



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:41 AM EDT

PDB ID : 2GER / pdb_00002ger
Title : Crystal Structure and Oxidative Mechanism of Human Pyrroline-5-carboxylate Reductase
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.
Deposited on : 2006-03-20
Resolution : 3.10 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

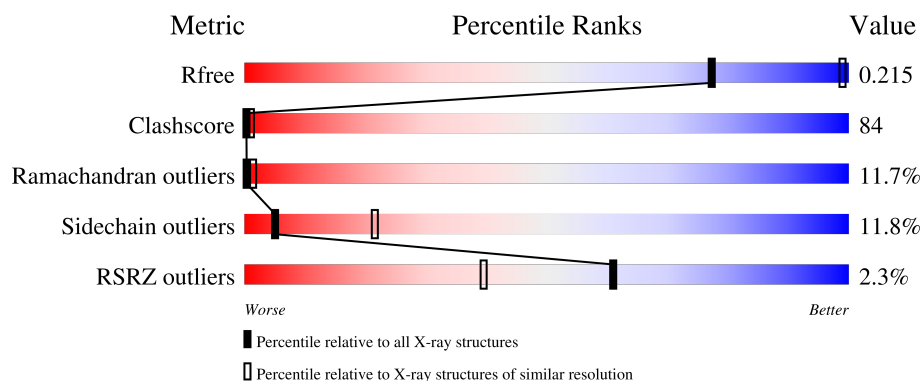
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	321	
1	B	321	
1	C	321	
1	D	321	
1	E	321	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10768 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 Pyrroline-5-carboxylate reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	B	276	Total	C	N	O	S	0	0	0
			2025	1271	359	382	13			
1	C	277	Total	C	N	O	S	0	0	0
			2032	1276	360	383	13			
1	D	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	E	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	cloning artifact	UNP P32322
A	0	ALA	-	cloning artifact	UNP P32322
B	-1	ARG	-	cloning artifact	UNP P32322
B	0	ALA	-	cloning artifact	UNP P32322
C	-1	ARG	-	cloning artifact	UNP P32322
C	0	ALA	-	cloning artifact	UNP P32322
D	-1	ARG	-	cloning artifact	UNP P32322
D	0	ALA	-	cloning artifact	UNP P32322
E	-1	ARG	-	cloning artifact	UNP P32322
E	0	ALA	-	cloning artifact	UNP P32322

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	118	Total	O	0	0
			118	118		

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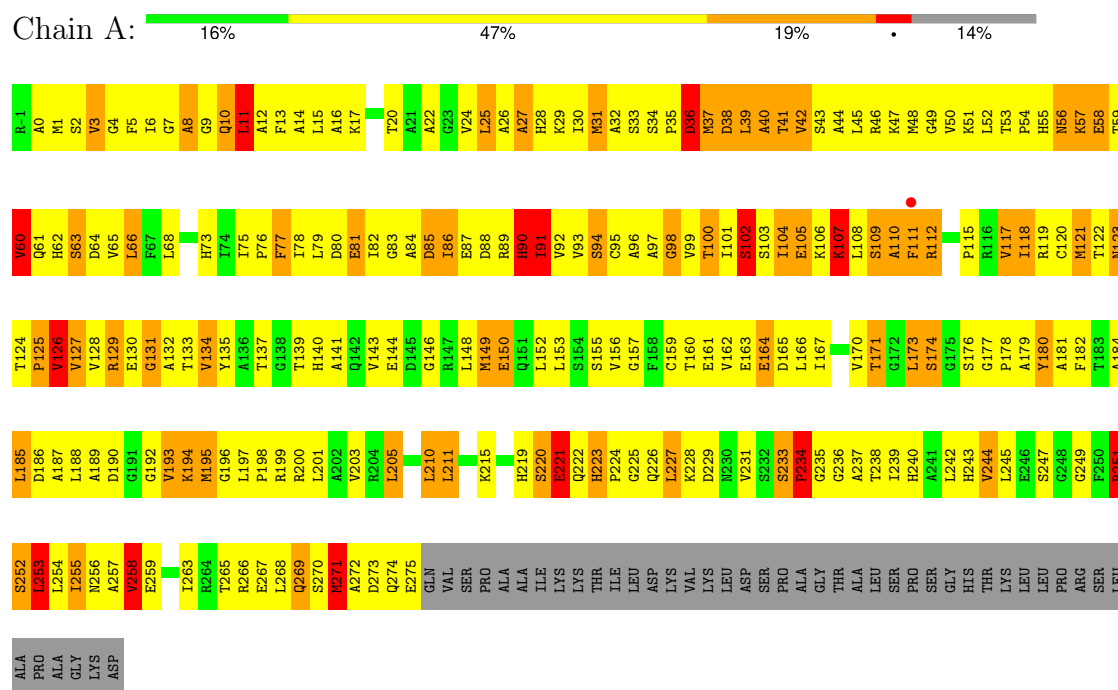
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	119	Total 119	O 119	0	0
2	D	126	Total 126	O 126	0	0
2	E	128	Total 128	O 128	0	0

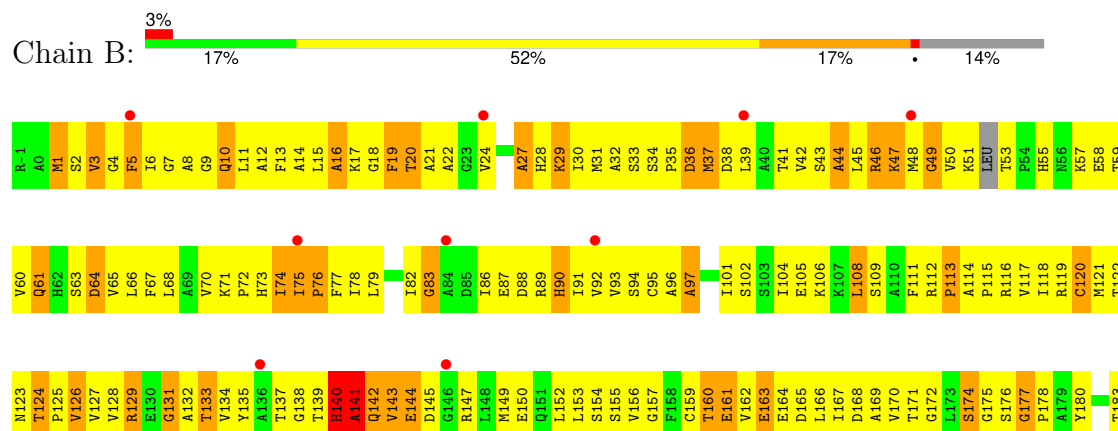
3 Residue-property plots

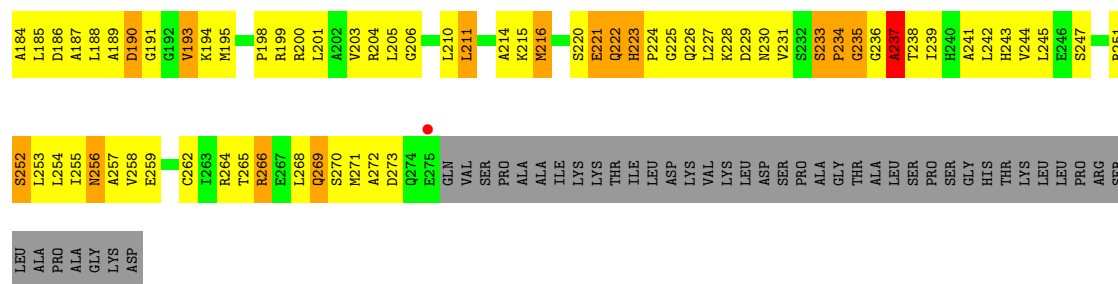
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

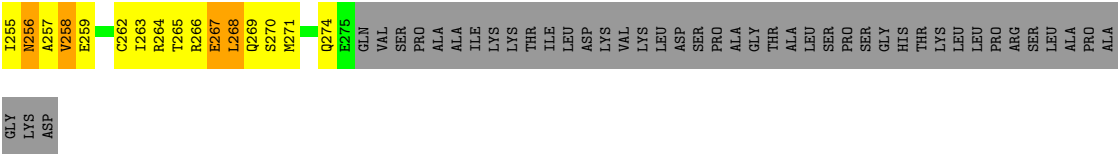
• Molecule 1: Pyrroline-5-carboxylate reductase 1



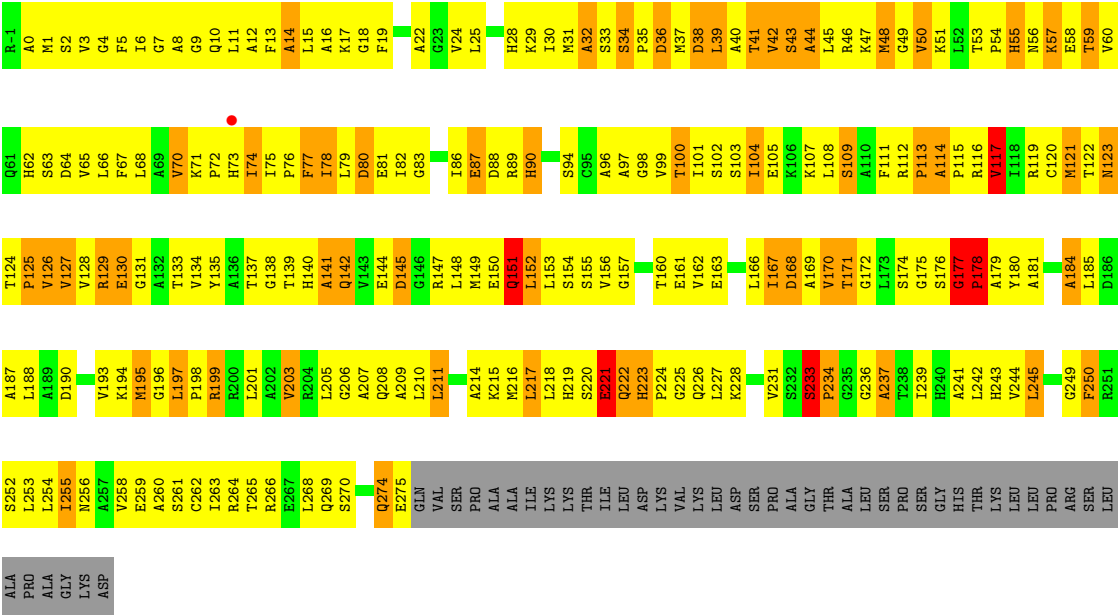
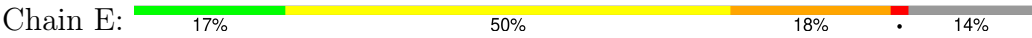
• Molecule 1: Pyrroline-5-carboxylate reductase 1







• Molecule 1: Pyrroline-5-carboxylate reductase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.61Å 123.81Å 120.79Å 90.00° 121.76° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 98.6 (50.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 3.11Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.261 0.221 , 0.215	Depositor DCC
R_{free} test set	2346 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 126.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.036 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-1,1/2*h-1/2*k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10768	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	0/2069	1.32	34/2800 (1.2%)
1	B	0.77	0/2055	1.24	20/2781 (0.7%)
1	C	0.82	0/2063	1.31	28/2793 (1.0%)
1	D	0.91	1/2069 (0.0%)	1.32	25/2800 (0.9%)
1	E	0.84	0/2069	1.34	28/2800 (1.0%)
All	All	0.84	1/10325 (0.0%)	1.31	135/13974 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	6	ILE	CA-CB	-5.47	1.47	1.54

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	39	LEU	N-CA-C	-13.02	97.39	113.28
1	D	101	ILE	N-CA-C	-10.67	100.47	110.82
1	B	193	VAL	N-CA-C	-10.47	100.14	110.72
1	B	1	MET	N-CA-C	9.35	119.24	108.49
1	A	0	ALA	N-CA-C	-9.31	101.85	113.02
1	D	245	LEU	N-CA-C	-9.15	101.28	111.07
1	B	21	ALA	N-CA-C	-9.11	102.15	113.18
1	C	221	GLU	N-CA-C	-8.99	102.46	113.97
1	C	159	CYS	N-CA-C	8.97	123.08	108.55
1	D	172	GLY	N-CA-C	-8.88	101.61	113.24
1	B	44	ALA	N-CA-C	-8.55	101.99	114.39
1	C	103	SER	N-CA-C	-8.43	102.02	111.71
1	D	222	GLN	N-CA-C	8.37	120.03	111.07
1	E	145	ASP	N-CA-C	-8.35	102.80	113.16
1	B	159	CYS	N-CA-C	8.35	121.40	108.96
1	C	180	TYR	N-CA-C	-8.13	102.36	111.14
1	A	271	MET	N-CA-C	-8.11	105.37	114.62
1	C	261	SER	N-CA-C	-8.02	102.23	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	VAL	N-CA-C	7.97	118.03	110.30
1	E	64	ASP	N-CA-C	-7.96	103.17	113.12
1	E	154	SER	N-CA-C	-7.90	103.53	113.01
1	C	245	LEU	N-CA-C	-7.74	102.17	111.69
1	A	255	ILE	N-CA-C	-7.58	103.29	110.42
1	E	0	ALA	N-CA-C	-7.41	102.78	112.41
1	A	3	VAL	N-CA-C	7.34	119.72	109.29
1	A	58	GLU	N-CA-C	-7.34	103.27	111.71
1	D	109	SER	N-CA-C	-7.30	103.33	111.28
1	E	32	ALA	N-CA-C	-7.19	98.14	109.50
1	C	130	GLU	N-CA-C	7.18	118.67	108.54
1	E	197	LEU	N-CA-C	7.16	120.50	110.20
1	E	177	GLY	CA-C-N	7.09	128.71	119.84
1	E	177	GLY	C-N-CA	7.09	128.71	119.84
1	A	180	TYR	N-CA-C	-7.00	103.72	111.36
1	D	64	ASP	N-CA-C	-6.99	103.09	111.69
1	D	3	VAL	N-CA-C	6.98	118.54	108.48
1	D	154	SER	N-CA-C	-6.90	105.40	113.88
1	D	228	LYS	N-CA-C	-6.88	102.63	111.02
1	A	66	LEU	N-CA-C	6.86	120.64	109.59
1	E	184	ALA	N-CA-C	-6.84	103.51	110.97
1	D	117	VAL	N-CA-C	6.81	117.85	107.77
1	B	49	GLY	N-CA-C	-6.81	100.55	114.16
1	D	112	ARG	CA-C-N	6.74	128.26	119.84
1	D	112	ARG	C-N-CA	6.74	128.26	119.84
1	C	80	ASP	N-CA-C	-6.72	104.55	112.89
1	B	131	GLY	N-CA-C	-6.71	102.24	112.51
1	D	34	SER	CA-C-N	-6.71	112.72	119.56
1	D	34	SER	C-N-CA	-6.71	112.72	119.56
1	C	177	GLY	CA-C-N	6.69	128.20	119.84
1	C	177	GLY	C-N-CA	6.69	128.20	119.84
1	A	81	GLU	N-CA-C	-6.62	105.77	114.31
1	E	233	SER	CA-C-N	6.57	128.05	119.84
1	E	233	SER	C-N-CA	6.57	128.05	119.84
1	C	92	VAL	N-CA-C	6.54	116.66	107.37
1	C	191	GLY	N-CA-C	-6.43	97.94	113.18
1	B	88	ASP	N-CA-C	-6.43	105.82	113.21
1	A	233	SER	CA-C-N	6.39	127.83	119.84
1	A	233	SER	C-N-CA	6.39	127.83	119.84
1	C	23	GLY	N-CA-C	-6.37	106.53	115.32
1	E	63	SER	N-CA-C	6.37	120.26	110.20
1	C	1	MET	N-CA-C	6.33	118.14	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	SER	N-CA-C	6.31	119.98	109.95
1	B	74	ILE	N-CA-C	-6.30	104.81	113.00
1	A	34	SER	CA-C-N	-6.29	111.98	119.84
1	A	34	SER	C-N-CA	-6.29	111.98	119.84
1	E	152	LEU	N-CA-C	6.26	117.90	111.14
1	E	255	ILE	N-CA-C	-6.20	103.79	110.23
1	D	108	LEU	N-CA-C	-6.17	105.01	112.54
1	B	256	ASN	N-CA-C	-6.14	105.79	113.28
1	E	117	VAL	N-CA-C	6.14	116.76	108.17
1	A	117	VAL	N-CA-C	6.13	117.53	108.45
1	C	6	ILE	N-CA-C	-6.12	104.38	110.62
1	B	269	GLN	N-CA-C	-6.11	104.70	111.36
1	D	52	LEU	N-CA-C	6.11	118.90	109.07
1	A	258	VAL	N-CA-C	-6.10	104.69	110.42
1	A	90	HIS	N-CA-C	6.10	119.87	110.42
1	E	245	LEU	N-CA-C	-6.09	104.27	111.03
1	C	179	ALA	N-CA-C	-6.01	105.78	113.23
1	D	56	ASN	N-CA-C	5.98	117.80	111.28
1	A	112	ARG	CA-C-N	5.93	125.41	119.24
1	A	112	ARG	C-N-CA	5.93	125.41	119.24
1	B	266	ARG	N-CA-C	-5.92	104.17	111.40
1	C	197	LEU	N-CA-C	5.91	122.86	109.81
1	A	126	VAL	N-CA-C	-5.90	104.60	110.62
1	A	185	LEU	N-CA-C	5.88	117.36	111.07
1	D	93	VAL	N-CA-C	-5.83	100.03	108.36
1	E	109	SER	N-CA-C	-5.76	105.51	112.54
1	B	141	ALA	N-CA-C	-5.74	98.58	110.80
1	D	178	PRO	N-CA-C	-5.73	105.91	113.65
1	C	29	LYS	N-CA-C	-5.67	106.69	113.21
1	A	174	SER	N-CA-C	5.65	118.98	111.75
1	B	3	VAL	N-CA-C	5.63	115.26	108.06
1	D	91	ILE	N-CA-C	-5.63	100.37	108.53
1	D	0	ALA	N-CA-C	-5.61	103.96	111.87
1	E	38	ASP	N-CA-C	5.59	118.52	109.40
1	C	228	LYS	N-CA-C	-5.58	105.19	111.28
1	E	114	ALA	CA-C-N	5.58	125.56	120.03
1	E	114	ALA	C-N-CA	5.58	125.56	120.03
1	E	221	GLU	N-CA-C	-5.58	98.92	110.80
1	A	100	THR	N-CA-C	5.56	118.34	110.50
1	D	145	ASP	N-CA-C	-5.52	105.18	111.14
1	A	86	ILE	N-CA-C	5.51	115.25	106.88
1	A	272	ALA	N-CA-C	-5.51	106.33	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	ALA	N-CA-C	-5.50	104.80	112.45
1	B	1	MET	CB-CA-C	-5.50	106.57	114.87
1	B	108	LEU	N-CA-C	-5.49	106.74	113.50
1	D	43	SER	N-CA-C	5.48	117.33	111.36
1	C	117	VAL	N-CA-C	5.42	115.91	107.99
1	C	92	VAL	CB-CA-C	-5.42	106.05	111.80
1	E	87	GLU	N-CA-C	5.38	118.51	107.37
1	B	190	ASP	N-CA-C	-5.35	99.41	110.80
1	E	90	HIS	N-CA-C	5.34	117.83	110.35
1	A	91	ILE	CB-CA-C	-5.30	102.42	110.95
1	E	55	HIS	N-CA-C	5.27	117.33	108.73
1	A	109	SER	N-CA-C	-5.25	106.82	113.18
1	A	193	VAL	CB-CA-C	-5.25	104.39	112.05
1	E	171	THR	N-CA-C	-5.23	106.02	112.72
1	A	131	GLY	N-CA-C	-5.23	105.85	112.54
1	E	126	VAL	N-CA-C	-5.22	104.38	111.89
1	C	71	LYS	CA-C-N	5.21	126.36	119.84
1	C	71	LYS	C-N-CA	5.21	126.36	119.84
1	A	144	GLU	N-CA-C	-5.20	106.96	113.72
1	C	126	VAL	N-CA-C	-5.20	104.56	111.05
1	B	126	VAL	N-CA-C	-5.16	104.60	111.05
1	D	37	MET	N-CA-C	5.15	117.02	107.60
1	A	251	ARG	N-CA-C	-5.14	105.36	110.97
1	B	237	ALA	N-CA-C	-5.14	99.85	110.80
1	A	221	GLU	N-CA-C	-5.13	99.86	110.80
1	D	268	LEU	N-CA-C	-5.13	105.34	111.03
1	A	227	LEU	N-CA-C	-5.11	106.31	112.54
1	C	5	PHE	N-CA-C	5.10	118.33	107.67
1	A	31	MET	N-CA-C	5.06	117.58	108.48
1	B	46	ARG	N-CA-C	-5.01	103.11	111.37
1	A	57	LYS	N-CA-C	-5.01	107.12	113.43
1	C	37	MET	N-CA-C	5.01	115.91	108.60
1	E	196	GLY	N-CA-C	5.01	120.76	114.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2038	0	2082	339	0
1	B	2025	0	2063	376	0
1	C	2032	0	2071	375	0
1	D	2038	0	2082	318	0
1	E	2038	0	2082	336	0
2	A	106	0	0	48	0
2	B	118	0	0	53	0
2	C	119	0	0	55	0
2	D	126	0	0	49	0
2	E	128	0	0	63	0
All	All	10768	0	10380	1726	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 84.

All (1726) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ILE:HD12	1:D:239:ILE:H	1.08	1.16
1:C:75:ILE:HD12	1:C:99:VAL:HG21	1.27	1.16
1:B:75:ILE:HB	1:B:76:PRO:HD3	1.22	1.14
1:E:101:ILE:HD11	1:E:138:GLY:HA2	1.28	1.14
1:C:86:ILE:HD11	1:C:108:LEU:HD22	1.34	1.09
1:B:9:GLY:H	1:B:12:ALA:HB3	1.17	1.08
1:D:37:MET:HG2	1:D:42:VAL:HG11	1.35	1.06
1:A:86:ILE:HD12	1:A:108:LEU:HD11	1.35	1.06
1:B:74:ILE:HA	1:B:78:ILE:HD12	1.06	1.06
1:C:122:THR:HB	1:C:133:THR:HG22	1.38	1.06
1:C:270:SER:O	1:C:274:GLN:HB2	1.55	1.06
1:B:160:THR:HG22	1:B:161:GLU:H	1.17	1.06
1:B:6:ILE:HA	1:B:33:SER:HB3	1.35	1.04
1:D:31:MET:HG2	1:D:59:THR:HA	1.37	1.04
1:C:112:ARG:HH11	1:C:113:PRO:HD2	1.20	1.03
1:A:133:THR:HG21	1:A:153:LEU:HD13	1.41	1.02
1:E:75:ILE:HA	1:E:78:ILE:HD12	1.42	1.01
1:A:234:PRO:HB3	1:C:196:GLY:O	1.62	1.00
1:B:5:PHE:HZ	1:B:15:LEU:HB2	1.25	1.00
1:D:9:GLY:H	1:D:41:THR:HG21	1.27	1.00
1:D:239:ILE:H	1:D:239:ILE:CD1	1.73	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLN:HG2	1:B:143:VAL:H	1.26	0.99
1:E:195:MET:HA	1:E:195:MET:HE3	1.45	0.98
1:E:180:TYR:HA	2:E:381:HOH:O	1.63	0.97
1:B:200:ARG:HH11	1:B:204:ARG:HH21	1.11	0.97
1:E:241:ALA:O	1:E:244:VAL:HG12	1.65	0.97
1:C:126:VAL:HA	2:C:334:HOH:O	1.64	0.96
1:C:135:TYR:CE1	1:C:161:GLU:HB3	2.00	0.96
1:B:195:MET:HE2	1:B:195:MET:HA	1.46	0.96
1:C:236:GLY:HA2	1:C:239:ILE:HG22	1.48	0.96
1:A:123:ASN:HD21	1:A:132:ALA:H	1.07	0.95
1:D:122:THR:HG23	1:D:133:THR:HB	1.49	0.94
1:D:121:MET:CE	1:D:171:THR:HG23	1.97	0.94
1:A:75:ILE:HG22	1:A:76:PRO:HD3	1.47	0.94
1:A:153:LEU:HB2	1:A:159:CYS:SG	2.08	0.94
1:B:74:ILE:HA	1:B:78:ILE:CD1	1.98	0.93
1:A:258:VAL:HA	2:A:419:HOH:O	1.66	0.93
1:A:91:ILE:HD12	1:A:91:ILE:H	1.34	0.93
1:D:122:THR:CG2	1:D:133:THR:HB	2.00	0.91
1:D:239:ILE:HD12	1:D:239:ILE:N	1.86	0.91
1:E:228:LYS:HE3	1:E:242:LEU:HD13	1.50	0.91
1:C:112:ARG:HG3	1:C:113:PRO:HD2	1.51	0.91
1:B:7:GLY:O	1:B:12:ALA:HB2	1.70	0.90
1:E:101:ILE:CD1	1:E:138:GLY:HA2	2.00	0.90
1:B:143:VAL:HG12	1:B:144:GLU:H	1.36	0.90
1:D:178:PRO:HD3	2:D:416:HOH:O	1.68	0.90
1:D:97:ALA:HB1	1:D:265:THR:HG23	1.51	0.90
1:B:71:LYS:HB3	1:B:72:PRO:HD2	1.55	0.89
1:B:121:MET:O	1:B:133:THR:HB	1.72	0.89
1:B:63:SER:HB2	1:B:89:ARG:HH12	1.36	0.89
1:A:6:ILE:HG23	1:A:56:ASN:HB2	1.55	0.88
1:A:121:MET:HG2	1:A:171:THR:HG23	1.55	0.88
1:E:236:GLY:HA2	1:E:239:ILE:HG22	1.56	0.88
1:C:31:MET:HB3	1:C:59:THR:HG23	1.56	0.87
1:B:3:VAL:H	1:B:30:ILE:HG23	1.37	0.87
1:E:53:THR:HG22	1:E:55:HIS:H	1.37	0.87
1:E:122:THR:HG22	1:E:133:THR:HB	1.57	0.87
1:E:86:ILE:HD11	1:E:108:LEU:HD22	1.54	0.86
1:A:79:LEU:HD11	1:A:104:ILE:CD1	2.05	0.86
1:C:258:VAL:HG12	1:C:258:VAL:O	1.75	0.86
1:C:252:SER:O	1:C:254:LEU:N	2.08	0.86
1:B:243:HIS:HB3	2:B:400:HOH:O	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:MET:HE3	1:D:42:VAL:HG12	1.58	0.86
1:E:220:SER:HB2	1:E:222:GLN:HG2	1.56	0.86
1:D:83:GLY:O	1:D:86:ILE:HG22	1.75	0.86
1:B:160:THR:HG22	1:B:161:GLU:N	1.87	0.86
1:E:221:GLU:O	1:E:223:HIS:N	2.07	0.86
1:B:5:PHE:CZ	1:B:15:LEU:HB2	2.10	0.86
1:B:79:LEU:HD13	1:B:104:ILE:HG23	1.57	0.86
1:A:33:SER:OG	1:A:56:ASN:HB3	1.76	0.85
1:B:185:LEU:HD21	1:B:210:LEU:HD12	1.58	0.85
1:C:160:THR:HG21	2:C:421:HOH:O	1.76	0.85
1:E:217:LEU:HD21	1:E:224:PRO:HG3	1.58	0.85
1:C:112:ARG:HH11	1:C:113:PRO:CD	1.89	0.85
1:E:68:LEU:HG	2:E:358:HOH:O	1.76	0.84
1:B:58:GLU:O	1:B:61:GLN:HG3	1.77	0.84
1:E:68:LEU:HB2	1:E:94:SER:HA	1.60	0.84
1:B:74:ILE:CA	1:B:78:ILE:HD12	2.00	0.84
1:C:123:ASN:HB2	1:C:125:PRO:HD2	1.60	0.84
1:B:160:THR:CG2	1:B:161:GLU:H	1.91	0.84
1:E:114:ALA:HB1	1:E:140:HIS:CG	2.13	0.84
1:E:203:VAL:HG23	2:E:422:HOH:O	1.76	0.83
1:D:32:ALA:HB3	1:D:52:LEU:HD23	1.60	0.83
1:D:129:ARG:HD3	1:D:155:SER:O	1.77	0.83
1:D:67:PHE:C	1:D:68:LEU:HD23	2.04	0.83
1:E:9:GLY:H	1:E:41:THR:HG21	1.42	0.82
1:D:162:VAL:HG13	1:D:166:LEU:HD12	1.60	0.82
1:E:101:ILE:HD11	1:E:138:GLY:CA	2.09	0.82
1:A:124:THR:O	1:A:127:VAL:HG23	1.79	0.82
1:A:88:ASP:CB	1:A:112:ARG:HH21	1.92	0.82
1:D:170:VAL:HG12	1:D:170:VAL:O	1.76	0.82
1:A:123:ASN:HD21	1:A:132:ALA:N	1.77	0.82
1:D:98:GLY:HA3	1:D:269:GLN:HB2	1.60	0.82
1:B:71:LYS:HB2	1:B:73:HIS:CE1	2.14	0.81
1:D:262:CYS:HA	2:D:364:HOH:O	1.81	0.81
1:A:123:ASN:ND2	1:A:132:ALA:H	1.79	0.81
1:B:75:ILE:HB	1:B:76:PRO:CD	2.07	0.81
1:D:101:ILE:HD13	1:D:138:GLY:HA2	1.63	0.81
1:B:29:LYS:O	1:B:30:ILE:HG13	1.80	0.81
1:C:24:VAL:O	1:C:25:LEU:HB2	1.81	0.81
1:E:199:ARG:HG3	2:E:422:HOH:O	1.81	0.81
1:E:147:ARG:O	1:E:151:GLN:HB2	1.81	0.81
1:E:194:LYS:HA	2:E:363:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLY:H	1:A:41:THR:HG21	1.45	0.80
1:C:172:GLY:HA2	1:C:261:SER:OG	1.81	0.80
1:B:60:VAL:HG12	1:B:89:ARG:NH2	1.96	0.80
1:C:45:LEU:O	1:C:48:MET:HB3	1.81	0.80
1:C:122:THR:HG22	1:C:133:THR:HB	1.63	0.80
1:D:169:ALA:C	1:D:171:THR:H	1.89	0.80
1:C:223:HIS:ND1	1:C:224:PRO:HD2	1.96	0.80
1:C:122:THR:CB	1:C:133:THR:HG22	2.11	0.79
1:E:162:VAL:HG13	1:E:166:LEU:HD12	1.62	0.79
1:E:205:LEU:HA	2:E:408:HOH:O	1.81	0.79
1:A:3:VAL:HG12	1:A:4:GLY:H	1.47	0.79
1:A:244:VAL:HG23	2:A:387:HOH:O	1.83	0.79
1:B:29:LYS:C	1:B:30:ILE:HG13	2.08	0.79
1:D:3:VAL:HG22	1:D:65:VAL:HG13	1.62	0.79
1:A:9:GLY:N	1:A:41:THR:HG21	1.98	0.79
1:E:124:THR:O	1:E:127:VAL:HG23	1.83	0.79
1:A:115:PRO:HG3	2:A:354:HOH:O	1.83	0.79
1:C:71:LYS:H	1:C:71:LYS:HD3	1.48	0.78
1:A:123:ASN:H	1:A:123:ASN:HD22	1.31	0.78
1:A:239:ILE:HD11	1:C:190:ASP:O	1.83	0.78
1:A:253:LEU:C	2:A:390:HOH:O	2.26	0.78
1:E:53:THR:HG21	1:E:58:GLU:HB2	1.66	0.78
1:D:32:ALA:HB3	1:D:52:LEU:CD2	2.13	0.78
1:C:201:LEU:HA	2:C:337:HOH:O	1.83	0.78
1:D:133:THR:HG21	1:D:153:LEU:HB3	1.64	0.78
1:B:14:ALA:HA	1:B:127:VAL:HG22	1.66	0.78
1:B:79:LEU:HD11	1:B:104:ILE:HG12	1.66	0.78
1:C:101:ILE:CD1	1:C:138:GLY:HA3	2.14	0.78
1:E:25:LEU:HD23	1:E:25:LEU:H	1.49	0.77
1:B:82:ILE:HG22	1:B:86:ILE:HD11	1.65	0.77
1:B:8:ALA:HA	1:B:12:ALA:CB	2.13	0.77
1:B:78:ILE:O	1:B:82:ILE:HG13	1.84	0.77
1:C:101:ILE:O	1:C:105:GLU:HG3	1.85	0.77
1:D:30:ILE:HB	1:D:50:VAL:HG22	1.67	0.77
1:A:166:LEU:O	1:A:170:VAL:HG23	1.83	0.77
1:D:166:LEU:O	1:D:168:ASP:N	2.18	0.77
1:A:239:ILE:HG21	2:C:344:HOH:O	1.84	0.77
1:E:123:ASN:O	1:E:126:VAL:HG23	1.83	0.77
1:C:4:GLY:C	1:C:66:LEU:HG	2.09	0.77
1:A:115:PRO:O	1:A:140:HIS:HB2	1.85	0.77
1:B:60:VAL:O	1:B:89:ARG:NH2	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:THR:HG22	2:B:393:HOH:O	1.85	0.77
1:B:128:VAL:HB	2:B:340:HOH:O	1.85	0.77
1:A:79:LEU:HD11	1:A:104:ILE:HD12	1.67	0.77
1:E:4:GLY:O	1:E:66:LEU:HD12	1.84	0.76
1:E:172:GLY:HA2	1:E:261:SER:OG	1.84	0.76
1:C:122:THR:HB	1:C:133:THR:CG2	2.15	0.76
1:A:73:HIS:O	1:A:76:PRO:HD2	1.86	0.76
1:B:122:THR:HG22	1:B:133:THR:HB	1.66	0.76
1:E:122:THR:HB	1:E:133:THR:HG22	1.67	0.76
1:C:6:ILE:H	1:C:66:LEU:HD21	1.51	0.76
1:C:79:LEU:HD22	1:C:108:LEU:HD11	1.66	0.76
1:A:3:VAL:HG12	1:A:4:GLY:N	2.00	0.76
1:A:201:LEU:O	1:A:205:LEU:HG	1.86	0.76
1:D:80:ASP:O	1:D:82:ILE:N	2.18	0.76
1:C:72:PRO:HG2	1:C:97:ALA:O	1.86	0.76
1:B:264:ARG:O	1:B:268:LEU:HG	1.86	0.75
1:C:116:ARG:HA	1:C:140:HIS:HB2	1.67	0.75
1:D:9:GLY:N	1:D:41:THR:HG21	2.00	0.75
1:C:202:ALA:HB2	2:C:371:HOH:O	1.85	0.75
1:D:124:THR:O	1:D:127:VAL:HG23	1.86	0.75
1:D:92:VAL:HA	2:D:420:HOH:O	1.86	0.75
1:B:191:GLY:O	1:B:194:LYS:HB3	1.87	0.75
1:B:135:TYR:CE1	1:B:161:GLU:HB3	2.22	0.75
1:C:48:MET:HE3	1:C:48:MET:O	1.87	0.75
1:C:128:VAL:HG12	1:C:129:ARG:N	2.01	0.75
1:E:60:VAL:HG21	1:E:82:ILE:HD13	1.69	0.75
1:A:28:HIS:CE1	1:A:29:LYS:HG3	2.21	0.74
1:A:20:THR:HG21	1:A:48:MET:HE3	1.67	0.74
1:A:225:GLY:O	1:A:228:LYS:HB3	1.87	0.74
1:B:259:GLU:N	2:B:336:HOH:O	2.19	0.74
1:C:75:ILE:CD1	1:C:99:VAL:HG21	2.14	0.74
1:B:142:GLN:HG2	1:B:143:VAL:N	2.01	0.74
1:A:121:MET:HE3	1:A:171:THR:HG22	1.69	0.74
1:E:169:ALA:C	1:E:171:THR:H	1.94	0.74
1:A:118:ILE:HD12	1:A:149:MET:SD	2.27	0.74
1:B:141:ALA:O	1:B:145:ASP:HB3	1.87	0.74
1:E:274:GLN:HG3	1:E:275:GLU:H	1.52	0.74
1:B:9:GLY:H	1:B:12:ALA:CB	1.96	0.73
1:E:55:HIS:HB3	1:E:57:LYS:HG2	1.70	0.73
1:A:107:LYS:HB3	2:A:357:HOH:O	1.89	0.73
1:C:114:ALA:HB1	1:C:140:HIS:ND1	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:MET:HE3	2:C:370:HOH:O	1.88	0.73
1:E:122:THR:HG22	1:E:133:THR:CB	2.17	0.73
1:A:6:ILE:HD11	1:A:66:LEU:HD21	1.71	0.73
1:A:14:ALA:HA	1:A:127:VAL:HG22	1.69	0.73
1:B:200:ARG:O	1:B:204:ARG:HG2	1.89	0.73
1:E:129:ARG:HG2	1:E:130:GLU:N	2.02	0.73
1:B:93:VAL:HA	1:B:118:ILE:O	1.87	0.73
1:D:20:THR:OG1	1:D:48:MET:HE3	1.89	0.73
1:E:55:HIS:HB3	1:E:57:LYS:HE2	1.70	0.73
1:B:162:VAL:HB	1:B:166:LEU:HD12	1.70	0.73
1:C:89:ARG:HD2	1:C:90:HIS:N	2.04	0.73
1:A:88:ASP:HB2	1:A:112:ARG:HH21	1.54	0.73
1:B:176:SER:HA	2:B:410:HOH:O	1.89	0.73
1:D:93:VAL:HG12	1:D:118:ILE:HG13	1.71	0.73
1:B:82:ILE:O	1:B:86:ILE:HG13	1.89	0.72
1:D:70:VAL:HG12	1:D:74:ILE:HB	1.69	0.72
1:D:227:LEU:O	1:D:231:VAL:HG23	1.89	0.72
1:B:70:VAL:HG12	1:B:71:LYS:H	1.54	0.72
1:B:27:ALA:HB1	1:B:49:GLY:O	1.89	0.72
1:A:93:VAL:HG23	2:A:368:HOH:O	1.89	0.72
1:A:149:MET:HE3	1:A:149:MET:HA	1.71	0.72
1:B:186:ASP:HB3	2:B:388:HOH:O	1.89	0.72
1:D:3:VAL:HG22	1:D:65:VAL:CG1	2.19	0.72
1:A:275:GLU:HB2	2:A:353:HOH:O	1.89	0.72
1:C:68:LEU:HD21	2:C:332:HOH:O	1.88	0.72
1:C:95:CYS:HB2	2:C:412:HOH:O	1.88	0.72
1:D:75:ILE:HB	1:D:76:PRO:HD3	1.72	0.71
1:E:125:PRO:HG2	2:E:325:HOH:O	1.89	0.71
1:A:91:ILE:HD12	1:A:91:ILE:N	2.06	0.71
1:A:121:MET:HG2	1:A:171:THR:CG2	2.21	0.71
1:A:43:SER:HA	1:A:46:ARG:HG3	1.72	0.71
1:B:2:SER:HA	1:B:30:ILE:HG12	1.71	0.71
1:B:251:ARG:O	1:B:254:LEU:N	2.24	0.71
1:E:83:GLY:HA2	1:E:86:ILE:CD1	2.19	0.71
1:B:29:LYS:HD3	2:B:333:HOH:O	1.89	0.71
1:B:198:PRO:HG2	1:B:201:LEU:HB3	1.71	0.71
1:C:124:THR:N	1:C:125:PRO:HD2	2.05	0.71
1:E:169:ALA:O	1:E:171:THR:N	2.24	0.71
1:E:195:MET:HA	1:E:195:MET:CE	2.19	0.71
1:B:124:THR:O	1:B:127:VAL:HG23	1.90	0.71
1:C:185:LEU:HD21	1:C:210:LEU:HD12	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLY:O	1:C:253:LEU:HD13	1.91	0.71
1:E:72:PRO:HG3	1:E:96:ALA:HB1	1.73	0.71
1:A:26:ALA:HB3	1:A:29:LYS:HE2	1.70	0.71
1:C:51:LYS:H	1:C:51:LYS:HD3	1.55	0.71
1:A:211:LEU:HB2	2:A:328:HOH:O	1.90	0.71
1:A:79:LEU:HD11	1:A:104:ILE:HD13	1.71	0.71
1:B:236:GLY:HA2	1:B:239:ILE:HG22	1.71	0.71
1:C:29:LYS:C	1:C:30:ILE:HG13	2.15	0.71
1:D:170:VAL:HG23	2:D:393:HOH:O	1.90	0.71
1:D:185:LEU:HD21	1:D:210:LEU:HD12	1.70	0.71
1:D:211:LEU:HD12	1:D:211:LEU:O	1.91	0.71
1:A:196:GLY:O	1:E:234:PRO:HB3	1.90	0.70
1:C:269:GLN:HG3	1:C:270:SER:H	1.56	0.70
1:B:70:VAL:HG11	1:B:78:ILE:HD11	1.74	0.70
1:B:228:LYS:HA	2:B:339:HOH:O	1.91	0.70
1:C:53:THR:HG22	1:C:55:HIS:H	1.57	0.70
1:D:258:VAL:HG12	1:D:259:GLU:N	2.07	0.70
1:B:5:PHE:CE1	1:B:12:ALA:HA	2.26	0.70
1:E:3:VAL:HG22	1:E:65:VAL:HB	1.73	0.70
1:E:180:TYR:HB2	2:E:391:HOH:O	1.91	0.70
1:C:262:CYS:O	1:C:265:THR:N	2.24	0.70
1:A:128:VAL:HG12	1:A:129:ARG:N	2.07	0.69
1:B:105:GLU:OE2	1:B:139:THR:HB	1.92	0.69
1:D:122:THR:HG23	1:D:133:THR:CB	2.21	0.69
1:D:185:LEU:HD21	1:D:210:LEU:CD1	2.22	0.69
1:A:171:THR:HA	2:A:410:HOH:O	1.93	0.69
1:E:126:VAL:HB	2:E:376:HOH:O	1.91	0.69
1:B:19:PHE:HA	1:B:22:ALA:HB3	1.72	0.69
1:C:4:GLY:O	1:C:66:LEU:HG	1.92	0.69
1:C:101:ILE:HB	1:C:164:GLU:OE1	1.92	0.69
1:C:177:GLY:HA2	1:C:180:TYR:CD1	2.28	0.69
1:B:33:SER:HB2	1:B:59:THR:OG1	1.92	0.69
1:B:256:ASN:C	2:B:336:HOH:O	2.35	0.69
1:E:77:PHE:HD1	1:E:77:PHE:H	1.40	0.69
1:E:31:MET:HG2	1:E:51:LYS:HB2	1.74	0.69
1:D:6:ILE:N	2:D:344:HOH:O	2.26	0.69
1:E:3:VAL:HG13	1:E:65:VAL:O	1.92	0.69
1:A:3:VAL:HG13	1:A:65:VAL:O	1.93	0.69
1:A:215:LYS:HD2	1:A:219:HIS:CE1	2.28	0.69
1:A:233:SER:O	1:A:235:GLY:N	2.26	0.69
1:C:5:PHE:HE2	1:C:15:LEU:HD12	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:GLY:H	1:D:33:SER:HB2	1.57	0.69
1:B:123:ASN:HB2	1:B:125:PRO:HD2	1.75	0.69
1:B:222:GLN:O	1:B:223:HIS:HB2	1.92	0.69
1:C:82:ILE:O	1:C:86:ILE:HG13	1.93	0.69
1:C:204:ARG:HB2	2:C:337:HOH:O	1.92	0.69
1:C:241:ALA:O	1:C:244:VAL:HG12	1.93	0.69
1:E:34:SER:HB3	1:E:54:PRO:HA	1.72	0.69
1:A:222:GLN:HB3	2:A:340:HOH:O	1.93	0.69
1:E:57:LYS:H	1:E:57:LYS:HD3	1.58	0.69
1:C:51:LYS:HE2	2:C:355:HOH:O	1.92	0.68
1:C:240:HIS:CE1	1:D:194:LYS:HE2	2.28	0.68
1:C:92:VAL:HA	2:C:420:HOH:O	1.93	0.68
1:B:3:VAL:N	1:B:30:ILE:HG23	2.06	0.68
1:A:190:ASP:OD1	1:A:199:ARG:NH1	2.26	0.68
1:D:79:LEU:HD21	1:D:104:ILE:HA	1.76	0.68
1:B:200:ARG:NH1	1:B:204:ARG:HH21	1.89	0.68
1:B:258:VAL:HG13	1:B:259:GLU:N	2.09	0.68
1:C:271:MET:HA	1:C:274:GLN:HB3	1.76	0.68
1:E:53:THR:HG22	1:E:55:HIS:N	2.09	0.68
1:B:13:PHE:HB2	1:B:41:THR:HG21	1.76	0.68
1:B:164:GLU:HG3	1:B:167:ILE:HD12	1.76	0.68
1:C:43:SER:O	1:C:46:ARG:HB2	1.94	0.68
1:B:109:SER:OG	1:B:115:PRO:HD2	1.93	0.67
1:C:13:PHE:HE2	1:C:17:LYS:HE3	1.58	0.67
1:C:53:THR:HG21	1:C:58:GLU:HB2	1.76	0.67
1:D:22:ALA:HB3	1:D:24:VAL:HG23	1.77	0.67
1:D:238:THR:HB	1:D:239:ILE:HD12	1.76	0.67
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.60	0.67
1:D:123:ASN:HB2	1:D:125:PRO:HD2	1.76	0.67
1:E:217:LEU:C	1:E:219:HIS:H	2.01	0.67
1:D:118:ILE:HG22	1:D:137:THR:HA	1.76	0.67
1:E:220:SER:CB	1:E:222:GLN:HG2	2.24	0.67
1:B:221:GLU:O	1:B:223:HIS:N	2.27	0.67
1:D:171:THR:HB	2:D:364:HOH:O	1.95	0.67
1:A:141:ALA:HA	2:A:350:HOH:O	1.95	0.67
1:C:251:ARG:O	1:C:252:SER:O	2.13	0.67
1:D:64:ASP:O	1:D:90:HIS:HA	1.94	0.67
1:A:88:ASP:HB3	1:A:112:ARG:HH21	1.59	0.67
1:D:72:PRO:HG3	1:D:96:ALA:HB1	1.77	0.67
1:E:198:PRO:HG2	1:E:201:LEU:HB3	1.77	0.67
1:E:266:ARG:HD2	2:E:388:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:LYS:HB2	2:E:412:HOH:O	1.95	0.67
1:E:68:LEU:HA	2:E:322:HOH:O	1.95	0.67
1:B:78:ILE:HG22	1:B:82:ILE:HD11	1.75	0.66
1:E:9:GLY:N	1:E:41:THR:HG21	2.10	0.66
1:A:20:THR:CG2	1:A:48:MET:HE3	2.25	0.66
1:B:1:MET:HE1	1:B:65:VAL:HG21	1.76	0.66
1:C:41:THR:O	1:C:45:LEU:HB2	1.95	0.66
1:C:173:LEU:HD12	1:C:258:VAL:HG21	1.77	0.66
1:E:3:VAL:HG12	1:E:4:GLY:N	2.08	0.66
1:A:160:THR:HG22	1:A:161:GLU:O	1.95	0.66
1:A:270:SER:HA	1:A:273:ASP:OD2	1.96	0.66
1:B:101:ILE:HD12	1:B:138:GLY:HA2	1.78	0.66
1:C:134:VAL:HG11	1:C:162:VAL:HG22	1.77	0.66
1:B:124:THR:N	1:B:125:PRO:HD2	2.11	0.66
1:C:266:ARG:HD2	2:C:361:HOH:O	1.96	0.66
1:C:7:GLY:HA2	1:C:70:VAL:HG22	1.77	0.66
1:D:37:MET:HA	1:D:42:VAL:HG21	1.76	0.66
1:D:169:ALA:O	1:D:171:THR:N	2.29	0.66
1:A:86:ILE:HD12	1:A:108:LEU:CD1	2.20	0.66
1:B:105:GLU:HG2	1:B:139:THR:OG1	1.94	0.66
1:E:86:ILE:CD1	1:E:108:LEU:HD22	2.25	0.66
1:D:15:LEU:HG	1:D:126:VAL:HG11	1.77	0.66
1:B:67:PHE:CD2	1:B:93:VAL:HB	2.31	0.66
1:C:166:LEU:O	1:C:169:ALA:N	2.29	0.66
1:E:39:LEU:HD23	1:E:39:LEU:H	1.61	0.66
1:A:121:MET:HE3	1:A:171:THR:CG2	2.26	0.66
1:A:156:VAL:HG12	1:A:156:VAL:O	1.95	0.66
1:B:185:LEU:HD21	1:B:210:LEU:CD1	2.26	0.66
1:D:269:GLN:C	1:D:271:MET:H	2.04	0.66
1:A:252:SER:O	1:A:254:LEU:N	2.29	0.65
1:B:108:LEU:HB2	2:B:331:HOH:O	1.94	0.65
1:C:108:LEU:HB2	2:C:377:HOH:O	1.96	0.65
1:A:109:SER:C	1:A:111:PHE:H	2.05	0.65
1:B:198:PRO:HD2	1:B:201:LEU:HD23	1.78	0.65
1:D:66:LEU:HB3	2:D:420:HOH:O	1.97	0.65
1:D:93:VAL:CG1	1:D:118:ILE:HG13	2.26	0.65
1:D:105:GLU:O	1:D:107:LYS:N	2.21	0.65
1:E:179:ALA:HB1	2:E:333:HOH:O	1.96	0.65
1:B:9:GLY:N	1:B:12:ALA:HB3	2.02	0.65
1:C:71:LYS:HE2	1:C:73:HIS:HE1	1.61	0.65
1:A:5:PHE:O	1:A:32:ALA:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:SER:O	1:B:235:GLY:N	2.29	0.65
1:B:236:GLY:O	1:B:238:THR:N	2.29	0.65
1:C:35:PRO:O	1:C:36:ASP:HB2	1.95	0.65
1:D:68:LEU:HD23	1:D:68:LEU:N	2.07	0.65
1:E:75:ILE:HG21	1:E:104:ILE:HD11	1.78	0.65
1:A:61:GLN:O	1:A:89:ARG:NH2	2.30	0.65
1:B:22:ALA:HB2	2:B:323:HOH:O	1.97	0.65
1:C:199:ARG:HD3	2:C:349:HOH:O	1.96	0.65
1:E:197:LEU:HD23	1:E:201:LEU:HD23	1.78	0.65
1:B:122:THR:HG22	1:B:133:THR:CB	2.27	0.65
1:D:124:THR:HG23	2:D:425:HOH:O	1.97	0.65
1:B:176:SER:HB2	2:B:341:HOH:O	1.97	0.65
1:C:198:PRO:HG2	1:C:201:LEU:HB3	1.79	0.65
1:D:53:THR:HG22	1:D:55:HIS:H	1.61	0.65
1:D:109:SER:C	1:D:111:PHE:H	2.05	0.65
1:E:1:MET:HE3	1:E:3:VAL:HG23	1.79	0.65
1:B:75:ILE:CB	1:B:76:PRO:HD3	2.13	0.65
1:C:134:VAL:HG13	1:C:160:THR:O	1.97	0.65
1:D:271:MET:HE2	2:D:395:HOH:O	1.97	0.65
1:E:122:THR:CB	1:E:133:THR:HG22	2.26	0.65
1:E:124:THR:N	1:E:125:PRO:HD2	2.12	0.65
1:A:3:VAL:HG22	2:A:365:HOH:O	1.97	0.65
1:C:221:GLU:OE2	1:C:221:GLU:HA	1.97	0.65
1:E:3:VAL:CG1	1:E:4:GLY:N	2.59	0.65
1:E:220:SER:O	1:E:221:GLU:HB2	1.97	0.65
1:A:128:VAL:HB	2:A:331:HOH:O	1.96	0.64
1:C:3:VAL:HB	1:C:30:ILE:HG12	1.79	0.64
1:C:100:THR:HB	1:C:103:SER:HB2	1.78	0.64
1:E:172:GLY:HA2	1:E:261:SER:CB	2.26	0.64
1:A:65:VAL:HG22	1:A:91:ILE:HD13	1.79	0.64
1:C:101:ILE:HD11	1:C:138:GLY:HA3	1.78	0.64
1:D:70:VAL:CG1	1:D:74:ILE:HB	2.27	0.64
1:A:256:ASN:HB2	2:A:390:HOH:O	1.97	0.64
1:D:192:GLY:O	1:D:197:LEU:HB2	1.96	0.64
1:C:152:LEU:HD12	1:C:152:LEU:O	1.97	0.64
1:A:38:ASP:O	1:A:39:LEU:C	2.40	0.64
1:D:182:PHE:HA	2:D:351:HOH:O	1.96	0.64
1:E:1:MET:HE3	1:E:3:VAL:CG2	2.28	0.64
1:B:15:LEU:O	1:B:19:PHE:CE1	2.51	0.64
1:B:264:ARG:O	1:B:264:ARG:HD2	1.99	0.64
1:E:121:MET:HE3	1:E:121:MET:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ARG:NE	1:C:90:HIS:CD2	2.66	0.63
1:C:118:ILE:HG22	1:C:137:THR:HA	1.79	0.63
1:A:115:PRO:HD2	1:A:140:HIS:CD2	2.32	0.63
1:C:186:ASP:O	1:C:190:ASP:HB2	1.98	0.63
1:C:269:GLN:HG3	1:C:270:SER:N	2.13	0.63
1:A:123:ASN:ND2	1:A:123:ASN:H	1.95	0.63
1:D:204:ARG:HB3	2:D:383:HOH:O	1.97	0.63
1:A:33:SER:O	1:A:35:PRO:HD3	1.98	0.63
1:A:126:VAL:HG13	1:A:156:VAL:HG11	1.79	0.63
1:B:143:VAL:HG12	1:B:144:GLU:N	2.11	0.63
1:E:3:VAL:O	1:E:30:ILE:HA	1.98	0.63
1:A:68:LEU:HB2	1:A:94:SER:HA	1.79	0.63
1:B:70:VAL:HG12	1:B:71:LYS:N	2.13	0.63
1:B:114:ALA:HB1	2:B:393:HOH:O	1.98	0.63
1:B:194:LYS:HG3	2:D:331:HOH:O	1.99	0.63
1:C:65:VAL:HG23	1:C:91:ILE:O	1.98	0.63
1:D:39:LEU:O	1:D:43:SER:HB3	1.98	0.63
1:E:222:GLN:O	1:E:223:HIS:HB3	1.98	0.63
1:A:269:GLN:HG2	1:A:270:SER:N	2.13	0.63
1:B:125:PRO:HG2	1:B:131:GLY:HA2	1.80	0.63
1:C:128:VAL:HG12	1:C:129:ARG:H	1.62	0.63
1:C:262:CYS:O	1:C:265:THR:HG22	1.99	0.63
1:A:45:LEU:HD21	2:A:333:HOH:O	1.99	0.63
1:A:86:ILE:CD1	1:A:108:LEU:HD11	2.20	0.63
1:B:15:LEU:HB3	1:B:19:PHE:CZ	2.33	0.63
1:D:114:ALA:HB1	1:D:140:HIS:CG	2.34	0.63
1:A:153:LEU:CB	1:A:159:CYS:SG	2.84	0.63
1:A:189:ALA:O	1:A:193:VAL:HG23	1.97	0.63
1:D:231:VAL:HG12	2:D:357:HOH:O	1.99	0.63
1:E:101:ILE:CG2	1:E:102:SER:N	2.62	0.63
1:A:135:TYR:CE1	1:A:161:GLU:HG2	2.34	0.63
1:B:101:ILE:HB	2:B:405:HOH:O	1.98	0.63
1:C:79:LEU:HD11	1:C:104:ILE:HG13	1.81	0.63
1:E:56:ASN:O	1:E:60:VAL:HG23	1.97	0.63
1:E:79:LEU:O	1:E:81:GLU:N	2.28	0.63
1:A:198:PRO:HG2	1:A:201:LEU:CB	2.29	0.62
1:B:269:GLN:C	1:B:271:MET:H	2.06	0.62
1:D:60:VAL:HG21	1:D:82:ILE:HG21	1.81	0.62
1:D:89:ARG:HG3	1:D:90:HIS:H	1.63	0.62
1:E:128:VAL:HG12	1:E:128:VAL:O	1.99	0.62
1:D:13:PHE:HZ	1:D:17:LYS:HZ1	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ALA:O	1:D:193:VAL:HG23	1.99	0.62
1:D:239:ILE:N	2:D:435:HOH:O	2.32	0.62
1:C:101:ILE:HD13	1:C:138:GLY:HA3	1.81	0.62
1:E:231:VAL:HG12	2:E:339:HOH:O	1.99	0.62
1:D:128:VAL:O	1:D:129:ARG:HB2	1.99	0.62
1:D:232:SER:HB3	1:D:239:ILE:HG13	1.81	0.62
1:E:25:LEU:HD23	1:E:25:LEU:N	2.12	0.62
1:E:128:VAL:O	1:E:129:ARG:HB3	1.99	0.62
1:E:126:VAL:HA	1:E:129:ARG:O	2.00	0.62
1:E:227:LEU:HD23	2:E:442:HOH:O	1.99	0.62
1:A:15:LEU:HD23	1:A:126:VAL:HG11	1.82	0.62
1:B:198:PRO:HG2	1:B:201:LEU:CB	2.28	0.62
1:C:6:ILE:HG13	1:C:66:LEU:HD11	1.80	0.62
1:D:143:VAL:HB	2:D:349:HOH:O	2.00	0.62
1:D:170:VAL:O	1:D:170:VAL:CG1	2.46	0.62
1:A:198:PRO:HG2	1:A:201:LEU:HB3	1.81	0.62
1:B:11:LEU:O	1:B:15:LEU:HD12	1.99	0.62
1:C:149:MET:C	1:C:151:GLN:H	2.08	0.62
1:C:266:ARG:NH2	2:C:381:HOH:O	2.32	0.62
1:E:47:LYS:HG3	2:E:350:HOH:O	1.98	0.62
1:E:75:ILE:HA	1:E:78:ILE:CD1	2.26	0.62
1:E:96:ALA:HB2	2:E:362:HOH:O	1.98	0.62
1:A:35:PRO:O	1:A:36:ASP:HB2	1.98	0.62
1:B:51:LYS:HG2	2:B:320:HOH:O	2.00	0.62
1:A:55:HIS:C	1:A:57:LYS:H	2.07	0.62
1:B:165:ASP:OD1	1:B:166:LEU:N	2.32	0.62
1:E:6:ILE:HD12	1:E:68:LEU:HD21	1.81	0.62
1:A:223:HIS:ND1	1:A:224:PRO:HD2	2.14	0.61
1:B:74:ILE:O	1:B:78:ILE:HB	1.99	0.61
1:A:123:ASN:HB2	1:A:178:PRO:HG2	1.81	0.61
1:A:6:ILE:HG23	1:A:56:ASN:CB	2.29	0.61
1:E:126:VAL:HG23	2:E:325:HOH:O	1.99	0.61
1:E:227:LEU:O	1:E:231:VAL:HG23	2.00	0.61
1:A:129:ARG:O	1:A:129:ARG:HG2	2.00	0.61
1:E:68:LEU:HB2	1:E:94:SER:CA	2.29	0.61
1:B:101:ILE:HD12	1:B:138:GLY:CA	2.30	0.61
1:E:36:ASP:OD1	1:E:37:MET:N	2.34	0.61
1:E:142:GLN:HB2	1:E:145:ASP:OD2	1.99	0.61
1:A:242:LEU:O	1:A:243:HIS:C	2.44	0.61
1:B:185:LEU:O	1:B:186:ASP:C	2.43	0.61
1:C:105:GLU:HA	2:C:377:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HG2	1:D:2:SER:N	2.16	0.61
1:A:184:ALA:O	1:A:187:ALA:HB3	1.99	0.61
1:C:3:VAL:HG12	1:C:4:GLY:N	2.16	0.61
1:C:3:VAL:HG13	1:C:65:VAL:O	2.00	0.61
1:D:211:LEU:HD12	1:D:211:LEU:C	2.25	0.61
1:E:129:ARG:O	1:E:131:GLY:N	2.34	0.61
1:B:70:VAL:HG22	2:B:364:HOH:O	2.01	0.61
1:C:69:ALA:HB2	2:C:412:HOH:O	2.00	0.61
1:C:93:VAL:HG12	1:C:118:ILE:HG13	1.82	0.61
1:C:217:LEU:O	1:C:220:SER:HB3	2.01	0.61
1:D:162:VAL:CG1	1:D:166:LEU:HB2	2.30	0.61
1:E:220:SER:HB2	1:E:222:GLN:CG	2.30	0.61
1:B:141:ALA:HB1	1:B:145:ASP:OD2	2.01	0.61
1:B:153:LEU:C	1:B:155:SER:H	2.09	0.61
1:D:153:LEU:HB2	1:D:159:CYS:SG	2.40	0.61
1:C:160:THR:HG22	1:C:161:GLU:N	2.16	0.60
1:A:89:ARG:HG3	1:A:90:HIS:N	2.16	0.60
1:B:225:GLY:O	1:B:228:LYS:HB3	2.01	0.60
1:A:16:ALA:C	1:A:48:MET:HE1	2.27	0.60
1:A:31:MET:HE3	1:A:51:LYS:HB3	1.83	0.60
1:C:112:ARG:NH1	1:C:113:PRO:HD2	2.04	0.60
1:C:170:VAL:HB	2:C:401:HOH:O	2.00	0.60
1:D:215:LYS:HG3	1:D:219:HIS:CE1	2.36	0.60
1:E:129:ARG:HG2	1:E:130:GLU:H	1.66	0.60
1:B:211:LEU:C	1:B:211:LEU:HD12	2.26	0.60
1:B:211:LEU:HD12	1:B:211:LEU:O	2.02	0.60
1:E:45:LEU:O	1:E:49:GLY:O	2.18	0.60
1:A:75:ILE:HG22	1:A:76:PRO:CD	2.28	0.60
1:B:2:SER:HA	1:B:30:ILE:CG1	2.30	0.60
1:C:11:LEU:HD12	1:C:14:ALA:HB3	1.82	0.60
1:D:133:THR:HG22	1:D:158:PHE:O	2.00	0.60
1:A:130:GLU:HB2	2:A:331:HOH:O	2.00	0.60
1:C:152:LEU:HD12	1:C:152:LEU:C	2.26	0.60
1:D:87:GLU:HB3	2:D:380:HOH:O	2.02	0.60
1:D:60:VAL:O	1:D:90:HIS:NE2	2.33	0.60
1:B:66:LEU:HB2	1:B:92:VAL:HG22	1.83	0.60
1:C:89:ARG:HE	1:C:90:HIS:CD2	2.17	0.60
1:C:115:PRO:HD2	2:C:379:HOH:O	2.02	0.60
1:A:101:ILE:O	1:A:102:SER:C	2.44	0.60
1:C:3:VAL:HA	1:C:65:VAL:O	2.02	0.60
1:C:51:LYS:HB2	2:C:324:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ARG:O	1:C:203:VAL:HG23	2.01	0.60
1:C:100:THR:HG22	1:C:101:ILE:N	2.16	0.60
1:D:38:ASP:O	1:D:39:LEU:C	2.44	0.60
1:D:44:ALA:HB3	2:D:413:HOH:O	2.02	0.60
1:D:121:MET:HE3	1:D:171:THR:HG23	1.83	0.60
1:D:263:ILE:O	1:D:267:GLU:HG3	2.00	0.60
1:A:77:PHE:N	1:A:77:PHE:CD1	2.70	0.59
1:D:122:THR:HG22	1:D:133:THR:HB	1.81	0.59
1:E:115:PRO:O	1:E:140:HIS:HB2	2.01	0.59
1:E:123:ASN:HB2	1:E:178:PRO:HG2	1.82	0.59
1:D:111:PHE:O	1:D:112:ARG:C	2.45	0.59
1:D:202:ALA:HB1	2:D:350:HOH:O	2.02	0.59
1:B:152:LEU:HD12	1:B:152:LEU:O	2.03	0.59
1:C:87:GLU:H	1:C:90:HIS:HE1	1.49	0.59
1:C:105:GLU:HB2	2:C:366:HOH:O	2.01	0.59
1:D:126:VAL:HG13	1:D:156:VAL:HG11	1.84	0.59
1:E:79:LEU:HD11	1:E:104:ILE:HG12	1.82	0.59
1:E:134:VAL:CG1	1:E:162:VAL:HB	2.32	0.59
1:A:3:VAL:CG1	1:A:4:GLY:H	2.15	0.59
1:D:1:MET:HG2	1:D:2:SER:H	1.68	0.59
1:D:59:THR:O	1:D:62:HIS:N	2.33	0.59
1:A:221:GLU:O	1:A:223:HIS:N	2.33	0.59
1:C:33:SER:HB2	1:C:59:THR:OG1	2.02	0.59
1:D:75:ILE:HD12	1:D:99:VAL:HG21	1.83	0.59
1:B:48:MET:O	1:B:50:VAL:HG23	2.03	0.59
1:E:223:HIS:ND1	1:E:224:PRO:HD2	2.18	0.59
1:C:128:VAL:HG23	2:C:417:HOH:O	2.03	0.59
1:E:68:LEU:N	2:E:358:HOH:O	2.35	0.59
1:E:73:HIS:O	1:E:74:ILE:HG13	2.02	0.59
1:E:79:LEU:HD12	1:E:107:LYS:HD2	1.85	0.59
1:A:222:GLN:O	1:A:223:HIS:CB	2.49	0.59
1:B:118:ILE:HG21	1:B:149:MET:SD	2.42	0.59
1:B:251:ARG:O	1:B:253:LEU:N	2.36	0.59
1:C:171:THR:HB	2:C:360:HOH:O	2.02	0.59
1:C:231:VAL:HG12	1:C:231:VAL:O	2.03	0.59
1:D:60:VAL:HG21	1:D:82:ILE:HD13	1.85	0.59
1:E:59:THR:O	1:E:62:HIS:HB3	2.03	0.59
1:A:194:LYS:O	1:A:195:MET:SD	2.61	0.59
1:A:194:LYS:HG2	1:E:239:ILE:HG23	1.85	0.59
1:B:241:ALA:O	1:B:242:LEU:C	2.44	0.59
1:C:255:ILE:C	1:C:257:ALA:H	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LEU:HD22	1:D:201:LEU:HD23	1.84	0.59
1:C:127:VAL:HG12	1:C:127:VAL:O	2.03	0.59
1:C:147:ARG:O	1:C:151:GLN:HG3	2.03	0.59
1:D:169:ALA:HB3	2:D:393:HOH:O	2.03	0.59
1:D:264:ARG:O	1:D:268:LEU:HB2	2.03	0.59
1:B:189:ALA:HB2	1:B:203:VAL:HA	1.85	0.58
1:E:122:THR:HG22	1:E:133:THR:CG2	2.33	0.58
1:B:71:LYS:HB3	1:B:72:PRO:CD	2.31	0.58
1:A:64:ASP:O	1:A:90:HIS:HB3	2.03	0.58
1:B:4:GLY:HA3	1:B:66:LEU:HD23	1.84	0.58
1:B:89:ARG:HD2	1:B:89:ARG:O	2.02	0.58
1:A:57:LYS:HA	1:A:60:VAL:HG23	1.84	0.58
1:A:77:PHE:N	1:A:77:PHE:HD1	2.00	0.58
1:C:28:HIS:ND1	1:C:51:LYS:HE3	2.17	0.58
1:C:155:SER:HB3	2:C:358:HOH:O	2.02	0.58
1:C:236:GLY:O	1:C:237:ALA:HB3	2.03	0.58
1:D:258:VAL:CG1	1:D:259:GLU:N	2.65	0.58
1:E:187:ALA:HB3	2:E:402:HOH:O	2.03	0.58
1:D:105:GLU:C	1:D:107:LYS:H	2.10	0.58
1:D:117:VAL:O	1:D:138:GLY:HA3	2.04	0.58
1:E:102:SER:O	1:E:103:SER:C	2.43	0.58
1:E:111:PHE:HB3	2:E:386:HOH:O	2.04	0.58
1:A:121:MET:CE	1:A:171:THR:HG22	2.33	0.58
1:B:41:THR:HA	1:B:44:ALA:HB3	1.85	0.58
1:B:83:GLY:HA3	1:B:111:PHE:CD2	2.38	0.58
1:D:210:LEU:O	1:D:211:LEU:C	2.46	0.58
1:E:80:ASP:HA	2:E:327:HOH:O	2.03	0.58
1:A:122:THR:CG2	1:A:123:ASN:N	2.66	0.58
1:B:8:ALA:HA	1:B:12:ALA:HB2	1.85	0.58
1:B:206:GLY:O	1:B:210:LEU:HG	2.04	0.58
1:E:170:VAL:HG12	1:E:170:VAL:O	2.04	0.58
1:B:82:ILE:CG2	1:B:86:ILE:HD11	2.32	0.58
1:E:38:ASP:HB3	1:E:40:ALA:HB3	1.86	0.58
1:A:101:ILE:HG22	1:A:105:GLU:HG3	1.85	0.58
1:A:152:LEU:O	1:A:155:SER:HB3	2.03	0.58
1:D:53:THR:HG22	1:D:55:HIS:N	2.17	0.58
1:A:121:MET:CG	1:A:171:THR:HG23	2.33	0.58
1:B:119:ARG:HB3	2:B:337:HOH:O	2.02	0.58
1:B:72:PRO:HB3	1:B:97:ALA:CB	2.34	0.57
1:C:39:LEU:HA	1:C:43:SER:HB2	1.84	0.57
1:C:86:ILE:HD11	1:C:108:LEU:CD2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLY:C	2:D:435:HOH:O	2.47	0.57
1:D:125:PRO:HB2	1:D:131:GLY:HA2	1.86	0.57
1:D:135:TYR:CE1	1:D:161:GLU:HB2	2.39	0.57
1:B:176:SER:O	1:B:177:GLY:C	2.47	0.57
1:D:143:VAL:C	1:D:145:ASP:H	2.10	0.57
1:A:37:MET:HA	1:A:42:VAL:HG21	1.85	0.57
1:A:121:MET:SD	1:A:171:THR:HG22	2.44	0.57
1:C:234:PRO:O	1:C:235:GLY:C	2.47	0.57
1:C:249:GLY:O	1:C:252:SER:HB2	2.04	0.57
1:E:68:LEU:HD12	1:E:94:SER:HB2	1.85	0.57
1:A:201:LEU:HG	1:A:205:LEU:HD11	1.85	0.57
1:B:2:SER:O	1:B:3:VAL:HG23	2.04	0.57
1:B:42:VAL:C	1:B:44:ALA:H	2.12	0.57
1:B:93:VAL:HG22	1:B:149:MET:HE1	1.86	0.57
1:B:143:VAL:C	1:B:145:ASP:H	2.11	0.57
1:E:180:TYR:O	2:E:372:HOH:O	2.17	0.57
1:A:25:LEU:HG	1:A:26:ALA:H	1.70	0.57
1:A:29:LYS:HG2	2:A:396:HOH:O	2.05	0.57
1:B:45:LEU:O	1:B:48:MET:HB2	2.05	0.57
1:B:87:GLU:C	1:B:89:ARG:H	2.13	0.57
1:B:258:VAL:CG1	1:B:259:GLU:N	2.68	0.57
1:D:164:GLU:HA	1:D:167:ILE:CG1	2.35	0.57
1:E:74:ILE:C	1:E:76:PRO:HD2	2.30	0.57
1:E:193:VAL:HG21	1:E:199:ARG:HD2	1.86	0.57
1:B:17:LYS:C	1:B:20:THR:HG23	2.28	0.57
1:B:72:PRO:HA	2:B:361:HOH:O	2.05	0.57
1:B:94:SER:HA	2:B:324:HOH:O	2.04	0.57
1:D:39:LEU:HA	1:D:43:SER:HB3	1.87	0.57
1:D:121:MET:HE1	1:D:171:THR:HG23	1.83	0.57
1:E:83:GLY:C	1:E:111:PHE:CD2	2.82	0.57
1:B:227:LEU:O	1:B:231:VAL:HG23	2.05	0.57
1:C:31:MET:HB2	1:C:62:HIS:CE1	2.39	0.57
1:D:115:PRO:O	1:D:140:HIS:HB2	2.05	0.57
1:D:118:ILE:CG2	1:D:137:THR:HA	2.34	0.57
1:D:129:ARG:CD	1:D:155:SER:O	2.51	0.57
1:D:146:GLY:O	1:D:149:MET:HB3	2.04	0.57
1:E:101:ILE:HG23	1:E:102:SER:N	2.19	0.57
1:E:233:SER:HB2	2:E:320:HOH:O	2.03	0.57
1:B:199:ARG:HD3	2:D:442:HOH:O	2.04	0.57
1:A:82:ILE:O	1:A:83:GLY:C	2.48	0.57
1:E:166:LEU:O	1:E:168:ASP:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:THR:N	2:A:369:HOH:O	2.36	0.56
1:B:57:LYS:HG3	1:B:58:GLU:N	2.20	0.56
1:B:186:ASP:HA	2:B:358:HOH:O	2.03	0.56
1:D:156:VAL:HG12	1:D:156:VAL:O	2.05	0.56
1:B:63:SER:HB2	1:B:89:ARG:NH1	2.13	0.56
1:C:127:VAL:HA	2:C:418:HOH:O	2.05	0.56
1:D:146:GLY:O	1:D:149:MET:N	2.38	0.56
1:E:35:PRO:HG2	2:E:401:HOH:O	2.05	0.56
1:E:45:LEU:HA	1:E:48:MET:HE3	1.86	0.56
1:E:119:ARG:HA	2:E:445:HOH:O	2.04	0.56
1:A:93:VAL:HG22	1:A:118:ILE:HD11	1.88	0.56
1:A:146:GLY:O	1:A:150:GLU:HB2	2.05	0.56
1:A:177:GLY:O	1:A:178:PRO:C	2.47	0.56
1:A:253:LEU:HD23	1:A:253:LEU:N	2.18	0.56
1:B:11:LEU:HA	1:B:14:ALA:HB3	1.87	0.56
1:B:147:ARG:NH1	1:B:150:GLU:OE2	2.38	0.56
1:C:124:THR:C	1:C:126:VAL:H	2.13	0.56
1:C:135:TYR:HE1	1:C:161:GLU:HB3	1.68	0.56
1:D:6:ILE:HG13	1:D:66:LEU:HD11	1.86	0.56
1:E:14:ALA:HB2	2:E:324:HOH:O	2.04	0.56
1:E:19:PHE:O	1:E:24:VAL:HG23	2.04	0.56
1:E:134:VAL:HG13	1:E:162:VAL:HB	1.86	0.56
1:E:166:LEU:O	1:E:167:ILE:C	2.49	0.56
1:E:264:ARG:CZ	1:E:268:LEU:HD21	2.35	0.56
1:A:64:ASP:O	1:A:90:HIS:CB	2.54	0.56
1:B:112:ARG:HB2	2:B:419:HOH:O	2.04	0.56
1:B:60:VAL:HG12	1:B:89:ARG:HH22	1.71	0.56
1:B:134:VAL:HG12	1:B:135:TYR:N	2.21	0.56
1:B:194:LYS:HG2	1:B:195:MET:HE3	1.87	0.56
1:C:19:PHE:CE2	1:C:152:LEU:HD11	2.40	0.56
1:C:251:ARG:C	1:C:252:SER:O	2.45	0.56
1:D:57:LYS:O	1:D:61:GLN:HG3	2.06	0.56
1:E:38:ASP:O	1:E:42:VAL:HB	2.05	0.56
1:E:126:VAL:O	1:E:156:VAL:HG12	2.05	0.56
1:E:222:GLN:O	1:E:223:HIS:CB	2.53	0.56
1:E:236:GLY:O	1:E:237:ALA:HB3	2.05	0.56
1:A:122:THR:HG22	1:A:123:ASN:N	2.20	0.56
1:A:269:GLN:C	1:A:271:MET:H	2.13	0.56
1:B:74:ILE:HG23	1:B:78:ILE:HG21	1.86	0.56
1:B:112:ARG:HG3	1:B:113:PRO:HD2	1.86	0.56
1:B:216:MET:HA	2:B:372:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:THR:O	1:C:127:VAL:HG23	2.05	0.56
1:E:129:ARG:HG3	1:E:157:GLY:N	2.20	0.56
1:D:94:SER:HA	2:D:422:HOH:O	2.06	0.56
1:E:45:LEU:HD23	1:E:48:MET:HE1	1.86	0.56
1:E:185:LEU:HD21	1:E:210:LEU:HD12	1.87	0.56
1:A:82:ILE:O	1:A:82:ILE:HG22	2.05	0.56
1:A:40:ALA:O	1:A:44:ALA:HB2	2.06	0.56
1:B:119:ARG:HD3	1:B:167:ILE:CD1	2.36	0.56
1:B:129:ARG:O	1:B:129:ARG:HD3	2.05	0.56
1:B:239:ILE:N	2:B:338:HOH:O	2.38	0.56
1:B:258:VAL:CG1	1:B:259:GLU:H	2.19	0.56
1:D:192:GLY:HA3	2:D:350:HOH:O	2.05	0.56
1:C:71:LYS:HE2	1:C:73:HIS:CE1	2.41	0.56
1:C:122:THR:HG22	1:C:133:THR:CB	2.35	0.56
1:D:93:VAL:HA	1:D:118:ILE:O	2.06	0.56
1:D:232:SER:HB3	1:D:239:ILE:CG1	2.36	0.56
1:C:45:LEU:CD2	1:C:50:VAL:HB	2.36	0.55
1:A:82:ILE:HG23	1:A:85:ASP:HB2	1.88	0.55
1:B:195:MET:HA	1:B:195:MET:CE	2.29	0.55
1:C:25:LEU:HD21	1:C:30:ILE:HD11	1.88	0.55
1:C:162:VAL:HB	1:C:166:LEU:HD12	1.87	0.55
1:E:6:ILE:HD12	1:E:68:LEU:CD2	2.36	0.55
1:D:34:SER:HB2	1:D:36:ASP:O	2.07	0.55
1:E:188:LEU:N	2:E:402:HOH:O	2.39	0.55
1:B:123:ASN:O	1:B:126:VAL:HG23	2.07	0.55
1:D:33:SER:O	1:D:35:PRO:HD2	2.06	0.55
1:A:33:SER:CB	1:A:56:ASN:HB3	2.36	0.55
1:C:31:MET:HB3	1:C:59:THR:CG2	2.32	0.55
1:D:128:VAL:O	1:D:129:ARG:CB	2.53	0.55
1:E:14:ALA:HB1	2:E:376:HOH:O	2.06	0.55
1:A:119:ARG:HD3	1:A:164:GLU:HG3	1.87	0.55
1:B:37:MET:SD	1:B:46:ARG:NH2	2.73	0.55
1:C:45:LEU:HD23	1:C:50:VAL:HB	1.88	0.55
1:E:42:VAL:O	1:E:43:SER:C	2.49	0.55
1:C:123:ASN:O	1:C:126:VAL:HG13	2.07	0.55
1:E:75:ILE:CA	1:E:78:ILE:HD12	2.29	0.55
1:C:128:VAL:CG1	1:C:129:ARG:N	2.69	0.55
1:D:5:PHE:CD2	1:D:67:PHE:HB2	2.42	0.55
1:D:107:LYS:HD2	2:D:329:HOH:O	2.07	0.55
1:E:80:ASP:OD2	1:E:107:LYS:NZ	2.35	0.55
1:E:126:VAL:HG22	1:E:131:GLY:HA3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LYS:HE2	1:D:85:ASP:OD2	2.07	0.55
1:B:139:THR:HG22	1:B:139:THR:O	2.07	0.55
1:B:239:ILE:HG21	2:E:363:HOH:O	2.05	0.55
1:B:13:PHE:HB2	1:B:41:THR:CG2	2.37	0.54
1:B:199:ARG:NH2	2:B:358:HOH:O	2.39	0.54
1:C:88:ASP:N	2:C:352:HOH:O	2.39	0.54
1:D:37:MET:HE3	1:D:42:VAL:CG1	2.35	0.54
1:E:5:PHE:O	1:E:32:ALA:HA	2.07	0.54
1:A:274:GLN:HB2	2:A:353:HOH:O	2.07	0.54
1:C:255:ILE:C	1:C:257:ALA:N	2.65	0.54
1:B:123:ASN:CB	1:B:125:PRO:HD2	2.37	0.54
1:C:83:GLY:HA2	1:C:86:ILE:CD1	2.37	0.54
1:D:89:ARG:NH2	2:D:370:HOH:O	2.40	0.54
1:D:121:MET:HE2	2:D:376:HOH:O	2.07	0.54
1:D:143:VAL:C	1:D:145:ASP:N	2.65	0.54
1:E:6:ILE:O	1:E:70:VAL:HG22	2.07	0.54
1:A:126:VAL:O	1:A:128:VAL:N	2.40	0.54
1:C:11:LEU:CD1	1:C:124:THR:HA	2.37	0.54
1:D:217:LEU:HD12	1:D:217:LEU:O	2.07	0.54
1:E:137:THR:HG23	2:E:330:HOH:O	2.05	0.54
1:C:15:LEU:O	1:C:19:PHE:CD1	2.61	0.54
1:C:109:SER:HA	1:C:115:PRO:CD	2.37	0.54
1:C:119:ARG:HG3	2:C:351:HOH:O	2.08	0.54
1:D:125:PRO:O	1:D:128:VAL:HG12	2.07	0.54
1:E:29:LYS:C	1:E:30:ILE:HG13	2.32	0.54
1:E:97:ALA:HB1	1:E:265:THR:HG23	1.89	0.54
1:E:205:LEU:HD23	2:E:408:HOH:O	2.08	0.54
1:A:88:ASP:HB2	1:A:112:ARG:NH2	2.22	0.54
1:A:149:MET:HA	1:A:149:MET:CE	2.37	0.54
1:B:73:HIS:C	1:B:75:ILE:H	2.15	0.54
1:B:180:TYR:N	1:B:180:TYR:CD2	2.75	0.54
1:B:239:ILE:HD11	1:E:190:ASP:O	2.08	0.54
1:C:78:ILE:HD11	2:C:380:HOH:O	2.07	0.54
1:C:194:LYS:HA	2:C:344:HOH:O	2.08	0.54
1:D:26:ALA:HB3	1:D:28:HIS:CD2	2.42	0.54
1:D:241:ALA:O	1:D:244:VAL:N	2.38	0.54
1:A:30:ILE:HG22	1:A:31:MET:N	2.23	0.54
1:A:233:SER:C	1:A:235:GLY:H	2.14	0.54
1:C:3:VAL:C	1:C:30:ILE:HG23	2.33	0.54
1:C:236:GLY:HA3	1:C:240:HIS:HD2	1.73	0.54
1:D:166:LEU:O	1:D:167:ILE:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LEU:HB2	2:D:419:HOH:O	2.08	0.54
1:E:1:MET:HG2	1:E:2:SER:N	2.23	0.54
1:A:112:ARG:HG3	2:A:407:HOH:O	2.08	0.54
1:B:75:ILE:CD1	1:B:272:ALA:HA	2.38	0.54
1:C:65:VAL:O	1:C:65:VAL:HG13	2.08	0.54
1:C:252:SER:HB3	2:C:321:HOH:O	2.07	0.54
1:C:262:CYS:HA	2:C:360:HOH:O	2.08	0.54
1:D:107:LYS:HB3	2:D:329:HOH:O	2.07	0.54
1:D:199:ARG:O	1:D:200:ARG:C	2.49	0.54
1:E:55:HIS:CB	1:E:57:LYS:HE2	2.34	0.54
1:E:126:VAL:N	2:E:325:HOH:O	2.41	0.54
1:C:61:GLN:C	1:C:63:SER:H	2.14	0.54
1:D:226:GLN:O	1:D:229:ASP:HB2	2.08	0.54
1:B:12:ALA:O	1:B:16:ALA:HB2	2.08	0.54
1:B:105:GLU:HG2	2:B:417:HOH:O	2.08	0.54
1:C:266:ARG:HA	2:C:323:HOH:O	2.08	0.54
1:D:6:ILE:HG21	1:D:78:ILE:HG21	1.88	0.54
1:E:217:LEU:O	1:E:219:HIS:N	2.40	0.54
1:A:39:LEU:O	1:A:40:ALA:C	2.51	0.53
1:A:68:LEU:HD12	1:A:94:SER:HB2	1.90	0.53
1:B:126:VAL:HA	2:B:328:HOH:O	2.08	0.53
1:B:251:ARG:O	1:B:252:SER:C	2.50	0.53
1:C:78:ILE:O	1:C:82:ILE:HG13	2.07	0.53
1:C:129:ARG:O	1:C:129:ARG:HG2	2.08	0.53
1:D:16:ALA:C	1:D:48:MET:HE1	2.33	0.53
1:D:98:GLY:HA2	2:D:336:HOH:O	2.07	0.53
1:A:88:ASP:CB	1:A:112:ARG:NH2	2.68	0.53
1:A:88:ASP:HB2	1:A:112:ARG:HE	1.73	0.53
1:A:123:ASN:HD22	1:A:123:ASN:N	1.94	0.53
1:C:3:VAL:HG22	1:C:65:VAL:HG13	1.90	0.53
1:C:66:LEU:N	2:C:420:HOH:O	2.40	0.53
1:D:265:THR:HG22	2:D:377:HOH:O	2.07	0.53
1:E:11:LEU:O	1:E:15:LEU:HD12	2.07	0.53
1:E:13:PHE:O	1:E:16:ALA:HB3	2.09	0.53
1:E:86:ILE:O	1:E:112:ARG:HD3	2.08	0.53
1:A:226:GLN:HB3	2:A:340:HOH:O	2.08	0.53
1:B:18:GLY:O	1:B:19:PHE:C	2.52	0.53
1:C:104:ILE:HG22	1:C:117:VAL:HG21	1.90	0.53
1:C:171:THR:O	1:C:175:GLY:HA3	2.09	0.53
1:C:223:HIS:ND1	1:C:224:PRO:CD	2.70	0.53
1:D:30:ILE:HB	1:D:50:VAL:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:LEU:C	1:E:219:HIS:N	2.67	0.53
1:B:1:MET:SD	1:B:2:SER:O	2.67	0.53
1:B:2:SER:CA	1:B:30:ILE:HG12	2.39	0.53
1:D:82:ILE:HG23	1:D:85:ASP:HB2	1.89	0.53
1:D:98:GLY:HA3	1:D:269:GLN:CB	2.37	0.53
1:D:222:GLN:O	1:D:223:HIS:HB3	2.08	0.53
1:E:55:HIS:HB3	1:E:57:LYS:CG	2.37	0.53
1:E:253:LEU:O	1:E:256:ASN:HB2	2.08	0.53
1:B:75:ILE:HD11	1:B:272:ALA:HA	1.91	0.53
1:B:255:ILE:HG22	1:B:255:ILE:O	2.09	0.53
1:C:29:LYS:O	1:C:30:ILE:HG13	2.09	0.53
1:C:75:ILE:N	1:C:76:PRO:CD	2.71	0.53
1:D:89:ARG:HG3	1:D:90:HIS:N	2.22	0.53
1:D:119:ARG:HB3	1:D:136:ALA:HB3	1.90	0.53
1:A:124:THR:N	1:A:125:PRO:HD2	2.24	0.53
1:A:167:ILE:O	1:A:167:ILE:HG22	2.09	0.53
1:B:63:SER:CB	1:B:89:ARG:HH12	2.15	0.53
1:C:173:LEU:HA	1:C:258:VAL:HG22	1.91	0.53
1:E:33:SER:O	1:E:35:PRO:HD2	2.09	0.53
1:B:12:ALA:O	1:B:16:ALA:N	2.41	0.53
1:B:233:SER:C	1:B:235:GLY:N	2.65	0.53
1:C:14:ALA:HB1	1:C:126:VAL:HG23	1.91	0.53
1:C:34:SER:O	1:C:36:ASP:N	2.41	0.53
1:E:113:PRO:HD2	2:E:342:HOH:O	2.07	0.53
1:A:193:VAL:HG13	1:E:234:PRO:HA	1.91	0.53
1:B:257:ALA:HA	2:B:418:HOH:O	2.08	0.53
1:C:33:SER:HA	1:C:53:THR:O	2.09	0.53
1:D:13:PHE:CZ	1:D:17:LYS:NZ	2.77	0.53
1:A:135:TYR:CD1	1:A:135:TYR:C	2.86	0.53
1:C:51:LYS:HD3	1:C:51:LYS:N	2.23	0.53
1:C:53:THR:HG23	1:C:58:GLU:OE2	2.09	0.53
1:C:57:LYS:O	1:C:60:VAL:HG23	2.07	0.53
1:D:77:PHE:HD1	1:D:77:PHE:N	2.06	0.53
1:E:117:VAL:O	1:E:138:GLY:HA3	2.09	0.53
1:E:211:LEU:HD13	1:E:211:LEU:C	2.34	0.53
1:B:2:SER:OG	1:B:30:ILE:HA	2.09	0.53
1:C:7:GLY:HA3	1:C:69:ALA:C	2.34	0.53
1:E:75:ILE:CG2	1:E:104:ILE:HD11	2.38	0.53
1:A:185:LEU:N	1:A:185:LEU:HD23	2.23	0.52
1:A:190:ASP:O	1:E:239:ILE:HD11	2.09	0.52
1:E:28:HIS:HB3	2:E:407:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:SER:C	1:B:235:GLY:H	2.17	0.52
1:C:61:GLN:N	1:C:61:GLN:OE1	2.42	0.52
1:E:162:VAL:HG12	1:E:163:GLU:O	2.09	0.52
1:A:124:THR:C	1:A:126:VAL:H	2.17	0.52
1:A:227:LEU:N	2:A:340:HOH:O	2.41	0.52
1:B:93:VAL:HG12	1:B:95:CYS:SG	2.50	0.52
1:C:3:VAL:O	1:C:30:ILE:HA	2.08	0.52
1:E:264:ARG:NE	1:E:268:LEU:HD21	2.24	0.52
1:A:93:VAL:HG22	1:A:118:ILE:CD1	2.39	0.52
1:B:123:ASN:HA	2:B:398:HOH:O	2.08	0.52
1:B:147:ARG:O	1:B:147:ARG:HG3	2.08	0.52
1:E:177:GLY:O	1:E:180:TYR:N	2.42	0.52
1:E:208:GLN:HB3	2:E:408:HOH:O	2.10	0.52
1:C:128:VAL:C	1:C:130:GLU:H	2.17	0.52
1:C:211:LEU:CD1	1:C:211:LEU:C	2.82	0.52
1:D:1:MET:HE3	1:D:3:VAL:HG23	1.91	0.52
1:D:13:PHE:CE1	1:D:17:LYS:HE3	2.43	0.52
1:D:103:SER:HA	2:D:342:HOH:O	2.10	0.52
1:D:123:ASN:O	1:D:126:VAL:HG23	2.10	0.52
1:D:233:SER:O	1:D:235:GLY:N	2.42	0.52
1:E:79:LEU:C	1:E:81:GLU:H	2.18	0.52
1:A:194:LYS:C	2:E:356:HOH:O	2.53	0.52
1:D:129:ARG:HA	1:D:156:VAL:HG13	1.92	0.52
1:D:164:GLU:HA	1:D:167:ILE:HG12	1.91	0.52
1:E:123:ASN:HB2	1:E:125:PRO:HD2	1.91	0.52
1:A:75:ILE:CG2	1:A:76:PRO:HD3	2.32	0.52
1:A:79:LEU:CD1	1:A:104:ILE:HA	2.39	0.52
1:A:256:ASN:N	2:A:390:HOH:O	2.43	0.52
1:B:45:LEU:HD22	1:B:48:MET:SD	2.50	0.52
1:B:79:LEU:CD1	1:B:104:ILE:HG23	2.36	0.52
1:C:112:ARG:CG	1:C:113:PRO:HD2	2.33	0.52
1:D:77:PHE:N	1:D:77:PHE:CD1	2.77	0.52
1:E:70:VAL:O	1:E:71:LYS:HB2	2.10	0.52
1:A:121:MET:CG	1:A:171:THR:CG2	2.88	0.52
1:B:50:VAL:HB	2:B:350:HOH:O	2.08	0.52
1:B:89:ARG:HD2	1:B:89:ARG:C	2.35	0.52
1:B:258:VAL:HG13	1:B:259:GLU:H	1.75	0.52
1:C:123:ASN:C	1:C:125:PRO:HD2	2.34	0.52
1:C:160:THR:CG2	1:C:161:GLU:N	2.73	0.52
1:D:133:THR:CG2	1:D:158:PHE:O	2.58	0.52
1:A:258:VAL:HG12	1:A:259:GLU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ASN:C	1:B:125:PRO:HD2	2.35	0.52
1:D:82:ILE:C	1:D:84:ALA:N	2.63	0.52
1:A:199:ARG:O	1:A:203:VAL:HG23	2.10	0.52
1:B:28:HIS:HA	2:B:320:HOH:O	2.09	0.52
1:C:3:VAL:HG12	1:C:4:GLY:H	1.75	0.52
1:C:4:GLY:HA2	1:C:30:ILE:HG23	1.92	0.52
1:C:27:ALA:HB1	1:C:50:VAL:HG22	1.92	0.52
1:C:173:LEU:CD1	1:C:258:VAL:HG21	2.40	0.52
1:E:162:VAL:CG1	1:E:166:LEU:HB2	2.39	0.52
1:C:262:CYS:O	1:C:263:ILE:C	2.54	0.51
1:D:67:PHE:CE2	1:D:93:VAL:HG21	2.45	0.51
1:E:129:ARG:O	1:E:130:GLU:C	2.52	0.51
1:B:70:VAL:HG11	1:B:78:ILE:CD1	2.39	0.51
1:B:101:ILE:O	1:B:105:GLU:HB2	2.10	0.51
1:C:169:ALA:O	1:C:170:VAL:C	2.51	0.51
1:A:33:SER:HA	1:A:53:THR:O	2.09	0.51
1:A:233:SER:C	1:A:235:GLY:N	2.69	0.51
1:B:1:MET:HG3	1:B:2:SER:N	2.25	0.51
1:B:119:ARG:HG2	1:B:120:CYS:N	2.25	0.51
1:C:35:PRO:O	1:C:36:ASP:CB	2.59	0.51
1:C:211:LEU:C	1:C:211:LEU:HD13	2.36	0.51
1:D:183:THR:N	2:D:415:HOH:O	2.43	0.51
1:D:258:VAL:O	1:D:259:GLU:C	2.51	0.51
1:E:8:ALA:HB1	1:E:41:THR:CG2	2.41	0.51
1:A:55:HIS:HA	2:A:374:HOH:O	2.11	0.51
1:D:153:LEU:N	1:D:153:LEU:HD23	2.25	0.51
1:D:252:SER:O	1:D:255:ILE:N	2.43	0.51
1:E:57:LYS:H	1:E:57:LYS:CD	2.18	0.51
1:A:102:SER:O	1:A:103:SER:C	2.54	0.51
1:B:4:GLY:HA3	1:B:66:LEU:CD2	2.40	0.51
1:C:66:LEU:C	1:C:66:LEU:HD23	2.36	0.51
1:C:269:GLN:C	1:C:271:MET:H	2.18	0.51
1:D:50:VAL:HG13	1:D:51:LYS:N	2.26	0.51
1:E:126:VAL:O	1:E:156:VAL:CG1	2.59	0.51
1:E:255:ILE:O	1:E:256:ASN:C	2.53	0.51
1:E:264:ARG:NH2	1:E:268:LEU:HD21	2.25	0.51
1:A:193:VAL:C	1:A:195:MET:H	2.17	0.51
1:B:124:THR:N	1:B:125:PRO:CD	2.73	0.51
1:C:55:HIS:C	1:C:57:LYS:H	2.19	0.51
1:E:134:VAL:HG21	1:E:170:VAL:HG11	1.91	0.51
1:C:149:MET:O	1:C:151:GLN:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLY:O	1:D:99:VAL:C	2.54	0.51
1:E:4:GLY:HA2	1:E:31:MET:O	2.11	0.51
1:E:114:ALA:HB1	1:E:140:HIS:ND1	2.25	0.51
1:E:264:ARG:O	1:E:268:LEU:HG	2.11	0.51
1:A:252:SER:C	1:A:254:LEU:H	2.18	0.51
1:B:39:LEU:HA	1:B:43:SER:HB2	1.93	0.51
1:B:45:LEU:O	1:B:46:ARG:C	2.53	0.51
1:B:266:ARG:O	1:B:269:GLN:HG2	2.11	0.51
1:C:50:VAL:HG13	2:C:343:HOH:O	2.10	0.51
1:D:142:GLN:HB3	2:D:375:HOH:O	2.11	0.51
1:E:119:ARG:NE	2:E:349:HOH:O	2.44	0.51
1:A:126:VAL:C	1:A:128:VAL:H	2.18	0.51
1:A:135:TYR:OH	1:A:150:GLU:CG	2.59	0.51
1:A:176:SER:O	1:A:179:ALA:N	2.40	0.51
1:B:13:PHE:O	1:B:16:ALA:HB3	2.11	0.51
1:C:13:PHE:O	1:C:16:ALA:HB3	2.11	0.51
1:C:208:GLN:HB2	2:C:354:HOH:O	2.11	0.51
1:C:258:VAL:O	1:C:258:VAL:CG1	2.47	0.51
1:D:82:ILE:O	1:D:85:ASP:N	2.44	0.51
1:D:172:GLY:C	1:D:258:VAL:HG22	2.36	0.51
1:E:8:ALA:HB1	1:E:41:THR:HG21	1.92	0.51
1:E:233:SER:N	2:E:320:HOH:O	2.43	0.51
1:E:250:PHE:N	2:E:341:HOH:O	2.44	0.51
1:C:105:GLU:O	1:C:109:SER:HB2	2.11	0.51
1:D:81:GLU:O	1:D:81:GLU:HG2	2.09	0.51
1:E:135:TYR:CZ	1:E:161:GLU:HB3	2.46	0.51
1:A:4:GLY:HA2	1:A:31:MET:O	2.10	0.50
1:A:6:ILE:HB	2:A:322:HOH:O	2.10	0.50
1:A:105:GLU:O	1:A:107:LYS:N	2.42	0.50
1:B:6:ILE:HB	2:B:325:HOH:O	2.11	0.50
1:C:210:LEU:O	1:C:211:LEU:C	2.54	0.50
1:E:15:LEU:HB3	1:E:19:PHE:CE1	2.46	0.50
1:E:99:VAL:HG12	1:E:99:VAL:O	2.11	0.50
1:A:24:VAL:HG21	1:A:155:SER:OG	2.11	0.50
1:B:184:ALA:O	1:B:188:LEU:HG	2.10	0.50
1:B:189:ALA:C	2:B:382:HOH:O	2.54	0.50
1:C:9:GLY:O	1:C:10:GLN:C	2.53	0.50
1:B:19:PHE:CD2	1:B:152:LEU:HD11	2.47	0.50
1:B:72:PRO:HB3	1:B:97:ALA:HB2	1.92	0.50
1:B:73:HIS:C	1:B:75:ILE:N	2.67	0.50
1:B:76:PRO:C	1:B:78:ILE:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:C	1:B:106:LYS:H	2.19	0.50
1:B:161:GLU:O	1:B:162:VAL:CG2	2.59	0.50
2:B:400:HOH:O	1:E:194:LYS:HE3	2.11	0.50
1:E:13:PHE:O	1:E:14:ALA:C	2.54	0.50
1:E:45:LEU:O	1:E:50:VAL:HB	2.11	0.50
1:E:60:VAL:CG2	1:E:82:ILE:HD13	2.39	0.50
1:E:153:LEU:C	1:E:155:SER:N	2.69	0.50
1:E:176:SER:O	1:E:177:GLY:C	2.55	0.50
1:A:93:VAL:HG22	1:A:118:ILE:HG13	1.94	0.50
1:A:125:PRO:HG2	1:A:131:GLY:HA2	1.92	0.50
1:B:101:ILE:HG12	1:B:164:GLU:OE1	2.11	0.50
1:B:121:MET:O	1:B:133:THR:CB	2.54	0.50
1:B:188:LEU:C	1:B:190:ASP:H	2.19	0.50
1:D:74:ILE:O	1:D:75:ILE:C	2.54	0.50
1:D:255:ILE:O	1:D:256:ASN:C	2.55	0.50
1:A:57:LYS:HA	1:A:60:VAL:CG2	2.41	0.50
1:B:121:MET:SD	1:B:122:THR:N	2.83	0.50
1:E:124:THR:O	1:E:126:VAL:N	2.44	0.50
1:E:249:GLY:O	1:E:252:SER:HB3	2.12	0.50
1:B:222:GLN:O	1:B:223:HIS:CB	2.58	0.50
1:C:269:GLN:O	1:C:272:ALA:N	2.45	0.50
1:E:49:GLY:O	1:E:50:VAL:O	2.30	0.50
1:E:89:ARG:O	1:E:116:ARG:NH2	2.42	0.50
1:A:1:MET:HG2	1:A:2:SER:N	2.27	0.50
1:A:123:ASN:ND2	1:A:123:ASN:N	2.50	0.50
1:C:124:THR:N	1:C:125:PRO:CD	2.74	0.50
1:E:18:GLY:HA3	1:E:156:VAL:HG11	1.94	0.50
1:C:25:LEU:HD21	1:C:30:ILE:CD1	2.42	0.50
1:C:262:CYS:SG	1:C:263:ILE:N	2.85	0.50
1:A:10:GLN:O	1:A:11:LEU:C	2.55	0.50
1:A:84:ALA:C	1:A:86:ILE:H	2.20	0.50
1:B:105:GLU:OE2	1:B:117:VAL:HB	2.11	0.50
1:B:220:SER:O	1:B:221:GLU:HB2	2.12	0.50
1:E:121:MET:HE2	1:E:122:THR:H	1.77	0.50
1:E:122:THR:CG2	1:E:133:THR:CG2	2.89	0.50
1:D:15:LEU:HA	1:D:126:VAL:HG11	1.93	0.49
1:A:8:ALA:HA	1:A:12:ALA:CB	2.42	0.49
1:B:45:LEU:HB3	2:B:350:HOH:O	2.11	0.49
1:B:172:GLY:O	1:B:258:VAL:HA	2.12	0.49
1:C:71:LYS:NZ	1:C:74:ILE:HD12	2.26	0.49
1:D:258:VAL:HG12	1:D:259:GLU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:LEU:N	1:E:25:LEU:CD2	2.75	0.49
1:B:228:LYS:HE2	1:B:229:ASP:OD1	2.12	0.49
1:C:198:PRO:HG2	1:C:201:LEU:CB	2.42	0.49
1:E:102:SER:C	1:E:104:ILE:N	2.67	0.49
1:B:71:LYS:H	1:B:71:LYS:HD2	1.77	0.49
1:B:193:VAL:N	2:B:382:HOH:O	2.44	0.49
1:C:86:ILE:HB	1:C:112:ARG:HB2	1.93	0.49
1:D:189:ALA:CB	1:D:203:VAL:HG23	2.42	0.49
1:A:186:ASP:HA	2:A:424:HOH:O	2.12	0.49
1:B:134:VAL:HG22	2:B:334:HOH:O	2.12	0.49
1:B:216:MET:HG3	2:B:372:HOH:O	2.12	0.49
1:B:236:GLY:O	1:B:237:ALA:HB3	2.12	0.49
1:B:262:CYS:HA	2:B:343:HOH:O	2.13	0.49
1:C:252:SER:O	1:C:253:LEU:C	2.54	0.49
1:C:271:MET:HA	1:C:274:GLN:CB	2.41	0.49
1:D:134:VAL:HA	2:D:384:HOH:O	2.11	0.49
1:D:194:LYS:HG2	1:D:194:LYS:O	2.12	0.49
1:D:204:ARG:HD3	2:D:404:HOH:O	2.11	0.49
1:E:149:MET:O	1:E:152:LEU:HB3	2.12	0.49
1:E:172:GLY:HA2	1:E:261:SER:HB3	1.93	0.49
1:A:197:LEU:HD22	1:A:201:LEU:HD23	1.94	0.49
1:B:168:ASP:HB2	2:B:375:HOH:O	2.12	0.49
1:C:152:LEU:HG	1:C:153:LEU:HG	1.95	0.49
1:E:22:ALA:HB3	1:E:24:VAL:HG23	1.94	0.49
1:A:65:VAL:HB	2:A:365:HOH:O	2.12	0.49
1:A:199:ARG:NH2	2:A:424:HOH:O	2.45	0.49
1:C:3:VAL:O	1:C:30:ILE:HG23	2.13	0.49
1:C:144:GLU:C	1:C:146:GLY:H	2.21	0.49
1:C:239:ILE:HD13	1:D:193:VAL:HG12	1.94	0.49
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.77	0.49
1:D:3:VAL:HG11	1:D:67:PHE:CE1	2.47	0.49
1:D:80:ASP:C	1:D:82:ILE:H	2.21	0.49
1:D:124:THR:O	1:D:126:VAL:N	2.46	0.49
1:A:100:THR:HG23	1:A:164:GLU:OE1	2.13	0.49
1:B:28:HIS:C	1:B:30:ILE:H	2.20	0.49
1:B:190:ASP:CG	1:B:199:ARG:HH12	2.21	0.49
1:C:46:ARG:O	1:C:48:MET:N	2.46	0.49
1:A:60:VAL:CG2	1:A:82:ILE:HD13	2.43	0.49
1:A:185:LEU:HA	1:A:188:LEU:HD12	1.94	0.49
1:A:239:ILE:N	2:A:369:HOH:O	2.46	0.49
1:D:38:ASP:OD2	1:D:40:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ASP:C	1:D:82:ILE:N	2.70	0.49
1:E:34:SER:HB3	1:E:54:PRO:CA	2.41	0.49
1:E:68:LEU:HB2	1:E:94:SER:CB	2.43	0.49
1:A:13:PHE:HA	2:A:333:HOH:O	2.13	0.49
1:C:7:GLY:HA3	1:C:69:ALA:O	2.13	0.49
1:D:69:ALA:N	2:D:344:HOH:O	2.25	0.49
1:E:227:LEU:HA	2:E:442:HOH:O	2.13	0.49
1:A:82:ILE:O	1:A:86:ILE:HG13	2.13	0.48
1:A:101:ILE:O	1:A:104:ILE:N	2.45	0.48
1:B:41:THR:HG22	2:B:367:HOH:O	2.12	0.48
1:B:71:LYS:CB	1:B:73:HIS:CE1	2.91	0.48
1:B:75:ILE:HD11	1:B:272:ALA:CB	2.43	0.48
1:C:112:ARG:HH11	1:C:112:ARG:HG3	1.77	0.48
1:C:148:LEU:HA	1:C:151:GLN:OE1	2.13	0.48
1:D:74:ILE:HG22	1:D:78:ILE:HG13	1.94	0.48
1:D:168:ASP:HB2	2:D:423:HOH:O	2.12	0.48
1:E:125:PRO:C	1:E:127:VAL:N	2.67	0.48
1:A:36:ASP:O	1:A:37:MET:CB	2.60	0.48
1:B:38:ASP:HB3	1:B:42:VAL:HB	1.94	0.48
1:B:41:THR:CA	1:B:44:ALA:HB3	2.43	0.48
1:B:94:SER:O	1:B:94:SER:OG	2.22	0.48
1:C:13:PHE:HE1	1:C:44:ALA:HB3	1.78	0.48
1:C:128:VAL:CG1	1:C:129:ARG:H	2.26	0.48
1:D:70:VAL:HG21	1:D:78:ILE:CD1	2.43	0.48
1:D:222:GLN:HG3	1:D:227:LEU:HD21	1.96	0.48
1:D:264:ARG:NE	2:D:321:HOH:O	2.29	0.48
1:E:144:GLU:HB3	2:E:352:HOH:O	2.13	0.48
1:A:104:ILE:O	1:A:105:GLU:C	2.56	0.48
1:A:178:PRO:O	1:A:181:ALA:HB3	2.14	0.48
1:B:119:ARG:HD2	1:B:164:GLU:OE2	2.13	0.48
1:C:67:PHE:HA	1:C:93:VAL:HG23	1.95	0.48
1:D:102:SER:HA	2:D:337:HOH:O	2.12	0.48
1:E:77:PHE:N	1:E:77:PHE:CD1	2.80	0.48
1:E:141:ALA:O	1:E:142:GLN:O	2.31	0.48
1:A:176:SER:HB3	1:A:180:TYR:CE2	2.48	0.48
1:B:3:VAL:HG13	1:B:65:VAL:O	2.14	0.48
1:C:102:SER:HB3	1:C:106:LYS:HG3	1.94	0.48
1:C:173:LEU:HB3	2:C:437:HOH:O	2.12	0.48
1:E:122:THR:CG2	1:E:133:THR:HG22	2.43	0.48
1:A:26:ALA:CB	1:A:29:LYS:HE2	2.40	0.48
1:A:98:GLY:O	1:A:269:GLN:OE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLU:OE1	1:B:117:VAL:HG21	2.13	0.48
1:B:166:LEU:O	1:B:169:ALA:N	2.44	0.48
1:B:183:THR:HA	2:B:388:HOH:O	2.12	0.48
1:C:11:LEU:HD12	1:C:14:ALA:CB	2.44	0.48
1:C:61:GLN:C	1:C:63:SER:N	2.66	0.48
1:E:77:PHE:O	1:E:78:ILE:C	2.56	0.48
1:E:185:LEU:HD21	1:E:210:LEU:CD1	2.44	0.48
1:A:10:GLN:O	1:A:12:ALA:N	2.46	0.48
1:A:127:VAL:HG12	1:A:127:VAL:O	2.14	0.48
1:A:219:HIS:O	1:A:220:SER:HB3	2.13	0.48
1:B:214:ALA:O	1:B:215:LYS:C	2.57	0.48
1:C:26:ALA:O	1:C:28:HIS:N	2.46	0.48
1:D:162:VAL:CG1	1:D:166:LEU:HD12	2.38	0.48
1:E:96:ALA:HA	2:E:447:HOH:O	2.14	0.48
1:A:26:ALA:O	1:A:27:ALA:C	2.56	0.48
1:A:165:ASP:OD2	1:A:166:LEU:N	2.47	0.48
1:A:173:LEU:HB3	1:A:174:SER:H	1.44	0.48
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.28	0.48
1:B:156:VAL:HG12	1:B:156:VAL:O	2.14	0.48
1:B:184:ALA:O	1:B:187:ALA:HB3	2.13	0.48
1:C:79:LEU:HG	2:C:332:HOH:O	2.14	0.48
1:C:112:ARG:HG3	1:C:113:PRO:CD	2.35	0.48
1:D:238:THR:O	1:D:241:ALA:HB3	2.13	0.48
1:E:134:VAL:CG2	1:E:170:VAL:HG11	2.43	0.48
1:E:206:GLY:O	1:E:209:ALA:HB3	2.13	0.48
1:E:269:GLN:HG3	2:E:373:HOH:O	2.13	0.48
1:A:26:ALA:O	1:A:29:LYS:N	2.46	0.48
1:A:153:LEU:C	1:A:155:SER:N	2.71	0.48
1:B:118:ILE:HD13	1:B:149:MET:SD	2.54	0.48
1:D:123:ASN:CB	1:D:125:PRO:HD2	2.43	0.48
1:E:220:SER:O	1:E:222:GLN:N	2.47	0.48
1:A:109:SER:C	1:A:111:PHE:N	2.70	0.48
1:A:129:ARG:O	1:A:157:GLY:HA2	2.14	0.48
1:B:135:TYR:HE1	1:B:161:GLU:OE1	1.97	0.48
1:C:68:LEU:HD11	1:C:78:ILE:HG21	1.95	0.48
1:C:86:ILE:CD1	1:C:108:LEU:HB3	2.44	0.48
1:C:269:GLN:C	1:C:271:MET:N	2.67	0.48
1:E:221:GLU:C	1:E:223:HIS:H	2.11	0.48
1:E:221:GLU:C	1:E:223:HIS:N	2.71	0.48
1:A:30:ILE:HB	1:A:50:VAL:HG13	1.96	0.48
1:B:82:ILE:HG22	1:B:86:ILE:CD1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:SER:O	1:B:221:GLU:CB	2.62	0.48
1:C:46:ARG:C	1:C:48:MET:N	2.71	0.48
1:D:33:SER:HB3	1:D:56:ASN:OD1	2.13	0.48
1:D:242:LEU:O	1:D:246:GLU:HB2	2.14	0.48
1:A:86:ILE:O	1:A:86:ILE:HG22	2.13	0.47
1:C:2:SER:C	1:C:3:VAL:HG23	2.39	0.47
1:E:12:ALA:O	1:E:13:PHE:C	2.56	0.47
1:E:70:VAL:O	1:E:74:ILE:HD12	2.14	0.47
1:E:181:ALA:O	1:E:184:ALA:N	2.45	0.47
1:B:234:PRO:HB3	1:E:197:LEU:O	2.13	0.47
1:C:43:SER:O	1:C:46:ARG:N	2.46	0.47
1:C:51:LYS:NZ	2:C:324:HOH:O	2.44	0.47
1:C:123:ASN:O	1:C:126:VAL:HG22	2.14	0.47
1:D:264:ARG:NH2	2:D:321:HOH:O	2.46	0.47
1:E:60:VAL:HG12	1:E:90:HIS:NE2	2.29	0.47
1:E:121:MET:CE	1:E:122:THR:H	2.26	0.47
1:E:137:THR:HG23	1:E:137:THR:O	2.15	0.47
1:A:92:VAL:HG12	1:A:117:VAL:HG23	1.96	0.47
1:A:135:TYR:HE1	1:A:161:GLU:HG2	1.77	0.47
1:B:93:VAL:CG2	1:B:149:MET:HE1	2.44	0.47
1:B:94:SER:OG	1:B:119:ARG:HG3	2.14	0.47
1:C:11:LEU:O	1:C:15:LEU:HG	2.14	0.47
1:C:230:ASN:HA	2:C:328:HOH:O	2.14	0.47
1:E:57:LYS:HD3	1:E:57:LYS:N	2.26	0.47
1:A:228:LYS:NZ	1:C:199:ARG:HH12	2.12	0.47
1:B:42:VAL:HA	1:B:45:LEU:HG	1.97	0.47
1:B:68:LEU:HA	2:B:325:HOH:O	2.14	0.47
1:B:119:ARG:HD3	1:B:167:ILE:HD12	1.95	0.47
1:B:143:VAL:O	1:B:145:ASP:N	2.42	0.47
1:A:17:LYS:HB3	1:A:127:VAL:HG13	1.97	0.47
1:A:188:LEU:O	1:A:192:GLY:N	2.45	0.47
1:C:64:ASP:O	1:C:65:VAL:HB	2.15	0.47
1:E:34:SER:C	1:E:36:ASP:H	2.23	0.47
1:A:57:LYS:HE3	2:A:374:HOH:O	2.14	0.47
1:A:100:THR:HG22	1:A:101:ILE:N	2.28	0.47
1:B:47:LYS:NZ	1:B:47:LYS:HB3	2.28	0.47
1:C:126:VAL:C	1:C:128:VAL:N	2.73	0.47
1:D:33:SER:O	1:D:35:PRO:CD	2.62	0.47
1:D:222:GLN:O	1:D:223:HIS:CB	2.62	0.47
1:E:17:LYS:CB	2:E:412:HOH:O	2.56	0.47
1:B:17:LYS:HA	1:B:20:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:MET:HG3	1:B:51:LYS:CB	2.45	0.47
1:B:41:THR:O	1:B:45:LEU:HG	2.14	0.47
1:B:91:ILE:HD11	1:B:145:ASP:OD1	2.14	0.47
1:B:112:ARG:O	1:B:113:PRO:C	2.58	0.47
1:C:10:GLN:O	1:C:12:ALA:N	2.48	0.47
1:C:93:VAL:HG12	1:C:118:ILE:CD1	2.44	0.47
1:C:100:THR:HG22	1:C:101:ILE:H	1.77	0.47
1:C:166:LEU:O	1:C:168:ASP:N	2.48	0.47
1:D:60:VAL:HG21	1:D:82:ILE:CG2	2.45	0.47
1:D:137:THR:O	1:D:137:THR:HG23	2.14	0.47
1:E:19:PHE:CE2	1:E:152:LEU:HG	2.50	0.47
1:E:43:SER:HB2	2:E:380:HOH:O	2.14	0.47
1:E:45:LEU:HD23	1:E:48:MET:CE	2.45	0.47
1:E:83:GLY:HA2	1:E:86:ILE:HD11	1.95	0.47
1:E:171:THR:HA	1:E:175:GLY:HA3	1.96	0.47
1:A:36:ASP:O	1:A:37:MET:HB2	2.15	0.47
1:A:133:THR:HG22	1:A:134:VAL:N	2.28	0.47
1:A:198:PRO:HG2	1:A:201:LEU:HB2	1.96	0.47
1:B:125:PRO:C	1:B:127:VAL:N	2.71	0.47
1:D:6:ILE:CD1	1:D:66:LEU:HD21	2.45	0.47
1:D:89:ARG:CG	1:D:90:HIS:H	2.28	0.47
1:E:17:LYS:O	1:E:18:GLY:C	2.58	0.47
1:E:262:CYS:O	1:E:263:ILE:C	2.56	0.47
1:A:13:PHE:N	2:A:333:HOH:O	2.48	0.47
1:A:181:ALA:O	1:A:184:ALA:HB3	2.13	0.47
1:A:198:PRO:HD2	1:A:201:LEU:HD23	1.97	0.47
1:B:46:ARG:HB2	2:B:345:HOH:O	2.15	0.47
1:C:46:ARG:O	1:C:49:GLY:N	2.45	0.47
1:D:45:LEU:O	1:D:46:ARG:C	2.58	0.47
1:D:121:MET:HE3	1:D:171:THR:HA	1.97	0.47
1:E:55:HIS:ND1	1:E:57:LYS:HE2	2.29	0.47
1:E:80:ASP:C	1:E:81:GLU:HG3	2.40	0.47
1:B:5:PHE:HZ	1:B:15:LEU:CB	2.10	0.47
1:C:6:ILE:HD11	1:C:60:VAL:HG22	1.97	0.47
1:D:3:VAL:HG11	1:D:67:PHE:HE1	1.80	0.47
1:D:60:VAL:CG2	1:D:82:ILE:HD13	2.44	0.47
1:D:75:ILE:CG2	1:D:79:LEU:HD22	2.45	0.47
1:D:82:ILE:O	1:D:83:GLY:C	2.57	0.47
1:D:135:TYR:CD1	1:D:135:TYR:C	2.92	0.47
1:D:167:ILE:HG22	2:D:397:HOH:O	2.14	0.47
1:D:217:LEU:HD13	2:D:323:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:O	1:A:186:ASP:C	2.55	0.46
1:B:76:PRO:O	1:B:78:ILE:N	2.47	0.46
1:B:239:ILE:HD13	1:E:194:LYS:N	2.30	0.46
1:C:10:GLN:C	1:C:12:ALA:H	2.23	0.46
1:C:70:VAL:HG21	1:C:78:ILE:HD12	1.96	0.46
1:E:112:ARG:HG3	2:E:342:HOH:O	2.13	0.46
1:E:228:LYS:HE3	1:E:242:LEU:CD1	2.35	0.46
1:A:10:GLN:O	1:A:13:PHE:N	2.49	0.46
1:A:33:SER:C	1:A:35:PRO:HD3	2.40	0.46
1:B:79:LEU:CD1	1:B:104:ILE:HG12	2.42	0.46
1:C:171:THR:HG21	2:C:423:HOH:O	2.14	0.46
1:E:99:VAL:O	1:E:100:THR:C	2.57	0.46
1:A:47:LYS:O	1:A:48:MET:C	2.59	0.46
1:B:27:ALA:CB	1:B:49:GLY:O	2.60	0.46
1:B:35:PRO:O	1:B:36:ASP:HB2	2.15	0.46
1:B:129:ARG:O	1:B:157:GLY:HA2	2.15	0.46
1:D:4:GLY:HA2	1:D:31:MET:O	2.16	0.46
1:D:150:GLU:O	1:D:150:GLU:HG2	2.15	0.46
1:D:164:GLU:HA	1:D:167:ILE:HG13	1.97	0.46
1:A:11:LEU:O	1:A:14:ALA:HB3	2.15	0.46
1:A:30:ILE:O	1:A:51:LYS:HB2	2.15	0.46
1:A:31:MET:HA	1:A:51:LYS:O	2.14	0.46
1:C:166:LEU:O	1:C:167:ILE:C	2.59	0.46
1:D:101:ILE:HG13	1:D:119:ARG:HB2	1.97	0.46
1:D:134:VAL:HG21	1:D:162:VAL:HG21	1.98	0.46
1:A:33:SER:HB3	1:A:56:ASN:HA	1.96	0.46
1:A:236:GLY:O	1:A:237:ALA:HB3	2.14	0.46
1:B:1:MET:CG	1:B:2:SER:N	2.77	0.46
1:B:74:ILE:HD11	1:B:96:ALA:HB3	1.98	0.46
1:C:124:THR:C	1:C:126:VAL:N	2.71	0.46
1:C:135:TYR:CD1	1:C:135:TYR:C	2.93	0.46
1:E:67:PHE:O	1:E:68:LEU:HD23	2.16	0.46
1:A:55:HIS:HB2	1:A:58:GLU:HG3	1.98	0.46
1:A:123:ASN:C	1:A:125:PRO:HD2	2.40	0.46
1:B:3:VAL:O	1:B:30:ILE:HG23	2.16	0.46
1:A:135:TYR:OH	1:A:150:GLU:HG3	2.16	0.46
1:B:60:VAL:O	1:B:63:SER:HB2	2.16	0.46
1:B:161:GLU:C	1:B:162:VAL:HG23	2.41	0.46
1:D:30:ILE:O	1:D:51:LYS:HB2	2.16	0.46
1:E:98:GLY:HA2	2:E:400:HOH:O	2.16	0.46
1:A:15:LEU:O	1:A:16:ALA:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:C	1:A:128:VAL:N	2.72	0.46
1:B:3:VAL:O	1:B:30:ILE:CG2	2.64	0.46
1:B:8:ALA:HA	1:B:12:ALA:HB1	1.93	0.46
1:B:161:GLU:O	1:B:162:VAL:HG22	2.16	0.46
1:C:172:GLY:O	1:C:258:VAL:HG22	2.15	0.46
1:D:252:SER:O	1:D:254:LEU:N	2.49	0.46
1:A:160:THR:HG22	1:A:161:GLU:N	2.30	0.46
1:B:34:SER:C	1:B:36:ASP:H	2.24	0.46
1:C:61:GLN:O	1:C:89:ARG:NH2	2.46	0.46
1:E:74:ILE:C	1:E:76:PRO:CD	2.89	0.46
1:A:79:LEU:HD21	1:A:104:ILE:HG23	1.97	0.46
1:A:159:CYS:O	1:A:160:THR:OG1	2.29	0.46
1:C:9:GLY:O	1:C:12:ALA:CB	2.63	0.46
1:C:83:GLY:HA2	1:C:108:LEU:HD22	1.98	0.46
1:C:264:ARG:O	1:C:268:LEU:HG	2.15	0.46
1:E:70:VAL:O	1:E:71:LYS:CB	2.63	0.46
1:B:5:PHE:HA	2:B:371:HOH:O	2.14	0.45
1:B:79:LEU:O	1:B:108:LEU:CD2	2.64	0.45
1:B:239:ILE:HD12	1:E:193:VAL:HG12	1.98	0.45
1:C:104:ILE:HG21	1:C:117:VAL:HG11	1.98	0.45
1:C:185:LEU:HD22	2:C:434:HOH:O	2.15	0.45
1:A:93:VAL:HG22	1:A:118:ILE:CG1	2.47	0.45
1:B:112:ARG:O	1:B:113:PRO:O	2.34	0.45
1:B:140:HIS:O	1:B:141:ALA:HB2	2.16	0.45
1:B:234:PRO:HA	1:E:193:VAL:HG13	1.98	0.45
1:C:6:ILE:HG21	1:C:78:ILE:HG21	1.97	0.45
1:C:61:GLN:O	1:C:63:SER:N	2.49	0.45
1:C:93:VAL:HG23	1:C:93:VAL:O	2.16	0.45
1:D:70:VAL:HG11	1:D:78:ILE:CD1	2.46	0.45
1:D:224:PRO:HA	2:D:419:HOH:O	2.15	0.45
1:E:236:GLY:HA2	1:E:239:ILE:CG2	2.39	0.45
1:A:27:ALA:HB1	1:A:49:GLY:C	2.42	0.45
1:A:92:VAL:CG1	1:A:117:VAL:HG23	2.46	0.45
1:A:101:ILE:O	1:A:104:ILE:HB	2.17	0.45
1:B:119:ARG:HD3	1:B:167:ILE:HD13	1.98	0.45
1:B:259:GLU:HB3	2:B:336:HOH:O	2.15	0.45
1:C:204:ARG:CB	2:C:337:HOH:O	2.59	0.45
1:D:99:VAL:HG12	1:D:104:ILE:HD11	1.98	0.45
1:D:193:VAL:C	1:D:195:MET:H	2.25	0.45
1:E:75:ILE:O	1:E:78:ILE:HB	2.16	0.45
1:B:185:LEU:C	1:B:187:ALA:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:PHE:CE2	1:C:17:LYS:HE3	2.47	0.45
1:C:71:LYS:HB2	1:C:73:HIS:CE1	2.52	0.45
1:C:143:VAL:HG12	1:C:143:VAL:O	2.16	0.45
1:C:238:THR:HB	2:C:326:HOH:O	2.17	0.45
1:D:31:MET:HA	1:D:51:LYS:O	2.15	0.45
1:E:111:PHE:O	1:E:112:ARG:C	2.60	0.45
1:E:153:LEU:C	1:E:155:SER:H	2.21	0.45
1:A:6:ILE:HG22	1:A:6:ILE:O	2.17	0.45
1:A:156:VAL:O	1:A:156:VAL:CG1	2.62	0.45
1:A:251:ARG:O	1:A:252:SER:C	2.57	0.45
1:D:4:GLY:O	1:D:66:LEU:HD12	2.16	0.45
1:D:266:ARG:O	1:D:268:LEU:N	2.50	0.45
1:E:169:ALA:HA	2:E:335:HOH:O	2.16	0.45
1:A:36:ASP:O	1:A:37:MET:HG3	2.17	0.45
1:B:132:ALA:C	1:B:133:THR:CG2	2.89	0.45
1:C:126:VAL:C	1:C:128:VAL:H	2.23	0.45
1:D:101:ILE:O	1:D:102:SER:C	2.60	0.45
1:E:82:ILE:O	1:E:82:ILE:HG22	2.16	0.45
1:B:161:GLU:HA	2:B:330:HOH:O	2.16	0.45
1:C:27:ALA:O	1:C:28:HIS:CG	2.70	0.45
1:C:164:GLU:O	1:C:164:GLU:HG2	2.16	0.45
1:C:210:LEU:HA	1:C:210:LEU:HD23	1.65	0.45
1:D:75:ILE:CD1	1:D:99:VAL:HG11	2.47	0.45
1:D:224:PRO:N	2:D:323:HOH:O	2.49	0.45
1:E:75:ILE:HD11	2:E:362:HOH:O	2.16	0.45
1:A:3:VAL:CG1	1:A:4:GLY:N	2.69	0.45
1:A:41:THR:O	1:A:42:VAL:C	2.60	0.45
1:A:160:THR:CG2	1:A:161:GLU:N	2.79	0.45
1:A:258:VAL:CG2	2:A:419:HOH:O	2.64	0.45
1:B:16:ALA:C	1:B:18:GLY:H	2.25	0.45
1:B:121:MET:HE2	1:B:121:MET:HA	1.99	0.45
1:C:87:GLU:H	1:C:90:HIS:CE1	2.33	0.45
1:C:122:THR:CG2	1:C:133:THR:CG2	2.95	0.45
1:C:177:GLY:HA2	1:C:180:TYR:CE1	2.50	0.45
1:C:253:LEU:HD12	1:C:253:LEU:N	2.32	0.45
1:D:70:VAL:O	1:D:71:LYS:C	2.59	0.45
1:A:135:TYR:CE2	1:A:150:GLU:HG2	2.51	0.45
1:B:16:ALA:C	1:B:18:GLY:N	2.74	0.45
1:C:83:GLY:HA2	1:C:86:ILE:HD11	1.99	0.45
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.69	0.45
1:D:101:ILE:HG22	1:D:102:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:VAL:HG22	1:D:162:VAL:HB	1.98	0.45
1:D:191:GLY:O	1:D:192:GLY:C	2.59	0.45
1:E:55:HIS:CG	1:E:57:LYS:HE2	2.52	0.45
1:A:122:THR:CG2	1:A:123:ASN:H	2.30	0.45
1:A:124:THR:O	1:A:126:VAL:N	2.50	0.45
1:A:222:GLN:O	1:A:223:HIS:HB3	2.16	0.45
1:C:53:THR:C	1:C:55:HIS:H	2.24	0.45
1:D:6:ILE:O	1:D:70:VAL:CG2	2.65	0.45
1:D:163:GLU:O	1:D:164:GLU:C	2.60	0.45
1:A:57:LYS:CA	1:A:60:VAL:HG23	2.48	0.44
1:B:239:ILE:HD13	1:E:194:LYS:CA	2.48	0.44
1:B:269:GLN:O	1:B:271:MET:N	2.48	0.44
1:C:93:VAL:HG12	1:C:118:ILE:CG1	2.47	0.44
1:C:147:ARG:HE	1:C:147:ARG:HB2	1.40	0.44
1:D:122:THR:HB	1:D:123:ASN:H	1.38	0.44
1:D:193:VAL:C	1:D:195:MET:N	2.73	0.44
1:E:172:GLY:O	1:E:258:VAL:HA	2.16	0.44
1:A:124:THR:C	1:A:126:VAL:N	2.75	0.44
1:C:121:MET:HE2	1:C:122:THR:H	1.82	0.44
1:D:38:ASP:O	1:D:38:ASP:CG	2.60	0.44
1:D:124:THR:N	1:D:125:PRO:CD	2.80	0.44
1:E:79:LEU:C	1:E:81:GLU:N	2.75	0.44
1:A:108:LEU:O	1:A:108:LEU:HG	2.17	0.44
1:A:259:GLU:O	1:A:263:ILE:HG13	2.18	0.44
1:B:57:LYS:O	1:B:58:GLU:C	2.60	0.44
1:B:122:THR:HG22	1:B:133:THR:CG2	2.47	0.44
1:B:244:VAL:HG12	1:B:245:LEU:N	2.30	0.44
1:C:124:THR:O	1:C:126:VAL:N	2.51	0.44
1:D:121:MET:O	1:D:133:THR:HA	2.18	0.44
1:E:188:LEU:HD23	1:E:188:LEU:HA	1.73	0.44
1:C:180:TYR:N	1:C:180:TYR:CD2	2.81	0.44
1:C:242:LEU:HA	1:C:242:LEU:HD23	1.60	0.44
1:C:249:GLY:C	1:C:253:LEU:HD13	2.41	0.44
1:D:107:LYS:O	1:D:110:ALA:HB3	2.16	0.44
1:E:55:HIS:HB3	1:E:57:LYS:CE	2.43	0.44
1:E:121:MET:HE2	1:E:122:THR:N	2.33	0.44
1:E:172:GLY:O	1:E:258:VAL:HG22	2.18	0.44
1:C:10:GLN:NE2	2:C:382:HOH:O	2.50	0.44
1:C:11:LEU:HD13	1:C:124:THR:HA	2.00	0.44
1:D:126:VAL:HG13	1:D:156:VAL:CG1	2.48	0.44
1:E:38:ASP:H	1:E:42:VAL:CG2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:PRO:N	2:E:404:HOH:O	2.50	0.44
1:B:176:SER:O	1:B:178:PRO:N	2.51	0.44
1:B:254:LEU:HB2	2:B:362:HOH:O	2.16	0.44
1:C:3:VAL:HB	1:C:30:ILE:CG1	2.47	0.44
1:C:17:LYS:O	1:C:20:THR:HB	2.18	0.44
1:C:28:HIS:C	1:C:30:ILE:H	2.25	0.44
1:C:265:THR:HG23	2:C:323:HOH:O	2.17	0.44
1:E:177:GLY:HA2	1:E:180:TYR:CD1	2.53	0.44
1:E:242:LEU:O	1:E:245:LEU:N	2.51	0.44
1:A:249:GLY:O	1:A:252:SER:HB3	2.17	0.44
1:B:104:ILE:C	1:B:106:LYS:N	2.76	0.44
1:B:190:ASP:O	1:B:191:GLY:C	2.60	0.44
1:C:167:ILE:HB	2:C:422:HOH:O	2.17	0.44
1:D:38:ASP:O	1:D:40:ALA:N	2.51	0.44
1:D:109:SER:C	1:D:111:PHE:N	2.73	0.44
1:E:83:GLY:HA2	1:E:86:ILE:HD12	1.97	0.44
1:E:124:THR:C	1:E:126:VAL:H	2.26	0.44
1:A:227:LEU:HG	2:A:340:HOH:O	2.16	0.44
1:B:128:VAL:O	1:B:129:ARG:HB2	2.16	0.44
1:C:75:ILE:HB	1:C:76:PRO:HD3	2.00	0.44
1:D:26:ALA:CB	1:D:28:HIS:CD2	3.01	0.44
1:E:6:ILE:HD11	1:E:66:LEU:HD21	2.00	0.44
1:C:173:LEU:HD13	1:C:258:VAL:HG11	1.99	0.44
1:D:95:CYS:O	1:D:96:ALA:HB2	2.16	0.44
1:E:75:ILE:O	1:E:79:LEU:HG	2.18	0.44
1:A:102:SER:OG	1:A:103:SER:N	2.49	0.43
1:B:86:ILE:HA	1:B:90:HIS:NE2	2.33	0.43
1:C:17:LYS:HA	1:C:20:THR:OG1	2.18	0.43
1:C:31:MET:HG2	1:C:53:THR:OG1	2.18	0.43
1:C:88:ASP:OD2	1:C:112:ARG:NH1	2.51	0.43
1:C:151:GLN:HA	2:C:335:HOH:O	2.17	0.43
1:D:135:TYR:CE1	1:D:161:GLU:CB	3.01	0.43
1:E:236:GLY:O	1:E:237:ALA:CB	2.65	0.43
1:A:77:PHE:HD1	1:A:77:PHE:H	1.66	0.43
1:B:66:LEU:N	1:B:91:ILE:O	2.51	0.43
1:B:91:ILE:HG12	1:B:116:ARG:CD	2.48	0.43
1:D:194:LYS:HD3	1:D:195:MET:HE3	2.00	0.43
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.85	0.43
1:A:79:LEU:HD11	1:A:104:ILE:HA	2.01	0.43
1:A:199:ARG:HD2	1:A:199:ARG:HA	1.86	0.43
1:A:252:SER:C	1:A:254:LEU:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HB2	1:B:73:HIS:ND1	2.33	0.43
1:B:121:MET:HG2	1:B:171:THR:OG1	2.18	0.43
1:B:161:GLU:C	1:B:162:VAL:CG2	2.91	0.43
1:C:35:PRO:HD3	2:C:380:HOH:O	2.17	0.43
1:C:257:ALA:C	1:C:259:GLU:H	2.26	0.43
1:E:33:SER:O	1:E:35:PRO:CD	2.66	0.43
1:E:242:LEU:O	1:E:243:HIS:C	2.59	0.43
1:A:13:PHE:CA	2:A:333:HOH:O	2.66	0.43
1:A:45:LEU:O	1:A:46:ARG:C	2.61	0.43
1:A:73:HIS:C	1:A:76:PRO:HD2	2.43	0.43
1:A:121:MET:SD	1:A:122:THR:N	2.91	0.43
1:A:123:ASN:HB2	1:A:125:PRO:HD2	2.00	0.43
1:A:134:VAL:CG1	1:A:135:TYR:N	2.81	0.43
1:A:153:LEU:C	1:A:155:SER:H	2.25	0.43
1:B:61:GLN:C	1:B:63:SER:H	2.27	0.43
1:B:140:HIS:CD2	1:B:142:GLN:HB2	2.53	0.43
1:C:51:LYS:HB2	1:C:51:LYS:NZ	2.33	0.43
1:C:172:GLY:HA2	1:C:261:SER:CB	2.48	0.43
1:E:49:GLY:CA	2:E:407:HOH:O	2.66	0.43
1:E:123:ASN:CB	1:E:178:PRO:HG2	2.48	0.43
1:A:126:VAL:O	1:A:156:VAL:CG1	2.66	0.43
1:A:134:VAL:HG12	2:A:373:HOH:O	2.18	0.43
1:A:257:ALA:N	2:A:390:HOH:O	2.51	0.43
1:B:132:ALA:O	1:B:133:THR:HG22	2.18	0.43
1:C:13:PHE:CE1	1:C:44:ALA:HB3	2.53	0.43
1:D:1:MET:HE2	1:D:25:LEU:HD21	2.00	0.43
1:E:34:SER:C	1:E:36:ASP:N	2.77	0.43
1:A:199:ARG:O	1:A:200:ARG:C	2.61	0.43
1:B:6:ILE:O	1:B:6:ILE:HG22	2.17	0.43
1:C:36:ASP:O	1:C:37:MET:CG	2.67	0.43
1:C:223:HIS:CE1	1:C:224:PRO:HD2	2.52	0.43
1:A:110:ALA:C	1:A:111:PHE:CD1	2.96	0.43
1:A:210:LEU:O	1:A:211:LEU:C	2.61	0.43
1:A:229:ASP:OD1	1:A:229:ASP:N	2.52	0.43
1:A:267:GLU:O	1:A:268:LEU:C	2.62	0.43
1:B:13:PHE:CD1	1:B:41:THR:HG23	2.53	0.43
1:B:32:ALA:O	1:B:53:THR:HB	2.19	0.43
1:B:60:VAL:C	1:B:89:ARG:HH22	2.16	0.43
1:B:115:PRO:HG3	2:B:331:HOH:O	2.18	0.43
1:C:45:LEU:HD23	1:C:45:LEU:C	2.43	0.43
1:C:171:THR:O	1:C:175:GLY:CA	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:C	1:D:84:ALA:H	2.26	0.43
1:D:197:LEU:HA	1:D:197:LEU:HD23	1.71	0.43
1:D:269:GLN:C	1:D:271:MET:N	2.74	0.43
2:A:405:HOH:O	1:E:228:LYS:HE2	2.17	0.43
1:B:124:THR:C	1:B:126:VAL:H	2.27	0.43
1:B:134:VAL:CG1	1:B:135:TYR:N	2.82	0.43
1:B:190:ASP:N	2:B:382:HOH:O	2.50	0.43
1:C:31:MET:CG	1:C:53:THR:OG1	2.66	0.43
1:C:196:GLY:O	1:C:197:LEU:O	2.37	0.43
1:C:228:LYS:NZ	1:C:229:ASP:OD1	2.52	0.43
1:D:110:ALA:C	1:D:111:PHE:CD1	2.97	0.43
1:D:148:LEU:HD12	1:D:148:LEU:O	2.19	0.43
1:D:245:LEU:O	1:D:246:GLU:C	2.61	0.43
1:E:43:SER:O	1:E:44:ALA:C	2.61	0.43
1:E:126:VAL:HG13	1:E:156:VAL:O	2.19	0.43
1:E:206:GLY:O	1:E:207:ALA:C	2.61	0.43
1:B:31:MET:HG3	1:B:51:LYS:HB2	2.01	0.43
1:B:68:LEU:C	1:B:70:VAL:H	2.26	0.43
1:B:105:GLU:O	1:B:109:SER:HB2	2.18	0.43
1:C:79:LEU:CD1	1:C:104:ILE:HG13	2.47	0.43
1:D:28:HIS:CD2	1:D:28:HIS:C	2.97	0.43
1:D:185:LEU:CD2	1:D:210:LEU:CD1	2.95	0.43
1:D:236:GLY:HA2	2:D:435:HOH:O	2.18	0.43
1:E:75:ILE:N	1:E:76:PRO:CD	2.82	0.43
1:A:133:THR:CG2	1:A:134:VAL:N	2.82	0.43
1:B:41:THR:O	1:B:45:LEU:N	2.52	0.43
1:B:134:VAL:HA	2:B:334:HOH:O	2.19	0.43
1:C:59:THR:HA	1:C:62:HIS:HE1	1.84	0.43
1:C:123:ASN:HB2	1:C:125:PRO:CD	2.42	0.43
1:C:213:ALA:O	1:C:216:MET:HB2	2.19	0.43
1:C:269:GLN:O	1:C:271:MET:N	2.52	0.43
1:D:105:GLU:C	1:D:107:LYS:N	2.71	0.43
1:D:210:LEU:C	1:D:212:GLY:N	2.77	0.43
1:E:59:THR:O	1:E:62:HIS:N	2.52	0.43
1:E:150:GLU:C	1:E:152:LEU:N	2.75	0.43
1:A:223:HIS:ND1	1:A:224:PRO:CD	2.82	0.42
1:B:102:SER:HA	1:B:105:GLU:CB	2.49	0.42
1:B:164:GLU:O	1:B:164:GLU:CG	2.67	0.42
2:B:390:HOH:O	1:D:239:ILE:CG2	2.67	0.42
1:C:3:VAL:HB	1:C:30:ILE:CD1	2.49	0.42
1:C:13:PHE:HE2	1:C:17:LYS:CE	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:GLN:HG2	1:C:274:GLN:O	2.18	0.42
1:D:27:ALA:HB1	1:D:49:GLY:HA3	2.01	0.42
1:D:266:ARG:C	1:D:268:LEU:N	2.75	0.42
1:E:46:ARG:C	1:E:48:MET:H	2.26	0.42
1:E:109:SER:C	1:E:111:PHE:H	2.26	0.42
1:E:223:HIS:ND1	1:E:223:HIS:C	2.77	0.42
1:B:18:GLY:O	1:B:20:THR:N	2.53	0.42
1:B:79:LEU:O	1:B:108:LEU:HD23	2.19	0.42
1:C:189:ALA:HA	1:C:202:ALA:HB1	2.01	0.42
1:D:143:VAL:O	1:D:145:ASP:N	2.52	0.42
1:A:20:THR:HG21	1:A:48:MET:CE	2.45	0.42
1:A:41:THR:O	1:A:44:ALA:HB3	2.19	0.42
1:A:41:THR:HG22	1:A:42:VAL:N	2.34	0.42
1:A:103:SER:HA	2:A:391:HOH:O	2.20	0.42
1:A:182:PHE:HB2	2:A:335:HOH:O	2.18	0.42
1:B:90:HIS:CD2	1:B:90:HIS:N	2.87	0.42
1:C:38:ASP:O	1:C:42:VAL:HB	2.18	0.42
1:C:45:LEU:O	1:C:45:LEU:HD23	2.20	0.42
1:D:16:ALA:HB3	2:D:365:HOH:O	2.19	0.42
1:A:25:LEU:CG	1:A:26:ALA:H	2.30	0.42
1:A:211:LEU:C	1:A:211:LEU:CD1	2.91	0.42
1:A:256:ASN:CB	2:A:390:HOH:O	2.60	0.42
1:B:57:LYS:CG	1:B:58:GLU:N	2.82	0.42
1:B:105:GLU:OE1	1:B:117:VAL:CG2	2.67	0.42
1:B:199:ARG:CZ	1:D:229:ASP:OD1	2.68	0.42
1:C:68:LEU:CD2	1:C:79:LEU:HD21	2.50	0.42
1:E:77:PHE:C	1:E:81:GLU:OE2	2.62	0.42
1:E:126:VAL:HG12	1:E:156:VAL:CG1	2.50	0.42
1:E:203:VAL:CG2	2:E:422:HOH:O	2.52	0.42
1:A:39:LEU:O	1:A:43:SER:HB3	2.19	0.42
1:B:174:SER:O	1:B:175:GLY:C	2.62	0.42
1:B:271:MET:HE2	1:B:271:MET:HB3	1.92	0.42
1:C:27:ALA:C	1:C:28:HIS:CG	2.98	0.42
1:C:99:VAL:CG1	1:C:104:ILE:HD11	2.49	0.42
1:C:201:LEU:O	1:C:205:LEU:HB2	2.19	0.42
1:D:99:VAL:CG1	1:D:104:ILE:HD11	2.50	0.42
1:D:214:ALA:O	1:D:215:LYS:C	2.62	0.42
1:D:217:LEU:HD12	1:D:217:LEU:C	2.45	0.42
1:D:220:SER:HB2	1:D:222:GLN:HG2	2.01	0.42
1:A:55:HIS:O	1:A:57:LYS:N	2.50	0.42
1:A:75:ILE:HD13	1:A:99:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:HG22	1:A:137:THR:HA	2.00	0.42
1:A:162:VAL:HG13	1:A:166:LEU:HD12	2.00	0.42
1:A:227:LEU:O	1:A:231:VAL:HG23	2.19	0.42
1:B:89:ARG:O	1:B:89:ARG:CD	2.67	0.42
1:B:239:ILE:HD12	1:E:193:VAL:CG1	2.50	0.42
1:B:244:VAL:O	1:B:247:SER:HB2	2.20	0.42
1:D:7:GLY:HA2	1:D:33:SER:O	2.18	0.42
1:D:13:PHE:HZ	1:D:17:LYS:NZ	2.12	0.42
1:D:34:SER:C	1:D:36:ASP:N	2.76	0.42
1:D:133:THR:O	1:D:159:CYS:HA	2.19	0.42
1:E:231:VAL:HG12	1:E:231:VAL:O	2.20	0.42
1:A:7:GLY:O	1:A:8:ALA:HB2	2.19	0.42
1:A:193:VAL:HA	1:A:197:LEU:O	2.20	0.42
1:B:79:LEU:HB3	1:B:108:LEU:HG	2.02	0.42
1:B:269:GLN:O	1:B:273:ASP:N	2.46	0.42
1:C:68:LEU:HD23	1:C:79:LEU:HD21	2.02	0.42
1:D:82:ILE:O	1:D:84:ALA:N	2.52	0.42
1:D:112:ARG:HA	1:D:113:PRO:HD3	1.93	0.42
1:D:154:SER:C	1:D:156:VAL:H	2.27	0.42
1:E:198:PRO:HG2	1:E:201:LEU:CB	2.48	0.42
1:E:259:GLU:O	1:E:260:ALA:C	2.62	0.42
1:A:61:GLN:O	1:A:63:SER:N	2.53	0.42
1:A:190:ASP:N	1:A:199:ARG:HH12	2.17	0.42
1:C:100:THR:CG2	1:C:101:ILE:N	2.83	0.42
1:C:257:ALA:C	1:C:259:GLU:N	2.77	0.42
1:D:75:ILE:O	1:D:76:PRO:C	2.62	0.42
1:E:105:GLU:OE1	1:E:139:THR:HB	2.20	0.42
1:A:245:LEU:HA	2:A:387:HOH:O	2.20	0.42
1:C:104:ILE:CG2	1:C:117:VAL:HG21	2.49	0.42
1:C:187:ALA:O	1:C:188:LEU:C	2.62	0.42
1:C:212:GLY:O	1:C:216:MET:HB2	2.20	0.42
1:C:249:GLY:O	1:C:253:LEU:CD1	2.64	0.42
1:D:83:GLY:O	1:D:86:ILE:CG2	2.59	0.42
1:D:121:MET:HG2	2:D:376:HOH:O	2.19	0.42
1:D:124:THR:C	1:D:126:VAL:N	2.76	0.42
1:A:78:ILE:C	1:A:80:ASP:N	2.78	0.42
1:B:70:VAL:CG1	1:B:71:LYS:N	2.83	0.42
1:B:87:GLU:C	1:B:89:ARG:N	2.78	0.42
1:C:142:GLN:HB2	1:C:145:ASP:OD2	2.20	0.42
1:C:266:ARG:HG2	2:C:323:HOH:O	2.19	0.42
1:D:17:LYS:O	1:D:20:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ILE:N	2:E:322:HOH:O	2.52	0.42
1:E:14:ALA:C	2:E:376:HOH:O	2.63	0.42
1:E:35:PRO:CG	2:E:401:HOH:O	2.65	0.42
1:E:179:ALA:C	2:E:333:HOH:O	2.63	0.42
1:E:270:SER:HA	2:E:373:HOH:O	2.19	0.42
1:A:42:VAL:HG13	1:A:52:LEU:HD13	2.02	0.41
2:B:390:HOH:O	1:D:239:ILE:HG23	2.20	0.41
1:C:19:PHE:HE2	1:C:153:LEU:HD23	1.85	0.41
1:C:185:LEU:O	1:C:186:ASP:C	2.59	0.41
1:E:121:MET:O	1:E:133:THR:HA	2.20	0.41
1:E:181:ALA:N	2:E:391:HOH:O	2.52	0.41
1:A:57:LYS:HE2	1:A:81:GLU:OE1	2.19	0.41
1:A:66:LEU:N	2:A:368:HOH:O	2.53	0.41
1:B:11:LEU:HB3	1:B:15:LEU:CD1	2.50	0.41
1:B:70:VAL:CG1	1:B:71:LYS:H	2.28	0.41
1:B:141:ALA:O	1:B:145:ASP:CB	2.62	0.41
1:B:198:PRO:CD	1:B:201:LEU:HD23	2.49	0.41
1:C:3:VAL:CG1	1:C:4:GLY:N	2.83	0.41
1:C:13:PHE:HE1	1:C:44:ALA:CB	2.33	0.41
1:D:270:SER:O	1:D:274:GLN:OE1	2.37	0.41
1:E:7:GLY:H	1:E:33:SER:HB2	1.85	0.41
1:E:75:ILE:HD12	1:E:99:VAL:HG21	2.02	0.41
1:E:124:THR:C	1:E:126:VAL:N	2.78	0.41
1:E:148:LEU:O	1:E:149:MET:C	2.64	0.41
1:E:214:ALA:O	1:E:215:LYS:C	2.62	0.41
1:E:225:GLY:O	1:E:226:GLN:C	2.62	0.41
1:A:97:ALA:O	1:A:99:VAL:N	2.53	0.41
1:A:176:SER:O	1:A:177:GLY:C	2.64	0.41
1:B:68:LEU:HG	1:B:92:VAL:CG1	2.50	0.41
1:B:101:ILE:HG13	1:B:102:SER:N	2.34	0.41
1:B:109:SER:OG	1:B:115:PRO:CD	2.65	0.41
1:B:119:ARG:NE	1:B:167:ILE:HG21	2.34	0.41
1:B:201:LEU:O	1:B:205:LEU:HG	2.20	0.41
1:C:213:ALA:O	1:C:216:MET:CB	2.68	0.41
1:D:192:GLY:C	1:D:197:LEU:HB2	2.45	0.41
1:D:236:GLY:O	1:D:237:ALA:HB3	2.20	0.41
2:A:422:HOH:O	1:C:199:ARG:HB2	2.18	0.41
1:B:226:GLN:O	1:B:230:ASN:OD1	2.38	0.41
1:C:251:ARG:HB2	2:C:340:HOH:O	2.19	0.41
1:D:33:SER:CB	1:D:56:ASN:OD1	2.69	0.41
1:D:39:LEU:O	1:D:40:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ARG:HG3	2:D:377:HOH:O	2.20	0.41
1:E:131:GLY:H	1:E:157:GLY:HA3	1.85	0.41
1:A:95:CYS:O	1:A:96:ALA:C	2.63	0.41
1:E:46:ARG:C	1:E:48:MET:N	2.78	0.41
1:E:135:TYR:CE1	1:E:161:GLU:HB3	2.56	0.41
1:E:150:GLU:O	1:E:152:LEU:N	2.53	0.41
1:A:59:THR:O	1:A:61:GLN:N	2.53	0.41
1:A:244:VAL:CG2	1:A:245:LEU:N	2.84	0.41
1:C:17:LYS:HE3	1:C:17:LYS:HB2	1.85	0.41
1:C:61:GLN:N	1:C:61:GLN:CD	2.79	0.41
1:C:122:THR:CB	1:C:133:THR:CG2	2.88	0.41
1:C:128:VAL:C	1:C:130:GLU:N	2.78	0.41
1:C:135:TYR:CZ	1:C:161:GLU:HB3	2.52	0.41
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.87	0.41
1:D:12:ALA:O	1:D:16:ALA:HB2	2.20	0.41
1:A:236:GLY:C	2:A:369:HOH:O	2.62	0.41
1:B:183:THR:O	1:B:184:ALA:C	2.63	0.41
1:C:2:SER:O	1:C:3:VAL:CG2	2.69	0.41
1:C:112:ARG:NH1	1:C:113:PRO:CD	2.68	0.41
1:C:161:GLU:C	1:C:162:VAL:HG13	2.44	0.41
1:C:233:SER:O	1:C:234:PRO:C	2.62	0.41
1:D:134:VAL:CG1	1:D:170:VAL:HG11	2.50	0.41
1:D:134:VAL:HG11	1:D:170:VAL:HG11	2.02	0.41
1:E:193:VAL:C	2:E:363:HOH:O	2.63	0.41
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.79	0.41
1:B:75:ILE:HD11	1:B:272:ALA:CA	2.51	0.41
1:B:143:VAL:C	1:B:145:ASP:N	2.78	0.41
1:C:168:ASP:HB2	1:C:266:ARG:NH1	2.36	0.41
1:D:45:LEU:O	1:D:48:MET:N	2.53	0.41
1:D:129:ARG:HG2	1:D:156:VAL:HG13	2.03	0.41
1:E:70:VAL:HB	1:E:78:ILE:HD11	2.03	0.41
1:E:87:GLU:O	1:E:89:ARG:N	2.54	0.41
1:E:121:MET:CE	2:E:405:HOH:O	2.68	0.41
1:A:56:ASN:O	1:A:82:ILE:HD11	2.21	0.41
1:A:92:VAL:HB	1:A:117:VAL:HG23	2.03	0.41
1:A:161:GLU:C	1:A:162:VAL:HG23	2.46	0.41
1:A:180:TYR:N	1:A:180:TYR:CD2	2.86	0.41
1:A:240:HIS:CD2	1:C:194:LYS:HG3	2.56	0.41
1:B:6:ILE:CA	1:B:33:SER:HB3	2.26	0.41
1:B:47:LYS:HB3	1:B:47:LYS:HZ3	1.86	0.41
1:B:176:SER:C	1:B:178:PRO:HD2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.87	0.41
1:B:223:HIS:ND1	1:B:224:PRO:HD2	2.35	0.41
1:B:245:LEU:C	1:B:247:SER:H	2.27	0.41
1:C:39:LEU:O	1:C:40:ALA:C	2.63	0.41
1:C:48:MET:HB3	1:C:50:VAL:HG23	2.03	0.41
1:D:33:SER:HA	1:D:53:THR:O	2.21	0.41
1:D:89:ARG:O	1:D:90:HIS:C	2.63	0.41
1:D:254:LEU:HD23	1:D:254:LEU:HA	1.83	0.41
1:E:116:ARG:HB2	2:E:396:HOH:O	2.20	0.41
1:E:125:PRO:C	1:E:127:VAL:H	2.29	0.41
1:E:131:GLY:HA2	2:E:325:HOH:O	2.20	0.41
1:A:163:GLU:O	1:A:164:GLU:C	2.64	0.41
1:A:187:ALA:O	1:A:190:ASP:N	2.53	0.41
1:B:124:THR:C	1:B:126:VAL:N	2.77	0.41
1:B:185:LEU:O	1:B:187:ALA:N	2.54	0.41
1:C:66:LEU:HB2	2:C:402:HOH:O	2.20	0.41
1:C:114:ALA:HA	2:C:379:HOH:O	2.21	0.41
1:D:125:PRO:O	1:D:126:VAL:C	2.64	0.41
1:D:203:VAL:HA	2:D:388:HOH:O	2.21	0.41
1:D:233:SER:C	1:D:235:GLY:N	2.79	0.41
1:D:252:SER:O	1:D:253:LEU:C	2.62	0.41
1:A:101:ILE:HG23	1:A:117:VAL:CG1	2.51	0.40
1:A:121:MET:SD	1:A:121:MET:C	3.04	0.40
1:C:31:MET:CG	1:C:53:THR:HG1	2.34	0.40
1:C:75:ILE:O	1:C:79:LEU:HG	2.21	0.40
1:C:125:PRO:HB2	1:C:130:GLU:O	2.22	0.40
1:C:126:VAL:O	1:C:128:VAL:O	2.39	0.40
1:D:86:ILE:HD12	1:D:108:LEU:HD13	2.03	0.40
1:D:252:SER:HA	1:D:255:ILE:HD12	2.02	0.40
1:E:53:THR:C	1:E:55:HIS:N	2.78	0.40
1:A:22:ALA:HA	2:A:379:HOH:O	2.21	0.40
1:B:53:THR:C	1:B:55:HIS:H	2.29	0.40
1:B:185:LEU:CD2	1:B:210:LEU:CD1	2.97	0.40
1:C:53:THR:HG22	1:C:55:HIS:O	2.21	0.40
1:C:93:VAL:HG11	1:C:149:MET:SD	2.61	0.40
1:C:99:VAL:HG11	1:C:104:ILE:HD11	2.03	0.40
1:C:119:ARG:NH2	2:C:339:HOH:O	2.48	0.40
1:E:28:HIS:O	1:E:51:LYS:HE3	2.21	0.40
1:E:254:LEU:HD23	1:E:254:LEU:HA	1.83	0.40
1:A:36:ASP:O	1:A:37:MET:CG	2.70	0.40
1:A:65:VAL:N	2:A:365:HOH:O	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:HA	1:A:255:ILE:HD12	2.03	0.40
1:B:17:LYS:HA	1:B:20:THR:CG2	2.52	0.40
1:B:94:SER:C	2:B:324:HOH:O	2.64	0.40
1:B:160:THR:CG2	1:B:161:GLU:N	2.56	0.40
1:C:70:VAL:CG1	1:C:74:ILE:HB	2.52	0.40
1:D:82:ILE:O	1:D:82:ILE:HG22	2.20	0.40
1:D:135:TYR:CE2	1:D:150:GLU:HB2	2.57	0.40
1:A:54:PRO:HG2	1:A:55:HIS:CD2	2.57	0.40
1:A:185:LEU:HD21	1:A:210:LEU:CD1	2.51	0.40
1:A:274:GLN:HB2	1:A:275:GLU:H	1.66	0.40
1:B:18:GLY:O	1:B:19:PHE:CD1	2.75	0.40
1:B:169:ALA:C	1:B:171:THR:N	2.77	0.40
1:C:31:MET:SD	1:C:53:THR:OG1	2.79	0.40
1:C:144:GLU:C	1:C:146:GLY:N	2.79	0.40
1:C:164:GLU:HG2	2:C:416:HOH:O	2.21	0.40
1:D:255:ILE:O	1:D:257:ALA:N	2.53	0.40
1:A:26:ALA:HB3	1:A:29:LYS:CE	2.46	0.40
1:A:51:LYS:NZ	2:A:415:HOH:O	2.54	0.40
1:A:129:ARG:O	1:A:129:ARG:CG	2.68	0.40
1:C:114:ALA:HB1	1:C:140:HIS:CE1	2.55	0.40
1:C:149:MET:C	1:C:151:GLN:N	2.76	0.40
1:C:193:VAL:HG12	2:C:344:HOH:O	2.21	0.40
1:D:154:SER:C	1:D:156:VAL:N	2.80	0.40
1:E:9:GLY:O	1:E:10:GLN:C	2.65	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	275/321 (86%)	182 (66%)	60 (22%)	33 (12%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	272/321 (85%)	168 (62%)	68 (25%)	36 (13%)	0	1
1	C	275/321 (86%)	183 (66%)	60 (22%)	32 (12%)	0	1
1	D	275/321 (86%)	183 (66%)	68 (25%)	24 (9%)	0	4
1	E	275/321 (86%)	183 (66%)	57 (21%)	35 (13%)	0	1
All	All	1372/1605 (86%)	899 (66%)	313 (23%)	160 (12%)	0	1

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	10	GLN
1	A	11	LEU
1	A	36	ASP
1	A	37	MET
1	A	39	LEU
1	A	40	ALA
1	A	41	THR
1	A	42	VAL
1	A	85	ASP
1	A	106	LYS
1	A	107	LYS
1	A	173	LEU
1	A	253	LEU
1	B	10	GLN
1	B	36	ASP
1	B	37	MET
1	B	61	GLN
1	B	75	ILE
1	B	77	PHE
1	B	97	ALA
1	B	113	PRO
1	B	129	ARG
1	B	137	THR
1	B	140	HIS
1	B	141	ALA
1	B	142	GLN
1	B	163	GLU
1	B	221	GLU
1	B	222	GLN
1	B	223	HIS
1	C	10	GLN

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Mol	Chain	Res	Type
1	C	11	LEU
1	C	16	ALA
1	C	27	ALA
1	C	36	ASP
1	C	63	SER
1	C	65	VAL
1	C	113	PRO
1	C	142	GLN
1	C	197	LEU
1	C	252	SER
1	C	253	LEU
1	D	40	ALA
1	D	81	GLU
1	D	99	VAL
1	D	106	LYS
1	D	129	ARG
1	D	167	ILE
1	D	170	VAL
1	E	42	VAL
1	E	43	SER
1	E	78	ILE
1	E	130	GLU
1	E	142	GLN
1	E	167	ILE
1	E	170	VAL
1	E	218	LEU
1	E	222	GLN
1	E	274	GLN
1	A	60	VAL
1	A	62	HIS
1	A	98	GLY
1	A	102	SER
1	A	105	GLU
1	A	127	VAL
1	A	129	ARG
1	A	164	GLU
1	A	223	HIS
1	A	234	PRO
1	B	19	PHE
1	B	24	VAL
1	B	29	LYS
1	B	76	PRO

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Mol	Chain	Res	Type
1	B	143	VAL
1	B	177	GLY
1	B	252	SER
1	B	270	SER
1	C	47	LYS
1	C	64	ASP
1	C	72	PRO
1	C	139	THR
1	C	150	GLU
1	C	262	CYS
1	D	39	LEU
1	D	90	HIS
1	D	164	GLU
1	D	199	ARG
1	D	223	HIS
1	E	14	ALA
1	E	50	VAL
1	E	59	THR
1	E	74	ILE
1	E	80	ASP
1	E	88	ASP
1	E	113	PRO
1	E	177	GLY
1	B	16	ALA
1	B	83	GLY
1	B	144	GLU
1	B	154	SER
1	B	160	THR
1	C	25	LEU
1	C	40	ALA
1	C	46	ARG
1	C	62	HIS
1	C	107	LYS
1	C	167	ILE
1	C	173	LEU
1	D	110	ALA
1	D	253	LEU
1	D	256	ASN
1	E	36	ASP
1	E	41	THR
1	E	44	ALA
1	E	129	ARG

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Mol	Chain	Res	Type
1	E	151	GLN
1	E	223	HIS
1	E	237	ALA
1	E	250	PHE
1	A	27	ALA
1	B	20	THR
1	B	64	ASP
1	B	234	PRO
1	B	237	ALA
1	C	61	GLN
1	C	140	HIS
1	C	263	ILE
1	D	41	THR
1	D	96	ALA
1	D	237	ALA
1	D	267	GLU
1	E	100	THR
1	E	125	PRO
1	E	199	ARG
1	A	25	LEU
1	A	111	PHE
1	A	125	PRO
1	A	220	SER
1	B	27	ALA
1	C	248	GLY
1	C	259	GLU
1	D	125	PRO
1	D	224	PRO
1	E	34	SER
1	E	141	ALA
1	E	221	GLU
1	A	56	ASN
1	A	110	ALA
1	A	252	SER
1	D	234	PRO
1	E	178	PRO
1	A	104	ILE
1	D	112	ARG
1	E	234	PRO
1	B	235	GLY
1	C	258	VAL
1	C	76	PRO

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Mol	Chain	Res	Type
1	D	156	VAL
1	E	203	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	215/250 (86%)	177 (82%)	38 (18%)	2	9
1	B	213/250 (85%)	196 (92%)	17 (8%)	11	37
1	C	214/250 (86%)	196 (92%)	18 (8%)	10	35
1	D	215/250 (86%)	181 (84%)	34 (16%)	2	12
1	E	215/250 (86%)	195 (91%)	20 (9%)	8	31
All	All	1072/1250 (86%)	945 (88%)	127 (12%)	5	21

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	36	ASP
1	A	38	ASP
1	A	60	VAL
1	A	77	PHE
1	A	87	GLU
1	A	90	HIS
1	A	91	ILE
1	A	94	SER
1	A	102	SER
1	A	107	LYS
1	A	118	ILE
1	A	120	CYS
1	A	121	MET
1	A	123	ASN
1	A	126	VAL
1	A	134	VAL

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Mol	Chain	Res	Type
1	A	139	THR
1	A	143	VAL
1	A	148	LEU
1	A	149	MET
1	A	150	GLU
1	A	171	THR
1	A	194	LYS
1	A	195	MET
1	A	205	LEU
1	A	210	LEU
1	A	211	LEU
1	A	221	GLU
1	A	234	PRO
1	A	244	VAL
1	A	247	SER
1	A	251	ARG
1	A	253	LEU
1	A	258	VAL
1	A	265	THR
1	A	269	GLN
1	A	271	MET
1	B	5	PHE
1	B	10	GLN
1	B	47	LYS
1	B	64	ASP
1	B	90	HIS
1	B	120	CYS
1	B	124	THR
1	B	133	THR
1	B	140	HIS
1	B	161	GLU
1	B	163	GLU
1	B	170	VAL
1	B	174	SER
1	B	211	LEU
1	B	216	MET
1	B	233	SER
1	B	265	THR
1	C	45	LEU
1	C	51	LYS
1	C	61	GLN
1	C	72	PRO

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Mol	Chain	Res	Type
1	C	90	HIS
1	C	121	MET
1	C	123	ASN
1	C	124	THR
1	C	152	LEU
1	C	190	ASP
1	C	195	MET
1	C	200	ARG
1	C	211	LEU
1	C	216	MET
1	C	228	LYS
1	C	232	SER
1	C	247	SER
1	C	273	ASP
1	D	2	SER
1	D	11	LEU
1	D	15	LEU
1	D	31	MET
1	D	37	MET
1	D	50	VAL
1	D	65	VAL
1	D	66	LEU
1	D	68	LEU
1	D	73	HIS
1	D	76	PRO
1	D	79	LEU
1	D	86	ILE
1	D	95	CYS
1	D	100	THR
1	D	101	ILE
1	D	118	ILE
1	D	120	CYS
1	D	122	THR
1	D	124	THR
1	D	127	VAL
1	D	142	GLN
1	D	144	GLU
1	D	153	LEU
1	D	159	CYS
1	D	203	VAL
1	D	208	GLN
1	D	211	LEU

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Mol	Chain	Res	Type
1	D	215	LYS
1	D	217	LEU
1	D	231	VAL
1	D	239	ILE
1	D	244	VAL
1	D	258	VAL
1	E	48	MET
1	E	57	LYS
1	E	70	VAL
1	E	77	PHE
1	E	104	ILE
1	E	117	VAL
1	E	120	CYS
1	E	121	MET
1	E	123	ASN
1	E	127	VAL
1	E	151	GLN
1	E	160	THR
1	E	168	ASP
1	E	174	SER
1	E	178	PRO
1	E	195	MET
1	E	211	LEU
1	E	216	MET
1	E	217	LEU
1	E	233	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	61	GLN
1	A	90	HIS
1	A	123	ASN
1	A	140	HIS
1	A	240	HIS
1	B	56	ASN
1	B	140	HIS
1	B	142	GLN
1	B	243	HIS
1	C	10	GLN
1	C	73	HIS

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Mol	Chain	Res	Type
1	C	90	HIS
1	C	142	GLN
1	C	240	HIS
1	C	243	HIS
1	C	269	GLN
1	D	28	HIS
1	D	140	HIS
1	D	240	HIS
1	E	28	HIS
1	E	222	GLN
1	E	226	GLN
1	E	240	HIS
1	E	274	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/321 (86%)	-0.16	1 (0%) 88 76	27, 79, 115, 154	0
1	B	276/321 (85%)	0.23	10 (3%) 46 26	26, 120, 172, 187	0
1	C	277/321 (86%)	0.28	19 (6%) 23 12	23, 117, 169, 183	0
1	D	277/321 (86%)	-0.23	1 (0%) 88 76	24, 70, 117, 163	0
1	E	277/321 (86%)	-0.19	1 (0%) 88 76	23, 78, 126, 156	0
All	All	1384/1605 (86%)	-0.01	32 (2%) 61 39	23, 82, 160, 187	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	ALA	3.9
1	B	136	ALA	3.6
1	B	75	ILE	3.6
1	B	92	VAL	3.5
1	E	73	HIS	2.8
1	C	41	THR	2.8
1	B	275	GLU	2.7
1	C	159	CYS	2.6
1	B	48	MET	2.6
1	C	25	LEU	2.6
1	D	39	LEU	2.6
1	B	146	GLY	2.5
1	C	98	GLY	2.4
1	C	54	PRO	2.4
1	B	24	VAL	2.4
1	C	6	ILE	2.3
1	C	118	ILE	2.3
1	C	92	VAL	2.3
1	B	84	ALA	2.2
1	C	24	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	26	ALA	2.2
1	C	153	LEU	2.1
1	C	96	ALA	2.1
1	C	32	ALA	2.1
1	C	136	ALA	2.1
1	B	5	PHE	2.1
1	C	146	GLY	2.0
1	C	94	SER	2.0
1	A	111	PHE	2.0
1	C	71	LYS	2.0
1	C	70	VAL	2.0
1	B	39	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.