Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:09 PM GMT

PDB ID	:	1SCU
Title	:	THE CRYSTAL STRUCTURE OF SUCCINYL-COA SYNTHETASE FROM ESCHERICHIA COLI AT 2.5 ANGSTROMS RESOLUTION
Authors	:	Wolodko, W.T.; Fraser, M.E.; James, M.N.G.; Bridger, W.A.
Deposited on	:	1993-11-18
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

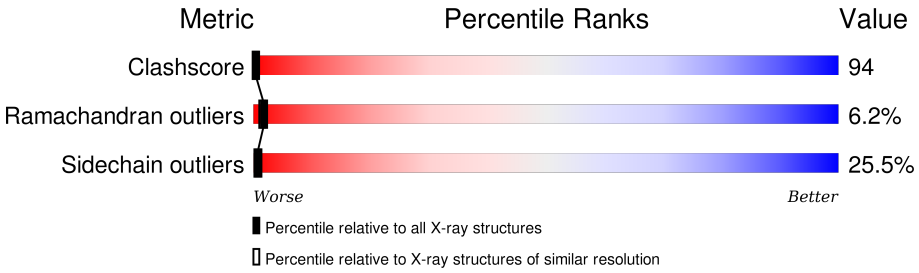
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	288	17% 50% 26% 7%
1	D	288	14% 51% 28% 6%
2	B	388	20% 49% 28% .
2	E	388	21% 41% 31% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10188 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.

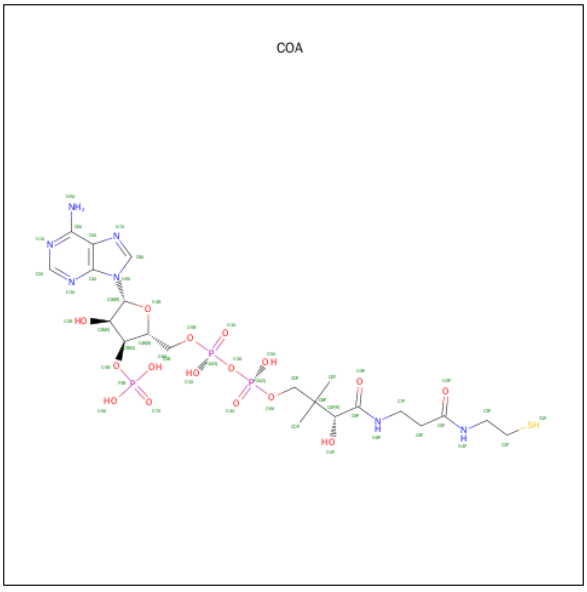
- Molecule 1 is a protein called SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	0
			2083	1319	348	404	1	11			
1	D	288	Total	C	N	O	P	S	0	0	0
			2083	1319	348	404	1	11			

- Molecule 2 is a protein called SUCCINYL-COA SYNTHETASE, BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	388	Total	C	N	O	S	0	0	0
			2908	1836	509	550	13			
2	E	388	Total	C	N	O	S	0	0	0
			2908	1836	509	550	13			

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	33	Total	O	0	0
			33	33		
4	D	25	Total	O	0	0
			25	25		
4	E	30	Total	O	0	0
			30	30		

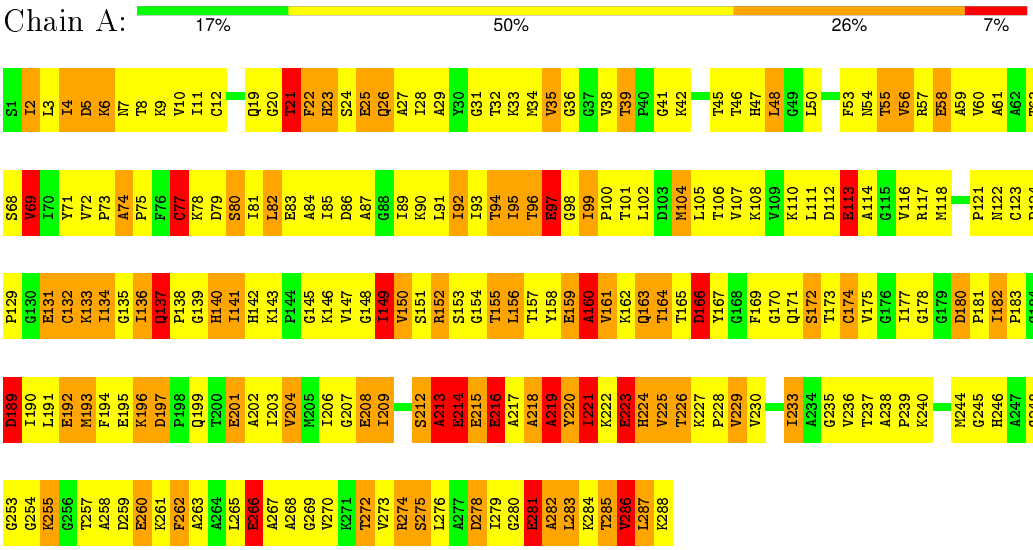
3 Residue-property plots (i)

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

Note EDS was not executed.

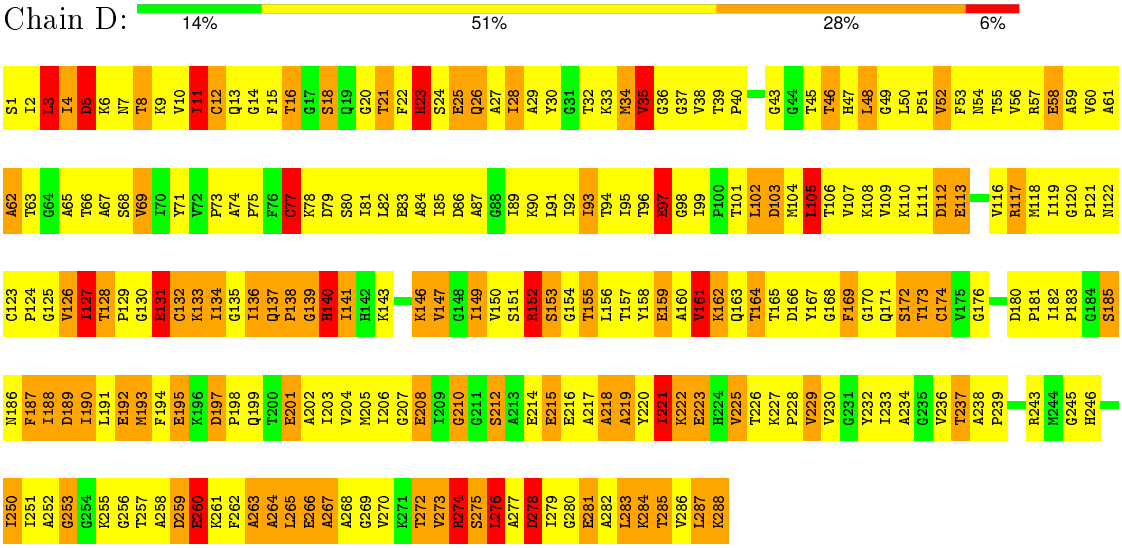
• Molecule 1: SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT

Chain A:



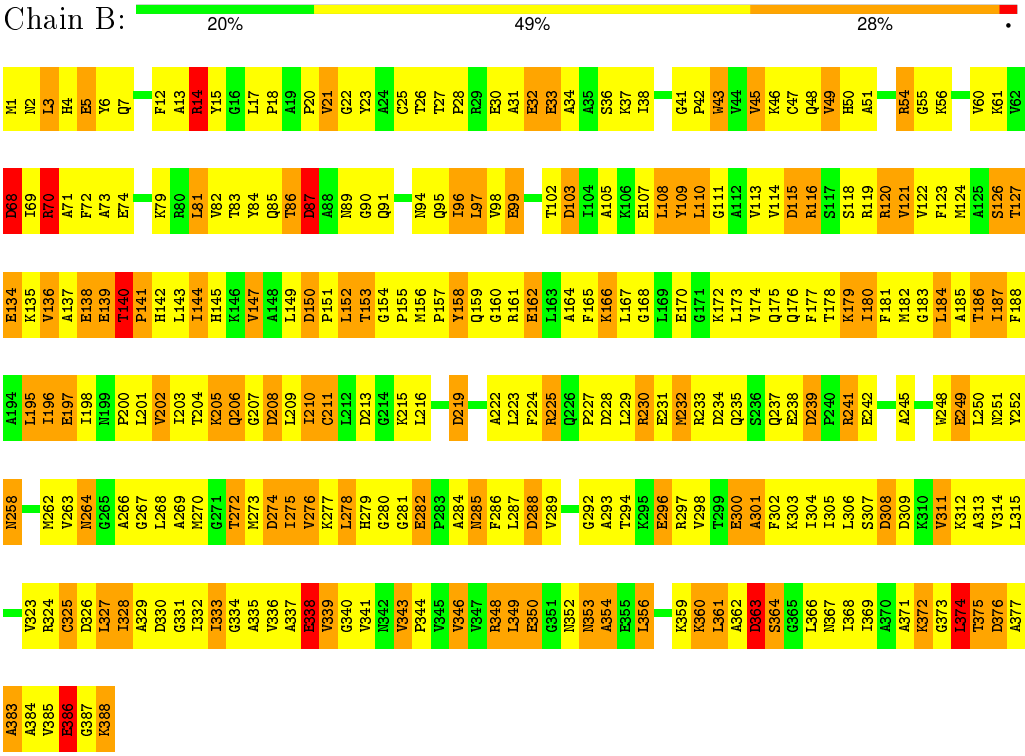
• Molecule 1: SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT

Chain D:



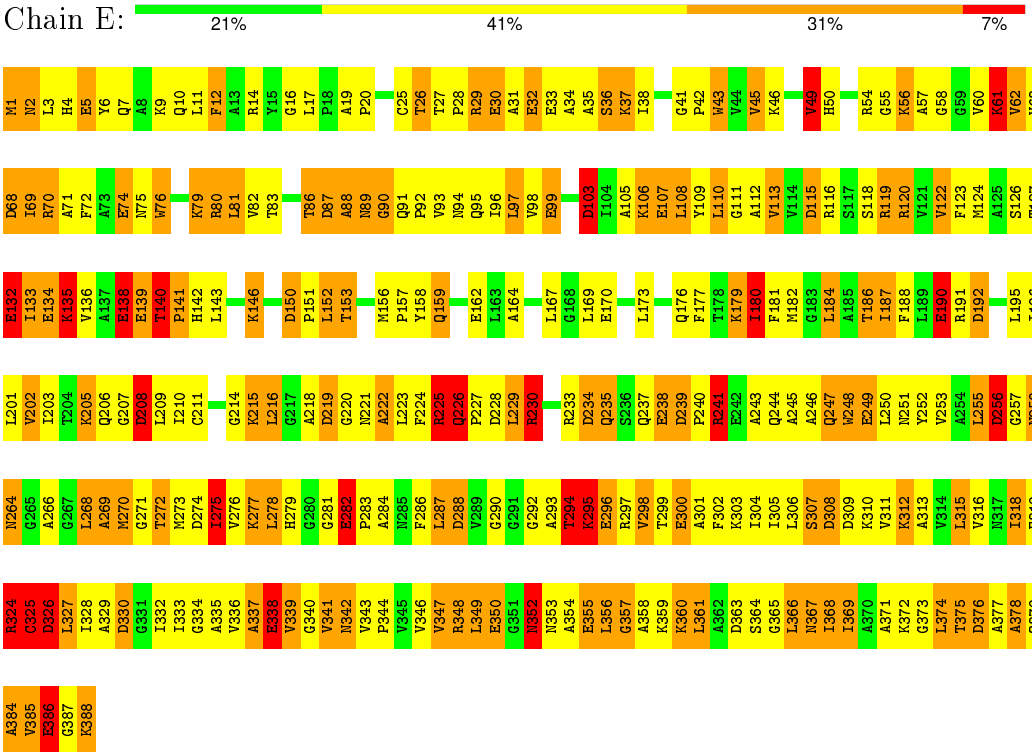
• Molecule 2: SUCCINYL-COA SYNTHETASE, BETA SUBUNIT

Chain B:



• Molecule 2: SUCCINYL-COA SYNTHETASE, BETA SUBUNIT

Chain E:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.47Å 98.47Å 400.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10188	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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: COA, NEP

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	1.38	16/2101 (0.8%)	1.82	46/2842 (1.6%)
1	D	1.38	18/2101 (0.9%)	1.79	42/2842 (1.5%)
2	B	1.42	26/2950 (0.9%)	1.79	55/3989 (1.4%)
2	E	1.43	26/2950 (0.9%)	1.85	89/3989 (2.2%)
All	All	1.41	86/10102 (0.9%)	1.81	232/13662 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
2	B	1	0
2	E	5	0
All	All	7	0

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	162	GLU	CD-OE2	10.37	1.37	1.25
2	E	350	GLU	CD-OE2	9.76	1.36	1.25
1	D	58	GLU	CD-OE2	9.60	1.36	1.25
2	E	132	GLU	CD-OE1	8.90	1.35	1.25
2	E	162	GLU	CD-OE2	8.88	1.35	1.25
1	A	223	GLU	CD-OE1	8.18	1.34	1.25
2	B	32	GLU	CD-OE2	7.91	1.34	1.25
2	E	67	GLU	CD-OE2	7.84	1.34	1.25
1	A	97	GLU	CD-OE2	7.80	1.34	1.25
1	D	266	GLU	CD-OE2	7.75	1.34	1.25
1	D	208	GLU	CD-OE2	7.75	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	GLU	CD-OE2	7.62	1.34	1.25
2	B	338	GLU	CD-OE2	7.57	1.33	1.25
1	D	192	GLU	CD-OE2	7.56	1.33	1.25
1	A	266	GLU	CD-OE2	7.53	1.33	1.25
2	B	249	GLU	CD-OE2	7.51	1.33	1.25
2	B	5	GLU	CD-OE2	7.50	1.33	1.25
2	B	197	GLU	CD-OE2	7.45	1.33	1.25
2	E	5	GLU	CD-OE2	7.33	1.33	1.25
2	E	30	GLU	CD-OE2	7.31	1.33	1.25
2	E	128	GLU	CD-OE2	7.20	1.33	1.25
2	B	242	GLU	CD-OE2	7.20	1.33	1.25
2	B	74	GLU	CD-OE2	7.17	1.33	1.25
2	E	197	GLU	CD-OE1	7.17	1.33	1.25
2	E	138	GLU	CD-OE2	7.15	1.33	1.25
1	D	215	GLU	CD-OE2	7.14	1.33	1.25
2	B	300	GLU	CD-OE2	7.14	1.33	1.25
1	D	159	GLU	CD-OE2	7.09	1.33	1.25
2	E	99	GLU	CD-OE2	7.05	1.33	1.25
1	A	25	GLU	CD-OE2	6.99	1.33	1.25
2	E	33	GLU	CD-OE2	6.96	1.33	1.25
2	E	338	GLU	CD-OE2	6.96	1.33	1.25
1	D	97	GLU	CD-OE1	6.93	1.33	1.25
2	B	170	GLU	CD-OE2	6.92	1.33	1.25
2	B	139	GLU	CD-OE2	6.84	1.33	1.25
2	B	231	GLU	CD-OE2	6.83	1.33	1.25
2	E	170	GLU	CD-OE2	6.81	1.33	1.25
2	E	238	GLU	CD-OE2	6.80	1.33	1.25
1	A	58	GLU	CD-OE2	6.74	1.33	1.25
2	B	132	GLU	CD-OE2	6.74	1.33	1.25
1	A	113	GLU	CD-OE2	6.73	1.33	1.25
1	A	159	GLU	CD-OE2	6.72	1.33	1.25
1	D	113	GLU	CD-OE2	6.68	1.32	1.25
2	B	282	GLU	CD-OE2	6.68	1.32	1.25
2	E	355	GLU	CD-OE2	6.68	1.32	1.25
2	B	238	GLU	CD-OE2	6.65	1.32	1.25
2	B	128	GLU	CD-OE1	6.52	1.32	1.25
2	E	32	GLU	CD-OE2	6.49	1.32	1.25
1	D	195	GLU	CD-OE2	6.47	1.32	1.25
2	E	134	GLU	CD-OE2	6.47	1.32	1.25
1	D	260	GLU	CD-OE2	6.45	1.32	1.25
2	E	107	GLU	CD-OE2	6.45	1.32	1.25
1	D	25	GLU	CD-OE2	6.42	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	386	GLU	CD-OE2	6.38	1.32	1.25
2	B	138	GLU	CD-OE2	6.35	1.32	1.25
1	D	131	GLU	CD-OE2	6.32	1.32	1.25
1	A	215	GLU	CD-OE2	6.30	1.32	1.25
1	A	216	GLU	CD-OE2	6.30	1.32	1.25
1	D	223	GLU	CD-OE2	6.28	1.32	1.25
1	A	201	GLU	CD-OE1	6.27	1.32	1.25
2	B	296	GLU	CD-OE2	6.24	1.32	1.25
2	B	134	GLU	CD-OE2	6.24	1.32	1.25
1	A	281	GLU	CD-OE2	6.21	1.32	1.25
1	D	216	GLU	CD-OE2	6.19	1.32	1.25
2	E	249	GLU	CD-OE2	6.18	1.32	1.25
2	B	190	GLU	CD-OE2	6.17	1.32	1.25
2	B	33	GLU	CD-OE2	6.16	1.32	1.25
2	E	300	GLU	CD-OE2	6.16	1.32	1.25
1	A	260	GLU	CD-OE2	6.14	1.32	1.25
2	B	386	GLU	CD-OE1	6.08	1.32	1.25
1	A	131	GLU	CD-OE2	6.02	1.32	1.25
2	B	99	GLU	CD-OE2	5.96	1.32	1.25
2	E	74	GLU	CD-OE2	5.95	1.32	1.25
2	E	139	GLU	CD-OE2	5.90	1.32	1.25
2	E	190	GLU	CD-OE2	5.76	1.31	1.25
1	D	83	GLU	CD-OE2	5.69	1.31	1.25
2	E	282	GLU	CD-OE2	5.67	1.31	1.25
1	D	201	GLU	CD-OE2	5.64	1.31	1.25
2	B	350	GLU	CD-OE2	5.64	1.31	1.25
2	B	192	ASP	CG-OD2	5.52	1.38	1.25
1	D	281	GLU	CD-OE2	5.40	1.31	1.25
1	A	192	GLU	CD-OE2	5.40	1.31	1.25
1	A	208	GLU	CD-OE1	-5.33	1.19	1.25
2	B	67	GLU	CD-OE2	5.27	1.31	1.25
2	E	296	GLU	CD-OE2	5.14	1.31	1.25
1	D	103	ASP	CG-OD2	5.03	1.36	1.25

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	140	THR	C-N-CD	-13.94	89.94	120.60
2	E	348	ARG	CD-NE-CZ	11.82	140.15	123.60
2	E	348	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	A	152	ARG	NE-CZ-NH2	-10.38	115.11	120.30
2	E	140	THR	C-N-CD	-9.88	98.86	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	226	GLN	C-N-CD	-9.86	98.90	120.60
1	A	79	ASP	CB-CG-OD1	9.76	127.08	118.30
1	A	213	ALA	N-CA-CB	-9.50	96.80	110.10
2	E	348	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	D	140	HIS	CA-CB-CG	-9.33	97.74	113.60
1	D	164	THR	CA-CB-CG2	-9.23	99.48	112.40
2	E	29	ARG	NE-CZ-NH2	-9.21	115.69	120.30
2	B	70	ARG	NE-CZ-NH1	9.21	124.90	120.30
2	B	225	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	D	166	ASP	CB-CG-OD2	-9.01	110.19	118.30
2	E	326	ASP	CB-CG-OD1	-8.93	110.27	118.30
2	B	363	ASP	CB-CG-OD2	-8.91	110.28	118.30
1	D	5	ASP	CB-CG-OD1	8.86	126.28	118.30
2	E	225	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	79	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	A	166	ASP	CB-CG-OD2	-8.77	110.41	118.30
2	E	219	ASP	CB-CG-OD2	-8.65	110.52	118.30
2	E	363	ASP	CB-CG-OD1	8.61	126.05	118.30
2	B	14	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	D	5	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	A	101	THR	CA-CB-CG2	-8.33	100.74	112.40
1	A	23	HIS	CA-CB-CG	-8.20	99.66	113.60
1	A	182	ILE	C-N-CD	-8.17	102.63	120.60
1	D	278	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	D	189	ASP	CB-CG-OD2	-8.03	111.08	118.30
2	B	288	ASP	CB-CG-OD2	-7.94	111.15	118.30
2	E	288	ASP	CB-CG-OD1	7.85	125.36	118.30
2	E	288	ASP	CB-CG-OD2	-7.82	111.27	118.30
2	B	68	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	D	197	ASP	CB-CG-OD1	7.77	125.30	118.30
2	B	325	CYS	CB-CA-C	7.73	125.87	110.40
1	A	152	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	E	308	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	D	79	ASP	CB-CG-OD1	7.58	125.12	118.30
1	D	79	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	77	CYS	CA-CB-SG	-7.53	100.44	114.00
1	A	275	SER	N-CA-CB	7.46	121.69	110.50
1	D	77	CYS	CA-CB-SG	-7.45	100.59	114.00
2	E	219	ASP	CB-CG-OD1	7.42	124.98	118.30
2	E	76	TRP	N-CA-CB	-7.41	97.25	110.60
2	E	120	ARG	NE-CZ-NH1	-7.41	116.60	120.30
2	E	202	VAL	CB-CA-C	-7.35	97.44	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	74	ALA	CB-CA-C	7.25	120.98	110.10
2	E	234	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	219	ALA	CB-CA-C	-7.21	99.29	110.10
1	A	137	GLN	N-CA-CB	-7.20	97.64	110.60
1	D	197	ASP	N-CA-CB	7.18	123.53	110.60
2	E	186	THR	CA-CB-CG2	-7.18	102.35	112.40
2	E	330	ASP	CB-CG-OD1	7.15	124.73	118.30
2	E	192	ASP	CB-CG-OD2	-7.13	111.88	118.30
2	E	208	ASP	CB-CG-OD1	-7.13	111.89	118.30
2	E	180	ILE	CB-CA-C	-7.08	97.45	111.60
1	A	56	VAL	CA-CB-CG1	-7.07	100.30	110.90
2	E	150	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	274	ARG	NE-CZ-NH1	6.97	123.78	120.30
2	B	308	ASP	CB-CG-OD2	-6.92	112.08	118.30
2	E	29	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	B	115	ASP	CB-CG-OD2	-6.87	112.12	118.30
2	E	80	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	D	23	HIS	CA-CB-CG	-6.85	101.95	113.60
1	A	5	ASP	CB-CG-OD1	6.81	124.43	118.30
2	B	288	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	278	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	2	ILE	C-N-CA	-6.75	104.83	121.70
1	A	180	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	259	ASP	CB-CG-OD2	-6.70	112.27	118.30
2	B	297	ARG	NE-CZ-NH2	-6.69	116.96	120.30
2	B	191	ARG	NE-CZ-NH1	-6.65	116.97	120.30
2	E	222	ALA	CB-CA-C	-6.61	100.19	110.10
1	A	69	VAL	CB-CA-C	-6.57	98.91	111.40
2	B	113	VAL	CB-CA-C	-6.55	98.95	111.40
2	E	122	VAL	CB-CA-C	-6.51	99.03	111.40
1	A	166	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	204	VAL	CA-CB-CG1	-6.48	101.17	110.90
2	B	256	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	189	ASP	CB-CG-OD2	-6.47	112.48	118.30
2	B	196	ILE	CB-CA-C	-6.46	98.69	111.60
2	B	153	THR	C-N-CA	-6.44	108.78	122.30
2	E	272	THR	CA-CB-CG2	-6.40	103.44	112.40
1	D	275	SER	N-CA-CB	6.38	120.06	110.50
2	B	225	ARG	CD-NE-CZ	6.35	132.49	123.60
1	A	278	ASP	CB-CG-OD1	6.34	124.01	118.30
2	B	309	ASP	CB-CG-OD2	-6.33	112.60	118.30
2	B	219	ASP	CB-CG-OD1	6.33	124.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	153	THR	C-N-CA	-6.32	109.02	122.30
2	E	363	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	69	VAL	CA-CB-CG2	-6.30	101.44	110.90
2	E	239	ASP	CB-CG-OD1	6.27	123.94	118.30
2	E	376	ASP	CB-CG-OD2	-6.24	112.68	118.30
2	B	150	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	21	THR	CA-CB-CG2	-6.20	103.72	112.40
2	E	309	ASP	CB-CG-OD2	-6.19	112.73	118.30
2	B	376	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	188	ILE	CA-CB-CG2	-6.17	98.56	110.90
2	B	213	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	D	11	ILE	CA-CB-CG2	-6.15	98.60	110.90
1	A	209	ILE	C-N-CA	-6.14	109.40	122.30
2	E	228	ASP	CA-CB-CG	-6.13	99.91	113.40
2	B	363	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	93	ILE	CB-CA-C	-6.12	99.36	111.60
1	D	11	ILE	N-CA-CB	-6.11	96.74	110.80
2	E	330	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	276	LEU	CB-CA-C	6.06	121.72	110.20
2	E	113	VAL	CB-CA-C	-6.06	99.88	111.40
2	E	275	ILE	CB-CA-C	-6.06	99.48	111.60
2	E	225	ARG	CB-CA-C	-6.06	98.28	110.40
2	B	297	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	E	324	ARG	NE-CZ-NH2	-6.03	117.28	120.30
2	B	230	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	E	184	LEU	CA-CB-CG	-6.02	101.46	115.30
1	D	152	ARG	N-CA-CB	-6.01	99.77	110.60
2	E	349	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	A	150	VAL	CB-CA-C	-6.01	99.98	111.40
2	B	68	ASP	CB-CG-OD1	6.01	123.71	118.30
2	E	376	ASP	CB-CG-OD1	6.01	123.70	118.30
2	B	354	ALA	CB-CA-C	6.00	119.10	110.10
2	E	62	VAL	CA-CB-CG1	-5.98	101.93	110.90
2	E	315	LEU	CA-CB-CG	-5.98	101.55	115.30
2	B	376	ASP	CB-CG-OD2	-5.98	112.92	118.30
2	B	274	ASP	CB-CG-OD1	5.98	123.68	118.30
2	B	114	VAL	CA-CB-CG1	-5.94	101.99	110.90
2	E	103	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	21	THR	CA-CB-CG2	-5.93	104.10	112.40
2	E	264	ASN	N-CA-CB	-5.93	99.93	110.60
2	E	115	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	E	198	ILE	CA-CB-CG1	-5.90	99.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	253	VAL	CA-CB-CG1	-5.89	102.06	110.90
1	D	126	VAL	CA-CB-CG1	-5.85	102.12	110.90
2	E	49	VAL	N-CA-CB	-5.85	98.64	111.50
2	E	256	ASP	N-CA-C	5.84	126.78	111.00
2	B	186	THR	CA-CB-CG2	-5.78	104.31	112.40
2	B	116	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	71	TYR	CB-CG-CD2	5.76	124.45	121.00
2	E	241	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	E	68	ASP	CB-CG-OD2	-5.75	113.12	118.30
2	E	87	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	D	221	ILE	CB-CA-C	-5.73	100.14	111.60
1	A	197	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	29	ALA	CB-CA-C	-5.72	101.52	110.10
2	E	266	ALA	N-CA-CB	5.71	118.10	110.10
1	A	39	THR	N-CA-CB	5.71	121.14	110.30
2	B	70	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	E	69	ILE	CB-CA-C	-5.67	100.26	111.60
1	D	225	VAL	CB-CA-C	5.67	122.16	111.40
2	B	119	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	B	328	ILE	CB-CA-C	-5.61	100.37	111.60
2	B	272	THR	CA-CB-CG2	-5.61	104.55	112.40
1	D	210	GLY	C-N-CA	-5.60	110.53	122.30
2	E	381	VAL	CA-CB-CG2	-5.59	102.51	110.90
2	E	120	ARG	CD-NE-CZ	-5.58	115.79	123.60
2	E	259	ILE	CB-CA-C	-5.58	100.44	111.60
2	E	167	LEU	CB-CA-C	-5.58	99.61	110.20
2	E	241	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	E	87	ASP	N-CA-CB	-5.56	100.59	110.60
1	A	229	VAL	CA-CB-CG2	-5.55	102.57	110.90
1	A	229	VAL	CB-CA-C	-5.54	100.86	111.40
1	A	97	GLU	CB-CA-C	5.54	121.48	110.40
1	A	45	THR	CA-CB-CG2	-5.53	104.65	112.40
2	B	301	ALA	CB-CA-C	-5.53	101.80	110.10
2	E	108	LEU	CA-CB-CG	-5.53	102.58	115.30
1	D	278	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	197	ASP	CB-CG-OD2	-5.52	113.33	118.30
2	E	349	LEU	N-CA-CB	5.52	121.45	110.40
2	B	308	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	138	PRO	N-CA-CB	5.52	109.92	103.30
1	A	92	ILE	CA-CB-CG2	-5.51	99.88	110.90
2	E	68	ASP	CB-CG-OD1	5.51	123.25	118.30
2	E	326	ASP	CB-CG-OD2	5.51	123.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	19	ALA	N-CA-CB	-5.48	102.43	110.10
2	E	140	THR	N-CA-CB	-5.46	99.93	110.30
1	A	55	THR	CB-CA-C	-5.45	96.89	111.60
1	A	160	ALA	CB-CA-C	-5.43	101.95	110.10
2	E	86	THR	N-CA-CB	5.43	120.61	110.30
1	D	94	THR	CA-CB-CG2	-5.42	104.81	112.40
2	E	1	MET	C-N-CA	-5.42	108.14	121.70
1	D	267	ALA	C-N-CA	-5.42	108.16	121.70
1	D	189	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	127	ILE	CA-C-N	-5.39	105.35	117.20
2	B	134	GLU	CB-CA-C	5.38	121.16	110.40
1	D	38	VAL	CB-CA-C	-5.37	101.19	111.40
2	E	103	ASP	CB-CG-OD1	5.37	123.13	118.30
2	E	256	ASP	CB-CG-OD2	-5.37	113.47	118.30
2	E	294	THR	CA-CB-CG2	-5.37	104.89	112.40
2	B	96	ILE	CA-CB-CG2	-5.35	100.20	110.90
2	E	225	ARG	CD-NE-CZ	5.34	131.07	123.60
2	B	219	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	E	229	LEU	CA-CB-CG	-5.33	103.04	115.30
2	E	298	VAL	CA-CB-CG1	-5.33	102.91	110.90
1	A	141	ILE	CB-CA-C	-5.32	100.96	111.60
2	E	153	THR	N-CA-C	-5.32	96.65	111.00
2	B	316	VAL	CB-CA-C	-5.31	101.31	111.40
1	A	224	HIS	CA-CB-CG	-5.29	104.62	113.60
1	A	65	ALA	O-C-N	-5.27	114.26	122.70
2	B	103	ASP	CB-CG-OD2	-5.26	113.56	118.30
2	B	239	ASP	CB-CG-OD2	-5.26	113.57	118.30
2	E	239	ASP	CB-CG-OD2	-5.25	113.57	118.30
2	E	378	ALA	N-CA-CB	-5.25	102.75	110.10
2	B	208	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	D	8	THR	CA-CB-CG2	-5.23	105.08	112.40
1	D	166	ASP	CB-CG-OD1	5.21	122.98	118.30
2	E	61	LYS	N-CA-CB	-5.19	101.25	110.60
2	B	353	ASN	CA-CB-CG	-5.18	101.99	113.40
1	A	149	ILE	CB-CA-C	-5.18	101.24	111.60
2	B	276	VAL	CB-CA-C	-5.18	101.55	111.40
2	B	21	VAL	CA-CB-CG2	-5.17	103.15	110.90
2	B	346	VAL	CA-CB-CG2	-5.14	103.18	110.90
2	E	200	PRO	CB-CA-C	-5.14	99.15	112.00
2	E	357	GLY	N-CA-C	-5.13	100.28	113.10
2	E	2	ASN	O-C-N	5.12	130.90	122.70
2	E	201	LEU	N-CA-C	-5.12	97.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	248	TRP	CA-CB-CG	-5.12	103.98	113.70
1	A	174	CYS	CA-CB-SG	-5.12	104.79	114.00
1	D	112	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	D	197	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	B	227	PRO	N-CA-CB	5.10	109.42	103.30
2	E	12	PHE	CB-CA-C	-5.09	100.22	110.40
1	A	156	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	E	120	ARG	CB-CA-C	-5.08	100.24	110.40
1	A	156	LEU	CA-CB-CG	-5.08	103.62	115.30
2	E	230	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	105	LEU	CB-CA-C	5.07	119.83	110.20
1	D	150	VAL	CB-CA-C	-5.06	101.79	111.40
2	B	108	LEU	CA-CB-CG	-5.06	103.67	115.30
2	B	274	ASP	CB-CG-OD2	-5.05	113.75	118.30
2	B	1	MET	CG-SD-CE	5.01	108.22	100.20
2	E	287	LEU	CB-CA-C	5.01	119.71	110.20
1	A	38	VAL	CA-CB-CG1	-5.00	103.39	110.90

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	99	ILE	CB
2	B	64	ASN	CA
2	E	64	ASN	CA
2	E	256	ASP	CA
2	E	287	LEU	CA
2	E	325	CYS	CA
2	E	352	ASN	CA

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	2083	0	2140	401	0
1	D	2083	0	2140	509	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2908	0	2962	465	0
2	E	2908	0	2963	563	0
3	A	48	0	32	13	0
3	D	48	0	32	17	0
4	A	22	0	0	8	0
4	B	33	0	0	13	0
4	D	25	0	0	6	0
4	E	30	0	0	9	0
All	All	10188	0	10269	1922	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 94.

All (1922) 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)
2:E:343:VAL:CG1	2:E:344:PRO:HD2	1.16	1.62
1:A:104:MET:HA	1:A:104:MET:CE	1.33	1.51
1:D:2:ILE:HD11	1:D:193:MET:CB	1.35	1.49
2:E:343:VAL:HG13	2:E:344:PRO:CD	1.40	1.49
1:A:4:ILE:HD11	1:A:132:CYS:SG	1.50	1.48
1:D:237:THR:CG2	2:E:274:ASP:OD1	1.65	1.43
1:D:2:ILE:CD1	1:D:193:MET:HB2	1.48	1.42
2:E:315:LEU:HD12	2:E:316:VAL:N	1.35	1.36
1:A:221:ILE:CG2	1:A:222:LYS:N	1.88	1.34
1:D:221:ILE:HA	1:D:225:VAL:CG1	1.59	1.31
1:A:104:MET:CA	1:A:104:MET:HE3	1.58	1.30
1:D:203:ILE:O	1:D:229:VAL:HG22	1.19	1.29
1:A:195:GLU:OE2	1:A:226:THR:HG23	1.26	1.26
1:A:97:GLU:OE1	1:A:98:GLY:N	1.69	1.26
2:B:380:GLN:O	2:B:383:ALA:HB3	1.36	1.26
2:E:343:VAL:CG1	2:E:344:PRO:CD	2.05	1.26
1:D:105:LEU:HD23	1:D:105:LEU:C	1.38	1.25
2:B:133:ILE:HD12	2:B:133:ILE:N	1.39	1.24
1:A:137:GLN:HE21	1:A:137:GLN:CA	1.40	1.24
2:E:352:ASN:HD22	2:E:352:ASN:C	1.33	1.24
2:E:136:VAL:O	2:E:140:THR:HG22	1.37	1.22
2:B:140:THR:OG1	2:B:143:LEU:HD12	1.39	1.20
2:B:270:MET:CB	4:B:419:HOH:O	1.88	1.20
2:E:287:LEU:C	2:E:287:LEU:HD23	1.60	1.20
1:D:149:ILE:CG1	1:D:174:CYS:HB3	1.73	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ILE:HG22	1:A:222:LYS:N	1.22	1.19
1:D:285:THR:O	1:D:288:LYS:HG3	1.39	1.18
1:A:4:ILE:CD1	1:A:132:CYS:SG	2.31	1.18
2:E:275:ILE:HG22	2:E:276:VAL:N	1.54	1.17
1:D:49:GLY:O	1:D:50:LEU:HD23	1.43	1.17
1:D:221:ILE:CA	1:D:225:VAL:HG12	1.74	1.17
2:E:108:LEU:N	2:E:108:LEU:HD23	1.55	1.17
2:E:82:VAL:HG22	2:E:90:GLY:H	1.00	1.16
1:D:203:ILE:O	1:D:229:VAL:CG2	1.95	1.15
2:E:319:PHE:CD2	2:E:350:GLU:HG2	1.80	1.15
1:D:97:GLU:OE1	1:D:98:GLY:N	1.79	1.15
2:E:369:ILE:N	2:E:369:ILE:CD1	2.08	1.15
2:E:275:ILE:CG2	2:E:276:VAL:N	2.09	1.14
1:D:221:ILE:HG22	1:D:222:LYS:N	1.42	1.14
2:E:82:VAL:HG22	2:E:90:GLY:N	1.63	1.14
1:A:21:THR:HG22	1:A:22:PHE:N	1.53	1.13
1:D:105:LEU:CD2	1:D:105:LEU:C	2.17	1.13
2:E:82:VAL:CG2	2:E:90:GLY:H	1.60	1.13
2:B:45:VAL:O	2:B:45:VAL:HG23	1.44	1.13
2:E:157:PRO:N	2:E:182:MET:HE2	1.59	1.13
1:D:136:ILE:HD13	1:D:136:ILE:H	1.12	1.13
1:D:6:LYS:O	1:D:33:LYS:HE3	1.45	1.13
2:E:368:ILE:C	2:E:369:ILE:HD12	1.68	1.13
1:A:2:ILE:HG23	1:A:3:LEU:N	1.62	1.13
2:E:277:LYS:HD2	2:E:278:LEU:N	1.62	1.13
2:E:87:ASP:O	2:E:89:ASN:N	1.82	1.12
1:D:257:THR:OG1	1:D:260:GLU:HB2	1.49	1.13
2:E:215:LYS:C	2:E:216:LEU:HD23	1.69	1.12
2:E:79:LYS:HB3	2:E:79:LYS:NZ	1.46	1.12
1:A:128:THR:O	1:A:128:THR:HG22	1.44	1.11
2:E:107:GLU:C	2:E:108:LEU:HD23	1.68	1.11
2:B:270:MET:HB3	4:B:419:HOH:O	1.44	1.11
1:D:124:PRO:HA	1:D:136:ILE:HD11	1.23	1.10
1:A:104:MET:CA	1:A:104:MET:CE	2.16	1.10
2:B:133:ILE:HD13	2:B:134:GLU:H	1.12	1.10
1:D:237:THR:HG23	2:E:274:ASP:OD1	0.92	1.10
3:A:289:COA:C6P	3:A:289:COA:O9P	2.00	1.10
2:B:215:LYS:O	2:B:216:LEU:HD23	1.49	1.10
1:D:203:ILE:HB	1:D:229:VAL:HG23	1.32	1.09
2:E:339:VAL:HG12	2:E:341:VAL:HG12	1.33	1.09
1:D:92:ILE:CG2	1:D:118:MET:HG3	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:CYS:HB3	2:B:349:LEU:HD13	1.33	1.09
2:E:356:LEU:HD22	2:E:357:GLY:N	1.66	1.08
1:D:221:ILE:CA	1:D:225:VAL:CG1	2.31	1.08
2:E:319:PHE:HA	2:E:350:GLU:CB	1.84	1.08
2:B:133:ILE:CD1	2:B:133:ILE:N	2.09	1.08
1:D:92:ILE:HG22	1:D:118:MET:HG3	1.16	1.08
1:A:137:GLN:HA	1:A:137:GLN:NE2	1.57	1.07
1:A:4:ILE:HD13	1:A:132:CYS:HB3	1.13	1.07
1:D:105:LEU:HD23	1:D:105:LEU:O	1.52	1.07
2:E:369:ILE:N	2:E:369:ILE:HD12	1.66	1.07
1:A:2:ILE:CG2	1:A:3:LEU:N	2.17	1.07
1:D:190:ILE:N	1:D:190:ILE:HD13	1.63	1.07
2:B:45:VAL:O	2:B:45:VAL:CG2	2.02	1.06
2:E:375:THR:O	2:E:378:ALA:HB3	1.55	1.06
2:B:133:ILE:CD1	2:B:133:ILE:H	1.56	1.06
2:B:215:LYS:C	2:B:216:LEU:HD23	1.75	1.06
1:D:229:VAL:HG12	1:D:270:VAL:CG1	1.86	1.05
2:B:63:VAL:CG1	2:B:68:ASP:HB3	1.86	1.05
2:B:328:ILE:HG22	2:B:329:ALA:N	1.70	1.05
2:B:272:THR:O	2:B:275:ILE:HG22	1.54	1.05
1:A:24:SER:HA	4:A:297:HOH:O	1.57	1.04
1:A:4:ILE:HD13	1:A:132:CYS:CB	1.86	1.04
1:D:2:ILE:C	4:D:293:HOH:O	1.96	1.04
2:E:315:LEU:CD1	2:E:316:VAL:N	2.19	1.04
1:D:229:VAL:HG12	1:D:270:VAL:HG13	1.31	1.04
1:D:157:THR:O	1:D:161:VAL:HG23	1.56	1.03
1:D:23:HIS:CE1	1:D:136:ILE:HG22	1.94	1.03
2:E:262:MET:HE1	2:E:301:ALA:HB3	1.38	1.02
1:A:2:ILE:HD12	1:A:194:PHE:CE1	1.94	1.02
1:D:266:GLU:HG2	1:D:272:THR:HG21	1.42	1.02
1:A:128:THR:O	1:A:128:THR:CG2	2.08	1.02
2:E:139:GLU:O	2:E:140:THR:HB	1.60	1.01
1:D:187:PHE:HE2	1:D:214:GLU:HG3	1.19	1.01
2:B:42:PRO:O	4:B:390:HOH:O	1.78	1.01
1:D:223:GLU:O	1:D:223:GLU:HG2	1.58	1.01
1:A:21:THR:CG2	1:A:22:PHE:N	2.21	1.01
1:D:221:ILE:CG2	1:D:222:LYS:N	2.13	1.01
2:E:319:PHE:HA	2:E:350:GLU:HB2	1.39	1.00
2:B:229:LEU:HA	2:B:232:MET:HE3	1.43	0.99
2:B:140:THR:CB	2:B:143:LEU:HD12	1.91	0.99
2:B:323:VAL:HG11	2:B:328:ILE:HG13	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HD22	2:B:98:VAL:N	1.78	0.99
2:E:287:LEU:O	2:E:287:LEU:HD23	1.62	0.99
2:E:312:LYS:NZ	2:E:388:LYS:HE3	1.77	0.99
2:E:81:LEU:O	2:E:90:GLY:HA3	1.61	0.99
2:E:87:ASP:C	2:E:89:ASN:H	1.60	0.99
1:D:10:VAL:O	1:D:34:MET:HE3	1.63	0.98
1:D:149:ILE:HG13	1:D:174:CYS:CB	1.93	0.98
2:E:315:LEU:CD1	2:E:316:VAL:H	1.76	0.98
1:D:10:VAL:C	1:D:34:MET:HE3	1.84	0.98
1:D:203:ILE:HB	1:D:229:VAL:CG2	1.91	0.98
2:E:339:VAL:CG1	2:E:341:VAL:HG12	1.92	0.98
2:E:315:LEU:HD12	2:E:316:VAL:H	0.87	0.98
2:E:83:THR:H	2:E:86:THR:HG23	1.29	0.98
2:E:352:ASN:C	2:E:352:ASN:ND2	2.12	0.97
1:D:124:PRO:HA	1:D:136:ILE:CD1	1.94	0.97
1:D:203:ILE:CB	1:D:229:VAL:HG23	1.93	0.97
1:D:23:HIS:NE2	1:D:136:ILE:HG22	1.81	0.96
1:A:124:PRO:O	1:A:135:GLY:HA3	1.65	0.96
1:A:137:GLN:HE21	1:A:137:GLN:HA	0.80	0.96
3:A:289:COA:H62	3:A:289:COA:O9P	1.64	0.96
2:B:109:TYR:C	2:B:109:TYR:CD1	2.39	0.96
2:E:277:LYS:HA	2:E:281:GLY:O	1.65	0.96
1:D:149:ILE:HG13	1:D:174:CYS:HB3	0.98	0.96
1:D:92:ILE:O	1:D:118:MET:HA	1.64	0.96
2:B:133:ILE:HD13	2:B:134:GLU:N	1.81	0.95
2:E:157:PRO:N	2:E:182:MET:CE	2.29	0.95
1:A:108:LYS:HE2	4:A:307:HOH:O	1.64	0.95
1:D:187:PHE:CE2	1:D:214:GLU:HG3	2.02	0.95
1:A:21:THR:HG22	1:A:22:PHE:H	1.17	0.95
2:E:292:GLY:O	2:E:294:THR:HG23	1.67	0.95
2:B:270:MET:CA	4:B:419:HOH:O	2.13	0.94
2:B:258:ASN:ND2	2:B:282:GLU:HB3	1.81	0.94
1:D:259:ASP:OD1	1:D:274:ARG:NH2	2.00	0.94
2:E:115:ASP:CG	4:E:395:HOH:O	2.05	0.94
1:D:190:ILE:HA	1:D:193:MET:HG3	1.50	0.94
1:D:28:ILE:HG22	1:D:29:ALA:N	1.81	0.94
1:A:4:ILE:CD1	1:A:132:CYS:HB3	1.98	0.93
1:D:123:CYS:N	3:D:289:COA:S1P	2.41	0.93
2:E:108:LEU:N	2:E:108:LEU:CD2	2.28	0.93
1:D:139:GLY:O	1:D:141:ILE:N	2.01	0.93
1:A:9:LYS:HB3	1:A:35:VAL:HG11	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:312:LYS:HZ3	2:E:388:LYS:HE3	1.34	0.92
1:A:167:TYR:HB3	1:A:169:PHE:CE2	2.04	0.92
2:E:346:VAL:HG21	2:E:381:VAL:HG22	1.50	0.92
2:B:140:THR:N	2:B:141:PRO:HD3	1.84	0.91
1:D:266:GLU:CG	1:D:272:THR:HG21	2.00	0.91
2:E:136:VAL:O	2:E:140:THR:CG2	2.20	0.90
2:B:63:VAL:HG13	2:B:68:ASP:HB3	1.53	0.90
1:A:223:GLU:O	1:A:224:HIS:CD2	2.25	0.90
2:B:82:VAL:HG22	2:B:86:THR:HG21	1.54	0.90
1:A:23:HIS:CE1	1:A:136:ILE:HG22	2.07	0.90
2:E:356:LEU:C	2:E:356:LEU:HD22	1.84	0.90
2:E:49:VAL:HG22	2:E:91:GLN:HB3	1.54	0.90
1:D:127:ILE:O	1:D:173:THR:HG22	1.71	0.89
2:B:133:ILE:HD12	2:B:133:ILE:H	0.75	0.89
1:D:157:THR:O	1:D:161:VAL:CG2	2.19	0.89
1:D:97:GLU:HB3	3:D:289:COA:C7P	2.00	0.89
2:E:357:GLY:O	2:E:361:LEU:HD22	1.72	0.89
1:A:4:ILE:CD1	1:A:132:CYS:CB	2.48	0.89
2:E:156:MET:C	2:E:182:MET:HE2	1.92	0.89
1:D:6:LYS:O	1:D:33:LYS:CE	2.21	0.89
2:B:258:ASN:H	2:B:258:ASN:ND2	1.69	0.89
2:E:312:LYS:NZ	2:E:388:LYS:CE	2.35	0.89
1:A:104:MET:CE	1:A:107:VAL:HB	2.01	0.89
2:E:157:PRO:CA	2:E:182:MET:HE2	2.01	0.89
2:E:326:ASP:O	2:E:328:ILE:N	2.05	0.89
2:E:352:ASN:HD22	2:E:353:ASN:N	1.68	0.89
2:E:252:TYR:C	2:E:253:VAL:HG23	1.92	0.89
2:E:262:MET:CE	2:E:301:ALA:CB	2.50	0.89
2:E:255:LEU:O	2:E:256:ASP:HB3	1.69	0.89
1:A:72:VAL:HG13	1:A:73:PRO:HD2	1.55	0.88
2:E:346:VAL:CG2	2:E:381:VAL:HG22	2.04	0.88
2:E:252:TYR:O	2:E:253:VAL:CG2	2.21	0.88
1:A:104:MET:HE2	1:A:104:MET:HA	1.55	0.88
2:E:107:GLU:O	2:E:129:GLY:HA3	1.72	0.88
2:B:97:LEU:HD22	2:B:98:VAL:H	1.39	0.88
1:A:55:THR:HG22	4:A:300:HOH:O	1.73	0.88
2:B:292:GLY:O	2:B:294:THR:HG23	1.73	0.88
2:E:79:LYS:HZ3	2:E:79:LYS:HB3	1.35	0.88
1:A:149:ILE:HG23	1:A:204:VAL:HB	1.54	0.88
1:D:116:VAL:CG1	1:D:117:ARG:N	2.37	0.88
1:A:10:VAL:HG12	1:A:11:ILE:N	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:CG2	4:A:300:HOH:O	2.22	0.87
2:B:195:LEU:HG	2:B:196:ILE:N	1.89	0.87
1:D:91:LEU:HD12	1:D:117:ARG:HG2	1.55	0.87
2:B:339:VAL:HG12	2:B:340:GLY:N	1.86	0.87
2:B:258:ASN:H	2:B:258:ASN:HD22	1.18	0.87
2:E:383:ALA:O	2:E:386:GLU:N	2.07	0.87
2:B:304:ILE:O	2:B:307:SER:OG	1.91	0.87
2:E:173:LEU:HD12	2:E:209:LEU:HG	1.56	0.87
1:D:203:ILE:C	1:D:229:VAL:HG22	1.95	0.87
1:D:123:CYS:HB2	1:D:124:PRO:HD2	1.55	0.87
2:E:275:ILE:HG22	2:E:276:VAL:H	1.40	0.86
2:E:75:ASN:O	2:E:79:LYS:CD	2.23	0.86
2:E:79:LYS:CB	2:E:79:LYS:NZ	2.35	0.86
2:E:257:GLY:HA3	2:E:282:GLU:O	1.75	0.86
2:B:385:VAL:HG12	2:B:386:GLU:N	1.87	0.86
2:B:263:VAL:HG11	2:B:268:LEU:HB3	1.55	0.86
2:E:79:LYS:HB3	2:E:79:LYS:HZ2	1.08	0.86
2:B:110:LEU:HD22	2:B:111:GLY:H	1.40	0.86
1:D:10:VAL:C	1:D:34:MET:CE	2.44	0.86
2:B:63:VAL:HG11	2:B:68:ASP:HB3	1.58	0.86
2:B:324:ARG:HB2	2:B:327:LEU:HD12	1.55	0.86
1:D:45:THR:O	1:D:52:VAL:HG23	1.75	0.86
1:A:92:ILE:HG22	1:A:93:ILE:N	1.91	0.86
2:E:62:VAL:HG13	2:E:63:VAL:N	1.90	0.86
2:B:223:LEU:O	2:B:230:ARG:NH1	2.08	0.86
1:A:233:ILE:HD12	1:A:261:LYS:HB3	1.57	0.85
2:B:248:TRP:O	2:B:250:LEU:HG	1.75	0.85
1:D:10:VAL:O	1:D:34:MET:CE	2.23	0.85
2:B:257:GLY:C	2:B:284:ALA:HB2	1.96	0.85
2:E:343:VAL:CB	2:E:344:PRO:HD2	2.04	0.85
2:E:383:ALA:O	2:E:384:ALA:C	2.13	0.85
2:E:352:ASN:ND2	2:E:353:ASN:N	2.24	0.85
2:E:156:MET:O	2:E:159:GLN:HG3	1.76	0.85
1:D:229:VAL:CG1	1:D:270:VAL:CG1	2.55	0.85
2:E:287:LEU:CD2	2:E:287:LEU:C	2.42	0.85
1:D:221:ILE:HG22	1:D:222:LYS:H	1.40	0.85
2:E:326:ASP:OD1	2:E:327:LEU:N	2.09	0.85
2:E:262:MET:CE	2:E:301:ALA:HB3	2.05	0.85
1:A:105:LEU:C	1:A:105:LEU:HD23	1.98	0.84
1:A:128:THR:CG2	1:A:131:GLU:HB2	2.07	0.84
2:B:239:ASP:OD1	2:B:241:ARG:HB2	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LYS:HB2	1:D:268:ALA:HB1	1.56	0.84
2:E:75:ASN:O	2:E:79:LYS:HD2	1.76	0.84
1:A:104:MET:HE2	1:A:104:MET:CA	2.08	0.84
2:B:270:MET:HA	4:B:419:HOH:O	1.73	0.84
2:B:140:THR:O	2:B:143:LEU:N	2.10	0.84
1:A:163:GLN:O	1:A:165:THR:N	2.10	0.84
1:D:2:ILE:O	4:D:293:HOH:O	1.90	0.84
1:D:203:ILE:C	1:D:229:VAL:CG2	2.45	0.84
2:B:180:ILE:HG22	2:B:181:PHE:N	1.91	0.84
2:B:82:VAL:HG12	2:B:82:VAL:O	1.77	0.83
1:D:203:ILE:CA	1:D:229:VAL:HG23	2.08	0.83
1:D:136:ILE:H	1:D:136:ILE:CD1	1.90	0.83
2:B:144:ILE:N	2:B:144:ILE:HD13	1.93	0.83
2:E:216:LEU:HD23	2:E:216:LEU:N	1.88	0.83
1:A:97:GLU:CD	1:A:97:GLU:C	2.38	0.83
2:B:279:HIS:O	2:B:382:VAL:HG21	1.78	0.83
2:E:49:VAL:CG2	2:E:91:GLN:HB3	2.09	0.83
2:B:49:VAL:HG13	2:B:51:ALA:H	1.44	0.83
2:E:277:LYS:HD2	2:E:278:LEU:CA	2.09	0.83
1:D:221:ILE:HG13	1:D:225:VAL:HG11	1.60	0.83
2:E:333:ILE:HG22	2:E:334:GLY:N	1.93	0.82
1:D:119:ILE:CD1	1:D:185:SER:OG	2.27	0.82
2:E:312:LYS:HZ3	2:E:388:LYS:CE	1.90	0.82
1:A:195:GLU:OE2	1:A:226:THR:CG2	2.20	0.82
2:B:139:GLU:C	2:B:141:PRO:HD3	2.00	0.82
1:D:265:LEU:O	1:D:270:VAL:HG23	1.79	0.82
2:E:369:ILE:HD13	2:E:369:ILE:N	1.92	0.82
2:E:302:PHE:O	2:E:306:LEU:HD12	1.80	0.82
1:A:97:GLU:CD	1:A:98:GLY:N	2.32	0.82
2:E:272:THR:HG22	2:E:273:MET:N	1.95	0.82
2:E:83:THR:H	2:E:86:THR:CG2	1.93	0.82
2:E:312:LYS:NZ	2:E:388:LYS:NZ	2.28	0.82
2:E:70:ARG:HG3	2:E:70:ARG:O	1.79	0.82
1:D:55:THR:HG22	1:D:57:ARG:H	1.42	0.82
2:E:343:VAL:HG12	2:E:344:PRO:CD	2.10	0.81
1:D:190:ILE:CD1	1:D:190:ILE:N	2.41	0.81
1:D:221:ILE:HA	1:D:225:VAL:HG12	0.84	0.81
1:A:181:PRO:HA	2:B:116:ARG:NH1	1.95	0.81
1:A:12:CYS:HA	1:A:69:VAL:HG23	1.62	0.81
2:B:287:LEU:HD23	2:B:288:ASP:N	1.96	0.81
1:D:21:THR:HG22	1:D:22:PHE:N	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:THR:HG22	1:D:50:LEU:O	1.81	0.81
1:A:6:LYS:HG2	1:A:131:GLU:O	1.80	0.81
1:D:10:VAL:HB	1:D:34:MET:CE	2.11	0.81
1:A:186:ASN:HD21	1:A:189:ASP:H	1.28	0.80
2:E:126:SER:HB2	2:E:143:LEU:O	1.81	0.80
1:D:218:ALA:O	1:D:221:ILE:HB	1.82	0.80
1:D:78:LYS:O	1:D:82:LEU:HB2	1.81	0.80
2:B:258:ASN:HD21	2:B:282:GLU:HB3	1.45	0.80
1:D:165:THR:O	1:D:168:GLY:N	2.14	0.80
2:E:319:PHE:HA	2:E:350:GLU:HB3	1.63	0.80
1:A:97:GLU:OE1	1:A:97:GLU:C	2.20	0.80
1:D:97:GLU:HB3	3:D:289:COA:H72	1.62	0.80
2:E:105:ALA:HB3	2:E:203:ILE:O	1.81	0.80
1:A:186:ASN:ND2	1:A:189:ASP:CG	2.35	0.80
2:B:263:VAL:O	2:B:289:VAL:HG23	1.80	0.80
2:B:86:THR:HG23	2:B:90:GLY:HA2	1.63	0.80
1:A:221:ILE:HG22	1:A:222:LYS:H	0.81	0.79
1:D:127:ILE:O	1:D:173:THR:CG2	2.30	0.79
1:D:266:GLU:O	1:D:269:GLY:N	2.13	0.79
2:E:251:ASN:HB2	2:E:288:ASP:HB3	1.65	0.79
2:E:326:ASP:O	2:E:327:LEU:C	2.20	0.79
2:B:275:ILE:O	2:B:278:LEU:HB3	1.83	0.79
1:D:127:ILE:HG12	1:D:128:THR:N	1.97	0.79
2:E:56:LYS:HD2	2:E:56:LYS:H	1.46	0.79
2:E:252:TYR:O	2:E:253:VAL:HG23	1.82	0.79
2:B:258:ASN:N	2:B:258:ASN:HD22	1.81	0.79
1:D:2:ILE:HD11	1:D:193:MET:HB3	1.62	0.79
1:A:137:GLN:CA	1:A:137:GLN:NE2	2.22	0.79
1:D:136:ILE:HD13	1:D:136:ILE:N	1.94	0.79
2:B:81:LEU:HD22	2:B:82:VAL:H	1.48	0.79
2:B:188:PHE:O	4:B:408:HOH:O	1.93	0.79
1:D:203:ILE:CB	1:D:229:VAL:CG2	2.57	0.79
2:B:110:LEU:HD22	2:B:111:GLY:N	1.97	0.79
1:D:221:ILE:HG22	1:D:222:LYS:CA	2.13	0.79
1:A:104:MET:HE1	1:A:107:VAL:HB	1.64	0.78
2:E:65:SER:HB2	2:E:67:GLU:OE1	1.82	0.78
2:E:262:MET:HE1	2:E:301:ALA:CB	2.13	0.78
2:B:105:ALA:HB3	2:B:203:ILE:HG22	1.66	0.78
2:E:70:ARG:O	2:E:74:GLU:HG3	1.82	0.78
1:D:10:VAL:HB	1:D:34:MET:HE3	1.63	0.78
2:E:330:ASP:O	2:E:333:ILE:HB	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:LEU:O	2:B:330:ASP:HB2	1.83	0.78
1:D:123:CYS:HB2	1:D:124:PRO:CD	2.13	0.78
2:E:315:LEU:C	2:E:315:LEU:HD12	1.91	0.78
1:D:91:LEU:CD1	1:D:117:ARG:HG2	2.13	0.78
2:B:257:GLY:O	2:B:284:ALA:HB2	1.83	0.78
3:A:289:COA:O9P	3:A:289:COA:H61	1.82	0.78
1:A:5:ASP:OD1	1:A:7:ASN:N	2.15	0.78
1:D:283:LEU:O	1:D:286:VAL:HG12	1.84	0.78
1:D:228:PRO:HB2	1:D:286:VAL:HG21	1.64	0.78
1:A:186:ASN:HD22	1:A:189:ASP:CG	1.87	0.78
1:A:197:ASP:O	1:A:227:LYS:NZ	2.15	0.78
2:E:262:MET:HE2	2:E:301:ALA:HB1	1.65	0.78
1:D:7:ASN:HA	1:D:33:LYS:NZ	1.99	0.78
2:E:296:GLU:OE1	2:E:296:GLU:N	2.12	0.78
1:A:92:ILE:CG2	1:A:93:ILE:N	2.47	0.78
1:A:2:ILE:CG2	1:A:3:LEU:H	1.94	0.77
1:D:53:PHE:CG	1:D:59:ALA:HB2	2.20	0.77
2:E:152:LEU:HD22	2:E:152:LEU:O	1.85	0.77
1:D:230:VAL:HG21	1:D:283:LEU:HD13	1.66	0.77
1:D:2:ILE:HG12	1:D:193:MET:HE2	1.65	0.77
2:B:141:PRO:HD2	2:B:142:HIS:HD2	1.47	0.77
1:A:106:THR:HG22	1:A:106:THR:O	1.83	0.77
2:B:126:SER:HB2	2:B:143:LEU:O	1.84	0.77
2:E:352:ASN:ND2	2:E:353:ASN:HB2	2.00	0.77
2:E:81:LEU:O	2:E:90:GLY:CA	2.31	0.77
2:E:119:ARG:O	2:E:120:ARG:HD3	1.85	0.77
1:D:172:SER:HB3	1:D:199:GLN:HG2	1.67	0.77
1:D:274:ARG:HG2	1:D:274:ARG:HH11	1.49	0.77
1:D:116:VAL:HG13	1:D:117:ARG:H	1.46	0.77
2:E:49:VAL:HG22	2:E:91:GLN:CB	2.13	0.77
1:A:123:CYS:HB2	1:A:124:PRO:HD2	1.64	0.77
2:B:249:GLU:OE2	2:E:70:ARG:NH2	2.17	0.77
1:A:221:ILE:CG2	1:A:222:LYS:H	1.68	0.77
2:B:361:LEU:O	2:B:364:SER:HB3	1.84	0.77
2:B:109:TYR:O	2:B:109:TYR:HD1	1.68	0.77
2:B:26:THR:HB	2:B:30:GLU:OE1	1.84	0.77
1:A:39:THR:HG22	1:A:42:LYS:HG3	1.65	0.77
2:E:316:VAL:HB	2:E:347:VAL:HG13	1.66	0.77
1:D:282:ALA:O	1:D:285:THR:HB	1.85	0.76
2:B:308:ASP:O	2:B:311:VAL:HG12	1.85	0.76
1:A:127:ILE:HD12	1:A:133:LYS:HG3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:C	1:A:224:HIS:CD2	2.59	0.76
2:E:246:ALA:O	2:E:248:TRP:N	2.17	0.76
1:D:169:PHE:CE2	1:D:283:LEU:HB3	2.20	0.76
1:A:10:VAL:CG1	1:A:11:ILE:N	2.47	0.76
2:E:300:GLU:O	2:E:304:ILE:HG12	1.85	0.76
2:B:375:THR:O	2:B:379:GLN:HG3	1.85	0.76
2:E:157:PRO:CA	2:E:182:MET:CE	2.62	0.76
2:E:319:PHE:O	2:E:320:GLY:O	2.03	0.76
2:B:274:ASP:OD2	4:B:420:HOH:O	2.03	0.76
3:D:289:COA:O8A	3:D:289:COA:O2B	2.02	0.76
2:B:110:LEU:CD2	2:B:111:GLY:H	1.98	0.76
2:E:150:ASP:O	2:E:153:THR:O	2.04	0.76
1:D:49:GLY:C	1:D:50:LEU:HD23	2.07	0.75
2:E:339:VAL:HG12	2:E:341:VAL:N	2.01	0.75
2:B:276:VAL:HG12	2:B:277:LYS:N	1.96	0.75
2:B:86:THR:CG2	2:B:90:GLY:HA2	2.16	0.75
1:D:221:ILE:CG1	1:D:225:VAL:HG11	2.17	0.75
2:E:97:LEU:HD23	2:E:98:VAL:N	2.01	0.75
2:E:319:PHE:CE2	2:E:350:GLU:HG2	2.20	0.75
1:D:252:ALA:O	1:D:253:GLY:C	2.24	0.75
2:B:380:GLN:O	2:B:383:ALA:CB	2.28	0.75
1:A:161:VAL:O	1:A:162:LYS:C	2.24	0.75
2:B:66:LYS:O	2:B:69:ILE:HB	1.85	0.75
2:E:63:VAL:HG12	2:E:64:ASN:N	2.02	0.75
2:B:201:LEU:HD12	2:B:202:VAL:H	1.51	0.75
1:D:203:ILE:O	1:D:230:VAL:N	2.15	0.75
1:A:221:ILE:HG22	1:A:222:LYS:CA	2.16	0.75
1:D:23:HIS:NE2	1:D:136:ILE:CG2	2.50	0.74
1:D:97:GLU:CB	3:D:289:COA:C7P	2.64	0.74
2:B:222:ALA:O	2:B:225:ARG:N	2.14	0.74
1:D:129:PRO:HD2	1:D:172:SER:O	1.86	0.74
1:D:11:ILE:HA	1:D:36:GLY:O	1.86	0.74
1:D:233:ILE:CD1	1:D:261:LYS:HB3	2.17	0.74
2:B:326:ASP:OD1	2:B:353:ASN:ND2	2.19	0.74
2:B:201:LEU:HD12	2:B:202:VAL:N	2.01	0.74
1:A:163:GLN:O	1:A:164:THR:C	2.25	0.74
2:E:72:PHE:CE1	2:E:76:TRP:CD1	2.76	0.74
2:B:325:CYS:HB2	2:B:352:ASN:O	1.88	0.74
1:D:180:ASP:HB3	1:D:181:PRO:HD2	1.68	0.74
1:D:116:VAL:HG12	1:D:117:ARG:N	2.02	0.74
2:E:324:ARG:NE	2:E:326:ASP:OD2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ILE:CG2	1:D:234:ALA:N	2.50	0.74
1:D:2:ILE:CD1	1:D:193:MET:CB	2.30	0.73
1:D:263:ALA:O	1:D:266:GLU:N	2.21	0.73
1:D:275:SER:HB3	1:D:278:ASP:OD2	1.87	0.73
2:E:262:MET:HE2	2:E:301:ALA:CB	2.16	0.73
1:D:180:ASP:HB3	1:D:181:PRO:CD	2.18	0.73
2:E:322:ILE:O	2:E:322:ILE:HG23	1.87	0.73
1:D:147:VAL:HG23	1:D:170:GLY:O	1.88	0.73
1:A:91:LEU:HD12	1:A:117:ARG:O	1.88	0.73
1:D:285:THR:HG22	1:D:286:VAL:N	2.01	0.73
1:A:236:VAL:HG23	4:B:420:HOH:O	1.88	0.73
1:A:265:LEU:O	1:A:270:VAL:HG23	1.88	0.73
1:D:215:GLU:OE1	1:D:261:LYS:HG2	1.89	0.73
2:B:109:TYR:C	2:B:109:TYR:HD1	1.91	0.73
1:A:2:ILE:HG22	1:A:3:LEU:H	1.54	0.73
2:B:150:ASP:OD1	2:B:152:LEU:N	2.18	0.73
1:A:218:ALA:HB1	1:A:268:ALA:HB2	1.69	0.73
1:A:207:GLY:O	1:A:233:ILE:HA	1.88	0.73
2:E:82:VAL:HG22	2:E:90:GLY:CA	2.18	0.73
1:A:195:GLU:OE1	1:A:225:VAL:HG23	1.89	0.73
2:E:63:VAL:HG11	2:E:68:ASP:HB3	1.71	0.72
2:E:253:VAL:HB	2:E:286:PHE:HB3	1.70	0.72
2:B:269:ALA:O	2:B:273:MET:HG3	1.88	0.72
1:D:233:ILE:HG22	1:D:234:ALA:N	2.03	0.72
1:A:219:ALA:O	1:A:220:TYR:C	2.26	0.72
1:A:97:GLU:OE1	1:A:97:GLU:CA	2.35	0.72
2:E:79:LYS:CB	2:E:79:LYS:HZ2	1.96	0.72
1:D:218:ALA:O	1:D:220:TYR:N	2.21	0.72
1:D:97:GLU:CB	3:D:289:COA:H71	2.20	0.72
2:E:215:LYS:O	2:E:216:LEU:HD23	1.88	0.72
2:E:262:MET:CE	2:E:301:ALA:HB1	2.20	0.72
1:D:2:ILE:HD11	1:D:193:MET:CG	2.17	0.72
1:D:123:CYS:CB	1:D:124:PRO:CD	2.66	0.72
2:E:252:TYR:O	2:E:253:VAL:HG22	1.89	0.72
2:B:133:ILE:O	2:B:134:GLU:C	2.26	0.71
2:E:79:LYS:O	2:E:93:VAL:HG23	1.89	0.71
2:B:296:GLU:OE1	2:B:296:GLU:N	2.18	0.71
2:B:352:ASN:O	2:B:353:ASN:CB	2.37	0.71
2:B:313:ALA:HA	2:B:343:VAL:HG13	1.71	0.71
2:E:86:THR:OG1	2:E:87:ASP:N	2.15	0.71
1:D:151:SER:HB2	1:D:206:ILE:HB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:ILE:N	2:B:144:ILE:CD1	2.53	0.71
2:B:22:GLY:HA2	2:B:98:VAL:O	1.91	0.71
2:E:45:VAL:HG22	2:E:61:LYS:O	1.90	0.71
1:D:223:GLU:O	1:D:223:GLU:CG	2.37	0.71
1:A:263:ALA:O	1:A:266:GLU:HG3	1.91	0.71
1:A:212:SER:O	1:A:215:GLU:N	2.23	0.71
2:B:142:HIS:CD2	2:B:142:HIS:H	2.08	0.71
1:A:146:LYS:HB2	1:A:201:GLU:HB2	1.72	0.71
1:A:214:GLU:OE1	1:A:261:LYS:HE3	1.90	0.71
1:D:143:LYS:O	1:D:171:GLN:N	2.22	0.71
1:A:136:ILE:H	1:A:136:ILE:HD13	1.56	0.71
2:B:287:LEU:HD23	2:B:287:LEU:C	2.11	0.71
1:D:97:GLU:OE1	1:D:97:GLU:C	2.28	0.71
1:A:150:VAL:HG23	1:A:150:VAL:O	1.88	0.71
2:B:97:LEU:CD2	2:B:98:VAL:H	2.04	0.71
2:E:239:ASP:OD1	2:E:241:ARG:N	2.18	0.71
2:E:150:ASP:OD1	2:E:151:PRO:HD2	1.89	0.71
2:E:364:SER:OG	2:E:366:LEU:HD22	1.91	0.71
2:E:366:LEU:HD22	2:E:366:LEU:N	2.05	0.71
2:B:316:VAL:CG1	2:B:317:ASN:N	2.53	0.70
2:E:287:LEU:O	2:E:287:LEU:CD2	2.39	0.70
2:E:87:ASP:C	2:E:89:ASN:N	2.31	0.70
1:D:97:GLU:HB2	3:D:289:COA:H71	1.72	0.70
2:E:326:ASP:HB3	2:E:356:LEU:HD13	1.72	0.70
1:A:152:ARG:HG3	1:A:177:ILE:HD11	1.73	0.70
2:E:269:ALA:O	2:E:272:THR:HB	1.92	0.70
2:B:325:CYS:HB3	2:B:349:LEU:CD1	2.17	0.70
1:A:182:ILE:N	1:A:183:PRO:HD3	2.05	0.70
1:A:153:SER:HB2	1:A:246:NEP:HE1	1.72	0.70
1:A:142:HIS:HB3	1:A:171:GLN:OE1	1.91	0.70
1:D:204:VAL:HA	1:D:230:VAL:O	1.92	0.70
1:D:285:THR:O	1:D:288:LYS:CG	2.29	0.70
2:B:143:LEU:C	2:B:144:ILE:HD13	2.12	0.70
1:A:218:ALA:O	1:A:219:ALA:C	2.29	0.70
2:E:140:THR:N	2:E:141:PRO:HD3	2.05	0.70
1:D:129:PRO:C	1:D:131:GLU:H	1.93	0.70
2:E:89:ASN:O	2:E:90:GLY:O	2.10	0.70
2:B:204:THR:O	2:B:207:GLY:N	2.25	0.70
1:D:123:CYS:CB	1:D:124:PRO:HD2	2.20	0.70
2:E:75:ASN:O	2:E:79:LYS:HD3	1.91	0.70
1:A:106:THR:O	1:A:106:THR:CG2	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:258:ASN:H	2:E:258:ASN:HD22	1.40	0.70
1:D:119:ILE:HD11	1:D:185:SER:OG	1.91	0.70
1:D:127:ILE:HG13	1:D:133:LYS:CB	2.21	0.69
1:D:218:ALA:O	1:D:219:ALA:C	2.29	0.69
1:A:229:VAL:O	1:A:229:VAL:HG22	1.89	0.69
2:B:377:ALA:O	2:B:381:VAL:HG23	1.91	0.69
1:D:128:THR:HG23	1:D:131:GLU:HB2	1.73	0.69
1:A:127:ILE:HG13	1:A:132:CYS:O	1.92	0.69
2:E:337:ALA:O	2:E:338:GLU:C	2.27	0.69
1:D:119:ILE:HD13	1:D:185:SER:OG	1.89	0.69
1:A:221:ILE:HA	1:A:225:VAL:CG1	2.22	0.69
1:D:154:GLY:O	1:D:157:THR:HB	1.92	0.69
1:D:188:ILE:O	1:D:189:ASP:C	2.25	0.69
2:B:140:THR:HB	2:B:143:LEU:HD12	1.74	0.69
2:E:282:GLU:O	2:E:282:GLU:HG3	1.91	0.69
2:B:26:THR:HG22	2:B:27:THR:HG23	1.74	0.69
2:E:278:LEU:O	2:E:278:LEU:HG	1.92	0.69
1:A:147:VAL:HG12	1:A:148:GLY:N	2.08	0.69
1:A:116:VAL:HG12	1:A:117:ARG:N	2.08	0.69
2:E:277:LYS:CD	2:E:278:LEU:N	2.48	0.69
2:B:298:VAL:O	2:B:298:VAL:HG12	1.93	0.69
1:D:128:THR:CG2	1:D:131:GLU:HB2	2.23	0.69
2:B:352:ASN:O	2:B:353:ASN:HB2	1.92	0.69
2:B:180:ILE:CG2	2:B:184:LEU:HD11	2.23	0.69
2:E:5:GLU:OE2	2:E:46:LYS:NZ	2.20	0.69
2:E:63:VAL:CG1	2:E:64:ASN:N	2.55	0.68
2:B:140:THR:N	2:B:141:PRO:CD	2.40	0.68
2:E:109:TYR:CD1	2:E:109:TYR:C	2.66	0.68
1:D:53:PHE:CD1	1:D:59:ALA:HB2	2.28	0.68
1:D:197:ASP:O	1:D:227:LYS:NZ	2.26	0.68
2:E:62:VAL:CG1	2:E:63:VAL:N	2.43	0.68
2:E:246:ALA:O	2:E:249:GLU:N	2.18	0.68
2:B:180:ILE:HG23	2:B:184:LEU:HD11	1.75	0.68
1:D:160:ALA:O	1:D:161:VAL:C	2.25	0.68
2:E:128:GLU:CA	2:E:128:GLU:OE1	2.41	0.68
1:D:27:ALA:HB1	1:D:32:THR:HB	1.75	0.68
1:A:97:GLU:HB3	3:A:289:COA:C7P	2.24	0.68
2:E:272:THR:O	2:E:273:MET:C	2.28	0.68
1:D:73:PRO:C	1:D:75:PRO:HD2	2.14	0.68
2:B:276:VAL:CG1	2:B:281:GLY:HA3	2.24	0.68
2:E:202:VAL:CG1	2:E:203:ILE:N	2.51	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ILE:O	1:D:4:ILE:N	2.26	0.68
1:D:3:LEU:HD23	1:D:193:MET:CE	2.23	0.68
1:D:5:ASP:OD1	1:D:7:ASN:N	2.23	0.68
2:E:76:TRP:HA	2:E:79:LYS:HG3	1.74	0.68
2:E:324:ARG:HB3	2:E:327:LEU:HD12	1.74	0.68
1:D:55:THR:HG22	1:D:57:ARG:N	2.08	0.68
1:D:250:ILE:HG12	1:D:251:ILE:N	2.06	0.68
2:E:383:ALA:O	2:E:385:VAL:N	2.26	0.68
1:D:221:ILE:CG1	1:D:225:VAL:CG1	2.72	0.68
2:B:278:LEU:O	2:B:278:LEU:HD12	1.94	0.68
2:B:103:ASP:O	2:B:204:THR:HA	1.93	0.68
1:D:128:THR:CA	1:D:173:THR:HG23	2.23	0.67
1:A:22:PHE:O	1:A:25:GLU:HB2	1.94	0.67
1:A:55:THR:HG22	1:A:57:ARG:H	1.59	0.67
1:A:199:GLN:HG3	1:A:199:GLN:O	1.93	0.67
2:E:364:SER:OG	2:E:366:LEU:CD2	2.42	0.67
2:E:50:HIS:CD2	2:E:237:GLN:HG3	2.29	0.67
2:E:27:THR:OG1	2:E:30:GLU:HG3	1.94	0.67
1:D:146:LYS:HB2	1:D:201:GLU:HB2	1.75	0.67
2:E:83:THR:N	2:E:86:THR:HG23	2.06	0.67
1:A:116:VAL:CG1	1:A:117:ARG:N	2.56	0.67
2:E:292:GLY:O	2:E:294:THR:N	2.27	0.67
1:D:2:ILE:HD11	1:D:193:MET:HB2	0.68	0.67
1:A:285:THR:O	1:A:287:LEU:N	2.28	0.67
1:D:286:VAL:HG13	1:D:287:LEU:N	2.08	0.67
2:B:324:ARG:O	2:B:327:LEU:HB2	1.94	0.67
2:E:34:ALA:HA	2:E:37:LYS:HG3	1.74	0.67
1:A:217:ALA:O	1:A:218:ALA:C	2.31	0.67
2:E:339:VAL:HG12	2:E:340:GLY:N	2.10	0.67
2:B:157:PRO:HG3	2:B:182:MET:HE2	1.76	0.67
2:B:2:ASN:C	2:B:3:LEU:HD23	2.14	0.67
1:D:147:VAL:O	1:D:172:SER:N	2.26	0.67
1:A:190:ILE:O	1:A:191:LEU:C	2.32	0.67
2:B:318:ILE:CG2	2:B:319:PHE:N	2.58	0.67
2:E:263:VAL:HG12	2:E:264:ASN:N	2.08	0.67
2:E:258:ASN:ND2	2:E:258:ASN:H	1.93	0.67
1:D:222:LYS:HB2	1:D:268:ALA:CB	2.25	0.66
1:A:229:VAL:HG13	1:A:270:VAL:HG13	1.77	0.66
2:B:63:VAL:HG13	2:B:68:ASP:CB	2.24	0.66
2:E:197:GLU:O	2:E:215:LYS:HE3	1.94	0.66
1:D:205:MET:HE1	1:D:217:ALA:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LEU:HD22	2:B:82:VAL:N	2.09	0.66
1:D:217:ALA:O	1:D:218:ALA:O	2.14	0.66
2:B:45:VAL:HG23	2:B:72:PHE:CE2	2.30	0.66
1:A:129:PRO:HD2	1:A:172:SER:O	1.95	0.66
2:E:152:LEU:CD2	2:E:152:LEU:O	2.43	0.66
2:E:323:VAL:O	2:E:324:ARG:HB2	1.96	0.66
1:A:9:LYS:HB3	1:A:35:VAL:CG1	2.23	0.66
1:D:251:ILE:HG22	1:D:251:ILE:O	1.95	0.66
2:B:68:ASP:O	2:B:71:ALA:HB3	1.95	0.66
1:A:167:TYR:CB	1:A:169:PHE:CE2	2.78	0.66
2:E:312:LYS:HZ2	2:E:388:LYS:HE3	1.61	0.66
1:D:2:ILE:HG23	1:D:3:LEU:HG	1.77	0.66
1:D:163:GLN:OE1	1:D:277:ALA:O	2.13	0.66
2:B:341:VAL:HG12	2:B:343:VAL:H	1.60	0.66
2:E:318:ILE:HG22	2:E:318:ILE:O	1.96	0.66
2:E:330:ASP:OD1	2:E:360:LYS:HE2	1.95	0.66
2:E:235:GLN:O	2:E:238:GLU:HG2	1.95	0.66
2:E:87:ASP:O	2:E:87:ASP:OD1	2.14	0.66
2:E:157:PRO:CD	2:E:182:MET:HE1	2.26	0.66
2:E:246:ALA:C	2:E:248:TRP:H	1.99	0.65
2:B:184:LEU:HA	2:B:187:ILE:HG13	1.77	0.65
2:B:84:TYR:CE1	2:B:85:GLN:HG3	2.30	0.65
1:D:275:SER:OG	1:D:277:ALA:HB3	1.97	0.65
1:A:216:GLU:O	1:A:219:ALA:HB3	1.96	0.65
2:E:368:ILE:C	2:E:369:ILE:CD1	2.51	0.65
2:B:258:ASN:HD21	2:B:282:GLU:CB	2.08	0.65
1:A:46:THR:HA	1:A:50:LEU:O	1.97	0.65
2:B:372:LYS:N	2:B:376:ASP:OD2	2.28	0.65
1:D:220:TYR:CD2	1:D:221:ILE:N	2.64	0.65
1:D:23:HIS:CE1	1:D:136:ILE:CG2	2.76	0.65
2:E:60:VAL:HG12	2:E:61:LYS:N	2.11	0.65
2:E:295:LYS:HB3	2:E:296:GLU:OE1	1.97	0.65
2:E:27:THR:O	2:E:30:GLU:HB2	1.97	0.65
1:A:283:LEU:O	1:A:287:LEU:N	2.27	0.65
2:E:70:ARG:O	2:E:70:ARG:CG	2.45	0.65
2:E:258:ASN:ND2	2:E:258:ASN:N	2.42	0.65
2:E:312:LYS:NZ	2:E:388:LYS:HZ1	1.92	0.65
1:D:128:THR:CG2	1:D:131:GLU:CB	2.73	0.65
2:E:103:ASP:HB3	2:E:205:LYS:HD2	1.79	0.65
1:A:104:MET:HE2	1:A:104:MET:O	1.97	0.65
2:E:255:LEU:O	2:E:256:ASP:CB	2.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:258:ASN:HD22	2:E:258:ASN:C	1.97	0.65
2:E:312:LYS:HZ1	2:E:388:LYS:NZ	1.95	0.64
2:B:21:VAL:O	2:B:99:GLU:HB2	1.97	0.64
2:E:258:ASN:N	2:E:258:ASN:HD22	1.93	0.64
2:E:374:LEU:C	2:E:374:LEU:HD12	2.18	0.64
1:D:55:THR:O	1:D:56:VAL:C	2.34	0.64
1:A:212:SER:O	1:A:215:GLU:OE1	2.15	0.64
2:E:263:VAL:HG11	2:E:268:LEU:HB3	1.79	0.64
2:B:188:PHE:HA	2:B:193:LEU:HD12	1.80	0.64
2:B:42:PRO:HA	2:B:64:ASN:ND2	2.12	0.64
2:E:257:GLY:HA3	2:E:282:GLU:HG3	1.80	0.64
2:B:239:ASP:OD1	2:B:239:ASP:C	2.36	0.64
2:E:41:GLY:CA	2:E:42:PRO:C	2.66	0.64
1:A:158:TYR:CD1	1:A:158:TYR:N	2.62	0.64
2:B:140:THR:O	2:B:142:HIS:N	2.30	0.64
2:B:165:PHE:O	2:B:167:LEU:N	2.31	0.64
2:E:199:ASN:HB3	2:E:215:LYS:HZ2	1.63	0.64
2:E:72:PHE:CE1	2:E:76:TRP:NE1	2.66	0.64
2:B:165:PHE:O	2:B:166:LYS:C	2.35	0.64
2:E:157:PRO:CD	2:E:182:MET:CE	2.74	0.64
2:E:326:ASP:C	2:E:328:ILE:N	2.49	0.64
1:A:104:MET:HE1	1:A:107:VAL:CB	2.28	0.64
2:B:143:LEU:C	2:B:144:ILE:CD1	2.67	0.64
1:D:127:ILE:HG13	1:D:133:LYS:HB3	1.80	0.63
2:B:296:GLU:H	2:B:296:GLU:CD	2.00	0.63
2:B:371:ALA:CB	2:B:377:ALA:HB2	2.27	0.63
2:E:248:TRP:O	2:E:249:GLU:HB2	1.97	0.63
1:D:153:SER:HB2	1:D:246:NEP:HE1	1.78	0.63
2:E:337:ALA:O	2:E:340:GLY:N	2.31	0.63
2:E:325:CYS:HB2	2:E:354:ALA:HA	1.79	0.63
1:A:94:THR:OG1	1:A:121:PRO:HB3	1.98	0.63
1:A:23:HIS:CE1	1:A:136:ILE:CG2	2.80	0.63
2:E:263:VAL:CG1	2:E:264:ASN:N	2.61	0.63
2:B:3:LEU:HD23	2:B:3:LEU:N	2.14	0.63
2:B:12:PHE:HB3	2:B:17:LEU:HB2	1.80	0.63
1:D:167:TYR:OH	1:D:281:GLU:HG2	1.97	0.63
2:E:249:GLU:O	2:E:290:GLY:HA3	1.99	0.63
1:D:159:GLU:O	1:D:160:ALA:C	2.30	0.63
2:B:97:LEU:CD2	2:B:98:VAL:N	2.56	0.63
2:B:150:ASP:OD1	2:B:151:PRO:N	2.31	0.63
2:E:17:LEU:N	2:E:17:LEU:HD23	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:PRO:HD2	2:B:142:HIS:CD2	2.32	0.63
1:D:10:VAL:CB	1:D:34:MET:HE3	2.27	0.63
2:B:48:GLN:NE2	2:B:48:GLN:HA	2.14	0.63
1:D:237:THR:HG21	2:E:274:ASP:OD1	1.90	0.63
2:E:128:GLU:HA	2:E:128:GLU:OE1	1.99	0.63
2:B:196:ILE:HG22	2:B:197:GLU:N	2.12	0.63
1:A:128:THR:HG21	1:A:131:GLU:HB2	1.78	0.63
2:E:45:VAL:CG2	2:E:61:LYS:O	2.45	0.63
2:B:292:GLY:O	2:B:294:THR:N	2.31	0.63
1:D:22:PHE:O	1:D:24:SER:N	2.32	0.63
1:A:244:MET:HE1	2:B:253:VAL:HG21	1.81	0.63
1:A:124:PRO:HA	1:A:136:ILE:HD13	1.80	0.62
2:B:69:ILE:O	2:B:70:ARG:C	2.35	0.62
2:B:109:TYR:CD1	2:B:110:LEU:N	2.66	0.62
2:E:258:ASN:HD22	2:E:259:ILE:N	1.96	0.62
1:A:123:CYS:HB3	1:A:178:GLY:CA	2.29	0.62
1:A:72:VAL:HG13	1:A:73:PRO:CD	2.27	0.62
2:E:246:ALA:C	2:E:248:TRP:N	2.52	0.62
2:E:252:TYR:C	2:E:253:VAL:CG2	2.56	0.62
1:A:253:GLY:O	1:A:255:LYS:N	2.32	0.62
1:A:158:TYR:HD1	1:A:158:TYR:N	1.96	0.62
1:A:195:GLU:O	1:A:227:LYS:HE3	1.98	0.62
2:E:369:ILE:HD13	2:E:369:ILE:H	1.61	0.62
2:E:156:MET:HB3	2:E:157:PRO:HD2	1.80	0.62
2:B:7:GLN:NE2	2:B:232:MET:HG2	2.13	0.62
1:D:57:ARG:O	1:D:58:GLU:C	2.32	0.62
1:D:30:TYR:OH	1:D:129:PRO:HA	1.99	0.62
1:A:124:PRO:O	1:A:135:GLY:CA	2.44	0.62
2:E:385:VAL:HG12	2:E:386:GLU:N	2.13	0.62
1:A:133:LYS:NZ	1:A:137:GLN:O	2.21	0.62
1:A:6:LYS:N	1:A:131:GLU:OE1	2.30	0.62
1:D:194:PHE:HB3	1:D:203:ILE:HD11	1.80	0.62
1:A:173:THR:HG22	1:A:174:CYS:N	2.14	0.62
2:E:152:LEU:HD22	2:E:152:LEU:C	2.20	0.62
1:A:104:MET:HA	1:A:104:MET:HE3	0.64	0.62
1:A:25:GLU:O	1:A:28:ILE:HB	1.99	0.62
1:D:156:LEU:O	1:D:157:THR:C	2.37	0.62
1:D:92:ILE:HG22	1:D:118:MET:CG	2.10	0.62
2:B:4:HIS:HB2	2:B:7:GLN:HG3	1.81	0.62
1:D:128:THR:O	1:D:128:THR:HG22	1.99	0.62
1:D:191:LEU:O	1:D:192:GLU:C	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ALA:O	1:D:265:LEU:N	2.32	0.62
2:E:109:TYR:CE2	2:E:197:GLU:OE1	2.52	0.62
1:D:127:ILE:C	1:D:173:THR:CG2	2.69	0.62
1:D:286:VAL:CG1	1:D:287:LEU:N	2.63	0.62
2:B:110:LEU:CD2	2:B:111:GLY:N	2.61	0.62
2:B:186:THR:HG23	2:B:190:GLU:HG3	1.82	0.62
1:A:248:GLY:O	2:B:116:ARG:NH2	2.33	0.62
1:D:217:ALA:O	1:D:221:ILE:HD12	1.99	0.61
1:D:23:HIS:CD2	1:D:136:ILE:HG22	2.35	0.61
1:A:221:ILE:HG23	1:A:222:LYS:N	2.03	0.61
1:A:26:GLN:O	1:A:27:ALA:C	2.37	0.61
2:E:184:LEU:HA	2:E:187:ILE:HG13	1.81	0.61
2:E:109:TYR:HE2	2:E:197:GLU:OE1	1.83	0.61
1:D:195:GLU:HA	1:D:227:LYS:HE3	1.81	0.61
2:B:380:GLN:C	2:B:383:ALA:HB3	2.19	0.61
2:E:72:PHE:CD1	2:E:76:TRP:CD1	2.89	0.61
2:E:126:SER:OG	2:E:128:GLU:N	2.28	0.61
2:B:83:THR:H	2:B:86:THR:HB	1.66	0.61
1:A:146:LYS:NZ	1:A:201:GLU:OE2	2.28	0.61
1:D:7:ASN:HA	1:D:33:LYS:HZ2	1.63	0.61
2:B:94:ASN:C	2:B:95:GLN:HG2	2.19	0.61
2:E:38:ILE:HG21	2:E:43:TRP:HD1	1.64	0.61
2:B:319:PHE:O	2:B:320:GLY:O	2.18	0.61
1:D:2:ILE:CG1	1:D:193:MET:HE2	2.31	0.61
1:A:124:PRO:HA	1:A:136:ILE:CD1	2.31	0.61
2:B:82:VAL:HG23	2:B:90:GLY:HA3	1.83	0.61
1:A:55:THR:HG22	1:A:57:ARG:N	2.15	0.61
2:E:343:VAL:HG13	2:E:344:PRO:CG	2.24	0.61
2:E:82:VAL:CG2	2:E:90:GLY:N	2.38	0.61
1:A:80:SER:O	1:A:83:GLU:HB3	2.00	0.61
1:A:97:GLU:HB3	3:A:289:COA:H71	1.83	0.61
1:D:77:CYS:HB3	1:D:99:ILE:HD11	1.83	0.61
2:B:186:THR:CG2	2:B:190:GLU:HG3	2.31	0.61
1:D:189:ASP:C	1:D:190:ILE:HD13	2.21	0.60
2:B:140:THR:HG1	2:B:143:LEU:HD12	1.64	0.60
1:A:172:SER:HB3	1:A:199:GLN:HG2	1.82	0.60
2:B:239:ASP:OD2	2:B:241:ARG:NH2	2.32	0.60
2:E:152:LEU:CD2	2:E:152:LEU:C	2.69	0.60
1:A:112:ASP:O	1:A:113:GLU:C	2.34	0.60
1:D:10:VAL:CB	1:D:34:MET:CE	2.80	0.60
1:A:127:ILE:O	1:A:127:ILE:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:O	1:A:141:ILE:HG22	1.99	0.60
1:D:275:SER:O	1:D:276:LEU:C	2.38	0.60
1:D:89:ILE:HG22	1:D:91:LEU:H	1.65	0.60
1:A:203:ILE:HG22	1:A:204:VAL:N	2.15	0.60
1:D:189:ASP:HB2	1:D:190:ILE:HD13	1.84	0.60
2:B:315:LEU:HD13	2:B:346:VAL:HB	1.84	0.60
1:A:21:THR:O	1:A:22:PHE:C	2.39	0.60
2:E:325:CYS:O	2:E:328:ILE:HB	2.02	0.60
1:D:250:ILE:CG1	1:D:251:ILE:N	2.63	0.60
1:D:127:ILE:HB	1:D:133:LYS:HB2	1.84	0.60
2:B:263:VAL:CG1	2:B:268:LEU:HB3	2.29	0.60
2:B:82:VAL:HG22	2:B:86:THR:CG2	2.28	0.60
2:B:343:VAL:HG22	2:B:344:PRO:HD2	1.83	0.60
1:D:228:PRO:HB2	1:D:286:VAL:CG2	2.32	0.60
1:D:252:ALA:O	1:D:253:GLY:O	2.20	0.60
2:B:316:VAL:HG12	2:B:317:ASN:N	2.13	0.60
2:E:67:GLU:H	2:E:67:GLU:CD	2.04	0.60
2:B:156:MET:HB3	2:B:157:PRO:HD2	1.82	0.60
2:B:181:PHE:O	2:B:182:MET:C	2.37	0.60
1:A:262:PHE:O	1:A:266:GLU:HG3	2.02	0.60
1:A:267:ALA:C	1:A:269:GLY:H	2.02	0.60
2:E:72:PHE:O	2:E:75:ASN:HB3	2.02	0.60
2:E:332:ILE:O	2:E:336:VAL:HG23	2.02	0.60
2:E:323:VAL:HG12	2:E:324:ARG:N	2.16	0.60
1:A:246:NEP:CD2	2:B:266:ALA:HB3	2.32	0.60
1:A:218:ALA:O	1:A:219:ALA:O	2.20	0.60
1:A:74:ALA:N	1:A:75:PRO:HD2	2.17	0.60
1:D:187:PHE:HE2	1:D:214:GLU:CG	2.04	0.60
1:A:148:GLY:C	1:A:149:ILE:HG12	2.22	0.60
2:B:202:VAL:HG13	2:B:203:ILE:N	2.17	0.60
2:B:140:THR:OG1	2:B:143:LEU:CD1	2.33	0.59
1:D:10:VAL:C	1:D:11:ILE:HG22	1.99	0.59
1:D:153:SER:HB3	4:D:309:HOH:O	2.01	0.59
2:E:312:LYS:HZ3	2:E:388:LYS:NZ	1.93	0.59
2:E:315:LEU:C	2:E:315:LEU:CD1	2.58	0.59
1:D:117:ARG:HG3	1:D:118:MET:N	2.15	0.59
1:A:35:VAL:CG2	1:A:65:ALA:HB2	2.33	0.59
2:E:49:VAL:CG2	2:E:91:GLN:CB	2.76	0.59
1:D:149:ILE:HD11	1:D:171:GLN:HG2	1.83	0.59
1:D:195:GLU:OE1	1:D:226:THR:N	2.35	0.59
1:A:218:ALA:O	1:A:221:ILE:HB	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:LEU:HD12	2:B:346:VAL:O	2.02	0.59
2:E:257:GLY:CA	2:E:282:GLU:HG3	2.32	0.59
2:E:63:VAL:HG11	2:E:68:ASP:CB	2.32	0.59
2:E:87:ASP:CG	2:E:87:ASP:O	2.41	0.59
2:E:158:TYR:CD1	2:E:158:TYR:C	2.76	0.59
1:D:116:VAL:CG1	1:D:117:ARG:H	2.05	0.59
2:B:333:ILE:HG22	2:B:334:GLY:N	2.08	0.59
2:B:275:ILE:HG23	2:B:276:VAL:N	2.15	0.59
1:A:86:ASP:O	1:A:86:ASP:OD1	2.21	0.59
1:A:39:THR:CG2	1:A:42:LYS:HG3	2.31	0.59
2:B:135:LYS:O	2:B:138:GLU:N	2.35	0.59
2:B:109:TYR:O	2:B:109:TYR:CD1	2.51	0.59
1:A:104:MET:C	1:A:104:MET:HE2	2.23	0.59
1:A:74:ALA:HB1	1:A:98:GLY:O	2.03	0.59
2:B:278:LEU:C	2:B:278:LEU:HD12	2.21	0.59
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.68	0.59
2:E:248:TRP:O	2:E:249:GLU:CB	2.50	0.59
1:A:35:VAL:HG21	1:A:65:ALA:HB2	1.84	0.59
1:A:97:GLU:HB3	3:A:289:COA:H72	1.84	0.58
2:B:141:PRO:HD2	2:B:142:HIS:H	1.66	0.58
2:E:106:LYS:HB3	2:E:203:ILE:HD12	1.84	0.58
2:E:348:ARG:NH1	2:E:374:LEU:H	2.01	0.58
1:D:128:THR:HA	1:D:173:THR:HG23	1.85	0.58
1:A:156:LEU:O	1:A:159:GLU:N	2.36	0.58
1:D:273:VAL:HG13	1:D:275:SER:H	1.68	0.58
2:E:371:ALA:CB	2:E:377:ALA:HA	2.34	0.58
1:D:50:LEU:HB3	1:D:51:PRO:HD2	1.84	0.58
1:A:21:THR:OG1	1:A:47:HIS:NE2	2.37	0.58
2:E:329:ALA:O	2:E:333:ILE:HD12	2.03	0.58
2:B:165:PHE:O	2:B:168:GLY:N	2.35	0.58
1:D:124:PRO:HG2	1:D:176:GLY:HA3	1.84	0.58
1:D:20:GLY:O	1:D:21:THR:C	2.41	0.58
2:E:157:PRO:CG	2:E:182:MET:CE	2.82	0.58
2:B:276:VAL:HG13	2:B:281:GLY:HA3	1.86	0.58
1:A:244:MET:CE	2:B:253:VAL:HG21	2.33	0.58
2:E:94:ASN:HB2	4:E:403:HOH:O	2.03	0.58
1:A:155:THR:O	1:A:156:LEU:C	2.40	0.58
2:E:335:ALA:O	2:E:336:VAL:C	2.40	0.58
2:B:275:ILE:CG2	2:B:276:VAL:N	2.66	0.58
1:D:180:ASP:CB	1:D:181:PRO:CD	2.80	0.58
1:D:218:ALA:O	1:D:221:ILE:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:CYS:N	3:A:289:COA:S1P	2.77	0.58
2:B:70:ARG:NH2	2:E:249:GLU:OE2	2.37	0.58
1:D:151:SER:CB	1:D:206:ILE:HB	2.33	0.58
1:A:105:LEU:HD23	1:A:106:THR:N	2.18	0.58
2:B:158:TYR:CE1	2:B:159:GLN:HG2	2.38	0.58
2:B:381:VAL:O	2:B:382:VAL:C	2.40	0.58
1:A:56:VAL:O	1:A:57:ARG:C	2.41	0.58
2:E:176:GLN:HE22	2:E:209:LEU:H	1.51	0.58
2:E:313:ALA:HA	2:E:343:VAL:HG11	1.86	0.58
1:A:229:VAL:CG2	1:A:230:VAL:N	2.56	0.58
2:E:195:LEU:HD23	2:E:195:LEU:C	2.24	0.58
1:D:7:ASN:HA	1:D:33:LYS:HZ1	1.67	0.58
2:B:362:ALA:O	2:B:364:SER:N	2.36	0.58
1:A:19:GLN:OE1	1:A:19:GLN:HA	2.02	0.58
2:B:263:VAL:CG1	2:B:264:ASN:N	2.66	0.58
1:D:280:GLY:O	1:D:281:GLU:C	2.42	0.58
2:E:157:PRO:HA	2:E:182:MET:HE2	1.84	0.58
2:E:294:THR:O	2:E:295:LYS:C	2.43	0.58
2:E:150:ASP:OD1	2:E:151:PRO:CD	2.51	0.58
1:D:267:ALA:C	1:D:269:GLY:H	2.07	0.57
2:B:319:PHE:C	2:B:319:PHE:CD1	2.78	0.57
1:D:55:THR:HB	1:D:58:GLU:H	1.69	0.57
2:B:373:GLY:O	2:B:376:ASP:HB3	2.04	0.57
2:B:13:ALA:O	2:B:14:ARG:C	2.40	0.57
2:B:263:VAL:HG12	2:B:264:ASN:N	2.19	0.57
1:A:155:THR:HG21	2:B:264:ASN:O	2.04	0.57
2:B:4:HIS:HD2	4:B:404:HOH:O	1.87	0.57
2:E:118:SER:C	2:E:119:ARG:HG3	2.24	0.57
1:A:262:PHE:O	1:A:263:ALA:C	2.43	0.57
2:B:115:ASP:OD2	2:B:118:SER:OG	2.22	0.57
2:E:176:GLN:HE21	2:E:209:LEU:HB2	1.68	0.57
1:D:26:GLN:O	1:D:27:ALA:C	2.43	0.57
2:B:252:TYR:HE2	2:B:254:ALA:HB2	1.69	0.57
2:E:364:SER:OG	2:E:365:GLY:N	2.33	0.57
2:B:13:ALA:O	2:B:15:TYR:N	2.38	0.57
1:D:203:ILE:C	1:D:229:VAL:HG23	2.20	0.57
1:D:221:ILE:CA	1:D:225:VAL:HG13	2.30	0.57
1:A:265:LEU:HB3	1:A:270:VAL:HB	1.86	0.57
2:B:152:LEU:O	2:B:152:LEU:CD2	2.52	0.57
2:E:94:ASN:C	2:E:95:GLN:HG2	2.23	0.57
1:D:202:ALA:C	1:D:203:ILE:HG13	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:MET:CE	1:D:34:MET:HA	2.34	0.57
2:E:364:SER:CB	2:E:366:LEU:CD2	2.83	0.57
2:E:140:THR:HG23	2:E:140:THR:O	2.02	0.57
2:B:277:LYS:HA	2:B:281:GLY:O	2.05	0.57
1:D:56:VAL:CG1	1:D:87:ALA:HB3	2.34	0.57
2:E:140:THR:N	2:E:141:PRO:CD	2.61	0.57
1:D:22:PHE:O	1:D:23:HIS:C	2.39	0.57
2:E:356:LEU:CD2	2:E:357:GLY:N	2.56	0.57
2:B:84:TYR:CE1	2:B:85:GLN:CG	2.88	0.57
1:D:203:ILE:HB	1:D:229:VAL:HG21	1.82	0.57
1:A:237:THR:HG23	2:B:274:ASP:OD1	2.03	0.57
2:E:32:GLU:OE1	2:E:70:ARG:NH1	2.38	0.57
2:E:264:ASN:HB2	2:E:318:ILE:HG13	1.86	0.57
1:D:22:PHE:C	1:D:24:SER:N	2.55	0.57
1:D:73:PRO:HA	3:D:289:COA:H143	1.87	0.57
1:A:149:ILE:HG23	1:A:204:VAL:CB	2.33	0.57
2:B:239:ASP:OD1	2:B:241:ARG:N	2.38	0.57
1:D:128:THR:HG22	1:D:131:GLU:CB	2.34	0.57
1:D:89:ILE:HG22	1:D:91:LEU:N	2.20	0.57
1:A:145:GLY:HA3	1:A:170:GLY:HA3	1.87	0.57
1:D:267:ALA:C	1:D:269:GLY:N	2.58	0.56
1:A:57:ARG:NH1	1:A:86:ASP:O	2.37	0.56
1:A:92:ILE:O	1:A:118:MET:HA	2.04	0.56
2:E:379:GLN:O	2:E:382:VAL:N	2.38	0.56
2:B:43:TRP:CE3	2:B:43:TRP:N	2.73	0.56
2:E:339:VAL:HG12	2:E:341:VAL:H	1.70	0.56
1:A:55:THR:HG22	1:A:56:VAL:N	2.20	0.56
1:A:159:GLU:O	1:A:160:ALA:C	2.43	0.56
1:A:159:GLU:OE2	2:B:319:PHE:HD2	1.87	0.56
2:B:250:LEU:CD2	2:B:289:VAL:HA	2.36	0.56
2:E:271:GLY:O	2:E:272:THR:C	2.41	0.56
1:D:158:TYR:HB3	2:E:319:PHE:CE1	2.40	0.56
2:E:281:GLY:H	2:E:382:VAL:HG21	1.70	0.56
2:E:132:GLU:OE1	2:E:134:GLU:HG3	2.04	0.56
2:E:57:ALA:HB2	2:E:83:THR:HG22	1.87	0.56
2:B:368:ILE:HG22	2:B:369:ILE:N	2.20	0.56
2:E:324:ARG:HG2	2:E:326:ASP:OD2	2.04	0.56
2:E:364:SER:HB2	2:E:366:LEU:CD2	2.35	0.56
2:E:20:PRO:HD3	2:E:210:ILE:HD11	1.88	0.56
1:A:6:LYS:HB2	1:A:131:GLU:OE1	2.06	0.56
2:B:348:ARG:HD3	2:B:348:ARG:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:ASP:O	2:E:71:ALA:HB3	2.06	0.56
2:E:127:THR:O	2:E:129:GLY:N	2.37	0.56
2:E:80:ARG:HD3	2:E:89:ASN:HD21	1.71	0.56
1:D:5:ASP:OD1	1:D:7:ASN:HB2	2.04	0.56
1:A:203:ILE:CG2	1:A:204:VAL:N	2.69	0.56
2:E:219:ASP:O	2:E:220:GLY:C	2.42	0.56
2:E:45:VAL:HB	2:E:72:PHE:CD2	2.39	0.56
2:E:79:LYS:CB	2:E:79:LYS:HZ3	2.12	0.56
2:B:152:LEU:O	2:B:152:LEU:HD23	2.05	0.56
1:D:186:ASN:ND2	1:D:186:ASN:H	2.01	0.56
1:D:89:ILE:HG22	1:D:90:LYS:N	2.19	0.56
2:B:257:GLY:O	2:B:284:ALA:CB	2.53	0.56
2:E:313:ALA:HA	2:E:343:VAL:CG1	2.36	0.56
1:A:161:VAL:HG12	1:A:162:LYS:N	2.19	0.56
2:B:386:GLU:O	2:B:388:LYS:NZ	2.39	0.56
1:D:10:VAL:O	1:D:35:VAL:HG23	2.06	0.56
2:E:45:VAL:HG23	2:E:45:VAL:O	2.05	0.56
1:D:129:PRO:C	1:D:131:GLU:N	2.59	0.56
1:A:195:GLU:CD	1:A:226:THR:H	2.09	0.56
2:E:258:ASN:ND2	2:E:258:ASN:C	2.58	0.56
1:D:140:HIS:ND1	1:D:140:HIS:N	2.53	0.56
1:D:2:ILE:CD1	1:D:193:MET:HE2	2.36	0.56
1:D:34:MET:HE3	1:D:34:MET:HA	1.88	0.56
1:D:123:CYS:CA	3:D:289:COA:S1P	2.94	0.56
2:E:156:MET:HB3	2:E:157:PRO:CD	2.36	0.56
2:E:343:VAL:HG12	2:E:344:PRO:N	2.20	0.55
2:B:82:VAL:HA	2:B:86:THR:HG21	1.88	0.55
1:D:169:PHE:CE2	1:D:283:LEU:CB	2.88	0.55
1:A:153:SER:OG	2:B:267:GLY:HA3	2.05	0.55
2:B:210:ILE:HG23	2:B:210:ILE:O	2.06	0.55
2:B:158:TYR:CD1	2:B:158:TYR:C	2.80	0.55
2:E:278:LEU:HD23	2:E:279:HIS:ND1	2.21	0.55
2:E:107:GLU:O	2:E:108:LEU:HD23	2.05	0.55
2:E:312:LYS:HZ3	2:E:388:LYS:HZ1	1.49	0.55
1:D:208:GLU:OE2	1:D:246:NEP:ND1	2.39	0.55
2:E:332:ILE:O	2:E:335:ALA:HB3	2.07	0.55
2:E:49:VAL:HG12	2:E:54:ARG:HD3	1.89	0.55
1:D:55:THR:HB	1:D:58:GLU:HG3	1.89	0.55
2:E:234:ASP:OD1	2:E:234:ASP:C	2.45	0.55
1:D:287:LEU:HD22	1:D:287:LEU:O	2.05	0.55
1:A:128:THR:HG22	1:A:131:GLU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:SER:O	2:B:68:ASP:HB2	2.07	0.55
2:E:294:THR:O	2:E:297:ARG:N	2.39	0.55
1:D:182:ILE:HB	4:D:302:HOH:O	2.07	0.55
1:D:110:LYS:HZ2	1:D:113:GLU:HG2	1.72	0.55
1:A:190:ILE:O	1:A:193:MET:N	2.39	0.55
2:E:377:ALA:O	2:E:381:VAL:HG23	2.06	0.55
1:D:122:ASN:C	3:D:289:COA:S1P	2.84	0.55
1:D:97:GLU:OE1	1:D:98:GLY:CA	2.53	0.55
2:B:234:ASP:OD2	2:B:237:GLN:HG2	2.06	0.55
2:E:164:ALA:HB1	2:E:169:LEU:HD12	1.87	0.55
1:D:128:THR:CG2	1:D:128:THR:O	2.54	0.55
2:E:271:GLY:O	2:E:274:ASP:N	2.39	0.55
2:E:126:SER:OG	2:E:127:THR:N	2.37	0.55
2:B:86:THR:HG23	2:B:87:ASP:N	2.22	0.55
2:B:324:ARG:CB	2:B:327:LEU:HD12	2.31	0.55
1:A:276:LEU:O	1:A:279:ILE:HG13	2.07	0.55
1:A:48:LEU:N	1:A:48:LEU:HD23	2.21	0.55
1:D:283:LEU:O	1:D:284:LYS:C	2.45	0.54
2:E:66:LYS:O	2:E:69:ILE:HB	2.06	0.54
2:E:133:ILE:HG23	2:E:134:GLU:N	2.21	0.54
2:B:45:VAL:HG22	2:B:45:VAL:O	2.01	0.54
1:A:129:PRO:HB3	1:A:142:HIS:HB2	1.88	0.54
2:E:41:GLY:HA3	2:E:42:PRO:C	2.24	0.54
2:E:346:VAL:HG21	2:E:381:VAL:CG2	2.30	0.54
2:B:165:PHE:C	2:B:167:LEU:N	2.58	0.54
2:B:63:VAL:CG1	2:B:68:ASP:CB	2.74	0.54
2:E:60:VAL:CG1	2:E:61:LYS:N	2.69	0.54
1:D:128:THR:CG2	1:D:131:GLU:HB3	2.36	0.54
1:A:95:ILE:HG13	1:A:123:CYS:O	2.07	0.54
1:A:138:PRO:HG2	1:A:141:ILE:HD11	1.89	0.54
2:B:229:LEU:HA	2:B:232:MET:CE	2.25	0.54
2:E:119:ARG:O	2:E:120:ARG:CD	2.55	0.54
1:D:181:PRO:O	2:E:116:ARG:HD3	2.06	0.54
1:A:110:LYS:HG3	1:A:110:LYS:O	2.07	0.54
1:D:285:THR:HG22	1:D:286:VAL:H	1.68	0.54
1:A:186:ASN:O	1:A:187:PHE:C	2.40	0.54
2:B:152:LEU:C	2:B:152:LEU:CD2	2.75	0.54
1:A:138:PRO:HD2	1:A:158:TYR:CZ	2.43	0.54
1:A:257:THR:OG1	1:A:260:GLU:HG3	2.06	0.54
2:E:352:ASN:HD21	2:E:353:ASN:HB2	1.70	0.54
2:B:356:LEU:CD2	2:B:356:LEU:C	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TYR:HB3	1:A:169:PHE:HE2	1.67	0.54
2:E:97:LEU:C	2:E:97:LEU:CD2	2.76	0.54
1:D:105:LEU:HD23	1:D:106:THR:N	2.15	0.54
1:D:257:THR:OG1	1:D:260:GLU:CB	2.39	0.54
1:D:66:THR:HG22	1:D:90:LYS:HD2	1.90	0.54
2:B:349:LEU:O	2:B:350:GLU:HB2	2.06	0.54
2:E:241:ARG:HB3	2:E:252:TYR:CE2	2.43	0.54
1:A:11:ILE:HD11	1:A:68:SER:HB2	1.89	0.54
1:A:229:VAL:HG23	1:A:230:VAL:N	2.21	0.54
1:D:136:ILE:N	1:D:136:ILE:CD1	2.62	0.54
2:E:176:GLN:NE2	2:E:209:LEU:H	2.05	0.54
2:B:252:TYR:CE2	2:B:254:ALA:HB2	2.41	0.54
2:B:176:GLN:O	2:B:179:LYS:HB3	2.08	0.54
1:D:195:GLU:OE2	1:D:226:THR:HG23	2.07	0.54
1:D:266:GLU:HG2	1:D:272:THR:CG2	2.26	0.54
1:D:287:LEU:O	1:D:287:LEU:CD2	2.55	0.54
1:A:173:THR:CG2	1:A:174:CYS:N	2.70	0.54
2:E:323:VAL:O	2:E:324:ARG:CB	2.53	0.54
2:E:180:ILE:O	2:E:181:PHE:C	2.42	0.54
1:D:283:LEU:HA	1:D:286:VAL:HG12	1.89	0.54
1:D:67:ALA:HB2	1:D:91:LEU:HB3	1.89	0.54
2:E:4:HIS:O	2:E:5:GLU:C	2.43	0.54
1:A:285:THR:C	1:A:287:LEU:N	2.61	0.54
1:A:212:SER:O	1:A:213:ALA:C	2.46	0.54
1:A:214:GLU:O	1:A:217:ALA:N	2.40	0.54
2:B:315:LEU:HD12	2:B:316:VAL:N	2.23	0.54
2:E:32:GLU:OE2	2:E:70:ARG:HD2	2.07	0.54
1:D:95:ILE:HD11	1:D:135:GLY:HA2	1.90	0.54
1:A:41:GLY:N	1:A:54:ASN:OD1	2.39	0.54
1:D:75:PRO:HB3	2:E:224:PHE:CE1	2.43	0.53
2:E:223:LEU:O	2:E:224:PHE:C	2.42	0.53
2:E:326:ASP:CG	2:E:327:LEU:H	2.09	0.53
1:A:11:ILE:HG13	1:A:67:ALA:O	2.08	0.53
2:B:205:LYS:C	2:B:207:GLY:H	2.10	0.53
1:D:186:ASN:HD21	1:D:189:ASP:CG	2.12	0.53
1:D:221:ILE:HG13	1:D:225:VAL:CG1	2.35	0.53
2:E:274:ASP:O	2:E:277:LYS:HG3	2.09	0.53
1:D:102:LEU:HD22	4:E:400:HOH:O	2.07	0.53
1:D:203:ILE:CG2	1:D:204:VAL:N	2.71	0.53
1:D:159:GLU:O	1:D:162:LYS:HB3	2.08	0.53
1:D:191:LEU:HD11	1:D:221:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ILE:O	1:D:222:LYS:C	2.41	0.53
1:D:287:LEU:C	1:D:287:LEU:HD23	2.28	0.53
1:A:160:ALA:O	1:A:161:VAL:C	2.45	0.53
1:A:2:ILE:CG2	1:A:173:THR:HG21	2.38	0.53
2:B:319:PHE:HD1	2:B:319:PHE:C	2.10	0.53
2:E:72:PHE:CD1	2:E:76:TRP:HD1	2.26	0.53
2:B:325:CYS:CB	2:B:349:LEU:HD13	2.23	0.53
2:B:184:LEU:O	2:B:185:ALA:C	2.45	0.53
2:E:373:GLY:O	2:E:376:ASP:HB3	2.09	0.53
3:D:289:COA:C6P	3:D:289:COA:O9P	2.57	0.53
1:D:59:ALA:O	1:D:60:VAL:C	2.44	0.53
1:D:283:LEU:O	1:D:287:LEU:N	2.28	0.53
2:E:346:VAL:HB	2:E:381:VAL:CG2	2.39	0.53
2:E:105:ALA:CB	2:E:203:ILE:O	2.53	0.53
1:A:202:ALA:HB2	1:A:228:PRO:HG2	1.90	0.53
1:D:169:PHE:HE2	1:D:283:LEU:CB	2.21	0.53
1:D:217:ALA:O	1:D:218:ALA:C	2.46	0.53
1:A:97:GLU:HA	1:A:97:GLU:OE1	2.08	0.53
2:E:330:ASP:HA	2:E:333:ILE:CD1	2.39	0.53
2:B:108:LEU:HD22	2:B:127:THR:HA	1.90	0.53
1:D:4:ILE:HG13	1:D:132:CYS:SG	2.48	0.53
2:E:346:VAL:C	2:E:347:VAL:CG2	2.72	0.53
2:E:375:THR:O	2:E:378:ALA:CB	2.43	0.53
2:E:128:GLU:N	2:E:128:GLU:OE1	2.40	0.53
1:A:48:LEU:H	1:A:48:LEU:HD23	1.74	0.53
2:E:131:VAL:HG12	2:E:132:GLU:N	2.24	0.53
1:D:34:MET:O	1:D:35:VAL:HG13	2.08	0.53
1:D:97:GLU:C	1:D:97:GLU:CD	2.68	0.53
2:E:45:VAL:HB	2:E:72:PHE:CE2	2.44	0.53
1:D:139:GLY:C	1:D:141:ILE:H	2.08	0.53
2:E:237:GLN:NE2	2:E:237:GLN:HA	2.24	0.53
2:E:16:GLY:C	2:E:17:LEU:HD23	2.29	0.53
1:D:232:TYR:HD1	1:D:273:VAL:O	1.92	0.52
1:D:105:LEU:CD2	1:D:106:THR:N	2.71	0.52
2:E:199:ASN:HB3	2:E:215:LYS:NZ	2.24	0.52
1:A:258:ALA:O	1:A:261:LYS:HB2	2.08	0.52
2:B:385:VAL:CG1	2:B:386:GLU:N	2.56	0.52
1:D:195:GLU:O	1:D:227:LYS:HE2	2.09	0.52
2:B:383:ALA:O	2:B:386:GLU:OE1	2.27	0.52
2:E:348:ARG:HH11	2:E:374:LEU:HB2	1.73	0.52
2:B:176:GLN:O	2:B:177:PHE:C	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:76:TRP:HA	2:E:79:LYS:CG	2.39	0.52
2:B:323:VAL:CG1	2:B:328:ILE:HG13	2.28	0.52
2:E:259:ILE:O	2:E:283:PRO:HA	2.08	0.52
1:A:273:VAL:HG11	1:A:278:ASP:HB2	1.91	0.52
1:D:13:GLN:N	1:D:69:VAL:O	2.33	0.52
2:B:121:VAL:HG22	2:B:149:LEU:HG	1.91	0.52
2:E:87:ASP:C	2:E:87:ASP:OD1	2.45	0.52
1:D:221:ILE:CB	1:D:225:VAL:CG1	2.86	0.52
3:A:289:COA:O9P	3:A:289:COA:CDP	2.55	0.52
2:E:66:LYS:O	2:E:67:GLU:C	2.48	0.52
1:D:108:LYS:HA	1:D:111:LEU:HD12	1.91	0.52
2:B:258:ASN:HD22	2:B:282:GLU:HB3	1.69	0.52
1:A:199:GLN:CG	1:A:199:GLN:O	2.55	0.52
2:E:38:ILE:HG21	2:E:43:TRP:CD1	2.45	0.52
1:D:12:CYS:O	1:D:15:PHE:HB2	2.09	0.52
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.92	0.52
2:E:276:VAL:HG13	2:E:281:GLY:HA3	1.91	0.52
2:B:144:ILE:HG22	2:B:145:HIS:N	2.25	0.52
2:B:34:ALA:O	2:B:38:ILE:HG13	2.10	0.52
1:A:185:SER:HA	1:A:189:ASP:OD2	2.10	0.52
1:A:192:GLU:O	1:A:196:LYS:HG3	2.09	0.52
2:E:376:ASP:O	2:E:379:GLN:HB2	2.10	0.52
2:B:135:LYS:O	2:B:138:GLU:HB3	2.10	0.52
1:A:35:VAL:CG2	1:A:63:THR:HB	2.40	0.52
2:B:105:ALA:HB3	2:B:203:ILE:CG2	2.39	0.52
1:A:259:ASP:O	1:A:260:GLU:C	2.48	0.52
2:B:248:TRP:O	2:B:249:GLU:C	2.49	0.52
2:B:285:ASN:HD22	2:B:286:PHE:N	2.07	0.52
1:A:145:GLY:HA3	1:A:170:GLY:C	2.29	0.52
1:A:11:ILE:HA	1:A:36:GLY:O	2.09	0.52
1:A:273:VAL:CG1	1:A:275:SER:O	2.58	0.52
1:D:4:ILE:CD1	1:D:126:VAL:HG22	2.40	0.52
1:D:266:GLU:CG	1:D:272:THR:CG2	2.81	0.52
1:D:77:CYS:HB3	1:D:99:ILE:CD1	2.40	0.52
2:E:202:VAL:HG13	2:E:203:ILE:N	2.23	0.52
1:D:15:PHE:CG	1:D:37:GLY:HA3	2.44	0.52
1:D:61:ALA:O	1:D:63:THR:N	2.43	0.52
2:E:346:VAL:C	2:E:347:VAL:HG22	2.29	0.51
2:E:262:MET:CE	2:E:302:PHE:N	2.73	0.51
1:A:123:CYS:HB3	1:A:178:GLY:HA2	1.91	0.51
1:A:195:GLU:O	1:A:227:LYS:CE	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:THR:O	1:D:109:VAL:HB	2.11	0.51
2:B:224:PHE:C	2:B:224:PHE:CD1	2.83	0.51
2:B:51:ALA:O	2:B:54:ARG:HD3	2.10	0.51
2:B:319:PHE:HD1	2:B:320:GLY:N	2.09	0.51
2:B:270:MET:CG	4:B:419:HOH:O	2.42	0.51
1:D:24:SER:O	1:D:25:GLU:C	2.48	0.51
2:B:23:TYR:HD2	2:B:34:ALA:HB1	1.75	0.51
2:B:202:VAL:CG1	2:B:203:ILE:N	2.70	0.51
2:B:205:LYS:C	2:B:207:GLY:N	2.63	0.51
2:B:17:LEU:HB3	2:B:18:PRO:HD2	1.93	0.51
2:B:208:ASP:HB2	4:B:392:HOH:O	2.08	0.51
1:A:163:GLN:O	1:A:166:ASP:N	2.43	0.51
2:E:336:VAL:HA	2:E:341:VAL:CG1	2.41	0.51
1:A:147:VAL:O	1:A:172:SER:N	2.34	0.51
1:A:251:ILE:O	1:A:252:ALA:O	2.28	0.51
1:D:127:ILE:C	1:D:173:THR:HG22	2.30	0.51
2:B:196:ILE:CG2	2:B:197:GLU:N	2.73	0.51
1:D:140:HIS:CD2	1:D:140:HIS:C	2.79	0.51
1:D:110:LYS:NZ	1:D:113:GLU:OE2	2.44	0.51
2:E:192:ASP:HB2	4:E:405:HOH:O	2.10	0.51
1:D:283:LEU:O	1:D:285:THR:N	2.44	0.51
2:E:132:GLU:O	2:E:135:LYS:HB3	2.11	0.51
2:B:6:TYR:HB3	2:B:48:GLN:OE1	2.11	0.51
1:A:128:THR:HG22	1:A:132:CYS:H	1.76	0.51
1:A:159:GLU:OE2	2:B:319:PHE:CD2	2.63	0.51
1:D:10:VAL:O	1:D:35:VAL:CG2	2.59	0.51
2:E:87:ASP:O	2:E:88:ALA:C	2.47	0.51
2:E:199:ASN:CB	2:E:215:LYS:HZ2	2.23	0.51
2:B:13:ALA:C	2:B:15:TYR:N	2.63	0.51
1:A:188:ILE:O	1:A:189:ASP:C	2.49	0.51
2:B:314:VAL:HG12	2:B:315:LEU:N	2.26	0.51
1:A:147:VAL:CG1	1:A:148:GLY:N	2.73	0.51
2:B:195:LEU:HD23	2:B:195:LEU:O	2.11	0.51
1:A:5:ASP:OD1	1:A:5:ASP:C	2.48	0.51
2:B:250:LEU:HD23	2:B:289:VAL:HA	1.92	0.51
1:D:276:LEU:HD12	1:D:276:LEU:C	2.31	0.51
1:D:10:VAL:CA	1:D:34:MET:HE3	2.40	0.51
2:E:224:PHE:CE1	2:E:225:ARG:HG2	2.45	0.51
1:A:33:LYS:HB2	4:A:291:HOH:O	2.11	0.51
1:D:263:ALA:O	1:D:264:ALA:C	2.49	0.51
2:E:139:GLU:O	2:E:139:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:ARG:HH11	1:D:274:ARG:CG	2.22	0.51
2:E:324:ARG:O	2:E:325:CYS:C	2.49	0.51
2:B:329:ALA:O	2:B:333:ILE:HD12	2.11	0.51
2:B:284:ALA:O	2:B:285:ASN:HB3	2.10	0.51
2:E:56:LYS:H	2:E:56:LYS:CD	2.21	0.51
2:E:97:LEU:HD23	2:E:97:LEU:C	2.29	0.51
2:E:9:LYS:O	2:E:10:GLN:C	2.48	0.51
1:A:218:ALA:O	1:A:221:ILE:CB	2.59	0.50
1:D:104:MET:CA	1:D:104:MET:CE	2.89	0.50
2:B:133:ILE:C	2:B:135:LYS:N	2.61	0.50
2:E:76:TRP:O	2:E:79:LYS:HG2	2.11	0.50
2:B:339:VAL:HG12	2:B:340:GLY:C	2.31	0.50
2:B:223:LEU:O	2:B:225:ARG:N	2.44	0.50
1:D:186:ASN:ND2	1:D:189:ASP:OD2	2.44	0.50
1:A:127:ILE:O	1:A:127:ILE:CG2	2.58	0.50
1:A:212:SER:O	1:A:215:GLU:HB2	2.11	0.50
2:B:263:VAL:HG22	2:B:317:ASN:HB3	1.92	0.50
1:D:124:PRO:O	1:D:136:ILE:HD13	2.10	0.50
2:E:302:PHE:C	2:E:306:LEU:HD12	2.31	0.50
2:E:176:GLN:O	2:E:179:LYS:HB3	2.11	0.50
2:E:26:THR:O	2:E:27:THR:HG23	2.11	0.50
1:D:48:LEU:N	1:D:48:LEU:HD23	2.24	0.50
1:D:203:ILE:HG22	1:D:204:VAL:N	2.27	0.50
1:D:3:LEU:C	1:D:4:ILE:CG2	2.80	0.50
2:B:318:ILE:HG23	2:B:319:PHE:N	2.25	0.50
2:B:140:THR:HB	2:B:143:LEU:CD1	2.40	0.50
2:B:356:LEU:O	2:B:360:LYS:CG	2.58	0.50
2:E:328:ILE:O	2:E:329:ALA:C	2.49	0.50
1:A:240:LYS:HD3	1:A:251:ILE:HG21	1.94	0.50
1:A:21:THR:OG1	1:A:47:HIS:CE1	2.64	0.50
2:E:142:HIS:CD2	2:E:142:HIS:H	2.29	0.50
2:B:38:ILE:CD1	2:B:98:VAL:HG12	2.41	0.50
2:B:326:ASP:H	2:B:353:ASN:HB3	1.77	0.50
2:E:210:ILE:HG12	2:E:211:CYS:N	2.26	0.50
2:B:206:GLN:CD	2:B:206:GLN:H	2.14	0.50
2:B:337:ALA:O	2:B:338:GLU:C	2.49	0.50
2:E:63:VAL:CG1	2:E:64:ASN:H	2.22	0.50
2:E:371:ALA:CB	2:E:377:ALA:HB2	2.41	0.50
2:E:80:ARG:HD3	2:E:89:ASN:ND2	2.25	0.50
1:D:124:PRO:CD	1:D:125:GLY:H	2.24	0.50
1:A:209:ILE:HG23	1:A:235:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:THR:HG23	2:E:143:LEU:HD12	1.94	0.50
2:E:82:VAL:CG2	2:E:90:GLY:CA	2.87	0.50
1:D:233:ILE:HD13	1:D:261:LYS:HB3	1.91	0.50
2:E:330:ASP:HA	2:E:333:ILE:HD12	1.94	0.50
2:E:150:ASP:OD1	2:E:151:PRO:N	2.44	0.50
2:E:243:ALA:O	2:E:244:GLN:C	2.49	0.50
1:D:30:TYR:OH	1:D:130:GLY:N	2.35	0.50
1:A:141:ILE:HG22	1:A:161:VAL:HG12	1.93	0.50
2:B:301:ALA:O	2:B:305:ILE:HG13	2.11	0.50
2:B:388:LYS:NZ	2:B:388:LYS:HB2	2.27	0.50
2:E:319:PHE:CG	2:E:350:GLU:HG2	2.40	0.50
1:D:50:LEU:HB3	1:D:51:PRO:CD	2.42	0.50
2:B:228:ASP:O	2:B:232:MET:HE2	2.12	0.50
2:B:82:VAL:CG2	2:B:86:THR:HG21	2.36	0.50
1:A:145:GLY:HA3	1:A:170:GLY:CA	2.42	0.50
1:A:80:SER:O	1:A:81:ILE:C	2.50	0.50
1:D:128:THR:HG22	1:D:131:GLU:HB3	1.92	0.50
2:B:248:TRP:CE2	2:B:300:GLU:HG3	2.47	0.50
2:E:352:ASN:ND2	2:E:353:ASN:CB	2.71	0.50
1:D:84:ALA:O	1:D:85:ILE:C	2.43	0.50
2:B:45:VAL:CG2	2:B:72:PHE:CE2	2.94	0.50
1:D:287:LEU:C	1:D:287:LEU:CD2	2.80	0.50
1:A:188:ILE:O	1:A:190:ILE:N	2.45	0.50
1:D:160:ALA:O	1:D:161:VAL:O	2.29	0.50
1:D:277:ALA:O	1:D:279:ILE:N	2.44	0.50
2:E:277:LYS:HD2	2:E:277:LYS:C	2.28	0.50
1:D:104:MET:CA	1:D:104:MET:HE3	2.42	0.50
2:E:339:VAL:HG11	2:E:341:VAL:HG12	1.87	0.50
2:B:82:VAL:CG2	2:B:90:GLY:HA3	2.40	0.50
2:B:156:MET:HB3	2:B:157:PRO:CD	2.41	0.50
2:B:308:ASP:OD1	2:B:308:ASP:C	2.50	0.50
2:E:43:TRP:HB3	2:E:99:GLU:O	2.12	0.50
1:A:150:VAL:O	1:A:150:VAL:CG2	2.59	0.49
1:A:220:TYR:O	1:A:221:ILE:C	2.48	0.49
2:B:356:LEU:O	2:B:360:LYS:HG3	2.12	0.49
2:E:357:GLY:O	2:E:361:LEU:N	2.45	0.49
2:B:332:ILE:O	2:B:333:ILE:C	2.47	0.49
2:B:86:THR:CG2	2:B:87:ASP:N	2.75	0.49
1:A:180:ASP:HB3	1:A:181:PRO:HD2	1.93	0.49
1:D:195:GLU:OE1	1:D:225:VAL:HG23	2.12	0.49
1:A:19:GLN:HB2	3:A:289:COA:O4A	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ILE:CA	1:D:36:GLY:O	2.58	0.49
1:D:9:LYS:HB2	1:D:65:ALA:HA	1.94	0.49
2:B:72:PHE:O	2:B:73:ALA:C	2.46	0.49
2:B:96:ILE:HG22	2:B:97:LEU:N	2.22	0.49
1:D:226:THR:OG1	1:D:227:LYS:N	2.46	0.49
1:A:2:ILE:HG22	1:A:3:LEU:N	2.08	0.49
2:E:241:ARG:HB3	2:E:252:TYR:CD2	2.47	0.49
2:E:300:GLU:O	2:E:301:ALA:C	2.47	0.49
2:B:228:ASP:O	2:B:232:MET:CE	2.60	0.49
2:B:48:GLN:CA	2:B:48:GLN:NE2	2.75	0.49
2:B:108:LEU:CD2	2:B:127:THR:HA	2.42	0.49
1:A:193:MET:O	1:A:194:PHE:C	2.47	0.49
1:D:46:THR:HA	1:D:50:LEU:O	2.12	0.49
2:E:156:MET:CB	2:E:157:PRO:CD	2.86	0.49
2:B:335:ALA:O	2:B:336:VAL:C	2.51	0.49
2:B:223:LEU:C	2:B:225:ARG:N	2.65	0.49
2:E:34:ALA:O	2:E:35:ALA:C	2.50	0.49
2:E:103:ASP:HB2	2:E:205:LYS:HB2	1.94	0.49
2:E:342:ASN:N	2:E:342:ASN:OD1	2.33	0.49
2:E:275:ILE:HG23	2:E:276:VAL:N	2.02	0.49
2:E:195:LEU:HD23	2:E:196:ILE:N	2.27	0.49
2:E:296:GLU:CD	2:E:296:GLU:H	2.01	0.49
2:B:285:ASN:ND2	2:B:286:PHE:N	2.60	0.49
1:A:35:VAL:HG21	1:A:63:THR:HB	1.95	0.49
2:B:50:HIS:CG	2:B:237:GLN:HG3	2.47	0.49
1:A:280:GLY:O	1:A:281:GLU:C	2.51	0.49
1:A:267:ALA:C	1:A:269:GLY:N	2.65	0.49
1:D:238:ALA:HB1	1:D:239:PRO:HD2	1.94	0.49
1:D:203:ILE:CA	1:D:229:VAL:CG2	2.81	0.49
1:A:6:LYS:HE2	1:A:31:GLY:O	2.12	0.49
2:B:133:ILE:O	2:B:135:LYS:N	2.46	0.49
1:D:152:ARG:NH2	1:D:208:GLU:O	2.46	0.49
1:A:157:THR:O	1:A:158:TYR:C	2.49	0.49
1:A:236:VAL:HG22	1:A:258:ALA:HB1	1.95	0.49
2:E:65:SER:O	2:E:66:LYS:C	2.51	0.49
1:D:104:MET:HA	1:D:104:MET:HE3	1.95	0.49
2:E:219:ASP:OD1	2:E:221:ASN:HB2	2.13	0.49
2:B:107:GLU:HG2	2:B:200:PRO:CB	2.43	0.49
2:E:157:PRO:CG	2:E:182:MET:HE1	2.42	0.49
1:D:2:ILE:HG12	1:D:193:MET:CE	2.39	0.49
2:E:269:ALA:O	2:E:272:THR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:CB	3:D:289:COA:H72	2.33	0.49
1:D:66:THR:CG2	1:D:90:LYS:HD2	2.42	0.49
1:D:67:ALA:HA	1:D:91:LEU:O	2.13	0.49
1:D:92:ILE:O	1:D:118:MET:CA	2.49	0.49
2:B:83:THR:N	2:B:86:THR:HB	2.28	0.49
1:D:230:VAL:HG21	1:D:283:LEU:CD1	2.41	0.49
2:B:140:THR:C	2:B:142:HIS:N	2.62	0.49
1:D:77:CYS:O	1:D:81:ILE:HD12	2.13	0.49
1:D:12:CYS:SG	1:D:15:PHE:HA	2.53	0.49
2:E:135:LYS:O	2:E:136:VAL:C	2.49	0.48
2:E:339:VAL:CG1	2:E:341:VAL:CG1	2.80	0.48
2:B:285:ASN:HD21	2:B:287:LEU:HB2	1.78	0.48
2:B:49:VAL:HG13	2:B:51:ALA:N	2.22	0.48
2:B:205:LYS:O	2:B:207:GLY:N	2.47	0.48
1:A:154:GLY:O	1:A:155:THR:C	2.51	0.48
1:D:277:ALA:C	1:D:279:ILE:H	2.16	0.48
1:D:46:THR:HG22	1:D:50:LEU:C	2.33	0.48
2:B:45:VAL:HA	2:B:97:LEU:O	2.14	0.48
2:E:56:LYS:HD2	2:E:56:LYS:N	2.22	0.48
1:D:3:LEU:O	1:D:4:ILE:HG22	2.12	0.48
1:A:194:PHE:O	1:A:195:GLU:C	2.52	0.48
1:A:151:SER:HA	1:A:206:ILE:O	2.14	0.48
2:B:216:LEU:N	2:B:216:LEU:HD23	2.11	0.48
1:A:92:ILE:CG2	1:A:118:MET:HG3	2.43	0.48
2:B:153:THR:C	2:B:154:GLY:O	2.50	0.48
1:D:129:PRO:HG2	1:D:171:GLN:O	2.12	0.48
1:A:150:VAL:HA	1:A:175:VAL:O	2.13	0.48
1:A:219:ALA:O	1:A:220:TYR:O	2.32	0.48
1:D:214:GLU:OE1	1:D:261:LYS:NZ	2.36	0.48
2:B:362:ALA:O	2:B:363:ASP:C	2.49	0.48
2:B:50:HIS:CE1	4:B:406:HOH:O	2.65	0.48
1:A:195:GLU:OE1	1:A:226:THR:N	2.46	0.48
1:D:11:ILE:HG21	1:D:65:ALA:HB1	1.96	0.48
1:A:108:LYS:O	1:A:111:LEU:HB2	2.14	0.48
1:A:105:LEU:C	1:A:105:LEU:CD2	2.74	0.48
2:B:174:VAL:O	2:B:175:GLN:C	2.52	0.48
1:D:127:ILE:C	1:D:173:THR:HG23	2.32	0.48
2:B:224:PHE:HA	2:B:230:ARG:NH1	2.28	0.48
1:D:190:ILE:HD13	1:D:190:ILE:H	1.70	0.48
1:D:195:GLU:CA	1:D:227:LYS:HE3	2.43	0.48
2:B:386:GLU:HA	2:B:388:LYS:HZ1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:371:ALA:HB1	2:E:377:ALA:CA	2.43	0.48
1:D:22:PHE:CD1	1:D:23:HIS:N	2.82	0.48
2:B:43:TRP:H	2:B:43:TRP:HE3	1.62	0.48
1:A:143:LYS:O	1:A:171:GLN:N	2.40	0.48
1:D:55:THR:HG22	1:D:56:VAL:N	2.28	0.48
2:B:94:ASN:O	2:B:95:GLN:HG2	2.14	0.48
2:E:229:LEU:O	2:E:230:ARG:C	2.49	0.48
2:E:343:VAL:HG13	2:E:344:PRO:HD2	0.50	0.48
1:A:104:MET:HE1	1:A:107:VAL:CG1	2.43	0.48
1:D:186:ASN:C	1:D:186:ASN:OD1	2.52	0.48
1:D:191:LEU:HD13	1:D:221:ILE:HG13	1.95	0.48
1:A:154:GLY:O	1:A:157:THR:HB	2.14	0.48
1:D:6:LYS:O	1:D:6:LYS:HG2	2.12	0.48
2:B:255:LEU:HD12	2:B:255:LEU:HA	1.58	0.48
2:E:322:ILE:O	2:E:322:ILE:CG2	2.57	0.48
2:B:210:ILE:O	2:B:210:ILE:CG2	2.61	0.48
1:D:127:ILE:HG12	1:D:128:THR:H	1.74	0.48
1:D:219:ALA:O	1:D:220:TYR:C	2.52	0.48
1:A:74:ALA:CB	1:A:98:GLY:O	2.62	0.48
1:A:167:TYR:CB	1:A:169:PHE:HE2	2.26	0.48
2:E:312:LYS:C	2:E:343:VAL:HG11	2.34	0.48
1:A:127:ILE:CD1	1:A:133:LYS:HG3	2.38	0.48
1:A:191:LEU:O	1:A:192:GLU:C	2.52	0.48
1:A:22:PHE:O	1:A:23:HIS:C	2.51	0.48
1:A:23:HIS:NE2	1:A:136:ILE:HG22	2.28	0.48
2:E:139:GLU:O	2:E:140:THR:CB	2.31	0.48
2:B:33:GLU:OE2	3:D:289:COA:H10	2.13	0.48
2:B:362:ALA:C	2:B:364:SER:N	2.66	0.48
1:A:281:GLU:O	1:A:284:LYS:HB2	2.14	0.48
1:A:253:GLY:C	1:A:255:LYS:H	2.16	0.48
2:E:367:ASN:HA	2:E:367:ASN:HD22	1.40	0.48
1:D:126:VAL:CG2	1:D:127:ILE:N	2.77	0.47
1:D:189:ASP:CB	1:D:190:ILE:HD13	2.43	0.47
1:A:186:ASN:ND2	1:A:189:ASP:H	2.05	0.47
2:B:318:ILE:N	2:B:348:ARG:O	2.47	0.47
2:B:65:SER:O	2:B:66:LYS:C	2.52	0.47
2:E:245:ALA:O	2:E:250:LEU:HB2	2.14	0.47
1:A:281:GLU:O	1:A:284:LYS:N	2.47	0.47
2:B:373:GLY:O	2:B:374:LEU:C	2.51	0.47
2:E:157:PRO:HD3	2:E:182:MET:HE1	1.96	0.47
2:E:186:THR:O	2:E:190:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:214:GLY:C	2:E:215:LYS:HG3	2.35	0.47
2:E:94:ASN:O	2:E:95:GLN:HG2	2.13	0.47
1:D:3:LEU:HD23	1:D:193:MET:HE1	1.95	0.47
1:A:77:CYS:O	1:A:78:LYS:C	2.51	0.47
2:B:268:LEU:HA	2:B:268:LEU:HD23	1.44	0.47
1:D:118:MET:HG2	1:D:119:ILE:N	2.30	0.47
1:D:89:ILE:CG2	1:D:90:LYS:N	2.76	0.47
2:B:4:HIS:CB	2:B:7:GLN:HG3	2.44	0.47
2:B:46:LYS:HG2	2:B:60:VAL:HG13	1.96	0.47
1:D:155:THR:HG21	2:E:264:ASN:O	2.14	0.47
1:D:164:THR:H	1:D:164:THR:HG23	1.21	0.47
2:E:57:ALA:CB	2:E:83:THR:HG22	2.45	0.47
2:E:115:ASP:O	2:E:119:ARG:N	2.46	0.47
1:D:127:ILE:HG23	1:D:127:ILE:O	2.13	0.47
1:A:11:ILE:O	1:A:69:VAL:CG2	2.62	0.47
1:A:287:LEU:HD22	1:A:287:LEU:O	2.14	0.47
2:B:172:LYS:HA	2:B:175:GLN:HG2	1.97	0.47
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.54	0.47
1:A:163:GLN:C	1:A:165:THR:N	2.64	0.47
2:E:110:LEU:HD22	2:E:111:GLY:N	2.28	0.47
1:D:189:ASP:O	1:D:193:MET:HG2	2.15	0.47
1:D:228:PRO:CB	1:D:286:VAL:CG2	2.92	0.47
2:E:29:ARG:O	2:E:32:GLU:HB3	2.14	0.47
1:A:215:GLU:O	1:A:216:GLU:C	2.52	0.47
2:E:277:LYS:HD2	2:E:278:LEU:H	1.70	0.47
2:E:346:VAL:CB	2:E:381:VAL:HG22	2.45	0.47
2:B:133:ILE:HA	2:B:136:VAL:HB	1.97	0.47
1:D:124:PRO:HD2	1:D:125:GLY:H	1.80	0.47
2:E:197:GLU:HG2	2:E:215:LYS:HD2	1.97	0.47
2:E:72:PHE:HE1	2:E:76:TRP:NE1	2.13	0.47
2:B:257:GLY:HA3	2:B:282:GLU:O	2.15	0.47
1:A:153:SER:CB	1:A:246:NEP:HE1	2.41	0.47
1:A:84:ALA:O	1:A:85:ILE:C	2.51	0.47
1:D:129:PRO:CD	1:D:172:SER:O	2.59	0.47
1:A:73:PRO:C	1:A:75:PRO:HD2	2.36	0.47
2:B:136:VAL:O	2:B:140:THR:N	2.41	0.47
2:B:140:THR:O	2:B:141:PRO:C	2.53	0.47
1:D:10:VAL:HG12	1:D:11:ILE:N	2.30	0.47
1:D:98:GLY:N	4:D:311:HOH:O	2.34	0.47
2:B:333:ILE:O	2:B:334:GLY:C	2.53	0.47
2:B:278:LEU:HA	2:B:278:LEU:HD13	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ILE:HG13	1:D:132:CYS:O	2.15	0.47
1:D:190:ILE:HA	1:D:193:MET:CG	2.32	0.47
1:A:4:ILE:HG12	1:A:8:THR:OG1	2.15	0.47
1:D:156:LEU:HA	1:D:156:LEU:HD23	1.49	0.47
2:E:287:LEU:HD23	2:E:288:ASP:N	2.24	0.47
1:D:18:SER:HB2	3:D:289:COA:O4A	2.15	0.47
2:B:65:SER:OG	2:B:68:ASP:HB2	2.15	0.47
2:E:157:PRO:O	2:E:158:TYR:C	2.52	0.47
2:B:232:MET:HE3	2:B:232:MET:HB2	1.78	0.47
1:A:11:ILE:HD12	1:A:68:SER:OG	2.15	0.47
2:B:172:LYS:O	2:B:176:GLN:HG3	2.14	0.47
1:D:191:LEU:O	1:D:194:PHE:N	2.42	0.47
1:A:174:CYS:C	1:A:175:VAL:CG2	2.84	0.47
1:D:156:LEU:O	1:D:159:GLU:N	2.45	0.47
2:E:188:PHE:HD2	2:E:196:ILE:HD12	1.80	0.47
2:E:202:VAL:HG12	2:E:203:ILE:N	2.18	0.47
1:A:262:PHE:O	1:A:266:GLU:CG	2.63	0.47
1:A:253:GLY:C	1:A:255:LYS:N	2.67	0.47
1:A:123:CYS:SG	1:A:123:CYS:O	2.73	0.46
1:A:190:ILE:HA	1:A:193:MET:HG3	1.97	0.46
1:D:158:TYR:HA	1:D:161:VAL:CG2	2.44	0.46
2:E:371:ALA:HB2	2:E:377:ALA:HA	1.97	0.46
2:E:176:GLN:HE22	2:E:208:ASP:HB3	1.80	0.46
1:D:43:GLY:N	1:D:54:ASN:OD1	2.47	0.46
1:D:198:PRO:O	1:D:199:GLN:C	2.54	0.46
2:E:277:LYS:HD2	2:E:278:LEU:HA	1.95	0.46
2:B:27:THR:HB	2:B:28:PRO:HD2	1.98	0.46
1:D:16:THR:OG1	1:D:39:THR:HG21	2.15	0.46
2:E:69:ILE:C	2:E:71:ALA:N	2.68	0.46
2:E:371:ALA:HB3	2:E:377:ALA:HB2	1.97	0.46
3:D:289:COA:P3B	3:D:289:COA:O2B	2.73	0.46
2:E:199:ASN:HA	2:E:200:PRO:HA	1.47	0.46
1:D:187:PHE:CE2	1:D:214:GLU:CG	2.88	0.46
1:D:152:ARG:NH2	1:D:210:GLY:O	2.45	0.46
2:E:150:ASP:C	2:E:150:ASP:OD1	2.51	0.46
2:E:191:ARG:NE	4:E:409:HOH:O	2.49	0.46
1:D:218:ALA:HB2	1:D:265:LEU:CD2	2.45	0.46
2:E:371:ALA:CB	2:E:377:ALA:CA	2.92	0.46
1:D:233:ILE:CG2	1:D:234:ALA:H	2.25	0.46
1:D:233:ILE:HG23	1:D:234:ALA:H	1.79	0.46
2:B:180:ILE:CG2	2:B:184:LEU:CD1	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ILE:O	2:B:203:ILE:HG22	2.07	0.46
2:E:10:GLN:O	2:E:11:LEU:C	2.54	0.46
1:D:126:VAL:HG22	1:D:127:ILE:N	2.30	0.46
2:B:348:ARG:CD	2:B:348:ARG:C	2.84	0.46
2:B:71:ALA:O	2:B:72:PHE:C	2.54	0.46
2:E:304:ILE:O	2:E:305:ILE:C	2.49	0.46
1:D:53:PHE:CE2	1:D:59:ALA:HA	2.50	0.46
1:D:146:LYS:HE2	1:D:287:LEU:HD11	1.97	0.46
1:A:186:ASN:OD1	1:A:188:ILE:N	2.48	0.46
3:D:289:COA:H61	3:D:289:COA:O9P	2.15	0.46
2:B:34:ALA:O	2:B:37:LYS:HB2	2.15	0.46
2:B:331:GLY:O	2:B:332:ILE:C	2.52	0.46
2:B:276:VAL:O	2:B:277:LYS:C	2.47	0.46
2:B:180:ILE:HG23	2:B:184:LEU:CD1	2.45	0.46
2:E:122:VAL:CG1	2:E:146:LYS:HB3	2.46	0.46
1:D:285:THR:HA	1:D:288:LYS:HD3	1.98	0.46
2:B:135:LYS:HB3	2:B:136:VAL:H	1.35	0.46
1:D:56:VAL:HG12	1:D:87:ALA:HB3	1.97	0.46
2:E:97:LEU:CD2	2:E:98:VAL:N	2.76	0.46
2:B:107:GLU:HB3	2:B:129:GLY:HA3	1.97	0.46
1:D:195:GLU:OE2	1:D:226:THR:CG2	2.62	0.46
1:D:195:GLU:CD	1:D:226:THR:H	2.20	0.46
1:D:236:VAL:N	2:E:274:ASP:OD2	2.48	0.46
1:D:107:VAL:O	1:D:108:LYS:C	2.51	0.46
2:B:23:TYR:CD2	2:B:34:ALA:HB1	2.50	0.46
2:E:195:LEU:HG	2:E:196:ILE:N	2.31	0.46
2:B:331:GLY:O	2:B:335:ALA:N	2.40	0.46
2:B:255:LEU:HD23	2:B:273:MET:CE	2.46	0.46
2:E:241:ARG:HE	2:E:241:ARG:HB2	1.41	0.46
2:E:252:TYR:CG	2:E:253:VAL:N	2.84	0.46
2:B:287:LEU:CD2	2:B:287:LEU:C	2.84	0.46
2:E:120:ARG:HD3	2:E:120:ARG:HA	1.51	0.46
2:E:257:GLY:C	2:E:284:ALA:HB2	2.35	0.46
2:E:110:LEU:CD2	2:E:111:GLY:N	2.79	0.46
2:E:312:LYS:O	2:E:385:VAL:HG23	2.16	0.46
1:A:2:ILE:HG21	1:A:173:THR:HG21	1.98	0.46
2:E:63:VAL:CG1	2:E:68:ASP:CB	2.94	0.46
2:E:329:ALA:HB1	2:E:361:LEU:CD1	2.46	0.46
1:A:55:THR:O	1:A:58:GLU:HB2	2.16	0.46
2:E:209:LEU:HA	2:E:209:LEU:HD23	1.53	0.46
2:B:308:ASP:HB3	4:B:410:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:O	1:A:284:LYS:C	2.54	0.46
1:A:285:THR:O	1:A:286:VAL:C	2.53	0.46
1:A:22:PHE:CD1	1:A:23:HIS:N	2.85	0.45
2:E:187:ILE:O	2:E:188:PHE:C	2.54	0.45
2:E:239:ASP:OD1	2:E:241:ARG:HB2	2.16	0.45
2:B:81:LEU:N	2:B:91:GLN:O	2.49	0.45
1:D:212:SER:HB3	1:D:255:LYS:NZ	2.31	0.45
2:B:204:THR:O	2:B:207:GLY:CA	2.64	0.45
2:E:50:HIS:NE2	2:E:237:GLN:HG3	2.31	0.45
1:D:283:LEU:C	1:D:285:THR:N	2.70	0.45
1:A:136:ILE:O	1:A:137:GLN:C	2.54	0.45
1:D:273:VAL:HG12	1:D:273:VAL:O	2.15	0.45
1:D:22:PHE:C	1:D:24:SER:H	2.19	0.45
1:A:108:LYS:CE	4:A:307:HOH:O	2.40	0.45
2:B:47:CYS:O	2:B:54:ARG:NH1	2.49	0.45
1:D:129:PRO:O	1:D:131:GLU:N	2.49	0.45
1:A:212:SER:O	1:A:214:GLU:N	2.49	0.45
2:E:28:PRO:O	2:E:29:ARG:C	2.53	0.45
2:E:69:ILE:HG22	2:E:70:ARG:N	2.28	0.45
1:A:69:VAL:HG23	1:A:69:VAL:O	2.16	0.45
2:E:192:ASP:CB	4:E:405:HOH:O	2.64	0.45
2:E:25:CYS:SG	2:E:31:ALA:HA	2.56	0.45
1:D:174:CYS:HB2	4:D:301:HOH:O	2.17	0.45
1:A:174:CYS:C	1:A:175:VAL:HG23	2.37	0.45
2:B:302:PHE:O	2:B:306:LEU:HB2	2.17	0.45
2:B:371:ALA:HB1	2:B:377:ALA:HB2	1.95	0.45
2:E:275:ILE:O	2:E:275:ILE:HG23	2.01	0.45
2:E:135:LYS:O	2:E:138:GLU:N	2.50	0.45
1:D:118:MET:O	1:D:119:ILE:HD13	2.16	0.45
2:B:277:LYS:O	2:B:280:GLY:N	2.49	0.45
2:B:224:PHE:C	2:B:230:ARG:HH12	2.19	0.45
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.26	0.45
2:E:191:ARG:HD2	2:E:226:GLN:NE2	2.32	0.45
1:D:186:ASN:ND2	1:D:189:ASP:CG	2.70	0.45
2:B:263:VAL:CG1	2:B:264:ASN:H	2.29	0.45
2:E:63:VAL:CG1	2:E:68:ASP:HB3	2.41	0.45
2:E:346:VAL:CB	2:E:381:VAL:CG2	2.95	0.45
2:E:300:GLU:HA	2:E:303:LYS:HG3	1.97	0.45
2:B:123:PHE:CZ	2:B:185:ALA:HA	2.52	0.45
1:D:53:PHE:CD1	1:D:53:PHE:N	2.85	0.45
1:A:244:MET:O	1:A:246:NEP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:348:ARG:HH11	2:E:374:LEU:CB	2.29	0.45
1:D:229:VAL:CG1	1:D:270:VAL:HG11	2.46	0.45
1:D:283:LEU:CA	1:D:286:VAL:HG12	2.47	0.45
2:E:315:LEU:CD1	2:E:346:VAL:O	2.65	0.45
2:B:182:MET:O	2:B:183:GLY:C	2.54	0.45
2:B:49:VAL:HG13	2:B:50:HIS:N	2.30	0.45
1:D:14:GLY:O	1:D:15:PHE:C	2.55	0.45
1:A:60:VAL:O	1:A:61:ALA:C	2.51	0.45
1:D:4:ILE:HD13	1:D:126:VAL:CG2	2.47	0.45
1:A:235:GLY:N	2:B:274:ASP:OD2	2.43	0.45
1:D:10:VAL:HG12	1:D:34:MET:HE1	1.99	0.45
2:B:22:GLY:CA	2:B:98:VAL:O	2.64	0.45
2:B:251:ASN:HB2	2:B:288:ASP:HB3	1.99	0.45
1:A:5:ASP:CG	1:A:7:ASN:H	2.16	0.45
1:A:20:GLY:HA2	1:A:71:TYR:CD2	2.52	0.45
2:B:161:ARG:O	2:B:162:GLU:C	2.53	0.45
1:A:154:GLY:O	1:A:157:THR:CB	2.65	0.45
1:A:186:ASN:O	1:A:189:ASP:HB2	2.16	0.45
1:A:19:GLN:HG3	3:A:289:COA:H132	1.98	0.45
2:B:38:ILE:HG21	2:B:43:TRP:HD1	1.82	0.45
2:E:79:LYS:H	2:E:79:LYS:HG2	1.51	0.45
2:B:331:GLY:O	2:B:335:ALA:CB	2.65	0.45
1:A:143:LYS:O	1:A:170:GLY:CA	2.65	0.45
2:B:25:CYS:HB3	2:B:30:GLU:HB2	1.99	0.45
2:E:36:SER:C	2:E:38:ILE:N	2.67	0.45
1:A:272:THR:HG22	1:A:272:THR:O	2.17	0.45
1:A:99:ILE:HA	1:A:100:PRO:HD3	1.59	0.45
1:A:127:ILE:HG22	1:A:174:CYS:HB2	1.98	0.45
2:E:346:VAL:HB	2:E:381:VAL:HG21	1.98	0.45
2:B:136:VAL:HG12	2:B:144:ILE:HD11	1.98	0.45
1:D:11:ILE:N	1:D:34:MET:CE	2.80	0.45
2:B:332:ILE:O	2:B:335:ALA:HB3	2.17	0.45
2:B:2:ASN:O	2:B:3:LEU:HD23	2.16	0.45
2:E:1:MET:HB3	2:E:218:ALA:HB3	1.99	0.45
2:B:301:ALA:O	2:B:302:PHE:C	2.55	0.44
1:D:124:PRO:O	1:D:135:GLY:HA3	2.17	0.44
2:E:341:VAL:HG22	2:E:341:VAL:O	2.17	0.44
2:B:187:ILE:HD12	2:B:187:ILE:HG21	1.65	0.44
1:A:181:PRO:C	1:A:183:PRO:HD3	2.38	0.44
1:D:229:VAL:HG22	1:D:230:VAL:H	1.79	0.44
1:D:3:LEU:HD23	1:D:193:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HG22	1:A:173:THR:HG21	1.99	0.44
1:A:72:VAL:O	1:A:96:THR:CG2	2.65	0.44
1:A:98:GLY:O	1:A:100:PRO:HD3	2.17	0.44
2:E:276:VAL:CG1	2:E:281:GLY:HA3	2.47	0.44
1:D:101:THR:O	1:D:105:LEU:N	2.47	0.44
2:E:81:LEU:HA	2:E:81:LEU:HD23	1.63	0.44
2:B:352:ASN:C	2:B:354:ALA:N	2.71	0.44
2:B:362:ALA:C	2:B:364:SER:H	2.20	0.44
2:E:49:VAL:HG22	2:E:91:GLN:HB2	1.97	0.44
1:A:55:THR:HB	1:A:58:GLU:HB2	1.99	0.44
1:A:239:PRO:HG3	2:B:255:LEU:HD11	1.98	0.44
2:E:4:HIS:O	2:E:7:GLN:N	2.49	0.44
2:E:50:HIS:CG	2:E:237:GLN:HG3	2.52	0.44
2:B:115:ASP:OD2	2:B:118:SER:CB	2.64	0.44
1:A:150:VAL:CG1	1:A:190:ILE:HG21	2.47	0.44
1:A:19:GLN:CA	1:A:19:GLN:OE1	2.65	0.44
1:A:77:CYS:HB3	1:A:99:ILE:HD11	1.99	0.44
1:D:104:MET:O	1:D:105:LEU:C	2.54	0.44
1:D:78:LYS:C	1:D:80:SER:H	2.20	0.44
2:B:43:TRP:HB3	2:B:99:GLU:O	2.17	0.44
2:E:257:GLY:O	2:E:284:ALA:HB2	2.18	0.44
1:A:92:ILE:HB	1:A:118:MET:HG3	1.99	0.44
1:A:238:ALA:HA	1:A:239:PRO:HD2	1.80	0.44
2:B:107:GLU:O	2:B:129:GLY:HA3	2.17	0.44
1:D:202:ALA:CB	1:D:228:PRO:HG2	2.47	0.44
1:D:136:ILE:C	1:D:137:GLN:O	2.54	0.44
2:B:368:ILE:CG2	2:B:369:ILE:N	2.81	0.44
2:E:255:LEU:HB3	2:E:256:ASP:H	1.48	0.44
1:A:11:ILE:HD11	1:A:68:SER:CB	2.47	0.44
2:B:255:LEU:CD2	2:B:273:MET:CE	2.96	0.44
2:E:12:PHE:CD1	2:E:12:PHE:N	2.83	0.44
1:A:273:VAL:CG1	1:A:278:ASP:HB2	2.48	0.44
2:B:20:PRO:HD3	2:B:210:ILE:HD11	1.99	0.44
1:A:19:GLN:HG2	3:A:289:COA:P2A	2.57	0.44
2:B:386:GLU:O	2:B:387:GLY:C	2.55	0.44
1:D:21:THR:CG2	1:D:22:PHE:N	2.63	0.44
1:A:10:VAL:CG1	1:A:11:ILE:H	2.26	0.44
2:B:153:THR:O	2:B:154:GLY:O	2.36	0.44
1:A:281:GLU:O	1:A:282:ALA:C	2.56	0.44
1:A:253:GLY:O	1:A:255:LYS:HB2	2.17	0.44
2:E:191:ARG:HA	2:E:191:ARG:HD2	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:O	1:A:220:TYR:HB3	2.18	0.44
2:B:316:VAL:HG13	2:B:317:ASN:N	2.30	0.44
2:B:386:GLU:C	2:B:388:LYS:HZ2	2.21	0.44
2:E:269:ALA:O	2:E:270:MET:C	2.53	0.44
2:E:133:ILE:CG2	2:E:134:GLU:N	2.81	0.44
2:E:336:VAL:HG13	2:E:341:VAL:HG13	1.99	0.44
2:E:299:THR:HG22	2:E:300:GLU:N	2.33	0.44
1:A:143:LYS:O	1:A:170:GLY:HA2	2.18	0.44
1:A:11:ILE:CD1	1:A:68:SER:OG	2.65	0.44
2:E:205:LYS:O	2:E:207:GLY:N	2.51	0.44
1:D:27:ALA:HB1	1:D:32:THR:CB	2.44	0.44
2:B:150:ASP:OD1	2:B:150:ASP:C	2.56	0.44
2:B:147:VAL:HG22	2:B:159:GLN:HE21	1.82	0.44
1:A:24:SER:O	1:A:25:GLU:C	2.53	0.44
1:A:2:ILE:HD12	1:A:194:PHE:CD1	2.50	0.44
2:B:346:VAL:HG21	2:B:381:VAL:HG22	1.98	0.44
1:D:158:TYR:HA	1:D:161:VAL:HG21	1.99	0.44
2:E:141:PRO:HD2	2:E:142:HIS:HD2	1.83	0.44
2:E:157:PRO:HG3	2:E:182:MET:HE1	2.00	0.44
2:E:239:ASP:OD1	2:E:240:PRO:HD2	2.18	0.44
2:B:6:TYR:CE1	2:B:7:GLN:HG2	2.52	0.44
1:A:280:GLY:O	1:A:283:LEU:HB2	2.18	0.44
1:A:285:THR:C	1:A:287:LEU:H	2.21	0.44
2:E:122:VAL:HG12	2:E:123:PHE:N	2.32	0.44
1:D:149:ILE:HG12	1:D:174:CYS:HB3	1.82	0.44
2:E:263:VAL:HG21	2:E:269:ALA:HA	1.99	0.44
2:E:277:LYS:CD	2:E:277:LYS:C	2.84	0.44
2:B:239:ASP:OD2	2:B:241:ARG:NE	2.50	0.44
1:A:181:PRO:HA	2:B:116:ARG:HH11	1.81	0.44
1:D:283:LEU:HA	1:D:286:VAL:CG1	2.48	0.43
2:E:62:VAL:O	2:E:63:VAL:CG2	2.66	0.43
2:B:138:GLU:O	2:B:138:GLU:HG2	2.18	0.43
1:D:259:ASP:O	1:D:260:GLU:C	2.56	0.43
2:E:94:ASN:C	2:E:95:GLN:CG	2.86	0.43
2:B:158:TYR:CD1	2:B:159:GLN:N	2.85	0.43
1:D:127:ILE:O	1:D:173:THR:HG23	2.14	0.43
1:D:229:VAL:HG13	1:D:230:VAL:N	2.29	0.43
1:A:136:ILE:O	1:A:138:PRO:HD3	2.18	0.43
2:B:139:GLU:O	2:B:141:PRO:HD3	2.16	0.43
1:D:11:ILE:CG2	1:D:65:ALA:HB1	2.48	0.43
1:D:103:ASP:O	1:D:107:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:246:ALA:O	2:E:247:GLN:C	2.52	0.43
2:B:325:CYS:CB	2:B:352:ASN:O	2.62	0.43
2:B:361:LEU:HG	2:B:368:ILE:HG21	2.00	0.43
2:B:241:ARG:NH2	2:B:254:ALA:CB	2.81	0.43
1:A:278:ASP:O	1:A:281:GLU:HB2	2.18	0.43
2:B:173:LEU:HA	2:B:173:LEU:HD23	1.65	0.43
2:B:315:LEU:HD12	2:B:315:LEU:HA	1.66	0.43
1:D:162:LYS:O	1:D:163:GLN:C	2.56	0.43
1:D:81:ILE:HG21	1:D:107:VAL:CG1	2.48	0.43
2:E:298:VAL:O	2:E:301:ALA:HB3	2.18	0.43
2:B:86:THR:HG21	2:B:90:GLY:HA2	1.98	0.43
2:E:105:ALA:N	2:E:203:ILE:O	2.46	0.43
2:E:5:GLU:O	2:E:6:TYR:C	2.56	0.43
2:E:9:LYS:O	2:E:12:PHE:HB2	2.18	0.43
1:A:100:PRO:HA	2:B:219:ASP:OD2	2.18	0.43
1:A:123:CYS:HB2	1:A:124:PRO:CD	2.41	0.43
1:A:19:GLN:O	1:A:23:HIS:HB2	2.17	0.43
1:D:77:CYS:CB	1:D:99:ILE:HD11	2.46	0.43
2:E:304:ILE:O	2:E:307:SER:OG	2.35	0.43
2:E:191:ARG:CD	4:E:409:HOH:O	2.65	0.43
2:E:308:ASP:C	2:E:308:ASP:OD1	2.55	0.43
1:D:205:MET:CE	1:D:217:ALA:CB	2.96	0.43
1:D:30:TYR:OH	1:D:127:ILE:HD11	2.18	0.43
1:A:58:GLU:O	1:A:59:ALA:C	2.53	0.43
1:D:256:GLY:O	1:D:261:LYS:HE2	2.18	0.43
2:B:215:LYS:O	2:B:216:LEU:CD2	2.42	0.43
2:B:87:ASP:OD2	2:B:89:ASN:OD1	2.37	0.43
2:B:223:LEU:C	2:B:230:ARG:HH11	2.22	0.43
2:E:205:LYS:C	2:E:207:GLY:H	2.22	0.43
1:A:81:ILE:HD11	1:A:94:THR:HG21	2.00	0.43
2:B:177:PHE:O	2:B:178:THR:C	2.57	0.43
1:D:126:VAL:HG13	1:D:126:VAL:O	2.18	0.43
1:D:2:ILE:HD12	1:D:193:MET:HB2	1.74	0.43
1:D:205:MET:CE	1:D:217:ALA:HB3	2.46	0.43
1:D:217:ALA:O	1:D:221:ILE:HB	2.18	0.43
1:A:162:LYS:O	1:A:163:GLN:O	2.37	0.43
1:A:213:ALA:O	1:A:214:GLU:C	2.54	0.43
2:E:371:ALA:CB	2:E:377:ALA:CB	2.97	0.43
2:E:226:GLN:HA	2:E:227:PRO:HD2	1.55	0.43
1:D:73:PRO:CA	3:D:289:COA:H143	2.49	0.43
1:D:233:ILE:HD13	1:D:261:LYS:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ASP:HB3	2:B:356:LEU:HD13	2.01	0.43
2:B:255:LEU:HB3	2:B:256:ASP:H	1.61	0.43
1:D:15:PHE:CE2	1:D:47:HIS:HB3	2.54	0.43
1:D:188:ILE:HA	1:D:191:LEU:HB2	2.01	0.43
1:D:220:TYR:HD2	1:D:221:ILE:N	2.15	0.43
1:D:288:LYS:HB2	1:D:288:LYS:HE3	1.68	0.43
2:E:379:GLN:O	2:E:380:GLN:C	2.57	0.43
2:E:107:GLU:O	2:E:129:GLY:CA	2.56	0.43
1:D:11:ILE:HG23	1:D:11:ILE:HD13	1.65	0.43
1:D:214:GLU:O	1:D:215:GLU:C	2.55	0.43
1:D:45:THR:C	1:D:52:VAL:HG23	2.37	0.43
2:B:152:LEU:O	2:B:152:LEU:HD22	2.19	0.43
1:D:266:GLU:O	1:D:269:GLY:CA	2.66	0.43
1:A:221:ILE:HA	1:A:225:VAL:HG12	1.99	0.43
1:A:123:CYS:C	3:A:289:COA:S1P	2.97	0.43
1:D:236:VAL:HA	1:D:258:ALA:HB3	2.01	0.43
2:E:371:ALA:HB1	2:E:377:ALA:HA	2.01	0.43
1:D:78:LYS:C	1:D:80:SER:N	2.72	0.43
2:E:184:LEU:C	2:E:186:THR:N	2.72	0.43
2:E:72:PHE:HE1	2:E:76:TRP:HE1	1.67	0.43
2:B:110:LEU:HD23	2:B:110:LEU:HA	1.35	0.43
2:B:254:ALA:O	2:B:255:LEU:HD13	2.19	0.43
2:E:5:GLU:HG2	2:E:9:LYS:HD2	2.01	0.43
1:A:150:VAL:HG12	1:A:190:ILE:HG21	2.00	0.42
1:A:226:THR:O	1:A:227:LYS:C	2.57	0.42
1:A:72:VAL:HA	1:A:73:PRO:HD3	1.64	0.42
2:B:317:ASN:OD1	2:B:317:ASN:C	2.54	0.42
1:D:276:LEU:O	1:D:279:ILE:HD12	2.18	0.42
2:E:140:THR:CG2	2:E:143:LEU:HD12	2.48	0.42
1:D:22:PHE:HD1	1:D:23:HIS:N	2.16	0.42
2:B:65:SER:O	2:B:68:ASP:N	2.52	0.42
2:E:245:ALA:HB1	2:E:250:LEU:HB2	2.00	0.42
2:E:157:PRO:CB	2:E:182:MET:CE	2.97	0.42
2:B:356:LEU:HD22	2:B:356:LEU:C	2.39	0.42
1:A:55:THR:CG2	1:A:56:VAL:N	2.82	0.42
2:E:55:GLY:O	2:E:56:LYS:C	2.56	0.42
1:A:116:VAL:CG1	1:A:117:ARG:H	2.31	0.42
2:B:55:GLY:O	2:B:56:LYS:C	2.58	0.42
2:B:120:ARG:HA	2:B:120:ARG:HD3	1.62	0.42
2:E:263:VAL:CG1	2:E:268:LEU:HB3	2.47	0.42
1:D:80:SER:O	1:D:81:ILE:C	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLY:C	1:D:141:ILE:N	2.65	0.42
2:B:156:MET:HA	2:B:157:PRO:HD3	1.39	0.42
1:A:182:ILE:HA	1:A:183:PRO:HD2	1.76	0.42
2:E:205:LYS:C	2:E:207:GLY:N	2.72	0.42
1:D:283:LEU:HD12	1:D:286:VAL:HG11	2.01	0.42
1:A:4:ILE:HD12	1:A:4:ILE:HG21	1.78	0.42
1:D:160:ALA:O	1:D:164:THR:HG23	2.20	0.42
2:B:165:PHE:C	2:B:167:LEU:H	2.22	0.42
1:D:32:THR:O	1:D:34:MET:N	2.47	0.42
2:E:329:ALA:C	2:E:333:ILE:HD12	2.40	0.42
2:E:241:ARG:HD2	2:E:307:SER:OG	2.17	0.42
2:B:254:ALA:C	2:B:255:LEU:HD13	2.40	0.42
2:B:204:THR:O	2:B:207:GLY:HA2	2.20	0.42
2:E:219:ASP:OD1	2:E:219:ASP:C	2.57	0.42
1:A:252:ALA:CB	4:A:308:HOH:O	2.67	0.42
1:D:120:GLY:HA3	1:D:121:PRO:HA	1.77	0.42
1:D:218:ALA:HB2	1:D:265:LEU:HD23	2.00	0.42
1:D:285:THR:CG2	1:D:286:VAL:N	2.69	0.42
1:D:275:SER:OG	1:D:277:ALA:CB	2.64	0.42
1:D:81:ILE:HG22	1:D:85:ILE:CD1	2.49	0.42
1:D:117:ARG:HH21	1:D:185:SER:HB3	1.83	0.42
2:B:184:LEU:HG	2:B:184:LEU:H	1.50	0.42
2:B:25:CYS:SG	2:B:31:ALA:HA	2.59	0.42
2:E:177:PHE:C	2:E:177:PHE:CD2	2.92	0.42
2:E:206:GLN:N	2:E:206:GLN:OE1	2.47	0.42
1:D:4:ILE:HD13	1:D:126:VAL:HG22	2.01	0.42
1:A:206:ILE:HG22	1:A:207:GLY:N	2.34	0.42
2:B:316:VAL:HG13	2:B:318:ILE:HD12	2.01	0.42
2:B:359:LYS:O	2:B:360:LYS:C	2.57	0.42
2:B:375:THR:O	2:B:378:ALA:HB3	2.19	0.42
2:B:160:GLY:O	2:B:161:ARG:C	2.56	0.42
1:A:140:HIS:N	1:A:140:HIS:ND1	2.65	0.42
1:D:3:LEU:HG	1:D:3:LEU:H	1.66	0.42
1:D:161:VAL:O	1:D:162:LYS:C	2.57	0.42
2:E:276:VAL:HG12	2:E:277:LYS:N	2.32	0.42
2:B:133:ILE:CD1	2:B:134:GLU:N	2.67	0.42
2:E:157:PRO:HG3	2:E:182:MET:CE	2.49	0.42
2:B:298:VAL:O	2:B:298:VAL:CG1	2.63	0.42
2:E:41:GLY:HA3	2:E:42:PRO:HA	1.82	0.42
1:A:186:ASN:O	1:A:187:PHE:O	2.38	0.42
1:A:27:ALA:CB	1:A:34:MET:HE1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:GLU:O	2:B:301:ALA:C	2.58	0.42
2:E:69:ILE:C	2:E:71:ALA:H	2.23	0.42
2:E:376:ASP:O	2:E:377:ALA:C	2.56	0.42
2:B:356:LEU:O	2:B:360:LYS:HG2	2.19	0.42
2:B:359:LYS:HE3	2:B:363:ASP:OD2	2.20	0.42
2:E:328:ILE:HG21	2:E:349:LEU:CD2	2.49	0.42
2:E:330:ASP:CA	2:E:333:ILE:HD12	2.48	0.42
2:E:356:LEU:HD22	2:E:357:GLY:H	1.72	0.42
2:B:312:LYS:O	2:B:343:VAL:HG22	2.19	0.42
1:A:112:ASP:O	1:A:114:ALA:N	2.53	0.42
1:D:112:ASP:O	1:D:113:GLU:C	2.54	0.42
1:A:220:TYR:HB3	1:A:221:ILE:H	1.46	0.42
1:A:78:LYS:HG3	1:A:82:LEU:HD22	2.01	0.42
2:E:377:ALA:O	2:E:378:ALA:C	2.58	0.42
1:D:35:VAL:C	1:D:50:LEU:HD13	2.40	0.42
2:E:157:PRO:HA	2:E:182:MET:CE	2.42	0.42
1:D:151:SER:C	1:D:153:SER:H	2.23	0.42
2:B:172:LYS:HA	2:B:175:GLN:CG	2.50	0.42
2:E:358:ALA:O	2:E:359:LYS:C	2.55	0.42
1:D:104:MET:HE2	1:D:104:MET:HB3	1.57	0.42
2:E:248:TRP:C	2:E:249:GLU:CG	2.86	0.42
1:D:5:ASP:O	1:D:8:THR:HB	2.20	0.42
1:D:207:GLY:O	1:D:208:GLU:HB3	2.19	0.42
2:B:356:LEU:CD2	2:B:356:LEU:O	2.68	0.42
2:B:4:HIS:HB2	2:B:7:GLN:CG	2.48	0.42
2:B:17:LEU:HD23	2:B:17:LEU:N	2.35	0.42
2:E:311:VAL:HG12	2:E:313:ALA:H	1.85	0.42
1:A:133:LYS:C	1:A:134:ILE:HG12	2.39	0.42
1:A:22:PHE:HD1	1:A:23:HIS:N	2.17	0.42
2:B:277:LYS:O	2:B:278:LEU:C	2.58	0.42
1:D:57:ARG:NH2	1:D:86:ASP:HB3	2.35	0.42
2:B:198:ILE:HG23	2:B:211:CYS:HB3	2.02	0.42
2:B:142:HIS:CD2	2:B:142:HIS:N	2.79	0.41
2:E:196:ILE:HA	2:E:216:LEU:HD22	2.02	0.41
2:E:76:TRP:O	2:E:79:LYS:CG	2.67	0.41
2:B:81:LEU:HA	2:B:81:LEU:HD23	1.65	0.41
1:A:145:GLY:O	1:A:199:GLN:NE2	2.43	0.41
1:D:220:TYR:O	1:D:221:ILE:C	2.58	0.41
1:D:236:VAL:O	1:D:236:VAL:HG12	2.19	0.41
2:E:315:LEU:HD12	2:E:346:VAL:O	2.20	0.41
1:D:25:GLU:O	1:D:28:ILE:HB	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ASP:CG	2:E:225:ARG:HH12	2.24	0.41
2:B:97:LEU:HD23	2:B:97:LEU:HA	1.33	0.41
2:B:96:ILE:CG2	2:B:97:LEU:N	2.79	0.41
1:D:208:GLU:O	1:D:261:LYS:HE3	2.20	0.41
1:A:223:GLU:O	1:A:224:HIS:CG	2.72	0.41
1:A:273:VAL:HG12	1:A:275:SER:O	2.19	0.41
2:E:233:ARG:HD3	2:E:235:GLN:HE21	1.84	0.41
1:A:84:ALA:O	1:A:87:ALA:N	2.54	0.41
2:E:343:VAL:HG12	2:E:344:PRO:O	2.20	0.41
1:A:214:GLU:OE1	1:A:261:LYS:CE	2.63	0.41
2:E:268:LEU:HA	2:E:268:LEU:HD23	1.70	0.41
2:E:80:ARG:NH2	2:E:92:PRO:HD3	2.35	0.41
1:D:117:ARG:HH11	1:D:117:ARG:HD2	1.75	0.41
2:E:326:ASP:O	2:E:329:ALA:N	2.54	0.41
2:E:26:THR:O	2:E:27:THR:CG2	2.68	0.41
1:A:281:GLU:O	1:A:283:LEU:N	2.53	0.41
1:A:285:THR:O	1:A:288:LYS:N	2.49	0.41
2:B:374:LEU:C	2:B:374:LEU:HD12	2.41	0.41
2:E:386:GLU:O	2:E:388:LYS:N	2.53	0.41
1:D:128:THR:HA	1:D:129:PRO:HD3	1.72	0.41
1:D:146:LYS:HB2	1:D:201:GLU:CB	2.49	0.41
1:D:259:ASP:C	1:D:261:LYS:N	2.72	0.41
2:B:224:PHE:CA	2:B:230:ARG:NH1	2.84	0.41
1:A:288:LYS:HB2	1:A:288:LYS:NZ	2.36	0.41
2:E:191:ARG:HD3	4:E:409:HOH:O	2.20	0.41
1:A:104:MET:HE2	1:A:107:VAL:HB	1.94	0.41
1:D:4:ILE:HD11	1:D:126:VAL:HG22	2.01	0.41
1:A:160:ALA:HB3	1:A:161:VAL:H	1.64	0.41
1:A:229:VAL:O	1:A:229:VAL:HG13	2.20	0.41
2:B:245:ALA:HB1	2:B:250:LEU:HB2	2.03	0.41
2:B:279:HIS:O	2:B:382:VAL:CG2	2.60	0.41
2:E:157:PRO:CB	2:E:182:MET:HE3	2.50	0.41
2:B:215:LYS:C	2:B:216:LEU:CD2	2.68	0.41
2:E:295:LYS:O	2:E:296:GLU:C	2.59	0.41
1:D:141:ILE:HG13	1:D:141:ILE:H	1.63	0.41
2:E:55:GLY:O	2:E:58:GLY:N	2.32	0.41
1:A:279:ILE:O	1:A:280:GLY:C	2.58	0.41
2:B:20:PRO:HD3	2:B:210:ILE:CD1	2.51	0.41
1:A:32:THR:HG23	1:A:132:CYS:SG	2.60	0.41
1:D:158:TYR:C	1:D:161:VAL:HG23	2.40	0.41
1:D:109:VAL:H	1:D:109:VAL:HG23	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLN:H	1:D:26:GLN:HG2	1.35	0.41
1:D:136:ILE:O	1:D:137:GLN:O	2.39	0.41
2:E:216:LEU:HD22	2:E:216:LEU:HA	1.85	0.41
1:A:54:ASN:N	1:A:58:GLU:OE1	2.54	0.41
2:B:241:ARG:NH2	2:B:254:ALA:HB2	2.35	0.41
2:B:186:THR:O	2:B:187:ILE:C	2.59	0.41
2:B:150:ASP:O	2:B:153:THR:O	2.38	0.41
1:D:39:THR:O	1:D:40:PRO:C	2.56	0.41
1:D:133:LYS:C	1:D:134:ILE:HG12	2.34	0.41
1:D:158:TYR:CD1	1:D:158:TYR:N	2.89	0.41
2:B:137:ALA:C	2:B:139:GLU:N	2.74	0.41
2:B:141:PRO:CD	2:B:142:HIS:H	2.33	0.41
1:D:257:THR:HG1	1:D:260:GLU:HB2	1.71	0.41
2:E:324:ARG:CG	2:E:326:ASP:OD2	2.68	0.41
2:B:82:VAL:CG2	2:B:90:GLY:CA	2.99	0.41
2:B:84:TYR:CZ	2:B:85:GLN:HG3	2.56	0.41
1:A:112:ASP:C	1:A:114:ALA:N	2.71	0.41
1:D:218:ALA:C	1:D:220:TYR:N	2.69	0.41
2:E:28:PRO:O	2:E:32:GLU:CB	2.69	0.41
2:E:325:CYS:HB2	2:E:354:ALA:CA	2.47	0.41
2:B:4:HIS:O	2:B:5:GLU:C	2.59	0.41
2:B:155:PRO:C	2:B:156:MET:HG2	2.40	0.41
1:D:53:PHE:CE2	1:D:62:ALA:HB3	2.55	0.41
1:A:104:MET:O	1:A:107:VAL:N	2.52	0.41
1:D:147:VAL:O	1:D:171:GLN:HA	2.21	0.41
1:A:95:ILE:O	1:A:122:ASN:HA	2.21	0.41
1:A:133:LYS:O	1:A:134:ILE:HG23	2.21	0.41
1:A:27:ALA:HB1	1:A:32:THR:HB	2.02	0.41
2:B:318:ILE:HG22	2:B:319:PHE:N	2.28	0.41
2:E:249:GLU:O	2:E:250:LEU:HD23	2.21	0.41
2:E:182:MET:O	2:E:186:THR:OG1	2.29	0.41
2:E:195:LEU:CD2	2:E:195:LEU:C	2.88	0.41
2:E:324:ARG:HD3	2:E:327:LEU:HD12	2.01	0.41
1:A:53:PHE:CD2	1:A:59:ALA:HA	2.56	0.41
1:A:172:SER:HA	1:A:199:GLN:NE2	2.36	0.41
2:B:313:ALA:HA	2:B:343:VAL:CG1	2.45	0.41
2:E:20:PRO:CD	2:E:210:ILE:HD11	2.51	0.41
1:D:13:GLN:HG3	1:D:68:SER:OG	2.21	0.41
1:A:208:GLU:H	1:A:208:GLU:HG2	1.77	0.41
1:A:89:ILE:HD12	1:A:89:ILE:HG23	1.73	0.41
1:A:72:VAL:CG1	1:A:73:PRO:CD	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:72:PHE:O	2:E:75:ASN:CB	2.69	0.41
1:D:119:ILE:HD13	1:D:119:ILE:HA	1.68	0.41
1:D:89:ILE:HA	1:D:89:ILE:HD13	1.86	0.41
1:D:69:VAL:HA	1:D:93:ILE:O	2.21	0.41
2:E:229:LEU:HD23	2:E:229:LEU:HA	1.45	0.41
2:B:191:ARG:O	2:B:192:ASP:C	2.60	0.41
1:D:283:LEU:O	1:D:286:VAL:CG1	2.63	0.40
1:A:123:CYS:CB	1:A:124:PRO:CD	2.96	0.40
1:D:155:THR:O	1:D:158:TYR:N	2.54	0.40
2:B:41:GLY:HA2	2:B:43:TRP:CE2	2.56	0.40
2:E:248:TRP:C	2:E:249:GLU:HG3	2.41	0.40
1:A:92:ILE:CB	1:A:118:MET:HG3	2.51	0.40
2:E:112:ALA:HB2	2:E:123:PHE:CD2	2.55	0.40
2:E:3:LEU:HA	2:E:3:LEU:HD23	1.81	0.40
2:E:343:VAL:CG1	2:E:344:PRO:CG	2.92	0.40
1:D:203:ILE:O	1:D:229:VAL:HG23	2.05	0.40
1:D:217:ALA:O	1:D:220:TYR:HB3	2.21	0.40
1:D:267:ALA:O	1:D:269:GLY:N	2.53	0.40
1:D:283:LEU:HA	1:D:283:LEU:HD12	1.70	0.40
1:A:265:LEU:O	1:A:268:ALA:N	2.54	0.40
2:B:382:VAL:O	2:B:383:ALA:O	2.40	0.40
1:D:278:ASP:HB3	1:D:281:GLU:HB2	2.03	0.40
2:B:143:LEU:C	2:B:144:ILE:HD12	2.40	0.40
2:B:145:HIS:ND1	2:B:166:LYS:HD2	2.36	0.40
2:B:164:ALA:HA	2:B:167:LEU:HD12	2.03	0.40
2:E:196:ILE:CG2	2:E:197:GLU:N	2.84	0.40
2:B:328:ILE:CG2	2:B:329:ALA:N	2.46	0.40
2:E:299:THR:O	2:E:302:PHE:HB2	2.20	0.40
1:A:257:THR:O	1:A:258:ALA:C	2.60	0.40
2:B:386:GLU:HA	2:B:388:LYS:NZ	2.36	0.40
1:D:274:ARG:HG2	1:D:274:ARG:NH1	2.27	0.40
2:B:328:ILE:O	2:B:332:ILE:HG13	2.22	0.40
2:E:298:VAL:O	2:E:299:THR:C	2.59	0.40
2:E:164:ALA:CB	2:E:169:LEU:HD12	2.50	0.40
2:E:222:ALA:HB3	4:E:405:HOH:O	2.20	0.40
1:D:195:GLU:O	1:D:227:LYS:CE	2.69	0.40
1:D:220:TYR:C	1:D:220:TYR:CD2	2.95	0.40
1:A:187:PHE:O	1:A:188:ILE:C	2.58	0.40
1:A:24:SER:CA	4:A:297:HOH:O	2.34	0.40
2:E:63:VAL:HG13	2:E:64:ASN:H	1.87	0.40
2:E:275:ILE:CG2	2:E:276:VAL:CA	2.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:372:LYS:HB3	2:E:376:ASP:OD2	2.21	0.40
2:E:381:VAL:HG23	2:E:381:VAL:H	1.60	0.40
2:E:262:MET:HE2	2:E:301:ALA:C	2.41	0.40
2:E:257:GLY:HA2	2:E:282:GLU:HG3	2.04	0.40
2:E:38:ILE:HD13	2:E:38:ILE:HG21	1.81	0.40
3:A:289:COA:O9P	3:A:289:COA:H131	2.18	0.40
1:D:50:LEU:CB	1:D:51:PRO:CD	2.97	0.40
2:B:103:ASP:HB3	2:B:205:LYS:HB2	2.04	0.40
2:E:11:LEU:HA	2:E:11:LEU:HD23	1.77	0.40
1:A:273:VAL:HG11	1:A:275:SER:O	2.22	0.40
2:B:209:LEU:HA	2:B:209:LEU:HD23	1.68	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	285/288 (99%)	209 (73%)	52 (18%)	24 (8%)	1	1
1	D	285/288 (99%)	207 (73%)	53 (19%)	25 (9%)	1	1
2	B	386/388 (100%)	315 (82%)	59 (15%)	12 (3%)	5	7
2	E	386/388 (100%)	307 (80%)	57 (15%)	22 (6%)	2	2
All	All	1342/1352 (99%)	1038 (77%)	221 (16%)	83 (6%)	2	1

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	164	THR
1	A	213	ALA
1	A	219	ALA

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Mol	Chain	Res	Type
1	A	221	ILE
1	A	252	ALA
1	A	281	GLU
1	A	285	THR
2	B	87	ASP
2	B	293	ALA
2	B	383	ALA
1	D	3	LEU
1	D	96	THR
1	D	140	HIS
1	D	161	VAL
1	D	218	ALA
1	D	219	ALA
2	E	88	ALA
2	E	90	GLY
2	E	140	THR
2	E	320	GLY
2	E	324	ARG
2	E	327	LEU
2	E	384	ALA
1	A	139	GLY
1	A	140	HIS
1	A	161	VAL
1	A	188	ILE
1	A	189	ASP
1	A	220	TYR
1	A	245	GLY
1	A	254	GLY
1	A	286	VAL
2	B	136	VAL
2	B	141	PRO
2	B	320	GLY
2	B	372	LYS
2	B	374	LEU
1	D	139	GLY
1	D	169	PHE
1	D	245	GLY
1	D	253	GLY
1	D	264	ALA
1	D	285	THR
2	E	247	GLN
2	E	269	ALA

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Mol	Chain	Res	Type
2	E	295	LYS
2	E	325	CYS
2	E	337	ALA
2	E	387	GLY
1	A	282	ALA
2	B	384	ALA
1	D	62	ALA
1	D	263	ALA
1	D	278	ASP
1	D	284	LYS
2	E	293	ALA
2	E	352	ASN
1	A	22	PHE
1	A	160	ALA
2	B	363	ASP
1	D	18	SER
2	E	132	GLU
2	E	135	LYS
2	E	141	PRO
2	E	326	ASP
2	E	338	GLU
2	E	383	ALA
2	B	206	GLN
1	D	23	HIS
1	D	138	PRO
1	D	187	PHE
1	D	212	SER
1	D	260	GLU
1	A	74	ALA
1	A	187	PHE
1	A	214	GLU
1	A	218	ALA
2	B	166	LYS
1	D	162	LYS
1	D	183	PRO
1	D	35	VAL
2	E	323	VAL

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	217/217 (100%)	169 (78%)	48 (22%)	1 2
1	D	217/217 (100%)	159 (73%)	58 (27%)	0 1
2	B	298/298 (100%)	221 (74%)	77 (26%)	0 1
2	E	298/298 (100%)	218 (73%)	80 (27%)	0 1
All	All	1030/1030 (100%)	767 (74%)	263 (26%)	1 1

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	6	LYS
1	A	21	THR
1	A	26	GLN
1	A	35	VAL
1	A	48	LEU
1	A	69	VAL
1	A	77	CYS
1	A	80	SER
1	A	82	LEU
1	A	90	LYS
1	A	94	THR
1	A	95	ILE
1	A	96	THR
1	A	97	GLU
1	A	99	ILE
1	A	102	LEU
1	A	104	MET
1	A	113	GLU
1	A	126	VAL
1	A	128	THR
1	A	132	CYS
1	A	133	LYS
1	A	134	ILE
1	A	136	ILE
1	A	137	GLN
1	A	149	ILE
1	A	155	THR

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Mol	Chain	Res	Type
1	A	166	ASP
1	A	172	SER
1	A	193	MET
1	A	196	LYS
1	A	212	SER
1	A	216	GLU
1	A	221	ILE
1	A	223	GLU
1	A	225	VAL
1	A	226	THR
1	A	233	ILE
1	A	250	ILE
1	A	255	LYS
1	A	262	PHE
1	A	266	GLU
1	A	272	THR
1	A	274	ARG
1	A	283	LEU
1	A	286	VAL
1	A	287	LEU
2	B	3	LEU
2	B	14	ARG
2	B	32	GLU
2	B	36	SER
2	B	43	TRP
2	B	45	VAL
2	B	49	VAL
2	B	54	ARG
2	B	61	LYS
2	B	64	ASN
2	B	67	GLU
2	B	68	ASP
2	B	70	ARG
2	B	79	LYS
2	B	81	LEU
2	B	86	THR
2	B	87	ASP
2	B	97	LEU
2	B	102	THR
2	B	109	TYR
2	B	110	LEU
2	B	120	ARG

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Mol	Chain	Res	Type
2	B	121	VAL
2	B	122	VAL
2	B	124	MET
2	B	126	SER
2	B	127	THR
2	B	128	GLU
2	B	133	ILE
2	B	140	THR
2	B	144	ILE
2	B	147	VAL
2	B	152	LEU
2	B	158	TYR
2	B	179	LYS
2	B	180	ILE
2	B	184	LEU
2	B	187	ILE
2	B	195	LEU
2	B	202	VAL
2	B	205	LYS
2	B	210	ILE
2	B	211	CYS
2	B	232	MET
2	B	233	ARG
2	B	235	GLN
2	B	241	ARG
2	B	255	LEU
2	B	258	ASN
2	B	262	MET
2	B	264	ASN
2	B	275	ILE
2	B	278	LEU
2	B	285	ASN
2	B	303	LYS
2	B	311	VAL
2	B	318	ILE
2	B	319	PHE
2	B	327	LEU
2	B	333	ILE
2	B	338	GLU
2	B	339	VAL
2	B	343	VAL
2	B	348	ARG

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Mol	Chain	Res	Type
2	B	349	LEU
2	B	356	LEU
2	B	360	LYS
2	B	361	LEU
2	B	364	SER
2	B	366	LEU
2	B	367	ASN
2	B	374	LEU
2	B	375	THR
2	B	380	GLN
2	B	381	VAL
2	B	386	GLU
2	B	388	LYS
1	D	1	SER
1	D	3	LEU
1	D	4	ILE
1	D	5	ASP
1	D	11	ILE
1	D	12	CYS
1	D	16	THR
1	D	26	GLN
1	D	28	ILE
1	D	34	MET
1	D	35	VAL
1	D	46	THR
1	D	48	LEU
1	D	52	VAL
1	D	69	VAL
1	D	77	CYS
1	D	97	GLU
1	D	102	LEU
1	D	105	LEU
1	D	117	ARG
1	D	127	ILE
1	D	128	THR
1	D	131	GLU
1	D	132	CYS
1	D	133	LYS
1	D	134	ILE
1	D	136	ILE
1	D	137	GLN
1	D	141	ILE

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Mol	Chain	Res	Type
1	D	146	LYS
1	D	147	VAL
1	D	149	ILE
1	D	152	ARG
1	D	153	SER
1	D	155	THR
1	D	161	VAL
1	D	172	SER
1	D	173	THR
1	D	174	CYS
1	D	185	SER
1	D	190	ILE
1	D	193	MET
1	D	221	ILE
1	D	222	LYS
1	D	229	VAL
1	D	237	THR
1	D	243	ARG
1	D	250	ILE
1	D	262	PHE
1	D	265	LEU
1	D	272	THR
1	D	273	VAL
1	D	274	ARG
1	D	276	LEU
1	D	278	ASP
1	D	283	LEU
1	D	287	LEU
1	D	288	LYS
2	E	2	ASN
2	E	14	ARG
2	E	26	THR
2	E	36	SER
2	E	37	LYS
2	E	43	TRP
2	E	45	VAL
2	E	49	VAL
2	E	56	LYS
2	E	61	LYS
2	E	70	ARG
2	E	79	LYS
2	E	81	LEU

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Mol	Chain	Res	Type
2	E	89	ASN
2	E	96	ILE
2	E	97	LEU
2	E	103	ASP
2	E	106	LYS
2	E	110	LEU
2	E	113	VAL
2	E	119	ARG
2	E	124	MET
2	E	128	GLU
2	E	132	GLU
2	E	133	ILE
2	E	135	LYS
2	E	138	GLU
2	E	146	LYS
2	E	152	LEU
2	E	159	GLN
2	E	179	LYS
2	E	180	ILE
2	E	187	ILE
2	E	190	GLU
2	E	205	LYS
2	E	208	ASP
2	E	215	LYS
2	E	216	LEU
2	E	225	ARG
2	E	226	GLN
2	E	230	ARG
2	E	235	GLN
2	E	241	ARG
2	E	255	LEU
2	E	256	ASP
2	E	258	ASN
2	E	262	MET
2	E	268	LEU
2	E	270	MET
2	E	275	ILE
2	E	277	LYS
2	E	278	LEU
2	E	282	GLU
2	E	294	THR
2	E	295	LYS

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Mol	Chain	Res	Type
2	E	307	SER
2	E	310	LYS
2	E	312	LYS
2	E	318	ILE
2	E	322	ILE
2	E	325	CYS
2	E	339	VAL
2	E	341	VAL
2	E	342	ASN
2	E	347	VAL
2	E	352	ASN
2	E	355	GLU
2	E	356	LEU
2	E	360	LYS
2	E	361	LEU
2	E	366	LEU
2	E	367	ASN
2	E	368	ILE
2	E	369	ILE
2	E	374	LEU
2	E	375	THR
2	E	380	GLN
2	E	385	VAL
2	E	386	GLU
2	E	388	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	137	GLN
1	A	224	HIS
2	B	4	HIS
2	B	64	ASN
2	B	95	GLN
2	B	142	HIS
2	B	159	GLN
2	B	235	GLN
2	B	258	ASN
2	B	285	ASN
2	B	367	ASN
2	B	380	GLN

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Mol	Chain	Res	Type
1	D	137	GLN
2	E	4	HIS
2	E	10	GLN
2	E	50	HIS
2	E	89	ASN
2	E	142	HIS
2	E	176	GLN
2	E	226	GLN
2	E	235	GLN
2	E	258	ASN
2	E	264	ASN
2	E	352	ASN
2	E	367	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	NEP	A	246	1	10,14,15	1.40	2 (20%)	4,20,22	1.03	0
1	NEP	D	246	1	10,14,15	1.58	2 (20%)	4,20,22	0.99	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
1	NEP	A	246	1	-	0/4/12/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NEP	D	246	1	-	0/4/12/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	NEP	P-O2P	-3.79	1.46	1.54
1	A	246	NEP	P-O2P	-2.70	1.48	1.54
1	D	246	NEP	P-O1P	-2.30	1.49	1.54
1	A	246	NEP	CD2-CG	2.27	1.39	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	246	NEP	4	0
1	D	246	NEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	COA	A	289	-	40,50,50	0.89	1 (2%)	50,75,75	2.69	8 (16%)
3	COA	D	289	-	40,50,50	0.88	1 (2%)	50,75,75	1.35	4 (8%)

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
3	COA	A	289	-	-	0/44/64/64	0/3/3/3
3	COA	D	289	-	-	0/44/64/64	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	289	COA	C4A-N3A	-2.04	1.32	1.35
3	D	289	COA	C6P-C5P	2.53	1.56	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	289	COA	O8A-P3B-O7A	-10.80	75.80	110.58
3	D	289	COA	P2A-O3A-P1A	-5.98	115.93	132.73
3	A	289	COA	C4B-O4B-C1B	-4.27	105.03	109.72
3	A	289	COA	C7P-N8P-C9P	-4.10	114.41	122.53
3	A	289	COA	CDP-CBP-CCP	-3.04	104.56	108.50
3	D	289	COA	C4B-O4B-C1B	-2.47	107.00	109.72
3	A	289	COA	O2B-C2B-C3B	2.45	118.25	111.16
3	D	289	COA	O8A-P3B-O7A	2.75	119.42	110.58
3	D	289	COA	O6A-CCP-CBP	2.78	115.01	110.55
3	A	289	COA	CEP-CBP-CCP	2.85	112.19	108.50
3	A	289	COA	O2A-P1A-O3A	4.34	124.78	105.09
3	A	289	COA	O9A-P3B-O7A	12.00	149.20	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	289	COA	13	0
3	D	289	COA	17	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.