



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:37 AM UTC

PDB ID : 1SCU / pdb_00001scu
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

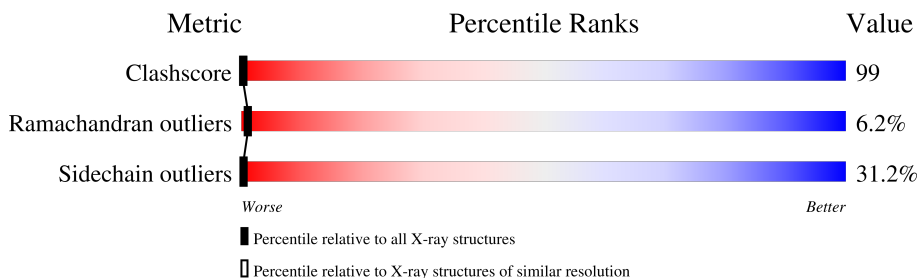
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	288	15% 40% 35% 9%
1	D	288	12% 39% 37% 11%
2	B	388	15% 46% 31% 8%
2	E	388	17% 39% 34% 11%

2 Entry composition [i](#)

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.

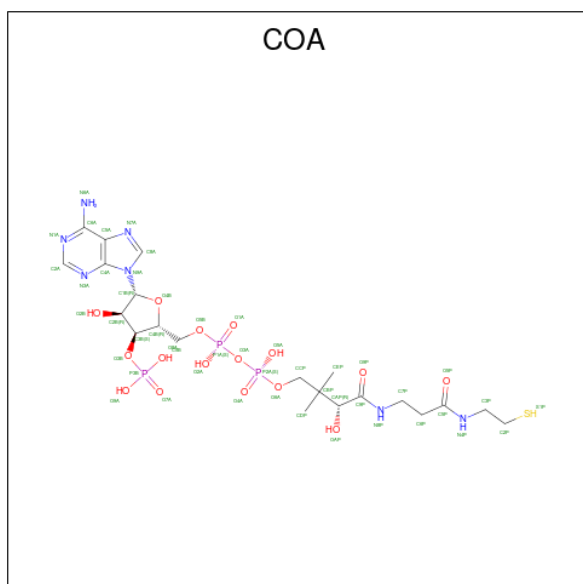
- Molecule 1 is a protein called SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT.

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 (CCD ID: 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.

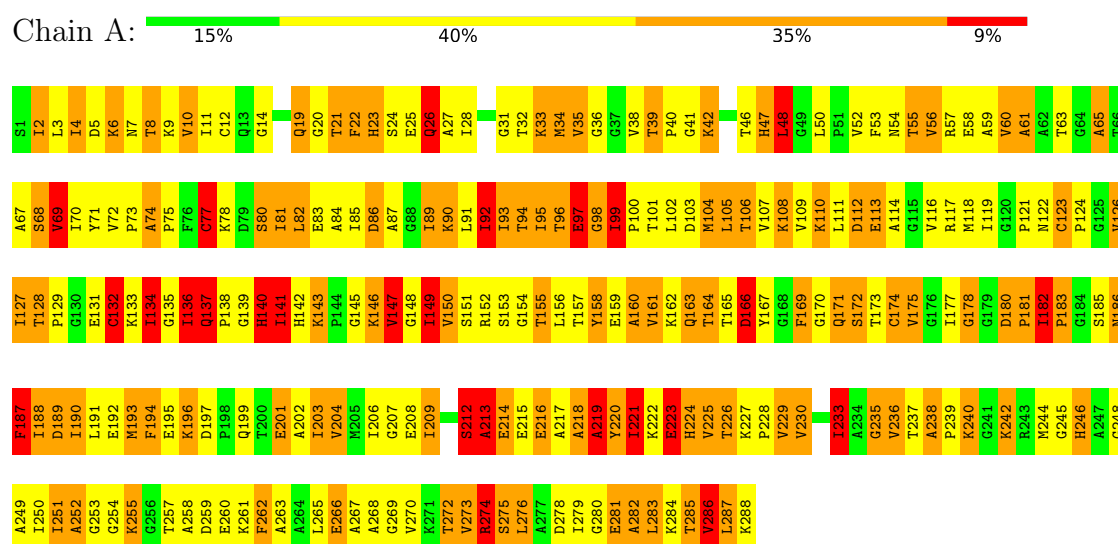
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	33	Total	O	0	0
			33	33		
4	D	25	Total	O	0	0
			25	25		
4	E	30	Total	O	0	0
			30	30		

3 Residue-property plots

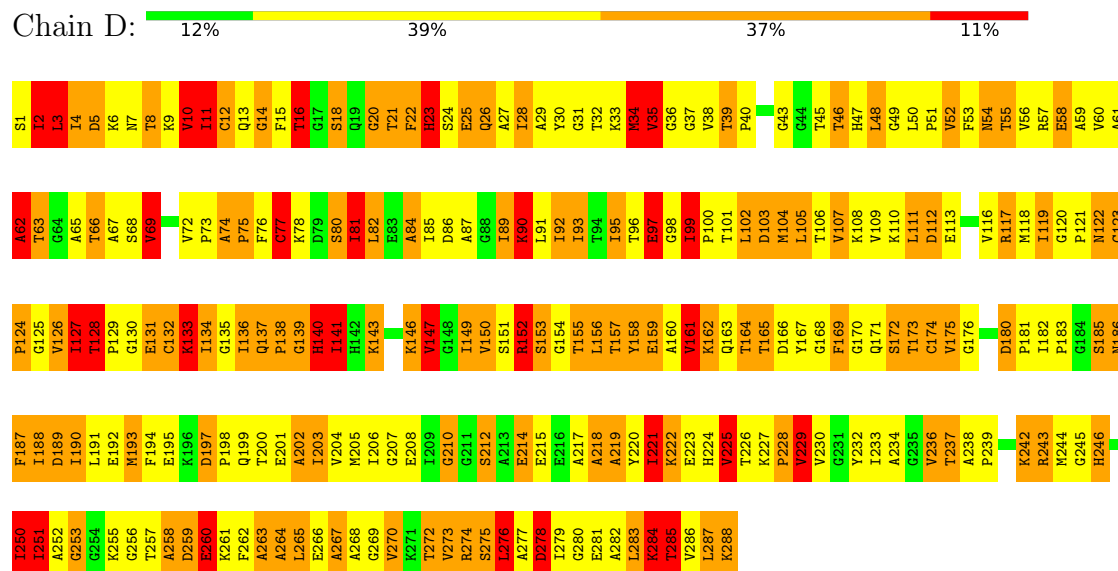
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

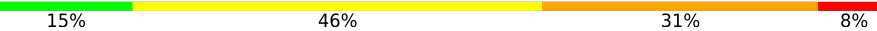
• Molecule 1: SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT

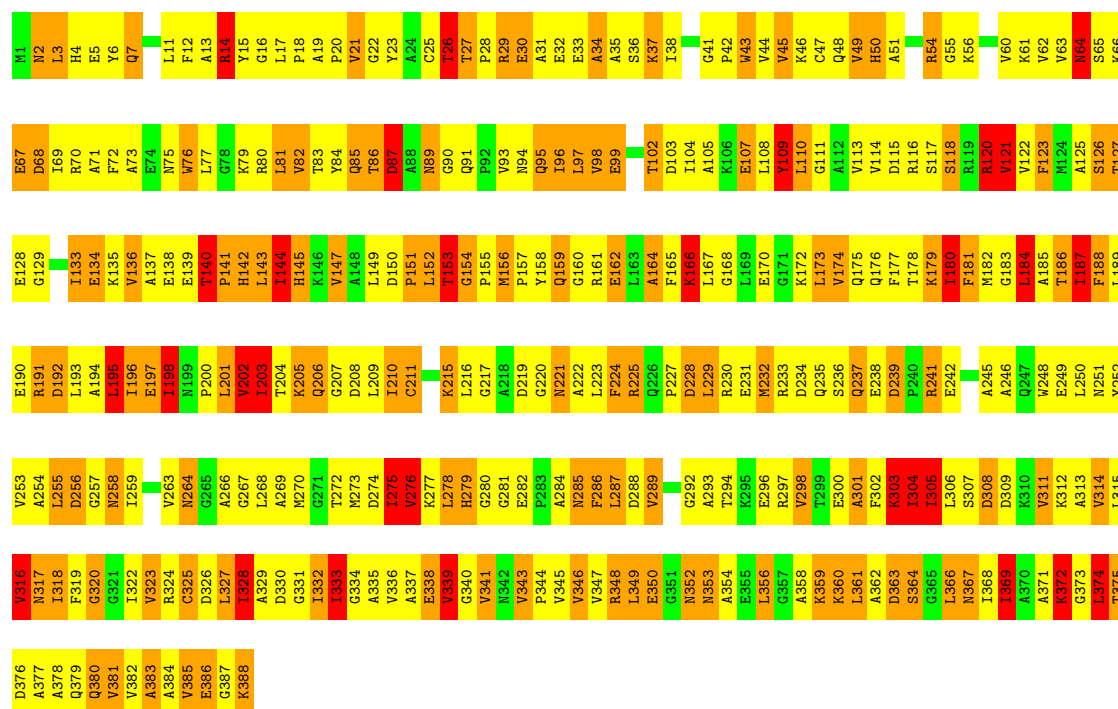


• Molecule 1: SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT

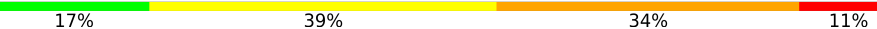


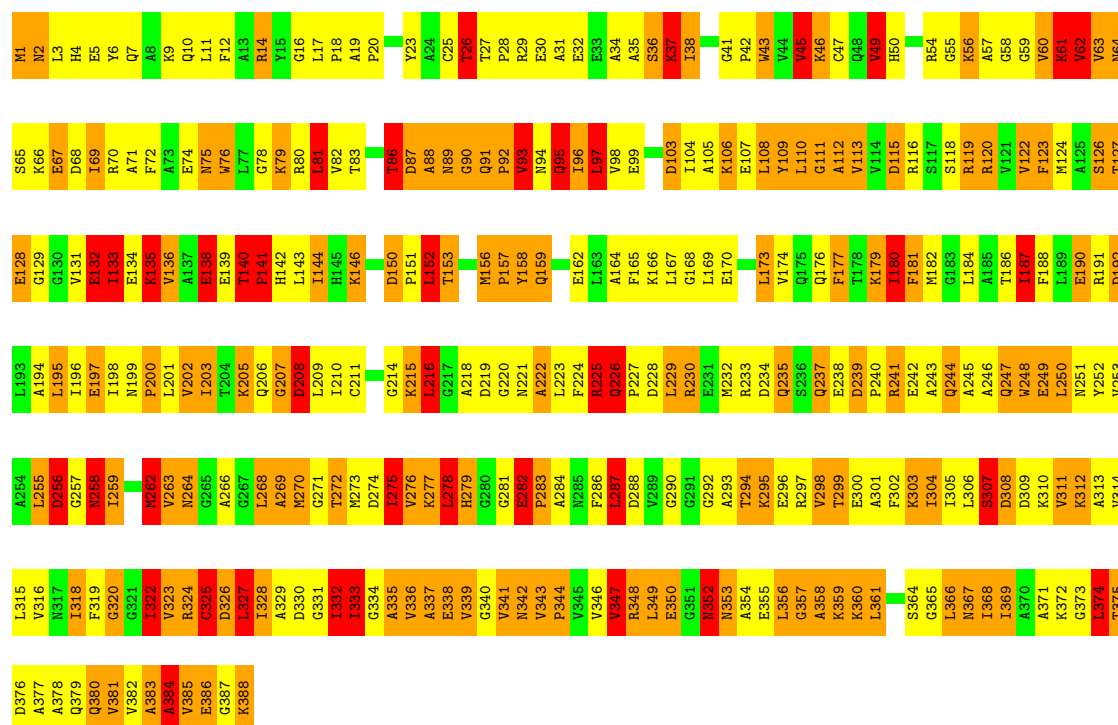
• Molecule 2: SUCCINYL-COA SYNTHETASE, BETA SUBUNIT

Chain B: 



● Molecule 2: SUCCINYL-COA SYNTHETASE, BETA SUBUNIT

Chain E: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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: NEP, COA

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	1.84	32/2101 (1.5%)	2.27	108/2842 (3.8%)
1	D	1.84	33/2101 (1.6%)	2.30	114/2842 (4.0%)
2	B	1.90	53/2950 (1.8%)	2.22	142/3989 (3.6%)
2	E	1.91	50/2950 (1.7%)	2.27	156/3989 (3.9%)
All	All	1.88	168/10102 (1.7%)	2.26	520/13662 (3.8%)

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 (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	THR	CA-C	-8.80	1.42	1.52
2	B	180	ILE	CA-CB	-8.52	1.44	1.54
2	E	180	ILE	CA-CB	-8.33	1.44	1.54
2	B	197	GLU	N-CA	-7.83	1.37	1.46
1	A	204	VAL	CA-CB	-7.81	1.44	1.54
2	E	19	ALA	N-CA	-7.66	1.38	1.45
2	E	203	ILE	CA-CB	-7.62	1.45	1.54
2	E	349	LEU	CA-C	-7.42	1.43	1.52
1	A	249	ALA	CA-C	-7.37	1.45	1.53
1	A	223	GLU	N-CA	-7.25	1.38	1.46
2	B	359	LYS	N-CA	-7.17	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	114	VAL	CA-CB	-7.12	1.45	1.54
1	A	2	ILE	CA-CB	-7.04	1.44	1.54
1	D	93	ILE	CA-CB	-6.99	1.44	1.54
2	B	95	GLN	CA-C	-6.88	1.44	1.52
2	B	96	ILE	CA-CB	-6.86	1.45	1.54
2	E	195	LEU	N-CA	-6.85	1.37	1.46
2	B	118	SER	CA-C	-6.79	1.43	1.52
2	B	188	PHE	CA-C	-6.72	1.43	1.52
2	B	192	ASP	CG-OD2	6.68	1.38	1.25
2	B	96	ILE	CA-C	-6.67	1.44	1.52
1	A	171	GLN	CA-C	-6.67	1.44	1.52
2	E	332	ILE	CA-CB	-6.67	1.46	1.54
1	A	2	ILE	N-CA	-6.66	1.38	1.46
1	D	39	THR	N-CA	-6.65	1.40	1.46
2	E	95	GLN	C-N	-6.65	1.24	1.33
1	D	74	ALA	C-N	-6.62	1.28	1.33
1	D	22	PHE	C-N	-6.59	1.25	1.33
2	E	2	ASN	CA-C	-6.58	1.44	1.52
2	E	298	VAL	CA-CB	-6.57	1.46	1.54
2	E	187	ILE	CA-CB	-6.46	1.46	1.54
2	B	195	LEU	N-CA	-6.42	1.38	1.46
1	A	68	SER	CA-C	-6.40	1.44	1.52
1	A	235	GLY	C-N	-6.36	1.25	1.33
2	B	333	ILE	N-CA	-6.33	1.39	1.46
1	D	156	LEU	C-N	-6.31	1.25	1.33
2	E	45	VAL	CA-CB	-6.29	1.46	1.54
2	E	174	VAL	CA-CB	-6.21	1.47	1.54
2	E	239	ASP	C-N	-6.21	1.26	1.34
2	E	87	ASP	N-CA	-6.18	1.38	1.46
2	E	198	ILE	CA-CB	-6.18	1.46	1.53
2	E	194	ALA	C-N	-6.17	1.25	1.33
2	B	162	GLU	CD-OE2	6.16	1.37	1.25
2	B	29	ARG	C-O	-6.14	1.17	1.24
1	D	112	ASP	CA-C	-6.13	1.45	1.52
2	E	350	GLU	N-CA	-6.10	1.38	1.46
1	D	180	ASP	CA-C	-6.09	1.45	1.53
1	D	103	ASP	CG-OD2	6.09	1.36	1.25
2	E	127	THR	N-CA	-6.08	1.38	1.46
1	A	81	ILE	CA-CB	-6.05	1.46	1.54
2	E	304	ILE	C-N	-6.05	1.26	1.33
1	A	183	PRO	CA-C	-6.04	1.46	1.52
2	E	86	THR	CA-C	-6.03	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	21	VAL	CA-C	-6.00	1.45	1.52
2	B	174	VAL	CA-CB	-5.96	1.47	1.54
2	B	164	ALA	CA-C	-5.93	1.45	1.52
2	E	120	ARG	CA-C	-5.91	1.45	1.52
1	A	101	THR	CA-CB	-5.89	1.44	1.53
1	D	10	VAL	C-N	-5.88	1.25	1.33
2	E	250	LEU	CA-C	-5.88	1.45	1.52
1	D	200	THR	CA-C	-5.88	1.45	1.52
2	E	229	LEU	CA-C	-5.84	1.44	1.52
1	A	175	VAL	CA-CB	-5.83	1.46	1.54
2	B	297	ARG	N-CA	-5.83	1.39	1.46
1	A	39	THR	CA-CB	5.83	1.58	1.53
1	A	180	ASP	CG-OD2	5.82	1.36	1.25
2	E	350	GLU	CD-OE2	5.81	1.36	1.25
2	E	263	VAL	N-CA	-5.80	1.39	1.46
1	A	90	LYS	C-N	-5.77	1.25	1.33
2	B	151	PRO	C-N	-5.76	1.26	1.33
1	D	80	SER	CA-C	-5.76	1.46	1.52
2	B	11	LEU	CA-C	-5.75	1.45	1.52
2	B	96	ILE	N-CA	-5.73	1.39	1.46
1	D	58	GLU	CD-OE2	5.71	1.36	1.25
2	E	46	LYS	CA-C	-5.71	1.45	1.52
2	E	141	PRO	N-CA	-5.71	1.40	1.47
1	D	188	ILE	CA-CB	-5.70	1.46	1.54
2	B	346	VAL	CA-CB	-5.68	1.47	1.54
2	B	62	VAL	CA-CB	-5.68	1.47	1.54
2	E	262	MET	CA-C	-5.68	1.46	1.53
2	E	60	VAL	CA-CB	-5.68	1.45	1.55
2	B	144	ILE	CA-C	-5.67	1.45	1.52
1	D	75	PRO	CA-C	-5.66	1.47	1.52
2	E	266	ALA	CA-C	-5.64	1.45	1.52
1	A	147	VAL	CA-C	-5.64	1.46	1.52
1	D	157	THR	N-CA	-5.64	1.39	1.46
1	D	221	ILE	N-CA	-5.64	1.39	1.46
1	A	108	LYS	CA-C	-5.61	1.45	1.52
2	B	75	ASN	N-CA	-5.61	1.39	1.46
1	D	23	HIS	N-CA	-5.59	1.39	1.46
1	D	104	MET	C-N	-5.59	1.26	1.34
2	B	353	ASN	N-CA	-5.58	1.39	1.46
2	B	341	VAL	CA-CB	-5.57	1.47	1.53
2	B	21	VAL	CA-CB	-5.56	1.47	1.54
2	B	317	ASN	CA-C	-5.56	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	23	TYR	CA-C	-5.56	1.45	1.52
1	D	127	ILE	N-CA	-5.54	1.39	1.46
2	B	308	ASP	CG-OD2	5.53	1.35	1.25
2	B	125	ALA	CA-C	-5.52	1.45	1.52
1	D	251	ILE	N-CA	-5.51	1.39	1.46
2	E	216	LEU	CA-C	-5.51	1.46	1.52
2	B	350	GLU	CA-C	-5.50	1.46	1.52
2	E	347	VAL	CA-CB	-5.50	1.47	1.54
1	A	34	MET	N-CA	-5.50	1.39	1.46
1	D	251	ILE	CA-C	-5.48	1.46	1.52
1	A	68	SER	N-CA	-5.46	1.39	1.46
1	D	236	VAL	CA-CB	-5.45	1.47	1.54
2	B	191	ARG	CA-C	-5.41	1.45	1.52
1	D	141	ILE	CA-CB	-5.39	1.49	1.54
2	B	174	VAL	N-CA	-5.39	1.40	1.46
2	B	303	LYS	C-N	-5.38	1.26	1.33
1	A	92	ILE	CA-CB	-5.38	1.46	1.55
2	E	104	ILE	CA-C	-5.38	1.47	1.53
2	B	347	VAL	CA-C	-5.38	1.46	1.52
2	E	314	VAL	CA-CB	-5.38	1.47	1.54
2	B	215	LYS	CA-C	-5.38	1.46	1.52
1	A	97	GLU	N-CA	-5.38	1.39	1.45
1	A	56	VAL	N-CA	-5.37	1.40	1.46
1	D	97	GLU	N-CA	-5.37	1.39	1.46
2	E	153	THR	CA-C	-5.36	1.45	1.53
1	A	56	VAL	CA-CB	-5.35	1.48	1.54
1	D	72	VAL	C-N	-5.32	1.27	1.33
2	B	159	GLN	N-CA	-5.31	1.39	1.46
1	D	89	ILE	CA-C	-5.31	1.47	1.52
2	E	132	GLU	CD-OE1	5.31	1.35	1.25
2	E	350	GLU	CA-C	-5.30	1.46	1.52
2	E	162	GLU	CD-OE2	5.30	1.35	1.25
1	D	127	ILE	CA-CB	-5.28	1.47	1.54
2	E	336	VAL	CA-CB	-5.28	1.47	1.54
2	B	314	VAL	CA-CB	-5.27	1.47	1.54
1	D	11	ILE	CA-CB	-5.26	1.45	1.55
1	D	63	THR	C-N	-5.26	1.26	1.33
2	B	93	VAL	N-CA	-5.26	1.40	1.46
2	E	208	ASP	CA-C	-5.26	1.45	1.53
1	A	61	ALA	N-CA	-5.25	1.39	1.46
2	B	333	ILE	CA-C	-5.24	1.46	1.52
2	E	298	VAL	C-N	-5.24	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLY	C-N	-5.22	1.28	1.33
2	B	173	LEU	C-N	-5.22	1.27	1.33
2	E	144	ILE	N-CA	-5.21	1.40	1.46
2	B	123	PHE	CA-C	-5.19	1.46	1.52
2	B	145	HIS	CA-C	-5.19	1.46	1.52
1	A	175	VAL	N-CA	-5.19	1.39	1.46
2	E	344	PRO	CA-C	-5.18	1.46	1.52
2	E	18	PRO	N-CA	-5.18	1.40	1.47
1	D	189	ASP	N-CA	-5.18	1.40	1.46
1	A	242	LYS	CA-C	-5.17	1.46	1.52
2	B	109	TYR	CA-C	-5.17	1.46	1.52
2	B	328	ILE	CA-CB	-5.17	1.47	1.54
1	A	55	THR	CA-C	-5.13	1.46	1.52
2	B	99	GLU	N-CA	-5.13	1.39	1.45
1	D	107	VAL	C-N	-5.13	1.27	1.33
1	D	180	ASP	C-N	-5.13	1.26	1.33
2	E	96	ILE	N-CA	-5.12	1.40	1.46
1	A	204	VAL	N-CA	-5.11	1.40	1.46
2	B	229	LEU	CA-C	-5.09	1.46	1.52
2	E	156	MET	CA-C	-5.09	1.45	1.53
1	A	105	LEU	C-N	-5.08	1.26	1.33
2	B	304	ILE	CA-CB	-5.08	1.47	1.54
2	B	332	ILE	CA-CB	-5.08	1.48	1.54
2	E	152	LEU	CA-C	-5.06	1.46	1.53
1	D	158	TYR	C-N	-5.06	1.27	1.33
2	E	109	TYR	N-CA	-5.06	1.39	1.46
1	A	86	ASP	CA-C	-5.04	1.46	1.52
1	A	127	ILE	CA-CB	-5.04	1.47	1.54
2	B	231	GLU	CA-C	-5.03	1.45	1.52
2	E	198	ILE	CA-C	-5.03	1.46	1.52
2	B	276	VAL	CA-CB	-5.02	1.48	1.54

All (520) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	HIS	CA-CB-CG	-16.06	97.74	113.80
1	A	23	HIS	CA-CB-CG	-14.14	99.66	113.80
2	E	228	ASP	CA-CB-CG	-12.69	99.91	112.60
1	D	23	HIS	CA-CB-CG	-11.85	101.95	113.80
2	E	348	ARG	CD-NE-CZ	11.25	140.15	124.40
2	E	180	ILE	CB-CA-C	-11.14	97.45	112.04
2	B	104	ILE	N-CA-C	10.84	122.76	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	353	ASN	CA-CB-CG	-10.61	101.99	112.60
1	D	72	VAL	CA-C-O	10.49	126.02	119.51
2	B	121	VAL	N-CA-CB	10.30	121.95	110.72
2	B	228	ASP	CA-CB-CG	-10.08	102.52	112.60
1	D	203	ILE	N-CA-C	9.95	123.28	108.46
1	A	2	ILE	CA-C-N	-9.94	104.83	122.42
1	A	2	ILE	C-N-CA	-9.94	104.83	122.42
1	D	140	HIS	CA-C-N	-9.80	109.81	122.16
1	D	140	HIS	C-N-CA	-9.80	109.81	122.16
1	D	186	ASN	CA-CB-CG	-9.78	102.82	112.60
1	D	93	ILE	CB-CA-C	-9.69	99.36	110.41
2	E	76	TRP	N-CA-CB	-9.65	97.25	110.67
2	B	325	CYS	CB-CA-C	9.41	125.87	110.81
2	E	275	ILE	CB-CA-C	-9.38	99.48	112.14
1	A	70	ILE	N-CA-CB	-9.37	99.45	111.64
2	B	37	LYS	N-CA-C	-9.35	102.00	113.50
1	D	197	ASP	N-CA-CB	9.26	123.53	110.01
1	A	224	HIS	CA-CB-CG	-9.18	104.62	113.80
2	E	69	ILE	CB-CA-C	-9.15	100.26	111.97
2	E	343	VAL	CA-C-N	9.13	129.21	119.90
2	E	343	VAL	C-N-CA	9.13	129.21	119.90
2	E	115	ASP	CA-CB-CG	-9.11	103.49	112.60
2	E	92	PRO	CB-CA-C	-9.04	100.53	111.11
1	A	178	GLY	CA-C-O	-9.00	116.37	122.22
2	E	153	THR	N-CA-C	-8.95	96.65	110.17
1	A	90	LYS	CA-C-O	8.88	128.62	118.77
1	A	175	VAL	N-CA-C	8.84	120.65	107.75
1	A	112	ASP	CA-CB-CG	-8.82	103.78	112.60
2	E	97	LEU	CA-C-N	-8.70	111.81	123.12
2	E	97	LEU	C-N-CA	-8.70	111.81	123.12
2	E	202	VAL	CB-CA-C	-8.69	97.44	110.82
2	E	180	ILE	N-CA-CB	-8.67	99.63	110.47
1	A	186	ASN	CA-CB-CG	-8.60	104.00	112.60
1	D	225	VAL	CB-CA-C	8.60	122.16	110.99
2	E	353	ASN	CA-CB-CG	-8.59	104.01	112.60
2	B	140	THR	C-N-CD	-8.55	89.94	125.00
1	A	99	ILE	N-CA-C	8.36	116.54	107.60
2	B	153	THR	CA-C-N	-8.34	108.78	121.87
2	B	153	THR	C-N-CA	-8.34	108.78	121.87
2	E	1	MET	CA-C-N	-8.33	108.14	123.05
2	E	1	MET	C-N-CA	-8.33	108.14	123.05
2	E	347	VAL	N-CA-C	8.22	119.96	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	153	THR	CA-C-N	-8.19	109.02	121.87
2	E	153	THR	C-N-CA	-8.19	109.02	121.87
2	B	333	ILE	CB-CA-C	-8.16	101.61	111.81
1	D	11	ILE	N-CA-CB	-8.12	96.74	111.92
2	E	309	ASP	CA-CB-CG	-8.12	104.48	112.60
1	A	213	ALA	N-CA-CB	-8.10	96.80	110.49
2	B	187	ILE	CB-CA-C	-8.02	101.61	111.88
2	B	276	VAL	CB-CA-C	-7.99	101.55	112.02
2	E	256	ASP	N-CA-C	7.99	126.78	114.64
1	D	104	MET	CA-C-O	7.90	129.03	120.10
2	E	122	VAL	CB-CA-C	-7.78	99.03	110.62
2	E	282	GLU	CA-C-N	7.67	127.68	119.78
2	E	282	GLU	C-N-CA	7.67	127.68	119.78
2	B	369	ILE	CB-CA-C	-7.65	101.63	110.73
2	E	225	ARG	CB-CA-C	-7.62	98.28	111.23
2	B	156	MET	CA-C-N	7.60	127.98	119.32
2	B	156	MET	C-N-CA	7.60	127.98	119.32
2	B	339	VAL	CB-CA-C	-7.57	102.10	112.02
2	B	120	ARG	CA-C-N	-7.53	112.65	122.37
2	B	120	ARG	C-N-CA	-7.53	112.65	122.37
2	B	113	VAL	CB-CA-C	-7.52	98.95	111.29
2	B	145	HIS	CA-CB-CG	-7.51	106.29	113.80
1	D	93	ILE	O-C-N	7.48	129.71	122.97
1	A	65	ALA	O-C-N	-7.48	114.26	122.79
1	A	69	VAL	CB-CA-C	-7.48	98.91	110.95
2	E	2	ASN	CA-CB-CG	-7.46	105.14	112.60
1	D	152	ARG	N-CA-CB	-7.45	99.77	110.57
2	E	89	ASN	CA-CB-CG	-7.43	105.17	112.60
2	E	49	VAL	N-CA-CB	-7.42	98.64	112.36
2	E	86	THR	N-CA-CB	7.41	120.61	109.94
1	A	229	VAL	N-CA-C	7.41	118.79	108.12
2	B	2	ASN	CA-CB-CG	-7.37	105.23	112.60
2	E	350	GLU	N-CA-C	7.37	120.93	109.07
2	B	196	ILE	CA-C-N	-7.34	110.67	121.76
2	B	196	ILE	C-N-CA	-7.34	110.67	121.76
1	D	210	GLY	CA-C-N	-7.34	110.53	122.05
1	D	210	GLY	C-N-CA	-7.34	110.53	122.05
2	E	123	PHE	CA-C-N	-7.34	110.48	122.81
2	E	123	PHE	C-N-CA	-7.34	110.48	122.81
2	B	279	HIS	CA-CB-CG	-7.33	106.47	113.80
1	D	259	ASP	CA-CB-CG	-7.32	105.28	112.60
2	E	259	ILE	CB-CA-C	-7.27	100.44	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	352	ASN	N-CA-C	7.25	121.01	110.28
2	E	14	ARG	N-CA-C	-7.23	103.55	112.38
2	B	369	ILE	CA-C-N	-7.21	110.86	121.24
2	B	369	ILE	C-N-CA	-7.21	110.86	121.24
1	A	137	GLN	N-CA-CB	-7.15	97.64	110.37
2	B	358	ALA	CA-C-N	-7.14	110.91	120.63
2	B	358	ALA	C-N-CA	-7.14	110.91	120.63
2	E	264	ASN	N-CA-CB	-7.14	99.93	110.49
2	E	304	ILE	CA-C-N	-7.11	111.60	120.56
2	E	304	ILE	C-N-CA	-7.11	111.60	120.56
1	A	275	SER	N-CA-CB	7.08	121.69	110.57
2	E	140	THR	CA-C-N	7.07	128.68	119.84
2	E	140	THR	C-N-CA	7.07	128.68	119.84
2	B	121	VAL	CA-C-N	-7.06	113.31	123.06
2	B	121	VAL	C-N-CA	-7.06	113.31	123.06
2	B	64	ASN	N-CA-C	7.06	122.06	113.38
1	A	47	HIS	CA-CB-CG	7.05	120.85	113.80
1	A	146	LYS	CA-C-N	-7.02	114.04	123.10
1	A	146	LYS	C-N-CA	-7.02	114.04	123.10
1	D	188	ILE	CA-CB-CG2	-7.02	98.56	110.50
1	A	90	LYS	CA-C-N	-7.01	110.55	122.33
1	A	90	LYS	C-N-CA	-7.01	110.55	122.33
1	D	188	ILE	CA-C-N	-7.01	111.05	120.79
1	D	188	ILE	C-N-CA	-7.01	111.05	120.79
2	E	37	LYS	N-CA-C	-7.01	104.60	113.01
2	E	157	PRO	CA-C-N	-7.00	109.39	120.60
2	E	157	PRO	C-N-CA	-7.00	109.39	120.60
1	D	11	ILE	CA-CB-CG2	-7.00	98.60	110.50
2	B	180	ILE	CB-CA-C	-6.99	103.02	111.97
2	B	102	THR	CB-CA-C	6.98	122.15	109.37
2	E	177	PHE	CA-CB-CG	-6.98	106.82	113.80
2	E	201	LEU	N-CA-C	-6.96	97.17	108.52
2	B	316	VAL	CB-CA-C	-6.96	101.31	111.68
2	E	113	VAL	CB-CA-C	-6.96	99.88	111.29
2	B	196	ILE	CB-CA-C	-6.95	98.69	110.71
1	A	262	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	132	CYS	N-CA-C	6.93	120.59	108.75
2	E	64	ASN	N-CA-C	6.90	122.69	113.72
1	A	169	PHE	N-CA-C	6.88	122.66	111.37
2	B	153	THR	N-CA-C	-6.86	99.51	110.14
1	D	250	ILE	CA-C-N	-6.85	113.51	123.10
1	D	250	ILE	C-N-CA	-6.85	113.51	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	189	LEU	CA-C-N	-6.83	111.12	120.28
2	B	189	LEU	C-N-CA	-6.83	111.12	120.28
1	A	140	HIS	CA-CB-CG	-6.82	106.98	113.80
2	B	26	THR	N-CA-CB	-6.80	101.86	110.90
1	D	221	ILE	CB-CA-C	-6.80	100.14	111.29
2	E	287	LEU	N-CA-C	6.78	121.98	107.67
2	B	188	PHE	O-C-N	6.77	130.39	122.20
2	E	349	LEU	N-CA-CB	6.76	121.45	110.43
2	B	287	LEU	CA-C-N	-6.73	113.24	123.07
2	B	287	LEU	C-N-CA	-6.73	113.24	123.07
1	D	259	ASP	O-C-N	6.73	129.36	122.09
2	B	317	ASN	CA-C-N	-6.71	114.44	123.10
2	B	317	ASN	C-N-CA	-6.71	114.44	123.10
1	A	150	VAL	CB-CA-C	-6.69	99.98	110.69
2	E	194	ALA	CA-C-O	6.69	126.26	118.90
1	A	89	ILE	N-CA-C	-6.68	98.57	109.12
2	B	328	ILE	CB-CA-C	-6.66	100.37	111.29
1	A	147	VAL	O-C-N	6.65	129.92	123.14
2	B	201	LEU	N-CA-C	-6.64	98.44	109.46
1	D	278	ASP	CA-CB-CG	-6.63	105.97	112.60
2	B	186	THR	N-CA-C	6.62	118.16	111.07
1	D	34	MET	N-CA-C	-6.61	101.80	110.53
1	D	175	VAL	N-CA-C	6.60	117.41	108.17
1	D	21	THR	CB-CA-C	-6.59	99.90	110.84
2	B	221	ASN	CA-C-N	-6.58	111.69	122.54
2	B	221	ASN	C-N-CA	-6.58	111.69	122.54
1	D	214	GLU	N-CA-C	-6.58	104.03	111.07
2	E	333	ILE	CB-CA-C	-6.57	103.28	111.70
1	D	224	HIS	CA-CB-CG	-6.57	107.23	113.80
1	D	54	ASN	N-CA-C	-6.55	104.52	113.30
1	D	76	PHE	CA-C-O	6.55	126.43	119.03
2	E	322	ILE	N-CA-C	-6.53	104.96	111.88
1	D	84	ALA	CA-C-N	-6.52	111.53	120.46
1	D	84	ALA	C-N-CA	-6.52	111.53	120.46
1	D	221	ILE	N-CA-CB	-6.51	100.48	111.23
1	A	149	ILE	N-CA-C	6.50	116.93	108.35
2	E	344	PRO	CB-CA-C	-6.50	103.31	111.56
1	A	212	SER	N-CA-C	-6.49	104.55	113.18
2	E	258	ASN	CA-CB-CG	-6.49	106.11	112.60
1	A	229	VAL	CB-CA-C	-6.48	100.86	110.33
1	D	164	THR	CA-CB-CG2	-6.48	99.48	110.50
2	E	226	GLN	CA-C-N	6.47	127.93	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	226	GLN	C-N-CA	6.47	127.93	119.84
2	E	314	VAL	N-CA-C	6.46	117.33	107.77
1	A	187	PHE	CA-CB-CG	-6.44	107.36	113.80
2	B	224	PHE	CA-C-N	-6.41	111.88	122.08
2	B	224	PHE	C-N-CA	-6.41	111.88	122.08
2	E	283	PRO	CB-CA-C	-6.41	103.03	111.23
1	A	273	VAL	N-CA-C	6.39	116.83	107.37
2	B	142	HIS	CA-CB-CG	-6.39	107.41	113.80
1	A	178	GLY	N-CA-C	-6.39	105.88	111.95
2	E	140	THR	C-N-CD	-6.38	98.86	125.00
2	E	226	GLN	C-N-CD	-6.37	98.90	125.00
1	D	123	CYS	CA-C-N	6.35	125.78	118.85
1	D	123	CYS	C-N-CA	6.35	125.78	118.85
1	D	138	PRO	N-CA-CB	6.35	109.92	103.25
1	D	81	ILE	CA-C-O	6.34	127.65	121.05
2	B	140	THR	CA-C-O	6.31	128.81	120.16
2	E	256	ASP	CA-CB-CG	-6.31	106.29	112.60
2	B	21	VAL	N-CA-C	-6.30	99.29	108.87
2	B	332	ILE	CB-CA-C	-6.30	103.63	112.14
2	B	358	ALA	CA-C-O	6.30	127.22	120.10
2	E	332	ILE	CB-CA-C	-6.30	103.91	111.97
1	D	89	ILE	CB-CA-C	-6.29	102.82	111.49
2	E	61	LYS	N-CA-CB	-6.28	101.25	111.24
2	E	62	VAL	CA-C-N	-6.28	113.19	122.23
2	E	62	VAL	C-N-CA	-6.28	113.19	122.23
1	D	180	ASP	CA-CB-CG	-6.27	106.33	112.60
2	E	78	GLY	CA-C-N	-6.27	111.82	122.67
2	E	78	GLY	C-N-CA	-6.27	111.82	122.67
1	A	60	VAL	N-CA-CB	6.27	117.47	110.51
2	E	262	MET	CA-C-N	-6.27	112.14	122.67
2	E	262	MET	C-N-CA	-6.27	112.14	122.67
1	A	203	ILE	N-CA-C	6.26	119.06	108.86
2	B	314	VAL	CA-C-N	-6.26	114.23	123.11
2	B	314	VAL	C-N-CA	-6.26	114.23	123.11
2	E	19	ALA	N-CA-CB	-6.26	102.43	111.25
2	E	384	ALA	CA-C-N	-6.25	112.69	120.56
2	E	384	ALA	C-N-CA	-6.25	112.69	120.56
1	A	92	ILE	CA-CB-CG2	-6.25	99.88	110.50
2	E	198	ILE	CA-CB-CG1	-6.25	99.78	110.40
2	B	143	LEU	CA-C-N	-6.24	114.96	123.14
2	B	143	LEU	C-N-CA	-6.24	114.96	123.14
1	D	89	ILE	N-CA-C	-6.21	100.81	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	278	LEU	CA-C-N	-6.21	112.65	122.95
2	E	278	LEU	C-N-CA	-6.21	112.65	122.95
2	B	298	VAL	CB-CA-C	-6.19	102.23	112.26
2	E	333	ILE	N-CA-CB	-6.17	104.14	110.62
1	A	97	GLU	CB-CA-C	6.17	121.48	109.33
1	A	101	THR	N-CA-C	6.17	118.79	111.33
2	E	358	ALA	CA-C-N	-6.16	112.52	120.65
2	E	358	ALA	C-N-CA	-6.16	112.52	120.65
2	E	120	ARG	CD-NE-CZ	-6.15	115.79	124.40
2	B	201	LEU	CA-C-N	-6.14	112.35	122.67
2	B	201	LEU	C-N-CA	-6.14	112.35	122.67
2	E	239	ASP	CA-C-O	6.14	125.94	119.80
1	A	123	CYS	O-C-N	6.13	126.23	121.88
1	A	209	ILE	CA-C-N	-6.13	109.40	121.41
1	A	209	ILE	C-N-CA	-6.13	109.40	121.41
2	E	150	ASP	CA-C-O	6.13	124.18	119.46
1	A	276	LEU	N-CA-CB	-6.10	100.85	109.94
1	A	8	THR	CA-CB-OG1	6.09	118.73	109.60
2	B	332	ILE	CA-C-N	-6.09	113.09	120.70
2	B	332	ILE	C-N-CA	-6.09	113.09	120.70
2	B	27	THR	O-C-N	6.08	126.20	121.88
1	A	123	CYS	CA-C-N	6.07	125.96	119.28
1	A	123	CYS	C-N-CA	6.07	125.96	119.28
1	D	275	SER	N-CA-CB	6.07	120.06	110.84
1	A	77	CYS	CA-CB-SG	-6.07	100.44	114.40
2	E	26	THR	N-CA-CB	-6.07	101.42	111.49
1	A	238	ALA	CA-C-N	6.06	126.25	120.31
1	A	238	ALA	C-N-CA	6.06	126.25	120.31
2	B	96	ILE	CA-CB-CG2	-6.06	100.20	110.50
1	D	38	VAL	CB-CA-C	-6.05	101.19	110.50
1	D	133	LYS	N-CA-C	6.03	118.57	109.23
2	B	21	VAL	O-C-N	6.02	129.82	122.83
1	A	174	CYS	CA-C-N	-6.02	115.10	123.10
1	A	174	CYS	C-N-CA	-6.02	115.10	123.10
2	E	181	PHE	CA-C-O	6.01	127.34	120.90
1	D	10	VAL	N-CA-C	6.01	118.66	108.86
2	B	256	ASP	CA-CB-CG	-6.00	106.60	112.60
1	D	77	CYS	CA-CB-SG	-6.00	100.59	114.40
2	B	347	VAL	N-CA-C	6.00	116.76	108.12
2	E	62	VAL	CB-CA-C	-6.00	102.74	111.68
2	B	191	ARG	CB-CA-C	-5.99	101.37	111.02
2	E	244	GLN	CB-CA-C	-5.97	101.27	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	GLY	N-CA-C	-5.96	107.09	115.32
1	A	249	ALA	CA-C-N	-5.96	112.89	122.25
1	A	249	ALA	C-N-CA	-5.96	112.89	122.25
2	B	239	ASP	CA-C-O	5.96	125.02	119.24
1	A	119	ILE	CB-CA-C	-5.95	102.27	110.96
2	E	298	VAL	N-CA-C	5.94	116.68	110.62
1	A	56	VAL	CA-CB-CG1	-5.94	100.30	110.40
2	B	156	MET	O-C-N	5.94	126.91	121.80
2	B	346	VAL	CA-C-N	-5.93	114.75	122.99
2	B	346	VAL	C-N-CA	-5.93	114.75	122.99
1	D	112	ASP	CA-CB-CG	-5.92	106.67	112.60
2	E	138	GLU	CA-C-N	-5.92	113.19	122.49
2	E	138	GLU	C-N-CA	-5.92	113.19	122.49
1	D	236	VAL	CB-CA-C	-5.92	104.15	112.14
1	D	126	VAL	CA-C-O	5.91	127.28	121.19
2	E	112	ALA	N-CA-C	5.91	117.50	108.52
2	B	117	SER	CA-C-N	-5.91	113.07	122.29
2	B	117	SER	C-N-CA	-5.91	113.07	122.29
2	E	222	ALA	CB-CA-C	-5.91	100.19	110.17
1	D	123	CYS	O-C-N	5.90	127.08	121.71
2	E	197	GLU	CA-C-N	-5.90	115.20	122.93
2	E	197	GLU	C-N-CA	-5.90	115.20	122.93
2	B	367	ASN	CA-CB-CG	-5.90	106.70	112.60
1	D	127	ILE	O-C-N	5.89	129.93	122.57
2	E	192	ASP	CB-CA-C	-5.87	103.56	111.89
2	E	140	THR	N-CA-CB	-5.87	99.93	110.37
1	A	90	LYS	N-CA-C	-5.86	106.75	114.31
2	E	133	ILE	N-CA-C	5.86	117.30	110.62
2	E	87	ASP	N-CA-CB	-5.86	100.59	110.49
2	E	308	ASP	CA-CB-CG	-5.85	106.75	112.60
2	E	352	ASN	N-CA-C	5.85	123.26	110.80
2	E	63	VAL	N-CA-C	5.84	116.78	108.42
2	E	76	TRP	N-CA-C	5.84	121.45	113.97
1	D	82	LEU	N-CA-C	5.84	117.65	111.28
2	E	307	SER	N-CA-C	-5.84	105.42	112.54
1	D	251	ILE	N-CA-C	5.83	115.13	106.85
1	A	10	VAL	CB-CA-C	-5.82	102.52	110.90
1	A	134	ILE	N-CA-CB	5.82	120.83	111.23
1	A	108	LYS	N-CA-C	-5.81	104.85	111.07
2	B	181	PHE	CA-C-N	-5.79	112.72	120.54
2	B	181	PHE	C-N-CA	-5.79	112.72	120.54
2	B	198	ILE	CB-CA-C	-5.79	104.41	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	243	ARG	N-CA-CB	5.79	118.93	109.95
2	B	217	GLY	CA-C-N	-5.79	112.74	122.92
2	B	217	GLY	C-N-CA	-5.79	112.74	122.92
2	B	225	ARG	CD-NE-CZ	5.78	132.49	124.40
2	B	259	ILE	N-CA-C	5.77	116.46	107.28
1	D	99	ILE	CB-CA-C	-5.76	104.05	110.68
2	B	345	VAL	N-CA-C	5.76	116.58	108.17
2	B	227	PRO	CA-C-N	-5.75	112.96	120.44
2	B	227	PRO	C-N-CA	-5.75	112.96	120.44
2	B	89	ASN	CA-CB-CG	-5.75	106.85	112.60
2	B	85	GLN	CB-CG-CD	-5.75	102.83	112.60
1	A	101	THR	CA-CB-CG2	-5.74	100.74	110.50
1	A	126	VAL	N-CA-C	5.74	118.22	108.86
1	D	55	THR	CB-CA-C	-5.74	99.53	109.86
1	D	62	ALA	CA-C-N	-5.73	113.31	122.08
1	D	62	ALA	C-N-CA	-5.73	113.31	122.08
2	E	333	ILE	O-C-N	5.71	128.13	121.96
2	B	144	ILE	CB-CA-C	-5.71	102.18	110.63
1	A	55	THR	CB-CA-C	-5.71	96.89	109.56
1	A	65	ALA	CA-C-N	-5.71	113.01	122.08
1	A	65	ALA	C-N-CA	-5.71	113.01	122.08
2	E	2	ASN	O-C-N	5.71	130.90	122.97
1	A	19	GLN	O-C-N	5.69	128.64	122.15
2	E	180	ILE	CA-C-N	-5.69	112.86	120.54
2	E	180	ILE	C-N-CA	-5.69	112.86	120.54
1	A	194	PHE	CA-CB-CG	-5.69	108.11	113.80
1	D	276	LEU	CB-CA-C	5.68	121.72	110.42
1	D	126	VAL	N-CA-C	5.66	116.52	108.42
1	A	141	ILE	CA-C-N	-5.65	113.03	122.64
1	A	141	ILE	C-N-CA	-5.65	113.03	122.64
2	B	203	ILE	CA-CB-CG2	-5.64	100.90	110.50
1	D	258	ALA	CA-C-N	-5.64	112.77	120.44
1	D	258	ALA	C-N-CA	-5.64	112.77	120.44
2	E	75	ASN	N-CA-C	5.64	117.43	111.28
2	B	76	TRP	N-CA-C	5.64	120.17	113.12
2	B	239	ASP	CA-C-N	5.63	126.88	119.84
2	B	239	ASP	C-N-CA	5.63	126.88	119.84
2	B	301	ALA	CB-CA-C	-5.63	101.80	110.81
1	D	229	VAL	N-CA-C	5.62	117.92	108.81
1	A	103	ASP	CA-C-O	5.62	126.48	120.70
1	A	251	ILE	N-CA-C	5.61	115.34	107.37
1	A	14	GLY	CA-C-N	5.60	128.10	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLY	C-N-CA	5.60	128.10	120.54
2	B	50	HIS	CA-CB-CG	5.60	119.40	113.80
1	A	26	GLN	CA-C-N	-5.59	112.72	120.38
1	A	26	GLN	C-N-CA	-5.59	112.72	120.38
1	A	219	ALA	CB-CA-C	-5.59	99.29	110.42
1	D	5	ASP	CA-CB-CG	5.59	118.19	112.60
2	B	227	PRO	N-CA-CB	5.58	109.42	103.39
1	D	128	THR	O-C-N	5.58	126.51	121.04
1	D	69	VAL	O-C-N	5.58	129.20	123.18
2	E	93	VAL	CB-CA-C	-5.57	104.18	111.25
2	B	14	ARG	CA-C-N	-5.56	112.30	121.92
2	B	14	ARG	C-N-CA	-5.56	112.30	121.92
2	E	14	ARG	CA-C-N	-5.56	113.36	122.54
2	E	14	ARG	C-N-CA	-5.56	113.36	122.54
1	D	202	ALA	CA-C-N	-5.56	115.21	122.94
1	D	202	ALA	C-N-CA	-5.56	115.21	122.94
2	B	89	ASN	N-CA-C	-5.54	106.10	112.92
2	E	358	ALA	N-CA-C	-5.53	105.25	111.28
1	D	100	PRO	N-CA-CB	5.52	108.24	103.27
2	E	347	VAL	N-CA-CB	-5.52	103.46	111.52
1	D	16	THR	N-CA-C	5.51	117.29	111.28
2	E	249	GLU	O-C-N	5.51	128.90	122.67
1	A	92	ILE	CB-CA-C	-5.50	102.35	110.82
2	B	144	ILE	CA-C-N	-5.50	114.02	122.87
2	B	144	ILE	C-N-CA	-5.50	114.02	122.87
2	E	167	LEU	CB-CA-C	-5.50	99.61	110.27
1	D	74	ALA	CB-CA-C	5.49	120.98	110.17
2	E	2	ASN	N-CA-CB	5.48	118.86	110.70
2	B	64	ASN	N-CA-CB	5.48	118.69	110.53
1	A	39	THR	N-CA-CB	5.47	121.14	111.78
1	D	147	VAL	O-C-N	5.47	129.18	122.83
1	A	182	ILE	C-N-CD	-5.46	102.63	125.00
1	D	123	CYS	CB-CA-C	-5.45	103.02	110.22
1	D	147	VAL	N-CA-CB	5.45	118.09	110.56
2	B	366	LEU	N-CA-CB	5.45	117.89	110.38
1	A	190	ILE	CB-CA-C	-5.44	102.36	111.29
2	B	34	ALA	N-CA-C	5.44	117.92	111.33
2	E	357	GLY	N-CA-C	-5.44	100.28	113.18
1	A	149	ILE	CB-CA-C	-5.44	101.24	111.30
2	B	309	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	204	VAL	CA-CB-CG1	-5.43	101.17	110.40
2	E	266	ALA	N-CA-CB	5.43	118.10	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	ILE	N-CA-C	5.42	116.91	111.00
2	E	64	ASN	N-CA-CB	5.42	118.61	110.65
1	D	124	PRO	CB-CA-C	-5.40	104.45	112.55
2	B	134	GLU	CB-CA-C	5.40	121.16	110.42
2	B	194	ALA	CA-C-N	-5.40	111.27	121.63
2	B	194	ALA	C-N-CA	-5.40	111.27	121.63
2	B	30	GLU	CB-CA-C	-5.39	101.52	110.68
1	D	93	ILE	CA-C-N	5.39	129.84	122.84
1	D	93	ILE	C-N-CA	5.39	129.84	122.84
2	E	158	TYR	CA-CB-CG	-5.38	104.21	113.90
2	B	188	PHE	CB-CA-C	-5.38	101.91	110.84
2	B	181	PHE	N-CA-CB	-5.38	101.93	109.94
1	D	150	VAL	CB-CA-C	-5.38	101.79	110.28
2	E	279	HIS	CB-CA-C	-5.38	103.67	111.14
2	B	64	ASN	CB-CA-C	5.37	119.00	109.65
2	E	350	GLU	CA-CB-CG	-5.37	103.36	114.10
1	D	82	LEU	N-CA-CB	-5.37	102.23	110.12
2	B	107	GLU	CA-C-N	-5.36	111.45	122.82
2	B	107	GLU	C-N-CA	-5.36	111.45	122.82
1	D	69	VAL	CB-CA-C	-5.36	102.63	110.62
2	E	352	ASN	N-CA-CB	5.36	119.55	110.49
2	E	187	ILE	CB-CA-C	-5.36	105.11	111.97
1	A	55	THR	CA-C-N	-5.35	113.81	120.56
1	A	55	THR	C-N-CA	-5.35	113.81	120.56
2	E	287	LEU	CB-CA-C	5.35	119.71	111.95
1	D	228	PRO	CB-CA-C	-5.33	103.01	110.63
2	E	91	GLN	CA-C-N	5.33	126.15	120.13
2	E	91	GLN	C-N-CA	5.33	126.15	120.13
1	A	99	ILE	N-CA-CB	-5.32	104.33	111.40
1	D	180	ASP	N-CA-CB	5.31	116.46	110.03
1	A	89	ILE	CA-C-O	-5.31	114.13	121.51
1	D	267	ALA	O-C-N	-5.31	116.49	122.12
1	D	76	PHE	CA-CB-CG	-5.31	108.49	113.80
2	E	335	ALA	CA-C-O	5.31	126.57	121.00
2	B	314	VAL	CB-CA-C	-5.30	102.33	110.50
1	D	31	GLY	CA-C-N	-5.30	113.83	121.42
1	D	31	GLY	C-N-CA	-5.30	113.83	121.42
1	D	119	ILE	N-CA-CB	-5.30	104.09	111.41
1	A	38	VAL	N-CA-C	5.30	115.49	107.75
1	D	275	SER	CB-CA-C	-5.29	102.63	110.62
1	A	112	ASP	CB-CA-C	5.29	119.14	110.95
1	A	110	LYS	CA-CB-CG	-5.29	103.53	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	ILE	CA-C-O	5.28	126.22	120.57
1	D	188	ILE	CB-CA-C	-5.28	102.64	111.29
2	E	87	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	69	VAL	CA-CB-CG2	-5.27	101.44	110.40
1	A	93	ILE	CA-C-N	-5.26	114.77	122.19
1	A	93	ILE	C-N-CA	-5.26	114.77	122.19
1	D	104	MET	CA-C-N	-5.26	112.70	120.28
1	D	104	MET	C-N-CA	-5.26	112.70	120.28
2	E	126	SER	N-CA-C	5.26	117.07	109.07
1	A	10	VAL	N-CA-C	5.26	117.20	108.99
2	E	67	GLU	N-CA-CB	-5.26	101.60	110.49
1	A	99	ILE	CA-C-N	5.25	126.40	119.84
1	A	99	ILE	C-N-CA	5.25	126.40	119.84
2	E	298	VAL	CA-C-O	5.24	126.40	120.95
2	E	374	LEU	N-CA-CB	-5.24	102.26	109.91
2	B	325	CYS	N-CA-CB	5.24	117.74	109.94
2	B	202	VAL	N-CA-C	5.23	116.91	108.85
1	D	2	ILE	CB-CA-C	5.23	119.87	111.29
1	A	38	VAL	CB-CA-C	-5.23	103.34	110.77
1	A	14	GLY	N-CA-C	-5.23	106.50	115.08
2	B	184	LEU	CA-C-N	-5.23	113.22	120.38
2	B	184	LEU	C-N-CA	-5.23	113.22	120.38
2	E	359	LYS	N-CA-C	-5.23	105.27	110.97
2	B	187	ILE	N-CA-CB	-5.23	104.71	110.51
1	D	93	ILE	CA-CB-CG2	-5.22	101.62	110.50
2	B	203	ILE	CB-CA-C	-5.22	103.34	110.96
2	B	275	ILE	CB-CA-C	-5.21	104.44	112.05
1	D	225	VAL	N-CA-C	5.21	115.56	107.28
2	E	81	LEU	CA-C-N	-5.21	116.32	123.14
2	E	81	LEU	C-N-CA	-5.21	116.32	123.14
1	A	209	ILE	O-C-N	-5.20	117.26	122.62
2	E	381	VAL	CA-C-N	-5.20	113.33	120.46
2	E	381	VAL	C-N-CA	-5.20	113.33	120.46
1	A	99	ILE	CA-C-O	5.19	125.55	119.89
2	E	96	ILE	N-CA-CB	-5.19	102.22	111.92
2	E	64	ASN	CB-CA-C	5.18	118.26	109.55
1	D	90	LYS	CA-C-O	5.18	124.75	119.05
2	E	47	CYS	CA-C-N	-5.18	115.51	123.07
2	E	47	CYS	C-N-CA	-5.18	115.51	123.07
1	A	181	PRO	CB-CA-C	-5.18	104.13	112.21
2	E	276	VAL	CB-CA-C	-5.17	105.34	111.81
2	E	207	GLY	CA-C-N	-5.17	113.60	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	207	GLY	C-N-CA	-5.17	113.60	123.32
2	E	111	GLY	CA-C-O	-5.17	116.19	121.61
1	A	136	ILE	CB-CA-C	5.16	119.75	111.29
1	A	224	HIS	ND1-CG-CD2	5.16	111.26	106.10
2	B	95	GLN	CB-CG-CD	-5.15	103.84	112.60
2	E	275	ILE	CA-CB-CG2	-5.15	101.75	110.50
2	E	200	PRO	CB-CA-C	-5.14	99.15	112.00
2	E	311	VAL	CB-CA-C	-5.14	104.47	111.15
2	B	181	PHE	CA-C-O	5.13	126.39	120.90
1	A	233	ILE	N-CA-C	5.12	115.35	107.77
2	E	348	ARG	CB-CG-CD	5.12	123.06	111.30
1	D	197	ASP	CA-C-O	5.11	125.05	119.32
1	A	166	ASP	CA-C-N	-5.11	112.09	122.31
1	A	166	ASP	C-N-CA	-5.11	112.09	122.31
2	E	45	VAL	N-CA-CB	-5.11	104.36	111.41
2	B	80	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	D	20	GLY	CA-C-N	-5.11	113.07	121.19
1	D	20	GLY	C-N-CA	-5.11	113.07	121.19
1	A	221	ILE	CB-CA-C	-5.10	102.92	111.29
2	B	154	GLY	O-C-N	5.10	126.87	121.77
2	B	286	PHE	CA-C-N	-5.10	114.89	122.74
2	B	286	PHE	C-N-CA	-5.10	114.89	122.74
1	D	122	ASN	N-CA-CB	-5.08	103.62	111.65
1	D	156	LEU	CA-C-O	5.08	126.66	121.07
2	B	229	LEU	O-C-N	5.07	127.30	122.07
1	D	128	THR	CA-C-N	5.07	126.18	119.84
1	D	128	THR	C-N-CA	5.07	126.18	119.84
2	E	136	VAL	CB-CA-C	-5.07	102.97	111.29
2	E	248	TRP	CA-CB-CG	-5.07	103.98	113.60
1	D	165	THR	N-CA-C	-5.06	103.19	111.04
2	B	372	LYS	CA-C-N	-5.06	117.22	122.69
2	B	372	LYS	C-N-CA	-5.06	117.22	122.69
2	B	341	VAL	CB-CA-C	-5.06	104.83	111.25
2	B	67	GLU	CB-CA-C	-5.05	102.10	110.68
2	B	98	VAL	CA-C-O	5.05	125.26	120.31
1	D	111	LEU	N-CA-C	-5.04	105.67	111.07
1	A	48	LEU	N-CA-CB	5.04	119.69	112.08
1	A	274	ARG	N-CA-CB	5.04	117.53	110.12
2	B	19	ALA	O-C-N	5.03	125.82	121.54
1	D	97	GLU	N-CA-CB	-5.03	101.90	111.00
2	E	18	PRO	N-CA-CB	5.03	108.53	103.25
2	B	170	GLU	N-CA-CB	-5.02	102.18	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	353	ASN	O-C-N	5.02	128.28	122.00
1	D	159	GLU	CB-CA-C	5.02	118.73	110.95
1	D	202	ALA	N-CA-C	5.01	116.43	108.96
1	D	11	ILE	CA-C-N	-5.01	115.42	122.94
1	D	11	ILE	C-N-CA	-5.01	115.42	122.94
2	E	144	ILE	CA-C-N	-5.01	114.94	122.81
2	E	144	ILE	C-N-CA	-5.01	114.94	122.81
2	B	37	LYS	CA-C-O	5.00	124.64	119.14
2	E	173	LEU	CA-C-O	5.00	125.75	120.10

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	412	0
1	D	2083	0	2140	533	0
2	B	2908	0	2962	493	0
2	E	2908	0	2963	591	0
3	A	48	0	32	13	0
3	D	48	0	32	19	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	2011	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 99.

All (2011) 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:CE	1:A:104:MET:HA	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:D:105:LEU:C	1:D:105:LEU:HD23	1.38	1.29
1:D:203:ILE:O	1:D:229:VAL:HG22	1.19	1.29
2:E:352:ASN:HD22	2:E:352:ASN:C	1.33	1.28
1:A:104:MET:CA	1:A:104:MET:HE2	1.62	1.27
2:E:262:MET:HE2	2:E:301:ALA:CB	1.64	1.27
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
2:B:133:ILE:HD12	2:B:133:ILE:N	1.39	1.24
2:E:287:LEU:HD23	2:E:287:LEU:C	1.60	1.24
1:A:137:GLN:HE21	1:A:137:GLN:CA	1.40	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
1:D:149:ILE:CG1	1:D:174:CYS:HB3	1.73	1.19
1:D:285:THR:O	1:D:288:LYS:HG3	1.39	1.18
1:A:104:MET:CE	1:A:104:MET:CA	2.16	1.18
1:A:4:ILE:CD1	1:A:132:CYS:SG	2.31	1.18
1:D:105:LEU:C	1:D:105:LEU:CD2	2.17	1.18
2:E:368:ILE:C	2:E:369:ILE:HD12	1.68	1.18
1:D:49:GLY:O	1:D:50:LEU:HD23	1.43	1.17
2:E:275:ILE:HG22	2:E:276:VAL:N	1.54	1.17
1:D:221:ILE:CA	1:D:225:VAL:HG12	1.74	1.17
2:E:215:LYS:C	2:E:216:LEU:HD23	1.69	1.17
2:E:107:GLU:C	2:E:108:LEU:HD23	1.68	1.16
2:E:82:VAL:HG22	2:E:90:GLY:H	1.00	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ILE:O	1:D:229:VAL:CG2	1.95	1.15
1:D:97:GLU:OE1	1:D:98:GLY:N	1.79	1.15
2:E:319:PHE:CD2	2:E:350:GLU:HG2	1.80	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
2:E:82:VAL:CG2	2:E:90:GLY:H	1.60	1.13
2:B:45:VAL:HG23	2:B:45:VAL:O	1.44	1.13
1:D:6:LYS:O	1:D:33:LYS:HE3	1.45	1.13
1:D:136:ILE:HD13	1:D:136:ILE:H	1.12	1.13
1:A:2:ILE:HG23	1:A:3:LEU:N	1.62	1.13
1:D:257:THR:OG1	1:D:260:GLU:HB2	1.49	1.13
2:E:79:LYS:HB3	2:E:79:LYS:NZ	1.46	1.12
2:E:87:ASP:O	2:E:89:ASN:N	1.82	1.12
2:E:277:LYS:HD2	2:E:278:LEU:N	1.62	1.13
1:A:128:THR:HG22	1:A:128:THR:O	1.44	1.11
1:D:10:VAL:O	1:D:34:MET:HE3	1.49	1.11
2:B:270:MET:HB3	4:B:419:HOH:O	1.44	1.11
1:A:104:MET:HA	1:A:104:MET:HE2	1.15	1.11
1:D:124:PRO:HA	1:D:136:ILE:HD11	1.23	1.10
2:B:215:LYS:C	2:B:216:LEU:HD23	1.75	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:A:221:ILE:HG22	1:A:222:LYS:N	1.22	1.09
1:D:203:ILE:HB	1:D:229:VAL:HG23	1.32	1.09
1:D:92:ILE:CG2	1:D:118:MET:HG3	1.83	1.09
2:E:339:VAL:HG12	2:E:341:VAL:HG12	1.33	1.09
2:E:262:MET:HE2	2:E:301:ALA:HB1	1.31	1.09
2:B:325:CYS:HB3	2:B:349:LEU:HD13	1.33	1.09
1:D:2:ILE:C	4:D:293:HOH:O	1.96	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:B:133:ILE:N	2:B:133:ILE:CD1	2.09	1.08
1:D:92:ILE:HG22	1:D:118:MET:HG3	1.16	1.08
2:E:319:PHE:HA	2:E:350:GLU:CB	1.84	1.08
1:A:4:ILE:HD13	1:A:132:CYS:HB3	1.13	1.07
1:A:137:GLN:NE2	1:A:137:GLN:HA	1.57	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HD23	1:D:105:LEU:O	1.52	1.07
1:A:2:ILE:CG2	1:A:3:LEU:N	2.17	1.07
1:D:190:ILE:HD13	1:D:190:ILE:N	1.63	1.07
2:B:45:VAL:O	2:B:45:VAL:CG2	2.02	1.06
1:A:104:MET:HA	1:A:104:MET:HE3	1.09	1.06
2:B:133:ILE:CD1	2:B:133:ILE:H	1.56	1.06
2:E:375:THR:O	2:E:378:ALA:HB3	1.55	1.06
2:B:63:VAL:CG1	2:B:68:ASP:HB3	1.86	1.05
1:D:229:VAL:HG12	1:D:270:VAL:CG1	1.86	1.05
2:B:272:THR:O	2:B:275:ILE:HG22	1.54	1.05
2:B:328:ILE:HG22	2:B:329:ALA:N	1.70	1.05
1:A:4:ILE:HD13	1:A:132:CYS:CB	1.86	1.04
1:A:24:SER:HA	4:A:297:HOH:O	1.57	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
2:E:369:ILE:HD12	2:E:369:ILE:N	1.66	1.03
2:E:87:ASP:C	2:E:89:ASN:H	1.60	1.03
1:D:23:HIS:CE1	1:D:136:ILE:HG22	1.94	1.03
1:A:2:ILE:HD12	1:A:194:PHE:CE1	1.94	1.02
2:E:108:LEU:HD23	2:E:108:LEU:N	1.55	1.02
1:A:128:THR:O	1:A:128:THR:CG2	2.08	1.02
1:D:266:GLU:HG2	1:D:272:THR:HG21	1.42	1.02
2:B:42:PRO:O	4:B:390:HOH:O	1.78	1.01
1:D:187:PHE:HE2	1:D:214:GLU:HG3	1.19	1.01
1:D:223:GLU:HG2	1:D:223:GLU:O	1.58	1.01
2:E:139:GLU:O	2:E:140:THR:HB	1.60	1.01
2:E:352:ASN:C	2:E:352:ASN:ND2	2.12	1.01
1:A:21:THR:CG2	1:A:22:PHE:N	2.21	1.01
2:B:109:TYR:CD1	2:B:109:TYR:C	2.39	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:E:157:PRO:CA	2:E:182:MET:HE2	1.90	1.00
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
2:B:97:LEU:HD22	2:B:98:VAL:N	1.78	0.99
2:E:287:LEU:HD23	2:E:287:LEU:O	1.62	0.99
2:E:81:LEU:O	2:E:90:GLY:HA3	1.61	0.99
2:E:312:LYS:NZ	2:E:388:LYS:HE3	1.77	0.99
2:E:115:ASP:CG	4:E:395:HOH:O	2.05	0.99
1:D:149:ILE:HG13	1:D:174:CYS:CB	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:LEU:CD1	2:E:316:VAL:H	1.76	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:356:LEU:HD22	2:E:356:LEU:C	1.84	0.98
2:E:83:THR:H	2:E:86:THR:HG23	1.29	0.98
2:E:315:LEU:HD12	2:E:316:VAL:H	0.87	0.98
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:O9P	3:A:289:COA:H62	1.64	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
1:D:28:ILE:HG22	1:D:29:ALA:N	1.81	0.94
1:D:190:ILE:HA	1:D:193:MET:HG3	1.50	0.94
1:D:205:MET:HE1	1:D:217:ALA:HB3	1.50	0.93
2:E:252:TYR:C	2:E:253:VAL:HG23	1.92	0.93
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
2:E:157:PRO:HA	2:E:182:MET:HE2	1.51	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
2:E:312:LYS:HZ3	2:E:388:LYS:HE3	1.34	0.92
1:A:97:GLU:C	1:A:97:GLU:CD	2.38	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
1:D:203:ILE:C	1:D:229:VAL:HG22	1.95	0.91
2:E:262:MET:HE2	2:E:301:ALA:HB3	1.48	0.91
1:D:10:VAL:C	1:D:34:MET:CE	2.44	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:63:VAL:HG13	2:B:68:ASP:HB3	1.53	0.90
2:E:136:VAL:O	2:E:140:THR:CG2	2.20	0.90
1:A:104:MET:HE2	1:A:104:MET:C	1.94	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
2:E:383:ALA:O	2:E:384:ALA:C	2.13	0.90
2:B:257:GLY:C	2:B:284:ALA:HB2	1.96	0.90
1:A:23:HIS:CE1	1:A:136:ILE:HG22	2.07	0.90
2:E:287:LEU:C	2:E:287:LEU:CD2	2.42	0.90
2:E:49:VAL:HG22	2:E:91:GLN:HB3	1.54	0.90
2:B:133:ILE:HD12	2:B:133:ILE:H	0.75	0.89
1:D:127:ILE:O	1:D:173:THR:HG22	1.71	0.89
1:A:105:LEU:C	1:A:105:LEU:HD23	1.98	0.89
1:D:97:GLU:HB3	3:D:289:COA:C7P	2.00	0.89
1:D:157:THR:O	1:D:161:VAL:CG2	2.19	0.89
1:D:203:ILE:C	1:D:229:VAL:CG2	2.45	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:B:258:ASN:ND2	2:B:258:ASN:H	1.69	0.89
1:D:6:LYS:O	1:D:33:LYS:CE	2.21	0.89
1:A:104:MET:CE	1:A:107:VAL:HB	2.01	0.89
2:E:312:LYS:NZ	2:E:388:LYS:CE	2.35	0.89
2:E:326:ASP:O	2:E:328:ILE:N	2.05	0.89
2:E:255:LEU:O	2:E:256:ASP:HB3	1.69	0.89
2:E:352:ASN:HD22	2:E:353:ASN:N	1.68	0.89
2:E:262:MET:CE	2:E:301:ALA:CB	2.50	0.89
1:A:72:VAL:HG13	1:A:73:PRO:HD2	1.55	0.88
2:E:252:TYR:O	2:E:253:VAL:CG2	2.21	0.88
2:E:346:VAL:CG2	2:E:381:VAL:HG22	2.04	0.88
2:E:107:GLU:O	2:E:129:GLY:HA3	1.72	0.88
1:A:55:THR:HG22	4:A:300:HOH:O	1.73	0.88
2:B:97:LEU:HD22	2:B:98:VAL:H	1.39	0.88
2:B:292:GLY:O	2:B:294:THR:HG23	1.73	0.88
1:A:149:ILE:HG23	1:A:204:VAL:HB	1.54	0.88
2:E:79:LYS:HB3	2:E:79:LYS:HZ3	1.35	0.88
1:A:10:VAL:HG12	1:A:11:ILE:N	1.87	0.88
2:B:229:LEU:HA	2:B:232:MET:HE3	1.56	0.88
1:D:116:VAL:CG1	1:D:117:ARG:N	2.37	0.88
1:A:55:THR:CG2	4:A:300:HOH:O	2.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:LEU:HG	2:B:196:ILE:N	1.89	0.87
2:B:339:VAL:HG12	2:B:340:GLY:N	1.86	0.87
1:D:91:LEU:HD12	1:D:117:ARG:HG2	1.55	0.87
2:B:258:ASN:H	2:B:258:ASN:HD22	1.18	0.87
2:B:304:ILE:O	2:B:307:SER:OG	1.91	0.87
2:E:383:ALA:O	2:E:386:GLU:N	2.07	0.87
2:B:139:GLU:C	2:B:141:PRO:HD3	2.00	0.87
2:E:173:LEU:HD12	2:E:209:LEU:HG	1.56	0.87
1:D:123:CYS:HB2	1:D:124:PRO:HD2	1.55	0.87
2:E:75:ASN:O	2:E:79:LYS:CD	2.23	0.86
2:E:79:LYS:NZ	2:E:79:LYS:CB	2.35	0.86
2:E:257:GLY:HA3	2:E:282:GLU:O	1.75	0.86
2:E:275:ILE:HG22	2:E:276:VAL:H	1.40	0.86
1:A:97:GLU:CD	1:A:98:GLY:N	2.32	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
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
2:B:223:LEU:O	2:B:230:ARG:NH1	2.08	0.86
2:E:62:VAL:HG13	2:E:63:VAL:N	1.90	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:E:156:MET:O	2:E:159:GLN:HG3	1.76	0.85
2:E:343:VAL:CB	2:E:344:PRO:HD2	2.04	0.85
2:E:352:ASN:ND2	2:E:353:ASN:N	2.24	0.85
1:D:229:VAL:CG1	1:D:270:VAL:CG1	2.55	0.85
2:E:157:PRO:N	2:E:182:MET:HE1	1.92	0.85
1:D:221:ILE:HG22	1:D:222:LYS:H	1.40	0.85
2:E:262:MET:CE	2:E:301:ALA:HB3	2.05	0.85
2:E:326:ASP:OD1	2:E:327:LEU:N	2.09	0.85
1:A:97:GLU:OE1	1:A:97:GLU:C	2.20	0.85
1:A:128:THR:CG2	1:A:131:GLU:HB2	2.07	0.84
1:A:186:ASN:ND2	1:A:189:ASP:CG	2.35	0.84
2:B:239:ASP:OD1	2:B:241:ARG:HB2	1.76	0.84
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
2:B:270:MET:HA	4:B:419:HOH:O	1.73	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:326:ASP:O	2:E:327:LEU:C	2.20	0.84
2:B:180:ILE:HG22	2:B:181:PHE:N	1.91	0.84
2:B:82:VAL:O	2:B:82:VAL:HG12	1.77	0.83
1:D:10:VAL:C	1:D:34:MET:HE3	2.02	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:HD13	2:B:144:ILE:N	1.93	0.83
2:E:216:LEU:HD23	2:E:216:LEU:N	1.88	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:315:LEU:HD12	2:E:315:LEU:C	1.91	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
1:D:205:MET:HE1	1:D:217:ALA:CB	2.09	0.82
2:E:157:PRO:N	2:E:182:MET:HE2	1.93	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
1:D:265:LEU:O	1:D:270:VAL:HG23	1.79	0.82
1:A:186:ASN:HD22	1:A:189:ASP:CG	1.87	0.82
2:E:302:PHE:O	2:E:306:LEU:HD12	1.80	0.82
2:E:369:ILE:N	2:E:369:ILE:HD13	1.92	0.82
1:D:2:ILE:HG12	1:D:193:MET:HE2	1.61	0.82
2:E:83:THR:H	2:E:86:THR:CG2	1.93	0.82
2:E:272:THR:HG22	2:E:273:MET:N	1.95	0.82
1:D:55:THR:HG22	1:D:57:ARG:H	1.42	0.82
2:E:70:ARG:HG3	2:E:70:ARG:O	1.79	0.82
2:E:312:LYS:NZ	2:E:388:LYS:NZ	2.28	0.82
1:A:104:MET:HE1	1:A:107:VAL:HB	1.59	0.81
2:E:343:VAL:HG12	2:E:344:PRO:CD	2.10	0.81
1:A:181:PRO:HA	2:B:116:ARG:NH1	1.95	0.81
1:D:190:ILE:N	1:D:190:ILE:CD1	2.41	0.81
1:D:221:ILE:HA	1:D:225:VAL:HG12	0.84	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
2:E:157:PRO:CD	2:E:182:MET:HE1	2.10	0.81

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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	0.81
1:D:21:THR:HG22	1:D:22:PHE:N	1.94	0.81
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:78:LYS:O	1:D:82:LEU:HB2	1.81	0.80
1:D:218:ALA:O	1:D:221:ILE:HB	1.82	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
1:D:49:GLY:C	1:D:50:LEU:HD23	2.07	0.80
2:E:319:PHE:HA	2:E:350:GLU:HB3	1.63	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:D:252:ALA:O	1:D:253:GLY:C	2.24	0.80
2:B:86:THR:HG23	2:B:90:GLY:HA2	1.63	0.80
2:B:263:VAL:O	2:B:289:VAL:HG23	1.80	0.80
1:D:10:VAL:CB	1:D:34:MET:HE1	2.12	0.80
1:A:161:VAL:O	1:A:162:LYS:C	2.24	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: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:H	2:E:56:LYS:HD2	1.46	0.79
2:B:258:ASN:HD22	2:B:258:ASN:N	1.81	0.79
1:A:137:GLN:CA	1:A:137:GLN:NE2	2.22	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:2:ILE:HD11	1:D:193:MET:HB3	1.62	0.79
1:D:136:ILE:HD13	1:D:136:ILE:N	1.94	0.79
2:B:110:LEU:HD22	2:B:111:GLY:N	1.97	0.79
1:D:203:ILE:CB	1:D:229:VAL:CG2	2.57	0.79
1:A:163:GLN:O	1:A:164:THR:C	2.25	0.79
1:D:221:ILE:HG22	1:D:222:LYS:CA	2.13	0.79
2:B:105:ALA:HB3	2:B:203:ILE:HG22	1.66	0.78
2:E:65:SER:HB2	2:E:67:GLU:OE1	1.82	0.78
2:B:327:LEU:O	2:B:330:ASP:HB2	1.83	0.78
1:D:104:MET:CA	1:D:104:MET:HE3	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:70:ARG:O	2:E:74:GLU:HG3	1.82	0.78
2:E:252:TYR:C	2:E:253:VAL:CG2	2.56	0.78
2:E:252:TYR:O	2:E:253:VAL:HG23	1.82	0.78
2:E:330:ASP:O	2:E:333:ILE:HB	1.82	0.78
1:A:92:ILE:HG22	1:A:93:ILE:N	1.91	0.78
1:D:123:CYS:HB2	1:D:124:PRO:CD	2.13	0.78
1:D:91:LEU:CD1	1:D:117:ARG:HG2	2.13	0.78
1:A:5:ASP:OD1	1:A:7:ASN:N	2.15	0.78
3:A:289:COA:O9P	3:A:289:COA:H61	1.82	0.78
1:D:228:PRO:HB2	1:D:286:VAL:HG21	1.64	0.78
1:D:283:LEU:O	1:D:286:VAL:HG12	1.84	0.78
2:E:368:ILE:C	2:E:369:ILE:CD1	2.51	0.78
1:A:197:ASP:O	1:A:227:LYS:NZ	2.15	0.78
2:B:257:GLY:O	2:B:284:ALA:HB2	1.83	0.78
1:A:92:ILE:CG2	1:A:93:ILE:N	2.47	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: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:O	2:E:152:LEU:HD22	1.85	0.77
1:A:106:THR:HG22	1:A:106:THR:O	1.83	0.77
2:B:141:PRO:HD2	2:B:142:HIS:HD2	1.47	0.77
1:D:230:VAL:HG21	1:D:283:LEU:HD13	1.66	0.77
2:B:126:SER:HB2	2:B:143:LEU:O	1.84	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
2:E:352:ASN:ND2	2:E:353:ASN:HB2	2.00	0.77
1:A:219:ALA:O	1:A:220:TYR:C	2.26	0.77
1:D:116:VAL:HG13	1:D:117:ARG:H	1.46	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
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:39:THR:HG22	1:A:42:LYS:HG3	1.65	0.77
1:A:221:ILE:CG2	1:A:222:LYS:H	1.68	0.77
2:B:26:THR:HB	2:B:30:GLU:OE1	1.84	0.77
2:B:109:TYR:HD1	2:B:109:TYR:O	1.68	0.77
2:B:361:LEU:O	2:B:364:SER:HB3	1.84	0.77
2:E:316:VAL:HB	2:E:347:VAL:HG13	1.66	0.77
2:B:308:ASP:O	2:B:311:VAL:HG12	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ALA:O	1:D:285:THR:HB	1.85	0.76
1:A:127:ILE:HD12	1:A:133:LYS:HG3	1.65	0.76
2:B:133:ILE:O	2:B:134:GLU:C	2.26	0.76
2:B:109:TYR:C	2:B:109:TYR:HD1	1.91	0.76
2:E:246:ALA:O	2:E:248:TRP:N	2.17	0.76
1:A:10:VAL:CG1	1:A:11:ILE:N	2.47	0.76
1:D:169:PHE:CE2	1:D:283:LEU:HB3	2.20	0.76
2:B:375:THR:O	2:B:379:GLN:HG3	1.85	0.76
2:E:300:GLU:O	2:E:304:ILE:HG12	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:110:LEU:CD2	2:B:111:GLY:H	1.98	0.76
2:B:274:ASP:OD2	4:B:420:HOH:O	2.03	0.76
2:B:287:LEU:HD23	2:B:287:LEU:C	2.11	0.76
3:D:289:COA:O2B	3:D:289:COA:O8A	2.02	0.76
2:E:150:ASP:O	2:E:153:THR:O	2.04	0.76
2:B:86:THR:CG2	2:B:90:GLY:HA2	2.16	0.75
1:D:97:GLU:OE1	1:D:97:GLU:C	2.28	0.75
2:E:339:VAL:HG12	2:E:341:VAL:N	2.01	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
2:B:380:GLN:O	2:B:383:ALA:CB	2.28	0.75
2:B:66:LYS:O	2:B:69:ILE:HB	1.85	0.75
2:B:143:LEU:C	2:B:144:ILE:HD13	2.12	0.75
1:A:218:ALA:O	1:A:219:ALA:C	2.29	0.75
2:B:201:LEU:HD12	2:B:202:VAL:H	1.51	0.75
2:E:63:VAL:HG12	2:E:64:ASN:N	2.02	0.75
1:A:221:ILE:HG22	1:A:222:LYS:CA	2.16	0.75
1:D:203:ILE:O	1:D:230:VAL:N	2.15	0.75
2:B:276:VAL:HG12	2:B:277:LYS:N	1.96	0.74
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:218:ALA:O	1:D:219:ALA:C	2.29	0.74
1:D:11:ILE:HA	1:D:36:GLY:O	1.86	0.74
1:D:129:PRO:C	1:D:131:GLU:H	1.93	0.74
2:E:337:ALA:O	2:E:338:GLU:C	2.27	0.74
2:B:326:ASP:OD1	2:B:353:ASN:ND2	2.19	0.74
1:D:233:ILE:CD1	1:D:261:LYS:HB3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:87:ASP:C	2:E:89:ASN:N	2.31	0.74
2:B:201:LEU:HD12	2:B:202:VAL:N	2.01	0.74
1:D:188:ILE:O	1:D:189:ASP:C	2.25	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
2:E:72:PHE:CE1	2:E:76:TRP:CD1	2.76	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
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:180:ASP:HB3	1:D:181:PRO:CD	2.18	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:322:ILE:HG23	2:E:322:ILE:O	1.87	0.73
1:A:91:LEU:HD12	1:A:117:ARG:O	1.88	0.73
1:D:147:VAL:HG23	1:D:170:GLY:O	1.88	0.73
1:A:236:VAL:HG23	4:B:420:HOH:O	1.88	0.73
1:D:285:THR:HG22	1:D:286:VAL:N	2.01	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:E:109:TYR:CD1	2:E:109:TYR:C	2.66	0.73
1:D:73:PRO:C	1:D:75:PRO:HD2	2.14	0.73
1:D:160:ALA:O	1:D:161:VAL:C	2.25	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
2:E:272:THR:O	2:E:273:MET:C	2.28	0.73
2:E:356:LEU:C	2:E:356:LEU:CD2	2.61	0.73
1:A:207:GLY:O	1:A:233:ILE:HA	1.88	0.73
1:A:218:ALA:HB1	1:A:268:ALA:HB2	1.69	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:B:269:ALA:O	2:B:273:MET:HG3	1.88	0.72
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
1:D:233:ILE:HG22	1:D:234:ALA:N	2.03	0.72
1:A:97:GLU:OE1	1:A:97:GLU:CA	2.35	0.72
1:D:10:VAL:HB	1:D:34:MET:HE1	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:296:GLU:OE1	2:B:296:GLU:N	2.18	0.71
2:E:79:LYS:O	2:E:93:VAL:HG23	1.89	0.71
1:A:217:ALA:O	1:A:218:ALA:C	2.31	0.71
2:B:313:ALA:HA	2:B:343:VAL:HG13	1.71	0.71
2:B:352:ASN:O	2:B:353:ASN:CB	2.37	0.71
1:A:190:ILE:O	1:A:191:LEU:C	2.32	0.71
2:B:2:ASN:C	2:B:3:LEU:HD23	2.14	0.71
1:D:151:SER:HB2	1:D:206:ILE:HB	1.71	0.71
2:E:86:THR:OG1	2:E:87:ASP:N	2.15	0.71
2:B:144:ILE:N	2:B:144:ILE:CD1	2.53	0.71
1:A:263:ALA:O	1:A:266:GLU:HG3	1.91	0.71
2:B:22:GLY:HA2	2:B:98:VAL:O	1.91	0.71
1:D:223:GLU:O	1:D:223:GLU:CG	2.37	0.71
2:E:45:VAL:HG22	2:E:61:LYS:O	1.90	0.71
1:A:146:LYS:HB2	1:A:201:GLU:HB2	1.72	0.71
1:A:212:SER:O	1:A:215:GLU:N	2.23	0.71
2:B:142:HIS:H	2:B:142:HIS:CD2	2.08	0.71
1:A:214:GLU:OE1	1:A:261:LYS:HE3	1.90	0.71
1:A:136:ILE:HD13	1:A:136:ILE:H	1.56	0.71
1:D:143:LYS:O	1:D:171:GLN:N	2.22	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:150:ASP:OD1	2:E:151:PRO:HD2	1.89	0.71
2:E:239:ASP:OD1	2:E:241:ARG:N	2.18	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
1:A:152:ARG:HG3	1:A:177:ILE:HD11	1.73	0.70
2:B:316:VAL:CG1	2:B:317:ASN:N	2.53	0.70
1:D:97:GLU:HB2	3:D:289:COA:H71	1.72	0.70
2:E:287:LEU:O	2:E:287:LEU:CD2	2.39	0.70
2:E:326:ASP:HB3	2:E:356:LEU:HD13	1.72	0.70
1:A:153:SER:HB2	1:A:246:NEP:HE1	1.72	0.70
1:A:182:ILE:N	1:A:183:PRO:HD3	2.05	0.70
2:B:325:CYS:HB3	2:B:349:LEU:CD1	2.17	0.70
2:E:269:ALA:O	2:E:272:THR:HB	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:246:ALA:C	2:E:248:TRP:H	1.99	0.70
2:E:140:THR:N	2:E:141:PRO:HD3	2.05	0.70
2:B:204:THR:O	2:B:207:GLY:N	2.25	0.70
2:E:89:ASN:O	2:E:90:GLY:O	2.10	0.70
1:D:123:CYS:CB	1:D:124:PRO:HD2	2.20	0.70
1:A:106:THR:O	1:A:106:THR:CG2	2.40	0.70
1:D:34:MET:HE3	1:D:34:MET:HA	1.74	0.70
2:E:75:ASN:O	2:E:79:LYS:HD3	1.91	0.70
2:E:258:ASN:HD22	2:E:258:ASN:H	1.40	0.70
1:D:119:ILE:HD11	1:D:185:SER:OG	1.91	0.70
2:B:377:ALA:O	2:B:381:VAL:HG23	1.91	0.69
1:D:127:ILE:HG13	1:D:133:LYS:CB	2.21	0.69
1:A:127:ILE:HG13	1:A:132:CYS:O	1.92	0.69
1:D:119:ILE:HD13	1:D:185:SER:OG	1.89	0.69
1:D:128:THR:HG23	1:D:131:GLU:HB2	1.73	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
2:B:26:THR:HG22	2:B:27:THR:HG23	1.74	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:E:374:LEU:C	2:E:374:LEU:HD12	2.18	0.69
1:A:116:VAL:HG12	1:A:117:ARG:N	2.08	0.69
1:D:55:THR:O	1:D:56:VAL:C	2.34	0.69
2:E:278:LEU:HG	2:E:278:LEU:O	1.92	0.69
2:B:298:VAL:O	2:B:298:VAL:HG12	1.93	0.69
2:E:258:ASN:HD22	2:E:258:ASN:C	1.97	0.69
2:E:277:LYS:CD	2:E:278:LEU:N	2.48	0.69
2:B:180:ILE:CG2	2:B:184:LEU:HD11	2.23	0.69
2:B:239:ASP:OD1	2:B:239:ASP:C	2.36	0.69
2:B:352:ASN:O	2:B:353:ASN:HB2	1.92	0.69
1:D:10:VAL:C	1:D:34:MET:HE1	2.18	0.69
1:D:128:THR:CG2	1:D:131:GLU:HB2	2.23	0.69
2:E:5:GLU:OE2	2:E:46:LYS:NZ	2.20	0.69
2:B:140:THR:N	2:B:141:PRO:CD	2.40	0.68
1:D:53:PHE:CD1	1:D:59:ALA:HB2	2.28	0.68
2:E:63:VAL:CG1	2:E:64:ASN:N	2.55	0.68
2:B:165:PHE:O	2:B:166:LYS:C	2.35	0.68
2:B:180:ILE:HG23	2:B:184:LEU:HD11	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:326:ASP:C	2:E:328:ILE:N	2.49	0.68
2:B:143:LEU:C	2:B:144:ILE:CD1	2.67	0.68
1:D:27:ALA:HB1	1:D:32:THR:HB	1.75	0.68
2:E:41:GLY:CA	2:E:42:PRO:C	2.66	0.68
2:E:128:GLU:CA	2:E:128:GLU:OE1	2.41	0.68
1:A:97:GLU:HB3	3:A:289:COA:C7P	2.24	0.68
2:B:276:VAL:CG1	2:B:281:GLY:HA3	2.24	0.68
2:B:296:GLU:H	2:B:296:GLU:CD	2.00	0.68
2:E:202:VAL:CG1	2:E:203:ILE:N	2.51	0.68
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
1:D:55:THR:HG22	1:D:57:ARG:N	2.08	0.68
1:D:159:GLU:O	1:D:160:ALA:C	2.30	0.68
1:D:250:ILE:HG12	1:D:251:ILE:N	2.06	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
2:B:103:ASP:O	2:B:204:THR:HA	1.93	0.68
2:B:278:LEU:HD12	2:B:278:LEU:O	1.94	0.68
1:D:221:ILE:CG1	1:D:225:VAL:CG1	2.72	0.68
2:E:383:ALA:O	2:E:385:VAL:N	2.26	0.68
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:D:128:THR:CA	1:D:173:THR:HG23	2.23	0.67
1:A:199:GLN:HG3	1:A:199:GLN:O	1.93	0.67
2:E:27:THR:OG1	2:E:30:GLU:HG3	1.94	0.67
2:E:50:HIS:CD2	2:E:237:GLN:HG3	2.29	0.67
2:E:364:SER:OG	2:E:366:LEU:CD2	2.42	0.67
1:A:104:MET:HE2	1:A:104:MET:O	1.94	0.67
1:A:116:VAL:CG1	1:A:117:ARG:N	2.56	0.67
2:B:69:ILE:O	2:B:70:ARG:C	2.35	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:147:VAL:HG12	1:A:148:GLY:N	2.08	0.67
2:E:292:GLY:O	2:E:294:THR:N	2.27	0.67
1:A:285:THR:O	1:A:287:LEU:N	2.28	0.67
2:B:157:PRO:HG3	2:B:182:MET:HE2	1.76	0.67
1:D:2:ILE:HD11	1:D:193:MET:HB2	0.68	0.67
1:D:57:ARG:O	1:D:58:GLU:C	2.32	0.67
2:B:324:ARG:O	2:B:327:LEU:HB2	1.94	0.67
1:D:286:VAL:HG13	1:D:287:LEU:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:ALA:HA	2:E:37:LYS:HG3	1.74	0.67
2:E:152:LEU:HD22	2:E:152:LEU:C	2.20	0.67
2:E:339:VAL:HG12	2:E:340:GLY:N	2.10	0.67
1:D:147:VAL:O	1:D:172:SER:N	2.26	0.67
1:D:156:LEU:O	1:D:157:THR:C	2.37	0.67
1:D:191:LEU:O	1:D:192:GLU:C	2.38	0.67
2:E:258:ASN:H	2:E:258:ASN:ND2	1.93	0.67
2:E:263:VAL:HG12	2:E:264:ASN:N	2.08	0.67
1:D:2:ILE:CG1	1:D:193:MET:HE2	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
1:D:127:ILE:C	1:D:173:THR:CG2	2.69	0.66
1:D:222:LYS:HB2	1:D:268:ALA:CB	2.25	0.66
2:E:197:GLU:O	2:E:215:LYS:HE3	1.94	0.66
1:A:26:GLN:O	1:A:27:ALA:C	2.37	0.66
2:B:81:LEU:HD22	2:B:82:VAL:N	2.09	0.66
1:A:129:PRO:HD2	1:A:172:SER:O	1.95	0.66
2:B:45:VAL:HG23	2:B:72:PHE:CE2	2.30	0.66
2:B:380:GLN:C	2:B:383:ALA:HB3	2.19	0.66
1:D:217:ALA:O	1:D:218:ALA:O	2.14	0.66
2:E:152:LEU:O	2:E:152:LEU:CD2	2.43	0.66
1:A:9:LYS:HB3	1:A:35:VAL:CG1	2.23	0.66
1:A:104:MET:CA	1:A:104:MET:HE3	2.04	0.66
1:D:203:ILE:C	1:D:229:VAL:HG23	2.20	0.66
1:D:251:ILE:O	1:D:251:ILE:HG22	1.95	0.66
1:A:167:TYR:CB	1:A:169:PHE:CE2	2.78	0.66
2:B:68:ASP:O	2:B:71:ALA:HB3	1.95	0.66
2:B:341:VAL:HG12	2:B:343:VAL:H	1.60	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:E:312:LYS:HZ2	2:E:388:LYS:HE3	1.61	0.66
2:B:94:ASN:C	2:B:95:GLN:HG2	2.19	0.66
1:D:10:VAL:C	1:D:11:ILE:HG22	1.99	0.66
2:E:235:GLN:O	2:E:238:GLU:HG2	1.95	0.66
2:E:318:ILE:O	2:E:318:ILE:HG22	1.96	0.66
2:E:330:ASP:OD1	2:E:360:LYS:HE2	1.95	0.66
1:A:267:ALA:C	1:A:269:GLY:H	2.02	0.66
2:E:87:ASP:O	2:E:87:ASP:OD1	2.14	0.66
2:B:84:TYR:CE1	2:B:85:GLN:HG3	2.30	0.65
2:B:184:LEU:HA	2:B:187:ILE:HG13	1.77	0.65
1:A:112:ASP:O	1:A:113:GLU:C	2.34	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:SER:OG	1:D:277:ALA:HB3	1.97	0.65
2:E:152:LEU:C	2:E:152:LEU:CD2	2.69	0.65
1:A:46:THR:HA	1:A:50:LEU:O	1.97	0.65
1:A:216:GLU:O	1:A:219:ALA:HB3	1.96	0.65
2:B:258:ASN:HD21	2:B:282:GLU:CB	2.08	0.65
1:D:189:ASP:C	1:D:190:ILE:HD13	2.21	0.65
2:B:372:LYS:N	2:B:376:ASP:OD2	2.28	0.65
1:A:283:LEU:O	1:A:287:LEU:N	2.27	0.65
1:D:23:HIS:CE1	1:D:136:ILE:CG2	2.76	0.65
1:D:220:TYR:CD2	1:D:221:ILE:N	2.64	0.65
1:D:275:SER:O	1:D:276:LEU:C	2.38	0.65
2:E:27:THR:O	2:E:30:GLU:HB2	1.97	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
1:A:21:THR:O	1:A:22:PHE:C	2.39	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
2:B:181:PHE:O	2:B:182:MET:C	2.37	0.65
2:E:255:LEU:O	2:E:256:ASP:CB	2.42	0.65
2:B:229:LEU:HA	2:B:232:MET:CE	2.25	0.64
2:B:21:VAL:O	2:B:99:GLU:HB2	1.97	0.64
2:E:258:ASN:HD22	2:E:258:ASN:N	1.93	0.64
2:E:312:LYS:HZ1	2:E:388:LYS:NZ	1.95	0.64
1:A:148:GLY:C	1:A:149:ILE:HG12	2.22	0.64
1:D:104:MET:HE3	1:D:104:MET:HA	1.80	0.64
2:E:323:VAL:O	2:E:324:ARG:HB2	1.96	0.64
2:E:315:LEU:CD1	2:E:315:LEU:C	2.58	0.64
1:A:212:SER:O	1:A:215:GLU:OE1	2.15	0.64
2:B:188:PHE:HA	2:B:193:LEU:HD12	1.80	0.64
2:E:263:VAL:HG11	2:E:268:LEU:HB3	1.79	0.64
2:B:42:PRO:HA	2:B:64:ASN:ND2	2.12	0.64
2:E:67:GLU:CD	2:E:67:GLU:H	2.04	0.64
2:E:257:GLY:HA3	2:E:282:GLU:HG3	1.80	0.64
1:A:104:MET:HE1	1:A:107:VAL:CB	2.26	0.64
1:A:158:TYR:N	1:A:158:TYR:CD1	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:72:PHE:CE1	2:E:76:TRP:NE1	2.66	0.64
1:D:10:VAL:CG1	1:D:34:MET:HE1	2.28	0.64
2:E:87:ASP:O	2:E:87:ASP:CG	2.41	0.64
2:E:158:TYR:C	2:E:158:TYR:CD1	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ILE:HG13	1:D:133:LYS:HB3	1.80	0.63
2:E:157:PRO:CD	2:E:182:MET:CE	2.74	0.63
1:A:94:THR:OG1	1:A:121:PRO:HB3	1.98	0.63
2:B:371:ALA:CB	2:B:377:ALA:HB2	2.27	0.63
1:D:153:SER:HB2	1:D:246:NEP:HE1	1.78	0.63
2:E:199:ASN:HB3	2:E:215:LYS:HZ2	1.63	0.63
2:E:248:TRP:O	2:E:249:GLU:HB2	1.97	0.63
2:E:325:CYS:HB2	2:E:354:ALA:HA	1.79	0.63
2:E:337:ALA:O	2:E:340:GLY:N	2.31	0.63
1:A:23:HIS:CE1	1:A:136:ILE:CG2	2.80	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
2:B:278:LEU:HD12	2:B:278:LEU:C	2.21	0.63
2:E:263:VAL:CG1	2:E:264:ASN:N	2.61	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
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
2:B:48:GLN:NE2	2:B:48:GLN:HA	2.14	0.63
2:B:141:PRO:HD2	2:B:142:HIS:CD2	2.32	0.63
2:E:312:LYS:NZ	2:E:388:LYS:HZ1	1.94	0.63
2:B:196:ILE:HG22	2:B:197:GLU:N	2.12	0.63
1:D:20:GLY:O	1:D:21:THR:C	2.41	0.63
1:D:237:THR:HG21	2:E:274:ASP:OD1	1.90	0.63
1:A:128:THR:HG21	1:A:131:GLU:HB2	1.78	0.63
1:A:155:THR:O	1:A:156:LEU:C	2.40	0.63
2:B:292:GLY:O	2:B:294:THR:N	2.31	0.63
2:E:45:VAL:CG2	2:E:61:LYS:O	2.45	0.63
2:E:335:ALA:O	2:E:336:VAL:C	2.40	0.63
1:D:22:PHE:O	1:D:24:SER:N	2.32	0.63
1:A:124:PRO:HA	1:A:136:ILE:HD13	1.80	0.62
2:B:109:TYR:CD1	2:B:110:LEU:N	2.66	0.62
2:B:381:VAL:O	2:B:382:VAL:C	2.40	0.62
2:E:258:ASN:HD22	2:E:259:ILE:N	1.96	0.62
1:A:72:VAL:HG13	1:A:73:PRO:CD	2.27	0.62
1:A:123:CYS:HB3	1:A:178:GLY:CA	2.29	0.62
1:A:253:GLY:O	1:A:255:LYS:N	2.32	0.62
2:B:273:MET:HE3	2:B:285:ASN:O	1.99	0.62
2:E:195:LEU:HD23	2:E:195:LEU:C	2.24	0.62
2:E:294:THR:O	2:E:295:LYS:C	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TYR:N	1:A:158:TYR:HD1	1.96	0.62
1:A:195:GLU:O	1:A:227:LYS:HE3	1.98	0.62
2:B:7:GLN:NE2	2:B:232:MET:HG2	2.13	0.62
2:B:319:PHE:CD1	2:B:319:PHE:C	2.78	0.62
1:D:280:GLY:O	1:D:281:GLU:C	2.42	0.62
2:E:156:MET:HB3	2:E:157:PRO:HD2	1.80	0.62
2:E:369:ILE:HD13	2:E:369:ILE:H	1.61	0.62
1:A:124:PRO:O	1:A:135:GLY:CA	2.44	0.62
2:B:13:ALA:O	2:B:14:ARG:C	2.40	0.62
1:D:30:TYR:OH	1:D:129:PRO:HA	1.99	0.62
1:A:6:LYS:N	1:A:131:GLU:OE1	2.30	0.62
1:A:133:LYS:NZ	1:A:137:GLN:O	2.21	0.62
1:A:262:PHE:O	1:A:263:ALA:C	2.43	0.62
1:D:267:ALA:C	1:D:269:GLY:H	2.07	0.62
2:E:385:VAL:HG12	2:E:386:GLU:N	2.13	0.62
1:A:173:THR:HG22	1:A:174:CYS:N	2.14	0.62
1:D:194:PHE:HB3	1:D:203:ILE:HD11	1.80	0.62
2:E:118:SER:C	2:E:119:ARG:HG3	2.24	0.62
1:A:25:GLU:O	1:A:28:ILE:HB	1.99	0.62
2:B:4:HIS:HB2	2:B:7:GLN:HG3	1.81	0.62
1:D:26:GLN:O	1:D:27:ALA:C	2.43	0.62
1:D:92:ILE:HG22	1:D:118:MET:CG	2.10	0.62
1:D:128:THR:HG22	1:D:128:THR:O	1.99	0.62
1:D:263:ALA:O	1:D:265:LEU:N	2.32	0.62
1:D:97:GLU:C	1:D:97:GLU:CD	2.68	0.62
2:E:109:TYR:CE2	2:E:197:GLU:OE1	2.52	0.62
1:A:248:GLY:O	2:B:116:ARG:NH2	2.33	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:D:202:ALA:C	1:D:203:ILE:HG13	2.24	0.62
1:D:286:VAL:CG1	1:D:287:LEU:N	2.63	0.62
1:D:22:PHE:O	1:D:23:HIS:C	2.39	0.61
1:D:23:HIS:CD2	1:D:136:ILE:HG22	2.35	0.61
1:D:217:ALA:O	1:D:221:ILE:HD12	1.99	0.61
1:A:221:ILE:HG23	1:A:222:LYS:N	2.03	0.61
2:E:109:TYR:HE2	2:E:197:GLU:OE1	1.83	0.61
2:E:184:LEU:HA	2:E:187:ILE:HG13	1.81	0.61
1:D:195:GLU:HA	1:D:227:LYS:HE3	1.81	0.61
2:E:72:PHE:CD1	2:E:76:TRP:CD1	2.89	0.61
2:E:246:ALA:C	2:E:248:TRP:N	2.52	0.61
1:A:146:LYS:NZ	1:A:201:GLU:OE2	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:THR:H	2:B:86:THR:HB	1.66	0.61
1:D:2:ILE:CD1	1:D:193:MET:HE2	2.30	0.61
2:E:94:ASN:C	2:E:95:GLN:HG2	2.23	0.61
2:E:126:SER:OG	2:E:128:GLU:N	2.28	0.61
1:D:7:ASN:HA	1:D:33:LYS:HZ2	1.63	0.61
2:E:38:ILE:HG21	2:E:43:TRP:HD1	1.64	0.61
1:A:159:GLU:O	1:A:160:ALA:C	2.43	0.61
2:B:318:ILE:CG2	2:B:319:PHE:N	2.58	0.61
2:B:319:PHE:O	2:B:320:GLY:O	2.18	0.61
1:A:55:THR:HG22	1:A:57:ARG:N	2.15	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:80:SER:O	1:A:83:GLU:HB3	2.00	0.61
2:B:348:ARG:HD3	2:B:348:ARG:C	2.26	0.61
2:E:82:VAL:CG2	2:E:90:GLY:N	2.38	0.61
2:E:219:ASP:O	2:E:220:GLY:C	2.42	0.61
2:E:343:VAL:HG13	2:E:344:PRO:CG	2.24	0.61
1:A:97:GLU:HB3	3:A:289:COA:H71	1.83	0.61
2:B:186:THR:CG2	2:B:190:GLU:HG3	2.31	0.61
1:D:77:CYS:HB3	1:D:99:ILE:HD11	1.83	0.61
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
1:A:195:GLU:CD	1:A:226:THR:H	2.09	0.60
1:D:129:PRO:C	1:D:131:GLU:N	2.59	0.60
1:D:237:THR:HG23	2:E:274:ASP:CG	2.05	0.60
1:A:127:ILE:HG23	1:A:127:ILE:O	2.01	0.60
1:A:141:ILE:HG22	1:A:141:ILE:O	1.99	0.60
1:A:203:ILE:HG22	1:A:204:VAL:N	2.15	0.60
1:D:89:ILE:HG22	1:D:91:LEU:H	1.65	0.60
2:B:315:LEU:HD13	2:B:346:VAL:HB	1.84	0.60
1:D:189:ASP:HB2	1:D:190:ILE:HD13	1.84	0.60
1:D:250:ILE:CG1	1:D:251:ILE:N	2.63	0.60
2:E:271:GLY:O	2:E:272:THR:C	2.41	0.60
2:E:325:CYS:O	2:E:328:ILE:HB	2.02	0.60
2:B:82:VAL:HG22	2:B:86:THR:CG2	2.28	0.60
2:B:263:VAL:CG1	2:B:268:LEU:HB3	2.29	0.60
2:B:343:VAL:HG22	2:B:344:PRO:HD2	1.83	0.60
1:D:127:ILE:HB	1:D:133:LYS:HB2	1.84	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:E:157:PRO:HD3	2:E:182:MET:HE1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:PHE:O	1:A:266:GLU:HG3	2.02	0.60
2:B:156:MET:HB3	2:B:157:PRO:HD2	1.82	0.60
2:B:158:TYR:C	2:B:158:TYR:CD1	2.80	0.60
2:B:316:VAL:HG12	2:B:317:ASN:N	2.13	0.60
1:A:246:NEP:CD2	2:B:266:ALA:HB3	2.32	0.60
2:E:72:PHE:O	2:E:75:ASN:HB3	2.02	0.60
2:E:323:VAL:HG12	2:E:324:ARG:N	2.16	0.60
2:E:332:ILE:O	2:E:336:VAL:HG23	2.02	0.60
1:A:74:ALA:N	1:A:75:PRO:HD2	2.17	0.60
1:A:218:ALA:O	1:A:219:ALA:O	2.20	0.60
2:B:202:VAL:HG13	2:B:203:ILE:N	2.17	0.60
1:D:187:PHE:HE2	1:D:214:GLU:CG	2.04	0.60
2:E:234:ASP:C	2:E:234:ASP:OD1	2.45	0.60
2:E:258:ASN:ND2	2:E:258:ASN:N	2.42	0.60
2:B:140:THR:OG1	2:B:143:LEU:CD1	2.33	0.59
1:D:153:SER:HB3	4:D:309:HOH:O	2.01	0.59
1:D:122:ASN:C	3:D:289:COA:S1P	2.84	0.59
2:E:312:LYS:HZ3	2:E:388:LYS:NZ	1.93	0.59
1:A:35:VAL:CG2	1:A:65:ALA:HB2	2.33	0.59
1:D:117:ARG:HG3	1:D:118:MET:N	2.15	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
1:D:283:LEU:O	1:D:284:LYS:C	2.45	0.59
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
1:A:39:THR:CG2	1:A:42:LYS:HG3	2.31	0.59
1:A:86:ASP:OD1	1:A:86:ASP:O	2.21	0.59
2:B:275:ILE:HG23	2:B:276:VAL:N	2.15	0.59
2:B:333:ILE:HG22	2:B:334:GLY:N	2.08	0.59
1:D:116:VAL:CG1	1:D:117:ARG:H	2.05	0.59
2:E:63:VAL:HG11	2:E:68:ASP:CB	2.32	0.59
1:A:186:ASN:O	1:A:187:PHE:C	2.40	0.59
2:B:135:LYS:O	2:B:138:GLU:N	2.35	0.59
1:A:74:ALA:HB1	1:A:98:GLY:O	2.03	0.59
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.68	0.59
1:A:35:VAL:HG21	1:A:65:ALA:HB2	1.84	0.59
2:B:152:LEU:C	2:B:152:LEU:CD2	2.75	0.59
1:D:22:PHE:C	1:D:24:SER:N	2.55	0.59
1:D:187:PHE:CG	1:D:205:MET:HE3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:GLY:HA3	2:E:42:PRO:C	2.24	0.59
2:E:248:TRP:O	2:E:249:GLU:CB	2.50	0.59
1:A:97:GLU:HB3	3:A:289:COA:H72	1.84	0.58
1:A:285:THR:C	1:A:287:LEU:N	2.61	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:180:ILE:O	2:E:181:PHE:C	2.42	0.58
2:E:348:ARG:NH1	2:E:374:LEU:H	2.01	0.58
1:A:56:VAL:O	1:A:57:ARG:C	2.41	0.58
1:A:156:LEU:O	1:A:159:GLU:N	2.36	0.58
1:D:50:LEU:HB3	1:D:51:PRO:HD2	1.84	0.58
1:D:128:THR:HA	1:D:173:THR:HG23	1.85	0.58
1:D:273:VAL:HG13	1:D:275:SER:H	1.68	0.58
2:E:4:HIS:O	2:E:5:GLU:C	2.43	0.58
2:E:97:LEU:C	2:E:97:LEU:CD2	2.76	0.58
2:E:371:ALA:CB	2:E:377:ALA:HA	2.34	0.58
1:A:21:THR:OG1	1:A:47:HIS:NE2	2.37	0.58
1:A:212:SER:O	1:A:213:ALA:C	2.46	0.58
2:B:165:PHE:C	2:B:167:LEU:N	2.58	0.58
2:E:329:ALA:O	2:E:333:ILE:HD12	2.03	0.58
1:A:244:MET:CE	2:B:253:VAL:HG21	2.33	0.58
2:B:165:PHE:O	2:B:168:GLY:N	2.35	0.58
2:B:276:VAL:HG13	2:B:281:GLY:HA3	1.86	0.58
1:D:124:PRO:HG2	1:D:176:GLY:HA3	1.84	0.58
2:E:94:ASN:HB2	4:E:403:HOH:O	2.03	0.58
2:E:157:PRO:CG	2:E:182:MET:CE	2.82	0.58
2:E:223:LEU:O	2:E:224:PHE:C	2.42	0.58
2:E:326:ASP:CG	2:E:327:LEU:H	2.09	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:186:ASN:HD21	1:D:189:ASP:CG	2.12	0.58
1:A:105:LEU:HD23	1:A:106:THR:N	2.18	0.58
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
2:B:158:TYR:CE1	2:B:159:GLN:HG2	2.38	0.58
1:D:151:SER:CB	1:D:206:ILE:HB	2.33	0.58
1:D:218:ALA:O	1:D:221:ILE:N	2.37	0.58
2:B:356:LEU:C	2:B:356:LEU:CD2	2.75	0.58
2:E:176:GLN:HE22	2:E:209:LEU:H	1.51	0.58
1:A:160:ALA:O	1:A:161:VAL:C	2.45	0.58
1:A:229:VAL:CG2	1:A:230:VAL:N	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:LEU:O	2:B:185:ALA:C	2.45	0.58
2:B:205:LYS:C	2:B:207:GLY:H	2.10	0.58
2:B:362:ALA:O	2:B:364:SER:N	2.36	0.58
1:D:7:ASN:HA	1:D:33:LYS:HZ1	1.67	0.58
2:E:313:ALA:HA	2:E:343:VAL:HG11	1.86	0.58
2:B:263:VAL:CG1	2:B:264:ASN:N	2.66	0.58
2:E:150:ASP:OD1	2:E:151:PRO:CD	2.51	0.58
2:B:319:PHE:C	2:B:319:PHE:HD1	2.10	0.57
2:B:373:GLY:O	2:B:376:ASP:HB3	2.04	0.57
1:D:55:THR:HB	1:D:58:GLU:H	1.69	0.57
2:E:262:MET:CE	2:E:301:ALA:HB1	2.20	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:B:115:ASP:OD2	2:B:118:SER:OG	2.22	0.57
2:B:263:VAL:HG12	2:B:264:ASN:N	2.19	0.57
1:D:217:ALA:O	1:D:218:ALA:C	2.46	0.57
1:D:221:ILE:O	1:D:222:LYS:C	2.41	0.57
2:E:176:GLN:HE21	2:E:209:LEU:HB2	1.68	0.57
2:B:13:ALA:O	2:B:15:TYR:N	2.38	0.57
2:B:252:TYR:HE2	2:B:254:ALA:HB2	1.69	0.57
1:D:139:GLY:C	1:D:141:ILE:H	2.08	0.57
2:E:16:GLY:C	2:E:17:LEU:HD23	2.29	0.57
2:E:364:SER:OG	2:E:365:GLY:N	2.33	0.57
1:A:265:LEU:HB3	1:A:270:VAL:HB	1.86	0.57
2:B:152:LEU:CD2	2:B:152:LEU:O	2.52	0.57
1:D:221:ILE:CA	1:D:225:VAL:HG13	2.30	0.57
2:E:156:MET:C	2:E:182:MET:CE	2.77	0.57
2:E:364:SER:CB	2:E:366:LEU:CD2	2.83	0.57
2:B:109:TYR:CD1	2:B:109:TYR:O	2.51	0.57
2:B:176:GLN:O	2:B:177:PHE:C	2.46	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
1:D:287:LEU:HD23	1:D:287:LEU:C	2.28	0.57
2:E:70:ARG:O	2:E:70:ARG:CG	2.45	0.57
2:E:140:THR:HG23	2:E:140:THR:O	2.02	0.57
2:B:84:TYR:CE1	2:B:85:GLN:CG	2.88	0.57
1:D:3:LEU:HD23	1:D:193:MET:HE1	1.86	0.57
2:E:140:THR:N	2:E:141:PRO:CD	2.61	0.57
2:E:356:LEU:CD2	2:E:357:GLY:N	2.56	0.57
1:A:149:ILE:HG23	1:A:204:VAL:CB	2.33	0.57
1:A:229:VAL:O	1:A:229:VAL:HG22	1.89	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:THR:HG23	2:B:274:ASP:OD1	2.03	0.57
2:B:239:ASP:OD1	2:B:241:ARG:N	2.38	0.57
2:B:255:LEU:CD2	2:B:273:MET:HE1	2.34	0.57
1:D:10:VAL:HG12	1:D:34:MET:HE1	1.85	0.57
1:D:73:PRO:HA	3:D:289:COA:H143	1.87	0.57
1:D:203:ILE:HB	1:D:229:VAL:HG21	1.82	0.57
2:E:32:GLU:OE1	2:E:70:ARG:NH1	2.38	0.57
2:E:87:ASP:C	2:E:87:ASP:OD1	2.45	0.57
2:E:264:ASN:HB2	2:E:318:ILE:HG13	1.86	0.57
1:A:145:GLY:HA3	1:A:170:GLY:C	2.29	0.57
1:A:145:GLY:HA3	1:A:170:GLY:HA3	1.87	0.57
1:D:89:ILE:HG22	1:D:91:LEU:N	2.20	0.57
1:D:128:THR:HG22	1:D:131:GLU:CB	2.34	0.57
2:E:66:LYS:O	2:E:67:GLU:C	2.48	0.57
2:E:346:VAL:C	2:E:347:VAL:CG2	2.72	0.57
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
1:A:55:THR:HG22	1:A:56:VAL:N	2.20	0.56
1:A:259:ASP:O	1:A:260:GLU:C	2.48	0.56
2:B:43:TRP:CE3	2:B:43:TRP:N	2.73	0.56
2:E:156:MET:C	2:E:182:MET:HE1	2.30	0.56
2:E:339:VAL:HG12	2:E:341:VAL:H	1.70	0.56
2:E:379:GLN:O	2:E:382:VAL:N	2.38	0.56
1:A:159:GLU:OE2	2:B:319:PHE:HD2	1.87	0.56
2:B:248:TRP:O	2:B:249:GLU:C	2.49	0.56
2:B:250:LEU:CD2	2:B:289:VAL:HA	2.36	0.56
2:B:368:ILE:HG22	2:B:369:ILE:N	2.20	0.56
1:D:59:ALA:O	1:D:60:VAL:C	2.44	0.56
1:D:104:MET:HE3	1:D:104:MET:C	2.30	0.56
1:D:158:TYR:HB3	2:E:319:PHE:CE1	2.40	0.56
2:E:20:PRO:HD3	2:E:210:ILE:HD11	1.88	0.56
2:E:57:ALA:HB2	2:E:83:THR:HG22	1.87	0.56
2:E:132:GLU:OE1	2:E:134:GLU:HG3	2.04	0.56
2:E:281:GLY:H	2:E:382:VAL:HG21	1.70	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
1:A:6:LYS:HB2	1:A:131:GLU:OE1	2.06	0.56
1:A:203:ILE:CG2	1:A:204:VAL:N	2.69	0.56
1:D:5:ASP:OD1	1:D:7:ASN:HB2	2.04	0.56
2:E:68:ASP:O	2:E:71:ALA:HB3	2.06	0.56
2:E:80:ARG:HD3	2:E:89:ASN:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:127:THR:O	2:E:129:GLY:N	2.37	0.56
2:B:152:LEU:O	2:B:152:LEU:HD23	2.05	0.56
2:B:224:PHE:C	2:B:224:PHE:CD1	2.83	0.56
1:D:34:MET:CE	1:D:34:MET:HA	2.34	0.56
2:E:45:VAL:HB	2:E:72:PHE:CD2	2.39	0.56
2:E:79:LYS:HZ3	2:E:79:LYS:CB	2.12	0.56
2:B:205:LYS:C	2:B:207:GLY:N	2.63	0.56
2:B:257:GLY:O	2:B:284:ALA:CB	2.53	0.56
1:D:24:SER:O	1:D:25:GLU:C	2.48	0.56
1:D:89:ILE:HG22	1:D:90:LYS:N	2.19	0.56
1:D:186:ASN:H	1:D:186:ASN:ND2	2.01	0.56
1:D:267:ALA:C	1:D:269:GLY:N	2.58	0.56
2:E:346:VAL:C	2:E:347:VAL:HG22	2.29	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
2:E:313:ALA:HA	2:E:343:VAL:CG1	2.36	0.56
1:D:127:ILE:C	1:D:173:THR:HG22	2.30	0.56
1:D:140:HIS:CD2	1:D:140:HIS:C	2.79	0.56
1:A:242:LYS:HB3	1:A:244:MET:HE3	1.87	0.56
1:D:140:HIS:N	1:D:140:HIS:ND1	2.53	0.56
1:A:5:ASP:OD1	1:A:5:ASP:C	2.48	0.56
1:D:123:CYS:CA	3:D:289:COA:S1P	2.94	0.56
2:E:87:ASP:O	2:E:88:ALA:C	2.47	0.56
2:E:156:MET:HB3	2:E:157:PRO:CD	2.36	0.56
1:A:188:ILE:O	1:A:189:ASP:C	2.49	0.55
2:B:82:VAL:HA	2:B:86:THR:HG21	1.88	0.55
2:E:343:VAL:HG12	2:E:344:PRO:N	2.20	0.55
1:D:169:PHE:CE2	1:D:283:LEU:CB	2.88	0.55
1:D:276:LEU:C	1:D:276:LEU:HD12	2.31	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:E:9:LYS:O	2:E:10:GLN:C	2.48	0.55
2:E:97:LEU:HD23	2:E:97:LEU:C	2.29	0.55
2:E:324:ARG:O	2:E:325:CYS:C	2.49	0.55
2:B:133:ILE:C	2:B:135:LYS:N	2.61	0.55
2:B:339:VAL:HG12	2:B:340:GLY:C	2.31	0.55
1:D:10:VAL:CB	1:D:34:MET:CE	2.80	0.55
1:A:19:GLN:OE1	1:A:19:GLN:HA	2.02	0.55
1:D:3:LEU:C	1:D:4:ILE:CG2	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:107:GLU:O	2:E:108:LEU:HD23	2.05	0.55
2:E:278:LEU:HD23	2:E:279:HIS:ND1	2.21	0.55
2:E:302:PHE:C	2:E:306:LEU:HD12	2.31	0.55
2:B:206:GLN:H	2:B:206:GLN:CD	2.14	0.55
1:D:55:THR:HB	1:D:58:GLU:HG3	1.89	0.55
1:D:208:GLU:OE2	1:D:246:NEP:ND1	2.39	0.55
2:E:49:VAL:HG12	2:E:54:ARG:HD3	1.89	0.55
2:E:258:ASN:C	2:E:258:ASN:ND2	2.58	0.55
2:E:328:ILE:O	2:E:329:ALA:C	2.49	0.55
2:E:332:ILE:O	2:E:335:ALA:HB3	2.07	0.55
1:A:128:THR:HG22	1:A:131:GLU:HB2	1.87	0.55
2:B:65:SER:O	2:B:68:ASP:HB2	2.07	0.55
2:B:337:ALA:O	2:B:338:GLU:C	2.49	0.55
1:D:110:LYS:HZ2	1:D:113:GLU:HG2	1.72	0.55
1:D:182:ILE:HB	4:D:302:HOH:O	2.07	0.55
1:D:287:LEU:O	1:D:287:LEU:HD22	2.05	0.55
2:E:294:THR:O	2:E:297:ARG:N	2.39	0.55
1:A:190:ILE:O	1:A:193:MET:N	2.39	0.55
2:B:234:ASP:OD2	2:B:237:GLN:HG2	2.06	0.55
1:D:97:GLU:OE1	1:D:98:GLY:CA	2.53	0.55
2:E:164:ALA:HB1	2:E:169:LEU:HD12	1.87	0.55
2:E:377:ALA:O	2:E:381:VAL:HG23	2.06	0.55
1:D:128:THR:CG2	1:D:128:THR:O	2.54	0.55
1:D:263:ALA:O	1:D:264:ALA:C	2.49	0.55
2:E:126:SER:OG	2:E:127:THR:N	2.37	0.55
2:E:157:PRO:HG3	2:E:182:MET:HE3	1.89	0.55
2:E:243:ALA:O	2:E:244:GLN:C	2.49	0.55
2:E:271:GLY:O	2:E:274:ASP:N	2.39	0.55
1:A:48:LEU:N	1:A:48:LEU:HD23	2.21	0.55
1:A:80:SER:O	1:A:81:ILE:C	2.50	0.55
1:A:104:MET:HE1	1:A:107:VAL:CG1	2.37	0.55
1:A:276:LEU:O	1:A:279:ILE:HG13	2.07	0.55
2:B:324:ARG:CB	2:B:327:LEU:HD12	2.31	0.55
1:A:129:PRO:HB3	1:A:142:HIS:HB2	1.88	0.54
2:B:45:VAL:O	2:B:45:VAL:HG22	2.01	0.54
2:B:86:THR:HG23	2:B:87:ASP:N	2.22	0.54
2:B:308:ASP:C	2:B:308:ASP:OD1	2.50	0.54
1:D:84:ALA:O	1:D:85:ILE:C	2.43	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:E:312:LYS:HZ3	2:E:388:LYS:HZ1	1.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:VAL:CG1	2:B:68:ASP:CB	2.74	0.54
1:D:287:LEU:C	1:D:287:LEU:CD2	2.80	0.54
2:E:60:VAL:CG1	2:E:61:LYS:N	2.69	0.54
2:E:277:LYS:HD2	2:E:277:LYS:C	2.28	0.54
2:E:346:VAL:HG21	2:E:381:VAL:CG2	2.30	0.54
1:A:95:ILE:HG13	1:A:123:CYS:O	2.07	0.54
1:A:110:LYS:HG3	1:A:110:LYS:O	2.07	0.54
1:A:138:PRO:HG2	1:A:141:ILE:HD11	1.89	0.54
1:A:220:TYR:O	1:A:221:ILE:C	2.48	0.54
2:B:332:ILE:O	2:B:333:ILE:C	2.47	0.54
1:D:128:THR:CG2	1:D:131:GLU:HB3	2.36	0.54
1:D:139:GLY:C	1:D:141:ILE:N	2.65	0.54
1:D:181:PRO:O	2:E:116:ARG:HD3	2.06	0.54
2:E:119:ARG:O	2:E:120:ARG:CD	2.55	0.54
2:E:262:MET:HE2	2:E:301:ALA:C	2.32	0.54
1:D:285:THR:HG22	1:D:286:VAL:H	1.68	0.54
1:A:138:PRO:HD2	1:A:158:TYR:CZ	2.43	0.54
1:A:167:TYR:HB3	1:A:169:PHE:HE2	1.67	0.54
1:A:257:THR:OG1	1:A:260:GLU:HG3	2.06	0.54
2:E:300:GLU:O	2:E:301:ALA:C	2.47	0.54
2:E:352:ASN:HD21	2:E:353:ASN:HB2	1.70	0.54
1:A:11:ILE:HD11	1:A:68:SER:HB2	1.89	0.54
1:A:193:MET:O	1:A:194:PHE:C	2.47	0.54
2:B:335:ALA:O	2:B:336:VAL:C	2.51	0.54
2:B:349:LEU:O	2:B:350:GLU:HB2	2.06	0.54
1:D:66:THR:HG22	1:D:90:LYS:HD2	1.90	0.54
1:D:257:THR:OG1	1:D:260:GLU:CB	2.39	0.54
2:E:34:ALA:O	2:E:35:ALA:C	2.50	0.54
2:E:241:ARG:HB3	2:E:252:TYR:CE2	2.43	0.54
1:A:229:VAL:HG23	1:A:230:VAL:N	2.21	0.54
1:A:280:GLY:O	1:A:281:GLU:C	2.51	0.54
2:B:176:GLN:O	2:B:179:LYS:HB3	2.08	0.54
2:B:252:TYR:CE2	2:B:254:ALA:HB2	2.41	0.54
1:D:136:ILE:CD1	1:D:136:ILE:N	2.62	0.54
2:E:176:GLN:NE2	2:E:209:LEU:H	2.05	0.54
2:E:296:GLU:H	2:E:296:GLU:CD	2.01	0.54
1:A:173:THR:CG2	1:A:174:CYS:N	2.70	0.54
1:A:267:ALA:C	1:A:269:GLY:N	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:323:VAL:O	2:E:324:ARG:CB	2.53	0.54
1:A:157:THR:O	1:A:158:TYR:C	2.49	0.54
1:D:67:ALA:HB2	1:D:91:LEU:HB3	1.89	0.54
1:D:283:LEU:HA	1:D:286:VAL:HG12	1.89	0.54
2:E:65:SER:O	2:E:66:LYS:C	2.51	0.54
2:E:199:ASN:CB	2:E:215:LYS:HZ2	2.21	0.54
1:A:41:GLY:N	1:A:54:ASN:OD1	2.39	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
1:D:95:ILE:HD11	1:D:135:GLY:HA2	1.90	0.54
2:E:32:GLU:OE2	2:E:70:ARG:HD2	2.07	0.54
1:D:75:PRO:HB3	2:E:224:PHE:CE1	2.43	0.53
1:D:127:ILE:C	1:D:173:THR:HG23	2.32	0.53
1:A:11:ILE:HG13	1:A:67:ALA:O	2.08	0.53
2:B:140:THR:C	2:B:142:HIS:N	2.62	0.53
1:D:102:LEU:HD22	4:E:400:HOH:O	2.07	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:A:253:GLY:C	1:A:255:LYS:H	2.16	0.53
1:D:46:THR:HG22	1:D:50:LEU:C	2.33	0.53
1:D:159:GLU:O	1:D:162:LYS:HB3	2.08	0.53
1:D:203:ILE:CG2	1:D:204:VAL:N	2.71	0.53
1:D:277:ALA:C	1:D:279:ILE:H	2.16	0.53
1:A:2:ILE:CG2	1:A:173:THR:HG21	2.38	0.53
1:A:194:PHE:O	1:A:195:GLU:C	2.52	0.53
2:B:153:THR:C	2:B:154:GLY:O	2.50	0.53
2:B:325:CYS:CB	2:B:349:LEU:HD13	2.23	0.53
1:D:191:LEU:HD11	1:D:221:ILE:HD11	1.89	0.53
2:E:72:PHE:CD1	2:E:76:TRP:HD1	2.26	0.53
2:E:135:LYS:O	2:E:136:VAL:C	2.49	0.53
1:A:244:MET:HE2	1:A:244:MET:HA	1.90	0.53
2:B:362:ALA:O	2:B:363:ASP:C	2.49	0.53
3:D:289:COA:O9P	3:D:289:COA:C6P	2.57	0.53
2:E:373:GLY:O	2:E:376:ASP:HB3	2.09	0.53
1:A:202:ALA:HB2	1:A:228:PRO:HG2	1.90	0.53
1:D:283:LEU:O	1:D:287:LEU:N	2.28	0.53
2:E:105:ALA:CB	2:E:203:ILE:O	2.53	0.53
2:E:346:VAL:HB	2:E:381:VAL:CG2	2.39	0.53
1:A:97:GLU:OE1	1:A:97:GLU:HA	2.08	0.53
2:B:108:LEU:HD22	2:B:127:THR:HA	1.90	0.53
1:D:169:PHE:HE2	1:D:283:LEU:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:330:ASP:HA	2:E:333:ILE:CD1	2.39	0.53
1:A:48:LEU:HD23	1:A:48:LEU:H	1.74	0.53
1:A:154:GLY:O	1:A:155:THR:C	2.51	0.53
1:D:4:ILE:HG13	1:D:132:CYS:SG	2.48	0.53
2:E:128:GLU:OE1	2:E:128:GLU:N	2.40	0.53
2:E:229:LEU:O	2:E:230:ARG:C	2.49	0.53
2:E:375:THR:O	2:E:378:ALA:CB	2.43	0.53
1:D:34:MET:O	1:D:35:VAL:HG13	2.08	0.53
1:D:186:ASN:OD1	1:D:186:ASN:C	2.52	0.53
1:D:219:ALA:O	1:D:220:TYR:C	2.52	0.53
2:E:45:VAL:HB	2:E:72:PHE:CE2	2.44	0.53
2:E:131:VAL:HG12	2:E:132:GLU:N	2.24	0.53
2:E:237:GLN:HA	2:E:237:GLN:NE2	2.24	0.53
1:D:105:LEU:CD2	1:D:106:THR:N	2.71	0.52
1:D:232:TYR:HD1	1:D:273:VAL:O	1.92	0.52
2:E:199:ASN:HB3	2:E:215:LYS:NZ	2.24	0.52
1:A:191:LEU:O	1:A:192:GLU:C	2.52	0.52
1:A:258:ALA:O	1:A:261:LYS:HB2	2.08	0.52
2:E:312:LYS:C	2:E:343:VAL:HG11	2.34	0.52
1:A:105:LEU:C	1:A:105:LEU:CD2	2.74	0.52
2:B:65:SER:O	2:B:66:LYS:C	2.52	0.52
2:B:362:ALA:C	2:B:364:SER:N	2.66	0.52
2:B:373:GLY:O	2:B:374:LEU:C	2.51	0.52
2:B:383:ALA:O	2:B:386:GLU:OE1	2.27	0.52
1:D:195:GLU:O	1:D:227:LYS:HE2	2.09	0.52
2:E:348:ARG:HH11	2:E:374:LEU:HB2	1.73	0.52
1:A:253:GLY:C	1:A:255:LYS:N	2.67	0.52
1:A:273:VAL:HG11	1:A:278:ASP:HB2	1.91	0.52
2:B:121:VAL:HG22	2:B:149:LEU:HG	1.91	0.52
2:B:323:VAL:CG1	2:B:328:ILE:HG13	2.28	0.52
1:D:13:GLN:N	1:D:69:VAL:O	2.33	0.52
2:E:76:TRP:HA	2:E:79:LYS:CG	2.39	0.52
2:E:214:GLY:C	2:E:215:LYS:HG3	2.35	0.52
2:E:259:ILE:O	2:E:283:PRO:HA	2.08	0.52
1:A:77:CYS:O	1:A:78:LYS:C	2.51	0.52
2:B:13:ALA:C	2:B:15:TYR:N	2.63	0.52
1:A:199:GLN:O	1:A:199:GLN:CG	2.55	0.52
3:A:289:COA:O9P	3:A:289:COA:CDP	2.55	0.52
2:B:258:ASN:HD22	2:B:282:GLU:HB3	1.69	0.52
1:D:12:CYS:O	1:D:15:PHE:HB2	2.09	0.52
1:D:108:LYS:HA	1:D:111:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ILE:CB	1:D:225:VAL:CG1	2.86	0.52
2:E:38:ILE:HG21	2:E:43:TRP:CD1	2.45	0.52
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.92	0.52
2:B:34:ALA:O	2:B:38:ILE:HG13	2.10	0.52
2:B:144:ILE:HG22	2:B:145:HIS:N	2.25	0.52
1:D:257:THR:HG1	1:D:260:GLU:HB2	1.71	0.52
2:E:276:VAL:HG13	2:E:281:GLY:HA3	1.91	0.52
1:A:35:VAL:CG2	1:A:63:THR:HB	2.40	0.52
1:A:163:GLN:C	1:A:165:THR:N	2.64	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:B:105:ALA:HB3	2:B:203:ILE:CG2	2.39	0.52
2:B:135:LYS:O	2:B:138:GLU:HB3	2.10	0.52
1:D:244:MET:HE1	2:E:253:VAL:HG11	1.91	0.52
2:E:376:ASP:O	2:E:379:GLN:HB2	2.10	0.52
1:A:11:ILE:HA	1:A:36:GLY:O	2.09	0.52
1:A:84:ALA:O	1:A:85:ILE:C	2.51	0.52
1:A:273:VAL:CG1	1:A:275:SER:O	2.58	0.52
2:B:285:ASN:HD22	2:B:286:PHE:N	2.07	0.52
2:E:262:MET:HE1	2:E:302:PHE:CD2	2.45	0.52
1:A:73:PRO:C	1:A:75:PRO:HD2	2.36	0.52
2:B:333:ILE:O	2:B:334:GLY:C	2.53	0.52
1:D:4:ILE:CD1	1:D:126:VAL:HG22	2.40	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
1:D:77:CYS:HB3	1:D:99:ILE:CD1	2.40	0.52
1:D:266:GLU:CG	1:D:272:THR:CG2	2.81	0.52
2:E:202:VAL:HG13	2:E:203:ILE:N	2.23	0.52
2:B:140:THR:O	2:B:141:PRO:C	2.53	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
2:B:51:ALA:O	2:B:54:ARG:HD3	2.10	0.51
1:D:106:THR:O	1:D:109:VAL:HB	2.11	0.51
1:A:174:CYS:C	1:A:175:VAL:CG2	2.84	0.51
2:B:17:LEU:HB3	2:B:18:PRO:HD2	1.93	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:208:ASP:HB2	4:B:392:HOH:O	2.08	0.51
2:B:270:MET:CG	4:B:419:HOH:O	2.42	0.51
2:B:319:PHE:HD1	2:B:320:GLY:N	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:O	1:A:172:SER:N	2.34	0.51
1:A:163:GLN:O	1:A:166:ASP:N	2.43	0.51
1:A:251:ILE:O	1:A:252:ALA:O	2.28	0.51
2:E:336:VAL:HA	2:E:341:VAL:CG1	2.41	0.51
2:B:72:PHE:O	2:B:73:ALA:C	2.46	0.51
2:B:196:ILE:CG2	2:B:197:GLU:N	2.73	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
2:B:6:TYR:HB3	2:B:48:GLN:OE1	2.11	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:E:150:ASP:OD1	2:E:150:ASP:C	2.51	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:128:GLU:OE1	2:E:128:GLU:HA	1.99	0.51
1:A:22:PHE:O	1:A:23:HIS:C	2.51	0.51
1:A:147:VAL:CG1	1:A:148:GLY:N	2.73	0.51
2:B:71:ALA:O	2:B:72:PHE:C	2.54	0.51
2:B:195:LEU:HD23	2:B:195:LEU:O	2.11	0.51
2:B:314:VAL:HG12	2:B:315:LEU:N	2.26	0.51
2:B:348:ARG:C	2:B:348:ARG:CD	2.84	0.51
2:E:277:LYS:CD	2:E:277:LYS:C	2.84	0.51
2:E:304:ILE:O	2:E:305:ILE:C	2.49	0.51
1:A:33:LYS:HB2	4:A:291:HOH:O	2.11	0.51
1:A:244:MET:HE1	2:B:253:VAL:HG21	1.92	0.51
2:B:250:LEU:HD23	2:B:289:VAL:HA	1.92	0.51
2:B:276:VAL:O	2:B:277:LYS:C	2.47	0.51
2:E:224:PHE:CE1	2:E:225:ARG:HG2	2.45	0.51
1:A:215:GLU:O	1:A:216:GLU:C	2.52	0.51
2:B:223:LEU:C	2:B:225:ARG:N	2.65	0.51
2:B:284:ALA:O	2:B:285:ASN:HB3	2.10	0.51
2:B:329:ALA:O	2:B:333:ILE:HD12	2.11	0.51
2:B:386:GLU:C	2:B:388:LYS:HZ1	2.19	0.51
1:D:22:PHE:C	1:D:24:SER:H	2.19	0.51
1:D:274:ARG:HH11	1:D:274:ARG:CG	2.22	0.51
2:E:56:LYS:H	2:E:56:LYS:CD	2.21	0.51
2:E:139:GLU:O	2:E:139:GLU:HG3	2.10	0.51
1:A:218:ALA:O	1:A:221:ILE:CB	2.59	0.50
2:B:223:LEU:O	2:B:225:ARG:N	2.44	0.50
1:D:107:VAL:O	1:D:108:LYS:C	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLU:CD	1:D:226:THR:H	2.20	0.50
2:E:76:TRP:O	2:E:79:LYS:HG2	2.11	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:48:LEU:N	1:D:48:LEU:HD23	2.24	0.50
1:D:124:PRO:O	1:D:136:ILE:HD13	2.10	0.50
1:D:186:ASN:ND2	1:D:189:ASP:OD2	2.44	0.50
2:E:26:THR:O	2:E:27:THR:HG23	2.11	0.50
2:E:176:GLN:O	2:E:179:LYS:HB3	2.11	0.50
2:E:257:GLY:C	2:E:284:ALA:HB2	2.35	0.50
1:A:240:LYS:HD3	1:A:251:ILE:HG21	1.94	0.50
1:A:283:LEU:O	1:A:284:LYS:C	2.54	0.50
1:A:285:THR:O	1:A:286:VAL:C	2.53	0.50
2:B:140:THR:HB	2:B:143:LEU:CD1	2.40	0.50
2:B:318:ILE:HG23	2:B:319:PHE:N	2.25	0.50
2:B:356:LEU:O	2:B:360:LYS:CG	2.58	0.50
1:D:203:ILE:HG22	1:D:204:VAL:N	2.27	0.50
1:A:21:THR:OG1	1:A:47:HIS:CE1	2.64	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:142:HIS:H	2:E:142:HIS:CD2	2.29	0.50
2:E:187:ILE:O	2:E:188:PHE:C	2.54	0.50
2:E:210:ILE:HG12	2:E:211:CYS:N	2.26	0.50
1:D:124:PRO:CD	1:D:125:GLY:H	2.24	0.50
2:E:63:VAL:CG1	2:E:64:ASN:H	2.22	0.50
2:E:80:ARG:HD3	2:E:89:ASN:ND2	2.25	0.50
2:E:371:ALA:CB	2:E:377:ALA:HB2	2.41	0.50
1:A:136:ILE:O	1:A:137:GLN:C	2.54	0.50
1:A:209:ILE:HG23	1:A:235:GLY:HA3	1.93	0.50
2:B:287:LEU:C	2:B:287:LEU:CD2	2.84	0.50
1:D:233:ILE:HD13	1:D:261:LYS:HB3	1.91	0.50
1:D:283:LEU:C	1:D:285:THR:N	2.70	0.50
2:E:82:VAL:CG2	2:E:90:GLY:CA	2.87	0.50
2:E:140:THR:HG23	2:E:143:LEU:HD12	1.94	0.50
2:E:150:ASP:OD1	2:E:151:PRO:N	2.44	0.50
2:E:330:ASP:HA	2:E:333:ILE:HD12	1.94	0.50
1:A:141:ILE:HG22	1:A:161:VAL:HG12	1.93	0.50
1:A:145:GLY:HA3	1:A:170:GLY:CA	2.42	0.50
2:B:82:VAL:CG2	2:B:86:THR:HG21	2.36	0.50
2:B:174:VAL:O	2:B:175:GLN:C	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:30:TYR:OH	1:D:130:GLY:N	2.35	0.50
1:D:50:LEU:HB3	1:D:51:PRO:CD	2.42	0.50
2:E:28:PRO:O	2:E:29:ARG:C	2.53	0.50
2:E:319:PHE:CG	2:E:350:GLU:HG2	2.40	0.50
2:B:45:VAL:CG2	2:B:72:PHE:CE2	2.94	0.50
2:B:224:PHE:C	2:B:230:ARG:HH12	2.19	0.50
2:B:248:TRP:CE2	2:B:300:GLU:HG3	2.47	0.50
1:D:128:THR:HG22	1:D:131:GLU:HB3	1.92	0.50
1:D:242:LYS:HB3	1:D:244:MET:HE3	1.94	0.50
2:E:352:ASN:ND2	2:E:353:ASN:CB	2.71	0.50
1:A:188:ILE:O	1:A:190:ILE:N	2.45	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
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:43:TRP:HB3	2:E:99:GLU:O	2.12	0.50
2:E:339:VAL:HG11	2:E:341:VAL:HG12	1.87	0.50
1:A:60:VAL:O	1:A:61:ALA:C	2.51	0.49
1:A:150:VAL:O	1:A:150:VAL:CG2	2.59	0.49
1:A:174:CYS:C	1:A:175:VAL:HG23	2.37	0.49
1:A:180:ASP:HB3	1:A:181:PRO:HD2	1.93	0.49
2:B:86:THR:CG2	2:B:87:ASP:N	2.75	0.49
2:B:182:MET:O	2:B:183:GLY:C	2.54	0.49
2:B:356:LEU:O	2:B:360:LYS:HG3	2.12	0.49
2:B:362:ALA:C	2:B:364:SER:H	2.20	0.49
2:E:357:GLY:O	2:E:361:LEU:N	2.45	0.49
1:A:5:ASP:CG	1:A:7:ASN:H	2.16	0.49
1:A:19:GLN:HB2	3:A:289:COA:O4A	2.12	0.49
2:B:96:ILE:HG22	2:B:97:LEU:N	2.22	0.49
2:B:161:ARG:O	2:B:162:GLU:C	2.53	0.49
1:D:9:LYS:HB2	1:D:65:ALA:HA	1.94	0.49
1:D:11:ILE:CA	1:D:36:GLY:O	2.58	0.49
1:D:195:GLU:OE1	1:D:225:VAL:HG23	2.12	0.49
1:A:2:ILE:HG22	1:A:3:LEU:N	2.08	0.49
2:B:48:GLN:NE2	2:B:48:GLN:CA	2.75	0.49
2:B:108:LEU:CD2	2:B:127:THR:HA	2.42	0.49
2:B:228:ASP:O	2:B:232:MET:CE	2.60	0.49
1:D:226:THR:OG1	1:D:227:LYS:N	2.46	0.49
2:E:36:SER:C	2:E:38:ILE:N	2.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:241:ARG:HB3	2:E:252:TYR:CD2	2.47	0.49
1:D:46:THR:HA	1:D:50:LEU:O	2.12	0.49
2:E:103:ASP:HB2	2:E:205:LYS:HB2	1.94	0.49
2:E:156:MET:CB	2:E:157:PRO:CD	2.86	0.49
2:E:342:ASN:OD1	2:E:342:ASN:N	2.33	0.49
1:A:35:VAL:HG21	1:A:63:THR:HB	1.95	0.49
1:A:181:PRO:C	1:A:183:PRO:HD3	2.38	0.49
2:B:50:HIS:CG	2:B:237:GLN:HG3	2.47	0.49
2:B:285:ASN:ND2	2:B:286:PHE:N	2.60	0.49
2:B:301:ALA:O	2:B:302:PHE:C	2.55	0.49
1:D:238:ALA:HB1	1:D:239:PRO:HD2	1.94	0.49
2:E:195:LEU:HD23	2:E:196:ILE:N	2.27	0.49
2:E:275:ILE:HG23	2:E:276:VAL:N	2.02	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:236:VAL:HG22	1:A:258:ALA:HB1	1.95	0.49
2:B:107:GLU:HG2	2:B:200:PRO:CB	2.43	0.49
2:B:215:LYS:C	2:B:216:LEU:CD2	2.68	0.49
2:E:219:ASP:OD1	2:E:221:ASN:HB2	2.13	0.49
1:D:78:LYS:C	1:D:80:SER:H	2.20	0.49
1:A:281:GLU:O	1:A:282:ALA:C	2.56	0.49
2:B:83:THR:N	2:B:86:THR:HB	2.28	0.49
2:B:228:ASP:O	2:B:232:MET:HE2	2.13	0.49
2:B:386:GLU:O	2:B:387:GLY:C	2.55	0.49
1:D:2:ILE:HG12	1:D:193:MET:CE	2.39	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
1:D:97:GLU:CB	3:D:289:COA:H72	2.33	0.49
1:D:104:MET:O	1:D:105:LEU:C	2.54	0.49
1:D:186:ASN:ND2	1:D:189:ASP:CG	2.70	0.49
2:E:269:ALA:O	2:E:270:MET:C	2.53	0.49
2:E:269:ALA:O	2:E:272:THR:N	2.46	0.49
1:D:12:CYS:SG	1:D:15:PHE:HA	2.53	0.49
1:D:14:GLY:O	1:D:15:PHE:C	2.55	0.49
1:D:77:CYS:O	1:D:81:ILE:HD12	2.13	0.49
1:D:230:VAL:HG21	1:D:283:LEU:CD1	2.41	0.49
2:E:89:ASN:ND2	2:E:89:ASN:C	2.71	0.49
2:E:292:GLY:C	2:E:294:THR:HG23	2.37	0.49
2:B:49:VAL:HG13	2:B:51:ALA:N	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:ASP:OD1	2:B:150:ASP:C	2.56	0.48
2:B:205:LYS:O	2:B:207:GLY:N	2.47	0.48
2:B:285:ASN:HD21	2:B:287:LEU:HB2	1.78	0.48
2:E:339:VAL:CG1	2:E:341:VAL:CG1	2.80	0.48
1:A:24:SER:O	1:A:25:GLU:C	2.53	0.48
1:A:285:THR:C	1:A:287:LEU:H	2.21	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
2:E:157:PRO:O	2:E:158:TYR:C	2.52	0.48
1:A:92:ILE:CG2	1:A:118:MET:HG3	2.43	0.48
1:A:151:SER:HA	1:A:206:ILE:O	2.14	0.48
1:D:3:LEU:O	1:D:4:ILE:HG22	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
2:B:50:HIS:CE1	4:B:406:HOH:O	2.65	0.48
1:D:129:PRO:HG2	1:D:171:GLN:O	2.12	0.48
1:D:214:GLU:OE1	1:D:261:LYS:NZ	2.36	0.48
1:D:259:ASP:O	1:D:260:GLU:C	2.56	0.48
2:E:94:ASN:C	2:E:95:GLN:CG	2.86	0.48
2:E:246:ALA:O	2:E:247:GLN:C	2.52	0.48
1:A:108:LYS:O	1:A:111:LEU:HB2	2.14	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
2:B:224:PHE:HA	2:B:230:ARG:NH1	2.28	0.48
1:D:162:LYS:O	1:D:163:GLN:C	2.56	0.48
1:D:218:ALA:C	1:D:220:TYR:N	2.69	0.48
1:A:143:LYS:O	1:A:171:GLN:N	2.40	0.48
2:B:43:TRP:H	2:B:43:TRP:HE3	1.62	0.48
2:B:94:ASN:O	2:B:95:GLN:HG2	2.14	0.48
1:D:22:PHE:CD1	1:D:23:HIS:N	2.82	0.48
1:D:55:THR:HG22	1:D:56:VAL:N	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:E:308:ASP:OD1	2:E:308:ASP:C	2.55	0.48
2:E:371:ALA:HB1	2:E:377:ALA:CA	2.43	0.48
1:A:58:GLU:O	1:A:59:ALA:C	2.53	0.48
1:A:154:GLY:O	1:A:157:THR:HB	2.14	0.48
2:B:210:ILE:O	2:B:210:ILE:CG2	2.61	0.48
2:B:255:LEU:HD12	2:B:255:LEU:HA	1.58	0.48
1:D:6:LYS:O	1:D:6:LYS:HG2	2.12	0.48
1:D:191:LEU:HD13	1:D:221:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:322:ILE:O	2:E:322:ILE:CG2	2.57	0.48
2:E:343:VAL:HG13	2:E:344:PRO:HD2	0.50	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
1:A:213:ALA:O	1:A:214:GLU:C	2.54	0.48
2:B:177:PHE:O	2:B:178:THR:C	2.57	0.48
2:B:223:LEU:C	2:B:230:ARG:HH11	2.22	0.48
1:D:127:ILE:HG12	1:D:128:THR:H	1.74	0.48
1:A:23:HIS:NE2	1:A:136:ILE:HG22	2.28	0.48
1:A:127:ILE:CD1	1:A:133:LYS:HG3	2.38	0.48
1:A:281:GLU:O	1:A:284:LYS:HB2	2.14	0.48
2:B:33:GLU:OE2	3:D:289:COA:H10	2.13	0.48
1:D:136:ILE:C	1:D:137:GLN:O	2.54	0.48
2:E:139:GLU:O	2:E:140:THR:CB	2.31	0.48
2:E:367:ASN:HD22	2:E:367:ASN:HA	1.40	0.48
1:A:186:ASN:ND2	1:A:189:ASP:H	2.05	0.47
1:A:281:GLU:O	1:A:284:LYS:N	2.47	0.47
2:B:318:ILE:N	2:B:348:ARG:O	2.47	0.47
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
2:E:245:ALA:O	2:E:250:LEU:HB2	2.14	0.47
1:D:45:THR:C	1:D:52:VAL:HG23	2.37	0.47
1:D:198:PRO:O	1:D:199:GLN:C	2.54	0.47
1:D:214:GLU:O	1:D:215:GLU:C	2.55	0.47
2:E:94:ASN:O	2:E:95:GLN:HG2	2.13	0.47
2:E:186:THR:O	2:E:190:GLU:HB2	2.14	0.47
2:E:379:GLN:O	2:E:380:GLN:C	2.57	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
2:B:268:LEU:HD23	2:B:268:LEU:HA	1.44	0.47
1:D:89:ILE:CG2	1:D:90:LYS:N	2.76	0.47
1:D:118:MET:HG2	1:D:119:ILE:N	2.30	0.47
1:A:226:THR:O	1:A:227:LYS:C	2.57	0.47
2:B:55:GLY:O	2:B:56:LYS:C	2.58	0.47
2:B:317:ASN:OD1	2:B:317:ASN:C	2.54	0.47
1:D:78:LYS:C	1:D:80:SER:N	2.72	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:55:GLY:O	2:E:56:LYS:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:O	1:A:69:VAL:CG2	2.62	0.47
1:A:287:LEU:O	1:A:287:LEU:HD22	2.14	0.47
2:B:172:LYS:HA	2:B:175:GLN:HG2	1.97	0.47
1:D:80:SER:O	1:D:81:ILE:C	2.54	0.47
1:D:127:ILE:O	1:D:127:ILE:HG23	2.13	0.47
2:E:329:ALA:C	2:E:333:ILE:HD12	2.40	0.47
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.54	0.47
2:B:254:ALA:C	2:B:255:LEU:HD13	2.40	0.47
2:E:110:LEU:HD22	2:E:111:GLY:N	2.28	0.47
2:E:219:ASP:OD1	2:E:219:ASP:C	2.57	0.47
1:A:123:CYS:C	3:A:289:COA:S1P	2.97	0.47
1:A:153:SER:CB	1:A:246:NEP:HE1	2.41	0.47
2:B:133:ILE:HA	2:B:136:VAL:HB	1.97	0.47
2:B:160:GLY:O	2:B:161:ARG:C	2.56	0.47
2:B:165:PHE:C	2:B:167:LEU:H	2.22	0.47
2:B:257:GLY:HA3	2:B:282:GLU:O	2.15	0.47
2:B:359:LYS:O	2:B:360:LYS:C	2.57	0.47
1:D:124:PRO:HD2	1:D:125:GLY:H	1.80	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
2:E:72:PHE:HE1	2:E:76:TRP:NE1	2.13	0.47
2:E:177:PHE:CD2	2:E:177:PHE:C	2.92	0.47
2:E:197:GLU:HG2	2:E:215:LYS:HD2	1.97	0.47
2:E:205:LYS:C	2:E:207:GLY:H	2.22	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:136:VAL:O	2:B:140:THR:N	2.41	0.47
2:B:278:LEU:HD13	2:B:278:LEU:HA	1.74	0.47
2:B:331:GLY:O	2:B:332:ILE:C	2.52	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
1:D:129:PRO:CD	1:D:172:SER:O	2.59	0.47
1:D:161:VAL:O	1:D:162:LYS:C	2.57	0.47
2:E:69:ILE:C	2:E:71:ALA:N	2.68	0.47
1:A:4:ILE:HG12	1:A:8:THR:OG1	2.15	0.47
1:A:11:ILE:HD12	1:A:68:SER:OG	2.15	0.47
2:B:65:SER:OG	2:B:68:ASP:HB2	2.15	0.47
2:B:172:LYS:O	2:B:176:GLN:HG3	2.14	0.47
2:B:300:GLU:O	2:B:301:ALA:C	2.58	0.47
1:D:18:SER:HB2	3:D:289:COA:O4A	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ASP:O	1:D:113:GLU:C	2.54	0.47
1:D:127:ILE:HG13	1:D:132:CYS:O	2.15	0.47
1:D:151:SER:C	1:D:153:SER:H	2.23	0.47
1:D:156:LEU:HD23	1:D:156:LEU:HA	1.49	0.47
1:D:190:ILE:HA	1:D:193:MET:CG	2.32	0.47
2:E:376:ASP:O	2:E:377:ALA:C	2.56	0.47
1:A:262:PHE:O	1:A:266:GLU:CG	2.63	0.47
2:B:356:LEU:C	2:B:356:LEU:HD22	2.39	0.47
1:D:35:VAL:C	1:D:50:LEU:HD13	2.40	0.47
1:D:156:LEU:O	1:D:159:GLU:N	2.45	0.47
1:D:191:LEU:O	1:D:194:PHE:N	2.42	0.47
2:E:188:PHE:HD2	2:E:196:ILE:HD12	1.80	0.47
2:E:377:ALA:O	2:E:378:ALA:C	2.58	0.47
1:A:123:CYS:O	1:A:123:CYS:SG	2.73	0.46
1:A:190:ILE:HA	1:A:193:MET:HG3	1.97	0.46
1:D:43:GLY:N	1:D:54:ASN:OD1	2.47	0.46
1:D:158:TYR:HA	1:D:161:VAL:CG2	2.44	0.46
2:E:176:GLN:HE22	2:E:208:ASP:HB3	1.80	0.46
2:E:248:TRP:C	2:E:249:GLU:CG	2.86	0.46
2:E:371:ALA:HB2	2:E:377:ALA:HA	1.97	0.46
2:B:27:THR:HB	2:B:28:PRO:HD2	1.98	0.46
2:B:277:LYS:O	2:B:278:LEU:C	2.58	0.46
1:D:16:THR:OG1	1:D:39:THR:HG21	2.15	0.46
2:E:277:LYS:HD2	2:E:278:LEU:HA	1.95	0.46
1:A:133:LYS:C	1:A:134:ILE:HG12	2.39	0.46
1:D:152:ARG:NH2	1:D:210:GLY:O	2.45	0.46
1:D:187:PHE:CE2	1:D:214:GLU:CG	2.88	0.46
3:D:289:COA:O2B	3:D:289:COA:P3B	2.73	0.46
2:E:191:ARG:NE	4:E:409:HOH:O	2.49	0.46
2:E:199:ASN:HA	2:E:200:PRO:HA	1.47	0.46
2:E:371:ALA:HB3	2:E:377:ALA:HB2	1.97	0.46
2:B:180:ILE:CG2	2:B:184:LEU:CD1	2.93	0.46
1:D:103:ASP:CG	2:E:225:ARG:HH12	2.24	0.46
1:D:218:ALA:HB2	1:D:265:LEU:CD2	2.45	0.46
1:D:220:TYR:O	1:D:221:ILE:C	2.58	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:E:156:MET:CA	2:E:182:MET:HE1	2.45	0.46
2:E:371:ALA:CB	2:E:377:ALA:CA	2.92	0.46
2:B:374:LEU:C	2:B:374:LEU:HD12	2.41	0.46
1:D:53:PHE:CE2	1:D:59:ALA:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:VAL:HG22	1:D:127:ILE:N	2.30	0.46
2:E:205:LYS:C	2:E:207:GLY:N	2.72	0.46
1:A:186:ASN:OD1	1:A:188:ILE:N	2.48	0.46
2:B:34:ALA:O	2:B:37:LYS:HB2	2.15	0.46
2:B:180:ILE:HG23	2:B:184:LEU:CD1	2.45	0.46
1:D:146:LYS:HE2	1:D:287:LEU:HD11	1.97	0.46
1:D:259:ASP:C	1:D:261:LYS:N	2.72	0.46
3:D:289:COA:O9P	3:D:289:COA:H61	2.15	0.46
2:E:122:VAL:CG1	2:E:146:LYS:HB3	2.46	0.46
1:A:279:ILE:O	1:A:280:GLY:C	2.58	0.46
2:B:107:GLU:HB3	2:B:129:GLY:HA3	1.97	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
1:D:158:TYR:C	1:D:161:VAL:HG23	2.40	0.46
1:D:267:ALA:O	1:D:268:ALA:C	2.56	0.46
1:D:285:THR:HA	1:D:288:LYS:HD3	1.98	0.46
2:E:157:PRO:CG	2:E:182:MET:HE3	2.45	0.46
2:E:287:LEU:HD23	2:E:288:ASP:N	2.24	0.46
2:E:295:LYS:O	2:E:296:GLU:C	2.59	0.46
2:B:23:TYR:CD2	2:B:34:ALA:HB1	2.50	0.46
2:B:186:THR:O	2:B:187:ILE:C	2.59	0.46
2:B:255:LEU:HD23	2:B:273:MET:CE	2.46	0.46
2:B:331:GLY:O	2:B:335:ALA:N	2.40	0.46
1:D:195:GLU:OE2	1:D:226:THR:CG2	2.62	0.46
1:D:236:VAL:N	2:E:274:ASP:OD2	2.48	0.46
2:E:195:LEU:HG	2:E:196:ILE:N	2.31	0.46
1:A:112:ASP:C	1:A:114:ALA:N	2.71	0.46
2:E:110:LEU:CD2	2:E:111:GLY:N	2.79	0.46
2:E:120:ARG:HD3	2:E:120:ARG:HA	1.51	0.46
2:E:241:ARG:HE	2:E:241:ARG:HB2	1.41	0.46
1:A:2:ILE:HG21	1:A:173:THR:HG21	1.98	0.46
1:A:55:THR:O	1:A:58:GLU:HB2	2.16	0.46
2:B:4:HIS:O	2:B:5:GLU:C	2.59	0.46
2:B:308:ASP:HB3	4:B:410:HOH:O	2.16	0.46
2:E:63:VAL:CG1	2:E:68:ASP:CB	2.94	0.46
2:E:209:LEU:HA	2:E:209:LEU:HD23	1.53	0.46
2:E:312:LYS:O	2:E:385:VAL:HG23	2.16	0.46
2:E:329:ALA:HB1	2:E:361:LEU:CD1	2.46	0.46
1:A:22:PHE:CD1	1:A:23:HIS:N	2.85	0.45
2:B:81:LEU:N	2:B:91:GLN:O	2.49	0.45
2:B:155:PRO:C	2:B:156:MET:HG2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:SER:HB3	1:D:255:LYS:NZ	2.31	0.45
2:E:239:ASP:OD1	2:E:241:ARG:HB2	2.16	0.45
2:B:204:THR:O	2:B:207:GLY:CA	2.64	0.45
2:E:10:GLN:O	2:E:11:LEU:C	2.54	0.45
2:E:50:HIS:NE2	2:E:237:GLN:HG3	2.31	0.45
2:E:195:LEU:C	2:E:195:LEU:CD2	2.88	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
2:B:191:ARG:O	2:B:192:ASP:C	2.60	0.45
1:D:273:VAL:O	1:D:273:VAL:HG12	2.15	0.45
2:E:358:ALA:O	2:E:359:LYS:C	2.55	0.45
1:A:69:VAL:HG23	1:A:69:VAL:O	2.16	0.45
1:A:212:SER:O	1:A:214:GLU:N	2.49	0.45
1:D:39:THR:O	1:D:40:PRO:C	2.56	0.45
1:D:129:PRO:O	1:D:131:GLU:N	2.49	0.45
2:E:25:CYS:SG	2:E:31:ALA:HA	2.56	0.45
2:E:69:ILE:HG22	2:E:70:ARG:N	2.28	0.45
2:E:192:ASP:CB	4:E:405:HOH:O	2.64	0.45
2:E:248:TRP:C	2:E:249:GLU:HG3	2.41	0.45
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.26	0.45
2:B:277:LYS:O	2:B:280:GLY:N	2.49	0.45
2:B:302:PHE:O	2:B:306:LEU:HB2	2.17	0.45
2:B:352:ASN:C	2:B:354:ALA:N	2.71	0.45
2:B:371:ALA:HB1	2:B:377:ALA:HB2	1.95	0.45
1:D:118:MET:O	1:D:119:ILE:HD13	2.16	0.45
1:D:133:LYS:C	1:D:134:ILE:HG12	2.34	0.45
1:D:174:CYS:HB2	4:D:301:HOH:O	2.17	0.45
2:E:69:ILE:C	2:E:71:ALA:H	2.23	0.45
2:E:135:LYS:O	2:E:138:GLU:N	2.50	0.45
2:E:191:ARG:HD2	2:E:226:GLN:NE2	2.32	0.45
2:E:262:MET:HE2	2:E:301:ALA:CA	2.41	0.45
1:A:187:PHE:O	1:A:188:ILE:C	2.58	0.45
1:A:244:MET:O	1:A:246:NEP:N	2.49	0.45
1:A:257:THR:O	1:A:258:ALA:C	2.60	0.45
2:B:123:PHE:CZ	2:B:185:ALA:HA	2.52	0.45
2:B:263:VAL:CG1	2:B:264:ASN:H	2.29	0.45
1:D:53:PHE:CD1	1:D:53:PHE:N	2.85	0.45
2:E:63:VAL:CG1	2:E:68:ASP:HB3	2.41	0.45
2:E:298:VAL:O	2:E:299:THR:C	2.59	0.45
2:E:300:GLU:HA	2:E:303:LYS:HG3	1.97	0.45
2:E:346:VAL:CB	2:E:381:VAL:CG2	2.95	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
2:B:49:VAL:HG13	2:B:50:HIS:N	2.30	0.45
1:D:220:TYR:CD2	1:D:220:TYR:C	2.95	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
1:A:20:GLY:HA2	1:A:71:TYR:CD2	2.52	0.45
1:A:235:GLY:N	2:B:274:ASP:OD2	2.43	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:D:4:ILE:HD13	1:D:126:VAL:CG2	2.47	0.45
1:A:19:GLN:HG3	3:A:289:COA:H132	1.98	0.45
1:A:143:LYS:O	1:A:170:GLY:CA	2.65	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:272:THR:O	1:A:272:THR:HG22	2.17	0.45
2:B:25:CYS:HB3	2:B:30:GLU:HB2	1.99	0.45
2:B:38:ILE:HG21	2:B:43:TRP:HD1	1.82	0.45
2:B:66:LYS:NZ	3:D:289:COA:O1A	2.47	0.45
2:B:331:GLY:O	2:B:335:ALA:CB	2.65	0.45
1:D:73:PRO:C	1:D:75:PRO:CD	2.88	0.45
2:E:79:LYS:HG2	2:E:79:LYS:H	1.51	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:B:2:ASN:O	2:B:3:LEU:HD23	2.16	0.45
2:B:136:VAL:HG12	2:B:144:ILE:HD11	1.98	0.45
2:B:332:ILE:O	2:B:335:ALA:HB3	2.17	0.45
1:D:11:ILE:N	1:D:34:MET:CE	2.80	0.45
2:E:1:MET:HB3	2:E:218:ALA:HB3	1.99	0.45
2:E:346:VAL:HB	2:E:381:VAL:HG21	1.98	0.45
2:B:29:ARG:O	2:B:30:GLU:C	2.59	0.44
2:B:187:ILE:HD12	2:B:187:ILE:HG21	1.65	0.44
1:D:104:MET:HE3	1:D:104:MET:O	2.17	0.44
1:D:124:PRO:O	1:D:135:GLY:HA3	2.17	0.44
1:D:265:LEU:O	1:D:266:GLU:C	2.59	0.44
2:E:341:VAL:O	2:E:341:VAL:HG22	2.17	0.44
1:A:2:ILE:HG22	1:A:173:THR:HG21	1.99	0.44
1:A:55:THR:HB	1:A:58:GLU:HB2	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
1:A:239:PRO:HG3	2:B:255:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:OD2	2:B:118:SER:CB	2.64	0.44
2:B:152:LEU:C	2:B:152:LEU:HD22	2.41	0.44
1:D:101:THR:O	1:D:105:LEU:N	2.47	0.44
1:D:226:THR:O	1:D:227:LYS:C	2.59	0.44
1:D:229:VAL:HG22	1:D:230:VAL:H	1.79	0.44
2:E:4:HIS:O	2:E:7:GLN:N	2.49	0.44
2:E:49:VAL:HG22	2:E:91:GLN:HB2	1.97	0.44
2:E:50:HIS:CG	2:E:237:GLN:HG3	2.52	0.44
2:E:81:LEU:HD23	2:E:81:LEU:HA	1.63	0.44
2:E:276:VAL:CG1	2:E:281:GLY:HA3	2.47	0.44
1:A:19:GLN:OE1	1:A:19:GLN:CA	2.65	0.44
1:A:77:CYS:HB3	1:A:99:ILE:HD11	1.99	0.44
1:A:92:ILE:HB	1:A:118:MET:HG3	1.99	0.44
1:A:150:VAL:CG1	1:A:190:ILE:HG21	2.47	0.44
1:A:238:ALA:HA	1:A:239:PRO:HD2	1.80	0.44
2:B:43:TRP:HB3	2:B:99:GLU:O	2.17	0.44
2:B:107:GLU:O	2:B:129:GLY:HA3	2.17	0.44
2:E:257:GLY:O	2:E:284:ALA:HB2	2.18	0.44
1:A:11:ILE:HD11	1:A:68:SER:CB	2.47	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
2:B:143:LEU:C	2:B:144:ILE:HD12	2.40	0.44
2:B:368:ILE:CG2	2:B:369:ILE:N	2.81	0.44
2:B:376:ASP:O	2:B:377:ALA:C	2.60	0.44
1:D:202:ALA:CB	1:D:228:PRO:HG2	2.47	0.44
2:E:12:PHE:N	2:E:12:PHE:CD1	2.83	0.44
2:E:184:LEU:C	2:E:186:THR:N	2.72	0.44
2:E:255:LEU:HB3	2:E:256:ASP:H	1.48	0.44
1:A:10:VAL:CG1	1:A:11:ILE:H	2.26	0.44
1:A:19:GLN:HG2	3:A:289:COA:P2A	2.57	0.44
1:A:253:GLY:O	1:A:255:LYS:HB2	2.17	0.44
2:B:153:THR:O	2:B:154:GLY:O	2.36	0.44
2:B:246:ALA:C	2:B:248:TRP:N	2.73	0.44
2:E:191:ARG:HD2	2:E:191:ARG:HA	1.71	0.44
1:A:11:ILE:CD1	1:A:68:SER:OG	2.65	0.44
1:A:143:LYS:O	1:A:170:GLY:HA2	2.18	0.44
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
1:D:266:GLU:O	1:D:267:ALA:C	2.59	0.44
2:E:133:ILE:CG2	2:E:134:GLU:N	2.81	0.44
2:E:156:MET:HA	2:E:182:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:205:LYS:O	2:E:207:GLY:N	2.51	0.44
2:E:299:THR:HG22	2:E:300:GLU:N	2.33	0.44
2:E:336:VAL:HG13	2:E:341:VAL:HG13	1.99	0.44
2:B:147:VAL:HG22	2:B:159:GLN:HE21	1.82	0.44
1:D:27:ALA:HB1	1:D:32:THR:CB	2.44	0.44
1:A:2:ILE:HD12	1:A:194:PHE:CD1	2.50	0.44
1:A:34:MET:HE2	1:A:34:MET:HB2	1.42	0.44
1:A:280:GLY:O	1:A:283:LEU:HB2	2.18	0.44
2:B:6:TYR:CE1	2:B:7:GLN:HG2	2.52	0.44
2:B:346:VAL:HG21	2:B:381:VAL:HG22	1.98	0.44
1:D:57:ARG:HH22	1:D:86:ASP:CG	2.26	0.44
1:D:61:ALA:C	1:D:63:THR:N	2.76	0.44
1:D:158:TYR:HA	1:D:161:VAL:HG21	1.99	0.44
2:E:122:VAL:HG12	2:E:123:PHE:N	2.32	0.44
2:E:141:PRO:HD2	2:E:142:HIS:HD2	1.83	0.44
2:E:239:ASP:OD1	2:E:240:PRO:HD2	2.18	0.44
2:E:249:GLU:C	2:E:250:LEU:HD23	2.43	0.44
1:A:181:PRO:HA	2:B:116:ARG:HH11	1.81	0.44
2:B:239:ASP:OD2	2:B:241:ARG:NE	2.50	0.44
2:B:255:LEU:CD2	2:B:273:MET:CE	2.96	0.44
1:D:149:ILE:HG12	1:D:174:CYS:HB3	1.82	0.44
2:E:252:TYR:CG	2:E:253:VAL:N	2.84	0.44
2:E:263:VAL:HG21	2:E:269:ALA:HA	1.99	0.44
2:B:138:GLU:HG2	2:B:138:GLU:O	2.18	0.43
2:B:158:TYR:CD1	2:B:159:GLN:N	2.85	0.43
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:E:330:ASP:O	2:E:331:GLY:C	2.60	0.43
1:A:136:ILE:O	1:A:138:PRO:HD3	2.18	0.43
1:A:278:ASP:O	1:A:281:GLU:HB2	2.18	0.43
2:B:76:TRP:O	2:B:77:LEU:C	2.55	0.43
2:B:139:GLU:O	2:B:141:PRO:HD3	2.16	0.43
2:B:173:LEU:HD23	2:B:173:LEU:HA	1.65	0.43
2:B:241:ARG:NH2	2:B:254:ALA:CB	2.81	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
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
1:D:127:ILE:O	1:D:173:THR:HG23	2.14	0.43
1:D:166:ASP:C	1:D:168:GLY:N	2.74	0.43
1:D:229:VAL:HG13	1:D:230:VAL:N	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:THR:HG21	2:B:90:GLY:HA2	1.98	0.43
2:B:315:LEU:HD12	2:B:315:LEU:HA	1.66	0.43
1:D:81:ILE:HG21	1:D:107:VAL:CG1	2.48	0.43
2:E:9:LYS:O	2:E:12:PHE:HB2	2.18	0.43
2:E:105:ALA:N	2:E:203:ILE:O	2.46	0.43
2:E:232:MET:O	2:E:233:ARG:C	2.61	0.43
2:E:298:VAL:O	2:E:301:ALA:HB3	2.18	0.43
1:A:19:GLN:O	1:A:23:HIS:HB2	2.17	0.43
1:A:73:PRO:O	1:A:74:ALA:C	2.61	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:214:GLU:O	1:A:215:GLU:C	2.61	0.43
2:B:377:ALA:O	2:B:378:ALA:C	2.60	0.43
1:D:77:CYS:CB	1:D:99:ILE:HD11	2.46	0.43
1:D:166:ASP:C	1:D:168:GLY:H	2.24	0.43
1:D:277:ALA:C	1:D:279:ILE:N	2.76	0.43
2:E:191:ARG:CD	4:E:409:HOH:O	2.65	0.43
2:E:304:ILE:O	2:E:307:SER:OG	2.35	0.43
2:B:137:ALA:C	2:B:139:GLU:N	2.74	0.43
1:D:30:TYR:OH	1:D:127:ILE:HD11	2.18	0.43
1:D:263:ALA:C	1:D:265:LEU:N	2.73	0.43
1:A:81:ILE:HD11	1:A:94:THR:HG21	2.00	0.43
2:B:64:ASN:C	2:B:64:ASN:HD22	2.26	0.43
2:B:87:ASP:OD2	2:B:89:ASN:OD1	2.37	0.43
2:B:215:LYS:O	2:B:216:LEU:CD2	2.42	0.43
1:D:3:LEU:C	1:D:4:ILE:HG23	2.43	0.43
1:D:256:GLY:O	1:D:261:LYS:HE2	2.18	0.43
1:A:162:LYS:O	1:A:163:GLN:O	2.37	0.43
2:B:195:LEU:HD23	2:B:195:LEU:C	2.43	0.43
2:B:382:VAL:O	2:B:383:ALA:C	2.62	0.43
1:D:2:ILE:HD12	1:D:193:MET:HB2	1.74	0.43
1:D:126:VAL:O	1:D:126:VAL:HG13	2.18	0.43
1:D:217:ALA:O	1:D:221:ILE:HB	2.18	0.43
1:D:275:SER:C	1:D:277:ALA:N	2.73	0.43
2:E:89:ASN:O	2:E:90:GLY:C	2.61	0.43
2:E:226:GLN:HA	2:E:227:PRO:HD2	1.55	0.43
2:E:371:ALA:CB	2:E:377:ALA:CB	2.97	0.43
2:B:255:LEU:HB3	2:B:256:ASP:H	1.61	0.43
2:B:326:ASP:HB3	2:B:356:LEU:HD13	2.01	0.43
1:D:15:PHE:CE2	1:D:47:HIS:HB3	2.54	0.43
1:D:73:PRO:CA	3:D:289:COA:H143	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ILE:HD13	1:D:261:LYS:CB	2.49	0.43
2:B:152:LEU:O	2:B:152:LEU:HD22	2.19	0.43
1:D:11:ILE:HD13	1:D:11:ILE:HG23	1.65	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:107:GLU:O	2:E:129:GLY:CA	2.56	0.43
2:E:140:THR:C	2:E:142:HIS:N	2.77	0.43
1:A:39:THR:O	1:A:40:PRO:C	2.62	0.43
1:A:221:ILE:HA	1:A:225:VAL:HG12	1.99	0.43
2:B:30:GLU:O	2:B:31:ALA:C	2.61	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
1:D:11:ILE:N	1:D:34:MET:HE1	2.34	0.43
1:D:136:ILE:O	1:D:137:GLN:C	2.61	0.43
1:D:236:VAL:HA	1:D:258:ALA:HB3	2.01	0.43
1:D:266:GLU:O	1:D:269:GLY:CA	2.66	0.43
2:E:5:GLU:HG2	2:E:9:LYS:HD2	2.01	0.43
2:E:72:PHE:HE1	2:E:76:TRP:HE1	1.67	0.43
2:E:371:ALA:HB1	2:E:377:ALA:HA	2.01	0.43
1:A:55:THR:CG2	1:A:56:VAL:N	2.82	0.42
1:A:72:VAL:HA	1:A:73:PRO:HD3	1.64	0.42
1:A:116:VAL:CG1	1:A:117:ARG:H	2.31	0.42
1:A:150:VAL:HG12	1:A:190:ILE:HG21	2.00	0.42
2:B:65:SER:O	2:B:68:ASP:N	2.52	0.42
2:B:120:ARG:HA	2:B:120:ARG:HD3	1.62	0.42
2:B:246:ALA:C	2:B:248:TRP:H	2.25	0.42
1:D:22:PHE:HD1	1:D:23:HIS:N	2.16	0.42
1:D:276:LEU:O	1:D:279:ILE:HD12	2.18	0.42
2:E:136:VAL:C	2:E:140:THR:HG22	2.32	0.42
2:E:140:THR:CG2	2:E:143:LEU:HD12	2.48	0.42
2:E:157:PRO:CB	2:E:182:MET:CE	2.97	0.42
2:E:202:VAL:HG12	2:E:203:ILE:C	2.44	0.42
2:E:245:ALA:HB1	2:E:250:LEU:HB2	2.00	0.42
2:E:338:GLU:O	2:E:339:VAL:C	2.61	0.42
1:A:182:ILE:HA	1:A:183:PRO:HD2	1.76	0.42
2:B:156:MET:HA	2:B:157:PRO:HD3	1.39	0.42
2:E:263:VAL:CG1	2:E:268:LEU:HB3	2.47	0.42
1:A:4:ILE:HD12	1:A:4:ILE:HG21	1.78	0.42
1:A:252:ALA:CB	4:A:308:HOH:O	2.67	0.42
2:B:204:THR:O	2:B:207:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:ASN:C	2:B:354:ALA:H	2.26	0.42
1:D:21:THR:CG2	1:D:22:PHE:N	2.63	0.42
1:D:32:THR:O	1:D:34:MET:N	2.47	0.42
1:D:104:MET:CA	1:D:104:MET:CE	2.89	0.42
1:D:120:GLY:HA3	1:D:121:PRO:HA	1.77	0.42
1:D:160:ALA:O	1:D:164:THR:HG23	2.20	0.42
1:D:283:LEU:HD12	1:D:286:VAL:HG11	2.01	0.42
2:E:241:ARG:HD2	2:E:307:SER:OG	2.17	0.42
2:E:326:ASP:C	2:E:328:ILE:H	2.25	0.42
2:B:25:CYS:SG	2:B:31:ALA:HA	2.59	0.42
2:B:184:LEU:H	2:B:184:LEU:HG	1.50	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
1:D:218:ALA:HB2	1:D:265:LEU:HD23	2.00	0.42
1:D:275:SER:OG	1:D:277:ALA:CB	2.64	0.42
2:E:206:GLN:OE1	2:E:206:GLN:N	2.47	0.42
1:A:11:ILE:HD12	1:A:11:ILE:C	2.44	0.42
1:A:140:HIS:ND1	1:A:140:HIS:N	2.65	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:375:THR:O	2:B:378:ALA:HB3	2.19	0.42
1:D:4:ILE:HD13	1:D:126:VAL:HG22	2.01	0.42
1:D:24:SER:C	1:D:26:GLN:N	2.73	0.42
2:E:332:ILE:O	2:E:333:ILE:C	2.63	0.42
2:B:133:ILE:CD1	2:B:134:GLU:N	2.67	0.42
2:B:298:VAL:O	2:B:298:VAL:CG1	2.63	0.42
2:B:302:PHE:O	2:B:303:LYS:C	2.59	0.42
2:B:381:VAL:C	2:B:383:ALA:N	2.78	0.42
1:D:3:LEU:HG	1:D:3:LEU:H	1.66	0.42
2:E:41:GLY:HA3	2:E:42:PRO:HA	1.82	0.42
2:E:89:ASN:C	2:E:89:ASN:HD22	2.18	0.42
2:E:276:VAL:HG12	2:E:277:LYS:N	2.32	0.42
1:A:112:ASP:O	1:A:114:ALA:N	2.53	0.42
1:A:186:ASN:O	1:A:187:PHE:O	2.38	0.42
2:B:312:LYS:O	2:B:343:VAL:HG22	2.19	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:5:GLU:O	2:E:6:TYR:C	2.56	0.42
2:E:36:SER:C	2:E:38:ILE:H	2.24	0.42
2:E:202:VAL:HG12	2:E:203:ILE:N	2.18	0.42
2:E:328:ILE:HG21	2:E:349:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:78:LYS:HG3	1:A:82:LEU:HD22	2.01	0.42
1:A:220:TYR:HB3	1:A:221:ILE:H	1.46	0.42
2:B:16:GLY:C	2:B:17:LEU:HD23	2.44	0.42
2:B:172:LYS:HA	2:B:175:GLN:CG	2.50	0.42
2:B:276:VAL:C	2:B:278:LEU:N	2.73	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:B:267:GLY:O	2:B:268:LEU:C	2.62	0.42
2:B:356:LEU:CD2	2:B:356:LEU:O	2.68	0.42
2:B:386:GLU:HA	2:B:388:LYS:HZ3	1.85	0.42
1:D:5:ASP:O	1:D:8:THR:HB	2.20	0.42
1:D:111:LEU:O	1:D:112:ASP:C	2.56	0.42
1:D:207:GLY:O	1:D:208:GLU:HB3	2.19	0.42
1:A:22:PHE:HD1	1:A:23:HIS:N	2.17	0.42
2:B:198:ILE:HG23	2:B:211:CYS:HB3	2.02	0.42
1:D:57:ARG:NH2	1:D:86:ASP:HB3	2.35	0.42
2:E:311:VAL:HG12	2:E:313:ALA:H	1.85	0.42
1:A:145:GLY:O	1:A:199:GLN:NE2	2.43	0.41
2:B:34:ALA:O	2:B:35:ALA:C	2.62	0.41
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.65	0.41
2:B:142:HIS:CD2	2:B:142:HIS:N	2.79	0.41
2:B:152:LEU:C	2:B:152:LEU:HD23	2.44	0.41
2:E:76:TRP:O	2:E:79:LYS:CG	2.67	0.41
2:E:196:ILE:HA	2:E:216:LEU:HD22	2.02	0.41
1:A:84:ALA:O	1:A:87:ALA:N	2.54	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:B:96:ILE:CG2	2:B:97:LEU:N	2.79	0.41
2:B:97:LEU:HD23	2:B:97:LEU:HA	1.33	0.41
1:D:25:GLU:O	1:D:28:ILE:HB	2.19	0.41
1:D:208:GLU:O	1:D:261:LYS:HE3	2.20	0.41
2:E:233:ARG:HD3	2:E:235:GLN:HE21	1.84	0.41
2:E:315:LEU:HD12	2:E:346:VAL:O	2.20	0.41
1:A:214:GLU:OE1	1:A:261:LYS:CE	2.63	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
1:D:102:LEU:O	1:D:103:ASP:C	2.63	0.41
1:D:117:ARG:HH11	1:D:117:ARG:HD2	1.75	0.41
2:E:26:THR:O	2:E:27:THR:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:80:ARG:NH2	2:E:92:PRO:HD3	2.35	0.41
2:E:268:LEU:HA	2:E:268:LEU:HD23	1.70	0.41
2:E:326:ASP:O	2:E:329:ALA:N	2.54	0.41
2:E:343:VAL:HG12	2:E:344:PRO:O	2.20	0.41
1:A:22:PHE:C	1:A:22:PHE:CD1	2.98	0.41
1:A:288:LYS:NZ	1:A:288:LYS:HB2	2.36	0.41
2:B:224:PHE:CA	2:B:230:ARG:NH1	2.84	0.41
2:B:319:PHE:O	2:B:320:GLY:C	2.61	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:283:LEU:C	1:D:286:VAL:HG12	2.42	0.41
2:E:191:ARG:HD3	4:E:409:HOH:O	2.20	0.41
2:E:386:GLU:O	2:E:388:LYS:N	2.53	0.41
1:A:160:ALA:HB3	1:A:161:VAL:H	1.64	0.41
1:A:229:VAL:HG13	1:A:229:VAL:O	2.20	0.41
2:B:20:PRO:HD3	2:B:210:ILE:CD1	2.51	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
1:D:4:ILE:HD11	1:D:126:VAL:HG22	2.01	0.41
1:D:141:ILE:H	1:D:141:ILE:HG13	1.63	0.41
2:E:55:GLY:O	2:E:58:GLY:N	2.32	0.41
1:A:32:THR:HG23	1:A:132:CYS:SG	2.60	0.41
1:A:54:ASN:N	1:A:58:GLU:OE1	2.54	0.41
1:A:104:MET:C	1:A:107:VAL:H	2.28	0.41
2:B:150:ASP:O	2:B:153:THR:O	2.38	0.41
2:B:241:ARG:NH2	2:B:254:ALA:HB2	2.35	0.41
2:B:241:ARG:O	2:B:242:GLU:C	2.63	0.41
1:D:26:GLN:H	1:D:26:GLN:HG2	1.35	0.41
1:D:109:VAL:H	1:D:109:VAL:HG23	1.63	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
2:E:302:PHE:O	2:E:303:LYS:C	2.58	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
2:B:141:PRO:CD	2:B:142:HIS:H	2.33	0.41
1:D:123:CYS:C	3:D:289:COA:S1P	3.03	0.41
1:D:158:TYR:N	1:D:158:TYR:CD1	2.89	0.41
1:D:168:GLY:O	1:D:169:PHE:C	2.64	0.41
2:E:97:LEU:CD2	2:E:98:VAL:N	2.76	0.41
2:E:240:PRO:C	2:E:242:GLU:N	2.76	0.41
2:E:324:ARG:CG	2:E:326:ASP:OD2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:VAL:O	2:E:386:GLU:C	2.63	0.41
2:B:296:GLU:N	2:B:296:GLU:CD	2.74	0.41
2:B:330:ASP:O	2:B:331:GLY:C	2.62	0.41
1:D:53:PHE:CE2	1:D:62:ALA:HB3	2.55	0.41
2:E:28:PRO:O	2:E:32:GLU:CB	2.69	0.41
2:E:165:PHE:C	2:E:168:GLY:H	2.28	0.41
2:E:268:LEU:O	2:E:269:ALA:C	2.63	0.41
2:E:325:CYS:HB2	2:E:354:ALA:CA	2.47	0.41
1:A:27:ALA:HB1	1:A:32:THR:HB	2.02	0.41
1:A:53:PHE:CD2	1:A:59:ALA:HA	2.56	0.41
1:A:89:ILE:HG23	1:A:89:ILE:HD12	1.73	0.41
1:A:92:ILE:C	1:A:93:ILE:HG13	2.46	0.41
1:A:95:ILE:O	1:A:122:ASN:HA	2.21	0.41
1:A:104:MET:O	1:A:107:VAL:N	2.52	0.41
1:A:133:LYS:O	1:A:134:ILE:HG23	2.21	0.41
1:A:135:GLY:C	1:A:137:GLN:H	2.28	0.41
1:A:172:SER:HA	1:A:199:GLN:NE2	2.36	0.41
1:A:208:GLU:H	1:A:208:GLU:HG2	1.77	0.41
2:B:313:ALA:HA	2:B:343:VAL:CG1	2.45	0.41
2:B:318:ILE:HG22	2:B:319:PHE:N	2.28	0.41
1:D:13:GLN:HG3	1:D:68:SER:OG	2.21	0.41
1:D:147:VAL:O	1:D:171:GLN:HA	2.21	0.41
2:E:20:PRO:CD	2:E:210:ILE:HD11	2.51	0.41
2:E:59:GLY:C	2:E:60:VAL:HG23	2.45	0.41
2:E:182:MET:O	2:E:186:THR:OG1	2.29	0.41
2:E:249:GLU:O	2:E:250:LEU:HD23	2.21	0.41
2:E:324:ARG:HD3	2:E:327:LEU:HD12	2.01	0.41
1:A:72:VAL:CG1	1:A:73:PRO:CD	2.98	0.41
2:B:140:THR:C	2:B:142:HIS:H	2.29	0.41
1:D:69:VAL:HA	1:D:93:ILE:O	2.21	0.41
1:D:89:ILE:HD13	1:D:89:ILE:HA	1.86	0.41
1:D:119:ILE:HD13	1:D:119:ILE:HA	1.68	0.41
2:E:72:PHE:O	2:E:75:ASN:CB	2.69	0.41
2:E:229:LEU:HA	2:E:229:LEU:HD23	1.45	0.41
1:A:92:ILE:CB	1:A:118:MET:HG3	2.51	0.40
1:A:123:CYS:CB	1:A:124:PRO:CD	2.96	0.40
2:B:41:GLY:HA2	2:B:43:TRP:CE2	2.56	0.40
2:B:325:CYS:O	2:B:326:ASP:C	2.63	0.40
1:D:155:THR:O	1:D:158:TYR:N	2.54	0.40
1:D:217:ALA:C	1:D:221:ILE:HD12	2.46	0.40
1:D:283:LEU:O	1:D:286:VAL:CG1	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:LEU:HD23	2:E:3:LEU:HA	1.81	0.40
2:E:112:ALA:HB2	2:E:123:PHE:CD2	2.55	0.40
1:A:265:LEU:O	1:A:268:ALA:N	2.54	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:B:234:ASP:C	2:B:236:SER:N	2.77	0.40
2:B:326:ASP:CG	2:B:327:LEU:N	2.79	0.40
2:B:328:ILE:CG2	2:B:329:ALA:N	2.46	0.40
2:B:382:VAL:O	2:B:383:ALA:O	2.40	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:278:ASP:HB3	1:D:281:GLU:HB2	2.03	0.40
1:D:283:LEU:HA	1:D:283:LEU:HD12	1.70	0.40
2:E:166:LYS:C	2:E:168:GLY:H	2.28	0.40
2:E:196:ILE:CG2	2:E:197:GLU:N	2.84	0.40
2:E:299:THR:O	2:E:302:PHE:HB2	2.20	0.40
2:E:343:VAL:CG1	2:E:344:PRO:CG	2.92	0.40
1:A:109:VAL:O	1:A:110:LYS:C	2.60	0.40
2:B:328:ILE:O	2:B:332:ILE:HG13	2.22	0.40
2:B:386:GLU:HA	2:B:388:LYS:NZ	2.36	0.40
1:D:104:MET:HE2	1:D:104:MET:HB3	1.94	0.40
1:D:274:ARG:HG2	1:D:274:ARG:NH1	2.27	0.40
2:E:156:MET:C	2:E:182:MET:HE2	2.43	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:A:24:SER:CA	4:A:297:HOH:O	2.34	0.40
1:A:108:LYS:O	1:A:109:VAL:C	2.62	0.40
2:B:223:LEU:O	2:B:224:PHE:C	2.62	0.40
2:B:303:LYS:O	2:B:304:ILE:C	2.64	0.40
1:D:73:PRO:O	1:D:74:ALA:C	2.64	0.40
1:D:195:GLU:O	1:D:227:LYS:CE	2.69	0.40
2:E:32:GLU:CD	2:E:70:ARG:HH11	2.28	0.40
2:E:38:ILE:HG21	2:E:38:ILE:HD13	1.81	0.40
2:E:63:VAL:HG13	2:E:64:ASN:H	1.87	0.40
2:E:257:GLY:HA2	2:E:282:GLU:HG3	2.04	0.40
2:E:275:ILE:CG2	2:E:276:VAL:CA	2.96	0.40
2:E:357:GLY:C	2:E:361:LEU:HD22	2.40	0.40
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
1:A:273:VAL:HG11	1:A:275:SER:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:289:COA:O9P	3:A:289:COA:H131	2.18	0.40
2:B:103:ASP:HB3	2:B:205:LYS:HB2	2.04	0.40
2:B:209:LEU:HA	2:B:209:LEU:HD23	1.68	0.40
2:B:220:GLY:O	2:B:221:ASN:C	2.62	0.40
1:D:50:LEU:CB	1:D:51:PRO:CD	2.97	0.40
2:E:11:LEU:HD23	2:E:11:LEU:HA	1.77	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%)	0	0
1	D	285/288 (99%)	207 (73%)	53 (19%)	25 (9%)	0	0
2	B	386/388 (100%)	315 (82%)	59 (15%)	12 (3%)	3	5
2	E	386/388 (100%)	307 (80%)	57 (15%)	22 (6%)	1	1
All	All	1342/1352 (99%)	1038 (77%)	221 (16%)	83 (6%)	1	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
1	A	221	ILE
1	A	252	ALA
1	A	281	GLU
1	A	285	THR
2	B	87	ASP

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Mol	Chain	Res	Type
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
2	E	295	LYS
2	E	325	CYS
2	E	337	ALA
2	E	387	GLY
1	A	282	ALA

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Mol	Chain	Res	Type
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 ⓘ

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%)	157 (72%)	60 (28%)	0	1
1	D	217/217 (100%)	141 (65%)	76 (35%)	0	0
2	B	298/298 (100%)	206 (69%)	92 (31%)	0	0
2	E	298/298 (100%)	205 (69%)	93 (31%)	0	0
All	All	1030/1030 (100%)	709 (69%)	321 (31%)	0	0

All (321) 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	33	LYS
1	A	35	VAL
1	A	42	LYS
1	A	48	LEU
1	A	52	VAL
1	A	69	VAL
1	A	77	CYS
1	A	80	SER
1	A	82	LEU
1	A	90	LYS
1	A	92	ILE
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	106	THR
1	A	113	GLU
1	A	126	VAL
1	A	128	THR
1	A	132	CYS
1	A	134	ILE
1	A	136	ILE
1	A	137	GLN
1	A	141	ILE
1	A	143	LYS
1	A	147	VAL

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Mol	Chain	Res	Type
1	A	149	ILE
1	A	155	THR
1	A	158	TYR
1	A	166	ASP
1	A	172	SER
1	A	182	ILE
1	A	193	MET
1	A	196	LYS
1	A	201	GLU
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	230	VAL
1	A	233	ILE
1	A	236	VAL
1	A	240	LYS
1	A	250	ILE
1	A	255	LYS
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	7	GLN
2	B	14	ARG
2	B	26	THR
2	B	32	GLU
2	B	36	SER
2	B	43	TRP
2	B	44	VAL
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

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Mol	Chain	Res	Type
2	B	79	LYS
2	B	81	LEU
2	B	82	VAL
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
2	B	121	VAL
2	B	122	VAL
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	153	THR
2	B	166	LYS
2	B	179	LYS
2	B	180	ILE
2	B	184	LEU
2	B	187	ILE
2	B	195	LEU
2	B	198	ILE
2	B	202	VAL
2	B	203	ILE
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	237	GLN
2	B	238	GLU
2	B	241	ARG
2	B	255	LEU
2	B	258	ASN
2	B	264	ASN

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Mol	Chain	Res	Type
2	B	275	ILE
2	B	276	VAL
2	B	278	LEU
2	B	285	ASN
2	B	289	VAL
2	B	303	LYS
2	B	304	ILE
2	B	305	ILE
2	B	311	VAL
2	B	316	VAL
2	B	318	ILE
2	B	322	ILE
2	B	323	VAL
2	B	327	LEU
2	B	328	ILE
2	B	333	ILE
2	B	338	GLU
2	B	339	VAL
2	B	343	VAL
2	B	348	ARG
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	369	ILE
2	B	374	LEU
2	B	375	THR
2	B	380	GLN
2	B	381	VAL
2	B	385	VAL
2	B	386	GLU
2	B	388	LYS
1	D	1	SER
1	D	2	ILE
1	D	3	LEU
1	D	4	ILE
1	D	8	THR
1	D	10	VAL
1	D	11	ILE

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Mol	Chain	Res	Type
1	D	12	CYS
1	D	16	THR
1	D	25	GLU
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	66	THR
1	D	69	VAL
1	D	77	CYS
1	D	81	ILE
1	D	90	LYS
1	D	92	ILE
1	D	97	GLU
1	D	99	ILE
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
1	D	143	LYS
1	D	146	LYS
1	D	147	VAL
1	D	149	ILE
1	D	150	VAL
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

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Mol	Chain	Res	Type
1	D	175	VAL
1	D	185	SER
1	D	190	ILE
1	D	193	MET
1	D	221	ILE
1	D	222	LYS
1	D	225	VAL
1	D	229	VAL
1	D	237	THR
1	D	242	LYS
1	D	243	ARG
1	D	250	ILE
1	D	251	ILE
1	D	260	GLU
1	D	262	PHE
1	D	265	LEU
1	D	270	VAL
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	284	LYS
1	D	285	THR
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	38	ILE
2	E	43	TRP
2	E	45	VAL
2	E	49	VAL
2	E	56	LYS
2	E	61	LYS
2	E	62	VAL
2	E	79	LYS
2	E	81	LEU
2	E	86	THR

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Mol	Chain	Res	Type
2	E	93	VAL
2	E	95	GLN
2	E	96	ILE
2	E	97	LEU
2	E	103	ASP
2	E	106	LYS
2	E	108	LEU
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	144	ILE
2	E	146	LYS
2	E	152	LEU
2	E	159	GLN
2	E	170	GLU
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	237	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	272	THR

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Mol	Chain	Res	Type
2	E	275	ILE
2	E	277	LYS
2	E	278	LEU
2	E	282	GLU
2	E	287	LEU
2	E	294	THR
2	E	299	THR
2	E	303	LYS
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	327	LEU
2	E	328	ILE
2	E	332	ILE
2	E	333	ILE
2	E	339	VAL
2	E	341	VAL
2	E	342	ASN
2	E	347	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	224	HIS

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Mol	Chain	Res	Type
2	B	4	HIS
2	B	50	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
1	D	137	GLN
1	D	140	HIS
2	E	4	HIS
2	E	10	GLN
2	E	75	ASN
2	E	89	ASN
2	E	142	HIS
2	E	176	GLN
2	E	221	ASN
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	11,14,15	1.49	1 (9%)	8,20,22	1.77	2 (25%)
1	NEP	D	246	1	11,14,15	1.62	2 (18%)	8,20,22	1.59	2 (25%)

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	-	2/5/12/14	0/1/1/1
1	NEP	D	246	1	-	3/5/12/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	NEP	P-O2P	-3.92	1.46	1.56
1	A	246	NEP	P-O2P	-3.02	1.48	1.56
1	D	246	NEP	P-O1P	-2.69	1.49	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	NEP	CA-CB-CG	3.64	122.75	113.77
1	D	246	NEP	CA-CB-CG	3.04	121.27	113.77
1	D	246	NEP	O2P-P-O3P	-2.13	107.70	112.95
1	A	246	NEP	O1P-P-O3P	-2.08	107.84	112.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	246	NEP	O-C-CA-CB
1	D	246	NEP	CA-CB-CG-CD2
1	D	246	NEP	CA-CB-CG-ND1
1	A	246	NEP	CA-CB-CG-CD2
1	A	246	NEP	CA-CB-CG-ND1

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 oligosaccharides 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	D	289	-	47,50,50	1.14	4 (8%)	69,75,75	0.94	3 (4%)
3	COA	A	289	-	47,50,50	0.75	0	69,75,75	2.38	11 (15%)

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	D	289	-	-	17/48/64/64	0/3/3/3
3	COA	A	289	-	-	16/48/64/64	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	289	COA	P2A-O3A	3.96	1.63	1.59
3	D	289	COA	P1A-O3A	2.79	1.62	1.59
3	D	289	COA	C6P-C5P	2.46	1.56	1.51
3	D	289	COA	CCP-CBP	2.41	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	289	COA	O9A-P3B-O7A	9.85	149.20	110.83
3	A	289	COA	O3A-P1A-O1A	-9.11	83.31	110.70
3	A	289	COA	O8A-P3B-O7A	-8.99	75.80	110.83
3	A	289	COA	O2A-P1A-O3A	6.48	124.78	107.27
3	A	289	COA	C7P-N8P-C9P	-4.53	114.41	122.55
3	A	289	COA	OAP-CAP-CBP	3.42	118.11	110.18
3	D	289	COA	O6A-CCP-CBP	2.78	115.01	110.55
3	A	289	COA	O2B-C2B-C3B	2.52	118.25	111.19
3	A	289	COA	CEP-CBP-CCP	2.41	112.19	108.22
3	A	289	COA	O4B-C1B-C2B	-2.40	101.47	106.62
3	A	289	COA	CDP-CBP-CCP	-2.22	104.56	108.22
3	D	289	COA	O8A-P3B-O7A	2.20	119.42	110.83
3	D	289	COA	P3B-O3B-C3B	-2.05	117.96	123.43
3	A	289	COA	C4B-O4B-C1B	-2.01	105.03	109.47

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	289	COA	OAP-CAP-CBP-CCP
3	A	289	COA	C9P-CAP-CBP-CCP
3	A	289	COA	C9P-CAP-CBP-CDP
3	A	289	COA	OAP-CAP-CBP-CEP
3	A	289	COA	C9P-CAP-CBP-CEP
3	D	289	COA	CCP-O6A-P2A-O3A
3	D	289	COA	CCP-O6A-P2A-O4A
3	D	289	COA	CCP-O6A-P2A-O5A
3	D	289	COA	CDP-CBP-CCP-O6A
3	D	289	COA	CEP-CBP-CCP-O6A
3	D	289	COA	CAP-CBP-CCP-O6A
3	D	289	COA	OAP-CAP-CBP-CCP
3	D	289	COA	C9P-CAP-CBP-CCP
3	D	289	COA	OAP-CAP-CBP-CDP
3	D	289	COA	C9P-CAP-CBP-CDP
3	D	289	COA	OAP-CAP-CBP-CEP
3	D	289	COA	C9P-CAP-CBP-CEP
3	A	289	COA	C6P-C7P-N8P-C9P
3	D	289	COA	C6P-C7P-N8P-C9P
3	D	289	COA	C2B-C3B-O3B-P3B
3	D	289	COA	C4B-C3B-O3B-P3B
3	A	289	COA	OAP-CAP-CBP-CDP

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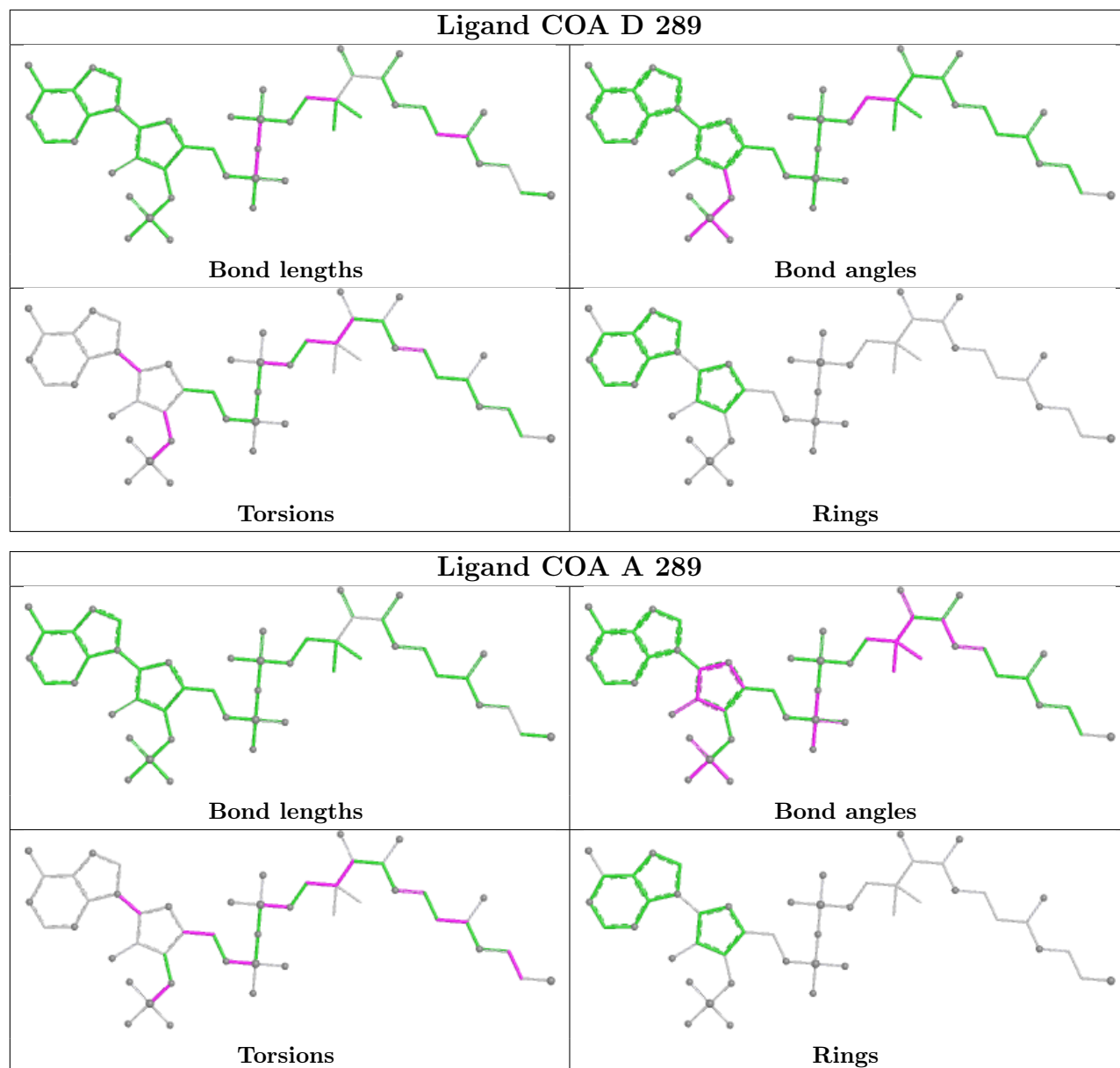
Mol	Chain	Res	Type	Atoms
3	D	289	COA	C2B-C1B-N9A-C8A
3	A	289	COA	CDP-CBP-CCP-O6A
3	A	289	COA	S1P-C2P-C3P-N4P
3	A	289	COA	C5B-O5B-P1A-O1A
3	A	289	COA	CCP-O6A-P2A-O4A
3	A	289	COA	O4B-C4B-C5B-O5B
3	A	289	COA	C3B-O3B-P3B-O7A
3	A	289	COA	O5P-C5P-C6P-C7P
3	A	289	COA	CEP-CBP-CCP-O6A
3	D	289	COA	C3B-O3B-P3B-O7A
3	A	289	COA	C2B-C1B-N9A-C4A

There are no ring outliers.

2 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	289	COA	19	0
3	A	289	COA	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.