Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:39 am BST

PDB ID	:	1GEH
Title	:	CRYSTAL STRUCTURE OF ARCHAEAL RUBISCO (RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE)
Authors	:	Kitano, K.; Maeda, N.; Fukui, T.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on	:	2000-11-13
Resolution	:	2.80 Å(reported)

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

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

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

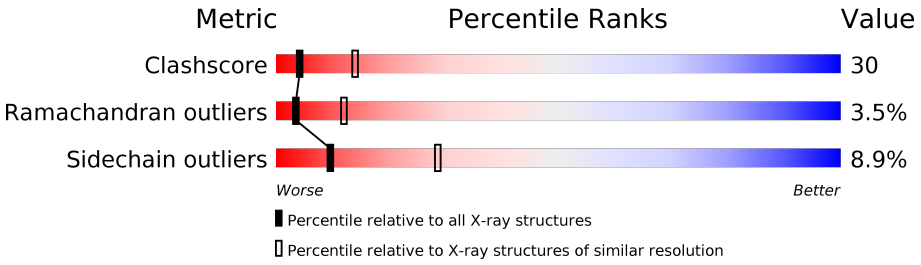
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	444	49% 41% 6%
1	B	444	49% 41% 6%
1	C	444	49% 41% 6%
1	D	444	49% 41% 6%
1	E	444	50% 40% 5%

2 Entry composition

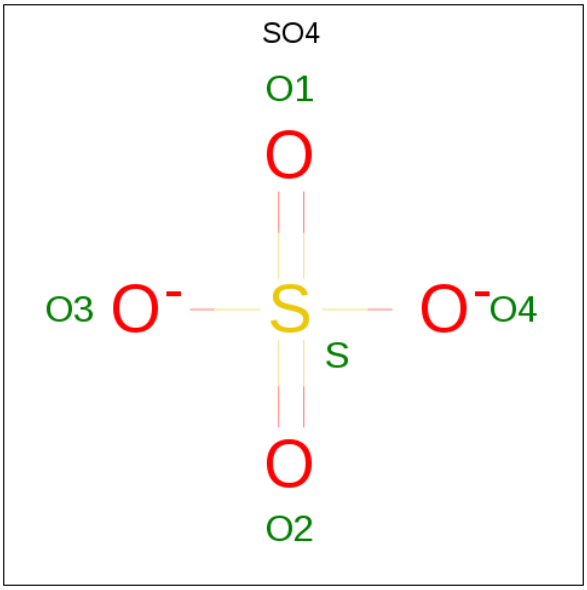
There are 2 unique types of molecules in this entry. The entry contains 16940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3378	2169	577	622	10			
1	B	427	Total	C	N	O	S	0	0	0
			3378	2169	577	622	10			
1	C	427	Total	C	N	O	S	0	0	0
			3378	2169	577	622	10			
1	D	427	Total	C	N	O	S	0	0	0
			3378	2169	577	622	10			
1	E	427	Total	C	N	O	S	0	0	0
			3378	2169	577	622	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

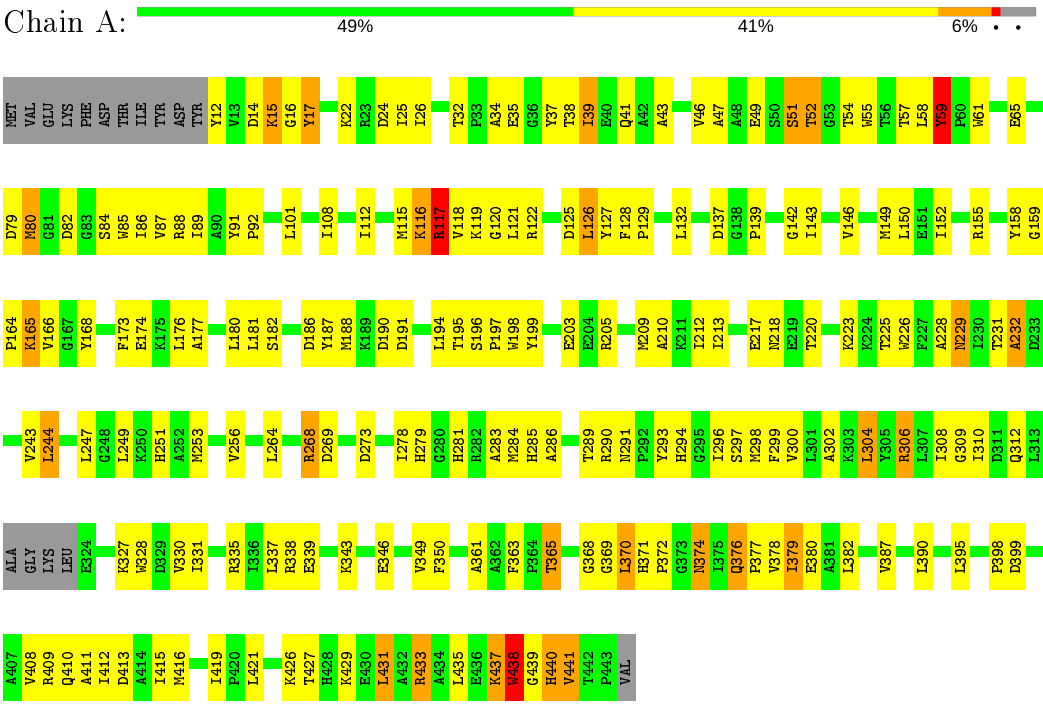
3 Residue-property plots (i)

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

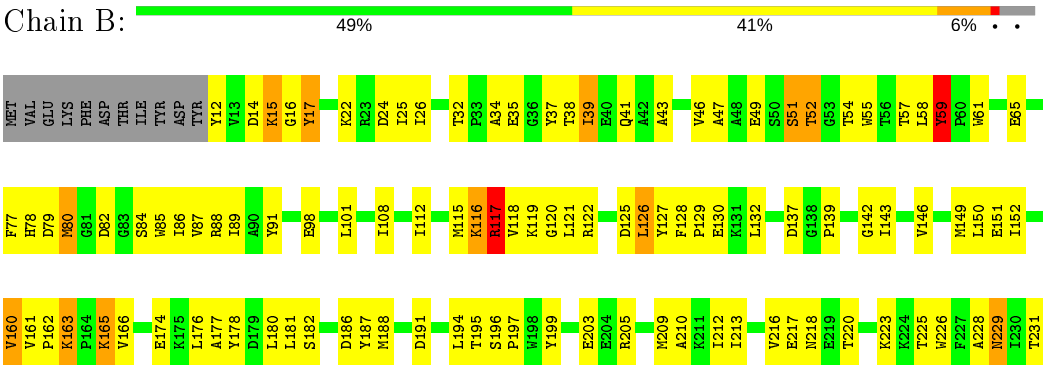
- Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

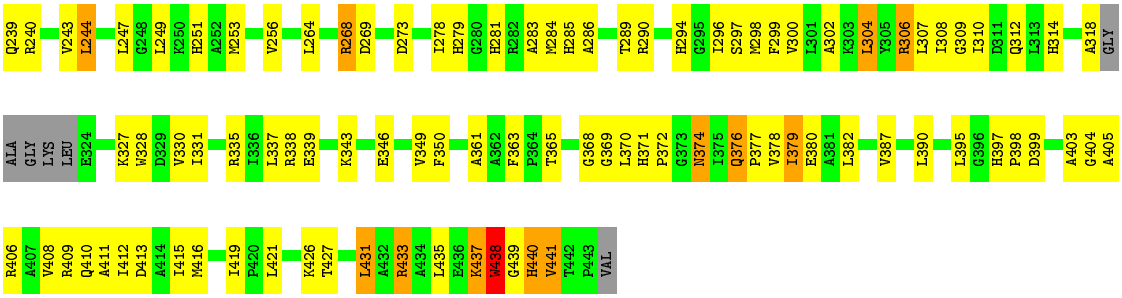
Chain A:



- Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

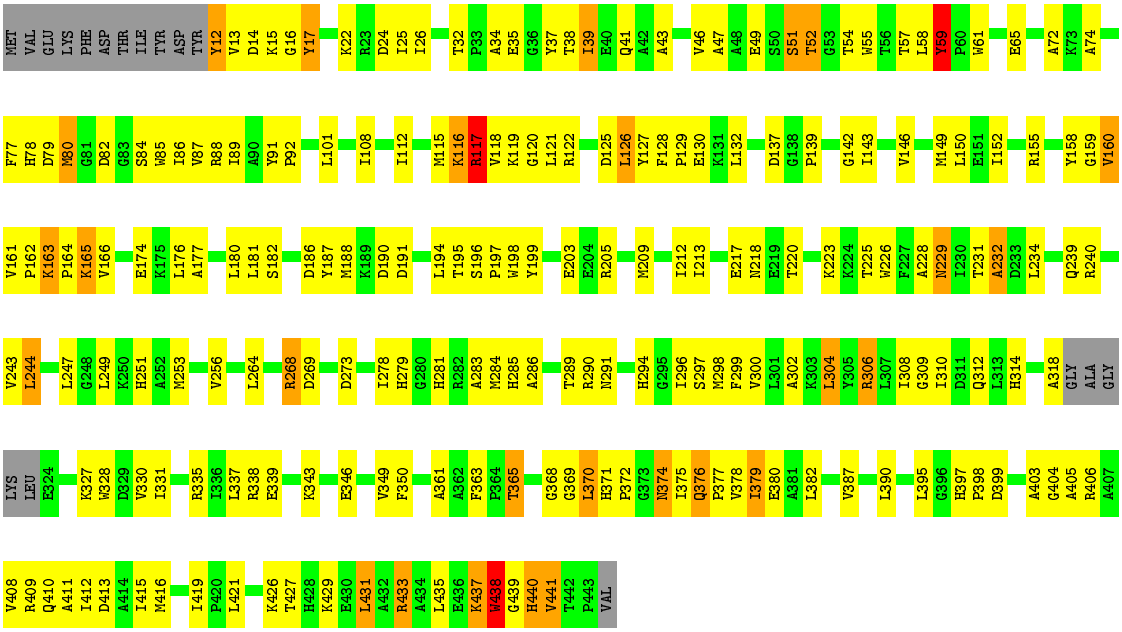
Chain B:





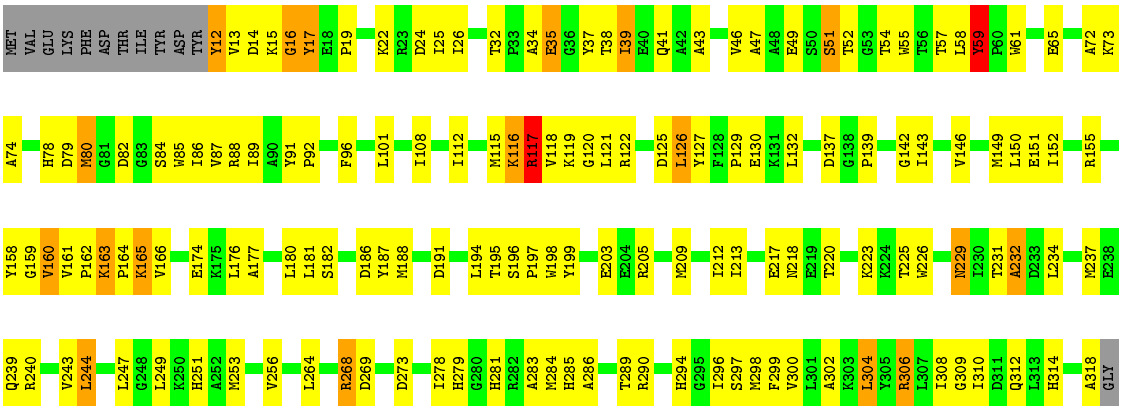
• Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

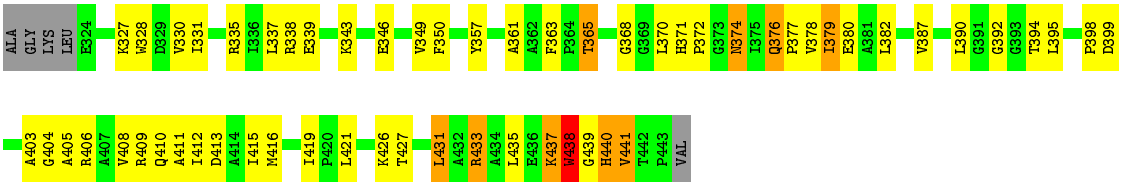
Chain C:



• Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

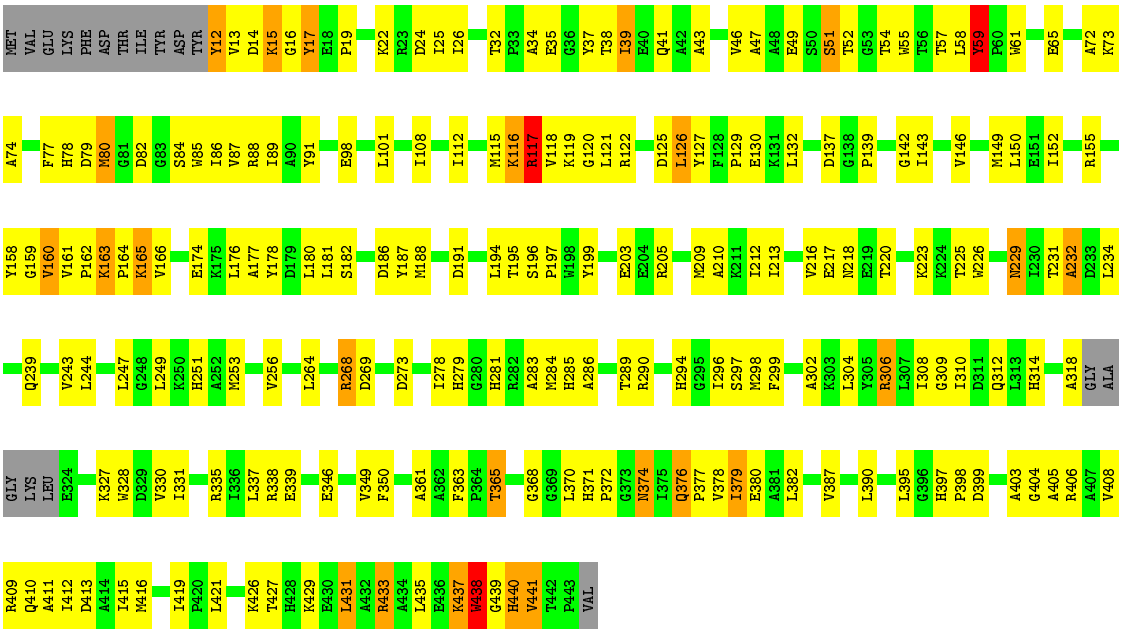
Chain D:





• Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain E:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	233.75Å 233.75Å 93.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16940	wwPDB-VP
Average B, all atoms (Å^2)	72.0	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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.38	0/3465	0.67	2/4695 (0.0%)
1	B	0.38	0/3465	0.67	2/4695 (0.0%)
1	C	0.37	0/3465	0.66	1/4695 (0.0%)
1	D	0.38	0/3465	0.67	1/4695 (0.0%)
1	E	0.38	0/3465	0.67	2/4695 (0.0%)
All	All	0.38	0/17325	0.67	8/23475 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	GLY	N-CA-C	-7.23	95.02	113.10
1	C	16	GLY	N-CA-C	-7.18	95.16	113.10
1	E	16	GLY	N-CA-C	-7.16	95.19	113.10
1	B	16	GLY	N-CA-C	-7.01	95.58	113.10
1	D	16	GLY	N-CA-C	-6.97	95.67	113.10
1	B	15	LYS	N-CA-C	5.12	124.82	111.00
1	A	15	LYS	N-CA-C	5.01	124.53	111.00
1	E	15	LYS	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3378	0	3316	198	0
1	B	3378	0	3316	200	0
1	C	3378	0	3316	203	0
1	D	3378	0	3316	199	0
1	E	3378	0	3316	194	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
All	All	16940	0	16580	991	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 30.

All (991) 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:B:435:LEU:HA	1:B:439:GLY:HA3	1.29	1.15
1:C:435:LEU:HA	1:C:439:GLY:HA3	1.30	1.11
1:E:435:LEU:HA	1:E:439:GLY:HA3	1.31	1.11
1:D:435:LEU:HA	1:D:439:GLY:HA3	1.30	1.09
1:A:435:LEU:HA	1:A:439:GLY:HA3	1.30	1.09
1:D:379:ILE:HD11	1:D:415:ILE:HD13	1.39	1.05
1:C:379:ILE:HD11	1:C:415:ILE:HD13	1.38	1.05
1:E:379:ILE:HD11	1:E:415:ILE:HD13	1.39	1.02
1:B:379:ILE:HD11	1:B:415:ILE:HD13	1.42	1.00
1:B:163:LYS:HA	1:B:163:LYS:HE2	1.44	0.98
1:A:379:ILE:HD11	1:A:415:ILE:HD13	1.41	0.98
1:A:403:ALA:HA	1:A:406:ARG:HH21	1.28	0.98
1:E:163:LYS:HE2	1:E:163:LYS:HA	1.43	0.97
1:C:163:LYS:HE2	1:C:163:LYS:HA	1.43	0.97
1:D:163:LYS:HA	1:D:163:LYS:HE2	1.43	0.96
1:A:163:LYS:HA	1:A:163:LYS:HE2	1.44	0.96
1:E:403:ALA:HA	1:E:406:ARG:HH21	1.31	0.94
1:B:403:ALA:HA	1:B:406:ARG:HH21	1.31	0.94
1:A:365:THR:HG23	1:A:387:VAL:HB	1.50	0.93
1:D:403:ALA:HA	1:D:406:ARG:HH21	1.30	0.93
1:C:403:ALA:HA	1:C:406:ARG:HH21	1.32	0.93
1:D:318:ALA:HB1	1:D:327:LYS:HG3	1.51	0.92
1:D:365:THR:HG23	1:D:387:VAL:HB	1.53	0.91
1:C:318:ALA:HB1	1:C:327:LYS:HG3	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:HB1	1:A:327:LYS:HG3	1.52	0.90
1:D:116:LYS:HD3	1:D:117:ARG:HD2	1.54	0.90
1:B:318:ALA:HB1	1:B:327:LYS:HG3	1.54	0.90
1:A:116:LYS:HD3	1:A:117:ARG:HD2	1.55	0.89
1:E:365:THR:HG23	1:E:387:VAL:HB	1.52	0.89
1:C:365:THR:HG23	1:C:387:VAL:HB	1.53	0.89
1:E:318:ALA:HB1	1:E:327:LYS:HG3	1.52	0.89
1:E:398:PRO:HG3	1:E:437:LYS:HD2	1.54	0.88
1:E:376:GLN:HB3	1:E:377:PRO:HD3	1.56	0.88
1:D:47:ALA:HB2	1:D:89:ILE:HD13	1.55	0.88
1:B:116:LYS:HD3	1:B:117:ARG:HD2	1.55	0.87
1:E:116:LYS:HD3	1:E:117:ARG:HD2	1.54	0.87
1:B:365:THR:HG23	1:B:387:VAL:HB	1.56	0.87
1:C:47:ALA:HB2	1:C:89:ILE:HD13	1.55	0.87
1:A:376:GLN:HB3	1:A:377:PRO:HD3	1.55	0.86
1:E:14:ASP:HB2	1:E:74:ALA:O	1.74	0.86
1:A:47:ALA:HB2	1:A:89:ILE:HD13	1.54	0.86
1:C:116:LYS:HD3	1:C:117:ARG:HD2	1.55	0.86
1:E:47:ALA:HB2	1:E:89:ILE:HD13	1.56	0.86
1:C:376:GLN:HB3	1:C:377:PRO:HD3	1.58	0.86
1:C:14:ASP:HB2	1:C:74:ALA:O	1.75	0.85
1:B:47:ALA:HB2	1:B:89:ILE:HD13	1.59	0.84
1:D:376:GLN:HB3	1:D:377:PRO:HD3	1.58	0.84
1:B:398:PRO:HG3	1:B:437:LYS:HD2	1.58	0.84
1:A:14:ASP:HB2	1:A:74:ALA:O	1.76	0.84
1:B:14:ASP:HB2	1:B:74:ALA:O	1.76	0.83
1:C:398:PRO:HG3	1:C:437:LYS:HD2	1.60	0.83
1:D:14:ASP:HB2	1:D:74:ALA:O	1.77	0.83
1:A:398:PRO:HG3	1:A:437:LYS:HD2	1.59	0.83
1:D:346:GLU:CD	1:D:346:GLU:H	1.83	0.83
1:B:376:GLN:HB3	1:B:377:PRO:HD3	1.60	0.82
1:A:346:GLU:CD	1:A:346:GLU:H	1.84	0.81
1:B:346:GLU:CD	1:B:346:GLU:H	1.84	0.81
1:D:398:PRO:HG3	1:D:437:LYS:HD2	1.60	0.81
1:E:346:GLU:H	1:E:346:GLU:CD	1.83	0.81
1:A:403:ALA:CA	1:A:406:ARG:HH21	1.96	0.79
1:D:38:THR:HG22	1:D:41:GLN:OE1	1.82	0.78
1:C:346:GLU:H	1:C:346:GLU:CD	1.84	0.78
1:E:38:THR:HG22	1:E:41:GLN:OE1	1.84	0.78
1:A:38:THR:HG22	1:A:41:GLN:OE1	1.83	0.78
1:A:251:HIS:HE1	1:A:312:GLN:HE22	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:MET:HA	1:D:80:MET:HE3	1.67	0.77
1:B:80:MET:HE3	1:B:80:MET:HA	1.66	0.76
1:A:80:MET:HE3	1:A:80:MET:HA	1.67	0.76
1:B:251:HIS:HE1	1:B:312:GLN:HE22	1.35	0.74
1:E:376:GLN:HA	1:E:415:ILE:HD11	1.69	0.74
1:C:38:THR:HG22	1:C:41:GLN:OE1	1.87	0.74
1:C:251:HIS:HE1	1:C:312:GLN:HE22	1.35	0.74
1:D:403:ALA:CA	1:D:406:ARG:HH21	2.00	0.74
1:C:376:GLN:HA	1:C:415:ILE:CD1	2.18	0.74
1:E:376:GLN:HA	1:E:415:ILE:CD1	2.18	0.74
1:A:116:LYS:HD2	1:A:116:LYS:N	2.03	0.74
1:B:116:LYS:HD2	1:B:116:LYS:N	2.03	0.74
1:A:174:GLU:HG3	1:A:212:ILE:HD11	1.70	0.74
1:D:376:GLN:HA	1:D:415:ILE:CD1	2.17	0.74
1:E:251:HIS:HE1	1:E:312:GLN:HE22	1.34	0.74
1:B:38:THR:HG22	1:B:41:GLN:OE1	1.87	0.73
1:D:376:GLN:HA	1:D:415:ILE:HD11	1.70	0.73
1:D:176:LEU:O	1:D:180:LEU:HD23	1.88	0.73
1:E:403:ALA:CA	1:E:406:ARG:HH21	1.99	0.73
1:B:376:GLN:HA	1:B:415:ILE:CD1	2.19	0.73
1:E:174:GLU:HG3	1:E:212:ILE:HD11	1.70	0.73
1:B:376:GLN:HA	1:B:415:ILE:HD11	1.70	0.73
1:C:174:GLU:HG3	1:C:212:ILE:HD11	1.70	0.73
1:C:376:GLN:HA	1:C:415:ILE:HD11	1.71	0.73
1:B:403:ALA:CA	1:B:406:ARG:HH21	2.02	0.73
1:A:376:GLN:HA	1:A:415:ILE:CD1	2.19	0.72
1:C:58:LEU:O	1:C:59:TYR:HB3	1.89	0.72
1:D:116:LYS:N	1:D:116:LYS:HD2	2.04	0.72
1:E:116:LYS:HD2	1:E:116:LYS:N	2.03	0.72
1:D:251:HIS:HE1	1:D:312:GLN:HE22	1.38	0.72
1:C:403:ALA:CA	1:C:406:ARG:HH21	2.00	0.72
1:D:58:LEU:O	1:D:59:TYR:HB3	1.90	0.72
1:E:80:MET:HE3	1:E:80:MET:HA	1.70	0.71
1:C:80:MET:HA	1:C:80:MET:HE3	1.70	0.71
1:B:58:LEU:O	1:B:59:TYR:HB3	1.89	0.71
1:C:116:LYS:HD2	1:C:116:LYS:N	2.06	0.71
1:C:268:ARG:HD3	1:C:309:GLY:HA3	1.73	0.71
1:E:117:ARG:HG2	1:E:117:ARG:HH11	1.55	0.71
1:E:268:ARG:HD3	1:E:309:GLY:HA3	1.72	0.71
1:E:58:LEU:O	1:E:59:TYR:HB3	1.90	0.71
1:A:176:LEU:O	1:A:180:LEU:HD23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:THR:O	1:C:205:ARG:NH2	2.24	0.70
1:D:268:ARG:HD3	1:D:309:GLY:HA3	1.73	0.70
1:A:251:HIS:CE1	1:A:312:GLN:HE22	2.09	0.70
1:B:213:ILE:O	1:B:217:GLU:HB2	1.92	0.70
1:A:195:THR:O	1:A:205:ARG:NH2	2.24	0.70
1:B:117:ARG:HG2	1:B:117:ARG:HH11	1.56	0.70
1:B:15:LYS:HD2	1:B:17:TYR:HB2	1.74	0.70
1:B:371:HIS:CE1	1:B:374:ASN:HB2	2.27	0.70
1:A:58:LEU:O	1:A:59:TYR:HB3	1.90	0.70
1:A:251:HIS:HE1	1:A:312:GLN:NE2	1.90	0.69
1:C:117:ARG:HG2	1:C:117:ARG:HH11	1.57	0.69
1:D:174:GLU:HG3	1:D:212:ILE:HD11	1.73	0.69
1:A:376:GLN:HA	1:A:415:ILE:HD11	1.74	0.69
1:B:176:LEU:O	1:B:180:LEU:HD23	1.92	0.69
1:A:371:HIS:CE1	1:A:374:ASN:HB2	2.28	0.69
1:E:176:LEU:O	1:E:180:LEU:HD23	1.93	0.69
1:D:117:ARG:HH11	1:D:117:ARG:HG2	1.57	0.69
1:E:251:HIS:CE1	1:E:312:GLN:HE22	2.10	0.69
1:E:251:HIS:HE1	1:E:312:GLN:NE2	1.91	0.69
1:C:176:LEU:O	1:C:180:LEU:HD23	1.93	0.69
1:B:174:GLU:HG3	1:B:212:ILE:HD11	1.73	0.69
1:B:268:ARG:HD3	1:B:309:GLY:HA3	1.75	0.68
1:D:371:HIS:CE1	1:D:374:ASN:HB2	2.28	0.68
1:E:371:HIS:CE1	1:E:374:ASN:HB2	2.28	0.68
1:E:410:GLN:HE21	1:E:431:LEU:HB2	1.57	0.68
1:D:195:THR:O	1:D:205:ARG:NH2	2.26	0.68
1:D:213:ILE:O	1:D:217:GLU:HB2	1.94	0.68
1:A:268:ARG:HD3	1:A:309:GLY:HA3	1.76	0.67
1:E:213:ILE:O	1:E:217:GLU:HB2	1.94	0.67
1:D:15:LYS:HD2	1:D:17:TYR:HB2	1.75	0.67
1:E:195:THR:O	1:E:205:ARG:NH2	2.25	0.67
1:A:117:ARG:HH11	1:A:117:ARG:HG2	1.59	0.67
1:B:370:LEU:N	1:B:370:LEU:HD12	2.10	0.67
1:B:410:GLN:HE21	1:B:431:LEU:HB2	1.59	0.67
1:E:438:TRP:HA	1:E:440:HIS:CE1	2.29	0.67
1:B:251:HIS:HE1	1:B:312:GLN:NE2	1.93	0.67
1:B:438:TRP:HA	1:B:440:HIS:CE1	2.29	0.67
1:C:438:TRP:HA	1:C:440:HIS:CE1	2.29	0.67
1:C:15:LYS:HD2	1:C:17:TYR:HB2	1.76	0.67
1:C:410:GLN:HE21	1:C:431:LEU:HB2	1.59	0.67
1:A:438:TRP:HA	1:A:440:HIS:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:HIS:CE1	1:B:312:GLN:HE22	2.13	0.66
1:C:116:LYS:CD	1:C:117:ARG:HD2	2.25	0.66
1:B:195:THR:O	1:B:205:ARG:NH2	2.27	0.66
1:C:213:ILE:O	1:C:217:GLU:HB2	1.95	0.66
1:C:251:HIS:HE1	1:C:312:GLN:NE2	1.94	0.66
1:D:410:GLN:HE21	1:D:431:LEU:HB2	1.59	0.66
1:D:438:TRP:HA	1:D:440:HIS:CE1	2.29	0.66
1:D:302:ALA:HB1	1:D:337:LEU:HD13	1.77	0.66
1:A:15:LYS:HD2	1:A:17:TYR:HB2	1.76	0.66
1:C:251:HIS:CE1	1:C:312:GLN:HE22	2.13	0.66
1:C:302:ALA:HB1	1:C:337:LEU:HD13	1.76	0.66
1:A:213:ILE:O	1:A:217:GLU:HB2	1.94	0.66
1:A:82:ASP:HB2	1:A:84:SER:OG	1.95	0.66
1:A:410:GLN:HE21	1:A:431:LEU:HB2	1.59	0.65
1:B:116:LYS:CD	1:B:117:ARG:HD2	2.26	0.65
1:D:370:LEU:HB2	1:D:390:LEU:HD22	1.78	0.65
1:C:370:LEU:HD12	1:C:370:LEU:N	2.11	0.65
1:C:82:ASP:HB2	1:C:84:SER:OG	1.97	0.65
1:D:205:ARG:HD2	1:D:226:TRP:HZ2	1.62	0.65
1:E:15:LYS:HD2	1:E:17:TYR:HB2	1.77	0.65
1:A:370:LEU:HB2	1:A:390:LEU:HD22	1.78	0.65
1:D:116:LYS:CD	1:D:117:ARG:HD2	2.25	0.65
1:A:370:LEU:HD12	1:A:370:LEU:N	2.11	0.65
1:E:370:LEU:HB2	1:E:390:LEU:HD22	1.79	0.65
1:C:371:HIS:CE1	1:C:374:ASN:HB2	2.31	0.65
1:E:82:ASP:HB2	1:E:84:SER:OG	1.96	0.65
1:A:116:LYS:HD2	1:A:116:LYS:H	1.62	0.65
1:D:251:HIS:CE1	1:D:312:GLN:HE22	2.14	0.65
1:E:302:ALA:HB1	1:E:337:LEU:HD13	1.79	0.65
1:B:34:ALA:HB3	1:B:37:TYR:CD1	2.33	0.64
1:E:370:LEU:N	1:E:370:LEU:HD12	2.12	0.64
1:A:116:LYS:CD	1:A:117:ARG:HD2	2.26	0.64
1:A:34:ALA:HB3	1:A:37:TYR:CD1	2.32	0.64
1:B:116:LYS:H	1:B:116:LYS:HD2	1.62	0.64
1:B:302:ALA:HB1	1:B:337:LEU:HD13	1.79	0.64
1:A:116:LYS:H	1:A:116:LYS:CD	2.09	0.64
1:E:34:ALA:HB3	1:E:37:TYR:CD1	2.32	0.64
1:B:82:ASP:HB2	1:B:84:SER:OG	1.98	0.64
1:E:116:LYS:HD2	1:E:116:LYS:H	1.62	0.64
1:A:158:TYR:O	1:A:186:ASP:HB2	1.98	0.64
1:D:251:HIS:HE1	1:D:312:GLN:NE2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ALA:HB3	1:C:37:TYR:CD1	2.33	0.64
1:D:158:TYR:O	1:D:186:ASP:HB2	1.97	0.64
1:C:160:VAL:HG11	1:C:180:LEU:HD12	1.80	0.63
1:D:34:ALA:HB3	1:D:37:TYR:CD1	2.33	0.63
1:E:116:LYS:CD	1:E:116:LYS:H	2.10	0.63
1:C:370:LEU:HB2	1:C:390:LEU:HD22	1.78	0.63
1:A:302:ALA:HB1	1:A:337:LEU:HD13	1.81	0.63
1:B:253:MET:HE3	1:B:281:HIS:HB2	1.81	0.63
1:B:370:LEU:HB2	1:B:390:LEU:HD22	1.80	0.63
1:C:205:ARG:HD2	1:C:226:TRP:HZ2	1.64	0.63
1:D:410:GLN:HE22	1:D:431:LEU:H	1.47	0.63
1:D:82:ASP:HB2	1:D:84:SER:OG	1.98	0.63
1:E:116:LYS:CD	1:E:117:ARG:HD2	2.26	0.63
1:E:398:PRO:CG	1:E:437:LYS:HD2	2.27	0.63
1:E:158:TYR:O	1:E:186:ASP:HB2	1.99	0.63
1:D:116:LYS:H	1:D:116:LYS:HD2	1.64	0.62
1:E:160:VAL:HG11	1:E:180:LEU:HD12	1.81	0.62
1:C:158:TYR:O	1:C:186:ASP:HB2	1.99	0.62
1:C:349:VAL:HG22	1:C:349:VAL:O	2.00	0.62
1:C:34:ALA:HB3	1:C:37:TYR:HD1	1.64	0.62
1:B:34:ALA:HB3	1:B:37:TYR:HD1	1.65	0.62
1:E:34:ALA:HB3	1:E:37:TYR:HD1	1.65	0.62
1:A:327:LYS:O	1:A:331:ILE:HG12	2.00	0.62
1:A:370:LEU:HB2	1:A:390:LEU:CD2	2.30	0.62
1:C:49:GLU:OE1	1:C:54:THR:HG21	1.99	0.62
1:D:116:LYS:CD	1:D:116:LYS:H	2.11	0.62
1:B:410:GLN:HE22	1:B:431:LEU:H	1.47	0.62
1:D:160:VAL:HG11	1:D:180:LEU:HD12	1.80	0.62
1:D:370:LEU:HB2	1:D:390:LEU:CD2	2.30	0.62
1:D:370:LEU:N	1:D:370:LEU:HD12	2.14	0.62
1:B:435:LEU:CA	1:B:439:GLY:HA3	2.18	0.62
1:A:160:VAL:HG11	1:A:180:LEU:HD12	1.82	0.62
1:A:49:GLU:OE1	1:A:54:THR:HG21	1.99	0.62
1:A:205:ARG:HD2	1:A:226:TRP:HZ2	1.65	0.61
1:A:331:ILE:HD13	1:A:382:LEU:HD13	1.82	0.61
1:D:268:ARG:HG3	1:D:269:ASP:N	2.15	0.61
1:B:158:TYR:O	1:B:186:ASP:HB2	2.00	0.61
1:C:410:GLN:HE22	1:C:431:LEU:H	1.49	0.61
1:E:370:LEU:HB2	1:E:390:LEU:CD2	2.30	0.61
1:A:34:ALA:HB3	1:A:37:TYR:HD1	1.65	0.61
1:C:116:LYS:HD2	1:C:116:LYS:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HD2	1:B:226:TRP:HZ2	1.65	0.61
1:E:410:GLN:HE22	1:E:431:LEU:H	1.47	0.61
1:C:327:LYS:O	1:C:331:ILE:HG12	2.01	0.61
1:D:435:LEU:CA	1:D:439:GLY:HA3	2.20	0.61
1:D:225:THR:OG1	1:D:251:HIS:HD2	1.84	0.61
1:E:349:VAL:O	1:E:349:VAL:HG22	2.00	0.61
1:B:160:VAL:HG11	1:B:180:LEU:HD12	1.82	0.60
1:C:370:LEU:HB2	1:C:390:LEU:CD2	2.30	0.60
1:C:116:LYS:CD	1:C:116:LYS:H	2.12	0.60
1:D:331:ILE:HD13	1:D:382:LEU:HD13	1.84	0.60
1:B:370:LEU:HB2	1:B:390:LEU:CD2	2.32	0.60
1:B:152:ILE:HD12	1:B:155:ARG:NH2	2.17	0.60
1:B:331:ILE:HD13	1:B:382:LEU:HD13	1.84	0.60
1:E:205:ARG:HD2	1:E:226:TRP:HZ2	1.67	0.60
1:B:349:VAL:HG22	1:B:349:VAL:O	2.01	0.60
1:E:435:LEU:CA	1:E:439:GLY:HA3	2.20	0.60
1:C:331:ILE:HD13	1:C:382:LEU:HD13	1.82	0.60
1:D:49:GLU:OE1	1:D:54:THR:HG21	2.02	0.60
1:E:331:ILE:HD13	1:E:382:LEU:HD13	1.84	0.60
1:E:49:GLU:OE1	1:E:54:THR:HG21	2.02	0.60
1:B:268:ARG:HG3	1:B:269:ASP:N	2.16	0.59
1:D:34:ALA:HB3	1:D:37:TYR:HD1	1.67	0.59
1:B:116:LYS:CD	1:B:116:LYS:H	2.09	0.59
1:D:327:LYS:O	1:D:331:ILE:HG12	2.02	0.59
1:D:349:VAL:HG22	1:D:349:VAL:O	2.01	0.59
1:B:327:LYS:O	1:B:331:ILE:HG12	2.02	0.59
1:B:374:ASN:O	1:B:377:PRO:HD2	2.02	0.59
1:A:435:LEU:CA	1:A:439:GLY:HA3	2.19	0.59
1:B:225:THR:OG1	1:B:251:HIS:HD2	1.85	0.59
1:A:410:GLN:HE22	1:A:431:LEU:H	1.49	0.59
1:E:327:LYS:O	1:E:331:ILE:HG12	2.03	0.59
1:A:152:ILE:HD12	1:A:155:ARG:NH2	2.18	0.59
1:E:139:PRO:HD3	1:E:306:ARG:O	2.03	0.59
1:E:225:THR:OG1	1:E:251:HIS:HD2	1.86	0.58
1:A:225:THR:OG1	1:A:251:HIS:HD2	1.85	0.58
1:A:349:VAL:O	1:A:349:VAL:HG22	2.03	0.58
1:C:225:THR:OG1	1:C:251:HIS:HD2	1.86	0.58
1:A:163:LYS:HA	1:A:163:LYS:CE	2.25	0.58
1:D:374:ASN:O	1:D:377:PRO:HD2	2.03	0.58
1:D:47:ALA:CB	1:D:89:ILE:HD13	2.31	0.58
1:E:152:ILE:HD12	1:E:155:ARG:NH2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:HG23	1:A:387:VAL:CB	2.31	0.58
1:A:378:VAL:HG13	1:A:382:LEU:HD23	1.86	0.58
1:A:398:PRO:CG	1:A:437:LYS:HD2	2.33	0.58
1:D:143:ILE:HD11	1:D:338:ARG:HG2	1.84	0.58
1:B:49:GLU:OE1	1:B:54:THR:HG21	2.03	0.58
1:E:268:ARG:HG3	1:E:269:ASP:N	2.19	0.58
1:A:408:VAL:O	1:A:412:ILE:HG12	2.04	0.58
1:B:378:VAL:HG13	1:B:382:LEU:HD23	1.86	0.58
1:C:165:LYS:HE3	1:C:191:ASP:OD2	2.04	0.58
1:E:378:VAL:HG13	1:E:382:LEU:HD23	1.86	0.58
1:A:139:PRO:HD3	1:A:306:ARG:O	2.04	0.58
1:C:310:ILE:HD12	1:C:310:ILE:N	2.19	0.57
1:A:268:ARG:HG3	1:A:269:ASP:N	2.19	0.57
1:B:117:ARG:HG2	1:B:117:ARG:NH1	2.18	0.57
1:A:163:LYS:HG2	1:A:395:LEU:HD23	1.86	0.57
1:B:112:ILE:HA	1:B:115:MET:HG3	1.86	0.57
1:C:79:ASP:HB2	1:C:85:TRP:CH2	2.40	0.57
1:A:47:ALA:CB	1:A:89:ILE:HD13	2.32	0.57
1:D:112:ILE:HA	1:D:115:MET:HG3	1.86	0.57
1:E:410:GLN:NE2	1:E:431:LEU:HB2	2.18	0.57
1:C:398:PRO:CG	1:C:437:LYS:HD2	2.34	0.57
1:A:253:MET:HE3	1:A:281:HIS:HB2	1.86	0.57
1:B:310:ILE:HD12	1:B:310:ILE:N	2.20	0.57
1:C:268:ARG:HG3	1:C:269:ASP:N	2.18	0.57
1:A:143:ILE:HD11	1:A:338:ARG:HG2	1.85	0.57
1:A:79:ASP:HB2	1:A:85:TRP:CH2	2.40	0.57
1:D:408:VAL:O	1:D:412:ILE:HG12	2.05	0.57
1:B:408:VAL:O	1:B:412:ILE:HG12	2.05	0.57
1:B:398:PRO:CG	1:B:437:LYS:HD2	2.32	0.57
1:C:49:GLU:HA	1:C:54:THR:HG22	1.87	0.57
1:C:47:ALA:CB	1:C:89:ILE:HD13	2.33	0.57
1:A:112:ILE:HA	1:A:115:MET:HG3	1.87	0.56
1:A:426:LYS:O	1:A:427:THR:OG1	2.22	0.56
1:C:152:ILE:HD12	1:C:155:ARG:NH2	2.19	0.56
1:C:410:GLN:NE2	1:C:431:LEU:HB2	2.20	0.56
1:C:435:LEU:CA	1:C:439:GLY:HA3	2.20	0.56
1:D:117:ARG:NH1	1:D:117:ARG:HG2	2.19	0.56
1:B:163:LYS:HG2	1:B:395:LEU:HD23	1.88	0.56
1:B:378:VAL:C	1:B:380:GLU:H	2.09	0.56
1:D:378:VAL:HG13	1:D:382:LEU:HD23	1.88	0.56
1:D:410:GLN:NE2	1:D:431:LEU:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:LEU:O	1:E:294:HIS:HA	2.06	0.56
1:A:421:LEU:HD12	1:A:441:VAL:HG13	1.86	0.56
1:A:403:ALA:HA	1:A:406:ARG:NH2	2.10	0.56
1:B:58:LEU:HD22	1:B:58:LEU:N	2.21	0.56
1:C:421:LEU:HD12	1:C:441:VAL:HG13	1.88	0.56
1:E:117:ARG:HG2	1:E:117:ARG:NH1	2.18	0.56
1:C:426:LYS:O	1:C:427:THR:OG1	2.21	0.56
1:C:253:MET:HE3	1:C:281:HIS:HB2	1.88	0.56
1:C:58:LEU:HD22	1:C:58:LEU:N	2.21	0.56
1:E:229:ASN:ND2	1:E:231:THR:H	2.03	0.56
1:A:229:ASN:ND2	1:A:231:THR:H	2.04	0.56
1:C:378:VAL:HG13	1:C:382:LEU:HD23	1.88	0.56
1:E:426:LYS:O	1:E:427:THR:OG1	2.20	0.56
1:A:49:GLU:HA	1:A:54:THR:HG22	1.88	0.56
1:D:152:ILE:HD12	1:D:155:ARG:NH2	2.21	0.56
1:E:112:ILE:HA	1:E:115:MET:HG3	1.87	0.56
1:A:410:GLN:NE2	1:A:431:LEU:HB2	2.20	0.55
1:B:143:ILE:HD11	1:B:338:ARG:HG2	1.88	0.55
1:B:79:ASP:HB2	1:B:85:TRP:CH2	2.41	0.55
1:C:121:LEU:O	1:C:294:HIS:HA	2.06	0.55
1:D:163:LYS:HG2	1:D:395:LEU:HD23	1.89	0.55
1:D:121:LEU:O	1:D:294:HIS:HA	2.06	0.55
1:D:421:LEU:HD12	1:D:441:VAL:HG13	1.87	0.55
1:E:408:VAL:O	1:E:412:ILE:HG12	2.06	0.55
1:A:58:LEU:HD22	1:A:58:LEU:N	2.22	0.55
1:D:163:LYS:HA	1:D:163:LYS:CE	2.25	0.55
1:E:163:LYS:HG2	1:E:395:LEU:HD23	1.88	0.55
1:B:57:THR:HG21	1:B:61:TRP:HD1	1.71	0.55
1:E:421:LEU:HD12	1:E:441:VAL:HG13	1.89	0.55
1:E:58:LEU:HD22	1:E:58:LEU:N	2.21	0.55
1:C:163:LYS:HG2	1:C:395:LEU:HD23	1.88	0.55
1:C:139:PRO:HD3	1:C:306:ARG:O	2.06	0.55
1:E:79:ASP:HB2	1:E:85:TRP:CH2	2.40	0.55
1:E:163:LYS:CE	1:E:163:LYS:HA	2.24	0.55
1:B:130:GLU:HG2	1:C:198:TRP:HZ3	1.72	0.55
1:C:57:THR:HG21	1:C:61:TRP:HD1	1.72	0.55
1:A:378:VAL:C	1:A:380:GLU:H	2.10	0.55
1:D:177:ALA:HA	1:D:188:MET:HE3	1.89	0.55
1:D:205:ARG:HD2	1:D:226:TRP:CZ2	2.42	0.55
1:C:408:VAL:O	1:C:412:ILE:HG12	2.06	0.55
1:D:49:GLU:HA	1:D:54:THR:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HG2	1:A:117:ARG:NH1	2.20	0.54
1:C:112:ILE:HA	1:C:115:MET:HG3	1.87	0.54
1:C:378:VAL:C	1:C:380:GLU:H	2.10	0.54
1:D:310:ILE:HD12	1:D:310:ILE:N	2.22	0.54
1:B:15:LYS:HB2	1:B:17:TYR:HB3	1.90	0.54
1:D:330:VAL:HG12	1:D:382:LEU:HD11	1.89	0.54
1:E:374:ASN:O	1:E:377:PRO:HD2	2.07	0.54
1:E:330:VAL:HG12	1:E:382:LEU:HD11	1.88	0.54
1:D:165:LYS:HE3	1:D:191:ASP:OD2	2.07	0.54
1:D:139:PRO:HD3	1:D:306:ARG:O	2.08	0.54
1:D:403:ALA:HA	1:D:406:ARG:NH2	2.12	0.54
1:C:403:ALA:HA	1:C:406:ARG:NH2	2.13	0.54
1:E:15:LYS:HB2	1:E:17:TYR:CB	2.38	0.54
1:E:143:ILE:HD11	1:E:338:ARG:HG2	1.89	0.54
1:B:410:GLN:NE2	1:B:431:LEU:HB2	2.21	0.54
1:D:376:GLN:CB	1:D:377:PRO:HD3	2.36	0.54
1:D:58:LEU:HD22	1:D:58:LEU:N	2.22	0.54
1:E:253:MET:HE3	1:E:281:HIS:HB2	1.89	0.54
1:E:57:THR:HG21	1:E:61:TRP:HD1	1.72	0.54
1:A:15:LYS:HB2	1:A:17:TYR:H	1.73	0.54
1:B:421:LEU:HD12	1:B:441:VAL:HG13	1.89	0.54
1:D:378:VAL:C	1:D:380:GLU:H	2.10	0.54
1:A:165:LYS:HE3	1:A:191:ASP:OD2	2.07	0.54
1:D:108:ILE:O	1:D:108:ILE:HG22	2.07	0.54
1:E:49:GLU:HA	1:E:54:THR:HG22	1.88	0.54
1:A:239:GLN:O	1:A:243:VAL:HG23	2.08	0.54
1:B:426:LYS:O	1:B:427:THR:OG1	2.22	0.54
1:E:15:LYS:HB2	1:E:17:TYR:H	1.73	0.54
1:E:378:VAL:C	1:E:380:GLU:H	2.11	0.54
1:A:15:LYS:HB2	1:A:17:TYR:CB	2.37	0.54
1:B:101:LEU:HD23	1:B:308:ILE:HD11	1.90	0.54
1:B:49:GLU:HA	1:B:54:THR:HG22	1.89	0.54
1:E:165:LYS:HE3	1:E:191:ASP:OD2	2.08	0.54
1:D:79:ASP:HB2	1:D:85:TRP:CH2	2.42	0.53
1:A:283:ALA:O	1:A:284:MET:HB3	2.06	0.53
1:A:57:THR:HG21	1:A:61:TRP:HD1	1.72	0.53
1:B:205:ARG:HD2	1:B:226:TRP:CZ2	2.43	0.53
1:A:15:LYS:HB2	1:A:17:TYR:HB3	1.90	0.53
1:B:139:PRO:HD3	1:B:306:ARG:O	2.09	0.53
1:C:289:THR:HG22	1:C:296:ILE:O	2.09	0.53
1:E:365:THR:HG23	1:E:387:VAL:CB	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ILE:HD11	1:C:338:ARG:HG2	1.90	0.53
1:C:374:ASN:O	1:C:377:PRO:HD2	2.08	0.53
1:A:376:GLN:CB	1:A:377:PRO:HD3	2.34	0.53
1:C:166:VAL:HG13	1:C:199:TYR:OH	2.09	0.53
1:D:57:THR:HG21	1:D:61:TRP:HD1	1.73	0.53
1:A:108:ILE:HG22	1:A:108:ILE:O	2.08	0.53
1:A:374:ASN:O	1:A:377:PRO:HD2	2.08	0.53
1:B:330:VAL:HG12	1:B:382:LEU:HD11	1.90	0.53
1:C:72:ALA:HB2	1:C:91:TYR:CD1	2.44	0.53
1:E:285:HIS:CG	1:E:286:ALA:N	2.76	0.53
1:A:310:ILE:HD12	1:A:310:ILE:N	2.23	0.53
1:B:24:ASP:O	1:B:129:PRO:HG3	2.09	0.53
1:B:437:LYS:C	1:B:439:GLY:H	2.11	0.53
1:A:409:ARG:HG2	1:A:409:ARG:HH11	1.73	0.53
1:B:108:ILE:HG22	1:B:108:ILE:O	2.09	0.53
1:C:205:ARG:HD2	1:C:226:TRP:CZ2	2.43	0.53
1:C:79:ASP:HB2	1:C:85:TRP:CZ3	2.44	0.53
1:E:283:ALA:O	1:E:284:MET:HB3	2.08	0.53
1:E:58:LEU:HD22	1:E:58:LEU:H	1.74	0.53
1:B:163:LYS:CE	1:B:163:LYS:HA	2.25	0.53
1:C:108:ILE:HG22	1:C:108:ILE:O	2.08	0.53
1:D:15:LYS:HB2	1:D:17:TYR:HB3	1.91	0.53
1:E:310:ILE:N	1:E:310:ILE:HD12	2.23	0.53
1:A:435:LEU:HA	1:A:439:GLY:CA	2.22	0.53
1:B:15:LYS:HB2	1:B:17:TYR:CB	2.39	0.53
1:D:15:LYS:HB2	1:D:17:TYR:CB	2.39	0.53
1:D:398:PRO:CG	1:D:437:LYS:HD2	2.34	0.53
1:E:166:VAL:HG13	1:E:199:TYR:OH	2.09	0.53
1:A:285:HIS:CG	1:A:286:ALA:N	2.77	0.52
1:A:121:LEU:O	1:A:294:HIS:HA	2.10	0.52
1:B:121:LEU:O	1:B:294:HIS:HA	2.09	0.52
1:E:108:ILE:HG22	1:E:108:ILE:O	2.10	0.52
1:B:165:LYS:HE3	1:B:191:ASP:OD2	2.09	0.52
1:C:130:GLU:HG2	1:D:198:TRP:HZ3	1.74	0.52
1:C:15:LYS:HB2	1:C:17:TYR:CB	2.39	0.52
1:D:32:THR:HG22	1:D:119:LYS:HB2	1.92	0.52
1:D:55:TRP:CZ3	1:D:57:THR:HA	2.44	0.52
1:A:289:THR:HG22	1:A:296:ILE:O	2.10	0.52
1:B:409:ARG:HH11	1:B:409:ARG:HG2	1.74	0.52
1:D:166:VAL:HG13	1:D:199:TYR:OH	2.09	0.52
1:D:289:THR:HG22	1:D:296:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:MET:CE	1:E:80:MET:HA	2.40	0.52
1:A:24:ASP:O	1:A:129:PRO:HG3	2.10	0.52
1:B:289:THR:HG22	1:B:296:ILE:O	2.09	0.52
1:C:365:THR:HG23	1:C:387:VAL:CB	2.33	0.52
1:C:330:VAL:HG12	1:C:382:LEU:HD11	1.92	0.52
1:E:409:ARG:HH11	1:E:409:ARG:HG2	1.75	0.52
1:B:283:ALA:O	1:B:284:MET:HB3	2.09	0.52
1:B:15:LYS:HB2	1:B:17:TYR:H	1.74	0.52
1:C:283:ALA:O	1:C:284:MET:HB3	2.09	0.52
1:D:285:HIS:CG	1:D:286:ALA:N	2.77	0.52
1:E:15:LYS:HB2	1:E:17:TYR:HB3	1.91	0.52
1:A:15:LYS:CB	1:A:17:TYR:H	2.22	0.52
1:C:58:LEU:HD22	1:C:58:LEU:H	1.74	0.52
1:A:72:ALA:HB2	1:A:91:TYR:CD1	2.45	0.52
1:C:15:LYS:HB2	1:C:17:TYR:H	1.73	0.52
1:E:47:ALA:CB	1:E:89:ILE:HD13	2.33	0.52
1:B:55:TRP:CZ3	1:B:57:THR:HA	2.44	0.52
1:A:437:LYS:C	1:A:439:GLY:H	2.12	0.52
1:A:59:TYR:O	1:A:59:TYR:CG	2.63	0.51
1:C:117:ARG:HG2	1:C:117:ARG:NH1	2.19	0.51
1:D:15:LYS:HB2	1:D:17:TYR:H	1.75	0.51
1:D:253:MET:HE3	1:D:281:HIS:HB2	1.92	0.51
1:D:58:LEU:HD22	1:D:58:LEU:H	1.75	0.51
1:E:403:ALA:HA	1:E:406:ARG:NH2	2.13	0.51
1:A:79:ASP:HB2	1:A:85:TRP:CZ3	2.45	0.51
1:D:39:ILE:HG12	1:D:85:TRP:CE2	2.45	0.51
1:D:59:TYR:CG	1:D:59:TYR:O	2.63	0.51
1:E:437:LYS:C	1:E:439:GLY:H	2.14	0.51
1:A:205:ARG:HD2	1:A:226:TRP:CZ2	2.43	0.51
1:B:58:LEU:H	1:B:58:LEU:HD22	1.74	0.51
1:E:177:ALA:HA	1:E:188:MET:HE3	1.92	0.51
1:E:39:ILE:HG12	1:E:85:TRP:CD1	2.46	0.51
1:C:15:LYS:HB2	1:C:17:TYR:HB3	1.91	0.51
1:D:116:LYS:HD3	1:D:117:ARG:CD	2.36	0.51
1:D:437:LYS:C	1:D:439:GLY:H	2.14	0.51
1:A:58:LEU:HD22	1:A:58:LEU:H	1.75	0.51
1:B:32:THR:HG22	1:B:119:LYS:HB2	1.91	0.51
1:D:239:GLN:O	1:D:243:VAL:HG23	2.11	0.51
1:E:15:LYS:CB	1:E:17:TYR:H	2.23	0.51
1:E:435:LEU:HA	1:E:439:GLY:CA	2.22	0.51
1:B:39:ILE:HG12	1:B:85:TRP:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HG12	1:B:85:TRP:CD1	2.45	0.51
1:E:209:MET:HG2	1:E:226:TRP:CD2	2.46	0.51
1:E:55:TRP:CZ3	1:E:57:THR:HA	2.46	0.51
1:B:166:VAL:HG13	1:B:199:TYR:OH	2.10	0.51
1:B:15:LYS:CB	1:B:17:TYR:H	2.23	0.51
1:B:247:LEU:HB2	1:B:249:LEU:HD23	1.93	0.51
1:B:285:HIS:CG	1:B:286:ALA:N	2.78	0.51
1:C:285:HIS:CG	1:C:286:ALA:N	2.79	0.51
1:C:32:THR:HG22	1:C:119:LYS:HB2	1.93	0.51
1:D:256:VAL:HG12	1:D:264:LEU:HD21	1.93	0.51
1:D:283:ALA:O	1:D:284:MET:HB3	2.11	0.51
1:D:229:ASN:ND2	1:D:231:THR:H	2.08	0.51
1:D:25:ILE:HD11	1:D:132:LEU:HD21	1.93	0.51
1:E:376:GLN:CB	1:E:377:PRO:HD3	2.35	0.51
1:B:43:ALA:HB1	1:B:87:VAL:HG11	1.93	0.50
1:C:39:ILE:HG12	1:C:85:TRP:CE2	2.47	0.50
1:E:24:ASP:O	1:E:129:PRO:HG3	2.11	0.50
1:C:376:GLN:CB	1:C:377:PRO:HD3	2.36	0.50
1:E:59:TYR:O	1:E:59:TYR:CG	2.64	0.50
1:E:87:VAL:HG12	1:E:88:ARG:N	2.27	0.50
1:B:79:ASP:HB2	1:B:85:TRP:CZ3	2.46	0.50
1:C:437:LYS:C	1:C:439:GLY:H	2.13	0.50
1:D:118:VAL:HG11	1:D:121:LEU:HB2	1.94	0.50
1:D:39:ILE:HG12	1:D:85:TRP:CD1	2.47	0.50
1:E:159:GLY:HA3	1:E:187:TYR:CZ	2.45	0.50
1:A:32:THR:HG22	1:A:119:LYS:HB2	1.94	0.50
1:B:80:MET:CE	1:B:80:MET:HA	2.40	0.50
1:D:24:ASP:O	1:D:129:PRO:HG3	2.12	0.50
1:A:101:LEU:HD23	1:A:308:ILE:HD11	1.94	0.50
1:A:55:TRP:CZ3	1:A:57:THR:HA	2.47	0.50
1:B:229:ASN:ND2	1:B:231:THR:H	2.09	0.50
1:B:59:TYR:CG	1:B:59:TYR:O	2.64	0.50
1:B:57:THR:HG21	1:B:61:TRP:CD1	2.47	0.50
1:C:231:THR:O	1:C:232:ALA:HB2	2.12	0.50
1:C:59:TYR:CG	1:C:59:TYR:O	2.64	0.50
1:D:15:LYS:CB	1:D:17:TYR:H	2.24	0.50
1:D:72:ALA:HB2	1:D:91:TYR:CD1	2.47	0.50
1:E:205:ARG:HD2	1:E:226:TRP:CZ2	2.45	0.50
1:A:43:ALA:HB1	1:A:87:VAL:HG11	1.93	0.50
1:B:47:ALA:CB	1:B:89:ILE:HD13	2.37	0.50
1:E:79:ASP:HB2	1:E:85:TRP:CZ3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG13	1:A:199:TYR:OH	2.11	0.50
1:B:137:ASP:HB2	1:B:268:ARG:HH12	1.77	0.50
1:B:435:LEU:HA	1:B:439:GLY:CA	2.20	0.50
1:C:15:LYS:CB	1:C:17:TYR:H	2.24	0.50
1:C:55:TRP:CZ3	1:C:57:THR:HA	2.47	0.50
1:A:39:ILE:HG12	1:A:85:TRP:CD1	2.47	0.50
1:B:118:VAL:HG11	1:B:121:LEU:HB2	1.93	0.50
1:C:24:ASP:O	1:C:129:PRO:HG3	2.12	0.50
1:A:137:ASP:HB2	1:A:268:ARG:HH12	1.77	0.50
1:A:39:ILE:HG12	1:A:85:TRP:CE2	2.46	0.50
1:C:268:ARG:HG2	1:C:268:ARG:HH11	1.77	0.49
1:E:247:LEU:HB2	1:E:249:LEU:HD23	1.94	0.49
1:A:330:VAL:HG12	1:A:382:LEU:HD11	1.92	0.49
1:A:411:ALA:O	1:A:415:ILE:HG22	2.12	0.49
1:C:229:ASN:ND2	1:C:231:THR:H	2.09	0.49
1:D:26:ILE:HB	1:D:127:TYR:HB3	1.94	0.49
1:C:26:ILE:HB	1:C:127:TYR:HB3	1.94	0.49
1:C:163:LYS:C	1:C:165:LYS:H	2.14	0.49
1:A:57:THR:HG21	1:A:61:TRP:CD1	2.47	0.49
1:A:22:LYS:HE2	1:A:22:LYS:HA	1.94	0.49
1:E:289:THR:HG22	1:E:296:ILE:O	2.11	0.49
1:A:26:ILE:HB	1:A:127:TYR:HB3	1.94	0.49
1:A:159:GLY:HA3	1:A:187:TYR:CZ	2.47	0.49
1:B:177:ALA:HA	1:B:188:MET:HE3	1.95	0.49
1:B:239:GLN:O	1:B:243:VAL:HG23	2.12	0.49
1:C:57:THR:HG21	1:C:61:TRP:CD1	2.47	0.49
1:C:87:VAL:HG12	1:C:88:ARG:N	2.27	0.49
1:E:39:ILE:HG12	1:E:85:TRP:CE2	2.47	0.49
1:E:72:ALA:HB2	1:E:91:TYR:CD1	2.47	0.49
1:A:87:VAL:HG12	1:A:88:ARG:N	2.28	0.49
1:B:163:LYS:C	1:B:165:LYS:H	2.16	0.49
1:D:87:VAL:HG12	1:D:88:ARG:N	2.27	0.49
1:E:239:GLN:O	1:E:243:VAL:HG23	2.13	0.49
1:A:163:LYS:C	1:A:165:LYS:N	2.67	0.49
1:C:247:LEU:HB2	1:C:249:LEU:HD23	1.94	0.49
1:E:43:ALA:HB1	1:E:87:VAL:HG11	1.95	0.49
1:B:209:MET:HG2	1:B:226:TRP:CD2	2.48	0.48
1:B:25:ILE:HD11	1:B:132:LEU:HD21	1.95	0.48
1:C:209:MET:HG2	1:C:226:TRP:CD2	2.48	0.48
1:D:181:LEU:HG	1:D:188:MET:CE	2.43	0.48
1:D:159:GLY:HA3	1:D:187:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLY:O	1:D:146:VAL:HG23	2.13	0.48
1:A:142:GLY:O	1:A:146:VAL:HG23	2.13	0.48
1:B:438:TRP:HA	1:B:440:HIS:HE1	1.77	0.48
1:B:72:ALA:HB2	1:B:91:TYR:CD1	2.48	0.48
1:B:87:VAL:HG12	1:B:88:ARG:N	2.28	0.48
1:C:163:LYS:C	1:C:165:LYS:N	2.65	0.48
1:C:163:LYS:CE	1:C:163:LYS:HA	2.25	0.48
1:C:409:ARG:HH11	1:C:409:ARG:HG2	1.78	0.48
1:D:247:LEU:HB2	1:D:249:LEU:HD23	1.95	0.48
1:D:268:ARG:HH11	1:D:268:ARG:HG2	1.78	0.48
1:D:79:ASP:HB2	1:D:85:TRP:CZ3	2.48	0.48
1:E:101:LEU:HD23	1:E:308:ILE:HD11	1.93	0.48
1:E:163:LYS:C	1:E:165:LYS:H	2.17	0.48
1:A:163:LYS:C	1:A:165:LYS:H	2.16	0.48
1:B:268:ARG:HH11	1:B:268:ARG:HG2	1.78	0.48
1:D:101:LEU:HD23	1:D:308:ILE:HD11	1.94	0.48
1:E:163:LYS:C	1:E:165:LYS:N	2.66	0.48
1:E:256:VAL:HG12	1:E:264:LEU:HD21	1.95	0.48
1:A:118:VAL:HG11	1:A:121:LEU:HB2	1.94	0.48
1:C:25:ILE:HD11	1:C:132:LEU:HD21	1.95	0.48
1:E:116:LYS:HD3	1:E:117:ARG:CD	2.36	0.48
1:E:65:GLU:N	1:E:65:GLU:OE1	2.44	0.48
1:A:209:MET:HG2	1:A:226:TRP:CD2	2.48	0.48
1:D:43:ALA:HB1	1:D:87:VAL:HG11	1.96	0.48
1:C:39:ILE:HG12	1:C:85:TRP:CD1	2.48	0.48
1:D:231:THR:O	1:D:232:ALA:HB2	2.14	0.48
1:E:268:ARG:HH11	1:E:268:ARG:HG2	1.79	0.48
1:B:403:ALA:HA	1:B:406:ARG:NH2	2.14	0.48
1:D:338:ARG:HA	1:D:361:ALA:HB1	1.96	0.48
1:C:116:LYS:HD3	1:C:117:ARG:CD	2.36	0.48
1:C:187:TYR:CD1	1:C:187:TYR:C	2.87	0.48
1:D:163:LYS:C	1:D:165:LYS:H	2.17	0.48
1:D:187:TYR:CD1	1:D:187:TYR:C	2.87	0.48
1:E:118:VAL:HG11	1:E:121:LEU:HB2	1.95	0.48
1:E:125:ASP:OD1	1:E:126:LEU:N	2.46	0.48
1:A:181:LEU:HG	1:A:188:MET:CE	2.44	0.48
1:A:86:ILE:HG21	1:A:349:VAL:O	2.13	0.48
1:B:376:GLN:CB	1:B:377:PRO:HD3	2.38	0.48
1:C:101:LEU:HD23	1:C:308:ILE:HD11	1.94	0.48
1:E:32:THR:HG22	1:E:119:LYS:HB2	1.95	0.48
1:E:22:LYS:HE2	1:E:22:LYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:ILE:HB	1:E:127:TYR:HB3	1.96	0.48
1:E:57:THR:HG21	1:E:61:TRP:CD1	2.47	0.48
1:C:159:GLY:HA3	1:C:187:TYR:CZ	2.49	0.47
1:C:268:ARG:HH11	1:C:268:ARG:CG	2.27	0.47
1:C:65:GLU:N	1:C:65:GLU:OE1	2.46	0.47
1:D:57:THR:HG21	1:D:61:TRP:CD1	2.48	0.47
1:E:159:GLY:HA3	1:E:187:TYR:CE1	2.49	0.47
1:B:411:ALA:O	1:B:415:ILE:HG22	2.14	0.47
1:C:43:ALA:HB1	1:C:87:VAL:HG11	1.96	0.47
1:D:163:LYS:C	1:D:165:LYS:N	2.67	0.47
1:D:209:MET:HG2	1:D:226:TRP:CD2	2.48	0.47
1:A:80:MET:HA	1:A:80:MET:CE	2.41	0.47
1:B:181:LEU:HG	1:B:188:MET:CE	2.45	0.47
1:B:22:LYS:HE2	1:B:22:LYS:HA	1.96	0.47
1:A:247:LEU:HB2	1:A:249:LEU:HD23	1.95	0.47
1:A:300:VAL:HG12	1:A:304:LEU:HD22	1.97	0.47
1:C:411:ALA:O	1:C:415:ILE:HG22	2.14	0.47
1:D:409:ARG:HH11	1:D:409:ARG:HG2	1.80	0.47
1:A:256:VAL:HG12	1:A:264:LEU:HD21	1.96	0.47
1:B:163:LYS:C	1:B:165:LYS:N	2.66	0.47
1:B:231:THR:O	1:B:232:ALA:HB2	2.14	0.47
1:B:256:VAL:HG12	1:B:264:LEU:HD21	1.96	0.47
1:C:137:ASP:HB2	1:C:268:ARG:HH12	1.80	0.47
1:D:137:ASP:HB2	1:D:268:ARG:HH12	1.79	0.47
1:E:182:SER:HA	1:E:220:THR:HG21	1.96	0.47
1:A:335:ARG:NH1	1:A:339:GLU:OE1	2.47	0.47
1:D:182:SER:HA	1:D:220:THR:HG21	1.96	0.47
1:D:435:LEU:HA	1:D:439:GLY:CA	2.21	0.47
1:B:26:ILE:HB	1:B:127:TYR:HB3	1.97	0.47
1:D:371:HIS:ND1	1:D:374:ASN:HB2	2.28	0.47
1:B:371:HIS:ND1	1:B:374:ASN:HB2	2.29	0.47
1:C:181:LEU:HG	1:C:188:MET:CE	2.44	0.47
1:C:182:SER:HA	1:C:220:THR:HG21	1.96	0.47
1:A:161:VAL:O	1:A:162:PRO:C	2.53	0.47
1:E:187:TYR:C	1:E:187:TYR:CD1	2.87	0.47
1:E:411:ALA:O	1:E:415:ILE:HG22	2.14	0.47
1:A:187:TYR:CD1	1:A:187:TYR:C	2.88	0.47
1:B:365:THR:HG23	1:B:387:VAL:CB	2.37	0.47
1:C:256:VAL:HG12	1:C:264:LEU:HD21	1.97	0.47
1:B:187:TYR:C	1:B:187:TYR:CD1	2.88	0.46
1:A:403:ALA:O	1:A:405:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ARG:HA	1:C:361:ALA:HB1	1.97	0.46
1:E:371:HIS:ND1	1:E:374:ASN:HB2	2.30	0.46
1:A:159:GLY:HA3	1:A:187:TYR:CE1	2.50	0.46
1:E:264:LEU:HA	1:E:264:LEU:HD23	1.80	0.46
1:E:268:ARG:HH11	1:E:268:ARG:CG	2.29	0.46
1:A:268:ARG:HH11	1:A:268:ARG:HG2	1.80	0.46
1:A:65:GLU:N	1:A:65:GLU:OE1	2.45	0.46
1:B:98:GLU:N	1:B:98:GLU:OE1	2.43	0.46
1:C:118:VAL:HG11	1:C:121:LEU:HB2	1.97	0.46
1:A:328:TRP:O	1:A:331:ILE:HB	2.15	0.46
1:A:438:TRP:HA	1:A:440:HIS:HE1	1.78	0.46
1:B:306:ARG:HH11	1:B:306:ARG:CG	2.29	0.46
1:B:39:ILE:HG12	1:B:85:TRP:NE1	2.31	0.46
1:E:297:SER:C	1:E:299:PHE:N	2.69	0.46
1:D:86:ILE:HG21	1:D:349:VAL:O	2.16	0.46
1:E:203:GLU:H	1:E:203:GLU:CD	2.19	0.46
1:E:338:ARG:HA	1:E:361:ALA:HB1	1.96	0.46
1:A:231:THR:O	1:A:232:ALA:HB2	2.15	0.46
1:B:338:ARG:HA	1:B:361:ALA:HB1	1.97	0.46
1:C:118:VAL:HG12	1:C:120:GLY:N	2.30	0.46
1:C:335:ARG:HG2	1:C:339:GLU:OE1	2.16	0.46
1:D:411:ALA:O	1:D:415:ILE:HG22	2.16	0.46
1:E:403:ALA:O	1:E:405:ALA:N	2.49	0.46
1:A:25:ILE:HD11	1:A:132:LEU:HD21	1.98	0.46
1:A:338:ARG:HA	1:A:361:ALA:HB1	1.96	0.46
1:A:371:HIS:ND1	1:A:374:ASN:HB2	2.29	0.46
1:C:379:ILE:HD11	1:C:415:ILE:HG21	1.98	0.46
1:C:390:LEU:HD12	1:C:408:VAL:HG21	1.98	0.46
1:E:251:HIS:CE1	1:E:312:GLN:NE2	2.75	0.46
1:D:390:LEU:HD12	1:D:408:VAL:HG21	1.97	0.46
1:E:231:THR:O	1:E:232:ALA:HB2	2.15	0.46
1:A:264:LEU:HA	1:A:264:LEU:HD23	1.79	0.46
1:D:372:PRO:HG3	1:D:408:VAL:HG22	1.98	0.46
1:D:268:ARG:HH11	1:D:268:ARG:CG	2.30	0.45
1:E:438:TRP:HA	1:E:440:HIS:HE1	1.76	0.45
1:C:403:ALA:O	1:C:405:ALA:N	2.49	0.45
1:E:306:ARG:HH11	1:E:306:ARG:CG	2.29	0.45
1:B:146:VAL:O	1:B:149:MET:HB3	2.16	0.45
1:C:306:ARG:HH11	1:C:306:ARG:CG	2.29	0.45
1:D:365:THR:HG23	1:D:387:VAL:CB	2.34	0.45
1:B:159:GLY:HA3	1:B:187:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ILE:HD11	1:B:350:PHE:HE1	1.82	0.45
1:C:435:LEU:HA	1:C:439:GLY:CA	2.22	0.45
1:D:159:GLY:HA3	1:D:187:TYR:CE1	2.52	0.45
1:A:182:SER:HA	1:A:220:THR:HG21	1.98	0.45
1:C:159:GLY:HA3	1:C:187:TYR:CE1	2.52	0.45
1:C:177:ALA:HA	1:C:188:MET:HE3	1.98	0.45
1:C:22:LYS:HA	1:C:22:LYS:HE2	1.98	0.45
1:E:51:SER:OG	1:E:52:THR:N	2.49	0.45
1:B:196:SER:N	1:B:197:PRO:HD3	2.31	0.45
1:B:399:ASP:OD2	1:B:433:ARG:HD3	2.16	0.45
1:D:203:GLU:CD	1:D:203:GLU:H	2.20	0.45
1:C:239:GLN:O	1:C:243:VAL:HG23	2.17	0.45
1:C:86:ILE:HG21	1:C:349:VAL:O	2.16	0.45
1:D:15:LYS:HB3	1:D:16:GLY:H	1.46	0.45
1:D:22:LYS:HA	1:D:22:LYS:HE2	1.99	0.45
1:E:379:ILE:HD11	1:E:415:ILE:HG21	1.99	0.45
1:E:412:ILE:O	1:E:416:MET:HB2	2.17	0.45
1:A:125:ASP:OD1	1:A:126:LEU:N	2.50	0.45
1:A:379:ILE:HD11	1:A:415:ILE:HG21	1.99	0.45
1:B:160:VAL:CG2	1:B:161:VAL:N	2.80	0.45
1:B:182:SER:HA	1:B:220:THR:HG21	1.98	0.45
1:B:268:ARG:HH11	1:B:268:ARG:CG	2.30	0.45
1:B:78:HIS:HE1	1:B:80:MET:HE3	1.82	0.45
1:C:142:GLY:O	1:C:146:VAL:HG23	2.17	0.45
1:E:314:HIS:CD2	1:E:365:THR:HB	2.52	0.45
1:E:399:ASP:OD2	1:E:433:ARG:HD3	2.17	0.45
1:A:251:HIS:CE1	1:A:312:GLN:NE2	2.76	0.45
1:A:372:PRO:HG3	1:A:408:VAL:HG22	1.99	0.45
1:C:80:MET:HA	1:C:80:MET:CE	2.44	0.45
1:D:379:ILE:HD11	1:D:415:ILE:CD1	2.29	0.45
1:D:38:THR:HG22	1:D:41:GLN:CD	2.37	0.45
1:D:403:ALA:O	1:D:405:ALA:N	2.50	0.45
1:E:146:VAL:O	1:E:149:MET:HB3	2.17	0.45
1:A:268:ARG:HA	1:A:278:ILE:HD11	1.99	0.44
1:A:268:ARG:HH11	1:A:268:ARG:CG	2.31	0.44
1:C:161:VAL:O	1:C:162:PRO:C	2.56	0.44
1:C:314:HIS:CD2	1:C:365:THR:HB	2.52	0.44
1:D:150:LEU:O	1:D:223:LYS:HB2	2.17	0.44
1:D:297:SER:C	1:D:299:PHE:N	2.70	0.44
1:E:161:VAL:O	1:E:162:PRO:C	2.54	0.44
1:A:118:VAL:HG12	1:A:120:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HD12	1:A:408:VAL:HG21	1.99	0.44
1:B:440:HIS:O	1:B:441:VAL:C	2.53	0.44
1:D:125:ASP:OD1	1:D:126:LEU:N	2.51	0.44
1:D:399:ASP:OD2	1:D:433:ARG:HD3	2.17	0.44
1:D:431:LEU:HD23	1:D:431:LEU:O	2.17	0.44
1:E:390:LEU:HD12	1:E:408:VAL:HG21	1.98	0.44
1:A:306:ARG:HH11	1:A:306:ARG:CG	2.29	0.44
1:A:38:THR:HG22	1:A:41:GLN:CD	2.38	0.44
1:B:390:LEU:HD12	1:B:408:VAL:HG21	1.99	0.44
1:C:397:HIS:HA	1:C:398:PRO:HD3	1.89	0.44
1:D:39:ILE:H	1:D:39:ILE:HG13	1.53	0.44
1:A:86:ILE:HD11	1:A:350:PHE:HE1	1.82	0.44
1:B:379:ILE:HD11	1:B:415:ILE:HG21	1.99	0.44
1:C:125:ASP:OD1	1:C:126:LEU:N	2.51	0.44
1:C:346:GLU:CD	1:C:346:GLU:N	2.63	0.44
1:C:399:ASP:OD2	1:C:433:ARG:HD3	2.18	0.44
1:C:78:HIS:HE1	1:C:80:MET:HE3	1.82	0.44
1:D:438:TRP:HA	1:D:440:HIS:HE1	1.77	0.44
1:E:181:LEU:HG	1:E:188:MET:CE	2.47	0.44
1:A:39:ILE:HG12	1:A:85:TRP:NE1	2.33	0.44
1:B:314:HIS:CD2	1:B:365:THR:HB	2.53	0.44
1:B:397:HIS:HA	1:B:398:PRO:HD3	1.88	0.44
1:C:371:HIS:ND1	1:C:374:ASN:HB2	2.32	0.44
1:D:196:SER:N	1:D:197:PRO:HD3	2.33	0.44
1:E:118:VAL:HG12	1:E:120:GLY:N	2.33	0.44
1:E:253:MET:HA	1:E:279:HIS:O	2.17	0.44
1:A:203:GLU:CD	1:A:203:GLU:H	2.21	0.44
1:A:409:ARG:NH1	1:A:409:ARG:HG2	2.32	0.44
1:A:431:LEU:O	1:A:431:LEU:HD23	2.17	0.44
1:E:116:LYS:O	1:E:118:VAL:N	2.50	0.44
1:E:86:ILE:HD11	1:E:350:PHE:HE1	1.83	0.44
1:A:46:VAL:HG12	1:A:47:ALA:N	2.32	0.44
1:B:161:VAL:O	1:B:162:PRO:C	2.56	0.44
1:C:117:ARG:H	1:C:117:ARG:HD2	1.82	0.44
1:C:39:ILE:HG12	1:C:85:TRP:NE1	2.33	0.44
1:D:253:MET:HA	1:D:279:HIS:O	2.17	0.44
1:D:426:LYS:O	1:D:427:THR:OG1	2.22	0.44
1:E:86:ILE:HG21	1:E:349:VAL:O	2.18	0.44
1:A:283:ALA:O	1:A:284:MET:CB	2.65	0.44
1:C:146:VAL:O	1:C:149:MET:HB3	2.17	0.44
1:C:310:ILE:CD1	1:C:310:ILE:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:SER:OG	1:C:52:THR:N	2.50	0.44
1:D:14:ASP:OD1	1:D:14:ASP:N	2.51	0.44
1:E:335:ARG:NH1	1:E:339:GLU:OE1	2.50	0.44
1:B:203:GLU:CD	1:B:203:GLU:H	2.21	0.44
1:C:297:SER:C	1:C:299:PHE:N	2.70	0.44
1:D:379:ILE:HD11	1:D:415:ILE:HG21	2.00	0.44
1:D:306:ARG:CG	1:D:306:ARG:HH11	2.30	0.43
1:D:412:ILE:O	1:D:416:MET:HB2	2.18	0.43
1:E:117:ARG:H	1:E:117:ARG:HD2	1.82	0.43
1:A:399:ASP:OD2	1:A:433:ARG:HD3	2.18	0.43
1:C:328:TRP:O	1:C:331:ILE:HB	2.18	0.43
1:C:335:ARG:NH2	1:C:343:LYS:O	2.51	0.43
1:E:335:ARG:HG2	1:E:339:GLU:OE1	2.17	0.43
1:A:440:HIS:O	1:A:441:VAL:C	2.57	0.43
1:B:412:ILE:O	1:B:416:MET:HB2	2.17	0.43
1:C:14:ASP:N	1:C:14:ASP:OD1	2.52	0.43
1:C:268:ARG:HA	1:C:278:ILE:HD11	2.00	0.43
1:D:39:ILE:HG12	1:D:85:TRP:NE1	2.32	0.43
1:E:39:ILE:HG13	1:E:39:ILE:H	1.53	0.43
1:A:253:MET:HA	1:A:279:HIS:O	2.18	0.43
1:A:314:HIS:CD2	1:A:365:THR:HB	2.54	0.43
1:B:253:MET:HA	1:B:279:HIS:O	2.17	0.43
1:B:65:GLU:OE1	1:B:65:GLU:N	2.46	0.43
1:C:440:HIS:O	1:C:441:VAL:C	2.57	0.43
1:D:431:LEU:HD22	1:D:435:LEU:CD1	2.49	0.43
1:E:25:ILE:HD11	1:E:132:LEU:HD21	2.00	0.43
1:B:116:LYS:O	1:B:118:VAL:N	2.52	0.43
1:B:297:SER:C	1:B:299:PHE:N	2.71	0.43
1:C:160:VAL:CG2	1:C:161:VAL:N	2.81	0.43
1:C:240:ARG:O	1:C:244:LEU:HD22	2.18	0.43
1:D:314:HIS:CD2	1:D:365:THR:HB	2.53	0.43
1:E:39:ILE:HG12	1:E:85:TRP:NE1	2.33	0.43
1:E:98:GLU:N	1:E:98:GLU:OE1	2.45	0.43
1:A:370:LEU:N	1:A:370:LEU:CD1	2.81	0.43
1:B:335:ARG:NH1	1:B:339:GLU:OE1	2.51	0.43
1:B:370:LEU:N	1:B:370:LEU:CD1	2.81	0.43
1:B:403:ALA:O	1:B:405:ALA:N	2.51	0.43
1:B:73:LYS:HE2	1:B:73:LYS:HB3	1.81	0.43
1:C:46:VAL:HG12	1:C:47:ALA:N	2.34	0.43
1:C:429:LYS:H	1:C:429:LYS:HG3	1.65	0.43
1:D:161:VAL:O	1:D:162:PRO:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:GLU:OE1	1:D:65:GLU:N	2.46	0.43
1:D:91:TYR:HA	1:D:92:PRO:HD3	1.88	0.43
1:E:440:HIS:O	1:E:441:VAL:C	2.57	0.43
1:A:73:LYS:HB3	1:A:73:LYS:HE2	1.81	0.43
1:B:117:ARG:H	1:B:117:ARG:HD2	1.84	0.43
1:B:118:VAL:HG12	1:B:120:GLY:N	2.33	0.43
1:B:125:ASP:OD1	1:B:126:LEU:N	2.52	0.43
1:B:86:ILE:HG21	1:B:349:VAL:O	2.19	0.43
1:D:73:LYS:HE2	1:D:73:LYS:HB3	1.83	0.43
1:E:137:ASP:HB2	1:E:268:ARG:HH12	1.84	0.43
1:E:429:LYS:H	1:E:429:LYS:HG3	1.64	0.43
1:A:51:SER:OG	1:A:52:THR:N	2.51	0.43
1:E:409:ARG:NH1	1:E:409:ARG:HG2	2.34	0.43
1:A:297:SER:C	1:A:299:PHE:N	2.70	0.43
1:B:310:ILE:CD1	1:B:310:ILE:N	2.82	0.43
1:D:440:HIS:O	1:D:441:VAL:C	2.57	0.43
1:E:328:TRP:O	1:E:331:ILE:HB	2.19	0.43
1:A:196:SER:N	1:A:197:PRO:HD3	2.33	0.42
1:B:181:LEU:HG	1:B:188:MET:HE1	2.01	0.42
1:B:150:LEU:O	1:B:223:LYS:HB2	2.18	0.42
1:B:378:VAL:C	1:B:380:GLU:N	2.72	0.42
1:B:409:ARG:HG2	1:B:409:ARG:NH1	2.33	0.42
1:B:51:SER:OG	1:B:52:THR:N	2.51	0.42
1:E:78:HIS:HE1	1:E:80:MET:HE3	1.82	0.42
1:B:116:LYS:HD3	1:B:117:ARG:CD	2.36	0.42
1:E:165:LYS:HE3	1:E:191:ASP:CG	2.39	0.42
1:E:72:ALA:O	1:E:73:LYS:HB3	2.19	0.42
1:A:177:ALA:HA	1:A:188:MET:HE3	2.00	0.42
1:A:150:LEU:O	1:A:223:LYS:HB2	2.20	0.42
1:A:376:GLN:HB3	1:A:377:PRO:CD	2.38	0.42
1:C:283:ALA:O	1:C:284:MET:CB	2.67	0.42
1:D:146:VAL:O	1:D:149:MET:HB3	2.18	0.42
1:E:142:GLY:O	1:E:146:VAL:HG23	2.19	0.42
1:E:150:LEU:O	1:E:223:LYS:HB2	2.19	0.42
1:A:331:ILE:HD13	1:A:382:LEU:CD1	2.49	0.42
1:A:403:ALA:C	1:A:405:ALA:N	2.71	0.42
1:B:142:GLY:O	1:B:146:VAL:HG23	2.19	0.42
1:D:403:ALA:C	1:D:405:ALA:N	2.72	0.42
1:E:164:PRO:O	1:E:165:LYS:HG2	2.19	0.42
1:E:268:ARG:HA	1:E:278:ILE:HD11	2.00	0.42
1:B:210:ALA:HB2	1:B:249:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:PRO:HG3	1:C:408:VAL:HG22	2.00	0.42
1:C:431:LEU:HD22	1:C:435:LEU:CD1	2.50	0.42
1:D:335:ARG:NH1	1:D:339:GLU:OE1	2.52	0.42
1:D:86:ILE:HD11	1:D:350:PHE:HE1	1.85	0.42
1:D:51:SER:OG	1:D:52:THR:N	2.51	0.42
1:A:146:VAL:O	1:A:149:MET:HB3	2.20	0.42
1:B:225:THR:OG1	1:B:251:HIS:CD2	2.70	0.42
1:C:150:LEU:O	1:C:223:LYS:HB2	2.19	0.42
1:C:165:LYS:HE3	1:C:191:ASP:CG	2.39	0.42
1:C:253:MET:HA	1:C:279:HIS:O	2.20	0.42
1:D:164:PRO:O	1:D:165:LYS:HG2	2.20	0.42
1:E:46:VAL:HG12	1:E:47:ALA:N	2.34	0.42
1:E:39:ILE:HD11	1:E:85:TRP:CZ2	2.55	0.42
1:B:335:ARG:NH2	1:B:343:LYS:O	2.52	0.42
1:B:369:GLY:C	1:B:370:LEU:HD12	2.39	0.42
1:D:117:ARG:H	1:D:117:ARG:HD2	1.84	0.42
1:D:118:VAL:HG12	1:D:120:GLY:N	2.34	0.42
1:D:181:LEU:HG	1:D:188:MET:HE1	2.02	0.42
1:E:12:TYR:HB3	1:E:13:VAL:H	1.72	0.42
1:B:150:LEU:O	1:B:151:GLU:HB2	2.20	0.42
1:B:372:PRO:HG3	1:B:408:VAL:HG22	2.02	0.42
1:B:77:PHE:N	1:B:77:PHE:CD1	2.88	0.42
1:D:328:TRP:O	1:D:331:ILE:HB	2.18	0.42
1:E:14:ASP:N	1:E:14:ASP:OD1	2.53	0.42
1:A:335:ARG:NH2	1:A:343:LYS:O	2.52	0.42
1:B:116:LYS:C	1:B:118:VAL:H	2.23	0.42
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.55	0.42
1:B:328:TRP:O	1:B:331:ILE:HB	2.19	0.42
1:C:369:GLY:C	1:C:370:LEU:HD12	2.39	0.42
1:C:39:ILE:HG13	1:C:39:ILE:H	1.50	0.42
1:C:77:PHE:CD1	1:C:77:PHE:N	2.88	0.42
1:D:335:ARG:HG2	1:D:339:GLU:OE1	2.20	0.42
1:A:376:GLN:O	1:A:380:GLU:HB2	2.20	0.42
1:A:72:ALA:O	1:A:73:LYS:HB3	2.19	0.42
1:D:39:ILE:HD11	1:D:85:TRP:CZ2	2.55	0.42
1:D:38:THR:CG2	1:D:41:GLN:HG3	2.50	0.42
1:D:410:GLN:NE2	1:D:431:LEU:H	2.15	0.42
1:A:198:TRP:HZ3	1:E:130:GLU:HG2	1.85	0.42
1:E:210:ALA:HB2	1:E:249:LEU:HD21	2.02	0.42
1:E:372:PRO:HG3	1:E:408:VAL:HG22	2.02	0.42
1:A:165:LYS:HE3	1:A:191:ASP:CG	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD22	1:A:435:LEU:CD1	2.49	0.41
1:B:410:GLN:NE2	1:B:431:LEU:H	2.15	0.41
1:D:378:VAL:C	1:D:380:GLU:N	2.73	0.41
1:B:14:ASP:N	1:B:14:ASP:OD1	2.52	0.41
1:C:196:SER:N	1:C:197:PRO:HD3	2.35	0.41
1:C:378:VAL:C	1:C:380:GLU:N	2.73	0.41
1:C:412:ILE:O	1:C:416:MET:HB2	2.19	0.41
1:E:403:ALA:C	1:E:405:ALA:N	2.72	0.41
1:A:335:ARG:HG2	1:A:339:GLU:OE1	2.20	0.41
1:A:91:TYR:HA	1:A:92:PRO:HD3	1.89	0.41
1:B:268:ARG:HA	1:B:278:ILE:HD11	2.02	0.41
1:C:86:ILE:HD11	1:C:350:PHE:HE1	1.84	0.41
1:E:196:SER:N	1:E:197:PRO:HD3	2.34	0.41
1:E:410:GLN:NE2	1:E:431:LEU:H	2.15	0.41
1:A:168:TYR:CD1	1:A:173:PHE:HB2	2.55	0.41
1:B:165:LYS:HE3	1:B:191:ASP:CG	2.40	0.41
1:B:178:TYR:CE1	1:B:216:VAL:HG22	2.55	0.41
1:B:378:VAL:O	1:B:380:GLU:N	2.53	0.41
1:C:181:LEU:HG	1:C:188:MET:HE1	2.03	0.41
1:D:130:GLU:HB2	1:D:357:TYR:CZ	2.56	0.41
1:D:232:ALA:O	1:D:237:MET:HE2	2.21	0.41
1:E:397:HIS:HA	1:E:398:PRO:HD3	1.88	0.41
1:E:409:ARG:HA	1:E:409:ARG:HD2	1.83	0.41
1:A:116:LYS:O	1:A:118:VAL:N	2.54	0.41
1:A:190:ASP:OD2	1:A:228:ALA:HA	2.19	0.41
1:A:210:ALA:HB2	1:A:249:LEU:HD21	2.01	0.41
1:C:300:VAL:HG12	1:C:304:LEU:HD22	2.02	0.41
1:A:369:GLY:C	1:A:370:LEU:HD12	2.41	0.41
1:A:429:LYS:H	1:A:429:LYS:HG3	1.63	0.41
1:B:46:VAL:HG12	1:B:47:ALA:N	2.35	0.41
1:C:302:ALA:HB1	1:C:337:LEU:CD1	2.46	0.41
1:C:39:ILE:HD11	1:C:85:TRP:CZ2	2.56	0.41
1:C:403:ALA:C	1:C:405:ALA:N	2.72	0.41
1:D:12:TYR:HB3	1:D:13:VAL:H	1.71	0.41
1:E:376:GLN:HB3	1:E:377:PRO:CD	2.39	0.41
1:A:240:ARG:O	1:A:244:LEU:HD22	2.21	0.41
1:B:128:PHE:HA	1:B:129:PRO:HD3	1.93	0.41
1:C:410:GLN:NE2	1:C:431:LEU:H	2.16	0.41
1:D:409:ARG:HA	1:D:409:ARG:HD2	1.85	0.41
1:E:116:LYS:C	1:E:118:VAL:H	2.24	0.41
1:E:178:TYR:CE1	1:E:216:VAL:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:TRP:HA	1:C:440:HIS:HE1	1.78	0.41
1:E:378:VAL:C	1:E:380:GLU:N	2.73	0.41
1:E:38:THR:HG22	1:E:41:GLN:CD	2.39	0.41
1:A:108:ILE:O	1:A:108:ILE:CG2	2.69	0.41
1:A:117:ARG:H	1:A:117:ARG:HD2	1.85	0.41
1:B:240:ARG:O	1:B:244:LEU:HD22	2.21	0.41
1:C:108:ILE:CG2	1:C:108:ILE:O	2.69	0.41
1:D:80:MET:HA	1:D:80:MET:CE	2.43	0.41
1:E:166:VAL:CG1	1:E:199:TYR:OH	2.69	0.41
1:C:164:PRO:O	1:C:165:LYS:HG2	2.21	0.41
1:C:190:ASP:OD2	1:C:228:ALA:HA	2.21	0.41
1:C:291:ASN:C	1:C:291:ASN:OD1	2.60	0.41
1:D:78:HIS:HE1	1:D:80:MET:HE3	1.84	0.41
1:E:310:ILE:N	1:E:310:ILE:CD1	2.84	0.41
1:A:128:PHE:HA	1:A:129:PRO:HD3	1.93	0.41
1:A:164:PRO:O	1:A:165:LYS:HG2	2.21	0.41
1:C:128:PHE:HA	1:C:129:PRO:HD3	1.91	0.41
1:C:268:ARG:NH1	1:C:268:ARG:CG	2.84	0.41
1:C:376:GLN:HB3	1:C:377:PRO:CD	2.41	0.41
1:C:91:TYR:HA	1:C:92:PRO:HD3	1.88	0.41
1:D:249:LEU:HA	1:D:249:LEU:HD13	1.94	0.41
1:D:35:GLU:O	1:D:37:TYR:N	2.48	0.41
1:A:116:LYS:C	1:A:118:VAL:H	2.25	0.40
1:A:412:ILE:O	1:A:416:MET:HB2	2.20	0.40
1:B:108:ILE:CG2	1:B:108:ILE:O	2.70	0.40
1:C:203:GLU:H	1:C:203:GLU:CD	2.23	0.40
1:C:431:LEU:O	1:C:431:LEU:HD23	2.21	0.40
1:D:108:ILE:O	1:D:108:ILE:CG2	2.68	0.40
1:D:268:ARG:HA	1:D:278:ILE:HD11	2.02	0.40
1:D:392:GLY:O	1:D:394:THR:N	2.54	0.40
1:E:77:PHE:N	1:E:77:PHE:CD1	2.88	0.40
1:A:209:MET:CE	1:A:209:MET:HA	2.52	0.40
1:A:291:ASN:OD1	1:A:293:TYR:N	2.44	0.40
1:C:38:THR:HG22	1:C:41:GLN:CD	2.41	0.40
1:D:150:LEU:O	1:D:151:GLU:HB2	2.21	0.40
1:D:160:VAL:CG2	1:D:161:VAL:N	2.84	0.40
1:D:240:ARG:O	1:D:244:LEU:HD22	2.21	0.40
1:D:46:VAL:HG12	1:D:47:ALA:N	2.35	0.40
1:A:17:TYR:C	1:A:17:TYR:CD2	2.95	0.40
1:A:39:ILE:H	1:A:39:ILE:HG13	1.52	0.40
1:B:300:VAL:HG12	1:B:304:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ARG:HA	1:B:409:ARG:HD2	1.83	0.40
1:B:431:LEU:O	1:B:431:LEU:HD23	2.21	0.40
1:C:375:ILE:H	1:C:375:ILE:HG13	1.67	0.40
1:C:379:ILE:HD11	1:C:415:ILE:CD1	2.28	0.40
1:C:378:VAL:O	1:C:380:GLU:N	2.54	0.40
1:C:409:ARG:NH1	1:C:409:ARG:HG2	2.37	0.40
1:A:310:ILE:CD1	1:A:310:ILE:N	2.85	0.40
1:B:226:TRP:CZ3	1:B:228:ALA:HB2	2.57	0.40
1:B:307:LEU:O	1:B:308:ILE:C	2.59	0.40
1:B:376:GLN:O	1:B:380:GLU:HB2	2.22	0.40
1:B:437:LYS:C	1:B:439:GLY:N	2.75	0.40
1:B:440:HIS:O	1:B:441:VAL:O	2.40	0.40
1:B:72:ALA:O	1:B:73:LYS:HB3	2.21	0.40
1:D:300:VAL:HG12	1:D:304:LEU:HD22	2.03	0.40
1:E:164:PRO:O	1:E:166:VAL:N	2.47	0.40
1:E:431:LEU:HD23	1:E:431:LEU:O	2.22	0.40
1:B:86:ILE:HD11	1:B:350:PHE:CE1	2.56	0.40
1:C:116:LYS:O	1:C:118:VAL:N	2.54	0.40
1:C:12:TYR:HB3	1:C:13:VAL:H	1.72	0.40
1:D:302:ALA:HB1	1:D:337:LEU:CD1	2.47	0.40
1:D:335:ARG:NH2	1:D:343:LYS:O	2.55	0.40
1:D:376:GLN:O	1:D:380:GLU:HB2	2.22	0.40
1:D:72:ALA:O	1:D:73:LYS:HB3	2.22	0.40
1:D:25:ILE:HD12	1:D:96:PHE:CE2	2.57	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	423/444 (95%)	354 (84%)	54 (13%)	15 (4%)	3 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	423/444 (95%)	352 (83%)	56 (13%)	15 (4%)	3	12
1	C	423/444 (95%)	354 (84%)	54 (13%)	15 (4%)	3	12
1	D	423/444 (95%)	350 (83%)	59 (14%)	14 (3%)	4	13
1	E	423/444 (95%)	351 (83%)	58 (14%)	14 (3%)	4	13
All	All	2115/2220 (95%)	1761 (83%)	281 (13%)	73 (4%)	3	12

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	B	59	TYR
1	C	59	TYR
1	D	59	TYR
1	E	59	TYR
1	A	35	GLU
1	A	117	ARG
1	A	165	LYS
1	A	368	GLY
1	A	437	LYS
1	B	35	GLU
1	B	117	ARG
1	B	165	LYS
1	B	368	GLY
1	B	437	LYS
1	B	441	VAL
1	C	35	GLU
1	C	117	ARG
1	C	165	LYS
1	C	232	ALA
1	C	368	GLY
1	C	437	LYS
1	D	35	GLU
1	D	117	ARG
1	D	165	LYS
1	D	368	GLY
1	D	437	LYS
1	E	35	GLU
1	E	117	ARG
1	E	165	LYS
1	E	368	GLY
1	E	437	LYS

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Mol	Chain	Res	Type
1	A	232	ALA
1	A	441	VAL
1	B	232	ALA
1	C	441	VAL
1	D	232	ALA
1	D	441	VAL
1	E	232	ALA
1	E	441	VAL
1	A	51	SER
1	B	51	SER
1	B	52	THR
1	C	51	SER
1	D	51	SER
1	E	51	SER
1	A	376	GLN
1	A	438	TRP
1	B	376	GLN
1	B	438	TRP
1	C	376	GLN
1	D	376	GLN
1	E	376	GLN
1	E	438	TRP
1	A	52	THR
1	A	379	ILE
1	A	419	ILE
1	B	379	ILE
1	C	52	THR
1	C	379	ILE
1	C	438	TRP
1	D	379	ILE
1	D	438	TRP
1	B	419	ILE
1	C	419	ILE
1	D	419	ILE
1	E	379	ILE
1	E	419	ILE
1	E	404	GLY
1	A	404	GLY
1	C	404	GLY
1	B	404	GLY
1	D	404	GLY

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	342/356 (96%)	311 (91%)	31 (9%)	9 27
1	B	342/356 (96%)	313 (92%)	29 (8%)	10 31
1	C	342/356 (96%)	311 (91%)	31 (9%)	9 27
1	D	342/356 (96%)	311 (91%)	31 (9%)	9 27
1	E	342/356 (96%)	311 (91%)	31 (9%)	9 27
All	All	1710/1780 (96%)	1557 (91%)	153 (9%)	9 28

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	17	TYR
1	A	39	ILE
1	A	59	TYR
1	A	80	MET
1	A	116	LYS
1	A	117	ARG
1	A	122	ARG
1	A	126	LEU
1	A	160	VAL
1	A	163	LYS
1	A	194	LEU
1	A	218	ASN
1	A	229	ASN
1	A	234	LEU
1	A	244	LEU
1	A	268	ARG
1	A	273	ASP
1	A	290	ARG
1	A	298	MET
1	A	304	LEU
1	A	306	ARG
1	A	363	PHE

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Mol	Chain	Res	Type
1	A	365	THR
1	A	370	LEU
1	A	374	ASN
1	A	413	ASP
1	A	431	LEU
1	A	433	ARG
1	A	438	TRP
1	A	440	HIS
1	B	12	TYR
1	B	17	TYR
1	B	39	ILE
1	B	59	TYR
1	B	80	MET
1	B	116	LYS
1	B	117	ARG
1	B	122	ARG
1	B	126	LEU
1	B	160	VAL
1	B	163	LYS
1	B	194	LEU
1	B	218	ASN
1	B	229	ASN
1	B	234	LEU
1	B	244	LEU
1	B	268	ARG
1	B	273	ASP
1	B	290	ARG
1	B	298	MET
1	B	304	LEU
1	B	306	ARG
1	B	363	PHE
1	B	374	ASN
1	B	413	ASP
1	B	431	LEU
1	B	433	ARG
1	B	438	TRP
1	B	440	HIS
1	C	12	TYR
1	C	17	TYR
1	C	39	ILE
1	C	59	TYR
1	C	80	MET

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Mol	Chain	Res	Type
1	C	116	LYS
1	C	117	ARG
1	C	122	ARG
1	C	126	LEU
1	C	160	VAL
1	C	163	LYS
1	C	194	LEU
1	C	218	ASN
1	C	229	ASN
1	C	234	LEU
1	C	244	LEU
1	C	268	ARG
1	C	273	ASP
1	C	290	ARG
1	C	298	MET
1	C	304	LEU
1	C	306	ARG
1	C	363	PHE
1	C	365	THR
1	C	370	LEU
1	C	374	ASN
1	C	413	ASP
1	C	431	LEU
1	C	433	ARG
1	C	438	TRP
1	C	440	HIS
1	D	12	TYR
1	D	17	TYR
1	D	19	PRO
1	D	39	ILE
1	D	59	TYR
1	D	80	MET
1	D	116	LYS
1	D	117	ARG
1	D	122	ARG
1	D	126	LEU
1	D	160	VAL
1	D	163	LYS
1	D	194	LEU
1	D	218	ASN
1	D	229	ASN
1	D	234	LEU

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Mol	Chain	Res	Type
1	D	244	LEU
1	D	268	ARG
1	D	273	ASP
1	D	290	ARG
1	D	298	MET
1	D	304	LEU
1	D	306	ARG
1	D	363	PHE
1	D	365	THR
1	D	374	ASN
1	D	413	ASP
1	D	431	LEU
1	D	433	ARG
1	D	438	TRP
1	D	440	HIS
1	E	12	TYR
1	E	17	TYR
1	E	19	PRO
1	E	39	ILE
1	E	59	TYR
1	E	80	MET
1	E	116	LYS
1	E	117	ARG
1	E	122	ARG
1	E	126	LEU
1	E	160	VAL
1	E	163	LYS
1	E	194	LEU
1	E	218	ASN
1	E	229	ASN
1	E	234	LEU
1	E	244	LEU
1	E	268	ARG
1	E	273	ASP
1	E	290	ARG
1	E	298	MET
1	E	304	LEU
1	E	306	ARG
1	E	363	PHE
1	E	365	THR
1	E	374	ASN
1	E	413	ASP

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Mol	Chain	Res	Type
1	E	431	LEU
1	E	433	ARG
1	E	438	TRP
1	E	440	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	78	HIS
1	A	183	ASN
1	A	229	ASN
1	A	251	HIS
1	A	312	GLN
1	A	374	ASN
1	A	410	GLN
1	A	440	HIS
1	B	64	GLN
1	B	78	HIS
1	B	183	ASN
1	B	229	ASN
1	B	251	HIS
1	B	312	GLN
1	B	374	ASN
1	B	410	GLN
1	B	440	HIS
1	C	64	GLN
1	C	78	HIS
1	C	183	ASN
1	C	229	ASN
1	C	251	HIS
1	C	312	GLN
1	C	374	ASN
1	C	410	GLN
1	C	440	HIS
1	D	64	GLN
1	D	78	HIS
1	D	183	ASN
1	D	229	ASN
1	D	251	HIS
1	D	312	GLN
1	D	374	ASN

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Mol	Chain	Res	Type
1	D	410	GLN
1	D	440	HIS
1	E	64	GLN
1	E	78	HIS
1	E	183	ASN
1	E	229	ASN
1	E	251	HIS
1	E	312	GLN
1	E	374	ASN
1	E	410	GLN
1	E	440	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	SO4	E	4446	-	4,4,4	0.44	0	6,6,6	0.18	0
2	SO4	C	2445	-	4,4,4	0.60	0	6,6,6	0.16	0
2	SO4	B	1446	-	4,4,4	0.45	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	3445	-	4,4,4	0.60	0	6,6,6	0.17	0
2	SO4	D	3446	-	4,4,4	0.35	0	6,6,6	0.24	0
2	SO4	A	445	-	4,4,4	0.66	0	6,6,6	0.20	0
2	SO4	E	4445	-	4,4,4	0.60	0	6,6,6	0.28	0
2	SO4	A	446	-	4,4,4	0.49	0	6,6,6	0.36	0
2	SO4	C	2446	-	4,4,4	0.48	0	6,6,6	0.25	0
2	SO4	B	1445	-	4,4,4	0.50	0	6,6,6	0.17	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.