL:HG13	1:D:514:MET:HE1	2.00	0.42
1:F:13:ARG:NH2	7:F:608:HOH:O	2.37	0.42
1:G:513:LEU:HD23	1:G:513:LEU:HA	1.78	0.42
1:H:44:PHE:N	1:H:44:PHE:CD1	2.88	0.42
1:H:205:ILE:HA	1:H:213:VAL:HG22	2.01	0.42
1:I:95:LEU:O	1:I:98:ALA:N	2.49	0.42
1:I:417:VAL:O	1:I:418:ALA:C	2.62	0.42
1:J:430:ARG:HA	1:J:430:ARG:HD3	1.72	0.42
1:K:40:LEU:HD12	1:L:521:VAL:HB	2.02	0.42
1:L:64:ASP:O	1:L:65:LYS:C	2.61	0.42
1:L:84:ALA:O	1:L:85:ALA:HB2	2.19	0.42
1:L:437:ASN:C	1:L:439:GLY:N	2.75	0.42
1:M:77:VAL:HG12	1:M:78:ALA:N	2.35	0.42
1:M:444:LEU:HA	1:M:444:LEU:HD23	1.86	0.42
1:N:119:GLY:O	1:N:120:ILE:C	2.63	0.42
2:P:7:HIS:O	2:P:8:ASP:CB	2.65	0.42
2:R:7:HIS:CE1	2:R:48:ILE:HD11	2.55	0.42
1:A:287:ALA:O	1:A:290:GLN:HB3	2.20	0.41
1:A:419:LEU:HD12	1:A:419:LEU:HA	1.82	0.41
1:B:429:LEU:HD12	1:B:429:LEU:HA	1.67	0.41
1:D:76:GLU:O	1:D:76:GLU:HG2	2.19	0.41
1:F:358:SER:HB3	1:F:361:ASP:OD1	2.19	0.41
1:G:74:VAL:C	1:G:76:GLU:H	2.27	0.41
1:H:417:VAL:HG21	1:H:488:MET:HG3	2.00	0.41
1:H:430:ARG:HD3	1:H:430:ARG:HA	1.57	0.41
1:L:166:MET:HE2	1:L:166:MET:HB3	1.92	0.41
1:L:315:GLU:O	1:L:315:GLU:HG2	2.19	0.41
1:N:21:ASN:HD22	1:N:21:ASN:HA	1.51	0.41
1:N:151:SER:C	1:N:153:ASN:H	2.28	0.41
1:N:163:ALA:O	1:N:167:ASP:HB2	2.20	0.41
1:A:146:GLN:O	1:A:147:VAL:C	2.62	0.41
1:C:233:MET:O	1:C:234:LEU:C	2.62	0.41
1:G:213:VAL:HB	1:G:325:ILE:HG12	2.02	0.41
1:H:64:ASP:OD1	1:H:65:LYS:O	2.38	0.41
1:I:205:ILE:HA	1:I:213:VAL:HG22	2.01	0.41
1:J:326:ASN:HB2	1:J:329:THR:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:449:ALA:HB3	1:L:450:PRO:HD3	2.01	0.41
1:D:74:VAL:C	1:D:76:GLU:N	2.78	0.41
1:D:88:GLY:HA2	5:D:600:ADP:O2B	2.20	0.41
1:D:266:THR:CG2	1:D:273:VAL:HB	2.51	0.41
1:G:18:ARG:NH1	1:G:18:ARG:CG	2.65	0.41
1:G:63:GLU:O	1:G:63:GLU:HG2	2.19	0.41
1:G:88:GLY:HA2	5:G:600:ADP:O2B	2.21	0.41
1:G:115:ASP:O	1:G:116:LEU:C	2.61	0.41
1:J:513:LEU:HA	1:J:513:LEU:HD12	1.73	0.41
1:K:43:SER:HB2	1:K:44:PHE:H	1.76	0.41
1:K:98:ALA:HB3	1:K:446:ALA:HB1	2.03	0.41
1:L:20:VAL:O	1:L:21:ASN:C	2.59	0.41
1:M:413:ALA:CB	1:M:417:VAL:HB	2.49	0.41
1:N:174:VAL:H	1:N:174:VAL:HG23	1.66	0.41
1:N:198:GLY:HA3	1:N:327:LYS:O	2.20	0.41
1:N:415:GLY:CA	1:N:417:VAL:HG23	2.51	0.41
2:S:41:LEU:O	2:S:61:VAL:HG13	2.20	0.41
2:T:3:ILE:H	2:T:3:ILE:CD1	2.31	0.41
1:A:206:ASN:HD21	1:A:214:GLU:N	2.10	0.41
1:A:237:LEU:HB3	2:O:26:VAL:HG21	2.02	0.41
1:A:522:THR:OG1	1:A:523:ASP:N	2.53	0.41
1:B:345:ARG:HE	1:B:349:ILE:HD11	1.85	0.41
1:C:69:MET:HE3	1:D:39:VAL:HG11	2.03	0.41
1:C:136:VAL:O	1:C:136:VAL:HG23	2.20	0.41
1:D:358:SER:HB3	1:D:361:ASP:HB2	2.02	0.41
1:D:358:SER:HB3	1:D:361:ASP:OD1	2.21	0.41
1:D:487:ASN:O	1:D:491:MET:HG3	2.20	0.41
1:E:193:MET:HE3	1:E:371:LYS:HD3	2.02	0.41
1:F:261:THR:O	1:F:262:LEU:C	2.64	0.41
1:H:513:LEU:HD12	1:H:513:LEU:HA	1.50	0.41
1:J:43:SER:HB2	1:J:44:PHE:H	1.68	0.41
1:J:107:VAL:HG11	1:J:515:ILE:HG23	2.02	0.41
1:J:222:LEU:HD23	1:J:250:ILE:HB	2.03	0.41
1:K:65:LYS:CA	7:K:528:HOH:O	2.64	0.41
1:L:15:LYS:NZ	1:L:64:ASP:OD2	2.53	0.41
1:L:413:ALA:CB	1:L:417:VAL:HB	2.49	0.41
1:L:497:THR:O	1:L:498:LYS:C	2.63	0.41
1:N:198:GLY:O	1:N:276:VAL:HG12	2.21	0.41
2:P:60:LYS:H	2:P:60:LYS:HG2	1.74	0.41
2:R:20:LYS:HB3	2:R:27:LEU:HG	2.03	0.41
2:S:51:ASN:O	2:S:52:GLY:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:HG13	1:A:74:VAL:HG11	2.01	0.41
1:A:213:VAL:HB	1:A:325:ILE:HG12	2.03	0.41
1:B:16:MET:SD	1:B:514:MET:HG3	2.59	0.41
1:B:16:MET:HE2	1:B:16:MET:CB	2.51	0.41
1:E:88:GLY:N	6:E:602:AF3:F2	2.44	0.41
1:E:358:SER:HB3	1:E:361:ASP:HB2	2.03	0.41
1:I:88:GLY:O	1:I:92:ALA:N	2.53	0.41
1:I:450:PRO:O	1:I:454:ILE:HG12	2.21	0.41
1:J:166:MET:HE3	1:J:171:LYS:HA	2.02	0.41
1:J:302:SER:H	1:J:307:MET:HE3	1.85	0.41
1:J:336:VAL:O	1:J:336:VAL:HG12	2.21	0.41
1:K:106:ALA:CB	1:K:111:MET:HE3	2.49	0.41
1:K:194:GLN:HB2	1:K:331:THR:HB	2.03	0.41
1:K:217:SER:N	1:K:218:PRO:CD	2.81	0.41
1:M:469:VAL:HG13	1:M:477:GLY:HA2	2.03	0.41
1:N:430:ARG:HA	1:N:430:ARG:HD3	1.61	0.41
1:N:437:ASN:O	1:N:438:VAL:C	2.63	0.41
1:A:512:GLY:O	1:A:515:ILE:HG13	2.21	0.41
1:B:63:GLU:O	1:B:63:GLU:HG2	2.19	0.41
1:B:234:LEU:HB2	1:B:235:PRO:CD	2.51	0.41
1:C:115:ASP:O	1:C:116:LEU:C	2.62	0.41
1:G:291:ASP:HB3	1:G:372:LEU:HD11	2.02	0.41
1:I:66:PHE:O	1:I:69:MET:N	2.52	0.41
1:I:166:MET:HE2	1:I:166:MET:HB3	1.87	0.41
1:I:216:GLU:C	1:I:218:PRO:HD3	2.44	0.41
1:J:64:ASP:OD1	1:J:65:LYS:O	2.38	0.41
1:K:415:GLY:C	1:K:417:VAL:N	2.78	0.41
1:M:126:ALA:CB	1:M:426:LEU:HD22	2.49	0.41
1:N:262:LEU:O	1:N:266:THR:HG23	2.21	0.41
2:P:95:VAL:CG1	2:Q:1:MET:HE2	2.49	0.41
2:S:20:LYS:HB3	2:S:27:LEU:HG	2.02	0.41
1:A:222:LEU:HB3	1:A:289:LEU:CD2	2.50	0.41
1:D:230:ILE:CD1	1:D:261:THR:HG21	2.43	0.41
1:F:266:THR:CG2	1:F:273:VAL:HB	2.50	0.41
1:G:324:VAL:HB	1:G:331:THR:HG23	2.03	0.41
1:G:524:LEU:CD2	1:G:525:PRO:HD2	2.50	0.41
1:H:84:ALA:O	1:H:85:ALA:HB2	2.21	0.41
1:H:116:LEU:HD23	1:H:116:LEU:HA	1.99	0.41
1:H:351:GLN:HE21	1:H:351:GLN:HB3	1.65	0.41
1:J:272:LYS:HZ1	1:K:228:SER:HB3	1.84	0.41
1:L:180:GLY:HA3	1:L:381:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:73:MET:HE2	1:M:514:MET:CE	2.49	0.41
1:M:174:VAL:HB	1:M:376:VAL:HG22	2.01	0.41
1:N:88:GLY:O	1:N:89:THR:C	2.64	0.41
1:N:432:GLN:H	1:N:436:GLN:NE2	2.19	0.41
2:Q:60:LYS:H	2:Q:60:LYS:HG2	1.71	0.41
1:A:238:GLU:OE2	2:O:23:GLY:C	2.63	0.41
1:B:287:ALA:O	1:B:290:GLN:HB3	2.20	0.41
1:B:511:ALA:O	1:B:515:ILE:HG12	2.21	0.41
1:C:103:GLY:O	1:C:104:LEU:C	2.62	0.41
1:E:400:LEU:O	1:E:400:LEU:HD13	2.20	0.41
1:G:117:LYS:O	1:G:118:ARG:C	2.62	0.41
1:H:43:SER:HB2	1:H:44:PHE:CD1	2.55	0.41
1:I:351:GLN:HE21	1:I:351:GLN:HB3	1.68	0.41
1:K:420:ILE:HD13	1:K:420:ILE:HG23	1.89	0.41
1:L:91:THR:O	1:L:92:ALA:C	2.63	0.41
1:L:455:VAL:CG1	1:L:462:PRO:HA	2.42	0.41
1:M:272:LYS:HZ3	1:N:228:SER:HB3	1.83	0.41
1:A:234:LEU:N	1:A:235:PRO:HD2	2.36	0.41
1:A:455:VAL:HG21	1:A:465:VAL:HG11	2.03	0.41
1:B:67:GLU:O	1:B:68:ASN:C	2.60	0.41
1:B:76:GLU:O	1:B:80:LYS:HB2	2.21	0.41
1:B:510:VAL:HG23	1:C:385:THR:HG21	2.02	0.41
1:C:234:LEU:HB2	1:C:235:PRO:CD	2.51	0.41
1:C:524:LEU:HD23	1:C:524:LEU:HA	1.84	0.41
1:D:147:VAL:HG23	1:D:148:GLY:N	2.34	0.41
1:D:514:MET:HE3	1:D:514:MET:HB2	1.49	0.41
1:F:100:ILE:HG13	1:F:511:ALA:HB1	2.03	0.41
1:G:131:LEU:HD23	1:G:131:LEU:HA	1.93	0.41
1:G:365:LEU:HD23	1:G:368:ARG:HH21	1.86	0.41
1:H:97:GLN:HE21	1:H:97:GLN:HB3	1.70	0.41
1:I:278:ALA:HB1	1:I:279:PRO:HD2	2.02	0.41
1:I:420:ILE:HD13	1:I:420:ILE:HG23	1.65	0.41
1:K:169:VAL:HG13	1:K:173:GLY:HA3	2.02	0.41
1:L:44:PHE:CD1	1:L:44:PHE:N	2.88	0.41
1:L:116:LEU:HD23	1:L:116:LEU:HA	1.85	0.41
1:L:128:VAL:HB	7:L:531:HOH:O	2.19	0.41
1:L:326:ASN:HD22	1:L:329:THR:CG2	2.34	0.41
1:M:193:MET:HE2	1:M:195:PHE:HD1	1.86	0.41
1:M:462:PRO:O	1:M:463:SER:C	2.63	0.41
1:N:270:ILE:HG22	1:N:271:VAL:HG23	2.02	0.41
2:Q:18:GLU:O	2:Q:19:THR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:20:LYS:HB3	2:Q:27:LEU:HG	2.03	0.41
2:Q:68:ASN:HD22	2:R:74:LYS:HD2	1.86	0.41
2:T:41:LEU:O	2:T:61:VAL:HG13	2.21	0.41
1:A:66:PHE:O	1:A:69:MET:HB2	2.21	0.41
1:B:40:LEU:HD22	1:B:59:GLU:HG3	2.02	0.41
1:B:114:MET:CE	1:B:114:MET:CG	2.95	0.41
1:C:240:VAL:HG21	1:C:247:LEU:HD22	2.02	0.41
1:D:33:PRO:HD3	5:D:600:ADP:C8	2.56	0.41
1:D:462:PRO:CD	7:D:608:HOH:O	2.51	0.41
1:E:455:VAL:HG11	1:E:462:PRO:HA	2.04	0.41
1:I:492:GLY:C	1:I:493:ILE:HD13	2.46	0.41
1:J:479:ASN:OD1	1:J:479:ASN:C	2.63	0.41
1:K:219:PHE:HB3	1:K:317:LEU:HD23	2.03	0.41
1:L:31:LEU:O	1:L:32:GLY:O	2.38	0.41
1:L:96:ALA:O	1:L:100:ILE:HG13	2.21	0.41
1:N:106:ALA:HB3	1:N:116:LEU:HD13	2.03	0.41
1:N:152:ALA:O	1:N:153:ASN:HB3	2.20	0.41
1:A:123:ALA:HB2	1:A:440:ILE:HG23	2.03	0.40
1:C:203:TYR:O	1:C:204:PHE:C	2.65	0.40
1:E:16:MET:HE2	1:E:16:MET:HB3	1.80	0.40
1:E:429:LEU:HA	1:E:429:LEU:HD12	1.84	0.40
1:F:219:PHE:C	1:F:220:ILE:HG13	2.45	0.40
5:F:600:ADP:O3B	6:F:602:AF3:F2	2.29	0.40
1:G:31:LEU:HD23	1:G:453:GLN:HB3	2.03	0.40
1:G:270:ILE:HD11	2:U:27:LEU:HB3	2.03	0.40
1:G:510:VAL:HG13	1:G:514:MET:HE1	2.00	0.40
1:G:522:THR:OG1	1:G:523:ASP:N	2.55	0.40
1:I:64:ASP:O	1:I:65:LYS:O	2.39	0.40
1:J:360:TYR:CZ	1:J:364:LYS:HE3	2.56	0.40
1:K:84:ALA:O	1:K:85:ALA:HB2	2.21	0.40
1:L:419:LEU:HD22	1:L:500:THR:CG2	2.51	0.40
1:M:508:ALA:O	1:M:509:SER:C	2.64	0.40
2:P:20:LYS:HB3	2:P:27:LEU:HG	2.03	0.40
1:C:74:VAL:C	1:C:76:GLU:N	2.79	0.40
1:C:213:VAL:HB	1:C:325:ILE:HG12	2.02	0.40
1:F:63:GLU:O	1:F:63:GLU:CG	2.70	0.40
1:G:6:VAL:O	1:G:6:VAL:HG23	2.18	0.40
1:H:73:MET:SD	1:H:514:MET:HE2	2.60	0.40
1:I:15:LYS:HD2	1:I:15:LYS:HA	1.83	0.40
1:I:193:MET:HE2	1:I:195:PHE:HD1	1.86	0.40
1:J:65:LYS:H	1:J:65:LYS:HG3	1.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:504:LEU:HD23	1:J:504:LEU:HA	1.84	0.40
1:K:10:ASN:O	1:K:11:ASP:C	2.64	0.40
1:K:49:ILE:HD13	1:L:73:MET:HE3	2.04	0.40
1:M:266:THR:HG21	1:M:273:VAL:O	2.22	0.40
1:N:30:THR:HB	1:N:51:LYS:O	2.22	0.40
1:N:421:ARG:HD2	1:N:421:ARG:HH11	1.69	0.40
1:A:151:SER:OG	1:A:399:ALA:HA	2.20	0.40
1:D:240:VAL:HG21	1:D:247:LEU:HD22	2.03	0.40
1:F:21:ASN:HD22	1:F:21:ASN:HA	1.73	0.40
1:F:114:MET:CE	1:F:114:MET:CG	2.98	0.40
1:F:291:ASP:HB3	1:F:372:LEU:HD11	2.03	0.40
1:G:127:ALA:HB1	1:G:422:VAL:HG21	2.02	0.40
1:G:146:GLN:HE21	1:G:146:GLN:HB2	1.56	0.40
1:H:452:ARG:HG2	1:H:452:ARG:NH1	2.37	0.40
1:J:19:GLY:HA3	1:J:67:GLU:O	2.20	0.40
1:K:433:ASN:HD22	1:K:433:ASN:HA	1.51	0.40
1:L:346:VAL:O	1:L:350:ARG:HB2	2.20	0.40
1:L:415:GLY:C	1:L:417:VAL:H	2.28	0.40
1:N:106:ALA:O	1:N:109:ALA:CB	2.62	0.40
1:A:493:ILE:O	1:A:493:ILE:HG22	2.21	0.40
1:B:146:GLN:O	1:B:147:VAL:C	2.62	0.40
1:D:486:GLY:CA	1:D:491:MET:CE	2.98	0.40
1:E:289:LEU:O	1:E:292:ILE:HB	2.21	0.40
1:E:448:GLU:HB3	1:E:452:ARG:HD2	2.03	0.40
1:G:9:GLY:O	1:G:10:ASN:C	2.63	0.40
1:G:54:VAL:O	1:G:54:VAL:HG22	2.20	0.40
1:G:123:ALA:HB2	1:G:440:ILE:HG23	2.03	0.40
1:H:419:LEU:HA	1:H:419:LEU:HD13	1.53	0.40
1:I:266:THR:HG21	1:I:273:VAL:O	2.20	0.40
1:J:205:ILE:HA	1:J:213:VAL:HG22	2.02	0.40
1:J:272:LYS:NZ	1:K:228:SER:HB3	2.36	0.40
1:K:302:SER:H	1:K:307:MET:HE3	1.87	0.40
1:L:106:ALA:HB1	1:L:111:MET:HE3	2.04	0.40
1:M:32:GLY:H	1:M:457:ASN:HD22	1.69	0.40
1:M:49:ILE:HD12	1:N:513:LEU:HD23	2.04	0.40
2:R:51:ASN:O	2:R:52:GLY:C	2.64	0.40
2:T:52:GLY:O	2:T:53:GLU:C	2.64	0.40
1:A:259:LEU:O	1:A:260:ALA:C	2.65	0.40
1:A:290:GLN:O	1:A:293:ALA:HB3	2.22	0.40
1:B:203:TYR:CD1	1:B:267:MET:HE1	2.56	0.40
1:B:358:SER:HB3	1:B:361:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:ASN:HD22	1:D:475:ASN:HA	1.55	0.40
1:E:67:GLU:O	1:E:68:ASN:C	2.61	0.40
1:E:69:MET:HE3	1:F:39:VAL:HG11	2.03	0.40
1:E:432:GLN:O	1:E:433:ASN:HB3	2.21	0.40
1:G:100:ILE:HG13	1:G:511:ALA:CB	2.52	0.40
1:I:315:GLU:O	1:I:315:GLU:HG2	2.20	0.40
1:J:360:TYR:CE1	1:J:364:LYS:HE3	2.57	0.40
1:K:13:ARG:HA	1:K:16:MET:HE3	2.04	0.40
1:K:20:VAL:O	1:K:21:ASN:C	2.61	0.40
1:K:413:ALA:CB	1:K:417:VAL:HB	2.51	0.40
1:L:24:ALA:HA	1:L:27:VAL:HG12	2.02	0.40
1:M:44:PHE:CD1	1:M:44:PHE:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/524 (100%)	472 (90%)	44 (8%)	6 (1%)	11	36
1	B	522/524 (100%)	476 (91%)	39 (8%)	7 (1%)	9	31
1	C	522/524 (100%)	473 (91%)	37 (7%)	12 (2%)	5	18
1	D	522/524 (100%)	475 (91%)	41 (8%)	6 (1%)	11	36
1	E	522/524 (100%)	474 (91%)	42 (8%)	6 (1%)	11	36
1	F	522/524 (100%)	478 (92%)	38 (7%)	6 (1%)	11	36
1	G	522/524 (100%)	479 (92%)	37 (7%)	6 (1%)	11	36
1	H	522/524 (100%)	477 (91%)	36 (7%)	9 (2%)	7	25
1	I	522/524 (100%)	471 (90%)	43 (8%)	8 (2%)	8	28
1	J	522/524 (100%)	473 (91%)	40 (8%)	9 (2%)	7	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	522/524 (100%)	473 (91%)	41 (8%)	8 (2%)	8	28
1	L	522/524 (100%)	479 (92%)	34 (6%)	9 (2%)	7	25
1	M	522/524 (100%)	477 (91%)	35 (7%)	10 (2%)	6	22
1	N	522/524 (100%)	471 (90%)	44 (8%)	7 (1%)	9	31
2	O	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0	1
2	P	95/97 (98%)	68 (72%)	16 (17%)	11 (12%)	0	1
2	Q	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0	1
2	R	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0	1
2	S	95/97 (98%)	70 (74%)	15 (16%)	10 (10%)	0	1
2	T	95/97 (98%)	69 (73%)	15 (16%)	11 (12%)	0	1
2	U	95/97 (98%)	68 (72%)	15 (16%)	12 (13%)	0	0
All	All	7973/8015 (100%)	7127 (89%)	663 (8%)	183 (2%)	5	18

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	B	44	PHE
1	C	44	PHE
1	D	44	PHE
1	E	44	PHE
1	F	44	PHE
1	G	44	PHE
1	H	85	ALA
1	I	85	ALA
1	J	85	ALA
1	K	85	ALA
1	L	43	SER
1	L	85	ALA
1	M	32	GLY
1	M	85	ALA
1	M	463	SER
1	N	85	ALA
2	O	7	HIS
2	P	7	HIS
2	Q	7	HIS
2	R	7	HIS
2	S	7	HIS

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Mol	Chain	Res	Type
2	T	7	HIS
2	U	7	HIS
1	A	225	LYS
1	C	58	ARG
1	C	256	GLY
1	D	256	GLY
1	D	373	ALA
1	F	225	LYS
1	G	256	GLY
1	G	373	ALA
1	H	32	GLY
1	H	256	GLY
1	I	32	GLY
1	I	43	SER
1	I	66	PHE
1	I	256	GLY
1	J	32	GLY
1	J	43	SER
1	J	65	LYS
1	J	256	GLY
1	J	457	ASN
1	K	32	GLY
1	K	66	PHE
1	K	256	GLY
1	L	32	GLY
1	L	256	GLY
1	M	256	GLY
1	M	457	ASN
1	M	462	PRO
1	N	32	GLY
1	N	43	SER
1	N	66	PHE
1	N	256	GLY
2	O	20	LYS
2	O	21	SER
2	O	52	GLY
2	P	20	LYS
2	P	21	SER
2	P	52	GLY
2	Q	20	LYS
2	Q	21	SER
2	Q	52	GLY

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Mol	Chain	Res	Type
2	Q	61	VAL
2	R	20	LYS
2	R	21	SER
2	R	52	GLY
2	S	20	LYS
2	S	21	SER
2	S	52	GLY
2	T	20	LYS
2	T	21	SER
2	T	52	GLY
2	U	20	LYS
2	U	21	SER
2	U	49	LEU
2	U	52	GLY
2	U	61	VAL
1	A	373	ALA
1	B	225	LYS
1	B	373	ALA
1	C	28	LYS
1	C	225	LYS
1	C	373	ALA
1	D	225	LYS
1	E	225	LYS
1	E	256	GLY
1	E	373	ALA
1	F	373	ALA
1	G	225	LYS
1	H	66	PHE
1	I	463	SER
1	J	66	PHE
1	L	65	LYS
1	L	66	PHE
1	M	43	SER
1	M	66	PHE
2	O	49	LEU
2	O	53	GLU
2	P	17	VAL
2	P	49	LEU
2	P	53	GLU
2	Q	49	LEU
2	Q	53	GLU
2	Q	80	ASN

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Mol	Chain	Res	Type
2	R	49	LEU
2	R	53	GLU
2	R	61	VAL
2	S	49	LEU
2	S	53	GLU
2	S	61	VAL
2	T	49	LEU
2	T	53	GLU
2	T	61	VAL
2	U	53	GLU
1	A	256	GLY
1	B	202	PRO
1	B	256	GLY
1	C	85	ALA
1	D	58	ARG
1	D	202	PRO
1	F	256	GLY
1	H	43	SER
1	H	202	PRO
1	H	462	PRO
1	J	202	PRO
1	K	43	SER
1	K	202	PRO
1	L	202	PRO
1	M	202	PRO
1	N	202	PRO
2	O	17	VAL
2	O	61	VAL
2	P	61	VAL
2	P	80	ASN
2	R	80	ASN
2	S	80	ASN
2	T	80	ASN
1	A	202	PRO
1	B	462	PRO
1	C	23	LEU
1	E	202	PRO
1	F	202	PRO
1	G	202	PRO
1	H	65	LYS
1	I	202	PRO
1	I	462	PRO

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Mol	Chain	Res	Type
1	J	462	PRO
1	K	462	PRO
1	L	462	PRO
1	L	463	SER
1	M	65	LYS
2	O	51	ASN
2	P	51	ASN
2	Q	17	VAL
2	Q	51	ASN
2	R	17	VAL
2	R	51	ASN
2	S	51	ASN
2	T	17	VAL
2	T	45	ASN
2	T	51	ASN
2	U	51	ASN
2	U	69	ASP
2	U	80	ASN
1	C	202	PRO
1	C	374	GLY
1	E	462	PRO
1	N	413	ALA
2	O	80	ASN
2	P	69	ASP
2	U	17	VAL
2	U	45	ASN
1	B	374	GLY
1	G	374	GLY
2	S	17	VAL
1	A	205	ILE
1	C	462	PRO
1	F	462	PRO
1	C	103	GLY
1	H	120	ILE
1	K	120	ILE

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	341 (84%)	63 (16%)	2	9
1	B	404/404 (100%)	346 (86%)	58 (14%)	3	11
1	C	404/404 (100%)	351 (87%)	53 (13%)	4	14
1	D	404/404 (100%)	345 (85%)	59 (15%)	3	11
1	E	404/404 (100%)	350 (87%)	54 (13%)	4	13
1	F	404/404 (100%)	340 (84%)	64 (16%)	2	9
1	G	404/404 (100%)	345 (85%)	59 (15%)	3	11
1	H	404/404 (100%)	323 (80%)	81 (20%)	1	4
1	I	404/404 (100%)	325 (80%)	79 (20%)	1	5
1	J	404/404 (100%)	320 (79%)	84 (21%)	1	4
1	K	404/404 (100%)	328 (81%)	76 (19%)	1	5
1	L	404/404 (100%)	327 (81%)	77 (19%)	1	5
1	M	404/404 (100%)	324 (80%)	80 (20%)	1	5
1	N	404/404 (100%)	329 (81%)	75 (19%)	1	5
2	O	80/80 (100%)	68 (85%)	12 (15%)	3	10
2	P	80/80 (100%)	67 (84%)	13 (16%)	2	8
2	Q	80/80 (100%)	67 (84%)	13 (16%)	2	8
2	R	80/80 (100%)	68 (85%)	12 (15%)	3	10
2	S	80/80 (100%)	68 (85%)	12 (15%)	3	10
2	T	80/80 (100%)	67 (84%)	13 (16%)	2	8
2	U	80/80 (100%)	69 (86%)	11 (14%)	3	12
All	All	6216/6216 (100%)	5168 (83%)	1048 (17%)	2	7

All (1048) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	LYS
1	A	18	ARG
1	A	23	LEU
1	A	28	LYS
1	A	43	SER
1	A	44	PHE
1	A	48	THR

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Mol	Chain	Res	Type
1	A	62	LEU
1	A	64	ASP
1	A	74	VAL
1	A	77	VAL
1	A	80	LYS
1	A	89	THR
1	A	97	GLN
1	A	111	MET
1	A	114	MET
1	A	129	GLU
1	A	134	LEU
1	A	138	CYS
1	A	147	VAL
1	A	150	ILE
1	A	153	ASN
1	A	176	THR
1	A	177	VAL
1	A	178	GLU
1	A	183	LEU
1	A	184	GLN
1	A	185	ASP
1	A	193	MET
1	A	230	ILE
1	A	231	ARG
1	A	284	ARG
1	A	289	LEU
1	A	322	ARG
1	A	328	ASP
1	A	331	THR
1	A	355	GLU
1	A	369	VAL
1	A	376	VAL
1	A	381	VAL
1	A	386	GLU
1	A	391	GLU
1	A	395	ARG
1	A	398	ASP
1	A	400	LEU
1	A	417	VAL
1	A	419	LEU
1	A	422	VAL
1	A	425	LYS

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Mol	Chain	Res	Type
1	A	430	ARG
1	A	432	GLN
1	A	445	ARG
1	A	447	MET
1	A	461	GLU
1	A	468	THR
1	A	491	MET
1	A	497	THR
1	A	499	VAL
1	A	504	LEU
1	A	514	MET
1	A	515	ILE
1	A	517	THR
1	B	6	VAL
1	B	18	ARG
1	B	23	LEU
1	B	28	LYS
1	B	43	SER
1	B	44	PHE
1	B	48	THR
1	B	62	LEU
1	B	73	MET
1	B	74	VAL
1	B	77	VAL
1	B	80	LYS
1	B	89	THR
1	B	97	GLN
1	B	111	MET
1	B	114	MET
1	B	120	ILE
1	B	129	GLU
1	B	134	LEU
1	B	135	SER
1	B	138	CYS
1	B	150	ILE
1	B	153	ASN
1	B	161	LEU
1	B	176	THR
1	B	177	VAL
1	B	178	GLU
1	B	183	LEU
1	B	184	GLN

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Mol	Chain	Res	Type
1	B	185	ASP
1	B	193	MET
1	B	209	GLU
1	B	230	ILE
1	B	231	ARG
1	B	284	ARG
1	B	289	LEU
1	B	322	ARG
1	B	328	ASP
1	B	331	THR
1	B	355	GLU
1	B	381	VAL
1	B	386	GLU
1	B	391	GLU
1	B	398	ASP
1	B	417	VAL
1	B	419	LEU
1	B	420	ILE
1	B	422	VAL
1	B	425	LYS
1	B	430	ARG
1	B	432	GLN
1	B	452	ARG
1	B	463	SER
1	B	491	MET
1	B	497	THR
1	B	499	VAL
1	B	504	LEU
1	B	515	ILE
1	C	6	VAL
1	C	7	LYS
1	C	18	ARG
1	C	23	LEU
1	C	43	SER
1	C	44	PHE
1	C	48	THR
1	C	62	LEU
1	C	74	VAL
1	C	77	VAL
1	C	80	LYS
1	C	89	THR
1	C	97	GLN

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Mol	Chain	Res	Type
1	C	111	MET
1	C	114	MET
1	C	129	GLU
1	C	134	LEU
1	C	138	CYS
1	C	150	ILE
1	C	161	LEU
1	C	176	THR
1	C	177	VAL
1	C	178	GLU
1	C	183	LEU
1	C	184	GLN
1	C	185	ASP
1	C	193	MET
1	C	230	ILE
1	C	231	ARG
1	C	284	ARG
1	C	289	LEU
1	C	322	ARG
1	C	328	ASP
1	C	331	THR
1	C	355	GLU
1	C	386	GLU
1	C	391	GLU
1	C	392	LYS
1	C	398	ASP
1	C	400	LEU
1	C	417	VAL
1	C	419	LEU
1	C	422	VAL
1	C	424	SER
1	C	425	LYS
1	C	430	ARG
1	C	452	ARG
1	C	461	GLU
1	C	491	MET
1	C	497	THR
1	C	499	VAL
1	C	504	LEU
1	C	517	THR
1	D	6	VAL
1	D	18	ARG

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Mol	Chain	Res	Type
1	D	23	LEU
1	D	28	LYS
1	D	43	SER
1	D	44	PHE
1	D	48	THR
1	D	62	LEU
1	D	73	MET
1	D	74	VAL
1	D	77	VAL
1	D	80	LYS
1	D	91	THR
1	D	97	GLN
1	D	102	GLU
1	D	111	MET
1	D	114	MET
1	D	120	ILE
1	D	129	GLU
1	D	134	LEU
1	D	135	SER
1	D	138	CYS
1	D	150	ILE
1	D	161	LEU
1	D	176	THR
1	D	177	VAL
1	D	178	GLU
1	D	183	LEU
1	D	184	GLN
1	D	185	ASP
1	D	193	MET
1	D	230	ILE
1	D	231	ARG
1	D	284	ARG
1	D	289	LEU
1	D	322	ARG
1	D	328	ASP
1	D	331	THR
1	D	355	GLU
1	D	376	VAL
1	D	381	VAL
1	D	386	GLU
1	D	390	LYS
1	D	391	GLU

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Mol	Chain	Res	Type
1	D	398	ASP
1	D	417	VAL
1	D	419	LEU
1	D	420	ILE
1	D	422	VAL
1	D	425	LYS
1	D	430	ARG
1	D	445	ARG
1	D	452	ARG
1	D	463	SER
1	D	491	MET
1	D	499	VAL
1	D	504	LEU
1	D	515	ILE
1	D	517	THR
1	E	6	VAL
1	E	18	ARG
1	E	23	LEU
1	E	43	SER
1	E	44	PHE
1	E	48	THR
1	E	62	LEU
1	E	74	VAL
1	E	77	VAL
1	E	80	LYS
1	E	97	GLN
1	E	111	MET
1	E	114	MET
1	E	129	GLU
1	E	134	LEU
1	E	135	SER
1	E	138	CYS
1	E	150	ILE
1	E	153	ASN
1	E	161	LEU
1	E	176	THR
1	E	177	VAL
1	E	178	GLU
1	E	183	LEU
1	E	184	GLN
1	E	185	ASP
1	E	193	MET

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Mol	Chain	Res	Type
1	E	230	ILE
1	E	231	ARG
1	E	284	ARG
1	E	289	LEU
1	E	295	LEU
1	E	322	ARG
1	E	328	ASP
1	E	331	THR
1	E	355	GLU
1	E	369	VAL
1	E	376	VAL
1	E	381	VAL
1	E	386	GLU
1	E	391	GLU
1	E	398	ASP
1	E	417	VAL
1	E	419	LEU
1	E	420	ILE
1	E	422	VAL
1	E	425	LYS
1	E	430	ARG
1	E	432	GLN
1	E	447	MET
1	E	499	VAL
1	E	504	LEU
1	E	515	ILE
1	E	517	THR
1	F	6	VAL
1	F	7	LYS
1	F	18	ARG
1	F	23	LEU
1	F	28	LYS
1	F	43	SER
1	F	44	PHE
1	F	48	THR
1	F	62	LEU
1	F	73	MET
1	F	74	VAL
1	F	77	VAL
1	F	80	LYS
1	F	83	ASP
1	F	91	THR

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Mol	Chain	Res	Type
1	F	97	GLN
1	F	111	MET
1	F	114	MET
1	F	120	ILE
1	F	129	GLU
1	F	134	LEU
1	F	135	SER
1	F	138	CYS
1	F	146	GLN
1	F	150	ILE
1	F	153	ASN
1	F	161	LEU
1	F	176	THR
1	F	177	VAL
1	F	178	GLU
1	F	183	LEU
1	F	184	GLN
1	F	185	ASP
1	F	193	MET
1	F	230	ILE
1	F	231	ARG
1	F	284	ARG
1	F	289	LEU
1	F	322	ARG
1	F	328	ASP
1	F	331	THR
1	F	355	GLU
1	F	376	VAL
1	F	381	VAL
1	F	386	GLU
1	F	391	GLU
1	F	398	ASP
1	F	400	LEU
1	F	417	VAL
1	F	419	LEU
1	F	422	VAL
1	F	425	LYS
1	F	430	ARG
1	F	432	GLN
1	F	442	VAL
1	F	452	ARG
1	F	461	GLU

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Mol	Chain	Res	Type
1	F	463	SER
1	F	468	THR
1	F	491	MET
1	F	499	VAL
1	F	504	LEU
1	F	514	MET
1	F	515	ILE
1	G	6	VAL
1	G	7	LYS
1	G	18	ARG
1	G	23	LEU
1	G	43	SER
1	G	44	PHE
1	G	48	THR
1	G	62	LEU
1	G	64	ASP
1	G	74	VAL
1	G	77	VAL
1	G	80	LYS
1	G	89	THR
1	G	97	GLN
1	G	111	MET
1	G	114	MET
1	G	129	GLU
1	G	138	CYS
1	G	146	GLN
1	G	147	VAL
1	G	150	ILE
1	G	153	ASN
1	G	161	LEU
1	G	162	ILE
1	G	176	THR
1	G	177	VAL
1	G	178	GLU
1	G	183	LEU
1	G	184	GLN
1	G	185	ASP
1	G	193	MET
1	G	230	ILE
1	G	231	ARG
1	G	284	ARG
1	G	289	LEU

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Mol	Chain	Res	Type
1	G	322	ARG
1	G	328	ASP
1	G	331	THR
1	G	355	GLU
1	G	376	VAL
1	G	381	VAL
1	G	386	GLU
1	G	391	GLU
1	G	398	ASP
1	G	417	VAL
1	G	419	LEU
1	G	420	ILE
1	G	422	VAL
1	G	425	LYS
1	G	430	ARG
1	G	432	GLN
1	G	461	GLU
1	G	463	SER
1	G	491	MET
1	G	499	VAL
1	G	504	LEU
1	G	514	MET
1	G	515	ILE
1	G	517	THR
1	H	7	LYS
1	H	11	ASP
1	H	15	LYS
1	H	16	MET
1	H	20	VAL
1	H	23	LEU
1	H	40	LEU
1	H	42	LYS
1	H	43	SER
1	H	44	PHE
1	H	48	THR
1	H	49	ILE
1	H	51	LYS
1	H	55	SER
1	H	59	GLU
1	H	65	LYS
1	H	77	VAL
1	H	79	SER

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Mol	Chain	Res	Type
1	H	87	ASP
1	H	101	THR
1	H	104	LEU
1	H	107	VAL
1	H	129	GLU
1	H	131	LEU
1	H	138	CYS
1	H	141	SER
1	H	147	VAL
1	H	150	ILE
1	H	151	SER
1	H	157	THR
1	H	161	LEU
1	H	172	GLU
1	H	189	VAL
1	H	201	SER
1	H	210	THR
1	H	217	SER
1	H	230	ILE
1	H	242	LYS
1	H	272	LYS
1	H	284	ARG
1	H	289	LEU
1	H	295	LEU
1	H	302	SER
1	H	307	MET
1	H	322	ARG
1	H	325	ILE
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	343	GLN
1	H	350	ARG
1	H	352	GLN
1	H	355	GLU
1	H	363	GLU
1	H	378	VAL
1	H	385	THR
1	H	389	MET
1	H	390	LYS
1	H	401	HIS
1	H	404	ARG

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Mol	Chain	Res	Type
1	H	419	LEU
1	H	420	ILE
1	H	421	ARG
1	H	422	VAL
1	H	426	LEU
1	H	430	ARG
1	H	433	ASN
1	H	434	GLU
1	H	441	LYS
1	H	452	ARG
1	H	454	ILE
1	H	464	VAL
1	H	467	ASN
1	H	468	THR
1	H	483	GLU
1	H	484	GLU
1	H	489	ILE
1	H	499	VAL
1	H	504	LEU
1	H	509	SER
1	H	513	LEU
1	I	7	LYS
1	I	11	ASP
1	I	16	MET
1	I	23	LEU
1	I	40	LEU
1	I	42	LYS
1	I	43	SER
1	I	44	PHE
1	I	48	THR
1	I	49	ILE
1	I	51	LYS
1	I	52	ASP
1	I	55	SER
1	I	59	GLU
1	I	65	LYS
1	I	77	VAL
1	I	79	SER
1	I	87	ASP
1	I	101	THR
1	I	104	LEU
1	I	107	VAL

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Mol	Chain	Res	Type
1	I	131	LEU
1	I	138	CYS
1	I	141	SER
1	I	147	VAL
1	I	150	ILE
1	I	157	THR
1	I	161	LEU
1	I	172	GLU
1	I	189	VAL
1	I	201	SER
1	I	210	THR
1	I	217	SER
1	I	230	ILE
1	I	242	LYS
1	I	272	LYS
1	I	284	ARG
1	I	289	LEU
1	I	295	LEU
1	I	302	SER
1	I	307	MET
1	I	322	ARG
1	I	325	ILE
1	I	328	ASP
1	I	329	THR
1	I	331	THR
1	I	343	GLN
1	I	350	ARG
1	I	351	GLN
1	I	352	GLN
1	I	355	GLU
1	I	363	GLU
1	I	378	VAL
1	I	385	THR
1	I	389	MET
1	I	390	LYS
1	I	404	ARG
1	I	411	VAL
1	I	419	LEU
1	I	420	ILE
1	I	421	ARG
1	I	426	LEU
1	I	430	ARG

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Mol	Chain	Res	Type
1	I	432	GLN
1	I	433	ASN
1	I	434	GLU
1	I	441	LYS
1	I	452	ARG
1	I	454	ILE
1	I	464	VAL
1	I	467	ASN
1	I	468	THR
1	I	483	GLU
1	I	484	GLU
1	I	489	ILE
1	I	498	LYS
1	I	499	VAL
1	I	504	LEU
1	I	513	LEU
1	J	7	LYS
1	J	11	ASP
1	J	15	LYS
1	J	16	MET
1	J	20	VAL
1	J	21	ASN
1	J	23	LEU
1	J	40	LEU
1	J	42	LYS
1	J	43	SER
1	J	44	PHE
1	J	49	ILE
1	J	51	LYS
1	J	52	ASP
1	J	55	SER
1	J	59	GLU
1	J	65	LYS
1	J	77	VAL
1	J	80	LYS
1	J	87	ASP
1	J	101	THR
1	J	104	LEU
1	J	107	VAL
1	J	129	GLU
1	J	131	LEU
1	J	138	CYS

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Mol	Chain	Res	Type
1	J	141	SER
1	J	147	VAL
1	J	150	ILE
1	J	151	SER
1	J	157	THR
1	J	161	LEU
1	J	172	GLU
1	J	189	VAL
1	J	201	SER
1	J	210	THR
1	J	217	SER
1	J	230	ILE
1	J	240	VAL
1	J	242	LYS
1	J	272	LYS
1	J	284	ARG
1	J	289	LEU
1	J	295	LEU
1	J	302	SER
1	J	307	MET
1	J	322	ARG
1	J	325	ILE
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	343	GLN
1	J	350	ARG
1	J	352	GLN
1	J	355	GLU
1	J	363	GLU
1	J	378	VAL
1	J	385	THR
1	J	389	MET
1	J	404	ARG
1	J	411	VAL
1	J	419	LEU
1	J	420	ILE
1	J	421	ARG
1	J	426	LEU
1	J	430	ARG
1	J	433	ASN
1	J	434	GLU

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Mol	Chain	Res	Type
1	J	441	LYS
1	J	452	ARG
1	J	454	ILE
1	J	463	SER
1	J	464	VAL
1	J	467	ASN
1	J	468	THR
1	J	483	GLU
1	J	484	GLU
1	J	489	ILE
1	J	494	LEU
1	J	498	LYS
1	J	499	VAL
1	J	504	LEU
1	J	509	SER
1	J	513	LEU
1	K	7	LYS
1	K	11	ASP
1	K	15	LYS
1	K	16	MET
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	49	ILE
1	K	51	LYS
1	K	52	ASP
1	K	55	SER
1	K	59	GLU
1	K	65	LYS
1	K	77	VAL
1	K	87	ASP
1	K	101	THR
1	K	104	LEU
1	K	107	VAL
1	K	129	GLU
1	K	131	LEU
1	K	138	CYS
1	K	141	SER
1	K	147	VAL

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Mol	Chain	Res	Type
1	K	150	ILE
1	K	151	SER
1	K	161	LEU
1	K	172	GLU
1	K	189	VAL
1	K	201	SER
1	K	217	SER
1	K	230	ILE
1	K	242	LYS
1	K	272	LYS
1	K	284	ARG
1	K	289	LEU
1	K	295	LEU
1	K	302	SER
1	K	307	MET
1	K	322	ARG
1	K	325	ILE
1	K	328	ASP
1	K	329	THR
1	K	331	THR
1	K	343	GLN
1	K	350	ARG
1	K	352	GLN
1	K	355	GLU
1	K	363	GLU
1	K	378	VAL
1	K	385	THR
1	K	389	MET
1	K	390	LYS
1	K	401	HIS
1	K	404	ARG
1	K	419	LEU
1	K	420	ILE
1	K	426	LEU
1	K	433	ASN
1	K	434	GLU
1	K	441	LYS
1	K	452	ARG
1	K	454	ILE
1	K	463	SER
1	K	464	VAL
1	K	467	ASN

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Mol	Chain	Res	Type
1	K	468	THR
1	K	483	GLU
1	K	489	ILE
1	K	494	LEU
1	K	499	VAL
1	K	504	LEU
1	K	509	SER
1	K	513	LEU
1	L	7	LYS
1	L	11	ASP
1	L	15	LYS
1	L	16	MET
1	L	20	VAL
1	L	23	LEU
1	L	40	LEU
1	L	42	LYS
1	L	43	SER
1	L	44	PHE
1	L	49	ILE
1	L	51	LYS
1	L	52	ASP
1	L	55	SER
1	L	59	GLU
1	L	65	LYS
1	L	77	VAL
1	L	87	ASP
1	L	101	THR
1	L	104	LEU
1	L	107	VAL
1	L	129	GLU
1	L	131	LEU
1	L	138	CYS
1	L	141	SER
1	L	147	VAL
1	L	150	ILE
1	L	161	LEU
1	L	172	GLU
1	L	189	VAL
1	L	201	SER
1	L	210	THR
1	L	217	SER
1	L	230	ILE

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Mol	Chain	Res	Type
1	L	242	LYS
1	L	272	LYS
1	L	284	ARG
1	L	289	LEU
1	L	295	LEU
1	L	302	SER
1	L	307	MET
1	L	322	ARG
1	L	325	ILE
1	L	328	ASP
1	L	329	THR
1	L	331	THR
1	L	343	GLN
1	L	350	ARG
1	L	352	GLN
1	L	355	GLU
1	L	363	GLU
1	L	378	VAL
1	L	385	THR
1	L	389	MET
1	L	390	LYS
1	L	401	HIS
1	L	404	ARG
1	L	419	LEU
1	L	420	ILE
1	L	426	LEU
1	L	430	ARG
1	L	432	GLN
1	L	433	ASN
1	L	434	GLU
1	L	441	LYS
1	L	452	ARG
1	L	454	ILE
1	L	464	VAL
1	L	467	ASN
1	L	468	THR
1	L	483	GLU
1	L	484	GLU
1	L	489	ILE
1	L	499	VAL
1	L	504	LEU
1	L	509	SER

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Mol	Chain	Res	Type
1	L	513	LEU
1	M	7	LYS
1	M	11	ASP
1	M	16	MET
1	M	20	VAL
1	M	21	ASN
1	M	23	LEU
1	M	40	LEU
1	M	42	LYS
1	M	43	SER
1	M	44	PHE
1	M	49	ILE
1	M	51	LYS
1	M	52	ASP
1	M	55	SER
1	M	59	GLU
1	M	65	LYS
1	M	77	VAL
1	M	87	ASP
1	M	101	THR
1	M	104	LEU
1	M	107	VAL
1	M	114	MET
1	M	120	ILE
1	M	129	GLU
1	M	131	LEU
1	M	138	CYS
1	M	141	SER
1	M	147	VAL
1	M	150	ILE
1	M	161	LEU
1	M	172	GLU
1	M	189	VAL
1	M	201	SER
1	M	210	THR
1	M	217	SER
1	M	230	ILE
1	M	242	LYS
1	M	272	LYS
1	M	284	ARG
1	M	289	LEU
1	M	295	LEU

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Mol	Chain	Res	Type
1	M	302	SER
1	M	307	MET
1	M	322	ARG
1	M	325	ILE
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	343	GLN
1	M	350	ARG
1	M	352	GLN
1	M	355	GLU
1	M	363	GLU
1	M	378	VAL
1	M	385	THR
1	M	389	MET
1	M	401	HIS
1	M	404	ARG
1	M	411	VAL
1	M	419	LEU
1	M	420	ILE
1	M	421	ARG
1	M	422	VAL
1	M	426	LEU
1	M	430	ARG
1	M	432	GLN
1	M	433	ASN
1	M	434	GLU
1	M	441	LYS
1	M	452	ARG
1	M	454	ILE
1	M	467	ASN
1	M	468	THR
1	M	483	GLU
1	M	489	ILE
1	M	498	LYS
1	M	499	VAL
1	M	504	LEU
1	M	509	SER
1	M	513	LEU
1	N	7	LYS
1	N	11	ASP
1	N	15	LYS

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Mol	Chain	Res	Type
1	N	16	MET
1	N	20	VAL
1	N	23	LEU
1	N	27	VAL
1	N	40	LEU
1	N	42	LYS
1	N	43	SER
1	N	44	PHE
1	N	49	ILE
1	N	51	LYS
1	N	55	SER
1	N	59	GLU
1	N	65	LYS
1	N	77	VAL
1	N	87	ASP
1	N	101	THR
1	N	104	LEU
1	N	107	VAL
1	N	129	GLU
1	N	131	LEU
1	N	138	CYS
1	N	141	SER
1	N	147	VAL
1	N	150	ILE
1	N	157	THR
1	N	161	LEU
1	N	172	GLU
1	N	189	VAL
1	N	201	SER
1	N	217	SER
1	N	230	ILE
1	N	242	LYS
1	N	272	LYS
1	N	284	ARG
1	N	289	LEU
1	N	295	LEU
1	N	302	SER
1	N	307	MET
1	N	322	ARG
1	N	325	ILE
1	N	328	ASP
1	N	329	THR

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Mol	Chain	Res	Type
1	N	331	THR
1	N	343	GLN
1	N	350	ARG
1	N	352	GLN
1	N	355	GLU
1	N	363	GLU
1	N	378	VAL
1	N	385	THR
1	N	389	MET
1	N	401	HIS
1	N	404	ARG
1	N	411	VAL
1	N	419	LEU
1	N	420	ILE
1	N	421	ARG
1	N	426	LEU
1	N	433	ASN
1	N	434	GLU
1	N	441	LYS
1	N	452	ARG
1	N	454	ILE
1	N	464	VAL
1	N	467	ASN
1	N	468	THR
1	N	483	GLU
1	N	489	ILE
1	N	494	LEU
1	N	499	VAL
1	N	504	LEU
1	N	513	LEU
2	O	1	MET
2	O	3	ILE
2	O	4	ARG
2	O	6	LEU
2	O	20	LYS
2	O	30	SER
2	O	55	LYS
2	O	60	LYS
2	O	78	ILE
2	O	80	ASN
2	O	86	MET
2	O	89	SER

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Mol	Chain	Res	Type
2	P	1	MET
2	P	3	ILE
2	P	4	ARG
2	P	6	LEU
2	P	20	LYS
2	P	28	THR
2	P	30	SER
2	P	55	LYS
2	P	60	LYS
2	P	78	ILE
2	P	80	ASN
2	P	86	MET
2	P	89	SER
2	Q	1	MET
2	Q	3	ILE
2	Q	4	ARG
2	Q	6	LEU
2	Q	20	LYS
2	Q	28	THR
2	Q	30	SER
2	Q	55	LYS
2	Q	60	LYS
2	Q	78	ILE
2	Q	80	ASN
2	Q	86	MET
2	Q	89	SER
2	R	1	MET
2	R	3	ILE
2	R	4	ARG
2	R	6	LEU
2	R	20	LYS
2	R	28	THR
2	R	30	SER
2	R	55	LYS
2	R	60	LYS
2	R	78	ILE
2	R	80	ASN
2	R	89	SER
2	S	1	MET
2	S	3	ILE
2	S	4	ARG
2	S	6	LEU

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Mol	Chain	Res	Type
2	S	20	LYS
2	S	30	SER
2	S	55	LYS
2	S	60	LYS
2	S	78	ILE
2	S	80	ASN
2	S	86	MET
2	S	89	SER
2	T	1	MET
2	T	3	ILE
2	T	4	ARG
2	T	6	LEU
2	T	20	LYS
2	T	28	THR
2	T	30	SER
2	T	55	LYS
2	T	60	LYS
2	T	78	ILE
2	T	80	ASN
2	T	86	MET
2	T	89	SER
2	U	1	MET
2	U	3	ILE
2	U	4	ARG
2	U	6	LEU
2	U	20	LYS
2	U	30	SER
2	U	55	LYS
2	U	60	LYS
2	U	78	ILE
2	U	80	ASN
2	U	89	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (199) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	37	ASN
1	A	97	GLN
1	A	146	GLN
1	A	153	ASN
1	A	194	GLN

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	326	ASN
1	A	348	GLN
1	A	351	GLN
1	A	366	GLN
1	A	453	GLN
1	A	457	ASN
1	A	475	ASN
1	B	21	ASN
1	B	37	ASN
1	B	146	GLN
1	B	153	ASN
1	B	194	GLN
1	B	206	ASN
1	B	265	ASN
1	B	326	ASN
1	B	348	GLN
1	B	351	GLN
1	B	366	GLN
1	B	401	HIS
1	B	457	ASN
1	B	475	ASN
1	C	21	ASN
1	C	37	ASN
1	C	146	GLN
1	C	153	ASN
1	C	194	GLN
1	C	206	ASN
1	C	265	ASN
1	C	326	ASN
1	C	348	GLN
1	C	351	GLN
1	C	366	GLN
1	C	453	GLN
1	C	457	ASN
1	C	475	ASN
1	D	10	ASN
1	D	21	ASN
1	D	37	ASN
1	D	146	GLN
1	D	153	ASN
1	D	194	GLN

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Mol	Chain	Res	Type
1	D	206	ASN
1	D	265	ASN
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	366	GLN
1	D	433	ASN
1	D	453	GLN
1	D	457	ASN
1	D	475	ASN
1	E	21	ASN
1	E	37	ASN
1	E	146	GLN
1	E	153	ASN
1	E	194	GLN
1	E	206	ASN
1	E	326	ASN
1	E	348	GLN
1	E	351	GLN
1	E	366	GLN
1	E	401	HIS
1	E	457	ASN
1	E	475	ASN
1	F	21	ASN
1	F	97	GLN
1	F	146	GLN
1	F	153	ASN
1	F	194	GLN
1	F	206	ASN
1	F	265	ASN
1	F	326	ASN
1	F	348	GLN
1	F	366	GLN
1	F	433	ASN
1	F	457	ASN
1	G	21	ASN
1	G	37	ASN
1	G	146	GLN
1	G	153	ASN
1	G	194	GLN
1	G	206	ASN
1	G	265	ASN

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Mol	Chain	Res	Type
1	G	326	ASN
1	G	348	GLN
1	G	351	GLN
1	G	366	GLN
1	G	453	GLN
1	G	457	ASN
1	G	475	ASN
1	H	21	ASN
1	H	72	GLN
1	H	82	ASN
1	H	97	GLN
1	H	153	ASN
1	H	265	ASN
1	H	326	ASN
1	H	351	GLN
1	H	433	ASN
1	H	436	GLN
1	H	453	GLN
1	H	467	ASN
1	I	10	ASN
1	I	21	ASN
1	I	72	GLN
1	I	97	GLN
1	I	265	ASN
1	I	326	ASN
1	I	351	GLN
1	I	433	ASN
1	I	436	GLN
1	I	453	GLN
1	I	467	ASN
1	I	475	ASN
1	J	10	ASN
1	J	21	ASN
1	J	72	GLN
1	J	97	GLN
1	J	153	ASN
1	J	194	GLN
1	J	229	ASN
1	J	265	ASN
1	J	326	ASN
1	J	351	GLN
1	J	433	ASN

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Mol	Chain	Res	Type
1	J	436	GLN
1	J	453	GLN
1	K	21	ASN
1	K	72	GLN
1	K	97	GLN
1	K	194	GLN
1	K	229	ASN
1	K	265	ASN
1	K	326	ASN
1	K	351	GLN
1	K	433	ASN
1	K	436	GLN
1	K	453	GLN
1	K	467	ASN
1	L	21	ASN
1	L	72	GLN
1	L	82	ASN
1	L	97	GLN
1	L	229	ASN
1	L	265	ASN
1	L	326	ASN
1	L	351	GLN
1	L	433	ASN
1	L	436	GLN
1	L	467	ASN
1	M	21	ASN
1	M	72	GLN
1	M	82	ASN
1	M	97	GLN
1	M	153	ASN
1	M	265	ASN
1	M	326	ASN
1	M	351	GLN
1	M	433	ASN
1	M	436	GLN
1	M	453	GLN
1	M	467	ASN
1	N	21	ASN
1	N	72	GLN
1	N	82	ASN
1	N	97	GLN
1	N	194	GLN

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Mol	Chain	Res	Type
1	N	229	ASN
1	N	265	ASN
1	N	326	ASN
1	N	348	GLN
1	N	351	GLN
1	N	433	ASN
1	N	436	GLN
1	N	467	ASN
2	O	45	ASN
2	O	68	ASN
2	O	80	ASN
2	P	45	ASN
2	P	68	ASN
2	Q	45	ASN
2	Q	51	ASN
2	Q	68	ASN
2	R	45	ASN
2	R	68	ASN
2	S	45	ASN
2	S	68	ASN
2	S	80	ASN
2	T	45	ASN
2	T	68	ASN
2	U	45	ASN
2	U	68	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	B	600	4,6,3	28,29,29	1.44	3 (10%)	43,45,45	2.31	16 (37%)
5	ADP	E	600	4,6,3	28,29,29	1.36	3 (10%)	43,45,45	2.29	17 (39%)
6	AF3	C	602	5	0,3,3	-	-	-		
6	AF3	F	602	5	0,3,3	-	-	-		
5	ADP	D	600	4,6	28,29,29	1.27	4 (14%)	43,45,45	2.07	10 (23%)
6	AF3	B	602	5	0,3,3	-	-	-		
5	ADP	A	600	4,6,3	28,29,29	1.10	3 (10%)	43,45,45	1.68	10 (23%)
6	AF3	D	602	5	0,3,3	-	-	-		
6	AF3	E	602	5	0,3,3	-	-	-		
5	ADP	F	600	4,6,3	28,29,29	1.34	3 (10%)	43,45,45	1.99	14 (32%)
6	AF3	A	602	5	0,3,3	-	-	-		
5	ADP	G	600	4,6,3	28,29,29	1.35	3 (10%)	43,45,45	1.99	13 (30%)
6	AF3	G	602	5	0,3,3	-	-	-		
5	ADP	C	600	4,6,3	28,29,29	1.08	1 (3%)	43,45,45	2.14	14 (32%)

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
5	ADP	B	600	4,6,3	-	5/16/32/32	0/3/3/3
5	ADP	E	600	4,6,3	-	4/16/32/32	0/3/3/3
5	ADP	D	600	4,6	-	5/16/32/32	0/3/3/3
5	ADP	A	600	4,6,3	-	4/16/32/32	0/3/3/3
5	ADP	F	600	4,6,3	-	4/16/32/32	0/3/3/3
5	ADP	G	600	4,6,3	-	4/16/32/32	0/3/3/3
5	ADP	C	600	4,6,3	-	4/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	ADP	PA-O3A	4.51	1.64	1.59
5	F	600	ADP	C5-N7	-3.99	1.31	1.39
5	G	600	ADP	C5-N7	-3.37	1.32	1.39
5	E	600	ADP	PA-O3A	3.33	1.63	1.59
5	G	600	ADP	O4'-C4'	-3.25	1.37	1.45
5	D	600	ADP	O4'-C4'	-2.77	1.38	1.45
5	B	600	ADP	O4'-C1'	-2.66	1.35	1.42
5	F	600	ADP	C2-N1	2.58	1.38	1.33
5	E	600	ADP	C5-N7	-2.58	1.34	1.39
5	A	600	ADP	C5-N7	-2.48	1.34	1.39
5	G	600	ADP	C5-C6	-2.39	1.34	1.41
5	C	600	ADP	O4'-C4'	-2.38	1.39	1.45
5	D	600	ADP	PA-O3A	2.36	1.62	1.59
5	A	600	ADP	C2-N1	2.29	1.38	1.33
5	D	600	ADP	C8-N7	2.24	1.36	1.31
5	D	600	ADP	C5-N7	-2.24	1.35	1.39
5	A	600	ADP	C4-N9	-2.21	1.33	1.37
5	F	600	ADP	C4-N9	-2.17	1.33	1.37
5	B	600	ADP	C5-N7	-2.16	1.35	1.39
5	E	600	ADP	O4'-C1'	-2.09	1.37	1.42

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	ADP	N3-C2-N1	-6.29	119.07	128.58
5	C	600	ADP	N9-C8-N7	-5.40	106.28	113.94
5	D	600	ADP	N3-C2-N1	-5.18	120.75	128.58
5	D	600	ADP	N9-C8-N7	-5.15	106.62	113.94
5	G	600	ADP	O4'-C1'-N9	4.92	117.53	108.09
5	C	600	ADP	C5-N7-C8	4.86	111.09	103.45
5	E	600	ADP	N3-C2-N1	-4.81	121.30	128.58
5	F	600	ADP	O4'-C1'-N9	4.76	117.24	108.09
5	E	600	ADP	C4-C5-N7	-4.70	105.21	110.58
5	B	600	ADP	C5-C4-N3	-4.68	120.27	126.72
5	F	600	ADP	N3-C2-N1	-4.61	121.61	128.58
5	E	600	ADP	N9-C8-N7	-4.61	107.40	113.94
5	G	600	ADP	N9-C8-N7	-4.53	107.51	113.94
5	D	600	ADP	C5-N7-C8	4.46	110.46	103.45
5	D	600	ADP	C5-C4-N3	-4.46	120.58	126.72
5	E	600	ADP	C5-N7-C8	4.43	110.42	103.45
5	C	600	ADP	C4-C5-N7	-4.38	105.57	110.58
5	B	600	ADP	C2-N3-C4	4.28	122.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	ADP	N3-C2-N1	-4.27	122.12	128.58
5	C	600	ADP	C5-C4-N3	-4.19	120.95	126.72
5	C	600	ADP	N3-C2-N1	-4.18	122.25	128.58
5	F	600	ADP	O3B-PB-O2B	-4.06	92.58	107.80
5	B	600	ADP	O4'-C1'-N9	3.99	115.75	108.09
5	G	600	ADP	N3-C2-N1	-3.98	122.56	128.58
5	B	600	ADP	N9-C8-N7	-3.92	108.37	113.94
5	E	600	ADP	C5-C4-N3	-3.89	121.36	126.72
5	G	600	ADP	O3B-PB-O2B	-3.84	93.42	107.80
5	D	600	ADP	C4-C5-N7	-3.83	106.20	110.58
5	E	600	ADP	O3'-C3'-C4'	-3.81	100.12	111.08
5	E	600	ADP	O4'-C1'-N9	3.79	115.36	108.09
5	F	600	ADP	N9-C8-N7	-3.73	108.65	113.94
5	E	600	ADP	C5-C4-N9	3.64	109.78	105.81
5	G	600	ADP	C5-N7-C8	3.60	109.11	103.45
5	B	600	ADP	C5-N7-C8	3.60	109.10	103.45
5	A	600	ADP	O4'-C1'-N9	3.55	114.91	108.09
5	D	600	ADP	C2-N3-C4	3.55	120.49	111.83
5	B	600	ADP	C4-C5-N7	-3.51	106.57	110.58
5	B	600	ADP	C5-C4-N9	3.49	109.61	105.81
5	E	600	ADP	C2-N3-C4	3.39	120.10	111.83
5	D	600	ADP	O4'-C1'-N9	3.34	114.50	108.09
5	D	600	ADP	C5-C4-N9	3.26	109.37	105.81
5	C	600	ADP	O3B-PB-O2B	-3.11	96.14	107.80
5	F	600	ADP	C5-C4-N3	-3.07	122.49	126.72
5	A	600	ADP	O2A-PA-O1A	3.05	126.64	112.44
5	B	600	ADP	C5'-C4'-C3'	-3.00	104.42	115.21
5	G	600	ADP	C2'-C3'-C4'	2.96	108.33	102.61
5	A	600	ADP	C5-C4-N3	-2.95	122.66	126.72
5	F	600	ADP	C5-N7-C8	2.93	108.05	103.45
5	C	600	ADP	O4'-C1'-N9	2.86	113.58	108.09
5	C	600	ADP	C6-C5-C4	2.85	121.07	117.18
5	B	600	ADP	O3B-PB-O1B	2.84	121.91	110.83
5	A	600	ADP	C2-N3-C4	2.79	118.66	111.83
5	B	600	ADP	O3'-C3'-C4'	-2.74	103.21	111.08
5	E	600	ADP	O3B-PB-O2B	-2.68	97.74	107.80
5	C	600	ADP	C4-N9-C8	2.66	108.54	105.74
5	F	600	ADP	O2B-PB-O3A	2.66	113.57	104.64
5	B	600	ADP	O3B-PB-O2B	-2.60	98.06	107.80
5	F	600	ADP	O3'-C3'-C4'	-2.58	103.68	111.08
5	F	600	ADP	C2-N3-C4	2.51	117.97	111.83
5	D	600	ADP	O2'-C2'-C1'	-2.49	101.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	ADP	N9-C8-N7	-2.49	110.41	113.94
5	C	600	ADP	C2-N3-C4	2.48	117.89	111.83
5	A	600	ADP	C5-C4-N9	2.47	108.51	105.81
5	C	600	ADP	C5-C4-N9	2.46	108.49	105.81
5	B	600	ADP	O2'-C2'-C3'	-2.43	104.02	111.82
5	E	600	ADP	C5'-C4'-C3'	-2.43	106.47	115.21
5	G	600	ADP	C4-C5-N7	-2.41	107.83	110.58
5	F	600	ADP	C5-C4-N9	2.37	108.39	105.81
5	E	600	ADP	O2B-PB-O3A	2.34	112.49	104.64
5	F	600	ADP	C6-C5-C4	2.33	120.36	117.18
5	E	600	ADP	O2A-PA-O1A	2.33	123.27	112.44
5	F	600	ADP	O3A-PA-O1A	2.32	117.70	110.70
5	E	600	ADP	C6-C5-C4	2.32	120.35	117.18
5	A	600	ADP	C4-C5-N7	-2.32	107.93	110.58
5	G	600	ADP	C3'-C2'-C1'	-2.29	97.13	101.46
5	E	600	ADP	O2'-C2'-C3'	-2.29	104.48	111.82
5	C	600	ADP	O2A-PA-O1A	2.28	123.07	112.44
5	A	600	ADP	O3B-PB-O2B	-2.24	99.39	107.80
5	G	600	ADP	C4-N9-C1'	-2.23	121.41	126.63
5	F	600	ADP	C4-C5-N7	-2.23	108.03	110.58
5	F	600	ADP	O5'-PA-O1A	-2.21	100.17	108.94
5	D	600	ADP	C6-C5-C4	2.20	120.18	117.18
5	C	600	ADP	O3'-C3'-C4'	-2.19	104.79	111.08
5	G	600	ADP	C5-C4-N3	-2.18	123.71	126.72
5	G	600	ADP	C4-N9-C8	2.11	107.95	105.74
5	G	600	ADP	O2B-PB-O3A	2.10	111.66	104.64
5	G	600	ADP	O2B-PB-O1B	2.09	119.00	110.83
5	B	600	ADP	O2'-C2'-C1'	-2.08	102.95	110.10
5	A	600	ADP	C5-N7-C8	2.08	106.71	103.45
5	B	600	ADP	O4'-C1'-C2'	-2.06	102.21	106.62
5	E	600	ADP	O3B-PB-O1B	2.05	118.82	110.83
5	C	600	ADP	C2'-C3'-C4'	2.03	106.54	102.61
5	B	600	ADP	O2A-PA-O1A	2.03	121.89	112.44
5	E	600	ADP	C4-N9-C1'	-2.02	121.91	126.63

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	600	ADP	PA-O3A-PB-O2B
5	D	600	ADP	PA-O3A-PB-O2B
5	F	600	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
5	G	600	ADP	PA-O3A-PB-O2B
5	E	600	ADP	PA-O3A-PB-O1B
5	F	600	ADP	PA-O3A-PB-O1B
5	G	600	ADP	PA-O3A-PB-O1B
5	B	600	ADP	PA-O3A-PB-O2B
5	E	600	ADP	PA-O3A-PB-O2B
5	G	600	ADP	PA-O3A-PB-O3B
5	C	600	ADP	PB-O3A-PA-O1A
5	B	600	ADP	PB-O3A-PA-O1A
5	B	600	ADP	PB-O3A-PA-O2A
5	C	600	ADP	PB-O3A-PA-O2A
5	D	600	ADP	PB-O3A-PA-O1A
5	D	600	ADP	PB-O3A-PA-O2A
5	A	600	ADP	PA-O3A-PB-O1B
5	A	600	ADP	PB-O3A-PA-O2A
5	D	600	ADP	PA-O3A-PB-O1B
5	A	600	ADP	PA-O3A-PB-O2B
5	A	600	ADP	PA-O3A-PB-O3B
5	B	600	ADP	PA-O3A-PB-O3B
5	C	600	ADP	PA-O3A-PB-O3B
5	D	600	ADP	PA-O3A-PB-O3B
5	E	600	ADP	PA-O3A-PB-O3B
5	F	600	ADP	PA-O3A-PB-O3B
5	E	600	ADP	PB-O3A-PA-O2A
5	F	600	ADP	PB-O3A-PA-O2A
5	G	600	ADP	PB-O3A-PA-O2A
5	B	600	ADP	PA-O3A-PB-O1B

There are no ring outliers.

13 monomers are involved in 18 short contacts:

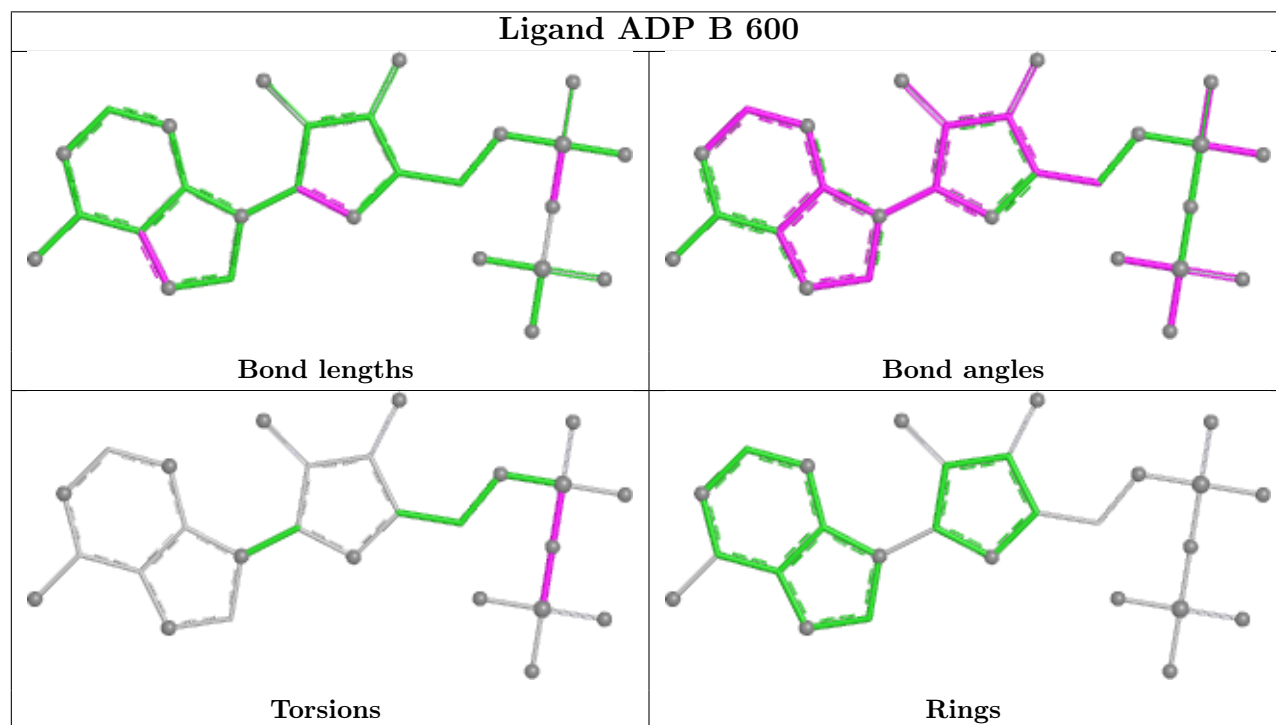
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	600	ADP	1	0
5	E	600	ADP	1	0
6	C	602	AF3	2	0
6	F	602	AF3	2	0
5	D	600	ADP	3	0
5	A	600	ADP	2	0
6	D	602	AF3	2	0
6	E	602	AF3	1	0
5	F	600	ADP	2	0
6	A	602	AF3	3	0

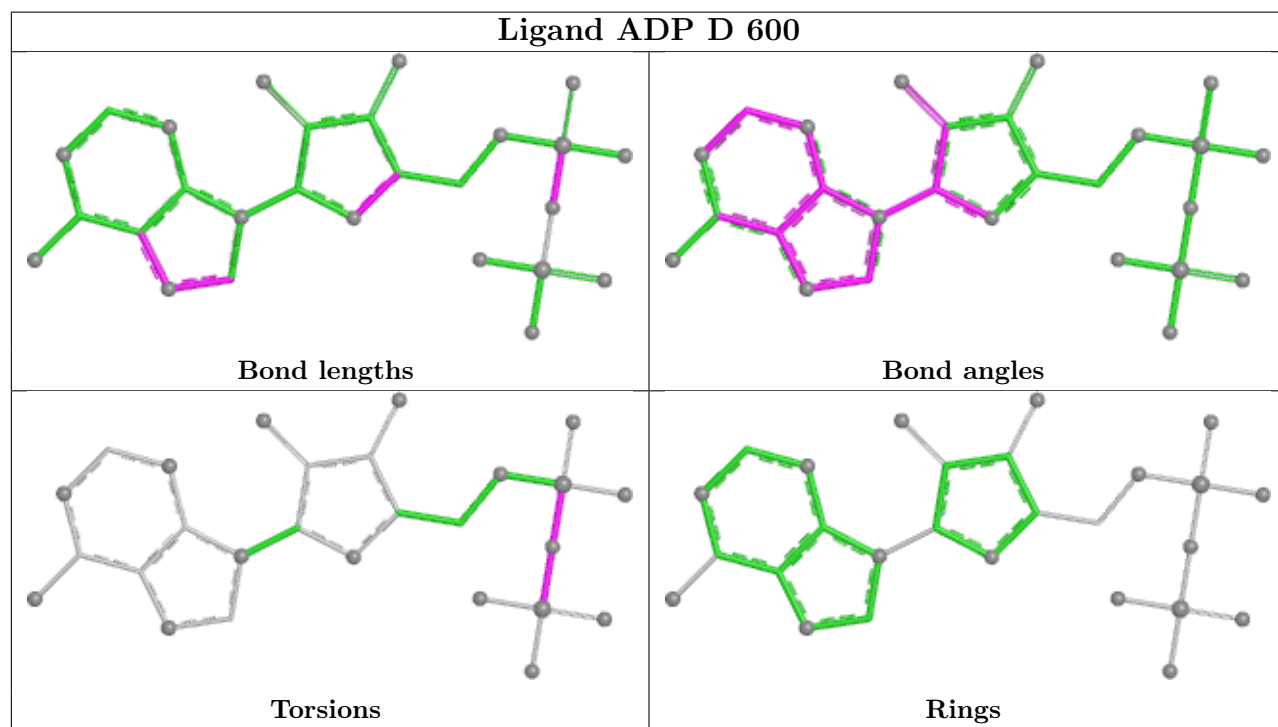
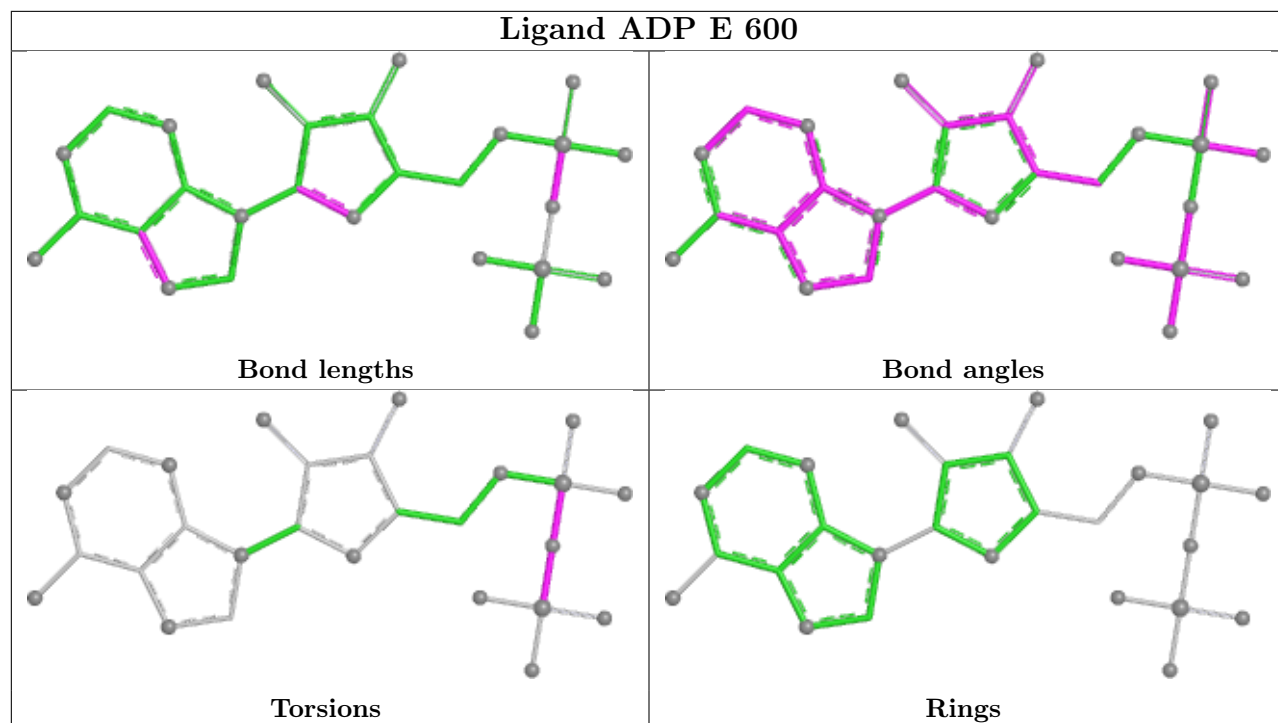
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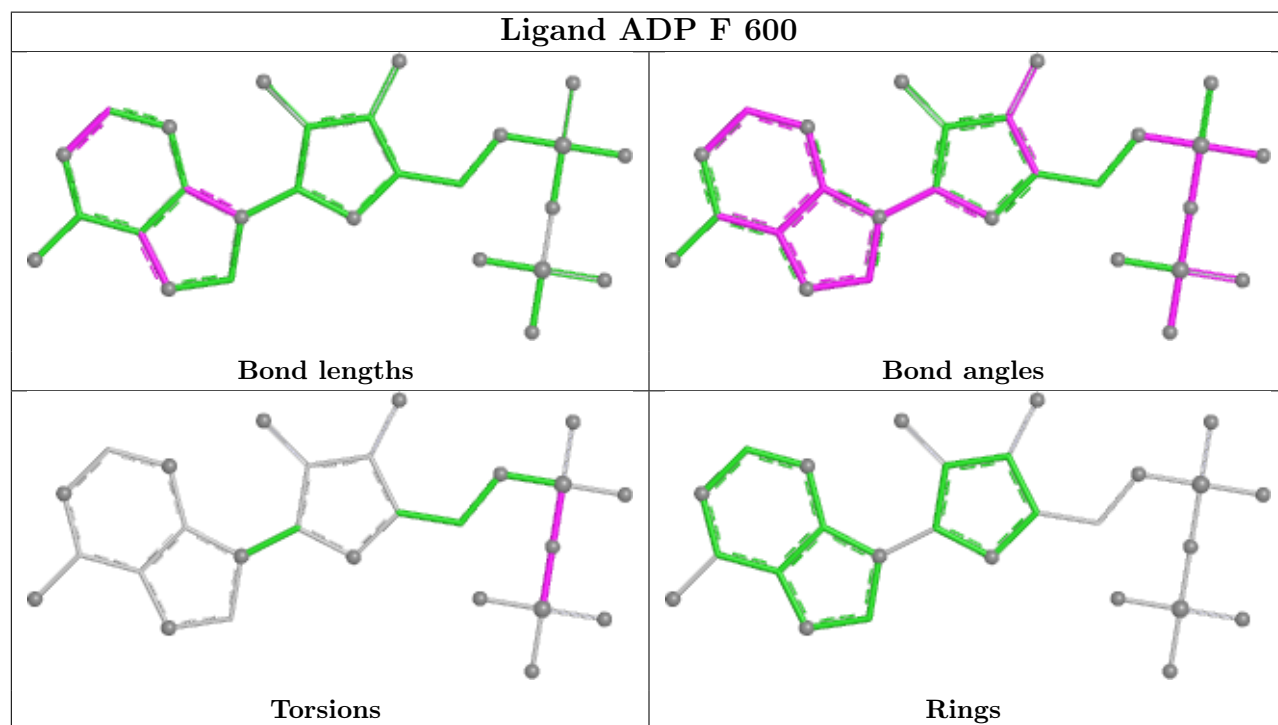
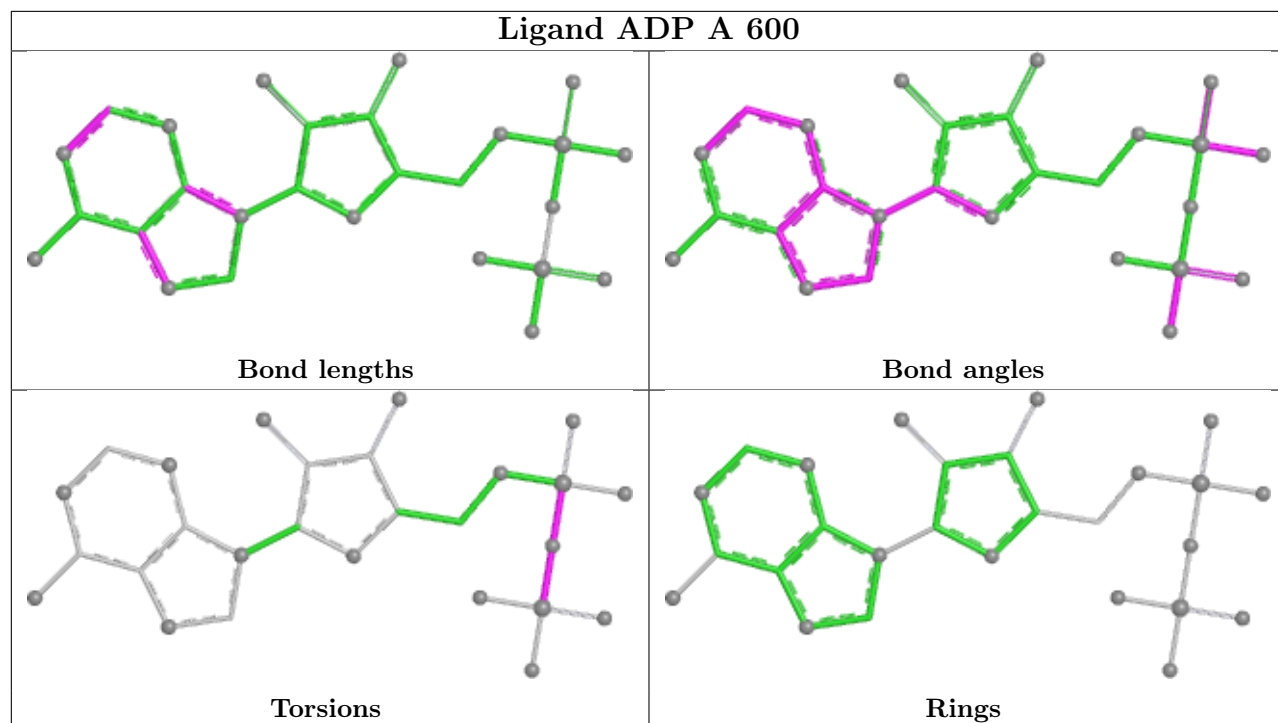
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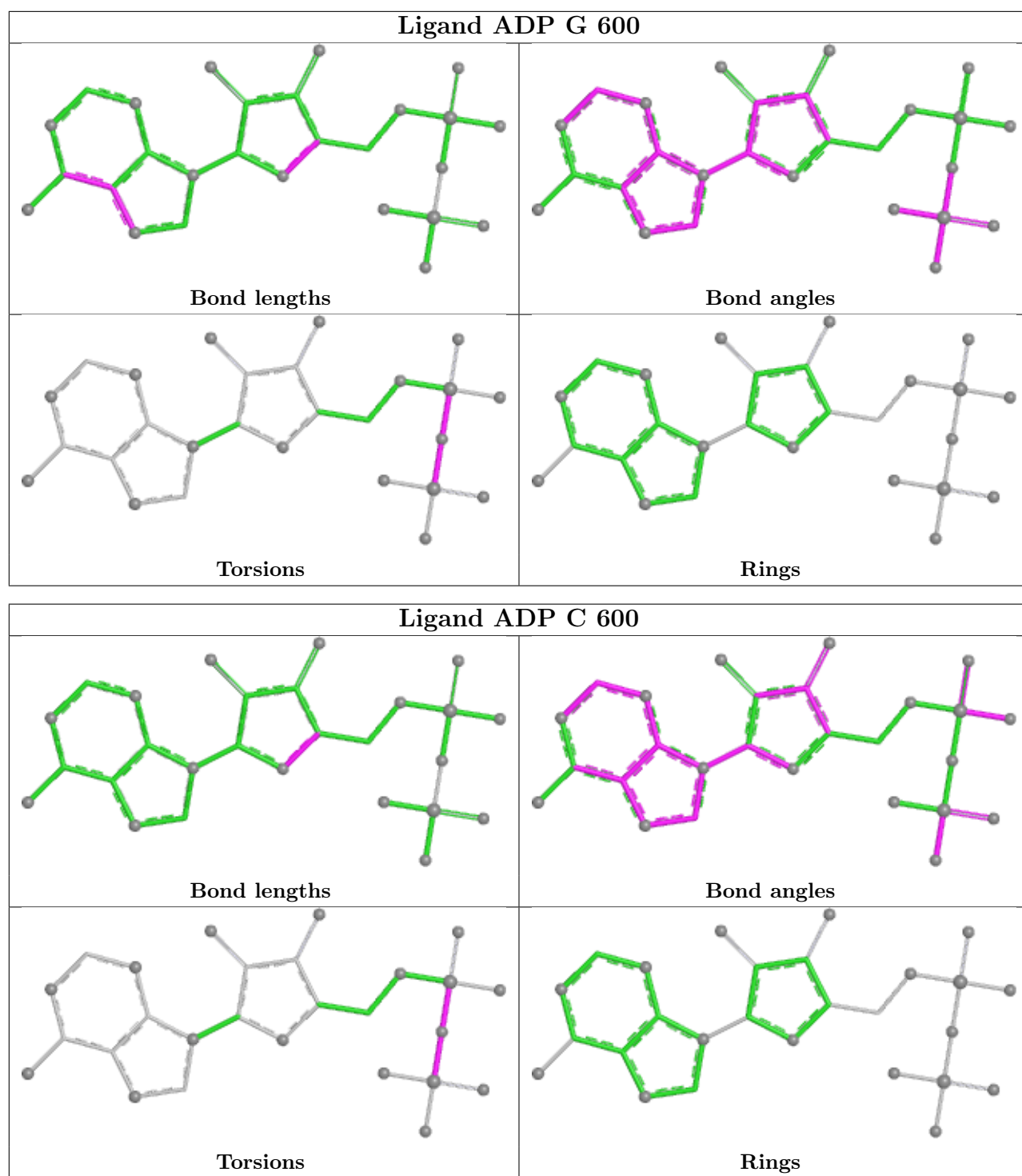
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	600	ADP	1	0
6	G	602	AF3	1	0
5	C	600	ADP	3	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.65	27 (5%)	33	25	2, 2, 4, 5	0
1	B	524/524 (100%)	-0.63	24 (4%)	37	29	2, 2, 4, 5	0
1	C	524/524 (100%)	-0.53	24 (4%)	37	29	2, 2, 4, 5	0
1	D	524/524 (100%)	-0.38	37 (7%)	22	16	2, 2, 4, 5	0
1	E	524/524 (100%)	-0.35	44 (8%)	17	12	2, 2, 4, 5	0
1	F	524/524 (100%)	-0.55	28 (5%)	32	24	2, 2, 4, 5	0
1	G	524/524 (100%)	-0.45	34 (6%)	25	18	2, 2, 4, 5	0
1	H	524/524 (100%)	-0.86	14 (2%)	56	46	2, 2, 4, 5	0
1	I	524/524 (100%)	-1.19	1 (0%)	91	88	2, 2, 4, 5	0
1	J	524/524 (100%)	-1.01	7 (1%)	75	66	2, 2, 4, 5	0
1	K	524/524 (100%)	-0.61	20 (3%)	44	35	2, 2, 4, 5	0
1	L	524/524 (100%)	-0.62	21 (4%)	42	33	2, 2, 3, 5	0
1	M	524/524 (100%)	-1.02	6 (1%)	78	70	2, 2, 4, 5	0
1	N	524/524 (100%)	-0.70	33 (6%)	26	19	2, 2, 4, 5	0
2	O	97/97 (100%)	-0.63	2 (2%)	63	54	2, 2, 2, 2	0
2	P	97/97 (100%)	-0.73	3 (3%)	51	41	2, 2, 2, 2	0
2	Q	97/97 (100%)	-0.70	2 (2%)	63	54	2, 2, 2, 2	0
2	R	97/97 (100%)	-0.61	2 (2%)	63	54	2, 2, 2, 2	0
2	S	97/97 (100%)	-0.64	2 (2%)	63	54	2, 2, 2, 2	0
2	T	97/97 (100%)	-0.45	6 (6%)	26	20	2, 2, 2, 2	0
2	U	97/97 (100%)	-0.72	0	100	100	2, 2, 2, 2	0
All	All	8015/8015 (100%)	-0.68	337 (4%)	40	32	2, 2, 4, 5	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	GLU	8.3
1	A	306	GLY	7.7
2	T	97	ALA	6.6
1	G	268	ARG	6.3
1	E	196	ASP	5.9
1	F	348	GLN	5.7
1	A	204	PHE	5.4
1	K	241	ALA	5.3
1	D	306	GLY	5.2
1	F	241	ALA	5.1
1	C	256	GLY	5.1
1	D	213	VAL	5.0
1	L	274	ALA	5.0
1	B	353	ILE	5.0
1	L	387	VAL	4.9
1	F	361	ASP	4.9
1	E	301	ILE	4.8
1	N	312	ALA	4.8
1	C	306	GLY	4.7
1	C	311	LYS	4.6
1	E	284	ARG	4.6
1	N	266	THR	4.5
1	D	346	VAL	4.4
1	C	183	LEU	4.3
1	G	260	ALA	4.3
1	G	199	TYR	4.3
1	F	353	ILE	4.3
1	N	268	ARG	4.3
1	D	359	ASP	4.2
1	E	266	THR	4.2
1	E	224	ASP	4.2
1	C	204	PHE	4.2
1	D	177	VAL	4.1
1	D	355	GLU	4.1
1	A	200	LEU	4.0
1	G	267	MET	4.0
1	K	239	ALA	4.0
1	C	258	ALA	3.9
1	E	306	GLY	3.9
1	E	227	ILE	3.9
1	N	330	THR	3.9
1	A	244	GLY	3.9
1	A	254	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	212	ALA	3.8
1	N	278	ALA	3.8
1	L	239	ALA	3.8
1	F	301	ILE	3.7
1	B	278	ALA	3.7
1	K	242	LYS	3.7
1	G	264	VAL	3.7
2	O	30	SER	3.7
1	F	239	ALA	3.7
1	E	204	PHE	3.7
1	E	354	GLU	3.7
1	F	231	ARG	3.7
1	K	308	GLU	3.7
1	G	212	ALA	3.7
1	A	211	GLY	3.6
1	G	232	GLU	3.6
1	E	294	THR	3.6
1	N	267	MET	3.6
1	B	256	GLY	3.6
1	H	254	VAL	3.6
1	E	244	GLY	3.5
1	F	242	LYS	3.5
1	A	268	ARG	3.5
1	B	313	THR	3.5
1	H	274	ALA	3.5
1	L	241	ALA	3.5
1	N	287	ALA	3.5
1	L	264	VAL	3.4
1	G	222	LEU	3.4
1	F	198	GLY	3.4
1	M	270	ILE	3.4
2	P	52	GLY	3.4
1	G	355	GLU	3.4
1	E	287	ALA	3.4
1	H	204	PHE	3.4
1	F	351	GLN	3.4
1	E	330	THR	3.3
2	T	52	GLY	3.3
1	A	272	LYS	3.3
1	G	228	SER	3.3
1	N	201	SER	3.3
1	D	377	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	247	LEU	3.3
1	K	280	GLY	3.3
1	L	260	ALA	3.3
1	D	271	VAL	3.3
1	D	211	GLY	3.3
1	D	256	GLY	3.3
1	D	255	GLU	3.2
1	K	310	GLU	3.2
1	D	383	ALA	3.2
1	G	274	ALA	3.2
1	A	230	ILE	3.2
1	D	231	ARG	3.2
1	E	350	ARG	3.2
1	B	267	MET	3.2
1	E	361	ASP	3.2
1	H	268	ARG	3.2
1	N	272	LYS	3.2
1	E	297	GLY	3.2
1	G	361	ASP	3.1
1	A	229	ASN	3.1
1	L	240	VAL	3.1
2	Q	50	GLU	3.1
1	N	230	ILE	3.1
1	C	305	ILE	3.1
1	F	172	GLU	3.1
1	G	209	GLU	3.1
1	E	268	ARG	3.1
1	D	243	ALA	3.1
2	P	31	ALA	3.1
1	N	254	VAL	3.1
1	B	268	ARG	3.1
2	T	71	TYR	3.0
1	D	259	LEU	3.0
1	E	209	GLU	3.0
1	N	229	ASN	3.0
1	E	360	TYR	3.0
1	E	353	ILE	3.0
1	B	391	GLU	3.0
1	A	271	VAL	3.0
1	N	300	VAL	3.0
1	B	205	ILE	3.0
1	C	228	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	228	SER	3.0
1	M	264	VAL	2.9
1	D	309	LEU	2.9
1	H	201	SER	2.9
1	A	353	ILE	2.9
1	F	205	ILE	2.9
1	N	200	LEU	2.9
1	F	217	SER	2.9
1	C	254	VAL	2.9
1	A	284	ARG	2.9
1	F	197	ARG	2.9
1	K	268	ARG	2.9
1	E	199	TYR	2.9
1	K	229	ASN	2.9
1	G	223	ALA	2.9
1	H	269	GLY	2.8
2	R	29	GLY	2.8
1	F	339	GLU	2.8
1	D	384	ALA	2.8
1	N	236	VAL	2.8
1	L	309	LEU	2.8
1	A	307	MET	2.8
1	G	244	GLY	2.8
1	C	212	ALA	2.8
1	G	243	ALA	2.8
1	H	240	VAL	2.8
1	A	227	ILE	2.8
1	E	250	ILE	2.8
1	C	235	PRO	2.8
1	A	312	ALA	2.8
1	L	275	ALA	2.8
1	E	385	THR	2.8
1	D	241	ALA	2.7
1	F	251	ALA	2.7
1	L	312	ALA	2.7
1	K	215	LEU	2.7
1	N	260	ALA	2.7
1	E	381	VAL	2.7
1	C	260	ALA	2.7
1	D	183	LEU	2.7
1	D	227	ILE	2.7
1	D	218	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	298	GLY	2.7
1	E	312	ALA	2.7
1	K	207	LYS	2.7
1	N	224	ASP	2.7
1	F	305	ILE	2.6
1	B	306	GLY	2.6
1	J	229	ASN	2.6
1	F	354	GLU	2.6
1	H	262	LEU	2.6
2	O	27	LEU	2.6
1	M	383	ALA	2.6
1	K	249	ILE	2.6
1	E	208	PRO	2.6
1	F	306	GLY	2.6
1	C	387	VAL	2.6
1	G	288	MET	2.6
1	K	303	GLU	2.6
1	D	281	PHE	2.6
1	E	347	ALA	2.6
1	C	361	ASP	2.6
1	J	256	GLY	2.5
1	E	267	MET	2.5
1	E	387	VAL	2.5
1	K	178	GLU	2.5
1	N	238	GLU	2.5
1	I	265	ASN	2.5
1	H	231	ARG	2.5
2	P	30	SER	2.5
1	M	234	LEU	2.5
1	D	307	MET	2.5
1	E	205	ILE	2.5
1	H	270	ILE	2.5
1	L	243	ALA	2.5
1	B	253	ASP	2.5
1	G	235	PRO	2.5
1	G	314	LEU	2.5
1	G	213	VAL	2.5
1	H	264	VAL	2.5
1	C	384	ALA	2.5
1	A	314	LEU	2.5
1	C	349	ILE	2.5
1	D	305	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	302	SER	2.5
1	D	376	VAL	2.5
1	E	195	PHE	2.5
1	H	310	GLU	2.5
1	N	290	GLN	2.5
1	N	299	THR	2.5
1	D	153	ASN	2.5
1	L	386	GLU	2.4
1	C	253	ASP	2.4
1	B	211	GLY	2.4
1	G	275	ALA	2.4
1	J	360	TYR	2.4
1	B	259	LEU	2.4
1	B	309	LEU	2.4
1	E	215	LEU	2.4
1	D	254	VAL	2.4
1	F	318	GLY	2.4
1	M	375	GLY	2.4
1	E	275	ALA	2.4
1	L	203	TYR	2.4
1	C	385	THR	2.4
1	D	266	THR	2.4
1	C	314	LEU	2.4
1	B	291	ASP	2.4
1	E	311	LYS	2.4
1	L	256	GLY	2.4
1	K	201	SER	2.4
1	C	261	THR	2.4
1	D	203	TYR	2.4
1	N	247	LEU	2.4
1	F	300	VAL	2.3
1	K	211	GLY	2.3
1	H	354	GLU	2.3
1	K	203	TYR	2.3
1	D	205	ILE	2.3
1	L	230	ILE	2.3
1	L	242	LYS	2.3
1	F	273	VAL	2.3
1	J	231	ARG	2.3
1	A	206	ASN	2.3
1	N	244	GLY	2.3
1	B	316	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	233	MET	2.3
1	N	313	THR	2.3
1	A	246	PRO	2.3
1	N	243	ALA	2.3
1	N	255	GLU	2.3
1	D	179	ASP	2.3
1	H	267	MET	2.3
1	G	319	GLN	2.3
1	J	230	ILE	2.3
1	L	268	ARG	2.3
1	D	326	ASN	2.3
1	J	223	ALA	2.3
1	L	308	GLU	2.3
2	Q	97	ALA	2.3
1	N	259	LEU	2.3
1	G	305	ILE	2.3
1	N	315	GLU	2.2
1	L	207	LYS	2.2
1	N	245	LYS	2.2
1	G	270	ILE	2.2
1	A	302	SER	2.2
1	F	254	VAL	2.2
1	N	271	VAL	2.2
1	A	327	LYS	2.2
1	E	200	LEU	2.2
1	L	227	ILE	2.2
1	D	268	ARG	2.2
1	L	254	VAL	2.2
2	R	30	SER	2.2
1	G	182	GLY	2.2
1	B	245	LYS	2.2
1	E	216	GLU	2.2
1	F	304	GLU	2.2
1	E	228	SER	2.2
1	G	297	GLY	2.2
1	K	245	LYS	2.2
1	E	248	LEU	2.2
1	G	295	LEU	2.2
1	A	257	GLU	2.2
1	F	349	ILE	2.2
1	E	300	VAL	2.2
1	A	313	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	S	27	LEU	2.2
1	G	287	ALA	2.2
1	K	238	GLU	2.2
1	F	218	PRO	2.1
1	G	363	GLU	2.1
1	C	220	ILE	2.1
2	T	51	ASN	2.1
1	C	213	VAL	2.1
2	T	26	VAL	2.1
1	N	277	LYS	2.1
1	B	357	THR	2.1
1	F	219	PHE	2.1
1	N	275	ALA	2.1
1	E	308	GLU	2.1
1	C	273	VAL	2.1
2	S	1	MET	2.1
1	G	198	GLY	2.1
1	D	357	THR	2.1
1	K	3	ALA	2.1
1	A	240	VAL	2.1
1	D	393	LYS	2.1
1	E	346	VAL	2.1
1	B	224	ASP	2.1
1	F	322	ARG	2.1
1	M	268	ARG	2.1
1	D	152	ALA	2.1
2	T	25	ILE	2.1
1	A	339	GLU	2.1
1	G	252	GLU	2.1
1	C	226	LYS	2.0
1	G	348	GLN	2.0
1	D	240	VAL	2.0
1	E	309	LEU	2.0
1	J	268	ARG	2.0
1	B	385	THR	2.0
1	B	315	GLU	2.0
1	G	216	GLU	2.0
1	K	208	PRO	2.0
1	B	350	ARG	2.0
1	A	287	ALA	2.0
1	B	307	MET	2.0
1	A	203	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

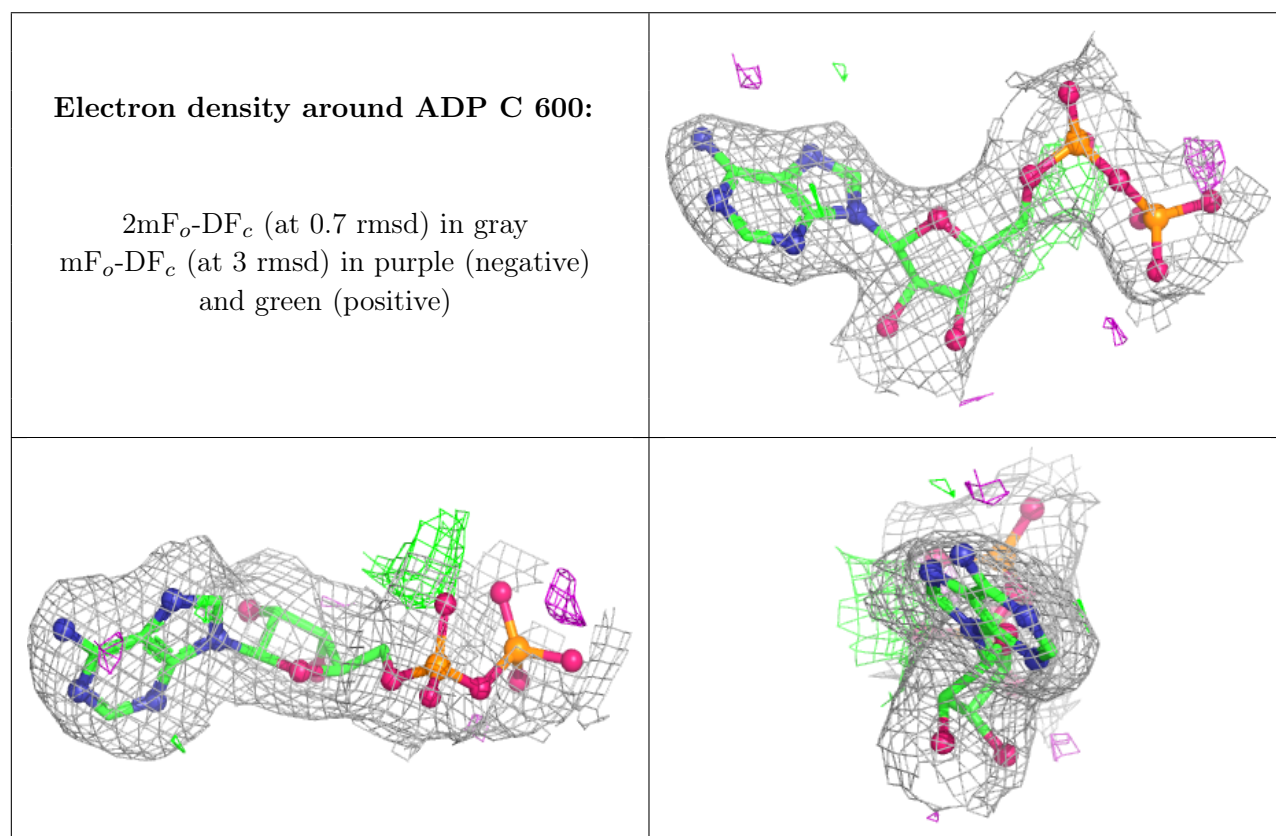
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	AF3	F	602	4/4	0.98	0.04	2,2,8,9	0
4	K	B	603	1/1	0.99	0.06	16,16,16,16	0
4	K	C	603	1/1	0.99	0.05	15,15,15,15	0
4	K	D	603	1/1	0.99	0.12	16,16,16,16	0
4	K	E	603	1/1	0.99	0.10	16,16,16,16	0
4	K	F	603	1/1	0.99	0.04	15,15,15,15	0
4	K	G	603	1/1	0.99	0.03	16,16,16,16	0
5	ADP	C	600	27/27	0.99	0.03	2,2,2,3	0
6	AF3	A	602	4/4	0.99	0.02	2,2,7,10	0
6	AF3	B	602	4/4	0.99	0.03	2,2,7,10	0
6	AF3	C	602	4/4	0.99	0.04	2,2,8,10	0
3	MG	C	601	1/1	0.99	0.05	2,2,2,2	0
3	MG	F	601	1/1	1.00	0.03	2,2,2,2	0
3	MG	G	601	1/1	1.00	0.03	2,2,2,2	0
5	ADP	A	600	27/27	1.00	0.03	2,2,2,3	0
5	ADP	B	600	27/27	1.00	0.02	2,2,3,3	0
4	K	A	603	1/1	1.00	0.09	16,16,16,16	0
5	ADP	D	600	27/27	1.00	0.03	2,2,2,3	0
5	ADP	E	600	27/27	1.00	0.04	2,2,2,3	0
5	ADP	F	600	27/27	1.00	0.02	2,2,2,3	0
5	ADP	G	600	27/27	1.00	0.02	2,2,2,3	0
3	MG	B	601	1/1	1.00	0.01	2,2,2,2	0
3	MG	A	601	1/1	1.00	0.04	2,2,2,2	0
3	MG	D	601	1/1	1.00	0.03	2,2,2,2	0
6	AF3	D	602	4/4	1.00	0.02	2,2,8,10	0
6	AF3	E	602	4/4	1.00	0.03	2,2,8,9	0
3	MG	E	601	1/1	1.00	0.01	2,2,2,2	0

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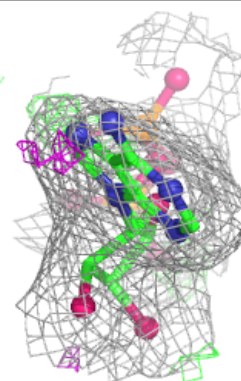
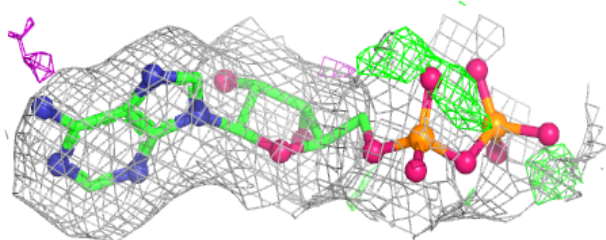
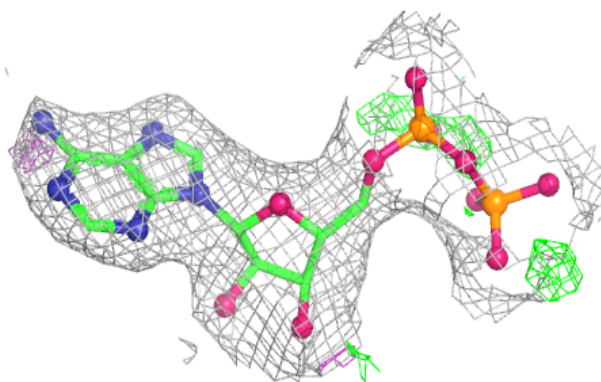
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	AF3	G	602	4/4	1.00	0.02	2,2,7,9	0

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.

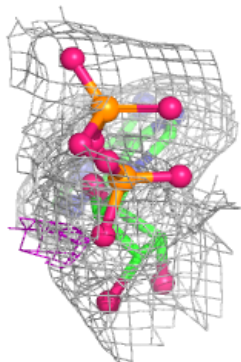
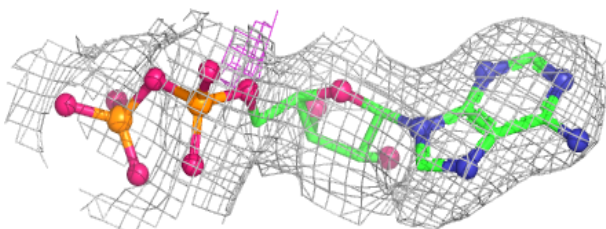
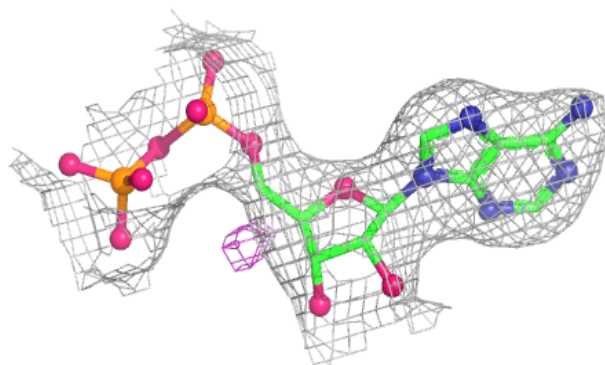


Electron density around ADP A 600:

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

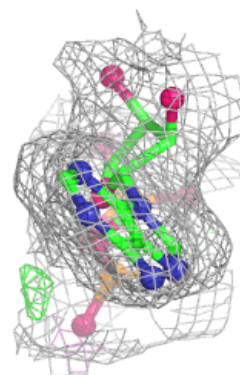
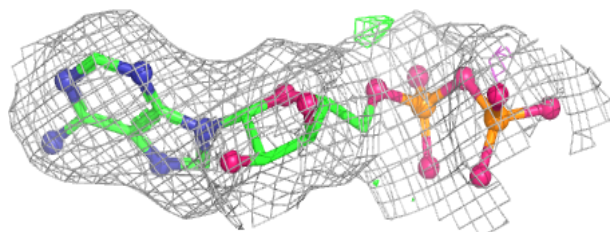
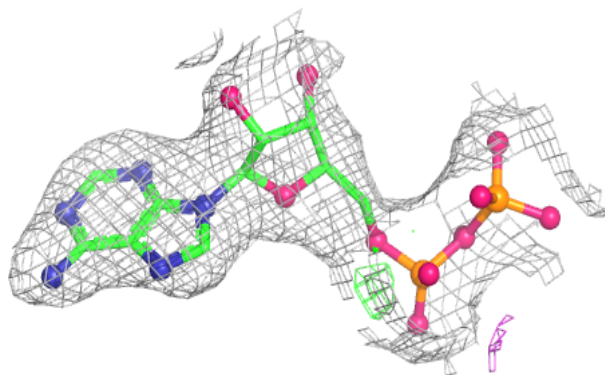
**Electron density around ADP B 600:**

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

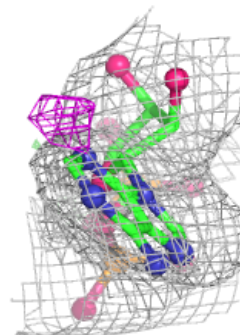
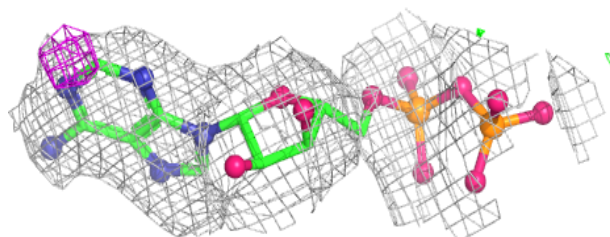
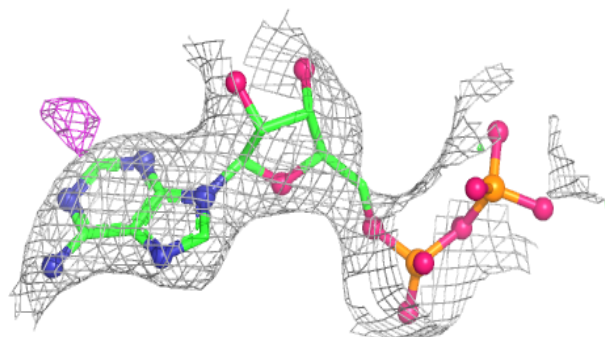


Electron density around ADP D 600:

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

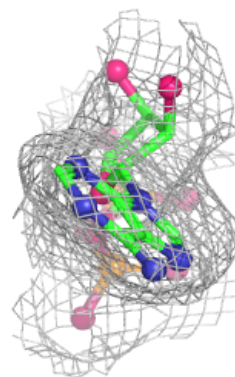
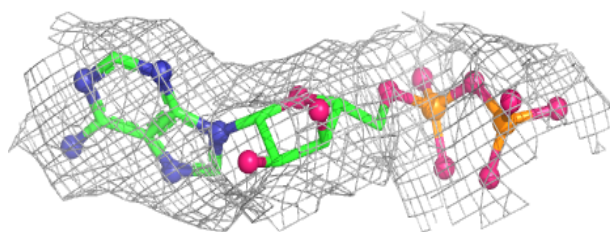
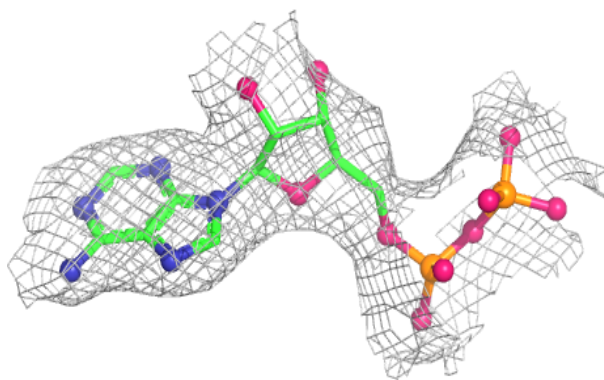
**Electron density around ADP E 600:**

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

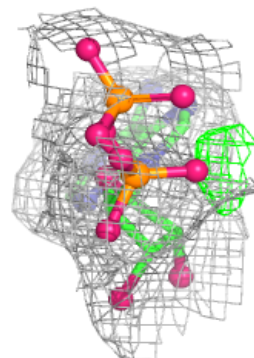
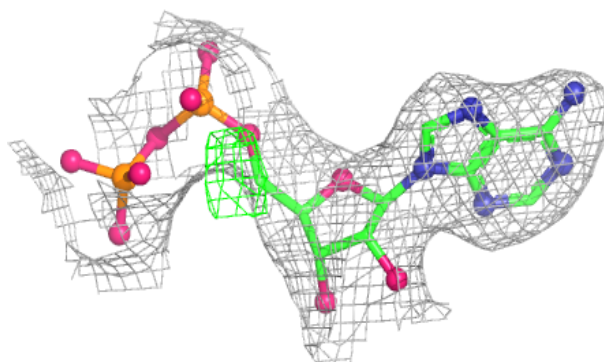


Electron density around ADP F 600:

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

**Electron density around ADP 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.