Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 10:27 AM EST

PDB ID	:	1AQF
Title	:	PYRUVATE KINASE FROM RABBIT MUSCLE WITH MG, K, AND L-PHOSPHOLACTATE
Authors	:	Larsen, T.M.; Benning, M.M.; Wesenberg, G.E.; Rayment, I.; Reed, G.H.
Deposited on	:	1997-07-29
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

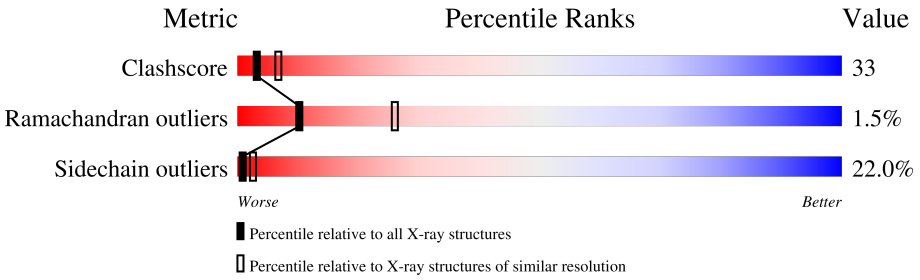
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	37% 47% 13%
1	B	530	33% 45% 18%
1	C	530	47% 40% 10%
1	D	530	42% 41% 14%
1	E	530	31% 34% 13% 20%
1	F	530	42% 39% 16%
1	G	530	32% 43% 22%
1	H	530	31% 45% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEQ	B	532	-	-	X	-
4	PEQ	F	532	-	-	X	-
4	PEQ	H	532	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31410 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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3979	2498	708	745	28			
1	B	519	Total	C	N	O	S	0	0	0
			3979	2498	708	745	28			
1	C	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	D	519	Total	C	N	O	S	0	0	0
			3979	2498	708	745	28			
1	E	426	Total	C	N	O	S	0	0	0
			3268	2045	592	606	25			
1	F	519	Total	C	N	O	S	0	0	0
			3979	2498	708	745	28			
1	G	519	Total	C	N	O	S	0	0	0
			3979	2498	708	745	28			
1	H	519	Total	C	N	O	S	0	0	0
			3979	2498	708	745	28			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		
2	F	1	Total	K	0	0
			1	1		

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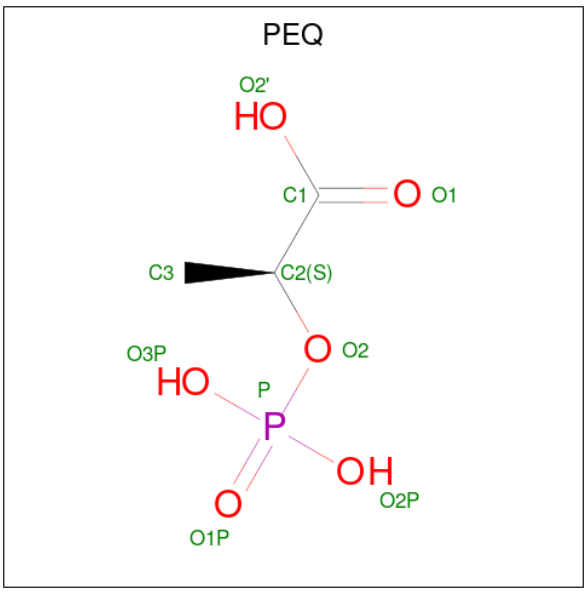
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is L-PHOSPHOLACTATE (three-letter code: PEQ) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		
4	B	1	Total	C	O	P	0	0
			10	3	6	1		
4	C	1	Total	C	O	P	0	0
			10	3	6	1		
4	D	1	Total	C	O	P	0	0
			10	3	6	1		
4	E	1	Total	C	O	P	0	0
			10	3	6	1		
4	F	1	Total	C	O	P	0	0
			10	3	6	1		
4	G	1	Total	C	O	P	0	0
			10	3	6	1		
4	H	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	25	Total	O	0	0
			25	25		
5	C	35	Total	O	0	0
			35	35		
5	D	35	Total	O	0	0
			35	35		
5	E	16	Total	O	0	0
			16	16		
5	F	18	Total	O	0	0
			18	18		
5	G	14	Total	O	0	0
			14	14		
5	H	15	Total	O	0	0
			15	15		

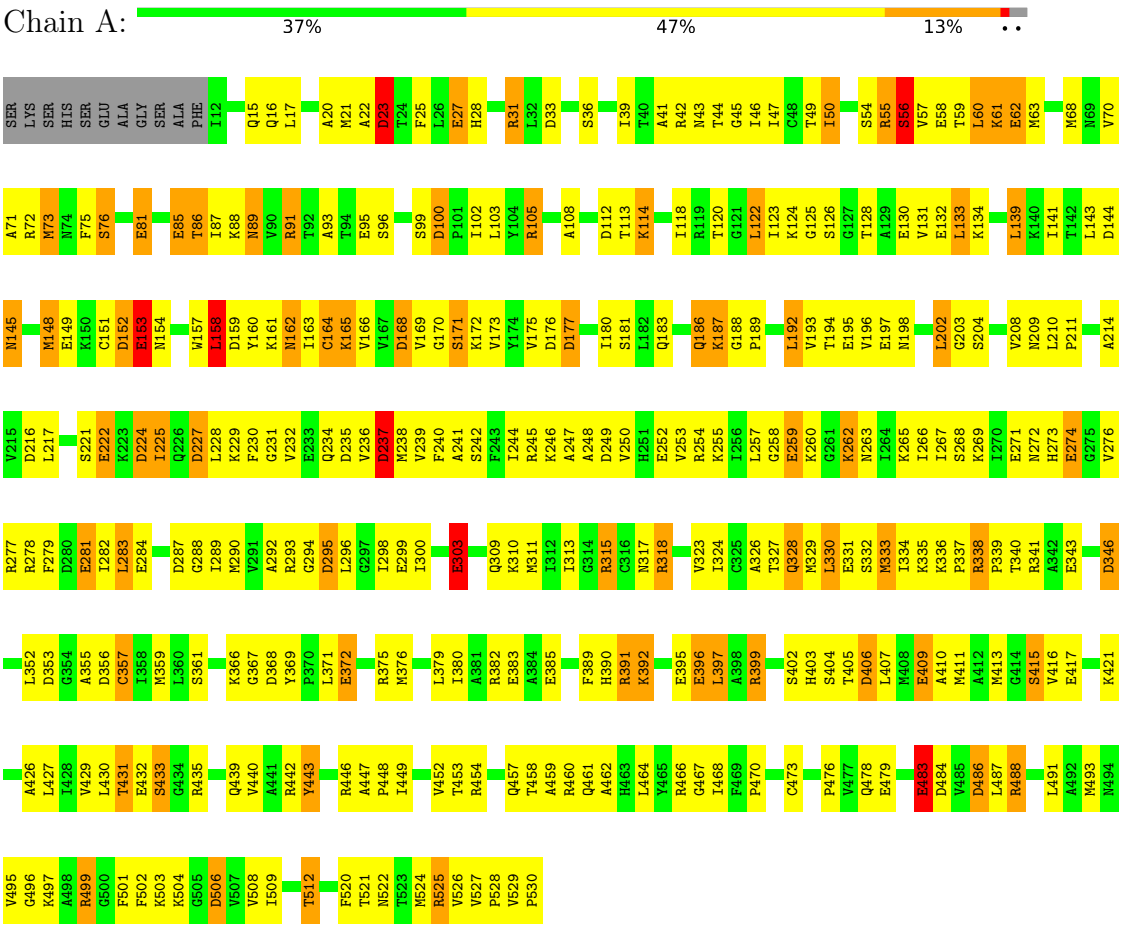
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

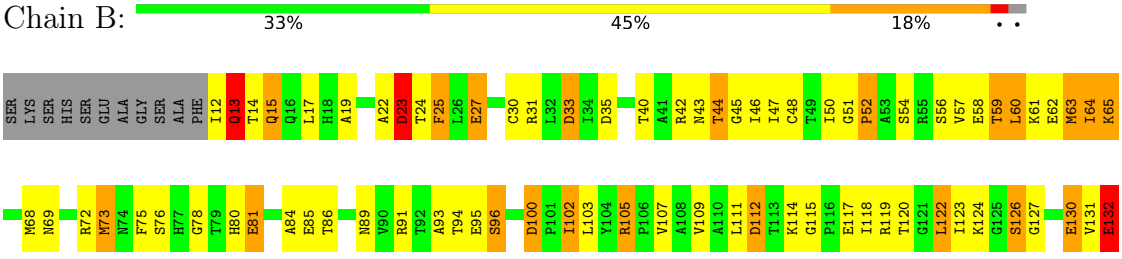
• Molecule 1: PYRUVATE KINASE

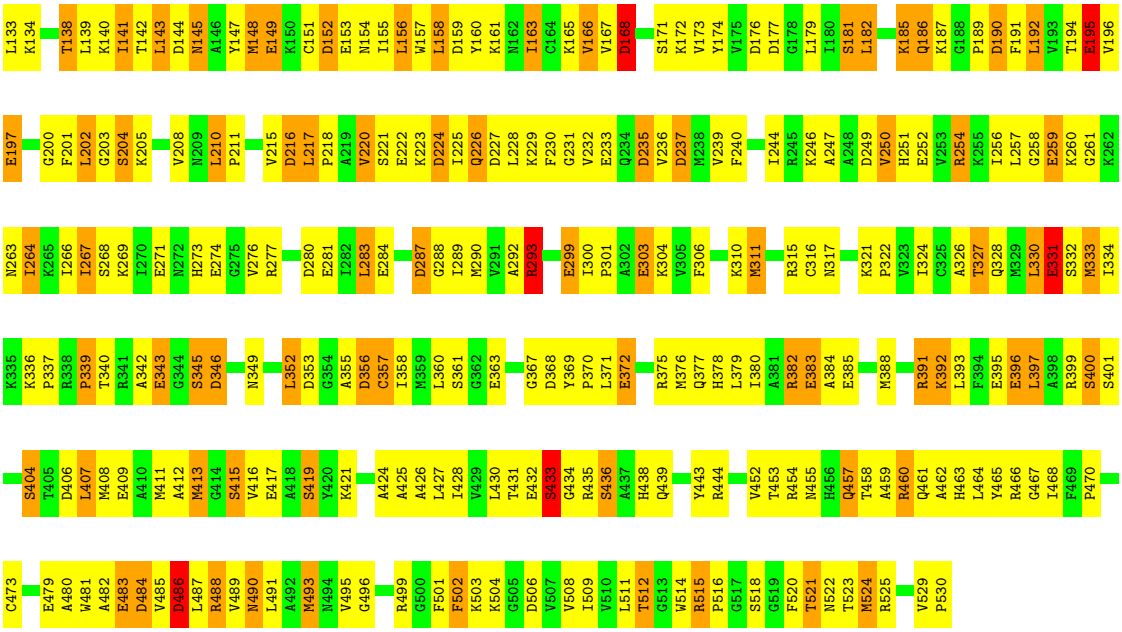
Chain A:



• Molecule 1: PYRUVATE KINASE

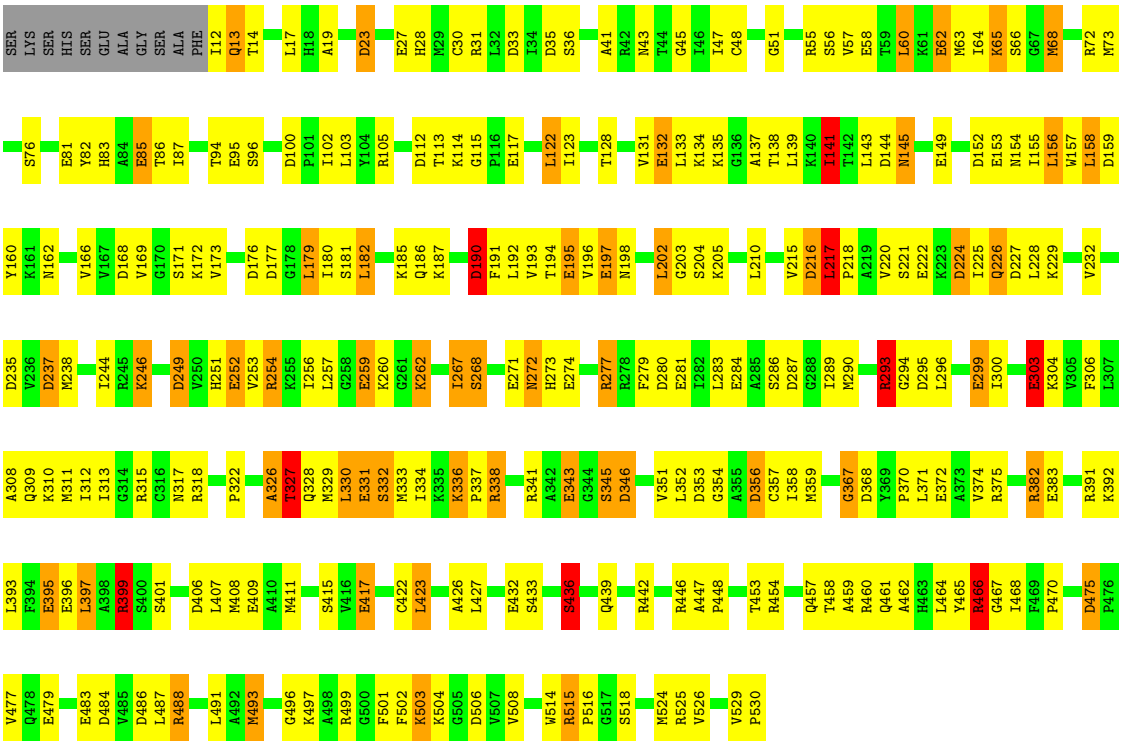
Chain B:





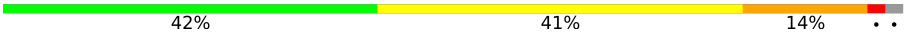
• Molecule 1: PYRUVATE KINASE

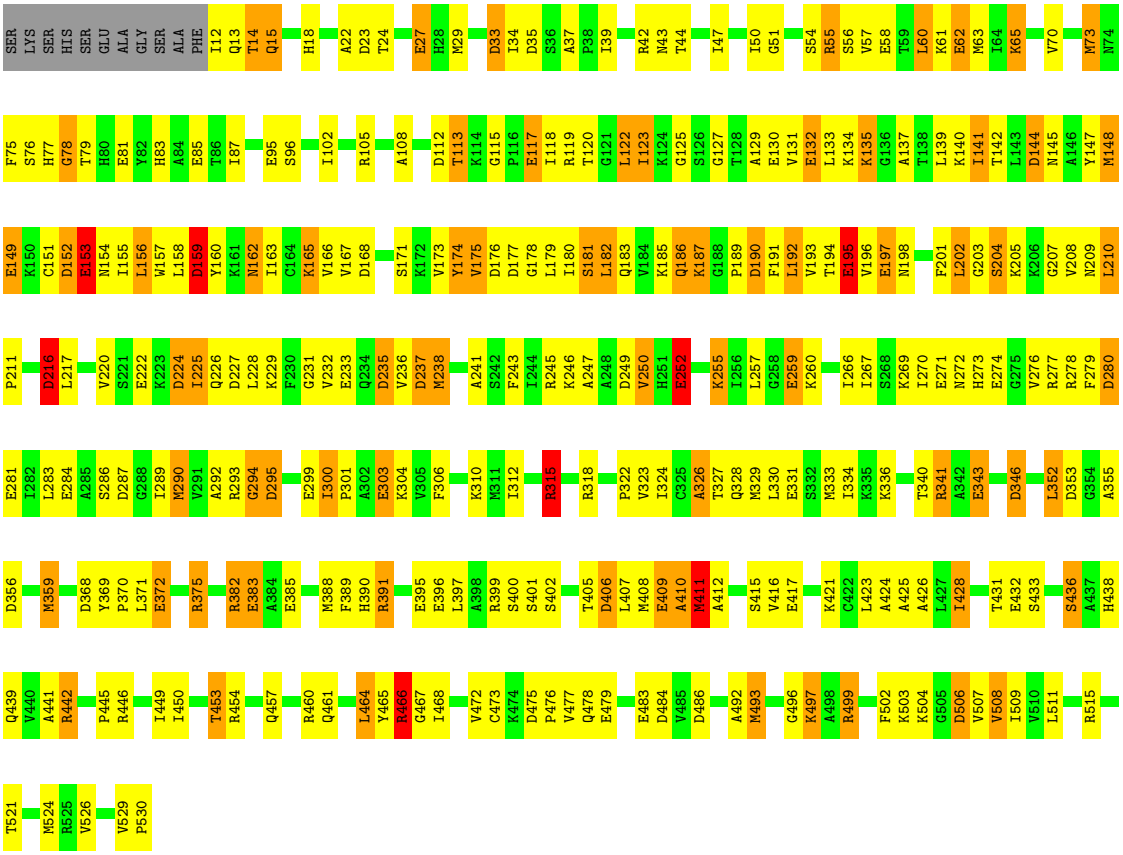
Chain C:



• Molecule 1: PYRUVATE KINASE

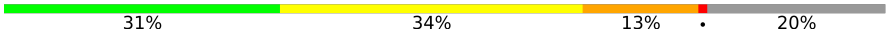
Chain D:

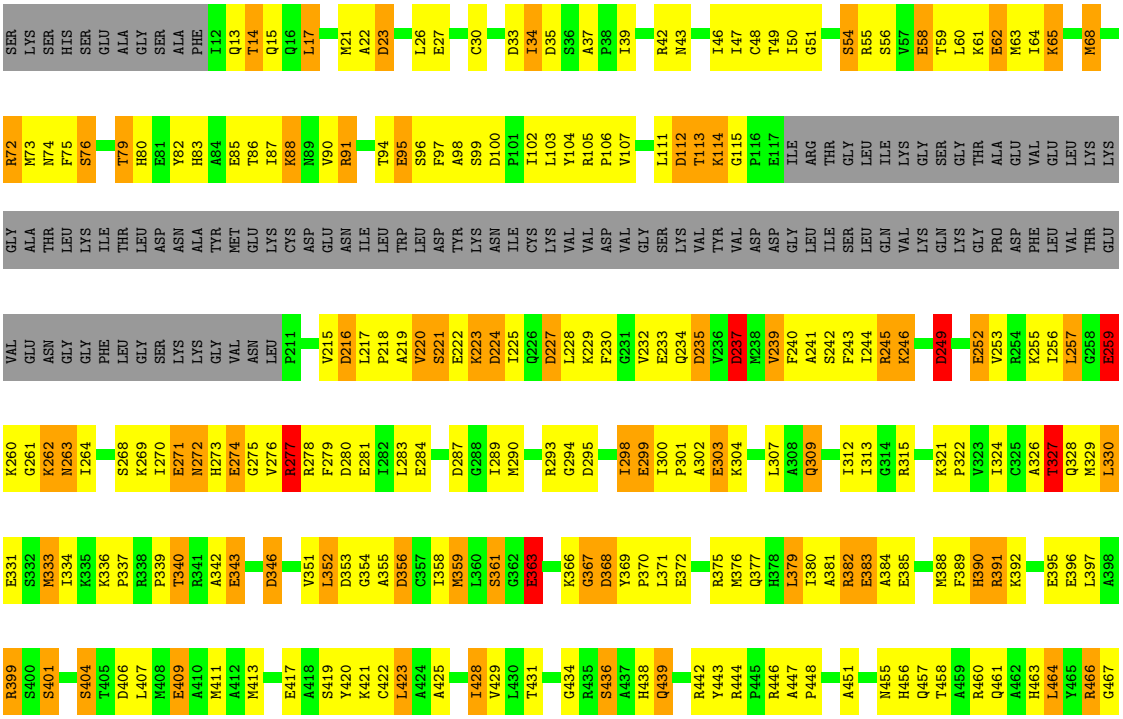


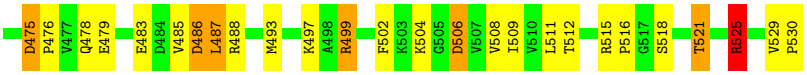


• Molecule 1: PYRUVATE KINASE

Chain E:

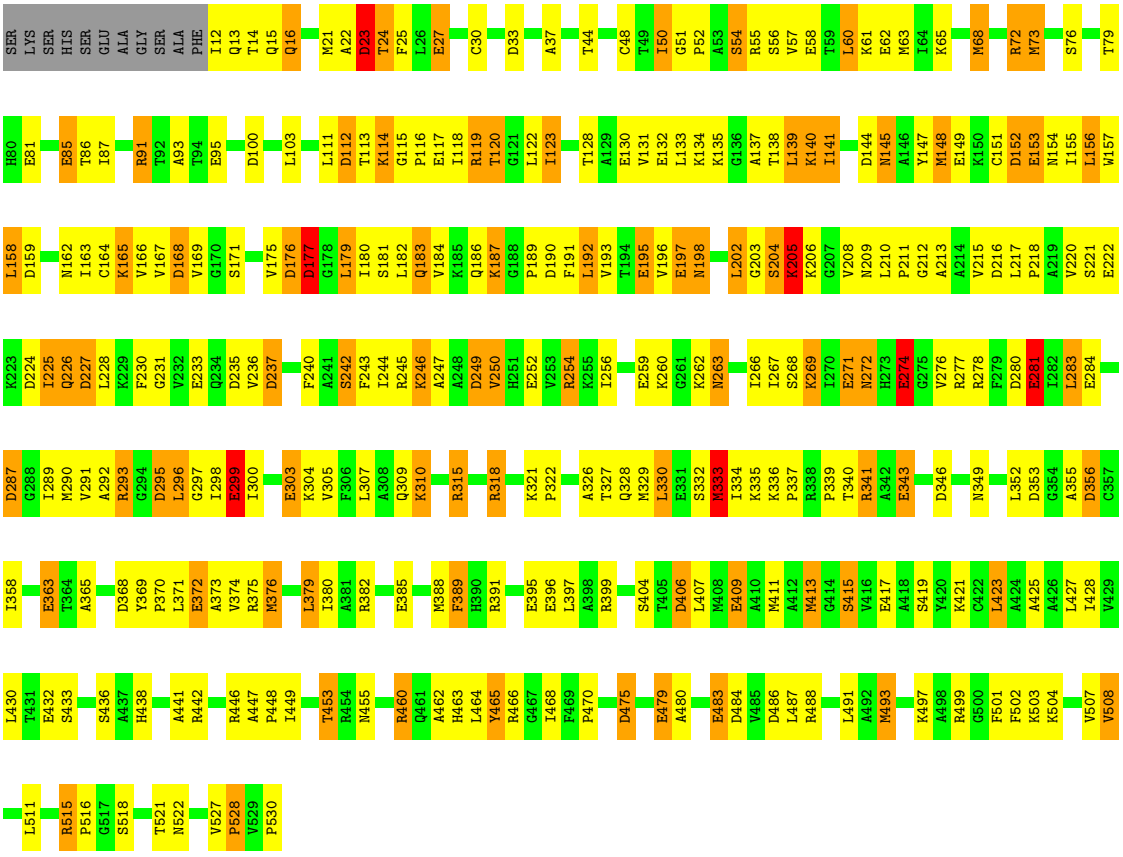






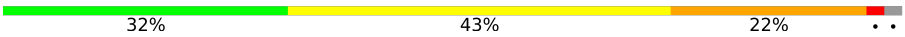
• Molecule 1: PYRUVATE KINASE

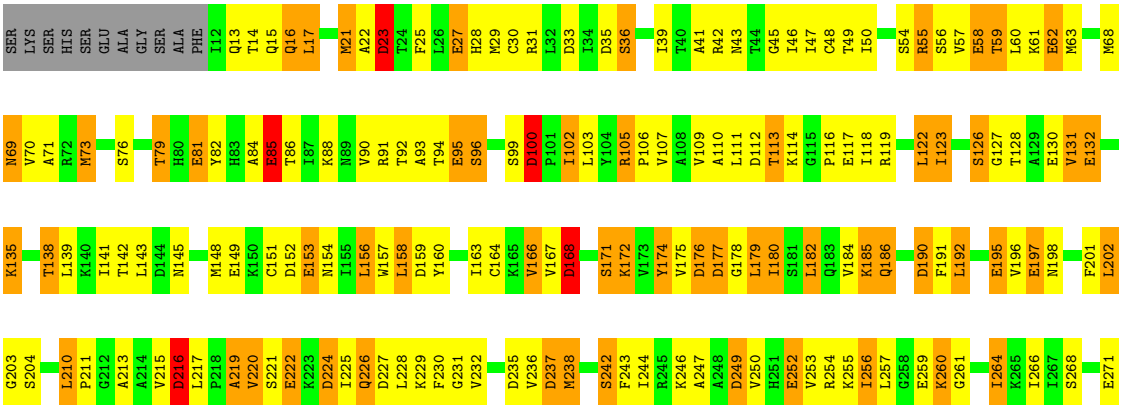
Chain F:

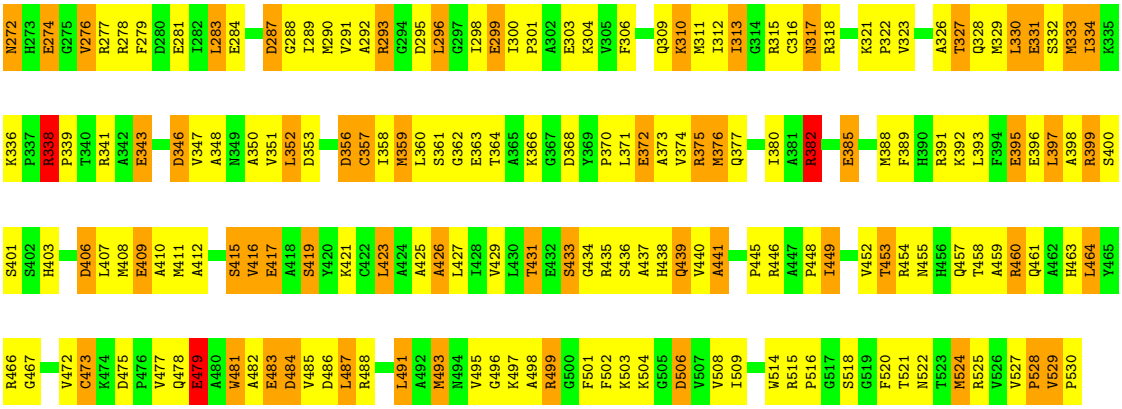


• Molecule 1: PYRUVATE KINASE

Chain G:

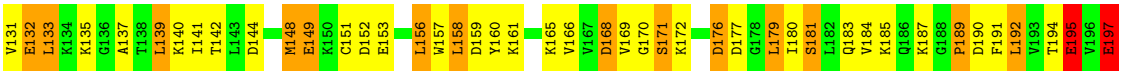


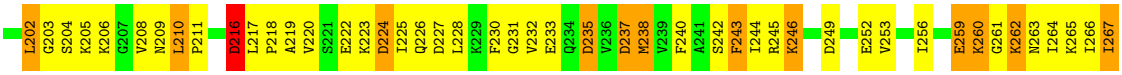


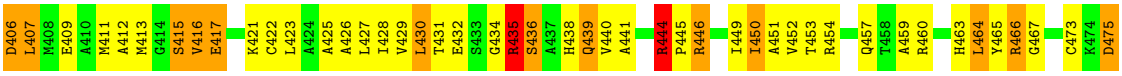


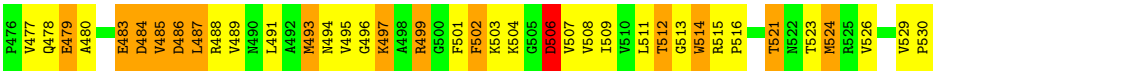
• Molecule 1: PYRUVATE KINASE

Chain H:









4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.40Å 112.60Å 171.20Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	93.0 (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31410	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.03	27/4042 (0.7%)	1.40	54/5452 (1.0%)
1	B	1.06	34/4042 (0.8%)	1.43	55/5452 (1.0%)
1	C	1.05	26/4041 (0.6%)	1.45	62/5452 (1.1%)
1	D	1.03	30/4042 (0.7%)	1.39	56/5452 (1.0%)
1	E	1.02	25/3322 (0.8%)	1.39	42/4482 (0.9%)
1	F	1.02	31/4042 (0.8%)	1.40	59/5452 (1.1%)
1	G	1.01	29/4042 (0.7%)	1.44	56/5452 (1.0%)
1	H	1.03	31/4042 (0.8%)	1.44	56/5452 (1.0%)
All	All	1.03	233/31615 (0.7%)	1.42	440/42646 (1.0%)

All (233) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	395	GLU	CD-OE1	9.26	1.35	1.25
1	F	372	GLU	CD-OE1	8.74	1.35	1.25
1	C	395	GLU	CD-OE1	8.68	1.35	1.25
1	B	396	GLU	CD-OE1	8.28	1.34	1.25
1	A	395	GLU	CD-OE1	8.23	1.34	1.25
1	H	117	GLU	CD-OE1	7.83	1.34	1.25
1	D	372	GLU	CD-OE1	7.55	1.33	1.25
1	B	274	GLU	CD-OE1	7.54	1.33	1.25
1	B	433	SER	CB-OG	7.48	1.51	1.42
1	B	432	GLU	CD-OE1	7.34	1.33	1.25
1	A	372	GLU	CD-OE1	7.29	1.33	1.25
1	F	395	GLU	CD-OE1	7.29	1.33	1.25
1	G	252	GLU	CD-OE2	7.24	1.33	1.25
1	A	396	GLU	CD-OE1	7.24	1.33	1.25
1	H	479	GLU	CD-OE1	7.12	1.33	1.25
1	E	396	GLU	CD-OE1	7.12	1.33	1.25
1	G	130	GLU	CD-OE1	7.07	1.33	1.25
1	C	58	GLU	CD-OE1	7.00	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	GLU	CD-OE1	6.99	1.33	1.25
1	C	372	GLU	CD-OE1	6.99	1.33	1.25
1	A	483	GLU	CD-OE1	6.96	1.33	1.25
1	C	331	GLU	CD-OE2	6.91	1.33	1.25
1	E	271	GLU	CD-OE2	6.89	1.33	1.25
1	G	222	GLU	CD-OE2	6.88	1.33	1.25
1	E	299	GLU	CD-OE1	6.88	1.33	1.25
1	C	271	GLU	CD-OE2	6.87	1.33	1.25
1	H	483	GLU	CD-OE1	6.85	1.33	1.25
1	H	372	GLU	CD-OE1	6.84	1.33	1.25
1	A	383	GLU	CD-OE1	6.82	1.33	1.25
1	F	483	GLU	CD-OE1	6.80	1.33	1.25
1	H	58	GLU	CD-OE2	6.79	1.33	1.25
1	C	252	GLU	CD-OE2	6.74	1.33	1.25
1	H	396	GLU	CD-OE1	6.72	1.33	1.25
1	H	222	GLU	CD-OE2	6.71	1.33	1.25
1	F	195	GLU	CD-OE2	6.71	1.33	1.25
1	F	303	GLU	CD-OE2	6.71	1.33	1.25
1	E	383	GLU	CD-OE1	6.68	1.32	1.25
1	C	222	GLU	CD-OE2	6.67	1.32	1.25
1	C	409	GLU	CD-OE2	6.67	1.32	1.25
1	E	259	GLU	CD-OE2	6.62	1.32	1.25
1	D	195	GLU	CD-OE2	6.60	1.32	1.25
1	H	284	GLU	CD-OE2	6.59	1.32	1.25
1	E	343	GLU	CD-OE2	6.57	1.32	1.25
1	B	222	GLU	CD-OE2	6.55	1.32	1.25
1	H	274	GLU	CD-OE1	6.55	1.32	1.25
1	F	432	GLU	CD-OE1	6.54	1.32	1.25
1	B	363	GLU	CD-OE1	6.53	1.32	1.25
1	F	409	GLU	CD-OE2	6.52	1.32	1.25
1	F	396	GLU	CD-OE1	6.52	1.32	1.25
1	B	331	GLU	CD-OE1	6.48	1.32	1.25
1	B	58	GLU	CD-OE1	6.47	1.32	1.25
1	D	233	GLU	CD-OE2	6.47	1.32	1.25
1	F	222	GLU	CD-OE2	6.46	1.32	1.25
1	B	95	GLU	CD-OE1	6.46	1.32	1.25
1	A	299	GLU	CD-OE1	6.44	1.32	1.25
1	G	274	GLU	CD-OE1	6.44	1.32	1.25
1	H	299	GLU	CD-OE1	6.37	1.32	1.25
1	D	117	GLU	CD-OE2	6.37	1.32	1.25
1	A	95	GLU	CD-OE1	6.36	1.32	1.25
1	D	58	GLU	CD-OE1	6.35	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	GLU	CD-OE2	6.33	1.32	1.25
1	C	85	GLU	CD-OE1	6.33	1.32	1.25
1	A	58	GLU	CD-OE1	6.29	1.32	1.25
1	C	149	GLU	CD-OE1	6.24	1.32	1.25
1	F	259	GLU	CD-OE1	6.24	1.32	1.25
1	H	81	GLU	CD-OE2	6.23	1.32	1.25
1	F	479	GLU	CD-OE2	6.23	1.32	1.25
1	D	281	GLU	CD-OE1	6.16	1.32	1.25
1	C	95	GLU	CD-OE1	6.16	1.32	1.25
1	D	62	GLU	CD-OE1	6.15	1.32	1.25
1	E	222	GLU	CD-OE2	6.15	1.32	1.25
1	H	195	GLU	CD-OE2	6.15	1.32	1.25
1	G	58	GLU	CD-OE2	6.15	1.32	1.25
1	H	85	GLU	CD-OE1	6.15	1.32	1.25
1	D	95	GLU	CD-OE1	6.14	1.32	1.25
1	B	81	GLU	CD-OE1	6.13	1.32	1.25
1	H	331	GLU	CD-OE1	6.12	1.32	1.25
1	E	483	GLU	CD-OE1	6.11	1.32	1.25
1	H	303	GLU	CD-OE2	6.11	1.32	1.25
1	B	479	GLU	CD-OE2	6.11	1.32	1.25
1	C	117	GLU	CD-OE1	6.11	1.32	1.25
1	D	432	GLU	CD-OE1	6.11	1.32	1.25
1	C	432	GLU	CD-OE1	6.09	1.32	1.25
1	F	62	GLU	CD-OE1	6.09	1.32	1.25
1	E	395	GLU	CD-OE1	6.09	1.32	1.25
1	G	95	GLU	CD-OE1	6.09	1.32	1.25
1	A	331	GLU	CD-OE1	6.08	1.32	1.25
1	F	274	GLU	CD-OE1	6.08	1.32	1.25
1	D	331	GLU	CD-OE1	6.07	1.32	1.25
1	B	130	GLU	CD-OE1	6.04	1.32	1.25
1	G	81	GLU	CD-OE2	6.02	1.32	1.25
1	F	281	GLU	CD-OE1	6.01	1.32	1.25
1	B	483	GLU	CD-OE1	6.00	1.32	1.25
1	B	233	GLU	CD-OE2	5.99	1.32	1.25
1	A	62	GLU	CD-OE1	5.99	1.32	1.25
1	B	303	GLU	CD-OE2	5.99	1.32	1.25
1	F	85	GLU	CD-OE1	5.99	1.32	1.25
1	G	479	GLU	CD-OE1	5.98	1.32	1.25
1	G	372	GLU	CD-OE1	5.98	1.32	1.25
1	D	343	GLU	CD-OE2	5.97	1.32	1.25
1	A	284	GLU	CD-OE2	5.97	1.32	1.25
1	C	284	GLU	CD-OE2	5.95	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	372	GLU	CD-OE1	5.95	1.32	1.25
1	A	153	GLU	CD-OE1	5.95	1.32	1.25
1	H	252	GLU	CD-OE2	5.95	1.32	1.25
1	D	130	GLU	CD-OE2	5.95	1.32	1.25
1	F	299	GLU	CD-OE1	5.94	1.32	1.25
1	H	383	GLU	CD-OE2	5.94	1.32	1.25
1	C	281	GLU	CD-OE1	5.94	1.32	1.25
1	H	149	GLU	CD-OE1	5.94	1.32	1.25
1	G	385	GLU	CD-OE1	5.94	1.32	1.25
1	D	479	GLU	CD-OE1	5.90	1.32	1.25
1	H	259	GLU	CD-OE1	5.89	1.32	1.25
1	G	299	GLU	CD-OE1	5.89	1.32	1.25
1	G	331	GLU	CD-OE1	5.88	1.32	1.25
1	C	274	GLU	CD-OE1	5.87	1.32	1.25
1	G	395	GLU	CD-OE1	5.87	1.32	1.25
1	G	27	GLU	CD-OE1	5.86	1.32	1.25
1	G	153	GLU	CD-OE1	5.86	1.32	1.25
1	E	479	GLU	CD-OE1	5.86	1.32	1.25
1	E	62	GLU	CD-OE1	5.85	1.32	1.25
1	F	271	GLU	CD-OE1	5.85	1.32	1.25
1	D	27	GLU	CD-OE1	5.85	1.32	1.25
1	G	259	GLU	CD-OE1	5.84	1.32	1.25
1	E	385	GLU	CD-OE1	5.84	1.32	1.25
1	F	284	GLU	CD-OE1	5.84	1.32	1.25
1	D	222	GLU	CD-OE2	5.83	1.32	1.25
1	E	95	GLU	CD-OE1	5.83	1.32	1.25
1	A	274	GLU	CD-OE1	5.82	1.32	1.25
1	D	81	GLU	CD-OE1	5.81	1.32	1.25
1	D	395	GLU	CD-OE1	5.80	1.32	1.25
1	G	284	GLU	CD-OE1	5.79	1.32	1.25
1	C	81	GLU	CD-OE1	5.79	1.32	1.25
1	C	343	GLU	CD-OE2	5.79	1.32	1.25
1	D	385	GLU	CD-OE1	5.79	1.32	1.25
1	F	132	GLU	CD-OE1	5.78	1.32	1.25
1	A	195	GLU	CD-OE2	5.77	1.32	1.25
1	C	479	GLU	CD-OE1	5.77	1.31	1.25
1	F	153	GLU	CD-OE1	5.77	1.31	1.25
1	B	195	GLU	CD-OE2	5.76	1.31	1.25
1	B	409	GLU	CD-OE2	5.75	1.31	1.25
1	B	85	GLU	CD-OE1	5.75	1.31	1.25
1	E	58	GLU	CD-OE1	5.75	1.31	1.25
1	G	149	GLU	CD-OE1	5.75	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	483	GLU	CD-OE1	5.74	1.31	1.25
1	H	197	GLU	CD-OE1	5.74	1.31	1.25
1	A	409	GLU	CD-OE2	5.73	1.31	1.25
1	A	252	GLU	CD-OE1	5.73	1.31	1.25
1	E	363	GLU	CD-OE1	5.71	1.31	1.25
1	E	409	GLU	CD-OE2	5.71	1.31	1.25
1	B	395	GLU	CD-OE1	5.71	1.31	1.25
1	H	385	GLU	CD-OE1	5.71	1.31	1.25
1	B	271	GLU	CD-OE2	5.70	1.31	1.25
1	E	274	GLU	CD-OE1	5.70	1.31	1.25
1	C	197	GLU	CD-OE1	5.70	1.31	1.25
1	A	259	GLU	CD-OE1	5.68	1.31	1.25
1	B	117	GLU	CD-OE1	5.66	1.31	1.25
1	B	149	GLU	CD-OE1	5.66	1.31	1.25
1	B	299	GLU	CD-OE1	5.65	1.31	1.25
1	A	85	GLU	CD-OE1	5.65	1.31	1.25
1	F	27	GLU	CD-OE1	5.65	1.31	1.25
1	D	396	GLU	CD-OE1	5.64	1.31	1.25
1	F	81	GLU	CD-OE2	5.63	1.31	1.25
1	A	479	GLU	CD-OE2	5.63	1.31	1.25
1	D	85	GLU	CD-OE1	5.62	1.31	1.25
1	E	281	GLU	CD-OE1	5.62	1.31	1.25
1	A	81	GLU	CD-OE2	5.62	1.31	1.25
1	F	197	GLU	CD-OE1	5.59	1.31	1.25
1	D	274	GLU	CD-OE1	5.59	1.31	1.25
1	H	132	GLU	CD-OE1	5.58	1.31	1.25
1	E	252	GLU	CD-OE2	5.58	1.31	1.25
1	G	409	GLU	CD-OE1	5.57	1.31	1.25
1	B	284	GLU	CD-OE1	5.57	1.31	1.25
1	G	132	GLU	CD-OE1	5.54	1.31	1.25
1	G	281	GLU	CD-OE1	5.52	1.31	1.25
1	F	363	GLU	CD-OE1	5.49	1.31	1.25
1	B	259	GLU	CD-OE1	5.48	1.31	1.25
1	D	259	GLU	CD-OE1	5.48	1.31	1.25
1	G	343	GLU	CD-OE2	5.48	1.31	1.25
1	H	417	GLU	CD-OE1	5.47	1.31	1.25
1	H	233	GLU	CD-OE2	5.46	1.31	1.25
1	F	417	GLU	CD-OE1	5.45	1.31	1.25
1	B	132	GLU	CD-OE1	5.44	1.31	1.25
1	F	58	GLU	CD-OE1	5.44	1.31	1.25
1	G	195	GLU	CD-OE2	5.42	1.31	1.25
1	A	385	GLU	CD-OE1	5.42	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	303	GLU	CD-OE2	5.42	1.31	1.25
1	G	483	GLU	CD-OE1	5.42	1.31	1.25
1	A	222	GLU	CD-OE1	5.41	1.31	1.25
1	F	117	GLU	CD-OE1	5.40	1.31	1.25
1	D	409	GLU	CD-OE2	5.40	1.31	1.25
1	C	62	GLU	CD-OE1	5.39	1.31	1.25
1	H	153	GLU	CD-OE1	5.39	1.31	1.25
1	F	130	GLU	CD-OE1	5.38	1.31	1.25
1	D	153	GLU	CD-OE2	5.38	1.31	1.25
1	F	95	GLU	CD-OE1	5.36	1.31	1.25
1	F	385	GLU	CD-OE1	5.35	1.31	1.25
1	B	281	GLU	CD-OE1	5.34	1.31	1.25
1	A	432	GLU	CD-OE1	5.31	1.31	1.25
1	C	259	GLU	CD-OE1	5.31	1.31	1.25
1	H	271	GLU	CD-OE2	5.30	1.31	1.25
1	E	331	GLU	CD-OE1	5.29	1.31	1.25
1	D	197	GLU	CD-OE1	5.29	1.31	1.25
1	B	197	GLU	CD-OE1	5.28	1.31	1.25
1	B	62	GLU	CD-OE1	5.27	1.31	1.25
1	H	281	GLU	CD-OE1	5.26	1.31	1.25
1	F	252	GLU	CD-OE1	5.25	1.31	1.25
1	A	130	GLU	CD-OE2	5.24	1.31	1.25
1	D	383	GLU	CD-OE1	5.23	1.31	1.25
1	C	132	GLU	CD-OE1	5.22	1.31	1.25
1	G	271	GLU	CD-OE1	5.22	1.31	1.25
1	G	62	GLU	CD-OE1	5.21	1.31	1.25
1	A	303	GLU	CD-OE2	5.21	1.31	1.25
1	G	85	GLU	CD-OE1	5.20	1.31	1.25
1	H	343	GLU	CD-OE2	5.18	1.31	1.25
1	D	252	GLU	CD-OE2	5.18	1.31	1.25
1	D	284	GLU	CD-OE2	5.17	1.31	1.25
1	C	195	GLU	CD-OE2	5.16	1.31	1.25
1	H	27	GLU	CD-OE1	5.13	1.31	1.25
1	B	383	GLU	CD-OE2	5.13	1.31	1.25
1	A	281	GLU	CD-OE1	5.13	1.31	1.25
1	B	343	GLU	CD-OE2	5.12	1.31	1.25
1	C	303	GLU	CD-OE2	5.12	1.31	1.25
1	A	385	GLU	CD-OE2	-5.11	1.20	1.25
1	E	85	GLU	CD-OE1	5.11	1.31	1.25
1	E	383	GLU	CD-OE2	-5.09	1.20	1.25
1	D	483	GLU	CD-OE1	5.08	1.31	1.25
1	G	417	GLU	CD-OE1	5.08	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	514	TRP	NE1-CE2	-5.07	1.30	1.37
1	D	132	GLU	CD-OE1	5.06	1.31	1.25
1	H	130	GLU	CD-OE1	5.05	1.31	1.25
1	E	417	GLU	CD-OE1	5.04	1.31	1.25
1	B	385	GLU	CD-OE2	-5.03	1.20	1.25

All (440) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	293	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	H	42	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	E	112	ASP	CB-CG-OD2	9.57	126.92	118.30
1	D	295	ASP	CB-CG-OD2	9.49	126.84	118.30
1	A	188	GLY	C-N-CD	-9.36	100.01	120.60
1	B	237	ASP	CB-CG-OD1	-9.15	110.07	118.30
1	C	168	ASP	CB-CG-OD2	-8.97	110.22	118.30
1	C	346	ASP	CB-CG-OD1	-8.86	110.32	118.30
1	E	391	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	488	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	G	382	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	B	249	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	B	488	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	H	168	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	E	346	ASP	CB-CG-OD1	-8.54	110.61	118.30
1	A	100	ASP	CB-CG-OD1	-8.54	110.62	118.30
1	C	168	ASP	CB-CG-OD1	8.47	125.92	118.30
1	H	318	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	D	295	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	F	237	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	C	249	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	B	177	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	D	391	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	C	391	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	E	488	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	A	356	ASP	CB-CG-OD1	-8.08	111.03	118.30
1	A	499	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	G	112	ASP	CB-CG-OD1	-7.98	111.11	118.30
1	A	488	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	H	227	ASP	CB-CG-OD1	-7.96	111.13	118.30
1	C	112	ASP	CB-CG-OD2	7.93	125.44	118.30
1	H	177	ASP	CB-CG-OD1	7.92	125.43	118.30
1	F	499	ARG	NE-CZ-NH1	7.84	124.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	341	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	G	356	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	G	431	THR	CA-CB-CG2	-7.83	101.44	112.40
1	E	280	ASP	CB-CG-OD1	-7.80	111.28	118.30
1	B	356	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	B	251	HIS	CA-CB-CG	-7.71	100.50	113.60
1	D	466	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	D	353	ASP	CB-CG-OD1	-7.64	111.43	118.30
1	C	488	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	D	33	ASP	CB-CG-OD1	-7.64	111.43	118.30
1	B	168	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	391	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	F	237	ASP	CB-CG-OD1	7.57	125.11	118.30
1	H	168	ASP	CB-CG-OD1	7.56	125.10	118.30
1	G	35	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	H	444	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	F	216	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	D	326	ALA	CB-CA-C	-7.52	98.82	110.10
1	G	176	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	A	144	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	H	237	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	C	499	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	224	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	C	224	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	235	ASP	CB-CG-OD1	-7.46	111.59	118.30
1	F	190	ASP	CB-CG-OD1	7.44	125.00	118.30
1	F	235	ASP	CB-CG-OD1	-7.42	111.62	118.30
1	E	100	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	B	177	ASP	CB-CG-OD1	7.39	124.96	118.30
1	B	249	ASP	CB-CG-OD1	7.38	124.94	118.30
1	H	216	ASP	CB-CG-OD1	-7.36	111.68	118.30
1	D	177	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	368	ASP	CB-CG-OD1	-7.35	111.69	118.30
1	F	235	ASP	CB-CG-OD2	7.33	124.89	118.30
1	G	224	ASP	CB-CG-OD1	-7.33	111.71	118.30
1	C	112	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	H	382	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	C	249	ASP	CB-CG-OD1	7.29	124.86	118.30
1	E	100	ASP	CB-CG-OD2	7.28	124.85	118.30
1	C	280	ASP	CB-CG-OD1	-7.27	111.76	118.30
1	H	119	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	B	444	ARG	NE-CZ-NH1	7.17	123.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	237	ASP	CB-CG-OD1	-7.14	111.87	118.30
1	G	42	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	287	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	D	112	ASP	CB-CG-OD1	-7.11	111.91	118.30
1	H	287	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	C	23	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	H	152	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	G	287	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	H	177	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	F	152	ASP	CB-CG-OD1	7.05	124.64	118.30
1	C	159	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	A	318	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	506	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	B	368	ASP	CB-CG-OD2	7.00	124.60	118.30
1	G	35	ASP	CB-CG-OD2	6.98	124.58	118.30
1	C	177	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	B	105	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	486	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	A	105	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	100	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	H	506	ASP	CB-CG-OD2	6.89	124.50	118.30
1	D	341	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	F	23	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	G	287	ASP	CB-CG-OD1	6.88	124.49	118.30
1	D	177	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	F	144	ASP	CB-CG-OD1	6.85	124.46	118.30
1	H	406	ASP	CB-CG-OD1	-6.82	112.16	118.30
1	F	144	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	H	112	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	H	190	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	216	ASP	CB-CG-OD1	-6.78	112.19	118.30
1	C	346	ASP	CB-CG-OD2	6.77	124.39	118.30
1	G	368	ASP	CB-CG-OD2	6.77	124.39	118.30
1	D	287	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	346	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	F	484	ASP	CB-CG-OD1	-6.74	112.23	118.30
1	F	152	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	C	287	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	119	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	E	525	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	F	356	ASP	CB-CG-OD2	6.65	124.29	118.30
1	G	317	ASN	CB-CA-C	-6.65	97.10	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	144	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	E	227	ASP	CB-CG-OD2	6.64	124.28	118.30
1	E	224	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	F	460	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	H	190	ASP	CB-CG-OD1	6.62	124.26	118.30
1	H	506	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	C	295	ASP	CB-CG-OD1	-6.59	112.36	118.30
1	E	488	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	406	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	D	190	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	G	318	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	237	ASP	CB-CG-OD2	6.57	124.21	118.30
1	D	315	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	E	112	ASP	CB-CG-OD1	-6.56	112.40	118.30
1	D	168	ASP	CB-CG-OD1	6.53	124.18	118.30
1	G	176	ASP	CB-CG-OD2	6.53	124.17	118.30
1	C	356	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	E	346	ASP	CB-CG-OD2	6.51	124.16	118.30
1	G	190	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	144	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	475	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	23	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	168	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	224	ASP	CB-CG-OD2	6.48	124.13	118.30
1	G	235	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	F	190	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	B	216	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	B	506	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	E	23	ASP	CB-CG-OD2	6.46	124.12	118.30
1	A	356	ASP	CB-CG-OD2	6.45	124.11	118.30
1	G	100	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	C	35	ASP	CB-CG-OD2	6.43	124.08	118.30
1	C	235	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	235	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	E	216	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	H	224	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	C	190	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	D	23	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	25	PHE	CB-CG-CD2	6.38	125.27	120.80
1	G	23	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	D	152	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	F	374	VAL	CA-CB-CG1	-6.37	101.35	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	295	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	287	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	295	ASP	CB-CG-OD2	6.35	124.02	118.30
1	C	100	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	H	235	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	G	460	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	H	72	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	33	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	G	506	ASP	CB-CG-OD2	6.32	123.99	118.30
1	F	159	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	33	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	A	506	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	E	33	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	G	249	ASP	CB-CG-OD1	6.28	123.95	118.30
1	E	235	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	C	177	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	287	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	33	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	B	126	SER	N-CA-CB	6.26	119.90	110.50
1	F	227	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	B	159	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	H	176	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	E	227	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	D	144	ASP	CB-CG-OD1	6.23	123.90	118.30
1	A	525	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	E	406	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	C	159	ASP	CB-CG-OD1	6.20	123.88	118.30
1	G	235	ASP	CB-CG-OD2	6.20	123.88	118.30
1	G	368	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	H	227	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	506	ASP	CB-CG-OD2	6.17	123.85	118.30
1	C	100	ASP	CB-CG-OD2	6.17	123.85	118.30
1	E	280	ASP	CB-CG-OD2	6.16	123.84	118.30
1	C	144	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	190	ASP	CB-CG-OD1	6.14	123.83	118.30
1	G	119	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	227	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	C	466	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	G	406	ASP	CB-CG-OD1	-6.11	112.81	118.30
1	F	295	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	A	216	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	318	ARG	NE-CZ-NH2	-6.09	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	249	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	177	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	235	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	224	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	506	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	F	295	ASP	CB-CG-OD2	6.05	123.75	118.30
1	F	406	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	G	23	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	216	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	C	144	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	152	ASP	CB-CG-OD1	6.02	123.72	118.30
1	E	442	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	F	176	ASP	CB-CG-OD1	-6.02	112.89	118.30
1	H	152	ASP	CB-CG-OD1	6.01	123.71	118.30
1	G	227	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	H	235	ASP	CB-CG-OD2	6.01	123.71	118.30
1	C	406	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	G	159	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	159	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	F	177	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	177	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	23	ASP	CB-CG-OD1	5.99	123.69	118.30
1	E	420	TYR	CA-CB-CG	5.99	124.78	113.40
1	H	391	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	227	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	A	382	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	D	42	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	224	ASP	CB-CG-OD2	5.95	123.66	118.30
1	D	353	ASP	CB-CG-OD2	5.95	123.66	118.30
1	F	33	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	C	368	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	338	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	144	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	356	ASP	CB-CG-OD2	5.93	123.63	118.30
1	B	152	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	466	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	E	287	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	E	428	ILE	CB-CA-C	-5.87	99.86	111.60
1	E	486	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	D	506	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	227	ASP	CB-CG-OD2	5.86	123.57	118.30
1	E	35	ASP	CB-CG-OD2	5.85	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	216	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	235	ASP	CB-CG-OD2	5.83	123.55	118.30
1	H	356	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	F	356	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	B	346	ASP	CB-CG-OD2	5.80	123.52	118.30
1	F	23	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	168	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	287	ASP	CB-CG-OD1	5.78	123.50	118.30
1	F	484	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	249	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	F	280	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	368	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	431	THR	CA-CB-CG2	-5.76	104.34	112.40
1	E	237	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	H	295	ASP	CB-CG-OD2	5.76	123.48	118.30
1	F	91	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	C	436	SER	CB-CA-C	5.75	121.02	110.10
1	F	249	ASP	CB-CG-OD1	5.74	123.46	118.30
1	H	475	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	100	ASP	CB-CG-OD2	5.73	123.45	118.30
1	D	346	ASP	CB-CG-OD1	-5.72	113.16	118.30
1	D	410	ALA	N-CA-CB	-5.72	102.10	110.10
1	F	72	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	F	277	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	159	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	237	ASP	CB-CG-OD2	5.69	123.42	118.30
1	G	227	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	237	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	B	112	ASP	CB-CG-OD1	-5.68	113.18	118.30
1	F	168	ASP	CB-CG-OD1	5.67	123.41	118.30
1	C	237	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	B	280	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	475	ASP	CB-CG-OD1	5.66	123.39	118.30
1	H	368	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	B	152	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	H	144	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	326	ALA	N-CA-CB	-5.62	102.22	110.10
1	E	35	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	A	338	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	341	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	112	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	D	237	ASP	CB-CG-OD1	-5.61	113.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	249	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	E	277	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	G	338	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	G	506	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	H	237	ASP	CB-CG-OD2	5.61	123.34	118.30
1	H	353	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	326	ALA	N-CA-CB	-5.59	102.27	110.10
1	E	391	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	158	LEU	CB-CA-C	-5.57	99.62	110.20
1	B	293	ARG	CD-NE-CZ	-5.56	115.82	123.60
1	F	168	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	G	159	ASP	CB-CG-OD1	5.56	123.30	118.30
1	H	484	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	H	224	ASP	CB-CG-OD2	5.55	123.30	118.30
1	E	356	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	A	100	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	406	ASP	CB-CG-OD1	5.55	123.29	118.30
1	G	237	ASP	CB-CG-OD2	5.55	123.29	118.30
1	G	177	ASP	CB-CG-OD1	5.54	123.29	118.30
1	H	356	ASP	CB-CG-OD1	5.54	123.29	118.30
1	H	382	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	E	475	ASP	CB-CG-OD2	5.52	123.27	118.30
1	G	174	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	G	382	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	H	287	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	486	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	506	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	159	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	F	100	ASP	CB-CG-OD2	5.50	123.25	118.30
1	F	353	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	G	484	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	G	353	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	280	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	C	484	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	B	112	ASP	CB-CG-OD2	5.48	123.23	118.30
1	E	249	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	159	ASP	CB-CG-OD1	5.47	123.23	118.30
1	C	235	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	H	48	CYS	N-CA-CB	5.46	120.43	110.60
1	H	524	MET	CG-SD-CE	-5.46	91.47	100.20
1	B	406	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	G	375	ARG	NE-CZ-NH1	5.44	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	315	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	H	100	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	235	ASP	CB-CG-OD2	5.43	123.18	118.30
1	D	224	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	H	35	ASP	CB-CG-OD1	-5.42	113.43	118.30
1	F	318	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	346	ASP	CB-CG-OD1	-5.41	113.44	118.30
1	D	235	ASP	CB-CG-OD1	-5.41	113.44	118.30
1	C	486	ASP	CB-CG-OD2	5.40	123.16	118.30
1	H	406	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	443	TYR	CA-CB-CG	-5.40	103.15	113.40
1	B	484	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	227	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	D	176	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	A	152	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	C	216	ASP	CB-CG-OD2	5.37	123.14	118.30
1	D	176	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	391	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	176	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	484	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	G	353	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	G	216	ASP	CB-CG-OD2	5.34	123.11	118.30
1	F	100	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	E	333	MET	CG-SD-CE	-5.33	91.68	100.20
1	D	23	ASP	CB-CG-OD1	5.33	123.09	118.30
1	H	33	ASP	CB-CG-OD2	5.32	123.09	118.30
1	D	280	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	486	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	H	119	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	35	ASP	CB-CA-C	5.31	121.03	110.40
1	D	406	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	295	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	C	399	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	368	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	F	315	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	G	295	ASP	CB-CG-OD2	5.28	123.06	118.30
1	F	254	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	168	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	346	ASP	CB-CG-OD2	5.27	123.05	118.30
1	F	460	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	H	216	ASP	CB-CA-C	-5.27	99.87	110.40
1	A	227	ASP	CB-CG-OD1	-5.26	113.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	368	ASP	CB-CG-OD2	5.26	123.03	118.30
1	G	100	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	23	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	295	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	475	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	D	216	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	H	475	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	H	72	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	F	72	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	55	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	G	177	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	406	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	35	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	290	MET	CG-SD-CE	-5.23	91.83	100.20
1	B	158	LEU	CB-CA-C	-5.23	100.27	110.20
1	F	368	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	G	216	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	D	174	TYR	CB-CG-CD1	5.21	124.12	121.00
1	B	224	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	B	460	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	280	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	F	159	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	23	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	C	35	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	D	287	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	346	ASP	CB-CG-OD1	5.18	122.96	118.30
1	H	159	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	216	ASP	CB-CG-OD2	5.18	122.96	118.30
1	G	276	VAL	CA-CB-CG1	-5.17	103.14	110.90
1	E	216	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	176	ASP	CB-CG-OD2	5.17	122.95	118.30
1	F	287	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	F	176	ASP	CB-CG-OD2	5.16	122.95	118.30
1	D	442	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	333	MET	CA-CB-CG	-5.15	104.54	113.30
1	G	293	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	486	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	353	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	327	THR	N-CA-CB	-5.13	100.55	110.30
1	E	506	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	F	446	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	H	23	ASP	CB-CG-OD2	5.12	122.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	216	ASP	CB-CA-C	-5.12	100.16	110.40
1	G	346	ASP	CB-CG-OD2	5.11	122.90	118.30
1	F	227	ASP	CB-CG-OD2	5.09	122.88	118.30
1	G	475	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	H	277	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	G	168	ASP	CB-CG-OD1	5.08	122.88	118.30
1	F	382	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	94	THR	CA-CB-CG2	-5.06	105.32	112.40
1	F	37	ALA	N-CA-CB	-5.06	103.02	110.10
1	C	152	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	D	375	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	368	ASP	CB-CG-OD2	5.05	122.84	118.30
1	G	441	ALA	CB-CA-C	-5.05	102.53	110.10
1	G	152	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	353	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	D	359	MET	N-CA-C	5.04	124.61	111.00
1	G	138	THR	CA-CB-CG2	-5.04	105.35	112.40
1	D	486	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	353	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	245	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	H	91	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	E	113	THR	N-CA-CB	-5.02	100.75	110.30
1	E	353	ASP	CB-CG-OD2	5.02	122.82	118.30
1	F	280	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	280	ASP	CB-CG-OD2	5.02	122.82	118.30
1	D	411	MET	CA-CB-CG	5.02	121.83	113.30
1	A	405	THR	CA-CB-CG2	-5.01	105.38	112.40
1	C	176	ASP	CB-CG-OD1	-5.00	113.80	118.30
1	C	141	ILE	N-CA-CB	5.00	122.31	110.80

There are no chirality outliers.

There are no planarity outliers.

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	3979	0	4055	259	0
1	B	3979	0	4055	321	0
1	C	3978	0	4055	208	0
1	D	3979	0	4056	230	0
1	E	3268	0	3315	222	0
1	F	3979	0	4055	266	0
1	G	3979	0	4056	347	0
1	H	3979	0	4056	352	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	10	0	4	1	0
4	B	10	0	4	4	0
4	C	10	0	4	2	0
4	D	10	0	4	3	0
4	E	10	0	4	1	0
4	F	10	0	4	4	0
4	G	10	0	4	1	0
4	H	10	0	4	6	0
5	A	36	0	0	3	0
5	B	25	0	0	2	0
5	C	35	0	0	7	0
5	D	35	0	0	3	0
5	E	16	0	0	0	0
5	F	18	0	0	2	0
5	G	14	0	0	1	0
5	H	15	0	0	0	0
All	All	31410	0	31735	2105	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 33.

All (2105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ILE:HG22	1:C:156:LEU:HB3	1.27	1.13
1:F:186:GLN:HB3	1:F:193:VAL:HB	1.30	1.12
1:E:47:ILE:HB	1:E:359:MET:HG2	1.27	1.12
1:H:15:GLN:HB3	1:H:17:LEU:HD23	1.29	1.09
1:E:391:ARG:NH1	1:F:399:ARG:HH21	1.51	1.09
1:G:123:ILE:HD11	1:G:202:LEU:HD13	1.33	1.06
1:E:114:LYS:HD3	1:E:223:LYS:HD3	1.37	1.05
1:H:24:THR:HG22	1:H:27:GLU:H	1.12	1.04
1:G:43:ASN:HB3	1:G:467:GLY:HA2	1.36	1.04
1:C:145:ASN:H	1:C:145:ASN:ND2	1.55	1.03
1:C:145:ASN:HD22	1:C:145:ASN:N	1.57	1.01
1:F:215:VAL:HG11	1:F:217:LEU:HD12	1.39	1.01
1:H:55:ARG:HG3	1:H:86:THR:HG23	1.40	1.01
1:E:220:VAL:HG22	1:E:224:ASP:HB2	1.43	1.00
1:E:257:LEU:HD21	1:E:264:ILE:HD12	1.44	0.99
1:C:273:HIS:HB3	1:C:277:ARG:HH11	1.26	0.99
1:H:105:ARG:HE	1:H:499:ARG:HH21	1.10	0.99
1:B:63:MET:HG3	1:B:371:LEU:HD23	1.45	0.97
1:G:272:ASN:HB2	1:G:299:GLU:HG2	1.47	0.96
1:H:187:LYS:HA	1:H:192:LEU:HD12	1.48	0.95
1:D:122:LEU:HD11	1:D:127:GLY:HA2	1.46	0.94
1:G:23:ASP:HB3	1:H:399:ARG:HH12	1.30	0.93
1:H:122:LEU:HB2	1:H:149:GLU:HA	1.49	0.93
1:F:328:GLN:HE21	1:H:341:ARG:H	1.16	0.93
1:A:328:GLN:HE21	1:C:341:ARG:H	1.03	0.92
1:H:43:ASN:HB3	1:H:467:GLY:HA2	1.51	0.92
1:H:123:ILE:HD13	1:H:131:VAL:HG23	1.51	0.91
1:H:24:THR:HG22	1:H:27:GLU:N	1.85	0.91
1:A:145:ASN:HB3	1:A:148:MET:HE3	1.53	0.90
1:F:511:LEU:HB3	1:F:521:THR:HG21	1.51	0.90
1:A:406:ASP:HB3	1:A:409:GLU:HG3	1.50	0.90
1:G:69:ASN:HB3	1:G:463:HIS:CD2	2.05	0.90
1:H:480:ALA:HB3	1:H:483:GLU:HG3	1.52	0.89
1:G:323:VAL:H	1:G:356:ASP:HB2	1.36	0.89
1:G:406:ASP:HB3	1:G:409:GLU:HB2	1.53	0.89
1:A:328:GLN:NE2	1:C:341:ARG:H	1.70	0.89
1:A:509:ILE:CD1	1:A:526:VAL:HG22	2.03	0.89
1:G:61:LYS:HG2	1:G:93:ALA:HB1	1.54	0.89
1:H:69:ASN:HB3	1:H:463:HIS:CD2	2.06	0.89
1:G:110:ALA:HB2	1:G:238:MET:HE2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:THR:HG21	1:B:459:ALA:HB2	1.56	0.88
1:E:328:GLN:HE21	1:G:341:ARG:H	1.22	0.87
1:B:379:LEU:HB3	1:D:303:GLU:HG2	1.56	0.87
1:G:454:ARG:NH1	1:G:477:VAL:HG22	1.88	0.87
1:B:102:ILE:HG22	1:B:103:LEU:HD12	1.57	0.86
1:H:15:GLN:HB3	1:H:17:LEU:CD2	2.04	0.86
1:A:145:ASN:HD22	1:A:145:ASN:H	1.21	0.86
1:H:430:LEU:CD1	1:H:452:VAL:HB	2.05	0.86
1:H:63:MET:HG3	1:H:371:LEU:HD23	1.57	0.86
1:B:57:VAL:HG22	1:B:89:ASN:HB3	1.56	0.86
1:B:428:ILE:HD12	1:B:508:VAL:HG11	1.58	0.86
1:H:60:LEU:HD21	1:H:90:VAL:HG23	1.57	0.86
1:E:391:ARG:HH12	1:F:399:ARG:HH21	1.17	0.86
1:B:63:MET:HG3	1:B:371:LEU:CD2	2.06	0.86
1:B:493:MET:HE2	1:B:530:PRO:HD2	1.55	0.85
1:A:340:THR:HB	1:C:328:GLN:HE21	1.42	0.85
1:E:47:ILE:CD1	1:E:324:ILE:HD13	2.06	0.85
1:F:133:LEU:HD13	1:F:139:LEU:HD13	1.57	0.85
1:A:493:MET:CE	1:A:529:VAL:HA	2.06	0.85
1:D:123:ILE:HG22	1:D:129:ALA:HB3	1.59	0.85
1:A:145:ASN:HD22	1:A:145:ASN:N	1.74	0.84
1:C:139:LEU:HD21	1:C:156:LEU:HB2	1.59	0.84
1:G:440:VAL:HG12	1:G:449:ILE:HD13	1.59	0.84
1:D:154:ASN:HB2	1:D:155:ILE:HD12	1.59	0.84
1:H:63:MET:HG3	1:H:371:LEU:CD2	2.07	0.84
1:G:46:ILE:HG23	1:G:377:GLN:NE2	1.93	0.84
1:A:43:ASN:HB3	1:A:467:GLY:HA2	1.59	0.84
1:F:242:SER:HA	1:F:269:LYS:HE2	1.59	0.84
1:G:102:ILE:HG22	1:G:103:LEU:HD12	1.60	0.84
1:C:123:ILE:HD12	1:C:131:VAL:CG2	2.08	0.84
1:B:145:ASN:HD22	1:B:145:ASN:N	1.75	0.83
1:G:382:ARG:HB2	1:G:382:ARG:HH11	1.41	0.83
1:G:23:ASP:HB3	1:H:399:ARG:NH1	1.92	0.83
1:G:43:ASN:HB3	1:G:467:GLY:CA	2.06	0.83
1:H:496:GLY:HA3	1:H:502:PHE:CZ	2.13	0.83
1:A:493:MET:HE2	1:A:530:PRO:HD2	1.59	0.83
1:D:132:GLU:HG3	1:D:201:PHE:HE1	1.42	0.83
1:A:273:HIS:CD2	1:A:277:ARG:HE	1.94	0.83
1:A:520:PHE:CE1	1:A:522:ASN:HB3	2.14	0.83
1:C:141:ILE:CG2	1:C:156:LEU:HB3	2.09	0.83
1:E:34:ILE:CD1	1:G:276:VAL:HG11	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ASN:HB3	1:B:467:GLY:HA2	1.59	0.82
1:B:292:ALA:HB1	4:B:532:PEQ:H21	1.61	0.82
1:A:493:MET:HE2	1:A:529:VAL:HA	1.59	0.82
1:E:511:LEU:HB3	1:E:521:THR:HG21	1.62	0.82
1:F:247:ALA:HB2	1:F:281:GLU:HG3	1.59	0.82
1:B:215:VAL:CG1	1:B:217:LEU:HD12	2.10	0.82
1:G:185:LYS:HG3	1:G:195:GLU:HB2	1.61	0.82
1:G:499:ARG:HD2	1:G:501:PHE:CZ	2.15	0.82
1:D:131:VAL:CG2	1:D:153:GLU:HB3	2.09	0.82
1:B:132:GLU:HG3	1:B:201:PHE:CE1	2.15	0.81
1:G:62:GLU:HB3	1:G:371:LEU:HD11	1.61	0.81
1:D:123:ILE:HG22	1:D:129:ALA:CB	2.10	0.81
1:H:55:ARG:CG	1:H:86:THR:HG23	2.09	0.81
1:E:47:ILE:HD11	1:E:324:ILE:HD13	1.60	0.81
1:E:301:PRO:HG2	1:E:304:LYS:HD2	1.63	0.81
1:C:515:ARG:HB3	1:C:516:PRO:HD2	1.63	0.80
1:E:46:ILE:HG23	1:E:377:GLN:NE2	1.96	0.80
1:H:43:ASN:HB3	1:H:467:GLY:CA	2.11	0.80
1:A:145:ASN:HB3	1:A:148:MET:CE	2.11	0.80
1:B:503:LYS:HG2	1:B:504:LYS:H	1.44	0.80
1:C:493:MET:HE1	1:C:529:VAL:HG22	1.63	0.80
1:F:333:MET:HE1	1:F:373:ALA:HA	1.63	0.80
1:G:343:GLU:O	1:G:347:VAL:HG23	1.82	0.80
1:A:328:GLN:NE2	1:C:341:ARG:HG2	1.97	0.80
1:F:328:GLN:NE2	1:H:341:ARG:H	1.80	0.80
1:B:43:ASN:HB3	1:B:467:GLY:CA	2.12	0.79
1:G:61:LYS:HG2	1:G:93:ALA:CB	2.11	0.79
1:H:242:SER:HA	1:H:269:LYS:HE2	1.64	0.79
1:F:511:LEU:HD22	1:F:521:THR:HG22	1.64	0.79
1:F:511:LEU:HB3	1:F:521:THR:CG2	2.12	0.79
1:G:524:MET:HG2	1:G:525:ARG:N	1.96	0.79
1:B:57:VAL:CG2	1:B:89:ASN:HB3	2.12	0.79
1:E:105:ARG:NE	1:E:499:ARG:HH12	1.80	0.79
1:B:261:GLY:CA	1:B:264:ILE:HG13	2.12	0.79
1:E:241:ALA:HB1	1:E:244:ILE:HD11	1.65	0.79
1:G:376:MET:O	1:G:380:ILE:HG13	1.83	0.79
1:G:360:LEU:HB3	1:G:363:GLU:HB2	1.65	0.79
1:C:465:TYR:HB2	1:C:468:ILE:HD12	1.64	0.78
1:A:241:ALA:HB1	1:A:244:ILE:HD11	1.65	0.78
1:B:328:GLN:HE21	1:D:340:THR:HB	1.46	0.78
1:G:382:ARG:HH11	1:G:382:ARG:CB	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:LEU:CD2	1:E:264:ILE:HD12	2.12	0.78
1:H:105:ARG:HE	1:H:499:ARG:NH2	1.81	0.78
1:B:393:LEU:HG	1:B:397:LEU:HD22	1.64	0.78
1:F:247:ALA:O	1:F:250:VAL:HG23	1.84	0.78
1:A:237:ASP:OD2	1:A:460:ARG:HD2	1.83	0.78
1:E:376:MET:O	1:E:380:ILE:HG13	1.82	0.78
1:E:221:SER:O	1:E:225:ILE:HG13	1.83	0.78
1:B:102:ILE:HG22	1:B:103:LEU:CD1	2.13	0.78
1:B:428:ILE:HD12	1:B:508:VAL:CG1	2.14	0.78
1:C:131:VAL:CG1	1:C:153:GLU:HB3	2.13	0.78
1:C:141:ILE:HG22	1:C:156:LEU:CB	2.10	0.78
1:A:273:HIS:HD2	1:A:277:ARG:HE	1.30	0.78
1:B:342:ALA:HB1	1:D:346:ASP:HB2	1.65	0.78
1:D:247:ALA:O	1:D:250:VAL:HG23	1.84	0.78
1:A:457:GLN:O	1:A:461:GLN:HG3	1.85	0.77
1:D:24:THR:HG23	1:D:27:GLU:H	1.48	0.77
1:F:371:LEU:O	1:F:375:ARG:HG3	1.85	0.77
1:B:411:MET:HG2	1:B:521:THR:O	1.84	0.77
1:F:315:ARG:HD2	1:H:30:CYS:HB3	1.67	0.77
1:F:493:MET:HG2	1:F:530:PRO:HD2	1.67	0.77
1:H:503:LYS:HG2	1:H:504:LYS:H	1.50	0.77
1:D:132:GLU:HG3	1:D:201:PHE:CE1	2.19	0.77
1:B:221:SER:H	1:B:224:ASP:HB2	1.50	0.76
1:D:226:GLN:HA	1:D:229:LYS:HE2	1.68	0.76
1:A:87:ILE:O	1:A:91:ARG:HG3	1.85	0.76
1:A:266:ILE:C	1:A:267:ILE:HD13	2.06	0.76
1:B:173:VAL:HB	1:B:182:LEU:HD12	1.65	0.76
1:C:462:ALA:HB1	1:C:468:ILE:HG21	1.68	0.76
1:F:187:LYS:HA	1:F:192:LEU:CD1	2.15	0.76
1:E:237:ASP:OD2	1:E:460:ARG:HD2	1.86	0.76
1:D:228:LEU:O	1:D:232:VAL:HG23	1.84	0.76
1:E:105:ARG:CZ	1:E:499:ARG:HH12	1.99	0.76
1:H:399:ARG:O	1:H:402:SER:HB3	1.86	0.76
1:C:237:ASP:OD1	1:C:460:ARG:HD2	1.85	0.76
1:E:391:ARG:NH1	1:F:399:ARG:NH2	2.33	0.76
1:G:61:LYS:HD3	1:G:93:ALA:HA	1.67	0.76
1:G:86:THR:O	1:G:90:VAL:HG23	1.86	0.76
1:G:412:ALA:O	1:G:416:VAL:HG23	1.86	0.75
1:B:261:GLY:HA3	1:B:264:ILE:HG13	1.66	0.75
1:A:433:SER:HB2	1:A:435:ARG:HG3	1.68	0.75
1:C:43:ASN:HB3	1:C:467:GLY:HA2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ALA:C	1:C:427:LEU:HD12	2.06	0.75
1:B:220:VAL:HG22	1:B:224:ASP:HB3	1.67	0.75
1:B:496:GLY:HA3	1:B:502:PHE:CZ	2.22	0.75
1:G:94:THR:HG22	1:G:95:GLU:HG2	1.68	0.75
1:G:338:ARG:HH22	1:G:341:ARG:HH22	1.34	0.75
1:E:224:ASP:O	1:E:228:LEU:HG	1.86	0.75
1:B:43:ASN:HB3	1:B:467:GLY:N	2.00	0.75
1:H:103:LEU:HA	1:H:499:ARG:HH12	1.51	0.75
1:G:416:VAL:HG13	1:G:445:PRO:HB3	1.69	0.75
1:F:237:ASP:OD2	1:F:460:ARG:HD2	1.86	0.74
1:G:328:GLN:HA	1:G:331:GLU:HG2	1.69	0.74
1:E:87:ILE:O	1:E:91:ARG:HG3	1.86	0.74
1:H:430:LEU:HD11	1:H:452:VAL:HB	1.70	0.74
1:B:141:ILE:CD1	1:B:192:LEU:HB2	2.18	0.74
1:H:376:MET:O	1:H:380:ILE:HG13	1.87	0.74
1:B:151:CYS:HB3	1:B:156:LEU:CD2	2.18	0.74
1:B:393:LEU:O	1:B:397:LEU:HB2	1.88	0.74
1:E:46:ILE:HG23	1:E:377:GLN:HE22	1.52	0.74
1:H:412:ALA:O	1:H:416:VAL:HG23	1.87	0.74
1:F:76:SER:HA	1:F:114:LYS:HB2	1.69	0.73
1:F:515:ARG:HB3	1:F:516:PRO:HD2	1.69	0.73
1:H:19:ALA:HA	1:H:31:ARG:HB3	1.70	0.73
1:H:430:LEU:HD12	1:H:452:VAL:HB	1.70	0.73
1:H:54:SER:O	1:H:60:LEU:HD13	1.87	0.73
1:D:406:ASP:HB3	1:D:409:GLU:HG3	1.69	0.73
1:E:115:GLY:HA2	1:E:224:ASP:OD2	1.89	0.73
1:G:288:GLY:O	1:G:289:ILE:HG12	1.87	0.73
1:H:328:GLN:HA	1:H:331:GLU:HG3	1.69	0.73
1:B:426:ALA:C	1:B:427:LEU:HD12	2.09	0.73
1:B:504:LYS:HG3	1:B:530:PRO:OXT	1.87	0.73
1:H:102:ILE:HG12	1:H:103:LEU:N	2.03	0.73
1:E:60:LEU:HD23	1:E:90:VAL:HA	1.69	0.73
1:G:440:VAL:CG1	1:G:449:ILE:HD13	2.19	0.73
1:H:209:ASN:O	1:H:211:PRO:HD3	1.88	0.73
1:B:151:CYS:HB3	1:B:156:LEU:HD23	1.68	0.73
1:B:382:ARG:HB2	1:B:382:ARG:HH11	1.52	0.73
1:C:300:ILE:HD12	1:C:304:LYS:HB2	1.70	0.73
1:H:246:LYS:HE2	1:H:249:ASP:OD1	1.88	0.73
1:G:293:ARG:HD3	1:G:326:ALA:O	1.89	0.73
1:D:24:THR:CG2	1:D:27:GLU:HB2	2.19	0.72
1:G:454:ARG:HG2	1:G:473:CYS:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:329:MET:O	1:G:343:GLU:HG2	1.89	0.72
1:H:493:MET:HE2	1:H:529:VAL:HG22	1.71	0.72
1:F:296:LEU:HD12	1:F:296:LEU:O	1.89	0.72
1:G:63:MET:HG2	1:G:371:LEU:HD21	1.71	0.72
1:H:202:LEU:HD22	1:H:203:GLY:N	2.04	0.72
1:G:123:ILE:HD11	1:G:202:LEU:CD1	2.16	0.72
1:H:328:GLN:HA	1:H:331:GLU:CG	2.19	0.72
1:H:503:LYS:HG2	1:H:504:LYS:N	2.04	0.72
1:C:55:ARG:HG3	1:C:86:THR:HG23	1.71	0.72
1:F:215:VAL:CG1	1:F:217:LEU:HD12	2.18	0.72
1:G:399:ARG:NH1	1:H:23:ASP:HB3	2.03	0.72
1:A:122:LEU:HD12	1:A:126:SER:O	1.89	0.72
1:C:370:PRO:O	1:C:374:VAL:HG23	1.90	0.72
1:G:49:THR:OG1	1:G:361:SER:HA	1.90	0.72
1:A:55:ARG:CG	1:A:86:THR:HG23	2.20	0.72
1:A:271:GLU:HG3	1:A:292:ALA:CB	2.19	0.72
1:D:160:TYR:OH	1:D:216:ASP:HB2	1.88	0.72
1:G:371:LEU:O	1:G:375:ARG:HD2	1.89	0.72
1:E:49:THR:HG23	1:E:72:ARG:HD3	1.71	0.72
1:E:391:ARG:HH12	1:F:399:ARG:NH2	1.86	0.72
1:G:322:PRO:HA	1:G:356:ASP:OD2	1.88	0.72
1:G:56:SER:OG	1:G:58:GLU:HB2	1.90	0.72
1:A:309:GLN:O	1:A:313:ILE:HD12	1.90	0.71
1:G:113:THR:HG22	1:G:242:SER:HB2	1.72	0.71
1:A:145:ASN:N	1:A:145:ASN:ND2	2.38	0.71
1:B:76:SER:HA	1:B:114:LYS:HB2	1.71	0.71
1:D:123:ILE:CD1	1:D:131:VAL:HB	2.21	0.71
1:E:504:LYS:HG3	1:E:530:PRO:O	1.89	0.71
1:G:202:LEU:HD22	1:G:203:GLY:N	2.04	0.71
1:E:352:LEU:HD22	1:E:384:ALA:HB1	1.71	0.71
1:G:452:VAL:HG11	1:G:488:ARG:HB3	1.71	0.71
1:D:131:VAL:HG21	1:D:153:GLU:HB3	1.71	0.71
1:G:493:MET:CE	1:G:529:VAL:HG13	2.20	0.71
1:C:83:HIS:O	1:C:87:ILE:HG13	1.90	0.71
1:H:426:ALA:C	1:H:427:LEU:HD12	2.10	0.71
1:B:369:TYR:HB3	1:B:372:GLU:HB2	1.72	0.71
1:C:123:ILE:HD12	1:C:131:VAL:HG23	1.72	0.71
1:D:461:GLN:O	1:D:464:LEU:HB2	1.91	0.71
1:E:421:LYS:HD3	1:F:413:MET:SD	2.31	0.71
1:H:123:ILE:HD13	1:H:131:VAL:CG2	2.21	0.71
1:H:330:LEU:HD12	1:H:339:PRO:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ALA:O	1:B:416:VAL:HG23	1.90	0.71
1:H:245:ARG:O	1:H:282:ILE:HD11	1.91	0.70
1:C:102:ILE:HG22	1:C:103:LEU:HD12	1.73	0.70
1:D:382:ARG:NH1	5:D:6191:HOH:O	2.25	0.70
1:E:102:ILE:HG22	1:E:103:LEU:CD1	2.21	0.70
1:F:154:ASN:C	1:F:155:ILE:HD12	2.11	0.70
1:F:179:LEU:HD13	1:H:338:ARG:NH2	2.06	0.70
1:G:410:ALA:HA	1:H:421:LYS:HG2	1.73	0.70
1:A:133:LEU:HD11	1:A:139:LEU:HD13	1.74	0.70
1:C:392:LYS:O	1:C:396:GLU:HG3	1.91	0.70
1:G:440:VAL:HG12	1:G:449:ILE:CD1	2.21	0.70
1:A:493:MET:HE2	1:A:529:VAL:HG13	1.72	0.70
1:B:493:MET:CE	1:B:529:VAL:HG13	2.21	0.70
1:E:340:THR:HB	1:G:328:GLN:HE21	1.57	0.70
1:B:328:GLN:HG2	1:B:331:GLU:HG3	1.74	0.70
1:B:480:ALA:HB3	1:B:483:GLU:HG3	1.72	0.70
1:F:202:LEU:HD23	1:F:203:GLY:H	1.56	0.70
1:A:89:ASN:HD22	1:A:89:ASN:N	1.86	0.70
1:E:330:LEU:HD12	1:E:343:GLU:HB3	1.74	0.70
1:E:515:ARG:HB3	1:E:516:PRO:HD2	1.74	0.70
1:G:338:ARG:NH2	1:G:341:ARG:HH12	1.89	0.70
1:A:27:GLU:O	1:A:31:ARG:HG3	1.91	0.69
1:G:338:ARG:NH2	1:G:341:ARG:HH22	1.89	0.69
1:B:160:TYR:O	1:B:163:ILE:HG22	1.92	0.69
1:B:433:SER:HB2	1:B:435:ARG:CD	2.22	0.69
1:C:156:LEU:HD22	1:C:157:TRP:N	2.07	0.69
1:G:43:ASN:CB	1:G:467:GLY:HA2	2.18	0.69
1:H:316:CYS:HB2	1:H:323:VAL:HG22	1.75	0.69
1:A:122:LEU:O	1:A:151:CYS:HB2	1.91	0.69
1:A:491:LEU:O	1:A:495:VAL:HG23	1.92	0.69
1:C:273:HIS:ND1	1:C:277:ARG:NH1	2.39	0.69
1:F:141:ILE:HG22	1:F:156:LEU:HB2	1.75	0.69
1:E:103:LEU:N	1:E:103:LEU:HD12	2.08	0.69
1:A:269:LYS:HD2	1:A:290:MET:SD	2.31	0.69
1:B:167:VAL:HG13	1:B:171:SER:CB	2.22	0.69
1:C:308:ALA:O	1:C:312:ILE:HD12	1.93	0.69
1:E:102:ILE:C	1:E:103:LEU:HD12	2.13	0.69
1:F:145:ASN:HD22	1:F:145:ASN:N	1.91	0.69
1:F:145:ASN:HB3	1:F:148:MET:CE	2.23	0.69
1:G:47:ILE:HB	1:G:359:MET:HB2	1.73	0.69
1:B:453:THR:CG2	1:B:459:ALA:HB2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLN:HE21	1:C:341:ARG:N	1.87	0.69
1:B:210:LEU:HD12	1:B:210:LEU:N	2.07	0.69
1:E:34:ILE:HD13	1:G:276:VAL:HG11	1.73	0.69
1:G:411:MET:SD	1:H:526:VAL:HG23	2.33	0.69
1:H:160:TYR:OH	1:H:216:ASP:HB2	1.93	0.69
1:H:267:ILE:HD13	1:H:267:ILE:N	2.08	0.69
1:B:141:ILE:HG13	1:B:158:LEU:CD2	2.23	0.68
1:C:328:GLN:HA	1:C:331:GLU:HG3	1.74	0.68
1:F:50:ILE:HB	1:F:73:MET:CE	2.23	0.68
1:G:132:GLU:HG3	1:G:201:PHE:CE1	2.28	0.68
1:B:244:ILE:HG13	1:B:268:SER:OG	1.93	0.68
1:C:76:SER:HA	1:C:114:LYS:HB2	1.74	0.68
1:C:123:ILE:HD12	1:C:131:VAL:HG21	1.75	0.68
1:H:358:ILE:HG13	1:H:377:GLN:NE2	2.08	0.68
1:A:42:ARG:NH1	1:A:46:ILE:HG13	2.08	0.68
1:E:51:GLY:O	1:E:55:ARG:HB2	1.92	0.68
1:H:72:ARG:NH2	4:H:532:PEQ:O1P	2.26	0.68
1:G:57:VAL:HG13	1:G:93:ALA:HB2	1.75	0.68
1:G:92:THR:HG22	1:G:93:ALA:N	2.08	0.68
1:H:529:VAL:HG13	1:H:530:PRO:HD2	1.74	0.68
1:A:447:ALA:HB1	1:A:448:PRO:HD2	1.74	0.68
1:B:141:ILE:HD13	1:B:192:LEU:HB2	1.75	0.68
1:H:328:GLN:HG2	1:H:331:GLU:HG3	1.74	0.68
1:D:187:LYS:HA	1:D:192:LEU:CD1	2.23	0.68
1:F:118:ILE:CG2	1:F:208:VAL:HB	2.24	0.68
1:F:293:ARG:HD3	1:F:326:ALA:O	1.93	0.68
1:H:360:LEU:HD11	1:H:377:GLN:CD	2.13	0.68
1:H:406:ASP:HB3	1:H:409:GLU:HB2	1.75	0.68
1:A:158:LEU:HD23	1:A:163:ILE:HD12	1.76	0.68
1:B:226:GLN:HA	1:B:229:LYS:HE2	1.74	0.68
1:B:489:VAL:O	1:B:493:MET:HG2	1.94	0.68
1:E:76:SER:HA	1:E:114:LYS:HB2	1.76	0.68
1:E:355:ALA:O	1:E:466:ARG:NH1	2.27	0.68
1:G:455:ASN:HB3	1:G:458:THR:HB	1.76	0.68
1:H:316:CYS:CB	1:H:323:VAL:HG22	2.24	0.68
1:H:370:PRO:O	1:H:374:VAL:HG23	1.94	0.68
1:B:328:GLN:NE2	1:D:341:ARG:H	1.92	0.67
1:E:75:PHE:HB2	1:E:112:ASP:O	1.94	0.67
1:E:431:THR:HG21	1:E:434:GLY:HA2	1.75	0.67
1:H:249:ASP:O	1:H:253:VAL:HG23	1.94	0.67
1:A:340:THR:HB	1:C:328:GLN:NE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PRO:HB2	1:B:220:VAL:O	1.93	0.67
1:D:241:ALA:O	1:D:269:LYS:HG3	1.94	0.67
1:E:309:GLN:O	1:E:313:ILE:HG13	1.94	0.67
1:E:329:MET:O	1:E:343:GLU:HB3	1.95	0.67
1:G:116:PRO:HB2	1:G:217:LEU:HD23	1.77	0.67
1:B:14:THR:O	1:B:17:LEU:HG	1.95	0.67
1:C:131:VAL:HG13	1:C:153:GLU:OE1	1.95	0.67
1:E:270:ILE:HD12	1:E:270:ILE:N	2.10	0.67
1:E:295:ASP:O	1:E:298:ILE:HB	1.94	0.67
1:E:425:ALA:HB1	1:E:502:PHE:HB3	1.77	0.67
1:F:140:LYS:HB2	1:F:193:VAL:HG22	1.76	0.67
1:H:43:ASN:CB	1:H:467:GLY:HA2	2.24	0.67
1:F:119:ARG:O	1:F:158:LEU:HD12	1.95	0.67
1:A:524:MET:HG2	1:A:525:ARG:N	2.07	0.67
1:B:493:MET:CE	1:B:530:PRO:HD2	2.25	0.67
1:D:293:ARG:HD3	1:D:326:ALA:O	1.95	0.67
1:F:406:ASP:HB3	1:F:409:GLU:HG3	1.75	0.67
1:H:360:LEU:N	1:H:360:LEU:HD12	2.10	0.67
1:B:54:SER:HA	1:B:59:THR:HG21	1.77	0.67
1:B:504:LYS:O	1:B:529:VAL:HB	1.95	0.67
1:E:457:GLN:HG2	1:E:461:GLN:HE21	1.59	0.67
1:G:135:LYS:HG3	1:G:198:ASN:H	1.59	0.67
1:H:512:THR:CA	1:H:521:THR:HG22	2.25	0.67
1:C:273:HIS:HB3	1:C:277:ARG:NH1	2.03	0.66
1:D:225:ILE:O	1:D:229:LYS:HG3	1.94	0.66
1:E:224:ASP:O	1:E:227:ASP:HB2	1.95	0.66
1:E:256:ILE:HG22	1:E:257:LEU:N	2.10	0.66
1:G:56:SER:HB3	1:G:59:THR:OG1	1.95	0.66
1:H:484:ASP:O	1:H:487:LEU:HB3	1.94	0.66
1:H:512:THR:N	1:H:521:THR:HG22	2.10	0.66
1:B:428:ILE:CD1	1:B:508:VAL:HG11	2.25	0.66
1:C:43:ASN:HB3	1:C:467:GLY:N	2.10	0.66
1:D:155:ILE:HD12	1:D:155:ILE:N	2.10	0.66
1:D:228:LEU:HD22	1:D:257:LEU:CD1	2.25	0.66
1:H:118:ILE:CG2	1:H:208:VAL:HB	2.25	0.66
1:H:118:ILE:HG22	1:H:208:VAL:HB	1.77	0.66
1:D:119:ARG:HH11	1:D:207:GLY:N	1.93	0.66
1:D:167:VAL:HG13	1:D:171:SER:OG	1.96	0.66
1:G:46:ILE:HG23	1:G:377:GLN:HE21	1.60	0.66
1:A:244:ILE:HG13	1:A:268:SER:HB3	1.77	0.66
1:B:355:ALA:O	1:B:466:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ILE:O	1:D:207:GLY:HA2	1.95	0.66
1:E:22:ALA:O	1:E:391:ARG:NH2	2.29	0.66
1:G:15:GLN:HG3	1:G:39:ILE:HG23	1.76	0.66
1:B:47:ILE:CD1	1:B:324:ILE:HD13	2.25	0.66
1:B:433:SER:HB2	1:B:435:ARG:HD2	1.78	0.66
1:B:515:ARG:HB3	1:B:516:PRO:HD2	1.77	0.66
1:C:43:ASN:HB3	1:C:467:GLY:CA	2.24	0.66
1:F:163:ILE:O	1:F:167:VAL:HG23	1.95	0.66
1:E:220:VAL:CG1	1:E:225:ILE:HD11	2.26	0.66
1:F:349:ASN:HD21	1:H:310:LYS:NZ	1.93	0.66
1:B:202:LEU:HD22	1:B:203:GLY:O	1.96	0.66
1:H:220:VAL:HG13	1:H:224:ASP:HB2	1.76	0.66
1:B:304:LYS:NZ	1:D:383:GLU:OE2	2.29	0.66
1:C:160:TYR:OH	1:C:216:ASP:HB2	1.95	0.66
1:D:122:LEU:HD12	1:D:123:ILE:H	1.58	0.66
1:F:329:MET:O	1:F:343:GLU:HB3	1.96	0.66
1:H:515:ARG:HB3	1:H:516:PRO:HD2	1.78	0.66
1:B:50:ILE:HB	1:B:73:MET:CE	2.26	0.66
1:B:333:MET:CE	1:B:339:PRO:HD3	2.26	0.66
1:D:63:MET:HG3	1:D:371:LEU:CD2	2.26	0.66
1:D:123:ILE:HB	1:D:204:SER:OG	1.96	0.66
1:E:220:VAL:HG22	1:E:224:ASP:CB	2.23	0.66
1:E:220:VAL:HG11	1:E:225:ILE:HD11	1.77	0.66
1:E:457:GLN:O	1:E:461:GLN:HG3	1.96	0.65
1:G:309:GLN:O	1:G:313:ILE:HG13	1.96	0.65
1:A:452:VAL:HG11	1:A:488:ARG:HB3	1.78	0.65
1:B:457:GLN:O	1:B:461:GLN:HG3	1.97	0.65
1:E:249:ASP:O	1:E:253:VAL:HG23	1.96	0.65
1:A:271:GLU:HG3	1:A:292:ALA:HB3	1.78	0.65
1:B:427:LEU:HD12	1:B:427:LEU:N	2.11	0.65
1:G:54:SER:O	1:G:60:LEU:HD11	1.97	0.65
1:A:328:GLN:NE2	1:C:341:ARG:N	2.42	0.65
1:C:131:VAL:HG12	1:C:153:GLU:HB3	1.77	0.65
1:F:409:GLU:O	1:F:413:MET:HG3	1.96	0.65
1:H:176:ASP:O	1:H:179:LEU:HB2	1.96	0.65
1:C:252:GLU:O	1:C:256:ILE:HG12	1.97	0.65
1:C:296:LEU:O	1:C:296:LEU:HD12	1.97	0.65
1:E:220:VAL:HG13	1:E:221:SER:N	2.11	0.65
1:E:298:ILE:HD13	1:E:298:ILE:N	2.12	0.65
1:F:227:ASP:O	1:F:230:PHE:HB3	1.95	0.65
1:H:330:LEU:CD2	1:H:377:GLN:HG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:O	1:A:267:ILE:HD13	1.95	0.65
1:B:123:ILE:HD11	1:B:202:LEU:HD13	1.78	0.65
1:F:25:PHE:N	1:H:396:GLU:OE2	2.29	0.65
1:F:247:ALA:CB	1:F:281:GLU:HG3	2.26	0.65
1:A:288:GLY:O	1:A:289:ILE:HG12	1.95	0.65
1:B:54:SER:O	1:B:60:LEU:HD11	1.96	0.65
1:G:392:LYS:O	1:G:396:GLU:HG3	1.97	0.65
1:C:27:GLU:O	1:C:31:ARG:HG3	1.96	0.65
1:G:220:VAL:HG22	1:G:224:ASP:HB3	1.78	0.65
1:H:64:ILE:HD13	1:H:107:VAL:HG21	1.78	0.65
1:B:514:TRP:C	1:B:515:ARG:HG2	2.17	0.65
1:E:485:VAL:HG12	1:E:486:ASP:N	2.11	0.65
1:F:118:ILE:HG22	1:F:208:VAL:CG2	2.26	0.65
1:F:507:VAL:HG12	1:F:508:VAL:H	1.62	0.65
1:F:511:LEU:HD22	1:F:521:THR:CG2	2.27	0.65
1:H:361:SER:N	1:H:363:GLU:OE1	2.28	0.65
1:D:306:PHE:O	1:D:310:LYS:HG3	1.97	0.64
1:F:154:ASN:O	1:F:155:ILE:HD12	1.97	0.64
1:H:23:ASP:OD1	1:H:23:ASP:N	2.30	0.64
1:A:278:ARG:O	1:A:282:ILE:HG13	1.96	0.64
1:B:156:LEU:HD22	1:B:157:TRP:H	1.62	0.64
1:C:493:MET:CE	1:C:529:VAL:HG13	2.28	0.64
1:E:47:ILE:HB	1:E:359:MET:CG	2.16	0.64
1:G:416:VAL:O	1:G:419:SER:HB3	1.96	0.64
1:A:315:ARG:NH1	1:C:30:CYS:O	2.30	0.64
1:F:186:GLN:O	1:F:192:LEU:HD12	1.98	0.64
1:F:336:LYS:HB3	1:F:337:PRO:HD2	1.80	0.64
1:B:141:ILE:HG13	1:B:158:LEU:HD21	1.78	0.64
1:F:191:PHE:O	1:F:192:LEU:HD13	1.97	0.64
1:G:485:VAL:HG12	1:G:486:ASP:N	2.10	0.64
1:E:246:LYS:HG2	1:E:249:ASP:OD2	1.97	0.64
1:E:326:ALA:CB	1:E:359:MET:HE2	2.27	0.64
1:G:496:GLY:HA3	1:G:502:PHE:CZ	2.33	0.64
1:G:497:LYS:NZ	1:G:530:PRO:O	2.30	0.64
1:H:381:ALA:HB1	1:H:385:GLU:OE2	1.96	0.64
1:A:293:ARG:HD3	1:A:326:ALA:O	1.98	0.64
1:B:43:ASN:CB	1:B:467:GLY:HA2	2.27	0.64
1:B:69:ASN:HB3	1:B:463:HIS:CD2	2.33	0.64
1:F:50:ILE:HG21	1:F:86:THR:CG2	2.27	0.64
1:A:43:ASN:HB3	1:A:467:GLY:CA	2.27	0.64
1:D:267:ILE:HD12	1:D:267:ILE:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:LYS:NZ	1:H:383:GLU:OE2	2.30	0.64
1:H:493:MET:O	1:H:497:LYS:HB2	1.98	0.64
1:A:102:ILE:HG22	1:A:103:LEU:HD12	1.79	0.64
1:G:48:CYS:HB3	1:G:364:THR:HG21	1.80	0.64
1:G:266:ILE:O	1:G:287:ASP:HB2	1.98	0.64
1:C:225:ILE:O	1:C:229:LYS:HG3	1.97	0.64
1:E:328:GLN:NE2	1:G:341:ARG:H	1.94	0.64
1:G:393:LEU:HG	1:G:397:LEU:HD22	1.80	0.64
1:G:215:VAL:CG1	1:G:217:LEU:HB2	2.28	0.63
1:H:55:ARG:CD	1:H:86:THR:HG23	2.27	0.63
1:C:427:LEU:HD12	1:C:427:LEU:N	2.13	0.63
1:D:202:LEU:HD22	1:D:203:GLY:O	1.98	0.63
1:G:431:THR:HG21	1:G:434:GLY:HA2	1.78	0.63
1:H:60:LEU:HD21	1:H:90:VAL:CG2	2.26	0.63
1:B:160:TYR:CD2	1:B:163:ILE:HB	2.33	0.63
1:C:217:LEU:HD23	1:C:218:PRO:HD2	1.78	0.63
1:D:185:LYS:HD3	1:D:195:GLU:HB3	1.79	0.63
1:D:243:PHE:N	1:D:271:GLU:OE1	2.29	0.63
1:F:217:LEU:HB3	1:F:218:PRO:HD2	1.79	0.63
1:F:507:VAL:HG12	1:F:508:VAL:N	2.13	0.63
1:G:57:VAL:HG11	1:G:92:THR:HG22	1.79	0.63
1:H:435:ARG:O	1:H:438:HIS:N	2.31	0.63
1:H:503:LYS:O	1:H:506:ASP:HB2	1.98	0.63
1:A:241:ALA:CB	1:A:244:ILE:HD11	2.27	0.63
1:B:254:ARG:CZ	1:B:266:ILE:HD12	2.29	0.63
1:C:279:PHE:HE2	1:C:315:ARG:HB3	1.63	0.63
1:C:293:ARG:NH2	1:C:346:ASP:OD1	2.30	0.63
1:E:105:ARG:NE	1:E:499:ARG:NH1	2.46	0.63
1:E:383:GLU:OE2	1:G:304:LYS:NZ	2.30	0.63
1:G:63:MET:HA	1:G:371:LEU:HD21	1.81	0.63
1:G:429:VAL:HG11	1:G:437:ALA:HB2	1.80	0.63
1:A:181:SER:HB3	1:A:198:ASN:HB2	1.79	0.63
1:E:56:SER:O	1:E:60:LEU:HD13	1.97	0.63
1:F:30:CYS:O	1:H:315:ARG:NH1	2.30	0.63
1:G:68:MET:O	1:G:69:ASN:ND2	2.31	0.63
1:G:431:THR:HG21	1:G:434:GLY:CA	2.28	0.63
1:C:279:PHE:HE1	1:C:289:ILE:HD12	1.64	0.63
1:D:329:MET:O	1:D:343:GLU:HB3	1.97	0.63
1:G:45:GLY:CA	1:G:357:CYS:HB3	2.29	0.63
1:H:382:ARG:HH11	1:H:382:ARG:HG3	1.62	0.63
1:A:221:SER:O	1:A:224:ASP:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:MET:HG2	1:D:148:MET:O	1.99	0.63
1:E:61:LYS:O	1:E:65:LYS:HB2	1.99	0.63
1:G:57:VAL:HG11	1:G:92:THR:CG2	2.29	0.63
1:A:25:PHE:O	1:A:28:HIS:HB3	1.99	0.63
1:B:50:ILE:HB	1:B:73:MET:HE1	1.80	0.63
1:B:231:GLY:O	1:B:236:VAL:HG22	1.99	0.63
1:H:148:MET:HG3	1:H:157:TRP:CZ3	2.34	0.63
1:D:123:ILE:O	1:D:129:ALA:HB3	1.99	0.62
1:G:60:LEU:HD23	1:G:90:VAL:HA	1.80	0.62
1:E:511:LEU:HB3	1:E:521:THR:CG2	2.28	0.62
1:D:187:LYS:HB2	1:D:192:LEU:HD11	1.80	0.62
1:H:292:ALA:HB1	4:H:532:PEQ:C1	2.28	0.62
1:B:47:ILE:HD11	1:B:324:ILE:HD13	1.81	0.62
1:B:293:ARG:HH22	1:B:346:ASP:CG	2.02	0.62
1:F:246:LYS:HG2	1:F:249:ASP:OD2	2.00	0.62
1:G:403:HIS:H	1:G:403:HIS:CD2	2.15	0.62
1:B:22:ALA:O	1:B:391:ARG:NH2	2.29	0.62
1:B:376:MET:HG3	1:B:376:MET:O	1.99	0.62
1:E:413:MET:HE2	1:E:443:TYR:CE1	2.35	0.62
1:B:45:GLY:O	1:B:357:CYS:HB3	2.00	0.62
1:F:328:GLN:HE22	1:H:340:THR:HA	1.64	0.62
1:F:333:MET:CE	1:F:373:ALA:HA	2.28	0.62
1:G:221:SER:O	1:G:224:ASP:HB2	2.00	0.62
1:H:217:LEU:HB3	1:H:218:PRO:HD2	1.81	0.62
1:B:13:GLN:HG2	1:B:17:LEU:HB2	1.80	0.62
1:D:24:THR:HG23	1:D:27:GLU:HB2	1.80	0.62
1:H:133:LEU:N	1:H:133:LEU:HD23	2.15	0.62
1:B:292:ALA:CB	4:B:532:PEQ:H21	2.29	0.62
1:D:131:VAL:HG12	1:D:202:LEU:HB3	1.82	0.62
1:D:493:MET:HE2	1:D:529:VAL:HA	1.81	0.62
1:A:230:PHE:CE2	1:A:234:GLN:HG3	2.35	0.62
1:B:167:VAL:HG13	1:B:171:SER:HB2	1.82	0.62
4:C:532:PEQ:O1P	4:C:532:PEQ:H33	2.00	0.62
1:E:252:GLU:O	1:E:256:ILE:HD13	2.00	0.62
1:G:228:LEU:O	1:G:231:GLY:N	2.33	0.62
4:G:532:PEQ:H33	4:G:532:PEQ:O1P	2.00	0.62
1:A:22:ALA:O	1:A:391:ARG:NH2	2.32	0.62
1:C:244:ILE:HG13	1:C:268:SER:OG	1.99	0.62
1:H:485:VAL:HG12	1:H:486:ASP:N	2.13	0.62
1:A:54:SER:HA	1:A:59:THR:HG21	1.81	0.61
1:D:131:VAL:HG22	1:D:153:GLU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:GLU:O	1:G:197:GLU:HG2	1.98	0.61
1:G:493:MET:HE3	1:G:529:VAL:HG13	1.82	0.61
1:H:132:GLU:C	1:H:133:LEU:HD23	2.20	0.61
1:H:139:LEU:HD21	1:H:156:LEU:HB2	1.82	0.61
1:B:217:LEU:HD23	1:B:218:PRO:HD2	1.82	0.61
1:E:14:THR:HG22	1:E:37:ALA:O	2.00	0.61
1:E:47:ILE:HD13	1:E:324:ILE:HD13	1.81	0.61
1:F:50:ILE:HB	1:F:73:MET:HE3	1.81	0.61
1:A:186:GLN:O	1:A:192:LEU:HD12	2.01	0.61
1:D:173:VAL:HB	1:D:182:LEU:HD12	1.83	0.61
1:D:189:PRO:HD2	1:D:191:PHE:CD1	2.35	0.61
1:E:102:ILE:HG22	1:E:103:LEU:HD12	1.81	0.61
1:E:399:ARG:HH12	1:F:23:ASP:HB3	1.64	0.61
1:F:340:THR:H	1:F:343:GLU:HG3	1.65	0.61
1:F:341:ARG:H	1:H:328:GLN:NE2	1.98	0.61
1:H:416:VAL:CG1	1:H:445:PRO:HA	2.31	0.61
1:A:240:PHE:HB3	1:A:269:LYS:HD3	1.83	0.61
1:B:400:SER:OG	1:B:401:SER:N	2.29	0.61
1:H:92:THR:HG22	1:H:93:ALA:N	2.14	0.61
1:H:266:ILE:C	1:H:267:ILE:HD13	2.21	0.61
1:C:290:MET:HE2	1:C:326:ALA:HB2	1.82	0.61
1:A:318:ARG:NH2	1:C:27:GLU:OE2	2.34	0.61
1:F:51:GLY:O	1:F:55:ARG:HB2	1.99	0.61
1:H:224:ASP:O	1:H:228:LEU:N	2.30	0.61
1:F:24:THR:OG1	1:H:396:GLU:HG2	2.01	0.61
1:H:43:ASN:HB3	1:H:467:GLY:N	2.16	0.61
4:H:532:PEQ:H33	4:H:532:PEQ:O3P	2.00	0.61
1:G:219:ALA:HB2	1:G:249:ASP:OD1	1.99	0.60
1:A:55:ARG:HG2	1:A:86:THR:HG23	1.83	0.60
1:A:392:LYS:O	1:A:396:GLU:HG3	2.01	0.60
1:B:221:SER:O	1:B:224:ASP:HB2	2.01	0.60
1:C:226:GLN:HB3	5:C:6127:HOH:O	2.01	0.60
1:C:256:ILE:HD13	1:C:256:ILE:N	2.16	0.60
1:D:446:ARG:HD3	5:D:6142:HOH:O	1.99	0.60
1:E:436:SER:HB3	1:E:521:THR:OG1	2.01	0.60
1:F:63:MET:HG2	1:F:371:LEU:CD2	2.31	0.60
1:F:339:PRO:HG3	1:F:376:MET:HG2	1.83	0.60
1:G:135:LYS:CG	1:G:198:ASN:H	2.14	0.60
1:G:219:ALA:HB3	1:G:252:GLU:OE2	2.00	0.60
1:B:215:VAL:HG11	1:B:217:LEU:HD12	1.83	0.60
1:B:360:LEU:HD11	1:B:377:GLN:NE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:HB3	1:C:180:ILE:HD12	1.83	0.60
1:E:245:ARG:HB2	1:E:246:LYS:HE2	1.83	0.60
1:G:399:ARG:HH12	1:H:23:ASP:HB3	1.66	0.60
1:A:49:THR:OG1	1:A:361:SER:HA	2.00	0.60
1:B:232:VAL:HG23	1:B:257:LEU:HD23	1.82	0.60
1:F:176:ASP:HB3	1:F:179:LEU:HB2	1.83	0.60
4:F:532:PEQ:O1P	4:F:532:PEQ:H33	2.01	0.60
1:G:358:ILE:HG13	1:G:377:GLN:NE2	2.16	0.60
1:G:395:GLU:O	1:G:398:ALA:HB3	2.01	0.60
1:E:245:ARG:O	1:E:278:ARG:HD3	2.02	0.60
1:H:55:ARG:HG3	1:H:86:THR:CG2	2.25	0.60
1:H:187:LYS:HA	1:H:192:LEU:CD1	2.28	0.60
1:A:503:LYS:N	1:A:506:ASP:OD2	2.34	0.60
1:C:202:LEU:HD22	1:C:203:GLY:N	2.16	0.60
1:D:123:ILE:N	1:D:204:SER:OG	2.35	0.60
1:G:481:TRP:O	1:G:484:ASP:N	2.35	0.60
1:A:55:ARG:HG3	1:A:86:THR:HG23	1.82	0.60
1:G:122:LEU:O	1:G:151:CYS:HB2	2.01	0.60
1:C:173:VAL:HB	1:C:182:LEU:HD12	1.83	0.60
1:E:49:THR:OG1	1:E:361:SER:HA	2.02	0.60
1:C:351:VAL:O	1:C:354:GLY:N	2.32	0.60
1:D:123:ILE:HD11	1:D:131:VAL:CG1	2.32	0.60
1:G:15:GLN:HB3	1:G:17:LEU:HD21	1.83	0.60
1:H:220:VAL:HG13	1:H:224:ASP:CB	2.32	0.60
1:G:109:VAL:N	1:G:237:ASP:OD2	2.29	0.60
1:G:110:ALA:HA	1:G:238:MET:O	2.01	0.60
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.38	0.59
1:B:126:SER:OG	1:B:127:GLY:N	2.35	0.59
1:D:24:THR:HG22	1:D:27:GLU:HB2	1.83	0.59
1:E:279:PHE:CZ	1:E:312:ILE:HG23	2.36	0.59
1:E:506:ASP:O	1:E:529:VAL:HG23	2.02	0.59
1:H:105:ARG:NE	1:H:499:ARG:HH21	1.91	0.59
1:B:336:LYS:HG2	1:B:337:PRO:HD2	1.84	0.59
1:D:208:VAL:HG12	1:D:209:ASN:N	2.17	0.59
1:E:322:PRO:HB3	1:E:464:LEU:O	2.01	0.59
1:E:421:LYS:HG3	1:E:421:LYS:O	2.00	0.59
1:B:424:ALA:CB	1:B:509:ILE:HD13	2.32	0.59
1:E:230:PHE:O	1:E:234:GLN:HG2	2.01	0.59
1:H:56:SER:O	1:H:60:LEU:HB2	2.02	0.59
1:H:382:ARG:HH11	1:H:382:ARG:CG	2.15	0.59
1:A:133:LEU:HD13	1:A:196:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:HIS:H	1:A:403:HIS:CD2	2.20	0.59
1:B:292:ALA:HB1	4:B:532:PEQ:C2	2.30	0.59
1:F:254:ARG:NH2	1:F:287:ASP:OD2	2.35	0.59
1:D:47:ILE:HB	1:D:359:MET:HB2	1.83	0.59
1:F:63:MET:CG	1:F:371:LEU:HD21	2.33	0.59
1:A:45:GLY:O	1:A:357:CYS:HB3	2.03	0.59
1:A:166:VAL:HG21	1:A:214:ALA:O	2.02	0.59
1:G:316:CYS:SG	1:G:323:VAL:HG22	2.43	0.59
1:C:504:LYS:HG3	1:C:530:PRO:O	2.01	0.59
1:D:50:ILE:HB	1:D:73:MET:CE	2.33	0.59
1:B:64:ILE:CD1	1:B:107:VAL:HG21	2.32	0.59
1:C:306:PHE:O	1:C:310:LYS:HG2	2.03	0.59
1:E:55:ARG:HG3	1:E:86:THR:HG23	1.84	0.59
1:A:23:ASP:OD2	1:B:399:ARG:NH1	2.36	0.59
1:A:293:ARG:HH22	1:A:346:ASP:CG	2.05	0.59
1:B:485:VAL:HG12	1:B:486:ASP:N	2.15	0.59
1:D:372:GLU:N	1:D:372:GLU:OE1	2.35	0.59
1:F:168:ASP:HA	1:F:187:LYS:HE2	1.84	0.59
1:F:369:TYR:HB3	1:F:372:GLU:HB2	1.84	0.59
1:G:50:ILE:HG21	1:G:86:THR:CG2	2.33	0.59
1:G:288:GLY:C	1:G:289:ILE:HG12	2.23	0.59
1:G:306:PHE:O	1:G:310:LYS:HG3	2.03	0.59
1:G:491:LEU:O	1:G:495:VAL:HG23	2.01	0.59
1:A:288:GLY:C	1:A:289:ILE:HG12	2.23	0.59
1:D:436:SER:CB	1:D:521:THR:HG23	2.33	0.59
1:D:411:MET:CE	1:D:524:MET:HB2	2.33	0.58
1:E:263:ASN:N	1:E:263:ASN:OD1	2.36	0.58
1:H:507:VAL:HG12	1:H:508:VAL:N	2.17	0.58
4:A:532:PEQ:O1P	4:A:532:PEQ:H33	2.03	0.58
1:E:48:CYS:SG	1:E:68:MET:HG3	2.43	0.58
1:G:70:VAL:HG11	1:G:238:MET:HE1	1.85	0.58
1:E:30:CYS:O	1:G:315:ARG:NH1	2.29	0.58
1:H:259:GLU:O	1:H:262:LYS:HG2	2.03	0.58
1:B:50:ILE:HG23	1:B:54:SER:O	2.03	0.58
1:F:118:ILE:HG21	1:F:208:VAL:HB	1.86	0.58
1:G:63:MET:HG2	1:G:371:LEU:CD2	2.32	0.58
1:H:172:LYS:O	1:H:211:PRO:HD2	2.03	0.58
1:A:410:ALA:HA	1:B:421:LYS:HG2	1.84	0.58
1:G:50:ILE:HG21	1:G:86:THR:HG23	1.85	0.58
1:B:232:VAL:CG2	1:B:257:LEU:HD23	2.33	0.58
1:B:382:ARG:HH11	1:B:382:ARG:CB	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LEU:HD13	1:C:194:THR:HG21	1.86	0.58
1:D:141:ILE:HG12	1:D:142:THR:N	2.18	0.58
1:E:293:ARG:HD3	1:E:326:ALA:O	2.03	0.58
1:G:63:MET:CG	1:G:371:LEU:HD21	2.33	0.58
1:A:89:ASN:N	1:A:89:ASN:ND2	2.52	0.58
1:B:43:ASN:HB3	1:B:467:GLY:H	1.69	0.58
1:B:182:LEU:HB2	1:B:194:THR:HB	1.85	0.58
1:D:12:ILE:HG21	1:D:33:ASP:OD2	2.03	0.58
1:D:174:TYR:HB3	1:D:178:GLY:HA2	1.84	0.58
1:F:181:SER:O	1:F:197:GLU:HB3	2.04	0.58
1:F:187:LYS:HA	1:F:192:LEU:HD11	1.84	0.58
1:G:261:GLY:HA2	1:G:264:ILE:HG13	1.86	0.58
1:B:383:GLU:OE2	1:D:304:LYS:HE2	2.03	0.58
1:C:268:SER:HB2	1:C:286:SER:OG	2.04	0.58
1:F:215:VAL:HG11	1:F:217:LEU:CD1	2.26	0.58
1:H:22:ALA:HB1	1:H:27:GLU:HB3	1.85	0.58
1:H:105:ARG:NE	1:H:499:ARG:NH2	2.50	0.58
1:H:202:LEU:HD22	1:H:203:GLY:H	1.67	0.58
1:D:63:MET:HG3	1:D:371:LEU:HD21	1.84	0.58
1:H:243:PHE:N	1:H:271:GLU:OE2	2.35	0.58
1:H:439:GLN:CA	1:H:439:GLN:HE21	2.14	0.58
1:A:102:ILE:CG2	1:A:103:LEU:HD12	2.34	0.58
1:C:19:ALA:O	1:C:28:HIS:HD2	1.86	0.57
1:H:210:LEU:HD13	1:H:210:LEU:N	2.18	0.57
1:H:293:ARG:HD3	1:H:326:ALA:O	2.04	0.57
1:A:63:MET:HG3	1:A:371:LEU:CD2	2.34	0.57
1:A:493:MET:CE	1:A:530:PRO:HD2	2.33	0.57
1:B:23:ASP:OD1	1:B:23:ASP:N	2.30	0.57
1:F:167:VAL:HG11	1:F:184:VAL:HG21	1.84	0.57
1:G:15:GLN:CG	1:G:39:ILE:HG23	2.34	0.57
1:H:369:TYR:HB3	1:H:372:GLU:HB2	1.86	0.57
1:C:51:GLY:O	1:C:55:ARG:HB2	2.04	0.57
1:C:293:ARG:HH22	1:C:346:ASP:CG	2.06	0.57
1:E:220:VAL:HG22	1:E:221:SER:H	1.69	0.57
1:D:54:SER:O	1:D:60:LEU:HD13	2.04	0.57
1:H:16:GLN:HG2	1:H:32:LEU:CD2	2.34	0.57
1:A:113:THR:HG22	1:A:114:LYS:N	2.20	0.57
1:C:156:LEU:HD22	1:C:157:TRP:H	1.68	0.57
1:C:336:LYS:HB3	1:C:337:PRO:HD2	1.86	0.57
1:G:22:ALA:O	1:G:391:ARG:NH2	2.37	0.57
1:G:172:LYS:O	1:G:211:PRO:HD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PHE:HB2	1:A:112:ASP:O	2.05	0.57
1:D:189:PRO:HG2	1:D:190:ASP:OD1	2.05	0.57
1:G:175:VAL:HG12	1:G:176:ASP:N	2.19	0.57
1:D:424:ALA:HB2	1:D:509:ILE:CD1	2.35	0.57
1:F:507:VAL:O	1:F:508:VAL:HG23	2.04	0.57
1:G:477:VAL:HG12	1:G:478:GLN:N	2.19	0.57
1:H:322:PRO:HB3	1:H:464:LEU:O	2.05	0.57
1:B:228:LEU:O	1:B:231:GLY:N	2.38	0.57
1:E:272:ASN:O	1:E:276:VAL:HG23	2.05	0.57
1:H:14:THR:O	1:H:17:LEU:HB2	2.04	0.57
1:A:512:THR:HG21	1:A:525:ARG:HH21	1.69	0.57
1:F:87:ILE:O	1:F:91:ARG:HG3	2.05	0.57
1:G:45:GLY:HA3	1:G:357:CYS:HB3	1.86	0.57
1:G:202:LEU:HD22	1:G:203:GLY:H	1.68	0.57
1:A:164:CYS:O	1:A:187:LYS:HE3	2.05	0.56
1:E:114:LYS:HD3	1:E:223:LYS:CD	2.25	0.56
1:E:220:VAL:HG11	1:E:225:ILE:CD1	2.35	0.56
1:E:322:PRO:HA	1:E:356:ASP:OD2	2.05	0.56
1:A:334:ILE:HG22	1:A:335:LYS:HG2	1.87	0.56
1:A:509:ILE:HD13	1:A:526:VAL:HG22	1.84	0.56
1:G:73:MET:HE2	1:G:86:THR:HG21	1.87	0.56
1:G:219:ALA:HB3	1:G:252:GLU:CD	2.25	0.56
1:A:45:GLY:C	1:A:357:CYS:HB3	2.25	0.56
1:A:141:ILE:HD12	1:A:194:THR:HG21	1.87	0.56
1:A:292:ALA:O	1:A:296:LEU:HB2	2.05	0.56
1:E:304:LYS:O	1:E:307:LEU:HB2	2.05	0.56
1:E:399:ARG:NH1	1:F:23:ASP:HB3	2.19	0.56
1:E:512:THR:N	1:E:521:THR:HG22	2.20	0.56
1:F:30:CYS:HB3	1:H:318:ARG:NH2	2.20	0.56
1:F:123:ILE:N	1:F:204:SER:OG	2.39	0.56
1:F:315:ARG:CD	1:H:30:CYS:HB3	2.35	0.56
1:G:55:ARG:NH2	1:G:82:TYR:O	2.38	0.56
1:G:164:CYS:SG	1:G:192:LEU:HD13	2.45	0.56
1:G:483:GLU:O	1:G:487:LEU:HB3	2.05	0.56
1:H:148:MET:O	1:H:148:MET:HG2	2.04	0.56
1:H:491:LEU:O	1:H:495:VAL:HG23	2.05	0.56
1:A:341:ARG:H	1:C:328:GLN:HE21	1.51	0.56
1:B:84:ALA:HB2	1:B:230:PHE:HZ	1.68	0.56
1:E:326:ALA:HB2	1:E:359:MET:HE2	1.86	0.56
1:G:63:MET:O	1:G:68:MET:HB2	2.05	0.56
1:A:158:LEU:HD23	1:A:163:ILE:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:SER:HB2	1:F:289:ILE:CD1	2.36	0.56
1:G:485:VAL:HG12	1:G:486:ASP:OD1	2.04	0.56
1:B:75:PHE:CD1	1:B:111:LEU:HG	2.40	0.56
1:D:122:LEU:HD12	1:D:204:SER:OG	2.05	0.56
1:D:189:PRO:CD	1:D:190:ASP:H	2.19	0.56
1:D:220:VAL:HG23	1:D:224:ASP:HB3	1.87	0.56
1:A:421:LYS:HD2	1:B:404:SER:O	2.05	0.56
1:F:204:SER:O	1:F:206:LYS:HD3	2.05	0.56
1:B:293:ARG:HD2	1:B:326:ALA:O	2.04	0.56
1:B:328:GLN:NE2	1:D:340:THR:HB	2.19	0.56
1:B:391:ARG:HG2	1:B:391:ARG:HH11	1.71	0.56
1:B:482:ALA:O	1:B:486:ASP:HB2	2.05	0.56
1:C:45:GLY:O	1:C:357:CYS:HB2	2.05	0.56
1:D:220:VAL:HG23	1:D:224:ASP:CB	2.36	0.56
1:D:326:ALA:O	1:D:327:THR:HB	2.04	0.56
1:F:315:ARG:HG3	1:H:30:CYS:HB3	1.86	0.56
1:G:228:LEU:HD12	1:G:256:ILE:HG21	1.88	0.56
1:H:157:TRP:C	1:H:158:LEU:HD13	2.25	0.56
1:H:316:CYS:HB2	1:H:323:VAL:CG2	2.36	0.56
1:A:332:SER:HB3	1:A:343:GLU:OE1	2.06	0.56
1:A:509:ILE:HD11	1:A:526:VAL:HG22	1.87	0.56
1:F:215:VAL:HG12	1:F:217:LEU:H	1.71	0.56
1:G:21:MET:HA	1:G:21:MET:CE	2.36	0.56
1:A:173:VAL:HG22	1:A:210:LEU:CD2	2.36	0.56
1:B:424:ALA:HB2	1:B:509:ILE:HD13	1.87	0.56
1:E:457:GLN:HG2	1:E:461:GLN:NE2	2.21	0.56
1:G:338:ARG:HH22	1:G:341:ARG:NH2	2.02	0.56
1:G:477:VAL:HG13	1:G:484:ASP:OD2	2.06	0.56
1:G:495:VAL:O	1:G:498:ALA:HB3	2.06	0.56
1:B:73:MET:HE1	1:B:86:THR:HG21	1.88	0.55
1:C:215:VAL:CG1	1:C:217:LEU:HD12	2.35	0.55
1:F:221:SER:O	1:F:224:ASP:HB2	2.06	0.55
1:G:105:ARG:HD3	1:G:499:ARG:HH21	1.71	0.55
1:G:323:VAL:N	1:G:356:ASP:HB2	2.14	0.55
1:G:382:ARG:HH11	1:G:382:ARG:CG	2.19	0.55
1:H:354:GLY:C	1:H:466:ARG:HH12	2.09	0.55
1:B:223:LYS:HA	1:B:226:GLN:OE1	2.06	0.55
1:C:220:VAL:HG13	1:C:224:ASP:HB2	1.88	0.55
1:C:246:LYS:HE2	1:C:249:ASP:OD1	2.07	0.55
1:D:83:HIS:O	1:D:87:ILE:HG13	2.06	0.55
1:G:515:ARG:HB2	1:G:516:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:ASN:HD22	1:H:272:ASN:H	1.55	0.55
1:B:138:THR:HG23	1:B:139:LEU:N	2.21	0.55
1:C:526:VAL:HG23	1:D:411:MET:SD	2.45	0.55
1:F:56:SER:O	1:F:60:LEU:HD22	2.06	0.55
1:H:15:GLN:CB	1:H:17:LEU:HD23	2.21	0.55
1:H:512:THR:OG1	1:H:513:GLY:N	2.35	0.55
1:B:56:SER:OG	1:B:59:THR:HB	2.06	0.55
1:F:16:GLN:NE2	5:F:6168:HOH:O	2.30	0.55
1:F:24:THR:HG22	1:F:27:GLU:HB2	1.88	0.55
1:F:175:VAL:HB	1:F:180:ILE:HB	1.88	0.55
1:F:231:GLY:O	1:F:236:VAL:HG22	2.06	0.55
1:A:131:VAL:HG12	1:A:202:LEU:HB3	1.89	0.55
1:A:341:ARG:N	1:C:328:GLN:NE2	2.55	0.55
1:B:215:VAL:HG13	1:B:217:LEU:HD12	1.85	0.55
1:F:202:LEU:HD23	1:F:203:GLY:N	2.21	0.55
1:F:376:MET:O	1:F:380:ILE:HG13	2.06	0.55
1:F:428:ILE:HD12	1:F:508:VAL:CG1	2.36	0.55
1:H:265:LYS:HA	1:H:287:ASP:OD2	2.06	0.55
1:A:454:ARG:NH2	1:A:484:ASP:OD1	2.31	0.55
1:B:109:VAL:HG12	1:B:236:VAL:HG12	1.89	0.55
1:B:122:LEU:HA	1:B:204:SER:OG	2.07	0.55
1:D:493:MET:CE	1:D:529:VAL:HA	2.36	0.55
1:A:186:GLN:HB2	1:A:193:VAL:HB	1.87	0.55
1:A:259:GLU:O	1:A:262:LYS:HG2	2.06	0.55
1:D:151:CYS:HB3	1:D:156:LEU:HD23	1.89	0.55
1:E:269:LYS:HD2	1:E:290:MET:SD	2.46	0.55
1:D:155:ILE:HG22	1:D:156:LEU:N	2.22	0.55
1:E:334:ILE:HD13	1:E:363:GLU:HA	1.89	0.55
1:G:160:TYR:OH	1:G:216:ASP:HB2	2.07	0.55
1:C:457:GLN:O	1:C:461:GLN:HG3	2.06	0.55
1:D:189:PRO:HD2	1:D:190:ASP:H	1.72	0.55
1:F:122:LEU:O	1:F:151:CYS:HB2	2.06	0.55
1:A:453:THR:CG2	1:A:459:ALA:HB2	2.37	0.55
1:A:484:ASP:O	1:A:488:ARG:HG3	2.06	0.55
1:B:105:ARG:HG2	5:B:6110:HOH:O	2.06	0.55
1:B:145:ASN:N	1:B:145:ASN:ND2	2.49	0.55
1:B:237:ASP:OD1	1:B:460:ARG:NH1	2.30	0.55
1:F:428:ILE:HD12	1:F:508:VAL:HG11	1.89	0.55
1:G:292:ALA:O	1:G:296:LEU:HB2	2.05	0.55
1:H:50:ILE:HB	1:H:73:MET:HE3	1.89	0.55
1:H:429:VAL:O	1:H:451:ALA:HA	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:ASP:OD2	1:F:460:ARG:NH1	2.29	0.54
1:G:416:VAL:CG1	1:G:445:PRO:HA	2.36	0.54
1:D:18:HIS:HB2	5:D:6141:HOH:O	2.07	0.54
1:G:493:MET:HE2	1:G:529:VAL:HG13	1.89	0.54
1:H:63:MET:HG3	1:H:371:LEU:HD21	1.87	0.54
1:A:267:ILE:HD12	1:A:288:GLY:HA3	1.89	0.54
1:E:431:THR:CG2	1:E:434:GLY:HA2	2.36	0.54
1:F:225:ILE:HG22	1:F:226:GLN:N	2.21	0.54
1:G:135:LYS:HG3	1:G:198:ASN:N	2.21	0.54
1:G:410:ALA:HB2	1:H:421:LYS:HG3	1.88	0.54
1:A:168:ASP:O	1:A:171:SER:HB2	2.07	0.54
1:B:30:CYS:O	1:D:315:ARG:NH1	2.36	0.54
1:B:61:LYS:O	1:B:65:LYS:HB2	2.07	0.54
1:B:433:SER:HB2	1:B:435:ARG:HD3	1.88	0.54
1:D:292:ALA:HB1	4:D:532:PEQ:C1	2.37	0.54
1:G:132:GLU:HG3	1:G:201:PHE:CZ	2.42	0.54
1:G:347:VAL:O	1:G:350:ALA:HB3	2.08	0.54
1:A:63:MET:HG3	1:A:371:LEU:HD21	1.90	0.54
1:A:73:MET:HB3	1:A:75:PHE:HE1	1.72	0.54
1:B:454:ARG:HG3	1:B:473:CYS:HB3	1.89	0.54
1:D:438:HIS:O	1:D:441:ALA:HB3	2.08	0.54
1:E:315:ARG:NH1	1:G:30:CYS:O	2.41	0.54
1:G:25:PHE:O	1:G:28:HIS:HB3	2.07	0.54
1:G:76:SER:HA	1:G:114:LYS:HB2	1.90	0.54
1:G:370:PRO:O	1:G:374:VAL:HG23	2.07	0.54
1:B:19:ALA:HA	1:B:31:ARG:HD3	1.89	0.54
1:B:167:VAL:CG2	1:B:210:LEU:HD23	2.38	0.54
1:B:322:PRO:HA	1:B:356:ASP:OD2	2.08	0.54
1:C:43:ASN:CB	1:C:467:GLY:HA2	2.37	0.54
1:G:410:ALA:HA	1:H:421:LYS:CG	2.36	0.54
1:B:290:MET:HE2	1:B:326:ALA:CB	2.38	0.54
1:G:410:ALA:HB2	1:H:422:CYS:HB3	1.88	0.54
1:H:382:ARG:HB2	1:H:382:ARG:NH1	2.23	0.54
1:B:352:LEU:HD22	1:B:384:ALA:HB1	1.90	0.54
1:B:512:THR:N	1:B:521:THR:HG22	2.23	0.54
1:C:122:LEU:HD12	1:C:204:SER:OG	2.07	0.54
1:G:220:VAL:HG22	1:G:224:ASP:CB	2.37	0.54
1:H:330:LEU:HG	1:H:333:MET:SD	2.48	0.54
1:H:453:THR:CG2	1:H:459:ALA:HB2	2.38	0.54
1:B:283:LEU:HD22	1:B:321:LYS:HD3	1.89	0.54
1:B:407:LEU:HB3	1:B:520:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:SER:OG	5:B:6001:HOH:O	2.18	0.54
1:D:50:ILE:HD13	1:D:50:ILE:N	2.23	0.54
1:G:316:CYS:HB2	1:G:323:VAL:CG2	2.38	0.54
1:A:330:LEU:O	1:A:333:MET:HB2	2.07	0.54
1:B:154:ASN:O	1:B:155:ILE:HG13	2.08	0.54
1:F:292:ALA:CB	4:F:532:PEQ:H21	2.38	0.54
1:H:63:MET:HB3	1:H:68:MET:HE3	1.89	0.54
1:A:525:ARG:HA	1:B:522:ASN:O	2.08	0.53
1:B:524:MET:HG2	1:B:525:ARG:N	2.21	0.53
1:D:175:VAL:CG2	1:D:182:LEU:HD11	2.38	0.53
1:F:332:SER:O	1:F:334:ILE:N	2.41	0.53
1:G:109:VAL:HG12	1:G:236:VAL:HG12	1.90	0.53
1:G:182:LEU:CD2	1:G:196:VAL:HG22	2.38	0.53
1:G:473:CYS:HB2	1:G:491:LEU:HD23	1.89	0.53
1:H:91:ARG:NH2	1:H:235:ASP:O	2.42	0.53
1:H:123:ILE:HD11	1:H:202:LEU:HD13	1.90	0.53
1:H:496:GLY:HA3	1:H:502:PHE:CE1	2.42	0.53
1:C:251:HIS:O	1:C:254:ARG:HB3	2.08	0.53
1:E:106:PRO:O	1:E:463:HIS:HE1	1.91	0.53
1:E:112:ASP:OD2	1:E:269:LYS:NZ	2.30	0.53
1:F:145:ASN:N	1:F:145:ASN:ND2	2.56	0.53
1:G:70:VAL:HG12	1:G:71:ALA:N	2.21	0.53
1:A:102:ILE:HG22	1:A:103:LEU:CD1	2.37	0.53
1:B:512:THR:O	1:B:523:THR:HB	2.09	0.53
1:D:196:VAL:HG12	1:D:196:VAL:O	2.08	0.53
1:H:58:GLU:O	1:H:61:LYS:HB2	2.09	0.53
1:H:428:ILE:HD12	1:H:508:VAL:HG11	1.90	0.53
1:A:341:ARG:H	1:C:328:GLN:NE2	2.06	0.53
1:G:109:VAL:HG23	1:G:237:ASP:OD2	2.08	0.53
1:H:328:GLN:HA	1:H:331:GLU:HG2	1.89	0.53
1:H:358:ILE:HG13	1:H:377:GLN:HE22	1.73	0.53
1:C:411:MET:SD	1:D:526:VAL:HG23	2.48	0.53
1:D:119:ARG:N	1:D:159:ASP:OD1	2.33	0.53
1:E:327:THR:HG22	1:E:328:GLN:HG3	1.90	0.53
1:F:292:ALA:HB1	4:F:532:PEQ:H21	1.89	0.53
1:F:328:GLN:NE2	1:H:341:ARG:N	2.53	0.53
1:G:293:ARG:NH1	1:G:327:THR:O	2.42	0.53
1:B:131:VAL:HG13	1:B:132:GLU:N	2.24	0.53
1:B:465:TYR:HB2	1:B:468:ILE:HD12	1.91	0.53
1:C:143:LEU:HD12	1:C:190:ASP:HA	1.90	0.53
1:D:141:ILE:HB	1:D:156:LEU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:THR:O	1:D:453:THR:HB	2.08	0.53
1:E:270:ILE:HD11	1:E:289:ILE:HD12	1.91	0.53
1:G:17:LEU:N	1:G:17:LEU:HD23	2.24	0.53
1:G:237:ASP:OD1	1:G:460:ARG:NH1	2.30	0.53
1:A:493:MET:HE2	1:A:530:PRO:CD	2.34	0.53
1:C:417:GLU:OE1	1:D:417:GLU:OE1	2.27	0.53
1:F:515:ARG:HB3	1:F:516:PRO:CD	2.36	0.53
1:H:65:LYS:HA	1:H:105:ARG:NH1	2.23	0.53
1:D:154:ASN:HB2	1:D:155:ILE:CD1	2.37	0.53
1:E:111:LEU:HB3	1:E:239:VAL:HG22	1.91	0.53
1:G:312:ILE:HG22	1:G:313:ILE:N	2.23	0.53
1:A:333:MET:HA	1:A:336:LYS:O	2.09	0.53
1:A:376:MET:O	1:A:380:ILE:HG13	2.08	0.53
1:A:503:LYS:O	1:A:529:VAL:HB	2.09	0.53
1:B:237:ASP:CG	1:B:460:ARG:HD2	2.29	0.53
1:F:138:THR:HG22	1:F:138:THR:O	2.09	0.53
1:A:175:VAL:HG12	1:A:176:ASP:N	2.24	0.52
1:A:224:ASP:O	1:A:227:ASP:HB2	2.08	0.52
1:A:506:ASP:HB2	1:A:529:VAL:HG21	1.91	0.52
1:D:118:ILE:CG2	1:D:208:VAL:HB	2.38	0.52
1:F:376:MET:HA	1:F:376:MET:CE	2.38	0.52
1:G:61:LYS:HD3	1:G:93:ALA:CA	2.37	0.52
1:H:220:VAL:CG1	1:H:224:ASP:HB2	2.39	0.52
1:E:54:SER:O	1:E:60:LEU:HD11	2.08	0.52
1:E:274:GLU:O	1:E:277:ARG:N	2.42	0.52
1:E:368:ASP:C	1:E:370:PRO:HD3	2.29	0.52
1:F:263:ASN:OD1	1:F:263:ASN:N	2.40	0.52
1:G:457:GLN:O	1:G:460:ARG:N	2.30	0.52
1:H:328:GLN:CA	1:H:331:GLU:HG3	2.38	0.52
1:A:123:ILE:HA	1:A:151:CYS:O	2.08	0.52
1:A:415:SER:HA	1:A:524:MET:CE	2.40	0.52
1:B:228:LEU:HD12	1:B:256:ILE:HG21	1.91	0.52
1:G:453:THR:CG2	1:G:459:ALA:HB2	2.39	0.52
1:B:42:ARG:HD2	1:B:44:THR:O	2.09	0.52
1:B:167:VAL:CG1	1:B:171:SER:HB2	2.39	0.52
1:D:139:LEU:HD11	1:D:153:GLU:O	2.09	0.52
1:D:202:LEU:HD22	1:D:203:GLY:N	2.24	0.52
1:E:328:GLN:NE2	1:G:341:ARG:HG2	2.25	0.52
1:G:126:SER:OG	1:G:127:GLY:N	2.40	0.52
1:G:261:GLY:CA	1:G:264:ILE:HG13	2.39	0.52
1:G:272:ASN:ND2	5:G:6179:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:290:MET:HE2	1:G:326:ALA:CB	2.39	0.52
1:H:122:LEU:HD23	1:H:149:GLU:HG3	1.91	0.52
1:A:172:LYS:NZ	1:A:197:GLU:OE1	2.40	0.52
1:A:253:VAL:O	1:A:257:LEU:HB2	2.10	0.52
1:B:328:GLN:CG	1:B:331:GLU:HG3	2.38	0.52
1:C:103:LEU:HD12	1:C:103:LEU:N	2.24	0.52
1:C:493:MET:HE2	1:C:529:VAL:HG13	1.90	0.52
1:D:70:VAL:HG22	1:D:108:ALA:HB3	1.92	0.52
1:H:316:CYS:HB3	1:H:321:LYS:O	2.09	0.52
1:B:316:CYS:HB3	1:B:321:LYS:O	2.09	0.52
1:C:334:ILE:HG23	1:C:367:GLY:HA2	1.92	0.52
1:C:439:GLN:O	1:C:442:ARG:HB3	2.10	0.52
1:E:54:SER:HA	1:E:59:THR:HG21	1.91	0.52
1:F:297:GLY:HA2	1:F:305:VAL:HG21	1.91	0.52
1:H:95:GLU:OE1	1:H:98:ALA:HB2	2.09	0.52
1:H:97:PHE:C	1:H:99:SER:H	2.11	0.52
1:A:311:MET:SD	1:A:315:ARG:HD3	2.49	0.52
1:B:455:ASN:HB3	1:B:458:THR:HB	1.91	0.52
1:A:50:ILE:HG13	1:A:71:ALA:HB1	1.92	0.52
1:B:122:LEU:HB2	1:B:149:GLU:HA	1.92	0.52
1:B:145:ASN:HD22	1:B:145:ASN:H	1.53	0.52
1:G:141:ILE:HG21	1:G:158:LEU:HD22	1.92	0.52
1:A:103:LEU:HD12	1:A:103:LEU:N	2.24	0.52
1:A:504:LYS:O	1:A:529:VAL:O	2.28	0.52
1:D:133:LEU:HD12	1:D:180:ILE:HG21	1.92	0.52
1:F:339:PRO:HG3	1:F:376:MET:CG	2.40	0.52
1:G:360:LEU:HA	1:G:363:GLU:OE1	2.09	0.52
1:H:334:ILE:HG22	1:H:335:LYS:HG3	1.90	0.52
1:A:228:LEU:HD22	1:A:257:LEU:HD11	1.92	0.52
1:A:250:VAL:O	1:A:250:VAL:HG12	2.10	0.52
1:D:266:ILE:C	1:D:267:ILE:HD12	2.31	0.52
1:E:369:TYR:N	1:E:370:PRO:HD3	2.25	0.52
1:G:385:GLU:O	1:G:388:MET:HG3	2.11	0.52
1:H:170:GLY:N	1:H:184:VAL:O	2.32	0.52
1:H:360:LEU:HD11	1:H:377:GLN:NE2	2.25	0.52
1:F:521:THR:HG22	1:F:521:THR:O	2.10	0.51
1:G:85:GLU:O	1:G:88:LYS:HB3	2.10	0.51
1:A:267:ILE:HD12	1:A:288:GLY:CA	2.39	0.51
1:D:50:ILE:HB	1:D:73:MET:HE2	1.91	0.51
1:F:274:GLU:OE2	1:F:278:ARG:HD2	2.10	0.51
1:G:493:MET:HE2	1:G:529:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:HG	1:B:190:ASP:O	2.10	0.51
1:B:283:LEU:CD2	1:B:321:LYS:HD3	2.40	0.51
1:H:45:GLY:O	1:H:357:CYS:HB3	2.10	0.51
1:H:169:VAL:HA	1:H:184:VAL:HG12	1.91	0.51
1:A:123:ILE:N	1:A:204:SER:OG	2.33	0.51
1:A:426:ALA:O	1:A:508:VAL:HG22	2.11	0.51
1:C:115:GLY:HA2	1:C:224:ASP:OD2	2.09	0.51
1:F:283:LEU:CD2	1:F:321:LYS:HD2	2.40	0.51
1:G:16:GLN:OE1	1:G:33:ASP:O	2.28	0.51
1:H:427:LEU:HD12	1:H:427:LEU:N	2.25	0.51
1:A:160:TYR:CE1	1:A:217:LEU:HD11	2.46	0.51
1:B:173:VAL:HB	1:B:182:LEU:CD1	2.38	0.51
1:C:393:LEU:O	1:C:397:LEU:HB2	2.11	0.51
1:E:390:HIS:NE2	1:E:446:ARG:HG3	2.26	0.51
1:H:16:GLN:O	1:H:20:ALA:HB2	2.10	0.51
1:H:292:ALA:HB1	4:H:532:PEQ:H21	1.92	0.51
1:A:162:ASN:HB3	1:A:165:LYS:HE3	1.92	0.51
1:A:246:LYS:HD2	1:A:248:ALA:HB3	1.92	0.51
1:A:281:GLU:HG3	1:A:282:ILE:N	2.24	0.51
1:A:355:ALA:O	1:A:466:ARG:NH1	2.44	0.51
1:C:48:CYS:SG	1:C:68:MET:HG3	2.50	0.51
1:C:215:VAL:HG11	1:C:217:LEU:HD12	1.93	0.51
1:E:220:VAL:HG11	1:E:225:ILE:CG1	2.41	0.51
1:F:157:TRP:O	1:F:158:LEU:HD13	2.10	0.51
1:F:310:LYS:NZ	1:H:349:ASN:HD21	2.09	0.51
1:F:327:THR:HG22	1:F:328:GLN:HG3	1.92	0.51
1:G:47:ILE:HG12	1:G:70:VAL:HB	1.92	0.51
1:G:417:GLU:OE1	1:H:417:GLU:OE1	2.29	0.51
1:G:504:LYS:O	1:G:529:VAL:O	2.29	0.51
1:H:66:SER:OG	1:H:375:ARG:NH2	2.44	0.51
1:A:421:LYS:NZ	1:B:404:SER:O	2.41	0.51
1:A:499:ARG:HB3	1:A:501:PHE:CE1	2.46	0.51
1:D:157:TRP:O	1:D:158:LEU:HD12	2.11	0.51
1:E:259:GLU:O	1:E:262:LYS:HG2	2.10	0.51
1:F:220:VAL:HG22	1:F:224:ASP:HB2	1.93	0.51
1:G:156:LEU:HD23	1:G:157:TRP:H	1.74	0.51
1:H:268:SER:HB2	1:H:286:SER:OG	2.10	0.51
1:H:485:VAL:O	1:H:489:VAL:HG23	2.11	0.51
1:H:504:LYS:O	1:H:529:VAL:O	2.29	0.51
1:A:483:GLU:O	1:A:487:LEU:HB2	2.11	0.51
1:B:276:VAL:HG11	1:D:34:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:MET:HA	1:B:336:LYS:O	2.10	0.51
1:B:408:MET:HE3	1:B:411:MET:HB3	1.93	0.51
1:C:139:LEU:HD23	1:C:139:LEU:C	2.31	0.51
1:F:141:ILE:HG22	1:F:156:LEU:CB	2.39	0.51
1:F:272:ASN:HB2	1:F:299:GLU:HG2	1.93	0.51
1:G:419:SER:HB2	1:G:427:LEU:HD11	1.92	0.51
1:H:56:SER:O	1:H:60:LEU:HD22	2.11	0.51
1:B:123:ILE:O	1:B:124:LYS:HB2	2.11	0.51
1:C:224:ASP:O	1:C:228:LEU:HG	2.11	0.51
1:F:72:ARG:NH2	4:F:532:PEQ:O1P	2.42	0.51
1:G:61:LYS:CG	1:G:93:ALA:HB1	2.35	0.51
1:H:242:SER:CA	1:H:269:LYS:HE2	2.37	0.51
1:H:328:GLN:HG2	1:H:331:GLU:CG	2.41	0.51
1:B:462:ALA:HB1	1:B:468:ILE:HG21	1.92	0.51
1:C:326:ALA:O	1:C:327:THR:HB	2.10	0.51
1:D:323:VAL:O	1:D:356:ASP:HB2	2.11	0.51
1:F:293:ARG:HH22	1:F:346:ASP:CG	2.11	0.51
1:G:123:ILE:HB	1:G:204:SER:OG	2.10	0.51
1:G:411:MET:O	1:G:415:SER:OG	2.29	0.51
1:H:15:GLN:OE1	1:H:446:ARG:HD2	2.10	0.51
1:C:138:THR:HG22	1:C:138:THR:O	2.10	0.50
1:E:55:ARG:NE	1:E:82:TYR:CE1	2.79	0.50
1:G:118:ILE:HG23	1:G:160:TYR:HB2	1.92	0.50
1:G:291:VAL:HG12	1:G:293:ARG:HG3	1.93	0.50
1:G:504:LYS:HG3	1:G:530:PRO:OXT	2.11	0.50
1:H:181:SER:O	1:H:197:GLU:O	2.30	0.50
1:B:186:GLN:HG3	1:B:187:LYS:O	2.11	0.50
1:B:224:ASP:O	1:B:228:LEU:HG	2.11	0.50
1:C:27:GLU:OE1	1:C:31:ARG:NH2	2.43	0.50
1:C:220:VAL:HG11	1:C:225:ILE:HG12	1.93	0.50
1:E:72:ARG:HG2	1:E:73:MET:N	2.26	0.50
1:E:217:LEU:HB3	1:E:218:PRO:HD2	1.93	0.50
1:G:113:THR:HG22	1:G:242:SER:H	1.76	0.50
1:G:333:MET:HE1	1:G:372:GLU:O	2.11	0.50
1:H:291:VAL:HG22	1:H:312:ILE:HG21	1.93	0.50
1:F:167:VAL:HG12	1:F:168:ASP:N	2.26	0.50
1:B:283:LEU:HD22	1:B:321:LYS:CD	2.40	0.50
1:C:395:GLU:O	1:C:399:ARG:HG2	2.11	0.50
1:C:401:SER:O	1:D:421:LYS:NZ	2.45	0.50
1:E:390:HIS:CD2	1:E:446:ARG:NH1	2.80	0.50
1:F:318:ARG:NH2	1:H:27:GLU:OE2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:300:ILE:HB	1:G:301:PRO:HD2	1.92	0.50
1:H:503:LYS:N	1:H:506:ASP:OD2	2.38	0.50
1:B:239:VAL:O	1:B:239:VAL:HG12	2.11	0.50
1:D:181:SER:O	1:D:197:GLU:O	2.30	0.50
1:D:237:ASP:OD2	1:D:460:ARG:HD2	2.12	0.50
1:D:333:MET:HA	1:D:336:LYS:O	2.12	0.50
1:H:286:SER:HB2	1:H:288:GLY:O	2.12	0.50
1:B:118:ILE:HB	1:B:208:VAL:HB	1.94	0.50
1:B:181:SER:O	1:B:197:GLU:O	2.29	0.50
1:E:42:ARG:HG3	1:E:381:ALA:HB3	1.93	0.50
1:E:334:ILE:HD11	1:E:363:GLU:N	2.26	0.50
1:A:289:ILE:O	1:A:323:VAL:HA	2.11	0.50
1:B:93:ALA:O	1:B:96:SER:HB3	2.10	0.50
1:B:340:THR:HA	1:D:328:GLN:OE1	2.11	0.50
1:E:227:ASP:O	1:E:230:PHE:HB3	2.12	0.50
1:F:349:ASN:HD21	1:H:310:LYS:HZ2	1.57	0.50
1:G:15:GLN:HB3	1:G:17:LEU:CD2	2.42	0.50
1:G:61:LYS:HE2	1:G:96:SER:OG	2.11	0.50
1:G:431:THR:CG2	1:G:434:GLY:HA2	2.41	0.50
1:G:493:MET:HG2	1:G:530:PRO:HD2	1.94	0.50
1:A:267:ILE:HD13	1:A:267:ILE:N	2.18	0.50
1:A:411:MET:O	1:A:415:SER:OG	2.30	0.50
1:B:167:VAL:HG12	1:B:168:ASP:N	2.26	0.50
1:C:447:ALA:HB1	1:C:448:PRO:HD2	1.94	0.50
1:E:75:PHE:CZ	1:E:83:HIS:CD2	3.00	0.50
1:E:339:PRO:HG3	1:E:376:MET:HG2	1.93	0.50
1:F:122:LEU:HA	1:F:204:SER:OG	2.11	0.50
1:G:158:LEU:HD23	1:G:163:ILE:HD13	1.93	0.50
1:G:228:LEU:CD1	1:G:256:ILE:HG21	2.42	0.50
1:H:80:HIS:HB3	1:H:230:PHE:CE1	2.47	0.50
1:H:403:HIS:H	1:H:403:HIS:CD2	2.29	0.50
1:A:54:SER:O	1:A:60:LEU:HD13	2.11	0.50
1:A:131:VAL:HG22	1:A:153:GLU:HB3	1.93	0.50
1:D:504:LYS:O	1:D:529:VAL:O	2.30	0.50
1:E:102:ILE:HG22	1:E:103:LEU:HD11	1.93	0.50
1:E:340:THR:HB	1:G:328:GLN:NE2	2.26	0.50
1:F:293:ARG:O	1:H:341:ARG:NE	2.43	0.50
1:H:272:ASN:HD22	1:H:272:ASN:N	2.09	0.50
1:B:25:PHE:CE1	1:B:392:LYS:HD3	2.47	0.49
1:B:237:ASP:OD1	1:B:460:ARG:HD2	2.11	0.49
1:D:271:GLU:HG2	1:D:295:ASP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:LYS:HE3	1:F:404:SER:O	2.12	0.49
1:E:504:LYS:O	1:E:529:VAL:O	2.30	0.49
1:G:14:THR:O	1:G:15:GLN:HB2	2.12	0.49
1:H:22:ALA:HA	1:H:31:ARG:NH1	2.27	0.49
1:A:417:GLU:OE1	1:B:417:GLU:OE1	2.30	0.49
1:B:481:TRP:CZ3	1:B:516:PRO:HA	2.47	0.49
1:C:504:LYS:O	1:C:529:VAL:O	2.29	0.49
1:D:113:THR:HG23	1:D:115:GLY:N	2.27	0.49
1:E:215:VAL:CG1	1:E:217:LEU:HD13	2.41	0.49
1:E:429:VAL:O	1:E:451:ALA:HA	2.12	0.49
1:G:55:ARG:NH1	1:G:82:TYR:CE1	2.80	0.49
1:G:215:VAL:HG13	1:G:217:LEU:H	1.77	0.49
1:G:527:VAL:CG1	1:G:528:PRO:HD2	2.42	0.49
1:H:77:HIS:O	1:H:78:GLY:O	2.30	0.49
1:A:43:ASN:CB	1:A:467:GLY:HA2	2.36	0.49
1:C:322:PRO:HB3	1:C:464:LEU:O	2.13	0.49
1:D:293:ARG:HH22	1:D:346:ASP:CG	2.15	0.49
1:E:75:PHE:CE2	1:E:83:HIS:CD2	3.00	0.49
1:F:63:MET:HG3	1:F:371:LEU:HD21	1.93	0.49
1:H:17:LEU:O	1:H:20:ALA:HB3	2.12	0.49
1:H:292:ALA:CB	4:H:532:PEQ:H21	2.41	0.49
1:H:316:CYS:O	1:H:320:GLY:N	2.45	0.49
5:A:6133:HOH:O	1:C:345:SER:HB2	2.12	0.49
1:B:221:SER:N	1:B:224:ASP:HB2	2.24	0.49
1:C:41:ALA:HB2	1:C:501:PHE:CE1	2.47	0.49
1:C:185:LYS:HG2	1:C:193:VAL:HG12	1.94	0.49
1:D:228:LEU:HD22	1:D:257:LEU:HD11	1.93	0.49
1:E:475:ASP:HB3	1:E:476:PRO:HD2	1.93	0.49
1:G:327:THR:HG22	1:G:328:GLN:HG3	1.93	0.49
1:G:461:GLN:O	1:G:464:LEU:HB2	2.12	0.49
1:H:332:SER:OG	1:H:343:GLU:OE1	2.29	0.49
1:B:221:SER:H	1:B:224:ASP:CB	2.22	0.49
1:F:22:ALA:O	1:F:389:PHE:HZ	1.96	0.49
1:G:63:MET:CA	1:G:371:LEU:HD21	2.42	0.49
1:B:273:HIS:CD2	1:B:277:ARG:HH21	2.29	0.49
1:D:497:LYS:HD2	1:D:529:VAL:CG1	2.42	0.49
4:D:532:PEQ:O1P	4:D:532:PEQ:H33	2.11	0.49
1:F:135:LYS:HA	1:F:196:VAL:HG12	1.94	0.49
1:F:242:SER:CA	1:F:269:LYS:HE2	2.38	0.49
1:G:182:LEU:HD23	1:G:196:VAL:HG22	1.94	0.49
1:H:279:PHE:HE1	1:H:289:ILE:HD13	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ASN:OD1	1:E:76:SER:OG	2.30	0.49
1:F:152:ASP:O	1:F:155:ILE:O	2.30	0.49
1:B:111:LEU:HD23	1:B:111:LEU:C	2.32	0.49
1:D:144:ASP:HB3	1:D:147:TYR:HD2	1.77	0.49
1:E:73:MET:HE3	1:E:87:ILE:HG13	1.93	0.49
1:G:109:VAL:CG1	1:G:236:VAL:HG12	2.42	0.49
1:A:276:VAL:O	1:A:279:PHE:HB2	2.13	0.49
1:A:283:LEU:O	1:A:283:LEU:HD22	2.13	0.49
1:B:326:ALA:O	1:B:327:THR:HB	2.12	0.49
1:B:503:LYS:HG2	1:B:504:LYS:N	2.22	0.49
1:C:279:PHE:CE1	1:C:289:ILE:HD12	2.46	0.49
1:E:419:SER:HB3	1:E:509:ILE:HD12	1.95	0.49
4:E:532:PEQ:O1P	4:E:532:PEQ:H33	2.13	0.49
1:F:50:ILE:HB	1:F:73:MET:HE1	1.94	0.49
1:G:48:CYS:SG	1:G:68:MET:HG3	2.52	0.49
1:G:105:ARG:HD3	1:G:499:ARG:NH2	2.27	0.49
1:G:334:ILE:HD11	1:G:362:GLY:C	2.33	0.49
1:G:503:LYS:O	1:G:529:VAL:HB	2.12	0.49
1:B:411:MET:O	1:B:415:SER:OG	2.31	0.49
4:B:532:PEQ:H33	4:B:532:PEQ:O1P	2.13	0.49
1:C:329:MET:O	1:C:330:LEU:HD12	2.12	0.49
1:D:493:MET:CE	1:D:529:VAL:HG22	2.43	0.49
1:F:328:GLN:NE2	1:H:340:THR:HA	2.27	0.49
1:F:411:MET:O	1:F:415:SER:OG	2.31	0.49
1:G:322:PRO:HA	1:G:356:ASP:CG	2.33	0.49
1:H:119:ARG:HA	1:H:206:LYS:O	2.12	0.49
1:A:16:GLN:HA	5:A:6092:HOH:O	2.12	0.48
1:A:329:MET:O	1:A:343:GLU:HG2	2.13	0.48
1:B:160:TYR:HE2	1:B:166:VAL:HG11	1.78	0.48
1:D:445:PRO:HG2	1:D:449:ILE:HD11	1.95	0.48
1:E:456:HIS:N	1:E:456:HIS:CD2	2.80	0.48
1:G:15:GLN:C	1:G:17:LEU:HD23	2.33	0.48
1:G:439:GLN:HE21	1:G:439:GLN:CA	2.26	0.48
1:H:103:LEU:HA	1:H:499:ARG:NH1	2.23	0.48
1:A:407:LEU:N	1:A:407:LEU:HD23	2.28	0.48
1:B:254:ARG:O	1:B:258:GLY:N	2.39	0.48
1:B:524:MET:HE3	1:B:524:MET:HB3	1.75	0.48
1:D:152:ASP:O	1:D:155:ILE:O	2.31	0.48
1:D:197:GLU:O	1:D:198:ASN:HB2	2.12	0.48
1:D:493:MET:HE2	1:D:529:VAL:HG22	1.95	0.48
1:F:167:VAL:HG12	1:F:168:ASP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:LEU:HA	1:H:338:ARG:HH22	1.78	0.48
1:B:115:GLY:HA2	1:B:224:ASP:OD2	2.13	0.48
1:E:220:VAL:HG11	1:E:225:ILE:HG12	1.96	0.48
1:F:24:THR:HG23	1:F:27:GLU:H	1.77	0.48
1:F:73:MET:HE2	1:F:86:THR:HG21	1.95	0.48
1:F:220:VAL:CG2	1:F:224:ASP:HB3	2.43	0.48
1:G:43:ASN:H	1:G:385:GLU:CD	2.15	0.48
1:G:61:LYS:HE2	1:G:96:SER:CB	2.44	0.48
1:H:515:ARG:HB3	1:H:516:PRO:CD	2.42	0.48
1:A:73:MET:HB3	1:A:75:PHE:CE1	2.47	0.48
1:A:326:ALA:O	1:A:327:THR:HB	2.13	0.48
1:B:100:ASP:OD1	1:B:102:ILE:HB	2.12	0.48
1:B:192:LEU:HD12	1:B:192:LEU:HA	1.70	0.48
1:B:254:ARG:NH2	1:B:266:ILE:HD12	2.29	0.48
1:C:102:ILE:CG2	1:C:103:LEU:HD12	2.40	0.48
1:D:22:ALA:HB1	1:D:27:GLU:HB3	1.95	0.48
1:F:52:PRO:HD2	1:F:365:ALA:O	2.13	0.48
1:H:19:ALA:HA	1:H:31:ARG:CB	2.42	0.48
1:A:47:ILE:HG12	1:A:70:VAL:HB	1.95	0.48
1:C:439:GLN:OE1	1:C:439:GLN:HA	2.13	0.48
1:C:462:ALA:HB3	1:C:470:PRO:HG3	1.96	0.48
1:D:220:VAL:O	1:D:220:VAL:HG13	2.12	0.48
1:E:240:PHE:CD2	1:E:290:MET:HE1	2.48	0.48
1:F:245:ARG:HB2	1:F:249:ASP:OD2	2.13	0.48
1:G:45:GLY:C	1:G:357:CYS:HB3	2.34	0.48
1:G:191:PHE:N	1:G:191:PHE:CD1	2.81	0.48
1:G:360:LEU:HD22	1:G:373:ALA:HB1	1.96	0.48
1:H:108:ALA:HA	1:H:237:ASP:OD2	2.12	0.48
1:A:143:LEU:O	1:A:145:ASN:ND2	2.47	0.48
1:A:209:ASN:ND2	1:A:298:ILE:HD13	2.28	0.48
1:A:271:GLU:HG2	1:A:295:ASP:HB2	1.96	0.48
1:C:66:SER:HB3	1:C:375:ARG:HG3	1.96	0.48
1:C:102:ILE:HG22	1:C:103:LEU:N	2.27	0.48
1:C:503:LYS:O	1:C:529:VAL:HG11	2.14	0.48
1:D:202:LEU:HD22	1:D:202:LEU:C	2.34	0.48
1:D:220:VAL:CG2	1:D:224:ASP:HB2	2.43	0.48
1:F:230:PHE:O	1:F:233:GLU:HB2	2.14	0.48
1:F:315:ARG:NH1	1:H:30:CYS:O	2.39	0.48
1:B:123:ILE:O	1:B:123:ILE:HG22	2.14	0.48
1:C:55:ARG:NH2	1:C:85:GLU:HB3	2.28	0.48
1:E:379:LEU:HD13	1:E:379:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:GLN:CA	1:E:439:GLN:HE21	2.25	0.48
1:F:266:ILE:O	1:F:266:ILE:HG22	2.11	0.48
1:G:179:LEU:C	1:G:180:ILE:HD13	2.33	0.48
1:G:439:GLN:HA	1:G:439:GLN:NE2	2.27	0.48
1:H:16:GLN:HG2	1:H:32:LEU:HD23	1.96	0.48
1:H:108:ALA:HB2	1:H:460:ARG:O	2.13	0.48
1:H:488:ARG:O	1:H:491:LEU:HB3	2.14	0.48
1:B:12:ILE:HG21	1:B:33:ASP:OD2	2.14	0.48
1:B:50:ILE:HB	1:B:73:MET:HE3	1.96	0.48
1:B:120:THR:HG22	1:B:156:LEU:CD1	2.43	0.48
1:B:133:LEU:HB2	1:B:200:GLY:O	2.14	0.48
1:B:288:GLY:O	1:B:289:ILE:HG12	2.14	0.48
1:D:62:GLU:OE2	1:D:65:LYS:NZ	2.40	0.48
1:D:369:TYR:HB3	1:D:372:GLU:HB2	1.96	0.48
1:E:269:LYS:HG2	1:E:290:MET:HB3	1.95	0.48
1:F:147:TYR:O	1:F:157:TRP:HB2	2.14	0.48
1:G:70:VAL:HG11	1:G:238:MET:CE	2.44	0.48
1:H:499:ARG:HB3	1:H:501:PHE:CD1	2.49	0.48
1:B:80:HIS:N	1:B:80:HIS:CD2	2.79	0.48
1:B:131:VAL:HG12	1:B:133:LEU:HD23	1.95	0.48
1:B:328:GLN:HG2	1:B:331:GLU:CG	2.41	0.48
1:B:375:ARG:O	1:B:378:HIS:HB3	2.13	0.48
1:C:145:ASN:H	1:C:145:ASN:HD22	0.74	0.48
1:G:63:MET:HA	1:G:371:LEU:CD2	2.41	0.48
1:G:110:ALA:CB	1:G:238:MET:HE2	2.36	0.48
1:G:111:LEU:HD23	1:G:111:LEU:C	2.34	0.48
1:G:237:ASP:OD1	1:G:460:ARG:HD2	2.14	0.48
1:A:296:LEU:O	1:A:300:ILE:HG12	2.13	0.48
1:A:501:PHE:N	1:A:501:PHE:CD1	2.79	0.48
1:B:328:GLN:HA	1:B:331:GLU:HG3	1.94	0.48
1:B:431:THR:HG21	1:B:434:GLY:HA2	1.96	0.48
1:C:465:TYR:CB	1:C:468:ILE:HD12	2.40	0.48
1:D:145:ASN:O	1:D:148:MET:HB3	2.14	0.48
1:D:185:LYS:HD3	1:D:195:GLU:CB	2.42	0.48
1:E:428:ILE:CD1	1:E:508:VAL:HG11	2.44	0.48
1:H:238:MET:HB2	1:H:265:LYS:O	2.14	0.48
1:B:154:ASN:C	1:B:155:ILE:HG13	2.33	0.47
1:B:240:PHE:N	1:B:240:PHE:CD1	2.80	0.47
1:C:272:ASN:HB2	1:C:299:GLU:HG2	1.96	0.47
1:C:273:HIS:CB	1:C:277:ARG:HH11	2.12	0.47
1:D:77:HIS:O	1:D:78:GLY:O	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:GLU:OE2	1:D:295:ASP:OD2	2.30	0.47
1:D:457:GLN:O	1:D:461:GLN:HG3	2.14	0.47
1:G:43:ASN:HB3	1:G:467:GLY:N	2.29	0.47
1:H:480:ALA:O	1:H:483:GLU:HB2	2.14	0.47
1:A:187:LYS:HA	1:A:192:LEU:CD1	2.44	0.47
1:B:266:ILE:O	1:B:287:ASP:HB2	2.14	0.47
1:B:337:PRO:HB3	1:B:369:TYR:CE2	2.50	0.47
1:B:382:ARG:HH11	1:B:382:ARG:CG	2.27	0.47
1:C:493:MET:HE1	1:C:529:VAL:HG13	1.96	0.47
1:D:472:VAL:HG12	1:D:473:CYS:N	2.28	0.47
1:E:43:ASN:HD21	1:E:448:PRO:HB3	1.79	0.47
1:E:268:SER:HB2	1:E:289:ILE:HD13	1.95	0.47
1:E:330:LEU:O	1:E:363:GLU:HG2	2.14	0.47
1:F:296:LEU:HD12	1:F:296:LEU:C	2.30	0.47
1:G:62:GLU:CB	1:G:371:LEU:HD11	2.39	0.47
1:H:266:ILE:N	1:H:287:ASP:OD2	2.40	0.47
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.60	0.47
1:B:84:ALA:HB2	1:B:230:PHE:CZ	2.47	0.47
1:C:514:TRP:HA	1:C:514:TRP:CE3	2.49	0.47
1:H:512:THR:C	1:H:521:THR:HG22	2.34	0.47
1:A:57:VAL:O	1:A:61:LYS:HG2	2.14	0.47
1:C:185:LYS:CD	1:C:195:GLU:HB2	2.44	0.47
1:D:158:LEU:HD23	1:D:163:ILE:HD13	1.96	0.47
1:G:145:ASN:O	1:G:148:MET:HB3	2.14	0.47
1:H:256:ILE:HA	1:H:256:ILE:HD13	1.72	0.47
1:A:118:ILE:HG23	1:A:160:TYR:HB2	1.95	0.47
1:B:50:ILE:HG23	1:B:50:ILE:HD12	1.45	0.47
1:F:453:THR:HG1	1:F:455:ASN:H	1.62	0.47
1:G:69:ASN:HB3	1:G:463:HIS:HD2	1.73	0.47
1:G:166:VAL:HG13	1:G:213:ALA:HB1	1.97	0.47
1:G:338:ARG:NH2	1:G:341:ARG:NH1	2.62	0.47
1:A:453:THR:HG21	1:A:459:ALA:HB2	1.97	0.47
1:C:122:LEU:HD11	1:C:205:LYS:HE2	1.95	0.47
1:E:88:LYS:O	1:E:88:LYS:HG2	2.11	0.47
1:E:334:ILE:HG23	1:E:367:GLY:HA2	1.96	0.47
1:F:171:SER:O	1:F:184:VAL:HG23	2.14	0.47
1:F:334:ILE:HG22	1:F:335:LYS:HG3	1.96	0.47
1:F:449:ILE:HB	1:F:468:ILE:HA	1.97	0.47
1:G:57:VAL:CG1	1:G:93:ALA:HB2	2.44	0.47
1:H:166:VAL:O	1:H:166:VAL:HG12	2.15	0.47
1:B:252:GLU:O	1:B:256:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:MET:CE	1:B:326:ALA:HB2	2.45	0.47
1:C:322:PRO:HA	1:C:356:ASP:OD2	2.14	0.47
1:D:135:LYS:HB2	1:D:135:LYS:HE3	1.77	0.47
1:D:181:SER:OG	1:D:198:ASN:HB2	2.14	0.47
1:D:424:ALA:HB2	1:D:509:ILE:HD12	1.97	0.47
1:F:211:PRO:C	1:F:213:ALA:H	2.17	0.47
1:F:487:LEU:C	1:F:487:LEU:HD12	2.35	0.47
1:G:184:VAL:O	1:G:184:VAL:HG12	2.14	0.47
1:H:279:PHE:CE1	1:H:289:ILE:CD1	2.98	0.47
1:B:111:LEU:HB3	1:B:239:VAL:HG22	1.97	0.47
1:B:342:ALA:HB1	1:D:346:ASP:CB	2.39	0.47
1:C:294:GLY:N	1:C:327:THR:HG21	2.29	0.47
1:D:122:LEU:HD13	1:D:122:LEU:HA	1.59	0.47
1:E:342:ALA:HA	1:G:346:ASP:OD2	2.15	0.47
1:E:354:GLY:O	1:E:444:ARG:NH2	2.48	0.47
1:G:333:MET:CE	1:G:373:ALA:HA	2.45	0.47
1:E:375:ARG:O	1:E:379:LEU:HD22	2.15	0.47
1:F:123:ILE:O	1:F:123:ILE:HG22	2.14	0.47
1:G:501:PHE:N	1:G:501:PHE:CD1	2.81	0.47
1:A:186:GLN:CB	1:A:193:VAL:HB	2.45	0.47
1:A:237:ASP:OD1	1:A:237:ASP:N	2.48	0.47
1:B:12:ILE:O	1:B:13:GLN:O	2.33	0.47
1:B:425:ALA:O	1:B:426:ALA:HB2	2.14	0.47
1:C:182:LEU:HB2	1:C:194:THR:HB	1.96	0.47
1:C:501:PHE:N	1:C:501:PHE:CD1	2.82	0.47
1:D:183:GLN:O	1:D:194:THR:HA	2.15	0.47
1:F:176:ASP:O	1:F:179:LEU:HB2	2.14	0.47
1:H:157:TRP:O	1:H:158:LEU:HD13	2.15	0.47
1:H:401:SER:O	1:H:403:HIS:N	2.48	0.47
1:B:187:LYS:HG3	1:B:192:LEU:HD11	1.97	0.46
1:B:220:VAL:HG13	1:B:221:SER:N	2.30	0.46
1:B:306:PHE:O	1:B:310:LYS:HG2	2.14	0.46
1:E:328:GLN:HE21	1:G:341:ARG:N	2.02	0.46
1:F:191:PHE:CD1	1:F:193:VAL:HG23	2.50	0.46
1:G:425:ALA:O	1:G:426:ALA:HB2	2.16	0.46
1:H:219:ALA:HB2	1:H:249:ASP:HA	1.97	0.46
1:H:382:ARG:HH11	1:H:382:ARG:HB2	1.81	0.46
1:B:131:VAL:HG12	1:B:133:LEU:CD2	2.45	0.46
1:D:14:THR:HG22	1:D:37:ALA:O	2.15	0.46
1:D:123:ILE:HD13	1:D:131:VAL:HB	1.97	0.46
1:E:390:HIS:HD2	1:E:446:ARG:NH1	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:PHE:HA	1:F:267:ILE:HB	1.97	0.46
1:H:160:TYR:OH	1:H:166:VAL:HG21	2.15	0.46
1:H:184:VAL:HA	1:H:194:THR:HG22	1.97	0.46
1:H:413:MET:HE2	1:H:413:MET:HB3	1.87	0.46
1:A:413:MET:SD	1:B:421:LYS:HE2	2.55	0.46
1:B:14:THR:HG22	1:B:15:GLN:HE21	1.79	0.46
1:B:152:ASP:C	1:B:154:ASN:H	2.18	0.46
1:B:290:MET:HE2	1:B:326:ALA:HB2	1.97	0.46
1:D:120:THR:HA	1:D:157:TRP:O	2.16	0.46
1:D:156:LEU:CD2	1:D:157:TRP:H	2.29	0.46
1:D:189:PRO:CD	1:D:191:PHE:CE1	2.99	0.46
1:D:369:TYR:N	1:D:370:PRO:HD3	2.30	0.46
1:D:453:THR:OG1	1:D:454:ARG:N	2.48	0.46
1:G:333:MET:HE1	1:G:373:ALA:HA	1.96	0.46
1:A:493:MET:CE	1:A:529:VAL:HG13	2.42	0.46
1:B:148:MET:HE3	1:B:148:MET:HB3	1.63	0.46
1:B:167:VAL:CG1	1:B:168:ASP:N	2.78	0.46
1:E:257:LEU:HD23	1:E:261:GLY:HA3	1.97	0.46
1:F:113:THR:O	1:F:242:SER:OG	2.25	0.46
1:G:527:VAL:HG13	1:G:528:PRO:HD2	1.97	0.46
1:H:333:MET:HA	1:H:336:LYS:O	2.14	0.46
1:A:55:ARG:HG3	1:A:86:THR:CG2	2.45	0.46
1:A:120:THR:HA	1:A:157:TRP:O	2.16	0.46
1:A:244:ILE:HG22	1:A:282:ILE:HD13	1.97	0.46
1:B:122:LEU:HA	1:B:122:LEU:HD12	1.51	0.46
1:D:113:THR:HG23	1:D:115:GLY:H	1.81	0.46
1:D:252:GLU:OE2	1:D:255:LYS:NZ	2.45	0.46
1:D:276:VAL:O	1:D:279:PHE:HB2	2.15	0.46
1:D:454:ARG:NH2	1:D:484:ASP:OD1	2.46	0.46
1:F:63:MET:HG2	1:F:371:LEU:HD23	1.98	0.46
1:F:140:LYS:HA	1:F:192:LEU:O	2.15	0.46
1:F:224:ASP:O	1:F:228:LEU:HG	2.15	0.46
1:F:465:TYR:N	1:F:465:TYR:CD1	2.84	0.46
1:G:409:GLU:O	1:G:412:ALA:HB3	2.15	0.46
1:H:63:MET:CG	1:H:371:LEU:HD23	2.38	0.46
1:H:123:ILE:CD1	1:H:131:VAL:HG23	2.36	0.46
1:H:363:GLU:OE1	1:H:363:GLU:N	2.39	0.46
1:H:371:LEU:O	1:H:374:VAL:N	2.49	0.46
1:B:141:ILE:HD13	1:B:141:ILE:O	2.16	0.46
1:B:514:TRP:O	1:B:515:ARG:HG2	2.16	0.46
1:E:47:ILE:CD1	1:E:324:ILE:HG23	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:LEU:CD2	1:G:163:ILE:HD13	2.45	0.46
1:H:228:LEU:O	1:H:231:GLY:N	2.48	0.46
1:H:411:MET:O	1:H:415:SER:OG	2.33	0.46
1:H:477:VAL:HG12	1:H:478:GLN:N	2.30	0.46
1:A:267:ILE:HG21	1:A:324:ILE:HD12	1.98	0.46
1:C:311:MET:HG2	1:C:315:ARG:HD3	1.96	0.46
1:C:487:LEU:HD23	1:C:488:ARG:N	2.31	0.46
1:D:43:ASN:ND2	1:D:467:GLY:HA2	2.31	0.46
1:D:355:ALA:O	1:D:466:ARG:NH1	2.49	0.46
1:D:436:SER:HB3	1:D:521:THR:HG23	1.96	0.46
1:E:63:MET:HG3	1:E:371:LEU:HD21	1.98	0.46
1:G:176:ASP:O	1:G:177:ASP:HB2	2.15	0.46
1:H:223:LYS:O	1:H:226:GLN:HB2	2.15	0.46
1:H:491:LEU:O	1:H:494:ASN:N	2.49	0.46
1:A:56:SER:O	1:A:60:LEU:HD22	2.16	0.46
1:B:182:LEU:HD13	1:B:194:THR:HG21	1.97	0.46
1:C:515:ARG:HB3	1:C:516:PRO:CD	2.40	0.46
1:D:189:PRO:HD3	1:D:191:PHE:CE1	2.50	0.46
1:D:503:LYS:O	1:D:529:VAL:HB	2.16	0.46
1:F:328:GLN:NE2	1:H:340:THR:CA	2.79	0.46
1:F:425:ALA:HB1	1:F:502:PHE:HB3	1.98	0.46
1:G:330:LEU:HD12	1:G:330:LEU:HA	1.75	0.46
1:H:113:THR:HG23	1:H:114:LYS:N	2.31	0.46
1:H:300:ILE:HB	1:H:301:PRO:HD2	1.97	0.46
1:H:327:THR:HG22	1:H:328:GLN:HG3	1.97	0.46
1:A:160:TYR:CE1	1:A:217:LEU:CD1	2.99	0.46
1:B:317:ASN:N	1:B:317:ASN:HD22	2.11	0.46
1:E:221:SER:H	1:E:224:ASP:HB2	1.81	0.46
1:F:501:PHE:N	1:F:501:PHE:CD1	2.82	0.46
1:G:33:ASP:HB3	1:G:36:SER:HB2	1.98	0.46
1:A:118:ILE:HB	1:A:208:VAL:HB	1.98	0.46
1:B:392:LYS:O	1:B:396:GLU:HG3	2.15	0.46
1:B:416:VAL:HG21	1:B:443:TYR:HB2	1.98	0.46
1:B:512:THR:CA	1:B:521:THR:HG22	2.46	0.46
1:C:156:LEU:HD23	1:C:156:LEU:HA	1.71	0.46
1:E:105:ARG:HD3	1:E:499:ARG:NH1	2.31	0.46
1:E:269:LYS:HG2	1:E:290:MET:SD	2.56	0.46
1:F:240:PHE:CD2	1:F:290:MET:CE	2.99	0.46
1:F:256:ILE:HD13	1:F:256:ILE:N	2.31	0.46
1:F:462:ALA:HB1	1:F:468:ILE:HG21	1.97	0.46
1:G:50:ILE:HB	1:G:73:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:MET:HG2	1:G:315:ARG:HD3	1.98	0.46
1:G:416:VAL:HG13	1:G:445:PRO:CB	2.43	0.46
1:H:51:GLY:O	1:H:55:ARG:HB2	2.16	0.46
1:H:158:LEU:HD12	1:H:158:LEU:HA	1.62	0.46
1:A:454:ARG:HG3	1:A:473:CYS:HB3	1.99	0.45
1:D:162:ASN:O	1:D:165:LYS:HB2	2.16	0.45
1:D:450:ILE:HG21	1:D:492:ALA:HB1	1.98	0.45
1:D:475:ASP:HB3	1:D:476:PRO:HD2	1.97	0.45
1:D:477:VAL:HG12	1:D:478:GLN:O	2.15	0.45
1:E:487:LEU:HD23	1:E:487:LEU:C	2.37	0.45
1:F:139:LEU:HD23	1:F:141:ILE:HG22	1.98	0.45
1:F:167:VAL:HG13	1:F:171:SER:HB2	1.98	0.45
1:F:330:LEU:HD12	1:F:343:GLU:HB2	1.99	0.45
1:G:84:ALA:HB2	1:G:230:PHE:HZ	1.81	0.45
1:H:148:MET:HE3	1:H:148:MET:HB3	1.77	0.45
1:H:170:GLY:HA2	1:H:183:GLN:HE21	1.79	0.45
1:A:340:THR:CA	1:C:328:GLN:NE2	2.79	0.45
1:E:413:MET:CE	1:E:443:TYR:CE1	3.00	0.45
1:G:156:LEU:CD2	1:G:157:TRP:N	2.79	0.45
1:G:352:LEU:HD12	1:G:352:LEU:HA	1.84	0.45
1:G:439:GLN:CA	1:G:439:GLN:NE2	2.80	0.45
1:A:525:ARG:HD3	1:B:514:TRP:CE3	2.52	0.45
1:B:189:PRO:HD2	1:B:191:PHE:CE1	2.51	0.45
1:B:340:THR:OG1	1:B:343:GLU:HG3	2.16	0.45
1:B:515:ARG:HB3	1:B:516:PRO:CD	2.46	0.45
1:C:493:MET:HE2	1:C:493:MET:HB3	1.53	0.45
1:D:125:GLY:HA2	1:D:149:GLU:O	2.15	0.45
1:E:428:ILE:HD13	1:E:508:VAL:HG11	1.98	0.45
1:F:247:ALA:HB2	1:F:281:GLU:CG	2.38	0.45
1:F:488:ARG:O	1:F:491:LEU:HB3	2.16	0.45
1:G:174:TYR:CD2	1:G:298:ILE:CG2	2.99	0.45
1:G:333:MET:O	1:G:336:LYS:O	2.34	0.45
1:H:431:THR:CG2	1:H:434:GLY:HA2	2.46	0.45
1:H:441:ALA:O	1:H:444:ARG:N	2.37	0.45
1:A:281:GLU:CG	1:A:282:ILE:N	2.79	0.45
1:B:185:LYS:HA	1:B:185:LYS:HD3	1.58	0.45
1:C:290:MET:HE3	1:C:359:MET:SD	2.56	0.45
1:D:57:VAL:O	1:D:61:LYS:HG3	2.17	0.45
1:E:240:PHE:CD2	1:E:290:MET:CE	2.99	0.45
1:F:147:TYR:CD2	1:F:155:ILE:HG21	2.52	0.45
1:H:102:ILE:HG12	1:H:103:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:328:GLN:CG	1:H:331:GLU:HG3	2.44	0.45
1:H:464:LEU:HD12	1:H:464:LEU:HA	1.79	0.45
1:H:507:VAL:CG1	1:H:508:VAL:N	2.79	0.45
1:A:460:ARG:NH2	5:A:6091:HOH:O	2.49	0.45
1:B:515:ARG:CB	1:B:516:PRO:HD2	2.44	0.45
1:C:318:ARG:HD2	5:C:6031:HOH:O	2.16	0.45
1:D:192:LEU:HD13	1:D:192:LEU:HA	1.74	0.45
1:F:139:LEU:HD21	1:F:156:LEU:HB2	1.98	0.45
1:G:508:VAL:CG1	1:G:509:ILE:N	2.79	0.45
1:H:477:VAL:CG1	1:H:478:GLN:N	2.80	0.45
1:A:22:ALA:HA	1:A:31:ARG:NH1	2.32	0.45
1:B:64:ILE:HD12	1:B:94:THR:HA	1.99	0.45
1:C:137:ALA:O	1:C:196:VAL:N	2.37	0.45
1:D:186:GLN:O	1:D:186:GLN:HG2	2.15	0.45
1:E:379:LEU:N	1:E:379:LEU:CD1	2.79	0.45
1:E:407:LEU:N	1:E:407:LEU:CD1	2.80	0.45
1:F:220:VAL:HG22	1:F:224:ASP:CB	2.46	0.45
1:F:369:TYR:N	1:F:370:PRO:CD	2.80	0.45
1:G:407:LEU:N	1:G:407:LEU:CD1	2.79	0.45
1:A:47:ILE:CG2	1:A:359:MET:HG3	2.47	0.45
1:A:520:PHE:HD1	1:A:521:THR:O	2.00	0.45
1:B:269:LYS:HD2	1:B:290:MET:SD	2.57	0.45
1:D:238:MET:HE2	1:D:238:MET:HB3	1.82	0.45
1:D:289:ILE:CG2	1:D:290:MET:N	2.80	0.45
1:F:202:LEU:CD2	1:F:203:GLY:N	2.80	0.45
1:G:256:ILE:HD13	1:G:256:ILE:N	2.31	0.45
1:G:351:VAL:HG12	1:G:351:VAL:O	2.17	0.45
1:G:410:ALA:CB	1:H:422:CYS:HB3	2.46	0.45
1:H:141:ILE:O	1:H:191:PHE:HA	2.16	0.45
1:H:430:LEU:HD21	1:H:488:ARG:HB2	1.99	0.45
1:A:124:LYS:C	1:A:126:SER:H	2.20	0.45
1:A:209:ASN:C	1:A:211:PRO:HD3	2.37	0.45
1:A:399:ARG:NH1	1:B:23:ASP:HB3	2.31	0.45
1:A:421:LYS:HE2	1:B:413:MET:SD	2.57	0.45
1:A:525:ARG:HB3	1:A:527:VAL:HG23	1.98	0.45
1:B:480:ALA:HB3	1:B:483:GLU:CG	2.44	0.45
1:C:62:GLU:O	1:C:65:LYS:HB2	2.16	0.45
1:C:407:LEU:N	1:C:407:LEU:CD1	2.80	0.45
1:D:123:ILE:HG22	1:D:123:ILE:O	2.15	0.45
1:D:154:ASN:CB	1:D:155:ILE:HD12	2.41	0.45
1:F:48:CYS:SG	1:F:68:MET:HG3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:VAL:HG12	1:F:61:LYS:HE2	1.98	0.45
1:F:145:ASN:HB3	1:F:148:MET:HE2	1.96	0.45
1:F:447:ALA:HB1	1:F:448:PRO:HD2	1.99	0.45
1:G:55:ARG:CZ	1:G:82:TYR:CE1	2.99	0.45
1:H:202:LEU:CD2	1:H:203:GLY:H	2.30	0.45
1:H:381:ALA:O	1:H:385:GLU:HG3	2.17	0.45
1:A:462:ALA:HB3	1:A:470:PRO:HG3	1.99	0.45
1:B:247:ALA:HA	1:B:250:VAL:HG23	1.99	0.45
1:B:430:LEU:N	1:B:430:LEU:CD1	2.80	0.45
1:C:303:GLU:H	1:C:303:GLU:HG3	1.24	0.45
1:D:47:ILE:HD13	1:D:324:ILE:HD13	1.99	0.45
1:F:133:LEU:HD11	1:F:202:LEU:HD12	1.98	0.45
1:F:296:LEU:O	1:F:300:ILE:HG12	2.17	0.45
1:F:355:ALA:O	1:F:466:ARG:NH1	2.46	0.45
1:H:100:ASP:OD1	1:H:102:ILE:HG23	2.17	0.45
1:H:141:ILE:HA	1:H:156:LEU:O	2.17	0.45
1:H:491:LEU:HA	1:H:491:LEU:HD12	1.54	0.45
1:A:162:ASN:H	1:A:162:ASN:ND2	2.14	0.45
1:B:138:THR:CG2	1:B:139:LEU:N	2.80	0.45
1:B:376:MET:O	1:B:380:ILE:HG13	2.17	0.45
1:C:57:VAL:O	1:C:60:LEU:HB2	2.16	0.45
1:C:244:ILE:HG21	1:C:268:SER:OG	2.17	0.45
1:C:262:LYS:H	1:C:262:LYS:HG3	1.46	0.45
1:C:330:LEU:HD12	1:C:330:LEU:HA	1.66	0.45
1:D:123:ILE:HD11	1:D:131:VAL:HG12	1.99	0.45
1:D:371:LEU:O	1:D:375:ARG:HD2	2.17	0.45
1:E:422:CYS:O	1:E:423:LEU:HB2	2.17	0.45
1:F:131:VAL:HG11	1:F:153:GLU:HA	1.99	0.45
1:F:183:GLN:HG3	1:F:184:VAL:N	2.31	0.45
1:F:322:PRO:HA	1:F:356:ASP:OD2	2.17	0.45
1:F:358:ILE:HD13	1:F:358:ILE:HG21	1.74	0.45
1:F:423:LEU:HD12	1:F:423:LEU:HA	1.53	0.45
1:G:46:ILE:HG23	1:G:377:GLN:HE22	1.78	0.45
1:G:327:THR:CG2	1:G:328:GLN:HG3	2.47	0.45
1:H:407:LEU:N	1:H:407:LEU:CD1	2.80	0.45
1:H:465:TYR:N	1:H:465:TYR:CD1	2.85	0.45
1:B:415:SER:O	1:B:419:SER:HB3	2.17	0.44
1:C:289:ILE:CG2	1:C:290:MET:N	2.79	0.44
1:D:189:PRO:CD	1:D:190:ASP:N	2.80	0.44
1:D:411:MET:HE1	1:D:524:MET:HB2	1.98	0.44
1:F:240:PHE:CD2	1:F:290:MET:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:LEU:HD22	1:G:321:LYS:HD2	1.98	0.44
1:H:160:TYR:CD1	1:H:217:LEU:HD21	2.53	0.44
1:H:314:GLY:O	1:H:318:ARG:HB2	2.17	0.44
1:A:415:SER:HA	1:A:524:MET:HE2	2.00	0.44
1:B:333:MET:HE1	1:B:339:PRO:HD3	1.97	0.44
1:B:491:LEU:O	1:B:495:VAL:HG23	2.16	0.44
1:C:173:VAL:HB	1:C:182:LEU:CD1	2.47	0.44
1:D:208:VAL:CG1	1:D:209:ASN:N	2.79	0.44
1:D:237:ASP:OD1	1:D:460:ARG:NH1	2.47	0.44
1:D:279:PHE:CE1	1:D:312:ILE:HD13	2.52	0.44
1:D:425:ALA:O	1:D:426:ALA:HB2	2.17	0.44
1:G:238:MET:O	1:G:238:MET:HG2	2.14	0.44
1:G:300:ILE:HB	1:G:301:PRO:CD	2.47	0.44
1:G:408:MET:O	1:G:408:MET:HG3	2.17	0.44
1:H:131:VAL:O	1:H:202:LEU:N	2.48	0.44
1:H:192:LEU:HD12	1:H:192:LEU:HA	1.82	0.44
1:H:493:MET:HG2	1:H:530:PRO:HD2	1.97	0.44
1:H:514:TRP:HA	1:H:514:TRP:HE3	1.82	0.44
1:A:310:LYS:HD3	1:A:353:ASP:OD2	2.17	0.44
1:A:508:VAL:CG1	1:A:509:ILE:N	2.80	0.44
1:C:221:SER:O	1:C:225:ILE:HG13	2.18	0.44
1:C:299:GLU:OE1	5:C:6192:HOH:O	2.21	0.44
1:D:134:LYS:O	1:D:196:VAL:HG11	2.17	0.44
1:E:26:LEU:HD12	1:E:26:LEU:HA	1.78	0.44
1:F:50:ILE:HD12	1:F:50:ILE:HA	1.65	0.44
1:F:507:VAL:HG13	1:F:527:VAL:O	2.17	0.44
1:G:488:ARG:O	1:G:491:LEU:HB3	2.16	0.44
1:H:232:VAL:HG11	1:H:260:LYS:HB3	2.00	0.44
1:H:397:LEU:O	1:H:400:SER:OG	2.35	0.44
1:H:453:THR:HG21	1:H:459:ALA:HB2	1.99	0.44
1:A:152:ASP:OD1	1:A:154:ASN:N	2.46	0.44
1:A:202:LEU:HA	1:A:202:LEU:HD23	1.76	0.44
1:A:274:GLU:OE2	1:A:278:ARG:NH1	2.42	0.44
1:A:338:ARG:HA	1:A:339:PRO:HD3	1.85	0.44
1:A:399:ARG:HH12	1:B:23:ASP:HB3	1.82	0.44
1:B:120:THR:CG2	1:B:156:LEU:HD11	2.47	0.44
1:B:436:SER:HB3	1:B:521:THR:OG1	2.18	0.44
1:D:160:TYR:O	1:D:163:ILE:HG22	2.18	0.44
1:D:324:ILE:HD13	1:D:324:ILE:HG21	1.58	0.44
1:D:388:MET:SD	1:D:466:ARG:NH2	2.90	0.44
1:F:272:ASN:O	1:F:276:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:507:VAL:CG1	1:F:508:VAL:N	2.80	0.44
1:F:527:VAL:HA	1:F:528:PRO:HD3	1.74	0.44
1:G:17:LEU:N	1:G:17:LEU:CD2	2.79	0.44
1:G:174:TYR:CD2	1:G:178:GLY:HA2	2.52	0.44
1:G:210:LEU:HA	1:G:210:LEU:HD12	1.76	0.44
1:G:477:VAL:CG1	1:G:478:GLN:N	2.79	0.44
1:B:158:LEU:HD22	1:B:158:LEU:N	2.31	0.44
1:B:499:ARG:HD3	1:B:499:ARG:HA	1.85	0.44
1:G:232:VAL:HG12	1:G:260:LYS:HD2	1.99	0.44
1:H:19:ALA:CA	1:H:31:ARG:HB3	2.46	0.44
1:H:133:LEU:N	1:H:133:LEU:CD2	2.80	0.44
1:H:428:ILE:HD12	1:H:508:VAL:CG1	2.47	0.44
1:A:222:GLU:HA	1:A:225:ILE:HG13	1.99	0.44
1:A:245:ARG:O	1:A:278:ARG:HD3	2.17	0.44
1:A:371:LEU:O	1:A:375:ARG:HD2	2.17	0.44
1:A:429:VAL:C	1:A:430:LEU:HD12	2.38	0.44
1:C:422:CYS:O	1:C:423:LEU:HB2	2.16	0.44
1:C:423:LEU:HD22	1:D:405:THR:HG21	2.00	0.44
1:D:105:ARG:CZ	1:D:499:ARG:NH2	2.81	0.44
1:D:231:GLY:O	1:D:236:VAL:HG22	2.18	0.44
1:F:155:ILE:CG2	1:F:156:LEU:N	2.80	0.44
1:F:156:LEU:HD23	1:F:156:LEU:HA	1.76	0.44
1:G:156:LEU:HD23	1:G:157:TRP:N	2.32	0.44
1:H:246:LYS:H	1:H:246:LYS:HG2	1.63	0.44
1:A:416:VAL:HG21	1:A:443:TYR:HB2	2.00	0.44
1:B:267:ILE:N	1:B:267:ILE:CD1	2.80	0.44
1:C:55:ARG:CZ	1:C:82:TYR:CE1	3.00	0.44
1:C:354:GLY:CA	1:C:466:ARG:HH12	2.31	0.44
1:D:210:LEU:HD13	1:D:210:LEU:N	2.33	0.44
1:F:120:THR:O	1:F:205:LYS:HA	2.17	0.44
1:F:243:PHE:N	1:F:271:GLU:OE1	2.37	0.44
1:F:336:LYS:HB3	1:F:337:PRO:CD	2.46	0.44
1:F:430:LEU:N	1:F:430:LEU:CD1	2.80	0.44
1:H:17:LEU:HA	1:H:17:LEU:HD22	1.74	0.44
1:B:73:MET:CE	1:B:86:THR:HG21	2.48	0.44
1:B:133:LEU:HD11	1:B:139:LEU:CD1	2.47	0.44
1:C:145:ASN:ND2	1:C:145:ASN:N	2.30	0.44
1:C:454:ARG:NE	1:C:475:ASP:O	2.41	0.44
1:E:334:ILE:CD1	1:E:363:GLU:N	2.79	0.44
1:F:315:ARG:CG	1:H:30:CYS:HB3	2.47	0.44
1:F:379:LEU:HD12	1:F:379:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:MET:HA	1:G:21:MET:HE2	1.98	0.44
1:G:253:VAL:O	1:G:257:LEU:HD13	2.18	0.44
1:H:279:PHE:CE1	1:H:289:ILE:HD13	2.53	0.44
1:H:292:ALA:HB1	4:H:532:PEQ:C2	2.47	0.44
1:H:508:VAL:O	1:H:509:ILE:HD13	2.18	0.44
1:A:246:LYS:HE2	1:A:249:ASP:OD1	2.18	0.44
1:C:47:ILE:O	1:C:359:MET:HG3	2.17	0.44
1:D:122:LEU:HD12	1:D:123:ILE:N	2.29	0.44
1:D:294:GLY:CA	1:D:327:THR:HG21	2.47	0.44
1:A:225:ILE:O	1:A:229:LYS:HG3	2.18	0.43
1:B:64:ILE:HD13	1:B:107:VAL:HG21	1.99	0.43
1:B:435:ARG:O	1:B:438:HIS:HB2	2.18	0.43
1:B:501:PHE:N	1:B:501:PHE:CD1	2.85	0.43
1:C:354:GLY:HA2	1:C:466:ARG:HH12	1.83	0.43
1:D:123:ILE:H	1:D:204:SER:HG	1.61	0.43
1:D:493:MET:HG2	1:D:530:PRO:HD2	1.99	0.43
1:E:98:ALA:HA	1:E:104:TYR:CD1	2.53	0.43
1:E:105:ARG:CD	1:E:499:ARG:NH1	2.81	0.43
1:E:371:LEU:O	1:E:375:ARG:HD2	2.18	0.43
1:F:141:ILE:H	1:F:141:ILE:HD13	1.83	0.43
1:F:328:GLN:NE2	1:H:340:THR:HB	2.33	0.43
1:G:174:TYR:CE2	1:G:298:ILE:HG23	2.53	0.43
1:G:226:GLN:H	1:G:226:GLN:HG3	1.63	0.43
1:G:520:PHE:CE1	1:G:522:ASN:HB3	2.53	0.43
1:H:42:ARG:HG2	1:H:381:ALA:HB3	2.00	0.43
1:H:202:LEU:CD2	1:H:203:GLY:N	2.79	0.43
1:A:183:GLN:O	1:A:194:THR:HA	2.18	0.43
1:A:528:PRO:O	1:A:530:PRO:HD3	2.18	0.43
1:B:160:TYR:OH	1:B:216:ASP:HB2	2.18	0.43
1:C:232:VAL:O	1:C:232:VAL:HG12	2.17	0.43
1:C:408:MET:HE2	1:C:436:SER:O	2.18	0.43
1:E:262:LYS:HE2	1:E:262:LYS:HB2	1.63	0.43
1:F:111:LEU:HD23	1:F:112:ASP:N	2.33	0.43
1:F:139:LEU:HD23	1:F:141:ILE:CG2	2.48	0.43
1:G:174:TYR:CD2	1:G:298:ILE:HG23	2.53	0.43
1:H:238:MET:HA	1:H:264:ILE:HG22	2.01	0.43
1:H:268:SER:HB2	1:H:286:SER:CB	2.48	0.43
1:B:375:ARG:O	1:B:379:LEU:HD13	2.19	0.43
1:B:503:LYS:O	1:B:529:VAL:HG11	2.18	0.43
1:C:338:ARG:HD3	5:C:6018:HOH:O	2.17	0.43
1:D:131:VAL:CG1	1:D:202:LEU:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:532:PEQ:O1P	4:D:532:PEQ:C3	2.66	0.43
1:F:463:HIS:CE1	1:F:470:PRO:HG2	2.53	0.43
1:G:141:ILE:CG2	1:G:158:LEU:HD22	2.49	0.43
1:H:440:VAL:HG12	1:H:449:ILE:HD13	1.99	0.43
1:B:202:LEU:HA	1:B:202:LEU:HD23	1.77	0.43
1:B:225:ILE:O	1:B:229:LYS:HG3	2.18	0.43
1:B:484:ASP:O	1:B:487:LEU:HB3	2.17	0.43
1:C:141:ILE:O	1:C:191:PHE:HA	2.18	0.43
1:C:415:SER:HA	1:C:524:MET:HE1	2.01	0.43
1:D:189:PRO:HD2	1:D:191:PHE:HD1	1.84	0.43
1:E:401:SER:O	1:F:421:LYS:NZ	2.51	0.43
1:F:50:ILE:N	1:F:50:ILE:CD1	2.79	0.43
1:F:328:GLN:O	1:H:342:ALA:HB2	2.18	0.43
1:G:57:VAL:O	1:G:57:VAL:HG12	2.17	0.43
1:G:334:ILE:HG12	1:G:363:GLU:HA	1.99	0.43
1:A:330:LEU:HD12	1:A:330:LEU:HA	1.77	0.43
1:A:340:THR:CB	1:C:328:GLN:NE2	2.81	0.43
1:B:496:GLY:HA3	1:B:502:PHE:CE1	2.53	0.43
1:C:123:ILE:HG23	1:C:131:VAL:CG2	2.48	0.43
1:D:190:ASP:OD1	1:D:190:ASP:N	2.51	0.43
1:E:60:LEU:O	1:E:63:MET:N	2.51	0.43
1:E:447:ALA:HB1	1:E:448:PRO:HD2	1.99	0.43
1:E:525:ARG:HB3	1:F:522:ASN:O	2.17	0.43
1:F:44:THR:CG2	1:F:358:ILE:HG12	2.49	0.43
1:F:50:ILE:N	1:F:50:ILE:HD13	2.33	0.43
1:G:202:LEU:HD23	1:G:202:LEU:HA	1.65	0.43
1:G:515:ARG:HB2	1:G:516:PRO:CD	2.47	0.43
1:H:156:LEU:HA	1:H:156:LEU:HD23	1.67	0.43
1:A:47:ILE:HG22	1:A:359:MET:HG3	2.00	0.43
1:A:122:LEU:HB2	1:A:149:GLU:HA	1.99	0.43
1:B:345:SER:O	1:B:349:ASN:HB2	2.18	0.43
1:D:209:ASN:C	1:D:211:PRO:HD3	2.38	0.43
1:D:322:PRO:HA	1:D:356:ASP:OD2	2.18	0.43
1:E:111:LEU:HD23	1:E:111:LEU:C	2.39	0.43
1:E:455:ASN:OD1	1:E:458:THR:N	2.47	0.43
1:F:24:THR:CG2	1:F:27:GLU:H	2.31	0.43
1:F:332:SER:C	1:F:334:ILE:H	2.22	0.43
1:A:76:SER:HA	1:A:114:LYS:HB2	2.00	0.43
1:B:44:THR:HG22	1:B:357:CYS:HA	2.00	0.43
1:B:102:ILE:HD12	1:B:102:ILE:HA	1.76	0.43
1:C:17:LEU:HA	1:C:17:LEU:HD23	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:LEU:HD11	1:C:300:ILE:HG23	2.01	0.43
1:G:15:GLN:CB	1:G:17:LEU:HD21	2.47	0.43
1:H:16:GLN:HG2	1:H:32:LEU:HD22	2.00	0.43
1:A:145:ASN:H	1:A:145:ASN:ND2	2.00	0.43
1:A:228:LEU:O	1:A:232:VAL:HG23	2.19	0.43
1:A:417:GLU:O	1:A:417:GLU:HG3	2.19	0.43
1:C:296:LEU:CD1	1:C:300:ILE:HG23	2.49	0.43
1:F:122:LEU:HB2	1:F:149:GLU:HG2	1.99	0.43
1:F:240:PHE:N	1:F:240:PHE:CD1	2.84	0.43
1:F:246:LYS:O	1:F:249:ASP:HB2	2.19	0.43
1:G:131:VAL:HG12	1:G:202:LEU:HB3	2.00	0.43
1:G:175:VAL:CG1	1:G:176:ASP:N	2.81	0.43
1:G:440:VAL:O	1:G:445:PRO:HD3	2.19	0.43
1:G:464:LEU:HD12	1:G:464:LEU:HA	1.76	0.43
1:H:432:GLU:HA	1:H:432:GLU:OE1	2.18	0.43
1:A:245:ARG:HG2	1:A:272:ASN:HD21	1.83	0.43
1:A:415:SER:HA	1:A:524:MET:HE1	2.01	0.43
1:B:328:GLN:CB	1:B:331:GLU:HG3	2.49	0.43
1:E:404:SER:OG	1:E:409:GLU:OE2	2.31	0.43
1:F:138:THR:CG2	1:F:193:VAL:HG13	2.49	0.43
1:F:276:VAL:HG11	1:H:34:ILE:HD13	2.00	0.43
1:G:45:GLY:O	1:G:357:CYS:HB3	2.18	0.43
1:G:106:PRO:C	1:G:107:VAL:HG23	2.39	0.43
1:G:317:ASN:N	1:G:317:ASN:HD22	2.16	0.43
1:H:16:GLN:CG	1:H:32:LEU:HD23	2.49	0.43
1:H:50:ILE:HD12	1:H:60:LEU:CD1	2.48	0.43
1:A:124:LYS:O	1:A:126:SER:N	2.51	0.43
1:C:60:LEU:O	1:C:64:ILE:N	2.47	0.43
1:C:427:LEU:N	1:C:427:LEU:CD1	2.82	0.43
1:D:210:LEU:N	1:D:210:LEU:CD1	2.82	0.43
1:E:39:ILE:O	1:E:382:ARG:HD3	2.19	0.43
1:E:293:ARG:HH22	1:E:346:ASP:CG	2.22	0.43
1:F:111:LEU:HD23	1:F:111:LEU:C	2.39	0.43
1:G:506:ASP:O	1:G:529:VAL:HG23	2.19	0.43
1:H:79:THR:HG22	1:H:80:HIS:N	2.34	0.43
1:H:328:GLN:CB	1:H:331:GLU:HG3	2.48	0.43
1:H:359:MET:C	1:H:360:LEU:HD12	2.39	0.43
1:B:118:ILE:CG2	1:B:208:VAL:HB	2.49	0.42
1:B:237:ASP:OD2	1:B:460:ARG:HD2	2.19	0.42
1:C:122:LEU:HD12	1:C:204:SER:CB	2.49	0.42
1:D:300:ILE:HB	1:D:301:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:GLU:OE1	1:G:58:GLU:HA	2.13	0.42
1:G:60:LEU:HD12	1:G:60:LEU:HA	1.49	0.42
1:G:132:GLU:HB2	1:G:201:PHE:HE1	1.84	0.42
1:G:184:VAL:HG13	1:G:186:GLN:O	2.19	0.42
1:H:40:THR:HG22	1:H:40:THR:O	2.17	0.42
1:H:109:VAL:N	1:H:237:ASP:OD2	2.49	0.42
1:H:261:GLY:HA3	1:H:264:ILE:HD12	2.00	0.42
1:A:55:ARG:NH2	1:A:85:GLU:HB3	2.34	0.42
1:A:303:GLU:H	1:A:303:GLU:HG3	1.09	0.42
1:C:504:LYS:O	1:C:504:LYS:HG2	2.18	0.42
1:D:301:PRO:HB3	1:D:303:GLU:OE2	2.19	0.42
1:D:468:ILE:HG21	1:D:468:ILE:HD13	1.73	0.42
1:E:47:ILE:HG21	1:E:359:MET:SD	2.59	0.42
1:E:351:VAL:HG12	1:E:352:LEU:N	2.33	0.42
1:F:158:LEU:HD12	1:F:158:LEU:HA	1.42	0.42
1:F:291:VAL:HG12	1:F:293:ARG:HG3	2.01	0.42
1:H:120:THR:HA	1:H:158:LEU:HD12	2.01	0.42
1:H:444:ARG:HA	1:H:445:PRO:HD2	1.81	0.42
1:A:42:ARG:NH1	1:A:44:THR:O	2.50	0.42
1:A:122:LEU:HA	1:A:122:LEU:HD13	1.63	0.42
1:B:488:ARG:O	1:B:491:LEU:HB3	2.19	0.42
1:E:75:PHE:CE2	1:E:83:HIS:HD2	2.37	0.42
1:E:529:VAL:HA	1:E:530:PRO:HD3	1.91	0.42
1:F:57:VAL:HG13	1:F:93:ALA:HB2	2.01	0.42
1:F:328:GLN:NE2	1:H:341:ARG:HG2	2.33	0.42
1:G:60:LEU:N	1:G:60:LEU:CD1	2.79	0.42
1:H:508:VAL:CG1	1:H:509:ILE:N	2.82	0.42
1:H:514:TRP:HA	1:H:514:TRP:CE3	2.54	0.42
1:B:300:ILE:HB	1:B:301:PRO:HD2	2.02	0.42
1:B:491:LEU:HA	1:B:491:LEU:HD12	1.76	0.42
1:C:123:ILE:HG21	1:C:131:VAL:HG23	2.00	0.42
1:C:202:LEU:HD23	1:C:202:LEU:HA	1.78	0.42
1:C:202:LEU:CD2	1:C:203:GLY:N	2.80	0.42
1:C:515:ARG:CB	1:C:516:PRO:HD2	2.41	0.42
1:D:390:HIS:CD2	1:D:390:HIS:H	2.36	0.42
1:E:17:LEU:N	1:E:17:LEU:HD23	2.34	0.42
1:E:86:THR:O	1:E:90:VAL:HG23	2.20	0.42
1:F:430:LEU:N	1:F:430:LEU:HD12	2.35	0.42
1:F:438:HIS:O	1:F:441:ALA:HB3	2.19	0.42
1:G:433:SER:HB2	1:G:435:ARG:HD2	2.01	0.42
1:H:278:ARG:O	1:H:281:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LYS:HE3	5:C:6127:HOH:O	2.19	0.42
1:E:49:THR:HG1	1:E:361:SER:HA	1.83	0.42
1:E:509:ILE:O	1:E:509:ILE:HG22	2.19	0.42
1:F:271:GLU:HG2	1:F:295:ASP:HB2	2.01	0.42
1:F:329:MET:O	1:F:330:LEU:HD13	2.19	0.42
1:G:421:LYS:HE2	1:H:413:MET:SD	2.60	0.42
1:A:242:SER:HA	1:A:269:LYS:HE2	2.01	0.42
1:B:370:PRO:HD2	1:B:371:LEU:H	1.83	0.42
1:B:407:LEU:HD12	1:B:407:LEU:HA	1.64	0.42
1:C:267:ILE:N	1:C:267:ILE:CD1	2.83	0.42
1:D:412:ALA:O	1:D:416:VAL:HG23	2.19	0.42
1:D:496:GLY:HA3	1:D:502:PHE:CZ	2.54	0.42
1:E:30:CYS:HB3	1:G:315:ARG:HD2	2.01	0.42
1:F:375:ARG:HH11	1:F:375:ARG:HD2	1.60	0.42
1:G:100:ASP:HB3	1:G:103:LEU:H	1.85	0.42
1:G:300:ILE:HG13	1:G:301:PRO:O	2.19	0.42
1:G:506:ASP:HB2	1:G:529:VAL:HG21	2.01	0.42
1:H:220:VAL:CG1	1:H:225:ILE:HG13	2.49	0.42
1:A:133:LEU:HD13	1:A:196:VAL:CG2	2.50	0.42
1:A:390:HIS:CD2	1:A:446:ARG:NH1	2.88	0.42
1:A:476:PRO:O	1:A:478:GLN:NE2	2.50	0.42
1:B:334:ILE:HG23	1:B:367:GLY:HA2	2.02	0.42
1:C:453:THR:CG2	1:C:459:ALA:HB2	2.49	0.42
1:C:465:TYR:HB2	1:C:468:ILE:CD1	2.42	0.42
1:D:123:ILE:HG12	1:D:151:CYS:O	2.20	0.42
1:D:270:ILE:O	1:D:270:ILE:HG22	2.18	0.42
1:D:289:ILE:HG22	1:D:290:MET:N	2.34	0.42
1:D:408:MET:O	1:D:408:MET:HG3	2.19	0.42
1:E:103:LEU:CD1	1:E:103:LEU:N	2.82	0.42
1:F:493:MET:HG2	1:F:530:PRO:CD	2.43	0.42
1:G:60:LEU:HD23	1:G:90:VAL:CA	2.48	0.42
1:G:180:ILE:HD13	1:G:180:ILE:N	2.34	0.42
1:H:120:THR:O	1:H:205:LYS:HA	2.20	0.42
1:H:137:ALA:O	1:H:195:GLU:HA	2.20	0.42
1:H:345:SER:O	1:H:349:ASN:HB2	2.20	0.42
1:A:163:ILE:HG23	1:A:164:CYS:N	2.35	0.42
1:A:247:ALA:O	1:A:250:VAL:HB	2.20	0.42
1:C:45:GLY:N	1:C:357:CYS:HB3	2.35	0.42
1:D:119:ARG:NH1	1:D:207:GLY:N	2.64	0.42
1:E:439:GLN:CA	1:E:439:GLN:NE2	2.83	0.42
1:F:217:LEU:HB3	1:F:218:PRO:CD	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:LEU:HD22	1:F:321:LYS:HD2	2.01	0.42
1:F:376:MET:O	1:F:376:MET:HE2	2.20	0.42
1:F:428:ILE:CD1	1:F:508:VAL:HG11	2.49	0.42
1:G:296:LEU:O	1:G:300:ILE:HG12	2.20	0.42
1:G:382:ARG:CG	1:G:382:ARG:NH1	2.80	0.42
1:H:407:LEU:N	1:H:407:LEU:HD13	2.35	0.42
1:B:14:THR:CG2	1:B:15:GLN:N	2.83	0.42
1:B:139:LEU:HD23	1:B:140:LYS:N	2.35	0.42
1:B:311:MET:SD	1:B:315:ARG:HD3	2.59	0.42
1:B:397:LEU:HD12	1:B:397:LEU:HA	1.96	0.42
1:D:472:VAL:CG1	1:D:473:CYS:N	2.80	0.42
1:E:94:THR:OG1	1:E:107:VAL:HB	2.19	0.42
1:E:95:GLU:C	1:E:97:PHE:H	2.23	0.42
1:E:456:HIS:CD2	1:E:456:HIS:H	2.36	0.42
1:F:118:ILE:HG22	1:F:208:VAL:HG21	2.01	0.42
1:G:93:ALA:O	1:G:96:SER:HB3	2.19	0.42
1:G:279:PHE:HE1	1:G:289:ILE:HG21	1.84	0.42
1:H:75:PHE:CZ	1:H:83:HIS:CB	3.03	0.42
1:H:104:TYR:O	1:H:106:PRO:HD3	2.19	0.42
1:A:131:VAL:CG2	1:A:153:GLU:HB3	2.50	0.42
1:A:283:LEU:HA	1:A:283:LEU:HD23	1.83	0.42
1:C:272:ASN:N	1:C:272:ASN:HD22	2.17	0.42
1:D:73:MET:HB3	1:D:75:PHE:HE1	1.83	0.42
1:E:23:ASP:OD1	1:E:23:ASP:N	2.43	0.42
1:E:340:THR:HG23	1:E:343:GLU:CD	2.40	0.42
1:F:162:ASN:HB3	1:F:165:LYS:HB3	2.02	0.42
1:G:84:ALA:HB2	1:G:230:PHE:CZ	2.55	0.42
1:G:276:VAL:O	1:G:279:PHE:HB2	2.19	0.42
1:H:189:PRO:HD2	1:H:191:PHE:CE2	2.55	0.42
1:H:499:ARG:HB3	1:H:501:PHE:CE1	2.55	0.42
1:A:237:ASP:O	1:A:461:GLN:NE2	2.52	0.41
1:B:328:GLN:HG2	1:B:331:GLU:CD	2.41	0.41
1:B:340:THR:O	1:B:343:GLU:HB2	2.20	0.41
1:C:14:THR:H	1:C:14:THR:HG22	1.58	0.41
1:C:55:ARG:NH2	1:C:82:TYR:CD1	2.88	0.41
1:C:196:VAL:CG1	1:C:197:GLU:N	2.82	0.41
1:D:228:LEU:CD2	1:D:257:LEU:HD11	2.49	0.41
1:D:303:GLU:H	1:D:303:GLU:HG3	1.40	0.41
1:E:225:ILE:O	1:E:229:LYS:HG3	2.19	0.41
1:F:16:GLN:HE21	1:F:16:GLN:HB2	1.54	0.41
1:F:21:MET:HE2	1:F:391:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ILE:HD13	1:F:151:CYS:O	2.20	0.41
1:F:162:ASN:OD1	1:F:165:LYS:HE3	2.20	0.41
1:G:348:ALA:O	1:G:352:LEU:HD22	2.20	0.41
1:A:17:LEU:O	1:A:20:ALA:HB3	2.20	0.41
1:B:156:LEU:HD22	1:B:157:TRP:N	2.32	0.41
1:B:182:LEU:H	1:B:182:LEU:HG	1.68	0.41
1:B:330:LEU:CD2	1:B:377:GLN:HG3	2.50	0.41
1:C:13:GLN:O	1:C:36:SER:OG	2.30	0.41
1:C:257:LEU:HD23	1:C:257:LEU:HA	1.89	0.41
1:C:468:ILE:HG22	1:C:470:PRO:HD3	2.02	0.41
1:D:51:GLY:O	1:D:55:ARG:HB2	2.20	0.41
1:E:324:ILE:HD12	1:E:324:ILE:HG21	1.82	0.41
1:F:54:SER:O	1:F:60:LEU:HD13	2.20	0.41
1:F:123:ILE:HA	1:F:151:CYS:HB2	2.01	0.41
1:F:244:ILE:HD13	1:F:244:ILE:HA	1.86	0.41
1:F:507:VAL:CG1	1:F:508:VAL:H	2.30	0.41
1:G:421:LYS:HA	1:G:421:LYS:HD3	1.86	0.41
1:G:423:LEU:N	1:G:423:LEU:CD1	2.80	0.41
1:G:503:LYS:N	1:G:506:ASP:OD2	2.50	0.41
1:H:24:THR:O	1:H:27:GLU:N	2.53	0.41
1:H:352:LEU:HD12	1:H:352:LEU:HA	1.67	0.41
1:A:369:TYR:HB3	1:A:372:GLU:HB2	2.01	0.41
1:B:464:LEU:HA	1:B:464:LEU:HD12	1.79	0.41
1:B:486:ASP:O	1:B:490:ASN:ND2	2.54	0.41
1:C:133:LEU:HD11	1:C:202:LEU:HB2	2.02	0.41
1:E:55:ARG:NH2	1:E:82:TYR:CD1	2.89	0.41
1:E:79:THR:OG1	1:E:80:HIS:N	2.48	0.41
1:F:145:ASN:HB3	1:F:148:MET:HE1	2.01	0.41
1:G:57:VAL:HG11	1:G:92:THR:HG21	2.02	0.41
1:G:524:MET:CE	1:H:524:MET:CE	2.99	0.41
1:H:168:ASP:O	1:H:171:SER:HB2	2.21	0.41
1:A:231:GLY:O	1:A:236:VAL:HG22	2.20	0.41
1:A:239:VAL:CG1	1:A:240:PHE:N	2.77	0.41
1:A:255:LYS:O	1:A:258:GLY:N	2.52	0.41
1:A:440:VAL:HG12	1:A:449:ILE:CD1	2.51	0.41
1:B:24:THR:HG22	1:B:27:GLU:HB2	2.02	0.41
1:B:413:MET:HE3	1:B:413:MET:HB3	1.92	0.41
1:B:424:ALA:HB2	1:B:509:ILE:CD1	2.50	0.41
1:D:155:ILE:CG2	1:D:156:LEU:N	2.83	0.41
1:E:388:MET:CE	1:E:466:ARG:NH2	2.83	0.41
1:G:138:THR:CG2	1:G:139:LEU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:ARG:HD2	1:H:86:THR:HG23	2.01	0.41
1:H:113:THR:CG2	1:H:114:LYS:N	2.80	0.41
1:H:209:ASN:C	1:H:210:LEU:HD13	2.40	0.41
1:H:253:VAL:O	1:H:253:VAL:HG12	2.18	0.41
1:H:382:ARG:HH11	1:H:382:ARG:CB	2.34	0.41
1:H:504:LYS:HA	1:H:530:PRO:OXT	2.20	0.41
1:B:380:ILE:HG13	1:B:380:ILE:H	1.53	0.41
1:C:56:SER:O	1:C:60:LEU:HD22	2.20	0.41
1:C:293:ARG:HD3	1:C:326:ALA:O	2.19	0.41
1:C:477:VAL:HG23	5:C:6139:HOH:O	2.20	0.41
1:D:60:LEU:HD12	1:D:60:LEU:HA	1.78	0.41
1:D:493:MET:HE2	1:D:529:VAL:HG13	2.02	0.41
1:E:390:HIS:CD2	1:E:446:ARG:HH11	2.39	0.41
1:F:341:ARG:HG2	1:H:328:GLN:NE2	2.35	0.41
1:G:168:ASP:O	1:G:171:SER:OG	2.38	0.41
1:G:316:CYS:HB3	1:G:321:LYS:O	2.21	0.41
1:G:504:LYS:O	1:G:529:VAL:HB	2.21	0.41
1:H:300:ILE:HG13	1:H:301:PRO:O	2.20	0.41
1:A:72:ARG:HH11	1:A:72:ARG:HD3	1.62	0.41
1:B:43:ASN:CG	1:B:467:GLY:HA2	2.40	0.41
1:B:72:ARG:NH2	1:B:112:ASP:OD2	2.48	0.41
1:G:50:ILE:N	1:G:50:ILE:HD13	2.34	0.41
1:G:166:VAL:HG13	1:G:166:VAL:O	2.20	0.41
1:G:244:ILE:HG13	1:G:268:SER:OG	2.20	0.41
1:G:279:PHE:HE2	1:G:315:ARG:HB3	1.86	0.41
1:G:438:HIS:O	1:G:441:ALA:HB3	2.20	0.41
1:H:49:THR:OG1	1:H:72:ARG:HD3	2.20	0.41
1:H:352:LEU:HD12	1:H:388:MET:HG2	2.02	0.41
1:H:430:LEU:HD12	1:H:430:LEU:HA	1.84	0.41
1:A:62:GLU:HG3	1:A:371:LEU:CD1	2.50	0.41
1:A:123:ILE:HB	1:A:204:SER:OG	2.20	0.41
1:A:294:GLY:CA	1:A:327:THR:HG21	2.51	0.41
1:B:160:TYR:HD2	1:B:163:ILE:HB	1.81	0.41
1:C:493:MET:O	1:C:497:LYS:HG3	2.21	0.41
1:D:142:THR:HG21	1:D:147:TYR:CD2	2.56	0.41
1:D:368:ASP:C	1:D:370:PRO:HD3	2.41	0.41
1:D:424:ALA:CB	1:D:509:ILE:HD12	2.50	0.41
1:E:428:ILE:O	1:E:428:ILE:HG22	2.15	0.41
1:E:436:SER:HB3	1:E:521:THR:HG1	1.86	0.41
1:G:481:TRP:O	1:G:483:GLU:N	2.53	0.41
1:H:50:ILE:HD12	1:H:60:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:ASP:HA	1:H:240:PHE:HB2	2.03	0.41
1:H:244:ILE:HD13	1:H:244:ILE:HA	1.93	0.41
1:H:449:ILE:HD13	1:H:449:ILE:HG21	1.76	0.41
1:A:39:ILE:HD12	1:A:41:ALA:HB3	2.02	0.41
1:A:72:ARG:NE	1:A:112:ASP:OD2	2.48	0.41
1:A:113:THR:CG2	1:A:114:LYS:N	2.83	0.41
1:B:48:CYS:SG	1:B:68:MET:HG3	2.61	0.41
1:B:133:LEU:CD2	1:B:133:LEU:N	2.83	0.41
1:B:283:LEU:HA	1:B:283:LEU:HD23	1.73	0.41
1:B:512:THR:C	1:B:521:THR:HG22	2.40	0.41
1:D:294:GLY:N	1:D:327:THR:HG21	2.36	0.41
1:E:17:LEU:HD22	1:E:17:LEU:HA	1.76	0.41
1:E:64:ILE:HG13	1:E:68:MET:CE	2.51	0.41
1:E:326:ALA:HB1	1:E:359:MET:CE	2.51	0.41
1:F:119:ARG:HA	1:F:119:ARG:HD2	1.84	0.41
1:F:327:THR:O	1:F:328:GLN:HB2	2.21	0.41
1:F:340:THR:OG1	1:F:343:GLU:HG2	2.20	0.41
5:F:6172:HOH:O	1:H:342:ALA:HB3	2.21	0.41
1:G:41:ALA:CB	1:G:448:PRO:HG3	2.51	0.41
1:G:529:VAL:O	1:G:530:PRO:OXT	2.39	0.41
1:H:122:LEU:O	1:H:151:CYS:HB2	2.21	0.41
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.52	0.41
1:A:60:LEU:HB3	1:A:93:ALA:CB	2.51	0.41
1:A:196:VAL:O	1:A:196:VAL:HG12	2.21	0.41
1:A:238:MET:HB2	1:A:265:LYS:O	2.20	0.41
1:B:46:ILE:HG23	1:B:377:GLN:NE2	2.35	0.41
1:B:111:LEU:HD23	1:B:112:ASP:N	2.36	0.41
1:B:147:TYR:CD1	1:B:147:TYR:N	2.89	0.41
1:B:342:ALA:CB	1:D:346:ASP:CB	2.99	0.41
1:C:51:GLY:O	1:C:55:ARG:N	2.54	0.41
1:C:63:MET:HG3	1:C:371:LEU:HD23	2.03	0.41
1:C:273:HIS:CB	1:C:277:ARG:NH1	2.80	0.41
1:D:162:ASN:OD1	1:D:162:ASN:N	2.54	0.41
1:D:245:ARG:O	1:D:278:ARG:HD3	2.20	0.41
1:E:102:ILE:CG2	1:E:103:LEU:HD12	2.49	0.41
1:E:104:TYR:CD2	1:E:106:PRO:HD3	2.56	0.41
1:E:270:ILE:N	1:E:270:ILE:CD1	2.79	0.41
1:F:133:LEU:CD1	1:F:139:LEU:HD13	2.41	0.41
1:F:145:ASN:HD22	1:F:157:TRP:HE1	1.69	0.41
1:F:192:LEU:HD13	1:F:192:LEU:HA	1.63	0.41
1:F:503:LYS:HB3	1:F:504:LYS:H	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:504:LYS:HG3	1:F:530:PRO:OXT	2.21	0.41
1:G:22:ALA:HB2	1:G:31:ARG:HD2	2.02	0.41
1:G:123:ILE:HA	1:G:151:CYS:O	2.20	0.41
1:G:316:CYS:CB	1:G:323:VAL:CG2	2.99	0.41
1:H:16:GLN:OE1	1:H:33:ASP:N	2.48	0.41
1:H:37:ALA:HA	1:H:38:PRO:HD3	1.97	0.41
1:H:63:MET:HB3	1:H:68:MET:CE	2.51	0.41
1:H:172:LYS:NZ	1:H:197:GLU:OE2	2.46	0.41
1:H:210:LEU:N	1:H:210:LEU:CD1	2.80	0.41
1:H:290:MET:CE	1:H:326:ALA:CB	2.99	0.41
1:H:290:MET:HE3	1:H:326:ALA:CB	2.51	0.41
1:H:507:VAL:HG12	1:H:508:VAL:H	1.84	0.41
1:A:100:ASP:OD2	1:A:103:LEU:HD13	2.20	0.41
1:A:169:VAL:CG1	1:A:170:GLY:N	2.84	0.41
1:A:461:GLN:O	1:A:464:LEU:HB2	2.21	0.41
1:B:336:LYS:CG	1:B:337:PRO:HD2	2.50	0.41
1:B:431:THR:CG2	1:B:434:GLY:HA2	2.51	0.41
1:D:247:ALA:C	1:D:250:VAL:HG23	2.42	0.41
1:D:267:ILE:N	1:D:267:ILE:CD1	2.80	0.41
1:D:352:LEU:HD12	1:D:352:LEU:HA	1.91	0.41
1:E:242:SER:HB3	1:E:271:GLU:OE2	2.21	0.41
1:F:480:ALA:HB3	1:F:483:GLU:HB2	2.02	0.41
1:G:90:VAL:HG23	1:G:90:VAL:H	1.63	0.41
1:G:329:MET:CE	1:G:347:VAL:HA	2.50	0.41
1:A:45:GLY:CA	1:A:357:CYS:HB3	2.51	0.40
1:A:60:LEU:HD23	1:A:89:ASN:C	2.42	0.40
1:A:429:VAL:O	1:A:430:LEU:HD12	2.21	0.40
1:A:503:LYS:HB2	1:A:506:ASP:OD2	2.22	0.40
1:B:50:ILE:HA	1:B:50:ILE:HD13	1.75	0.40
1:B:514:TRP:CD1	1:B:515:ARG:HG3	2.56	0.40
1:C:114:LYS:N	5:C:6126:HOH:O	2.49	0.40
1:C:382:ARG:HH11	1:C:382:ARG:HB2	1.86	0.40
1:C:491:LEU:HD12	1:C:491:LEU:HA	1.79	0.40
1:C:493:MET:HE1	1:C:529:VAL:CG2	2.44	0.40
1:E:232:VAL:HG12	1:E:233:GLU:N	2.36	0.40
1:E:328:GLN:NE2	1:G:341:ARG:N	2.65	0.40
1:F:115:GLY:HA2	1:F:116:PRO:HD3	1.64	0.40
1:F:289:ILE:HA	1:F:289:ILE:HD13	1.80	0.40
1:H:133:LEU:HD13	1:H:139:LEU:HD13	2.02	0.40
1:H:180:ILE:CG2	1:H:181:SER:N	2.84	0.40
1:C:496:GLY:HA3	1:C:502:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:PRO:HG3	1:D:465:TYR:CZ	2.57	0.40
1:E:50:ILE:HD13	1:E:50:ILE:HA	1.83	0.40
1:E:221:SER:HB3	1:E:224:ASP:OD2	2.20	0.40
1:E:515:ARG:HB3	1:E:516:PRO:CD	2.49	0.40
1:F:204:SER:O	1:F:206:LYS:HG2	2.21	0.40
1:F:333:MET:HE1	1:F:376:MET:HB2	2.03	0.40
1:G:247:ALA:O	1:G:250:VAL:N	2.54	0.40
1:G:330:LEU:HD23	1:G:360:LEU:HD21	2.03	0.40
1:H:60:LEU:HG	1:H:90:VAL:HG22	2.03	0.40
1:H:113:THR:HG22	1:H:242:SER:HB2	2.02	0.40
1:H:244:ILE:HG23	1:H:244:ILE:HD12	1.79	0.40
1:H:436:SER:HB3	1:H:521:THR:OG1	2.20	0.40
1:A:70:VAL:HG22	1:A:108:ALA:HB3	2.03	0.40
1:A:336:LYS:HB3	1:A:337:PRO:HD2	2.04	0.40
1:B:51:GLY:HA3	1:B:52:PRO:HD2	1.92	0.40
1:B:133:LEU:HD11	1:B:139:LEU:HD12	2.03	0.40
1:B:174:TYR:CE2	1:B:211:PRO:HG3	2.57	0.40
1:C:185:LYS:HG2	1:C:193:VAL:O	2.21	0.40
1:C:215:VAL:HG12	1:C:217:LEU:HB2	2.02	0.40
1:C:309:GLN:O	1:C:313:ILE:HG13	2.21	0.40
1:C:332:SER:HB3	1:C:343:GLU:OE1	2.22	0.40
1:E:43:ASN:ND2	1:E:467:GLY:HA2	2.36	0.40
1:E:219:ALA:HB2	1:E:252:GLU:OE2	2.22	0.40
1:G:316:CYS:CB	1:G:323:VAL:HG22	2.51	0.40
1:H:25:PHE:CE2	1:H:29:MET:CE	3.05	0.40
1:A:68:MET:HE3	1:A:68:MET:HB3	1.91	0.40
1:B:56:SER:O	1:B:60:LEU:HD22	2.21	0.40
1:B:64:ILE:CD1	1:B:94:THR:HA	2.51	0.40
1:B:80:HIS:CD2	1:B:80:HIS:H	2.39	0.40
1:B:195:GLU:HG3	1:B:196:VAL:N	2.36	0.40
1:B:342:ALA:HB2	1:D:346:ASP:OD2	2.22	0.40
1:C:487:LEU:HD23	1:C:487:LEU:C	2.42	0.40
1:D:134:LYS:HB3	1:D:134:LYS:HE3	1.58	0.40
1:D:185:LYS:NZ	1:D:195:GLU:HB2	2.36	0.40
1:D:428:ILE:HD12	1:D:508:VAL:CG1	2.51	0.40
1:E:105:ARG:HA	1:E:106:PRO:HD2	1.85	0.40
1:G:15:GLN:CB	1:G:17:LEU:CD2	2.99	0.40
1:G:79:THR:HG23	1:G:82:TYR:HB2	2.03	0.40
1:H:61:LYS:HE2	1:H:96:SER:OG	2.21	0.40
1:H:209:ASN:C	1:H:211:PRO:HD3	2.42	0.40
1:H:425:ALA:HB1	1:H:502:PHE:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HG3	1:A:499:ARG:HH21	1.87	0.40
1:A:123:ILE:HG13	1:A:203:GLY:O	2.21	0.40
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.62	0.40
1:C:289:ILE:HG22	1:C:290:MET:N	2.36	0.40
1:C:327:THR:OG1	4:C:532:PEQ:O2'	2.30	0.40
1:D:276:VAL:HG12	1:D:277:ARG:N	2.35	0.40
1:D:407:LEU:O	1:D:410:ALA:HB3	2.20	0.40
1:E:511:LEU:C	1:E:512:THR:HG23	2.42	0.40
1:F:177:ASP:HB3	1:F:298:ILE:CD1	2.51	0.40
1:F:330:LEU:O	1:F:363:GLU:HG2	2.22	0.40
1:G:221:SER:O	1:G:224:ASP:N	2.54	0.40
1:G:332:SER:OG	1:G:339:PRO:HA	2.21	0.40
1:H:267:ILE:HD12	1:H:267:ILE:HA	1.90	0.40
1:H:450:ILE:H	1:H:450:ILE:HG12	1.42	0.40
1:H:511:LEU:HA	1:H:523:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/530 (98%)	470 (91%)	41 (8%)	6 (1%)	13	32
1	B	517/530 (98%)	468 (90%)	43 (8%)	6 (1%)	13	32
1	C	517/530 (98%)	477 (92%)	37 (7%)	3 (1%)	25	50
1	D	517/530 (98%)	459 (89%)	49 (10%)	9 (2%)	9	23
1	E	422/530 (80%)	370 (88%)	43 (10%)	9 (2%)	7	18
1	F	517/530 (98%)	469 (91%)	39 (8%)	9 (2%)	9	23
1	G	517/530 (98%)	453 (88%)	56 (11%)	8 (2%)	10	26
1	H	517/530 (98%)	452 (87%)	56 (11%)	9 (2%)	9	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4041/4240 (95%)	3618 (90%)	364 (9%)	59 (2%)	10 26

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	GLY
1	B	13	GLN
1	D	15	GLN
1	D	137	ALA
1	F	137	ALA
1	H	13	GLN
1	H	506	ASP
1	A	189	PRO
1	A	328	GLN
1	D	78	GLY
1	D	148	MET
1	E	367	GLY
1	F	15	GLN
1	F	333	MET
1	G	482	ALA
1	H	78	GLY
1	H	402	SER
1	H	435	ARG
1	A	56	SER
1	A	148	MET
1	B	78	GLY
1	D	402	SER
1	E	302	ALA
1	F	177	ASP
1	F	198	ASN
1	F	205	LYS
1	F	212	GLY
1	G	219	ALA
1	G	479	GLU
1	G	521	THR
1	A	125	GLY
1	B	163	ILE
1	D	153	GLU
1	E	243	PHE
1	E	327	THR
1	G	481	TRP
1	C	327	THR

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Mol	Chain	Res	Type
1	E	96	SER
1	E	337	PRO
1	E	363	GLU
1	H	39	ILE
1	H	327	THR
1	B	327	THR
1	D	506	ASP
1	E	294	GLY
1	F	189	PRO
1	G	327	THR
1	G	426	ALA
1	B	52	PRO
1	D	217	LEU
1	E	275	GLY
1	F	528	PRO
1	G	528	PRO
1	H	189	PRO
1	B	339	PRO
1	C	217	LEU
1	C	367	GLY
1	D	294	GLY
1	H	444	ARG

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	426/434 (98%)	353 (83%)	73 (17%)	2	5
1	B	426/434 (98%)	331 (78%)	95 (22%)	1	2
1	C	426/434 (98%)	345 (81%)	81 (19%)	1	4
1	D	426/434 (98%)	336 (79%)	90 (21%)	1	3
1	E	347/434 (80%)	267 (77%)	80 (23%)	1	2
1	F	426/434 (98%)	333 (78%)	93 (22%)	1	2
1	G	426/434 (98%)	315 (74%)	111 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	426/434 (98%)	318 (75%)	108 (25%)	0 1
All	All	3329/3472 (96%)	2598 (78%)	731 (22%)	1 2

All (731) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	21	MET
1	A	23	ASP
1	A	27	GLU
1	A	31	ARG
1	A	36	SER
1	A	50	ILE
1	A	56	SER
1	A	60	LEU
1	A	61	LYS
1	A	73	MET
1	A	76	SER
1	A	81	GLU
1	A	86	THR
1	A	88	LYS
1	A	89	ASN
1	A	91	ARG
1	A	96	SER
1	A	99	SER
1	A	114	LYS
1	A	122	LEU
1	A	128	THR
1	A	132	GLU
1	A	133	LEU
1	A	134	LYS
1	A	139	LEU
1	A	145	ASN
1	A	153	GLU
1	A	158	LEU
1	A	161	LYS
1	A	162	ASN
1	A	164	CYS
1	A	165	LYS
1	A	171	SER
1	A	177	ASP
1	A	180	ILE

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Mol	Chain	Res	Type
1	A	186	GLN
1	A	187	LYS
1	A	192	LEU
1	A	202	LEU
1	A	225	ILE
1	A	237	ASP
1	A	254	ARG
1	A	260	LYS
1	A	262	LYS
1	A	263	ASN
1	A	283	LEU
1	A	303	GLU
1	A	315	ARG
1	A	317	ASN
1	A	330	LEU
1	A	352	LEU
1	A	357	CYS
1	A	366	LYS
1	A	379	LEU
1	A	389	PHE
1	A	392	LYS
1	A	397	LEU
1	A	399	ARG
1	A	402	SER
1	A	404	SER
1	A	415	SER
1	A	427	LEU
1	A	431	THR
1	A	433	SER
1	A	439	GLN
1	A	442	ARG
1	A	458	THR
1	A	468	ILE
1	A	483	GLU
1	A	486	ASP
1	A	497	LYS
1	A	512	THR
1	B	13	GLN
1	B	15	GLN
1	B	23	ASP
1	B	27	GLU
1	B	40	THR

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Mol	Chain	Res	Type
1	B	44	THR
1	B	59	THR
1	B	60	LEU
1	B	63	MET
1	B	64	ILE
1	B	65	LYS
1	B	73	MET
1	B	81	GLU
1	B	91	ARG
1	B	96	SER
1	B	102	ILE
1	B	122	LEU
1	B	130	GLU
1	B	132	GLU
1	B	134	LYS
1	B	138	THR
1	B	141	ILE
1	B	142	THR
1	B	143	LEU
1	B	145	ASN
1	B	148	MET
1	B	156	LEU
1	B	161	LYS
1	B	165	LYS
1	B	166	VAL
1	B	168	ASP
1	B	172	LYS
1	B	179	LEU
1	B	181	SER
1	B	182	LEU
1	B	185	LYS
1	B	186	GLN
1	B	192	LEU
1	B	195	GLU
1	B	202	LEU
1	B	204	SER
1	B	205	LYS
1	B	210	LEU
1	B	217	LEU
1	B	220	VAL
1	B	226	GLN
1	B	235	ASP

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Mol	Chain	Res	Type
1	B	246	LYS
1	B	250	VAL
1	B	254	ARG
1	B	259	GLU
1	B	260	LYS
1	B	263	ASN
1	B	264	ILE
1	B	267	ILE
1	B	283	LEU
1	B	293	ARG
1	B	299	GLU
1	B	303	GLU
1	B	311	MET
1	B	330	LEU
1	B	331	GLU
1	B	332	SER
1	B	333	MET
1	B	345	SER
1	B	352	LEU
1	B	357	CYS
1	B	358	ILE
1	B	361	SER
1	B	382	ARG
1	B	388	MET
1	B	392	LYS
1	B	397	LEU
1	B	400	SER
1	B	404	SER
1	B	407	LEU
1	B	413	MET
1	B	415	SER
1	B	419	SER
1	B	433	SER
1	B	436	SER
1	B	439	GLN
1	B	452	VAL
1	B	457	GLN
1	B	470	PRO
1	B	486	ASP
1	B	490	ASN
1	B	493	MET
1	B	502	PHE

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Mol	Chain	Res	Type
1	B	511	LEU
1	B	512	THR
1	B	515	ARG
1	B	518	SER
1	B	521	THR
1	B	524	MET
1	C	12	ILE
1	C	13	GLN
1	C	23	ASP
1	C	60	LEU
1	C	65	LYS
1	C	68	MET
1	C	72	ARG
1	C	73	MET
1	C	96	SER
1	C	105	ARG
1	C	113	THR
1	C	122	LEU
1	C	128	THR
1	C	132	GLU
1	C	134	LYS
1	C	135	LYS
1	C	141	ILE
1	C	145	ASN
1	C	154	ASN
1	C	155	ILE
1	C	156	LEU
1	C	158	LEU
1	C	162	ASN
1	C	166	VAL
1	C	169	VAL
1	C	171	SER
1	C	172	LYS
1	C	179	LEU
1	C	181	SER
1	C	182	LEU
1	C	186	GLN
1	C	187	LYS
1	C	190	ASP
1	C	192	LEU
1	C	198	ASN
1	C	202	LEU

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Mol	Chain	Res	Type
1	C	210	LEU
1	C	217	LEU
1	C	226	GLN
1	C	238	MET
1	C	246	LYS
1	C	253	VAL
1	C	254	ARG
1	C	259	GLU
1	C	260	LYS
1	C	262	LYS
1	C	267	ILE
1	C	268	SER
1	C	272	ASN
1	C	277	ARG
1	C	283	LEU
1	C	293	ARG
1	C	299	GLU
1	C	303	GLU
1	C	317	ASN
1	C	327	THR
1	C	330	LEU
1	C	332	SER
1	C	333	MET
1	C	336	LYS
1	C	338	ARG
1	C	345	SER
1	C	352	LEU
1	C	358	ILE
1	C	382	ARG
1	C	383	GLU
1	C	397	LEU
1	C	399	ARG
1	C	417	GLU
1	C	423	LEU
1	C	433	SER
1	C	436	SER
1	C	446	ARG
1	C	458	THR
1	C	466	ARG
1	C	493	MET
1	C	503	LYS
1	C	508	VAL

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Mol	Chain	Res	Type
1	C	515	ARG
1	C	518	SER
1	C	525	ARG
1	D	13	GLN
1	D	14	THR
1	D	15	GLN
1	D	29	MET
1	D	39	ILE
1	D	44	THR
1	D	55	ARG
1	D	56	SER
1	D	60	LEU
1	D	65	LYS
1	D	73	MET
1	D	76	SER
1	D	79	THR
1	D	96	SER
1	D	102	ILE
1	D	113	THR
1	D	117	GLU
1	D	122	LEU
1	D	123	ILE
1	D	135	LYS
1	D	140	LYS
1	D	141	ILE
1	D	149	GLU
1	D	153	GLU
1	D	156	LEU
1	D	159	ASP
1	D	162	ASN
1	D	165	LYS
1	D	166	VAL
1	D	175	VAL
1	D	179	LEU
1	D	181	SER
1	D	182	LEU
1	D	186	GLN
1	D	187	LYS
1	D	192	LEU
1	D	193	VAL
1	D	195	GLU
1	D	202	LEU

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Mol	Chain	Res	Type
1	D	204	SER
1	D	205	LYS
1	D	210	LEU
1	D	216	ASP
1	D	225	ILE
1	D	235	ASP
1	D	238	MET
1	D	246	LYS
1	D	250	VAL
1	D	252	GLU
1	D	255	LYS
1	D	259	GLU
1	D	260	LYS
1	D	272	ASN
1	D	273	HIS
1	D	280	ASP
1	D	283	LEU
1	D	286	SER
1	D	299	GLU
1	D	300	ILE
1	D	303	GLU
1	D	315	ARG
1	D	318	ARG
1	D	330	LEU
1	D	334	ILE
1	D	352	LEU
1	D	382	ARG
1	D	389	PHE
1	D	391	ARG
1	D	397	LEU
1	D	399	ARG
1	D	400	SER
1	D	401	SER
1	D	411	MET
1	D	415	SER
1	D	423	LEU
1	D	428	ILE
1	D	433	SER
1	D	436	SER
1	D	439	GLN
1	D	442	ARG
1	D	453	THR

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Mol	Chain	Res	Type
1	D	464	LEU
1	D	466	ARG
1	D	493	MET
1	D	497	LYS
1	D	499	ARG
1	D	507	VAL
1	D	508	VAL
1	D	511	LEU
1	D	515	ARG
1	E	13	GLN
1	E	14	THR
1	E	15	GLN
1	E	17	LEU
1	E	21	MET
1	E	27	GLU
1	E	34	ILE
1	E	54	SER
1	E	58	GLU
1	E	62	GLU
1	E	65	LYS
1	E	68	MET
1	E	72	ARG
1	E	76	SER
1	E	79	THR
1	E	88	LYS
1	E	91	ARG
1	E	99	SER
1	E	113	THR
1	E	114	LYS
1	E	216	ASP
1	E	220	VAL
1	E	221	SER
1	E	223	LYS
1	E	235	ASP
1	E	237	ASP
1	E	239	VAL
1	E	246	LYS
1	E	249	ASP
1	E	255	LYS
1	E	257	LEU
1	E	259	GLU
1	E	260	LYS

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Mol	Chain	Res	Type
1	E	262	LYS
1	E	263	ASN
1	E	272	ASN
1	E	273	HIS
1	E	277	ARG
1	E	283	LEU
1	E	284	GLU
1	E	298	ILE
1	E	299	GLU
1	E	300	ILE
1	E	303	GLU
1	E	309	GLN
1	E	321	LYS
1	E	327	THR
1	E	330	LEU
1	E	333	MET
1	E	336	LYS
1	E	340	THR
1	E	352	LEU
1	E	358	ILE
1	E	359	MET
1	E	361	SER
1	E	366	LYS
1	E	379	LEU
1	E	382	ARG
1	E	389	PHE
1	E	390	HIS
1	E	392	LYS
1	E	397	LEU
1	E	399	ARG
1	E	401	SER
1	E	404	SER
1	E	411	MET
1	E	423	LEU
1	E	436	SER
1	E	438	HIS
1	E	439	GLN
1	E	464	LEU
1	E	466	ARG
1	E	478	GLN
1	E	487	LEU
1	E	493	MET

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Mol	Chain	Res	Type
1	E	497	LYS
1	E	499	ARG
1	E	518	SER
1	E	521	THR
1	E	525	ARG
1	F	12	ILE
1	F	13	GLN
1	F	14	THR
1	F	16	GLN
1	F	23	ASP
1	F	24	THR
1	F	50	ILE
1	F	54	SER
1	F	60	LEU
1	F	65	LYS
1	F	68	MET
1	F	73	MET
1	F	79	THR
1	F	85	GLU
1	F	103	LEU
1	F	114	LYS
1	F	119	ARG
1	F	120	THR
1	F	123	ILE
1	F	128	THR
1	F	134	LYS
1	F	139	LEU
1	F	140	LYS
1	F	141	ILE
1	F	145	ASN
1	F	148	MET
1	F	156	LEU
1	F	158	LEU
1	F	164	CYS
1	F	165	LYS
1	F	166	VAL
1	F	169	VAL
1	F	179	LEU
1	F	182	LEU
1	F	183	GLN
1	F	187	LYS
1	F	192	LEU

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Mol	Chain	Res	Type
1	F	195	GLU
1	F	198	ASN
1	F	202	LEU
1	F	204	SER
1	F	205	LYS
1	F	209	ASN
1	F	210	LEU
1	F	225	ILE
1	F	226	GLN
1	F	242	SER
1	F	246	LYS
1	F	250	VAL
1	F	260	LYS
1	F	262	LYS
1	F	263	ASN
1	F	269	LYS
1	F	272	ASN
1	F	274	GLU
1	F	281	GLU
1	F	283	LEU
1	F	293	ARG
1	F	296	LEU
1	F	299	GLU
1	F	303	GLU
1	F	307	LEU
1	F	309	GLN
1	F	310	LYS
1	F	330	LEU
1	F	333	MET
1	F	343	GLU
1	F	352	LEU
1	F	376	MET
1	F	379	LEU
1	F	388	MET
1	F	389	PHE
1	F	397	LEU
1	F	407	LEU
1	F	413	MET
1	F	415	SER
1	F	419	SER
1	F	423	LEU
1	F	427	LEU

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Mol	Chain	Res	Type
1	F	433	SER
1	F	436	SER
1	F	442	ARG
1	F	453	THR
1	F	464	LEU
1	F	465	TYR
1	F	475	ASP
1	F	479	GLU
1	F	486	ASP
1	F	493	MET
1	F	497	LYS
1	F	508	VAL
1	F	515	ARG
1	F	518	SER
1	G	13	GLN
1	G	16	GLN
1	G	17	LEU
1	G	21	MET
1	G	23	ASP
1	G	27	GLU
1	G	29	MET
1	G	36	SER
1	G	55	ARG
1	G	59	THR
1	G	69	ASN
1	G	73	MET
1	G	79	THR
1	G	81	GLU
1	G	85	GLU
1	G	91	ARG
1	G	96	SER
1	G	99	SER
1	G	100	ASP
1	G	102	ILE
1	G	105	ARG
1	G	113	THR
1	G	117	GLU
1	G	122	LEU
1	G	123	ILE
1	G	126	SER
1	G	128	THR
1	G	131	VAL

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Mol	Chain	Res	Type
1	G	135	LYS
1	G	142	THR
1	G	143	LEU
1	G	153	GLU
1	G	154	ASN
1	G	156	LEU
1	G	158	LEU
1	G	166	VAL
1	G	167	VAL
1	G	168	ASP
1	G	171	SER
1	G	172	LYS
1	G	179	LEU
1	G	180	ILE
1	G	182	LEU
1	G	185	LYS
1	G	186	GLN
1	G	190	ASP
1	G	192	LEU
1	G	197	GLU
1	G	202	LEU
1	G	210	LEU
1	G	216	ASP
1	G	220	VAL
1	G	222	GLU
1	G	225	ILE
1	G	226	GLN
1	G	229	LYS
1	G	238	MET
1	G	242	SER
1	G	243	PHE
1	G	246	LYS
1	G	254	ARG
1	G	255	LYS
1	G	256	ILE
1	G	260	LYS
1	G	264	ILE
1	G	272	ASN
1	G	274	GLU
1	G	277	ARG
1	G	278	ARG
1	G	283	LEU

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Mol	Chain	Res	Type
1	G	296	LEU
1	G	303	GLU
1	G	310	LYS
1	G	313	ILE
1	G	330	LEU
1	G	333	MET
1	G	334	ILE
1	G	338	ARG
1	G	352	LEU
1	G	357	CYS
1	G	359	MET
1	G	366	LYS
1	G	376	MET
1	G	382	ARG
1	G	389	PHE
1	G	397	LEU
1	G	399	ARG
1	G	400	SER
1	G	401	SER
1	G	415	SER
1	G	416	VAL
1	G	419	SER
1	G	423	LEU
1	G	433	SER
1	G	436	SER
1	G	439	GLN
1	G	446	ARG
1	G	449	ILE
1	G	453	THR
1	G	464	LEU
1	G	466	ARG
1	G	472	VAL
1	G	473	CYS
1	G	479	GLU
1	G	487	LEU
1	G	491	LEU
1	G	493	MET
1	G	499	ARG
1	G	518	SER
1	G	524	MET
1	G	529	VAL
1	H	12	ILE

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Mol	Chain	Res	Type
1	H	13	GLN
1	H	14	THR
1	H	16	GLN
1	H	17	LEU
1	H	21	MET
1	H	23	ASP
1	H	24	THR
1	H	27	GLU
1	H	36	SER
1	H	44	THR
1	H	48	CYS
1	H	56	SER
1	H	60	LEU
1	H	62	GLU
1	H	64	ILE
1	H	65	LYS
1	H	69	ASN
1	H	72	ARG
1	H	73	MET
1	H	76	SER
1	H	86	THR
1	H	88	LYS
1	H	89	ASN
1	H	96	SER
1	H	100	ASP
1	H	102	ILE
1	H	113	THR
1	H	114	LYS
1	H	119	ARG
1	H	133	LEU
1	H	135	LYS
1	H	139	LEU
1	H	140	LYS
1	H	142	THR
1	H	148	MET
1	H	156	LEU
1	H	158	LEU
1	H	161	LYS
1	H	165	LYS
1	H	171	SER
1	H	179	LEU
1	H	181	SER

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Mol	Chain	Res	Type
1	H	185	LYS
1	H	192	LEU
1	H	195	GLU
1	H	197	GLU
1	H	202	LEU
1	H	204	SER
1	H	210	LEU
1	H	216	ASP
1	H	238	MET
1	H	243	PHE
1	H	246	LYS
1	H	260	LYS
1	H	262	LYS
1	H	263	ASN
1	H	267	ILE
1	H	268	SER
1	H	272	ASN
1	H	274	GLU
1	H	277	ARG
1	H	283	LEU
1	H	286	SER
1	H	299	GLU
1	H	300	ILE
1	H	303	GLU
1	H	323	VAL
1	H	330	LEU
1	H	345	SER
1	H	352	LEU
1	H	357	CYS
1	H	358	ILE
1	H	375	ARG
1	H	379	LEU
1	H	382	ARG
1	H	389	PHE
1	H	392	LYS
1	H	397	LEU
1	H	399	ARG
1	H	402	SER
1	H	407	LEU
1	H	415	SER
1	H	416	VAL
1	H	423	LEU

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Mol	Chain	Res	Type
1	H	430	LEU
1	H	435	ARG
1	H	436	SER
1	H	439	GLN
1	H	446	ARG
1	H	450	ILE
1	H	454	ARG
1	H	457	GLN
1	H	464	LEU
1	H	466	ARG
1	H	473	CYS
1	H	475	ASP
1	H	479	GLU
1	H	485	VAL
1	H	486	ASP
1	H	487	LEU
1	H	493	MET
1	H	497	LYS
1	H	499	ARG
1	H	502	PHE
1	H	512	THR
1	H	514	TRP
1	H	521	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	89	ASN
1	A	145	ASN
1	A	186	GLN
1	A	209	ASN
1	A	273	HIS
1	A	328	GLN
1	A	349	ASN
1	A	377	GLN
1	A	390	HIS
1	A	403	HIS
1	A	463	HIS
1	B	13	GLN
1	B	15	GLN
1	B	80	HIS

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Mol	Chain	Res	Type
1	B	145	ASN
1	B	186	GLN
1	B	273	HIS
1	B	317	ASN
1	B	328	GLN
1	B	349	ASN
1	B	377	GLN
1	B	390	HIS
1	B	439	GLN
1	B	456	HIS
1	B	457	GLN
1	B	463	HIS
1	B	490	ASN
1	B	494	ASN
1	C	13	GLN
1	C	15	GLN
1	C	28	HIS
1	C	77	HIS
1	C	89	ASN
1	C	145	ASN
1	C	186	GLN
1	C	198	ASN
1	C	226	GLN
1	C	272	ASN
1	C	328	GLN
1	C	377	GLN
1	C	390	HIS
1	C	457	GLN
1	C	494	ASN
1	D	13	GLN
1	D	15	GLN
1	D	43	ASN
1	D	89	ASN
1	D	186	GLN
1	D	377	GLN
1	D	390	HIS
1	D	457	GLN
1	D	463	HIS
1	D	494	ASN
1	E	15	GLN
1	E	43	ASN
1	E	77	HIS

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Mol	Chain	Res	Type
1	E	80	HIS
1	E	328	GLN
1	E	377	GLN
1	E	390	HIS
1	E	439	GLN
1	E	456	HIS
1	E	457	GLN
1	E	463	HIS
1	E	494	ASN
1	F	15	GLN
1	F	18	HIS
1	F	43	ASN
1	F	77	HIS
1	F	89	ASN
1	F	145	ASN
1	F	183	GLN
1	F	186	GLN
1	F	272	ASN
1	F	328	GLN
1	F	349	ASN
1	F	377	GLN
1	F	390	HIS
1	F	463	HIS
1	F	494	ASN
1	G	89	ASN
1	G	272	ASN
1	G	317	ASN
1	G	328	GLN
1	G	349	ASN
1	G	377	GLN
1	G	403	HIS
1	G	439	GLN
1	G	463	HIS
1	H	89	ASN
1	H	145	ASN
1	H	183	GLN
1	H	186	GLN
1	H	272	ASN
1	H	328	GLN
1	H	349	ASN
1	H	377	GLN
1	H	403	HIS

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Mol	Chain	Res	Type
1	H	439	GLN
1	H	457	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PEQ	A	532	3,2	8,9,9	1.11	0	11,13,13	0.88	0
4	PEQ	C	532	2	8,9,9	1.10	0	11,13,13	0.89	0
4	PEQ	H	532	2	8,9,9	1.12	0	11,13,13	0.89	0
4	PEQ	B	532	2	8,9,9	1.12	1 (12%)	11,13,13	0.89	0
4	PEQ	E	532	3,2	8,9,9	1.10	0	11,13,13	0.89	0
4	PEQ	D	532	2	8,9,9	1.12	1 (12%)	11,13,13	0.89	0
4	PEQ	G	532	2	8,9,9	1.10	0	11,13,13	0.88	0
4	PEQ	F	532	2	8,9,9	1.14	1 (12%)	11,13,13	0.90	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEQ	A	532	3,2	-	5/9/9/9	-
4	PEQ	C	532	2	-	6/9/9/9	-
4	PEQ	H	532	2	-	4/9/9/9	-
4	PEQ	B	532	2	-	6/9/9/9	-
4	PEQ	E	532	3,2	-	5/9/9/9	-
4	PEQ	D	532	2	-	5/9/9/9	-
4	PEQ	G	532	2	-	4/9/9/9	-
4	PEQ	F	532	2	-	5/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	532	PEQ	P-O2	2.08	1.63	1.59
4	D	532	PEQ	P-O2	2.04	1.63	1.59
4	B	532	PEQ	P-O2	2.00	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	532	PEQ	O1-C1-C2-C3
4	A	532	PEQ	O2'-C1-C2-O2
4	A	532	PEQ	C1-C2-O2-P
4	B	532	PEQ	O1-C1-C2-C3
4	B	532	PEQ	O2'-C1-C2-O2
4	B	532	PEQ	C1-C2-O2-P
4	C	532	PEQ	O1-C1-C2-C3
4	C	532	PEQ	O2'-C1-C2-O2
4	C	532	PEQ	C1-C2-O2-P
4	D	532	PEQ	O1-C1-C2-O2
4	D	532	PEQ	O2'-C1-C2-O2
4	D	532	PEQ	C3-C2-O2-P
4	E	532	PEQ	O1-C1-C2-C3
4	E	532	PEQ	O2'-C1-C2-O2
4	E	532	PEQ	C1-C2-O2-P
4	F	532	PEQ	O2'-C1-C2-O2
4	F	532	PEQ	C1-C2-O2-P

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Mol	Chain	Res	Type	Atoms
4	G	532	PEQ	O1-C1-C2-O2
4	G	532	PEQ	O2'-C1-C2-O2
4	H	532	PEQ	C3-C2-O2-P
4	A	532	PEQ	O1-C1-C2-O2
4	A	532	PEQ	O2'-C1-C2-C3
4	B	532	PEQ	O1-C1-C2-O2
4	B	532	PEQ	O2'-C1-C2-C3
4	C	532	PEQ	O1-C1-C2-O2
4	C	532	PEQ	O2'-C1-C2-C3
4	D	532	PEQ	O1-C1-C2-C3
4	D	532	PEQ	O2'-C1-C2-C3
4	E	532	PEQ	O1-C1-C2-O2
4	E	532	PEQ	O2'-C1-C2-C3
4	F	532	PEQ	O1-C1-C2-C3
4	F	532	PEQ	O1-C1-C2-O2
4	F	532	PEQ	O2'-C1-C2-C3
4	G	532	PEQ	O1-C1-C2-C3
4	G	532	PEQ	O2'-C1-C2-C3
4	H	532	PEQ	O1-C1-C2-C3
4	H	532	PEQ	O2'-C1-C2-O2
4	C	532	PEQ	C2-O2-P-O3P
4	H	532	PEQ	O2'-C1-C2-C3
4	B	532	PEQ	C2-O2-P-O2P

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	532	PEQ	1	0
4	C	532	PEQ	2	0
4	H	532	PEQ	6	0
4	B	532	PEQ	4	0
4	E	532	PEQ	1	0
4	D	532	PEQ	3	0
4	G	532	PEQ	1	0
4	F	532	PEQ	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.