



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:13 AM UTC

PDB ID : 2TMG / pdb_00002tmg
Title : THERMOTOGA MARITIMA GLUTAMATE DEHYDROGENASE MUTANT S128R, T158E, N117R, S160E
Authors : Knapp, S.; Lebbink, J.H.G.; van der Oost, J.; de Vos, W.M.; Rice, D.; Ladenstein, R.
Deposited on : 1998-12-04
Resolution : 2.90 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

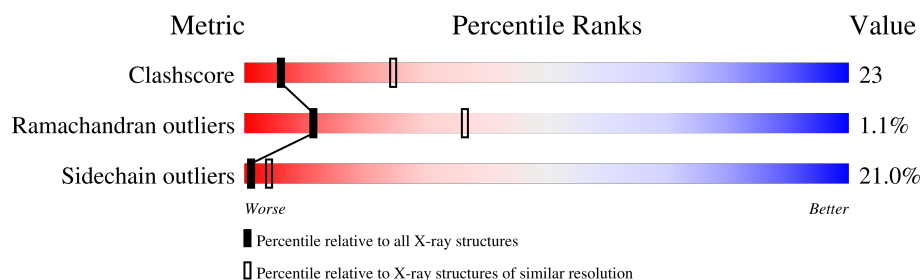
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	415	
1	B	415	
1	C	415	
1	D	415	
1	E	415	
1	F	415	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 19032 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 PROTEIN (GLUTAMATE DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3172	2013	556	590	13			
1	B	408	Total	C	N	O	S	0	0	0
			3172	2013	556	590	13			
1	C	408	Total	C	N	O	S	0	0	0
			3172	2013	556	590	13			
1	D	408	Total	C	N	O	S	0	0	0
			3172	2013	556	590	13			
1	E	408	Total	C	N	O	S	0	0	0
			3172	2013	556	590	13			
1	F	408	Total	C	N	O	S	0	0	0
			3172	2013	556	590	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	ASN	engineered mutation	UNP P96110
A	128	ARG	SER	engineered mutation	UNP P96110
A	158	GLU	THR	engineered mutation	UNP P96110
A	160	GLU	SER	engineered mutation	UNP P96110
B	117	ARG	ASN	engineered mutation	UNP P96110
B	128	ARG	SER	engineered mutation	UNP P96110
B	158	GLU	THR	engineered mutation	UNP P96110
B	160	GLU	SER	engineered mutation	UNP P96110
C	117	ARG	ASN	engineered mutation	UNP P96110
C	128	ARG	SER	engineered mutation	UNP P96110
C	158	GLU	THR	engineered mutation	UNP P96110
C	160	GLU	SER	engineered mutation	UNP P96110
D	117	ARG	ASN	engineered mutation	UNP P96110
D	128	ARG	SER	engineered mutation	UNP P96110
D	158	GLU	THR	engineered mutation	UNP P96110
D	160	GLU	SER	engineered mutation	UNP P96110
E	117	ARG	ASN	engineered mutation	UNP P96110

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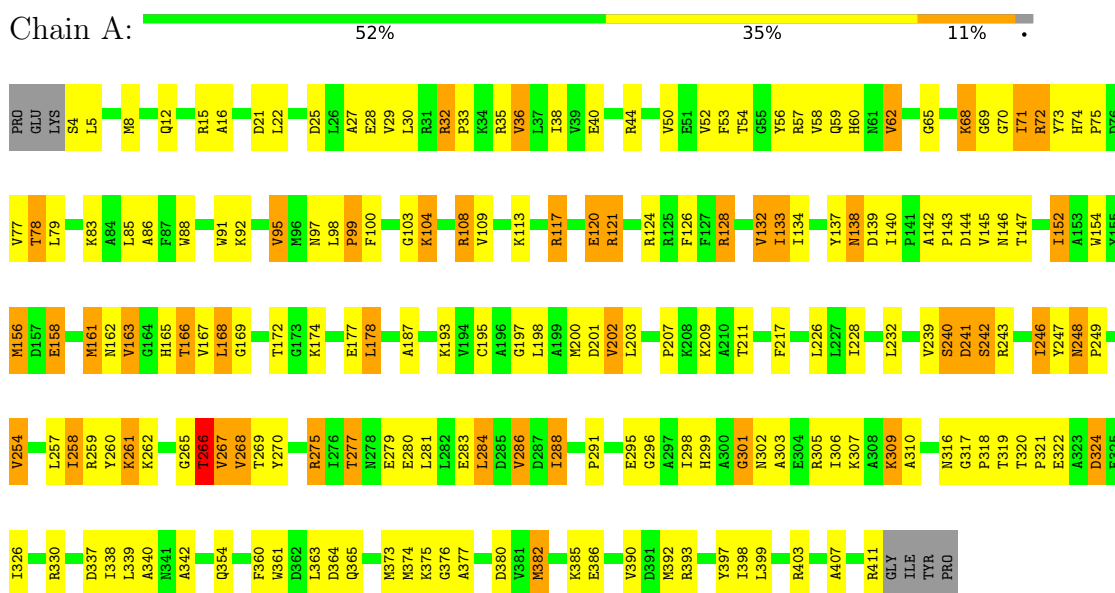
Chain	Residue	Modelled	Actual	Comment	Reference
E	128	ARG	SER	engineered mutation	UNP P96110
E	158	GLU	THR	engineered mutation	UNP P96110
E	160	GLU	SER	engineered mutation	UNP P96110
F	117	ARG	ASN	engineered mutation	UNP P96110
F	128	ARG	SER	engineered mutation	UNP P96110
F	158	GLU	THR	engineered mutation	UNP P96110
F	160	GLU	SER	engineered mutation	UNP P96110

3 Residue-property plots

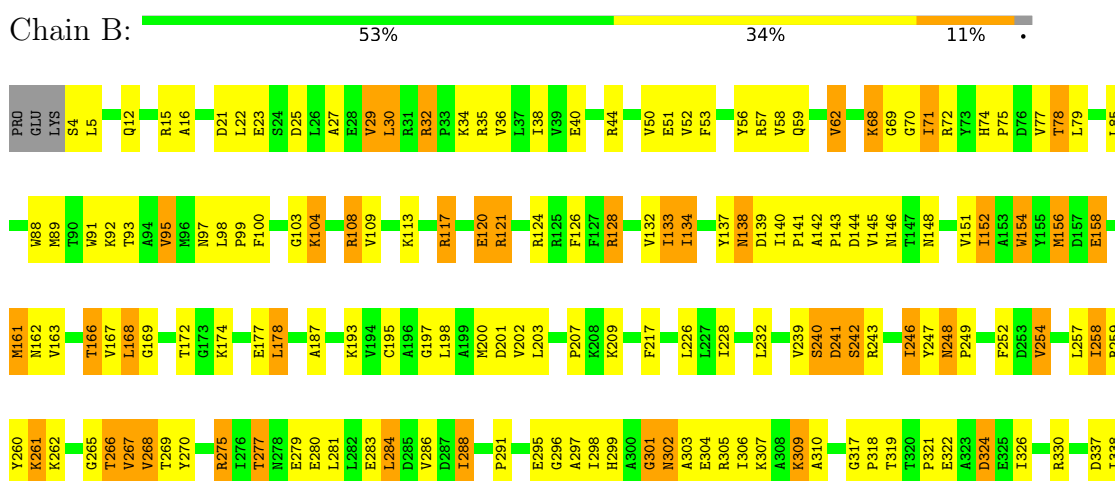
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

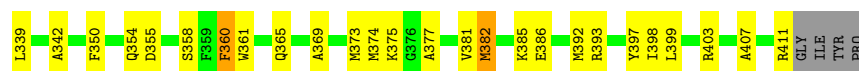
Note EDS was not executed.

• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)



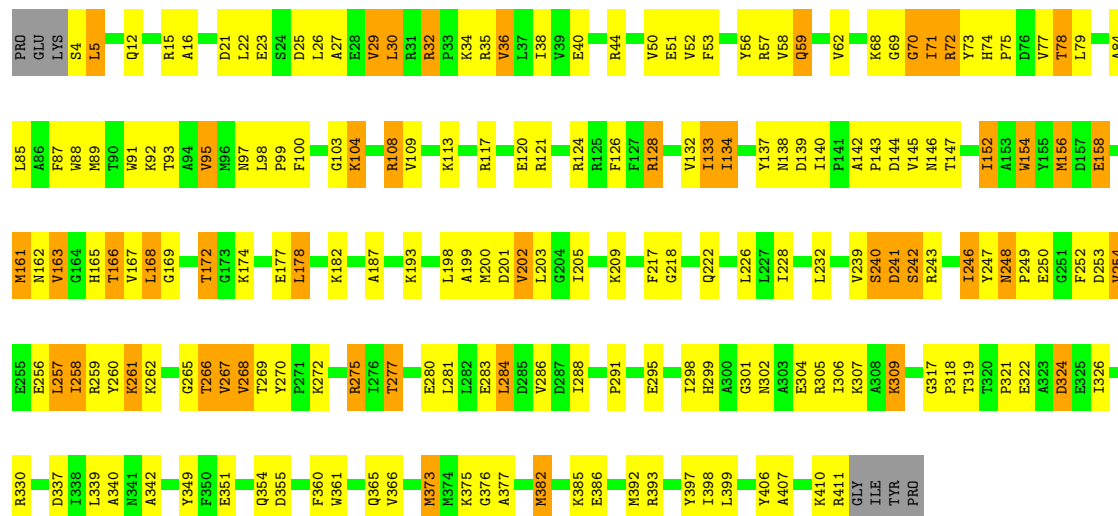
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)





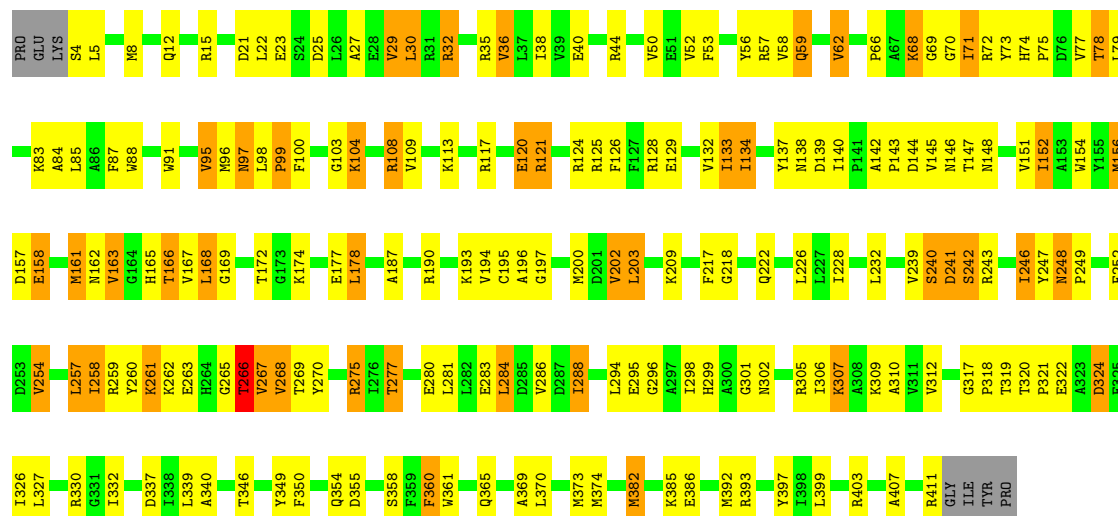
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

Chain C: 52% 35% 11%



• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

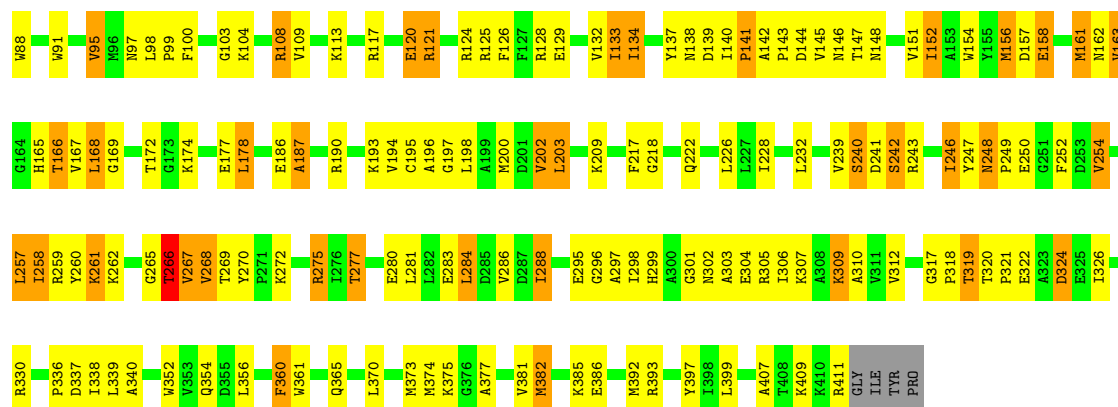
Chain D: 52% 35% 11%



• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

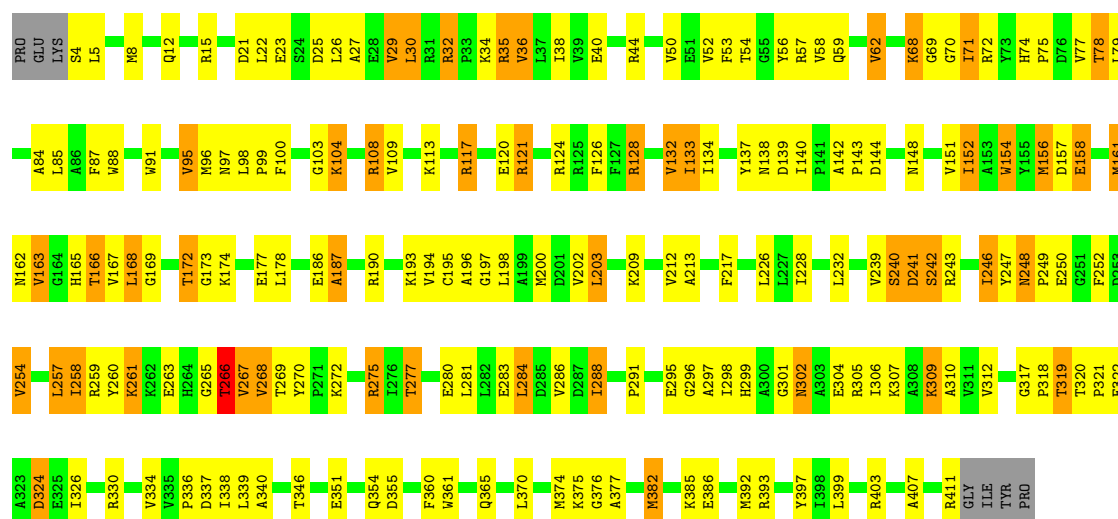
Chain E: 51% 37% 11%





• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

Chain F: 51% 35% 12% •



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.10Å 145.10Å 272.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	98.0 (8.00-2.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.211 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19032	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.51	0/3231	0.87	5/4371 (0.1%)
1	B	0.45	0/3231	0.87	5/4371 (0.1%)
1	C	0.46	0/3231	0.89	7/4371 (0.2%)
1	D	0.44	0/3231	0.87	7/4371 (0.2%)
1	E	0.50	0/3231	0.89	5/4371 (0.1%)
1	F	0.49	0/3231	0.88	4/4371 (0.1%)
All	All	0.48	0/19386	0.88	33/26226 (0.1%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	340	ALA	N-CA-C	6.55	118.08	111.07
1	A	242	SER	N-CA-C	-6.38	105.48	113.20
1	F	242	SER	N-CA-C	-6.11	105.80	113.20
1	C	242	SER	N-CA-C	-6.04	105.90	113.20
1	E	340	ALA	N-CA-C	5.95	118.25	111.11
1	E	242	SER	N-CA-C	-5.88	106.09	113.20
1	B	242	SER	N-CA-C	-5.83	106.15	113.20
1	D	242	SER	N-CA-C	-5.81	106.17	113.20
1	C	340	ALA	N-CA-C	5.79	117.27	111.07
1	B	360	PHE	N-CA-C	5.79	118.67	109.24
1	D	349	TYR	N-CA-C	-5.63	105.06	111.14
1	D	134	ILE	N-CA-C	5.50	117.10	109.29
1	D	340	ALA	N-CA-C	5.49	117.69	111.11
1	C	134	ILE	N-CA-C	5.41	116.97	109.29
1	C	154	TRP	N-CA-C	-5.38	105.58	111.82
1	D	360	PHE	N-CA-C	5.38	118.01	109.24
1	E	266	THR	N-CA-C	5.35	117.12	109.14
1	C	349	TYR	N-CA-C	-5.35	105.35	111.07
1	D	294	LEU	N-CA-C	-5.34	101.41	109.85
1	F	154	TRP	N-CA-C	-5.30	105.67	111.82
1	A	301	GLY	N-CA-C	5.29	119.29	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	THR	N-CA-C	5.28	117.00	109.14
1	B	154	TRP	N-CA-C	-5.25	105.72	111.82
1	B	301	GLY	N-CA-C	5.19	118.92	112.64
1	C	70	GLY	N-CA-C	5.12	120.35	112.51
1	E	360	PHE	N-CA-C	5.11	117.30	109.07
1	A	86	ALA	N-CA-C	-5.11	105.60	111.07
1	C	34	LYS	N-CA-C	5.11	116.53	111.07
1	D	266	THR	N-CA-C	5.11	116.75	109.14
1	F	266	THR	N-CA-C	5.08	116.71	109.14
1	A	340	ALA	N-CA-C	5.06	117.18	111.11
1	E	134	ILE	N-CA-C	5.03	116.43	109.29
1	B	134	ILE	N-CA-C	5.02	116.41	109.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3172	0	3196	144	0
1	B	3172	0	3196	140	0
1	C	3172	0	3196	143	0
1	D	3172	0	3196	152	0
1	E	3172	0	3196	163	0
1	F	3172	0	3196	148	0
All	All	19032	0	19176	866	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 23.

All (866) 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:243:ARG:HD3	1:D:266:THR:HG21	1.24	1.16
1:A:243:ARG:HD3	1:A:266:THR:HG21	1.29	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:HD3	1:B:266:THR:HG21	1.29	1.12
1:C:243:ARG:HD3	1:C:266:THR:HG21	1.25	1.09
1:F:243:ARG:HD3	1:F:266:THR:HG21	1.32	1.08
1:E:243:ARG:HD3	1:E:266:THR:HG21	1.33	1.08
1:E:156:MET:HE3	1:E:174:LYS:HD2	1.42	1.02
1:C:156:MET:HE3	1:C:174:LYS:HD2	1.43	0.97
1:D:156:MET:HE3	1:D:174:LYS:HD2	1.48	0.94
1:F:36:VAL:HG22	1:F:58:VAL:HG22	1.49	0.93
1:A:156:MET:HE3	1:A:174:LYS:HD2	1.51	0.93
1:B:156:MET:HE3	1:B:174:LYS:HD2	1.52	0.92
1:C:36:VAL:HG22	1:C:58:VAL:HG22	1.52	0.91
1:E:36:VAL:HG22	1:E:58:VAL:HG22	1.53	0.91
1:E:200:MET:HG3	1:E:288:ILE:HD11	1.55	0.88
1:D:36:VAL:HG22	1:D:58:VAL:HG22	1.55	0.87
1:A:36:VAL:HG22	1:A:58:VAL:HG22	1.55	0.87
1:C:88:TRP:HZ3	1:C:397:TYR:CE1	1.92	0.86
1:F:156:MET:HE3	1:F:174:LYS:HD2	1.55	0.86
1:B:36:VAL:HG22	1:B:58:VAL:HG22	1.54	0.86
1:A:88:TRP:HZ3	1:A:397:TYR:CE1	1.95	0.84
1:E:91:TRP:O	1:E:95:VAL:HG12	1.78	0.84
1:E:200:MET:HG3	1:E:288:ILE:CD1	2.10	0.82
1:D:277:THR:HG23	1:D:280:GLU:HB2	1.61	0.81
1:A:277:THR:HG23	1:A:280:GLU:HB2	1.60	0.81
1:A:88:TRP:HZ3	1:A:397:TYR:HE1	1.27	0.81
1:B:277:THR:HG23	1:B:280:GLU:HB2	1.62	0.80
1:F:200:MET:HG3	1:F:288:ILE:CD1	2.11	0.80
1:F:277:THR:HG23	1:F:280:GLU:HB2	1.62	0.80
1:D:200:MET:HG3	1:D:288:ILE:CD1	2.13	0.79
1:E:277:THR:HG23	1:E:280:GLU:HB2	1.63	0.79
1:C:88:TRP:HZ3	1:C:397:TYR:HE1	1.28	0.78
1:D:243:ARG:CD	1:D:266:THR:HG21	2.11	0.78
1:B:91:TRP:O	1:B:95:VAL:HG12	1.84	0.78
1:F:200:MET:HG3	1:F:288:ILE:HD11	1.67	0.77
1:C:243:ARG:CD	1:C:266:THR:HG21	2.10	0.77
1:D:91:TRP:O	1:D:95:VAL:HG12	1.85	0.76
1:E:124:ARG:HH11	1:E:158:GLU:HG2	1.50	0.76
1:C:277:THR:HG23	1:C:280:GLU:HB2	1.68	0.75
1:E:156:MET:HE2	1:E:168:LEU:HB2	1.69	0.75
1:C:91:TRP:O	1:C:95:VAL:HG12	1.86	0.75
1:D:200:MET:HG3	1:D:288:ILE:HD11	1.69	0.75
1:B:156:MET:HE2	1:B:168:LEU:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:HH11	1:D:158:GLU:HG2	1.54	0.72
1:E:243:ARG:CD	1:E:266:THR:HG21	2.17	0.72
1:E:166:THR:HG23	1:F:137:TYR:O	1.89	0.72
1:A:128:ARG:HH11	1:E:161:MET:HB3	1.55	0.72
1:C:124:ARG:HH11	1:C:158:GLU:HG2	1.55	0.72
1:B:124:ARG:HH11	1:B:158:GLU:HG2	1.55	0.71
1:C:156:MET:HE2	1:C:168:LEU:HB2	1.73	0.71
1:D:156:MET:HE2	1:D:168:LEU:HB2	1.72	0.71
1:A:91:TRP:O	1:A:95:VAL:HG12	1.91	0.71
1:F:326:ILE:O	1:F:330:ARG:HG3	1.91	0.70
1:E:59:GLN:HE22	1:E:133:ILE:CG2	2.05	0.70
1:C:88:TRP:CZ3	1:C:397:TYR:HE1	2.10	0.69
1:A:243:ARG:CD	1:A:266:THR:HG21	2.16	0.69
1:A:137:TYR:O	1:C:166:THR:HG23	1.93	0.69
1:A:166:THR:HG23	1:B:137:TYR:O	1.92	0.69
1:C:198:LEU:O	1:C:202:VAL:HG13	1.92	0.69
1:E:75:PRO:O	1:E:108:ARG:HD3	1.93	0.69
1:F:243:ARG:CD	1:F:266:THR:HG21	2.19	0.69
1:D:247:TYR:CE2	1:D:249:PRO:HD3	2.28	0.69
1:F:156:MET:HE2	1:F:168:LEU:HB2	1.73	0.68
1:F:247:TYR:CE2	1:F:249:PRO:HD3	2.28	0.68
1:A:120:GLU:HA	1:A:154:TRP:CE3	2.29	0.68
1:D:240:SER:HB3	1:D:281:LEU:HD13	1.75	0.68
1:A:88:TRP:CZ3	1:A:397:TYR:HE1	2.10	0.68
1:C:156:MET:HE3	1:C:174:LYS:CD	2.23	0.68
1:C:240:SER:HB3	1:C:281:LEU:HD13	1.74	0.67
1:D:393:ARG:HG2	1:D:397:TYR:HE2	1.59	0.67
1:E:32:ARG:HG2	1:E:32:ARG:HH11	1.59	0.67
1:B:88:TRP:HZ3	1:B:397:TYR:CE1	2.13	0.67
1:A:200:MET:HE1	1:A:232:LEU:HD13	1.77	0.67
1:A:393:ARG:HG2	1:A:397:TYR:HE2	1.60	0.67
1:F:75:PRO:O	1:F:108:ARG:HD3	1.95	0.67
1:A:75:PRO:O	1:A:108:ARG:HD3	1.93	0.67
1:C:317:GLY:N	1:C:318:PRO:HD3	2.10	0.67
1:D:137:TYR:O	1:F:166:THR:HG23	1.95	0.67
1:C:247:TYR:CE2	1:C:249:PRO:HD3	2.30	0.67
1:A:124:ARG:HH11	1:A:158:GLU:HG2	1.60	0.66
1:E:88:TRP:HZ3	1:E:397:TYR:HE1	1.44	0.66
1:A:240:SER:HB3	1:A:281:LEU:HD13	1.76	0.66
1:B:200:MET:HE1	1:B:232:LEU:HD13	1.76	0.66
1:E:32:ARG:HG2	1:E:32:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLY:N	1:A:318:PRO:HD3	2.10	0.66
1:B:59:GLN:HE22	1:B:133:ILE:CG2	2.08	0.66
1:C:22:LEU:HD23	1:C:27:ALA:HB2	1.76	0.66
1:E:22:LEU:HD23	1:E:27:ALA:HB2	1.78	0.65
1:A:217:PHE:HD2	1:A:261:LYS:HG3	1.62	0.65
1:C:88:TRP:CZ3	1:C:397:TYR:CE1	2.81	0.65
1:F:91:TRP:O	1:F:95:VAL:HG12	1.97	0.65
1:A:382:MET:O	1:A:385:LYS:HB3	1.97	0.65
1:B:393:ARG:HG2	1:B:397:TYR:HE2	1.60	0.65
1:C:217:PHE:HD2	1:C:261:LYS:HG3	1.62	0.65
1:E:156:MET:HE3	1:E:174:LYS:CD	2.23	0.64
1:A:88:TRP:CZ3	1:A:397:TYR:CE1	2.83	0.64
1:F:22:LEU:HD23	1:F:27:ALA:HB2	1.79	0.64
1:B:240:SER:HB3	1:B:281:LEU:HD13	1.77	0.64
1:B:243:ARG:CD	1:B:266:THR:HG21	2.16	0.64
1:E:326:ILE:O	1:E:330:ARG:HG3	1.97	0.64
1:B:88:TRP:HZ3	1:B:397:TYR:HE1	1.46	0.64
1:B:317:GLY:N	1:B:318:PRO:HD3	2.13	0.64
1:C:393:ARG:HG2	1:C:397:TYR:HE2	1.63	0.63
1:E:71:ILE:HD13	1:E:126:PHE:HE2	1.64	0.63
1:E:196:ALA:HA	1:E:312:VAL:HG21	1.79	0.63
1:B:268:VAL:O	1:B:269:THR:HB	1.98	0.63
1:F:240:SER:HB3	1:F:281:LEU:HD13	1.78	0.63
1:A:120:GLU:HG3	1:A:154:TRP:CE2	2.34	0.63
1:E:228:ILE:O	1:E:232:LEU:HB2	1.99	0.63
1:E:268:VAL:O	1:E:269:THR:HB	1.98	0.62
1:F:217:PHE:HD2	1:F:261:LYS:HG3	1.62	0.62
1:D:228:ILE:O	1:D:232:LEU:HB2	1.99	0.62
1:D:22:LEU:HD23	1:D:27:ALA:HB2	1.80	0.62
1:C:161:MET:HB3	1:F:128:ARG:HH11	1.64	0.62
1:C:120:GLU:HG3	1:C:154:TRP:CE2	2.35	0.62
1:B:228:ILE:O	1:B:232:LEU:HB2	1.99	0.62
1:E:247:TYR:CE2	1:E:249:PRO:HD3	2.35	0.62
1:F:196:ALA:HA	1:F:312:VAL:HG21	1.81	0.62
1:F:120:GLU:HG3	1:F:154:TRP:CE2	2.35	0.62
1:B:32:ARG:HG2	1:B:32:ARG:HH11	1.65	0.61
1:B:75:PRO:O	1:B:108:ARG:HD3	1.99	0.61
1:C:354:GLN:HG2	1:C:360:PHE:HA	1.81	0.61
1:B:120:GLU:HG3	1:B:154:TRP:CE2	2.34	0.61
1:B:247:TYR:CE2	1:B:249:PRO:HD3	2.35	0.61
1:B:266:THR:OG1	1:B:268:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:SER:HB3	1:E:281:LEU:HD13	1.81	0.61
1:F:317:GLY:N	1:F:318:PRO:HD3	2.15	0.61
1:B:124:ARG:HB3	1:B:158:GLU:HG3	1.82	0.61
1:A:247:TYR:CE2	1:A:249:PRO:HD3	2.35	0.61
1:D:166:THR:HG23	1:E:137:TYR:O	2.00	0.61
1:E:317:GLY:N	1:E:318:PRO:HD3	2.15	0.61
1:E:120:GLU:HG3	1:E:154:TRP:CE2	2.36	0.61
1:C:228:ILE:O	1:C:232:LEU:HB2	2.01	0.61
1:C:268:VAL:O	1:C:269:THR:HB	2.01	0.61
1:A:22:LEU:HD23	1:A:27:ALA:HB2	1.83	0.61
1:D:266:THR:OG1	1:D:268:VAL:HG23	1.99	0.61
1:A:268:VAL:O	1:A:269:THR:HB	2.00	0.61
1:E:53:PHE:HE2	1:E:109:VAL:HG23	1.66	0.61
1:A:120:GLU:O	1:A:124:ARG:HG3	2.01	0.60
1:A:156:MET:HE2	1:A:168:LEU:HB2	1.82	0.60
1:A:354:GLN:HG2	1:A:360:PHE:HA	1.82	0.60
1:D:217:PHE:HD2	1:D:261:LYS:HG3	1.65	0.60
1:E:59:GLN:HE21	1:E:139:ASP:CG	2.09	0.60
1:D:196:ALA:HA	1:D:312:VAL:HG21	1.84	0.60
1:C:53:PHE:HE2	1:C:109:VAL:HG23	1.66	0.60
1:D:120:GLU:HG3	1:D:154:TRP:CE2	2.36	0.60
1:B:124:ARG:NH1	1:B:158:GLU:HG2	2.15	0.60
1:D:71:ILE:HD13	1:D:126:PHE:HE2	1.66	0.60
1:B:354:GLN:HG2	1:B:360:PHE:HA	1.82	0.60
1:E:277:THR:HG22	1:E:280:GLU:OE1	2.02	0.60
1:C:16:ALA:HB1	1:C:398:ILE:HG13	1.84	0.60
1:C:71:ILE:HD13	1:C:126:PHE:HE2	1.67	0.60
1:E:200:MET:HE2	1:E:288:ILE:HD13	1.84	0.60
1:B:32:ARG:HG2	1:B:32:ARG:NH1	2.15	0.59
1:C:266:THR:OG1	1:C:268:VAL:HG23	2.01	0.59
1:D:317:GLY:N	1:D:318:PRO:HD3	2.17	0.59
1:E:217:PHE:HD2	1:E:261:LYS:HG3	1.67	0.59
1:D:134:ILE:HG22	1:D:139:ASP:HB3	1.83	0.59
1:D:59:GLN:HE22	1:D:133:ILE:CG2	2.15	0.59
1:D:88:TRP:HZ3	1:D:397:TYR:HE1	1.49	0.59
1:B:68:LYS:NZ	1:B:140:ILE:O	2.35	0.59
1:B:407:ALA:O	1:B:411:ARG:HG3	2.03	0.59
1:D:74:HIS:ND1	1:D:75:PRO:HD2	2.18	0.59
1:F:38:ILE:HG23	1:F:56:TYR:CD2	2.37	0.59
1:F:120:GLU:HA	1:F:154:TRP:CE3	2.38	0.59
1:A:198:LEU:HD11	1:A:375:LYS:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLU:O	1:B:307:LYS:HD2	2.02	0.59
1:C:72:ARG:HG3	1:C:144:ASP:OD1	2.03	0.59
1:E:59:GLN:HE22	1:E:133:ILE:HG23	1.68	0.59
1:F:268:VAL:O	1:F:269:THR:HB	2.02	0.59
1:A:59:GLN:HE21	1:A:139:ASP:HB2	1.65	0.59
1:D:53:PHE:HE2	1:D:109:VAL:HG23	1.66	0.59
1:B:22:LEU:HD23	1:B:27:ALA:HB2	1.84	0.59
1:B:156:MET:HE3	1:B:174:LYS:CD	2.30	0.59
1:C:361:TRP:HB3	1:C:365:GLN:NE2	2.17	0.59
1:D:268:VAL:O	1:D:269:THR:HB	2.02	0.59
1:F:354:GLN:HG2	1:F:360:PHE:HA	1.84	0.59
1:B:59:GLN:HE22	1:B:133:ILE:HG23	1.67	0.59
1:F:200:MET:HG3	1:F:288:ILE:HD13	1.85	0.59
1:B:326:ILE:O	1:B:330:ARG:HG3	2.03	0.58
1:C:59:GLN:HE21	1:C:139:ASP:CG	2.11	0.58
1:D:407:ALA:O	1:D:411:ARG:HG3	2.03	0.58
1:E:134:ILE:HG22	1:E:139:ASP:HB3	1.84	0.58
1:F:283:GLU:O	1:F:307:LYS:HD2	2.03	0.58
1:C:326:ILE:O	1:C:330:ARG:HG3	2.03	0.58
1:D:75:PRO:O	1:D:108:ARG:HD3	2.04	0.58
1:F:393:ARG:HG2	1:F:397:TYR:HE2	1.68	0.58
1:E:68:LYS:NZ	1:E:140:ILE:O	2.36	0.58
1:C:124:ARG:NH1	1:C:158:GLU:HG2	2.17	0.58
1:F:53:PHE:HE2	1:F:109:VAL:HG23	1.69	0.58
1:F:298:ILE:HG23	1:F:306:ILE:HD11	1.86	0.58
1:A:59:GLN:NE2	1:A:139:ASP:HB2	2.18	0.58
1:C:283:GLU:O	1:C:307:LYS:HD2	2.03	0.58
1:E:69:GLY:HA3	1:E:103:GLY:O	2.03	0.58
1:E:283:GLU:O	1:E:307:LYS:HD2	2.04	0.57
1:C:199:ALA:O	1:C:202:VAL:HG22	2.04	0.57
1:B:53:PHE:HE2	1:B:109:VAL:HG23	1.68	0.57
1:E:298:ILE:HG23	1:E:306:ILE:HD11	1.86	0.57
1:B:177:GLU:CD	1:B:177:GLU:H	2.12	0.57
1:C:32:ARG:NH1	1:C:32:ARG:HG2	2.19	0.57
1:E:254:VAL:O	1:E:258:ILE:HG13	2.04	0.57
1:F:59:GLN:NE2	1:F:139:ASP:HB2	2.20	0.57
1:F:71:ILE:HD13	1:F:126:PHE:HE2	1.70	0.57
1:A:132:VAL:HG12	1:F:132:VAL:HG12	1.87	0.57
1:D:326:ILE:O	1:D:330:ARG:HG3	2.03	0.57
1:C:198:LEU:O	1:C:201:ASP:HB2	2.04	0.57
1:D:68:LYS:NZ	1:D:140:ILE:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:THR:CG2	1:E:280:GLU:HB2	2.34	0.57
1:D:156:MET:HE3	1:D:174:LYS:CD	2.29	0.57
1:F:59:GLN:HE21	1:F:139:ASP:HB2	1.69	0.57
1:F:120:GLU:O	1:F:124:ARG:HG3	2.05	0.57
1:A:177:GLU:CD	1:A:177:GLU:H	2.13	0.57
1:D:124:ARG:NH1	1:D:158:GLU:HG2	2.19	0.57
1:F:228:ILE:O	1:F:232:LEU:HB2	2.05	0.57
1:D:200:MET:HG3	1:D:288:ILE:HD13	1.87	0.56
1:F:74:HIS:ND1	1:F:75:PRO:HD2	2.20	0.56
1:A:53:PHE:HE2	1:A:109:VAL:HG23	1.70	0.56
1:B:74:HIS:ND1	1:B:75:PRO:HD2	2.20	0.56
1:B:217:PHE:HD2	1:B:261:LYS:HG3	1.69	0.56
1:B:393:ARG:HG2	1:B:397:TYR:CE2	2.40	0.56
1:F:85:LEU:HB3	1:F:104:LYS:HE2	1.88	0.56
1:A:69:GLY:HA3	1:A:103:GLY:O	2.05	0.56
1:A:266:THR:OG1	1:A:268:VAL:HG23	2.04	0.56
1:C:59:GLN:HE22	1:C:133:ILE:CG2	2.18	0.56
1:E:124:ARG:NH1	1:E:158:GLU:HG2	2.18	0.56
1:E:266:THR:OG1	1:E:268:VAL:HG23	2.06	0.56
1:F:168:LEU:HD12	1:F:355:ASP:HB3	1.86	0.56
1:A:16:ALA:HB1	1:A:398:ILE:HG13	1.87	0.56
1:B:299:HIS:HD2	1:B:301:GLY:H	1.54	0.56
1:C:142:ALA:HB1	1:C:143:PRO:HD2	1.88	0.56
1:C:200:MET:HG2	1:C:205:ILE:HB	1.87	0.56
1:C:321:PRO:O	1:C:324:ASP:HB2	2.06	0.56
1:C:32:ARG:HG2	1:C:32:ARG:HH11	1.70	0.56
1:E:321:PRO:O	1:E:324:ASP:HB2	2.05	0.56
1:E:393:ARG:HG2	1:E:397:TYR:HE2	1.69	0.56
1:B:36:VAL:HG22	1:B:58:VAL:CG2	2.33	0.56
1:E:88:TRP:HZ3	1:E:397:TYR:CE1	2.23	0.56
1:E:120:GLU:HA	1:E:154:TRP:CE3	2.41	0.56
1:C:120:GLU:HA	1:C:154:TRP:CE3	2.40	0.56
1:C:134:ILE:HG22	1:C:139:ASP:HB3	1.87	0.56
1:F:382:MET:O	1:F:385:LYS:HB3	2.06	0.56
1:B:241:ASP:CG	1:B:266:THR:HB	2.31	0.56
1:D:393:ARG:HG2	1:D:397:TYR:CE2	2.39	0.56
1:E:36:VAL:HG22	1:E:58:VAL:CG2	2.33	0.56
1:E:124:ARG:HB3	1:E:158:GLU:HG3	1.88	0.56
1:E:382:MET:O	1:E:385:LYS:HB3	2.05	0.56
1:F:254:VAL:O	1:F:258:ILE:HG13	2.05	0.56
1:A:74:HIS:ND1	1:A:75:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:CYS:SG	1:A:374:MET:HE2	2.45	0.55
1:A:393:ARG:HG2	1:A:397:TYR:CE2	2.41	0.55
1:C:59:GLN:HE22	1:C:133:ILE:HG23	1.71	0.55
1:D:382:MET:O	1:D:385:LYS:HB3	2.06	0.55
1:E:120:GLU:O	1:E:124:ARG:HG3	2.05	0.55
1:F:32:ARG:NH1	1:F:32:ARG:HG2	2.20	0.55
1:C:69:GLY:HA3	1:C:103:GLY:O	2.07	0.55
1:D:32:ARG:NH1	1:D:32:ARG:HG2	2.21	0.55
1:B:38:ILE:HG23	1:B:56:TYR:CD2	2.42	0.55
1:C:124:ARG:HB3	1:C:158:GLU:HG3	1.87	0.55
1:D:59:GLN:HE22	1:D:133:ILE:HG23	1.71	0.55
1:D:354:GLN:HG2	1:D:360:PHE:HA	1.89	0.55
1:E:128:ARG:HD3	1:E:162:ASN:HD21	1.70	0.55
1:E:74:HIS:ND1	1:E:75:PRO:HD2	2.22	0.55
1:A:326:ILE:O	1:A:330:ARG:HG3	2.06	0.55
1:C:382:MET:O	1:C:385:LYS:HB3	2.07	0.55
1:C:68:LYS:NZ	1:C:140:ILE:O	2.40	0.55
1:D:280:GLU:O	1:D:284:LEU:HD23	2.06	0.55
1:E:361:TRP:HB3	1:E:365:GLN:NE2	2.22	0.55
1:F:399:LEU:O	1:F:399:LEU:HD12	2.06	0.55
1:A:198:LEU:O	1:A:201:ASP:HB2	2.06	0.55
1:B:71:ILE:HD13	1:B:126:PHE:HE2	1.72	0.55
1:C:75:PRO:O	1:C:108:ARG:HD3	2.06	0.54
1:B:128:ARG:HH11	1:D:161:MET:HB3	1.72	0.54
1:D:124:ARG:HB3	1:D:158:GLU:HG3	1.88	0.54
1:C:393:ARG:HG2	1:C:397:TYR:CE2	2.42	0.54
1:E:354:GLN:HG2	1:E:360:PHE:HA	1.90	0.54
1:B:120:GLU:HA	1:B:154:TRP:CE3	2.43	0.54
1:B:167:VAL:HG12	1:B:169:GLY:H	1.72	0.54
1:B:277:THR:HG22	1:B:280:GLU:OE1	2.07	0.54
1:A:277:THR:HG22	1:A:280:GLU:OE1	2.08	0.54
1:D:59:GLN:HE21	1:D:139:ASP:HB2	1.73	0.54
1:D:241:ASP:CG	1:D:266:THR:HB	2.32	0.54
1:A:167:VAL:O	1:A:168:LEU:HG	2.06	0.54
1:B:382:MET:O	1:B:385:LYS:HB3	2.08	0.54
1:E:246:ILE:HD11	1:E:257:LEU:HD21	1.90	0.54
1:F:32:ARG:HG2	1:F:32:ARG:HH11	1.73	0.54
1:A:197:GLY:HA2	1:A:200:MET:HE3	1.89	0.54
1:D:88:TRP:HZ3	1:D:397:TYR:CE1	2.25	0.54
1:D:277:THR:HG22	1:D:280:GLU:OE1	2.08	0.54
1:C:74:HIS:ND1	1:C:75:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ARG:HG2	1:D:32:ARG:HH11	1.73	0.54
1:E:177:GLU:H	1:E:177:GLU:CD	2.15	0.54
1:B:120:GLU:O	1:B:124:ARG:HG3	2.08	0.53
1:D:120:GLU:HA	1:D:154:TRP:CE3	2.43	0.53
1:C:59:GLN:NE2	1:C:139:ASP:HB2	2.23	0.53
1:C:120:GLU:O	1:C:124:ARG:HG3	2.07	0.53
1:D:59:GLN:NE2	1:D:139:ASP:HB2	2.24	0.53
1:B:277:THR:CG2	1:B:280:GLU:HB2	2.36	0.53
1:C:177:GLU:H	1:C:177:GLU:CD	2.16	0.53
1:F:246:ILE:HD11	1:F:257:LEU:HD21	1.91	0.53
1:F:407:ALA:O	1:F:411:ARG:HG3	2.08	0.53
1:A:59:GLN:HE21	1:A:139:ASP:CB	2.21	0.53
1:C:254:VAL:O	1:C:258:ILE:HG13	2.08	0.53
1:F:266:THR:OG1	1:F:268:VAL:HG23	2.08	0.53
1:C:198:LEU:HD11	1:C:375:LYS:HA	1.91	0.53
1:D:246:ILE:HD11	1:D:257:LEU:HD21	1.90	0.53
1:A:277:THR:CG2	1:A:280:GLU:HB2	2.35	0.53
1:D:241:ASP:OD2	1:D:267:VAL:HG22	2.09	0.53
1:D:361:TRP:HB3	1:D:365:GLN:NE2	2.23	0.53
1:B:59:GLN:HE21	1:B:139:ASP:CG	2.16	0.53
1:A:361:TRP:HB3	1:A:365:GLN:NE2	2.24	0.53
1:D:120:GLU:O	1:D:124:ARG:HG3	2.09	0.53
1:F:361:TRP:HB3	1:F:365:GLN:NE2	2.24	0.53
1:C:168:LEU:HD12	1:C:355:ASP:CG	2.34	0.52
1:F:142:ALA:HB1	1:F:143:PRO:HD2	1.91	0.52
1:B:268:VAL:O	1:B:269:THR:CB	2.56	0.52
1:D:283:GLU:O	1:D:307:LYS:HD2	2.10	0.52
1:F:195:CYS:SG	1:F:374:MET:HE2	2.49	0.52
1:A:228:ILE:O	1:A:232:LEU:HB2	2.09	0.52
1:C:59:GLN:HE21	1:C:139:ASP:HB2	1.73	0.52
1:D:98:LEU:C	1:D:100:PHE:H	2.15	0.52
1:A:321:PRO:O	1:A:324:ASP:HB2	2.08	0.52
1:F:36:VAL:HG22	1:F:58:VAL:CG2	2.31	0.52
1:F:124:ARG:HH11	1:F:158:GLU:HG2	1.75	0.52
1:F:152:ILE:HG23	1:F:174:LYS:HG2	1.91	0.52
1:A:280:GLU:O	1:A:284:LEU:HD23	2.10	0.52
1:D:254:VAL:O	1:D:258:ILE:HG13	2.09	0.52
1:F:277:THR:HG22	1:F:280:GLU:OE1	2.10	0.52
1:A:317:GLY:N	1:A:318:PRO:CD	2.72	0.52
1:B:198:LEU:O	1:B:201:ASP:HB2	2.09	0.52
1:B:198:LEU:HD11	1:B:375:LYS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ILE:HD11	1:C:257:LEU:HD21	1.90	0.52
1:E:268:VAL:O	1:E:269:THR:CB	2.56	0.52
1:F:241:ASP:CG	1:F:266:THR:HB	2.35	0.52
1:C:36:VAL:HG22	1:C:58:VAL:CG2	2.34	0.52
1:C:268:VAL:O	1:C:269:THR:CB	2.58	0.52
1:D:59:GLN:HE21	1:D:139:ASP:CG	2.17	0.52
1:E:142:ALA:HB1	1:E:143:PRO:HD2	1.91	0.52
1:F:59:GLN:HE22	1:F:133:ILE:HG23	1.75	0.52
1:D:298:ILE:HG23	1:D:306:ILE:HD11	1.92	0.52
1:F:268:VAL:O	1:F:269:THR:CB	2.57	0.52
1:A:98:LEU:O	1:A:100:PHE:N	2.41	0.52
1:D:98:LEU:O	1:D:100:PHE:N	2.36	0.52
1:E:59:GLN:OE1	1:E:133:ILE:HG23	2.09	0.52
1:E:194:VAL:HG11	1:E:374:MET:HB3	1.92	0.52
1:A:32:ARG:NH1	1:A:32:ARG:HG2	2.26	0.51
1:B:62:VAL:O	1:B:62:VAL:HG13	2.11	0.51
1:B:195:CYS:SG	1:B:374:MET:HE2	2.49	0.51
1:A:98:LEU:C	1:A:100:PHE:H	2.18	0.51
1:B:167:VAL:O	1:B:168:LEU:HG	2.10	0.51
1:D:277:THR:CG2	1:D:280:GLU:HB2	2.37	0.51
1:B:361:TRP:HB3	1:B:365:GLN:NE2	2.26	0.51
1:E:59:GLN:NE2	1:E:133:ILE:CG2	2.72	0.51
1:E:98:LEU:C	1:E:100:PHE:H	2.17	0.51
1:E:241:ASP:OD2	1:E:267:VAL:HG22	2.11	0.51
1:F:173:GLY:H	1:F:351:GLU:CD	2.19	0.51
1:A:85:LEU:HB3	1:A:104:LYS:HE2	1.91	0.51
1:D:36:VAL:HG22	1:D:58:VAL:CG2	2.36	0.51
1:E:382:MET:SD	1:E:392:MET:HE3	2.51	0.51
1:B:134:ILE:HG22	1:B:139:ASP:HB3	1.91	0.51
1:A:124:ARG:NH1	1:A:158:GLU:HG2	2.25	0.51
1:C:298:ILE:HG23	1:C:306:ILE:HD11	1.93	0.51
1:D:321:PRO:O	1:D:324:ASP:HB2	2.10	0.51
1:A:59:GLN:HE22	1:A:133:ILE:HG23	1.76	0.51
1:D:268:VAL:O	1:D:269:THR:CB	2.58	0.51
1:A:59:GLN:HE21	1:A:139:ASP:CG	2.17	0.51
1:C:128:ARG:HD3	1:C:162:ASN:HD21	1.76	0.51
1:C:241:ASP:OD2	1:C:267:VAL:HG22	2.11	0.51
1:B:254:VAL:O	1:B:258:ILE:HG13	2.11	0.51
1:F:177:GLU:CD	1:F:177:GLU:H	2.19	0.51
1:A:68:LYS:NZ	1:A:140:ILE:O	2.44	0.51
1:B:59:GLN:NE2	1:B:133:ILE:CG2	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:O	1:B:62:VAL:CG1	2.58	0.51
1:C:241:ASP:CG	1:C:266:THR:HB	2.36	0.51
1:A:299:HIS:HD2	1:A:301:GLY:H	1.59	0.50
1:B:166:THR:HG23	1:C:137:TYR:O	2.11	0.50
1:F:268:VAL:CG1	1:F:275:ARG:HD3	2.41	0.50
1:A:124:ARG:HB3	1:A:158:GLU:HG3	1.94	0.50
1:F:88:TRP:HZ3	1:F:397:TYR:HE1	1.59	0.50
1:E:59:GLN:NE2	1:E:139:ASP:HB2	2.27	0.50
1:E:167:VAL:HG12	1:E:169:GLY:H	1.76	0.50
1:E:393:ARG:HG2	1:E:397:TYR:CE2	2.46	0.50
1:F:98:LEU:C	1:F:100:PHE:H	2.19	0.50
1:E:59:GLN:NE2	1:E:133:ILE:HG23	2.26	0.50
1:E:163:VAL:HG12	1:E:165:HIS:H	1.76	0.50
1:B:59:GLN:NE2	1:B:133:ILE:HG23	2.26	0.50
1:C:277:THR:CG2	1:C:280:GLU:HB2	2.40	0.50
1:D:177:GLU:CD	1:D:177:GLU:H	2.19	0.50
1:F:35:ARG:NH1	1:F:59:GLN:OE1	2.44	0.50
1:A:241:ASP:CG	1:A:266:THR:HB	2.37	0.50
1:A:268:VAL:CG1	1:A:275:ARG:HD3	2.42	0.50
1:A:298:ILE:HG23	1:A:306:ILE:HD11	1.94	0.50
1:B:246:ILE:HD11	1:B:257:LEU:HD21	1.92	0.50
1:E:59:GLN:HE22	1:E:133:ILE:HG22	1.76	0.50
1:F:38:ILE:HG23	1:F:56:TYR:CE2	2.47	0.50
1:F:59:GLN:HE21	1:F:139:ASP:CG	2.18	0.50
1:F:167:VAL:O	1:F:168:LEU:HG	2.11	0.50
1:A:254:VAL:O	1:A:258:ILE:HG13	2.12	0.49
1:E:98:LEU:O	1:E:100:PHE:N	2.39	0.49
1:F:134:ILE:HG22	1:F:139:ASP:HB3	1.93	0.49
1:B:98:LEU:C	1:B:100:PHE:H	2.19	0.49
1:C:71:ILE:O	1:C:144:ASP:HB3	2.12	0.49
1:F:69:GLY:HA3	1:F:103:GLY:O	2.11	0.49
1:F:124:ARG:HB3	1:F:158:GLU:HG3	1.94	0.49
1:B:85:LEU:HB3	1:B:104:LYS:HE2	1.93	0.49
1:B:247:TYR:O	1:B:248:ASN:HB2	2.13	0.49
1:C:128:ARG:HH11	1:F:161:MET:HB3	1.76	0.49
1:C:277:THR:HG22	1:C:280:GLU:OE1	2.13	0.49
1:C:280:GLU:O	1:C:284:LEU:HD23	2.12	0.49
1:B:161:MET:HB3	1:D:128:ARG:HH11	1.76	0.49
1:F:128:ARG:HD3	1:F:162:ASN:HD21	1.77	0.49
1:F:197:GLY:O	1:F:200:MET:HB2	2.11	0.49
1:A:38:ILE:HG23	1:A:56:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ILE:HG23	1:B:306:ILE:HD11	1.94	0.49
1:D:35:ARG:NH1	1:D:59:GLN:OE1	2.46	0.49
1:D:148:ASN:OD1	1:D:151:VAL:HG23	2.13	0.49
1:F:59:GLN:HE21	1:F:139:ASP:CB	2.25	0.49
1:F:68:LYS:NZ	1:F:140:ILE:O	2.45	0.49
1:F:280:GLU:O	1:F:284:LEU:HD23	2.11	0.49
1:C:98:LEU:C	1:C:100:PHE:H	2.19	0.49
1:B:92:LYS:HE2	1:B:342:ALA:HA	1.94	0.49
1:B:280:GLU:O	1:B:284:LEU:HD23	2.13	0.49
1:D:59:GLN:HE21	1:D:139:ASP:CB	2.25	0.49
1:A:407:ALA:O	1:A:411:ARG:HG3	2.13	0.49
1:C:317:GLY:N	1:C:318:PRO:CD	2.76	0.49
1:D:411:ARG:HB3	1:F:157:ASP:OD1	2.12	0.49
1:E:393:ARG:O	1:E:397:TYR:HD2	1.95	0.49
1:F:393:ARG:HG2	1:F:397:TYR:CE2	2.47	0.49
1:A:35:ARG:NH1	1:A:59:GLN:OE1	2.46	0.49
1:B:25:ASP:OD1	1:B:25:ASP:N	2.45	0.49
1:F:321:PRO:O	1:F:324:ASP:HB2	2.12	0.49
1:A:134:ILE:HG22	1:A:139:ASP:HB3	1.95	0.49
1:B:200:MET:SD	1:B:207:PRO:HA	2.53	0.48
1:C:59:GLN:HE21	1:C:139:ASP:CB	2.26	0.48
1:D:85:LEU:HB3	1:D:104:LYS:HE2	1.93	0.48
1:B:298:ILE:HD12	1:B:319:THR:HG22	1.95	0.48
1:C:167:VAL:O	1:C:168:LEU:HG	2.13	0.48
1:D:152:ILE:HG23	1:D:174:LYS:HG2	1.95	0.48
1:D:247:TYR:O	1:D:248:ASN:HB2	2.13	0.48
1:F:277:THR:CG2	1:F:280:GLU:HB2	2.37	0.48
1:A:241:ASP:OD2	1:A:267:VAL:HG22	2.13	0.48
1:F:167:VAL:HG12	1:F:169:GLY:H	1.77	0.48
1:A:71:ILE:O	1:A:144:ASP:HB3	2.13	0.48
1:C:152:ILE:HG23	1:C:174:LYS:HG2	1.96	0.48
1:E:268:VAL:CG1	1:E:275:ARG:HD3	2.43	0.48
1:C:217:PHE:CD2	1:C:261:LYS:HG3	2.48	0.48
1:D:168:LEU:HD12	1:D:355:ASP:HB3	1.95	0.48
1:E:73:TYR:CD1	1:E:147:THR:HG22	2.48	0.48
1:F:98:LEU:O	1:F:100:PHE:N	2.39	0.48
1:B:40:GLU:HA	1:B:53:PHE:O	2.13	0.48
1:C:172:THR:HA	1:C:351:GLU:OE1	2.14	0.48
1:E:88:TRP:CZ3	1:E:397:TYR:HE1	2.26	0.48
1:A:268:VAL:C	1:A:270:TYR:H	2.21	0.48
1:B:32:ARG:HH11	1:B:32:ARG:CG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:O	1:B:100:PHE:N	2.41	0.48
1:B:241:ASP:OD2	1:B:267:VAL:HG22	2.14	0.48
1:C:218:GLY:O	1:C:222:GLN:HG3	2.14	0.48
1:D:69:GLY:HA3	1:D:103:GLY:O	2.13	0.48
1:F:298:ILE:HD12	1:F:319:THR:HG22	1.95	0.48
1:F:299:HIS:HD2	1:F:301:GLY:H	1.62	0.48
1:A:32:ARG:HG2	1:A:32:ARG:HH11	1.78	0.47
1:A:128:ARG:HD3	1:A:162:ASN:HD21	1.79	0.47
1:B:32:ARG:HD3	1:E:52:VAL:HG11	1.96	0.47
1:B:152:ILE:HG23	1:B:174:LYS:HG2	1.96	0.47
1:D:62:VAL:O	1:D:62:VAL:CG1	2.60	0.47
1:F:59:GLN:HE22	1:F:133:ILE:CG2	2.28	0.47
1:F:168:LEU:HD12	1:F:168:LEU:O	2.13	0.47
1:B:268:VAL:CG1	1:B:275:ARG:HD3	2.45	0.47
1:C:22:LEU:O	1:C:23:GLU:C	2.55	0.47
1:D:268:VAL:C	1:D:270:TYR:H	2.21	0.47
1:D:298:ILE:HD12	1:D:319:THR:HG22	1.97	0.47
1:F:194:VAL:HG11	1:F:374:MET:HB3	1.97	0.47
1:A:283:GLU:O	1:A:307:LYS:HD2	2.15	0.47
1:B:321:PRO:O	1:B:324:ASP:HB2	2.14	0.47
1:D:73:TYR:CD1	1:D:147:THR:HG22	2.48	0.47
1:B:361:TRP:CD1	1:B:361:TRP:N	2.82	0.47
1:A:32:ARG:HD3	1:F:52:VAL:HG11	1.95	0.47
1:A:25:ASP:N	1:A:25:ASP:OD1	2.47	0.47
1:A:71:ILE:HD13	1:A:126:PHE:HE2	1.79	0.47
1:C:168:LEU:HD12	1:C:168:LEU:O	2.15	0.47
1:C:182:LYS:O	1:C:366:VAL:HG11	2.15	0.47
1:C:258:ILE:O	1:C:262:LYS:HG3	2.15	0.47
1:C:382:MET:SD	1:C:392:MET:HE3	2.54	0.47
1:F:241:ASP:OD2	1:F:267:VAL:HG22	2.15	0.47
1:F:268:VAL:C	1:F:270:TYR:H	2.21	0.47
1:C:337:ASP:OD2	1:C:337:ASP:N	2.45	0.47
1:E:156:MET:HE2	1:E:168:LEU:CB	2.42	0.47
1:A:243:ARG:HD3	1:A:266:THR:CG2	2.22	0.47
1:A:382:MET:SD	1:A:392:MET:HE3	2.55	0.47
1:B:52:VAL:HG11	1:E:32:ARG:HD3	1.97	0.47
1:D:157:ASP:OD1	1:E:411:ARG:HB3	2.15	0.47
1:E:337:ASP:N	1:E:337:ASP:OD2	2.47	0.47
1:D:59:GLN:NE2	1:D:133:ILE:HG23	2.30	0.47
1:E:32:ARG:HH11	1:E:32:ARG:CG	2.24	0.47
1:D:217:PHE:CD2	1:D:261:LYS:HG3	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:LEU:O	1:D:403:ARG:HG3	2.15	0.46
1:B:268:VAL:C	1:B:270:TYR:H	2.23	0.46
1:D:167:VAL:O	1:D:168:LEU:HG	2.14	0.46
1:E:299:HIS:HD2	1:E:301:GLY:H	1.63	0.46
1:F:291:PRO:HB2	1:F:318:PRO:HB3	1.97	0.46
1:A:40:GLU:OE1	1:A:54:THR:OG1	2.25	0.46
1:C:84:ALA:O	1:C:87:PHE:HB3	2.16	0.46
1:D:268:VAL:CG1	1:D:275:ARG:HD3	2.45	0.46
1:D:299:HIS:HD2	1:D:301:GLY:H	1.64	0.46
1:B:373:MET:HE2	1:B:373:MET:HB3	1.84	0.46
1:C:268:VAL:CG1	1:C:275:ARG:HD3	2.44	0.46
1:D:258:ILE:O	1:D:262:LYS:HG3	2.15	0.46
1:D:288:ILE:HG13	1:D:310:ALA:HB3	1.97	0.46
1:D:337:ASP:OD2	1:D:337:ASP:N	2.47	0.46
1:D:393:ARG:CG	1:D:397:TYR:HE2	2.27	0.46
1:A:142:ALA:HB1	1:A:143:PRO:HD2	1.97	0.46
1:A:277:THR:HG23	1:A:280:GLU:CB	2.38	0.46
1:F:96:MET:HE2	1:F:346:THR:OG1	2.15	0.46
1:F:399:LEU:O	1:F:403:ARG:HG3	2.14	0.46
1:A:70:GLY:HA2	1:A:142:ALA:O	2.16	0.46
1:A:163:VAL:HG12	1:A:165:HIS:H	1.81	0.46
1:C:203:LEU:HD23	1:C:309:LYS:HB2	1.98	0.46
1:C:299:HIS:HD2	1:C:301:GLY:H	1.64	0.46
1:D:197:GLY:O	1:D:200:MET:HB2	2.16	0.46
1:F:288:ILE:HG13	1:F:310:ALA:HB3	1.97	0.46
1:C:156:MET:HE2	1:C:168:LEU:CB	2.44	0.46
1:D:59:GLN:NE2	1:D:133:ILE:CG2	2.79	0.46
1:D:167:VAL:HG12	1:D:169:GLY:H	1.80	0.46
1:D:252:PHE:HB3	1:D:257:LEU:HD12	1.98	0.46
1:E:268:VAL:C	1:E:270:TYR:H	2.23	0.46
1:E:320:THR:HB	1:E:321:PRO:HD2	1.98	0.46
1:E:393:ARG:CG	1:E:397:TYR:HE2	2.28	0.46
1:A:62:VAL:O	1:A:62:VAL:CG1	2.64	0.46
1:B:317:GLY:N	1:B:318:PRO:CD	2.79	0.46
1:C:52:VAL:HG11	1:D:32:ARG:HD3	1.98	0.46
1:C:268:VAL:C	1:C:270:TYR:H	2.24	0.46
1:D:142:ALA:HB1	1:D:143:PRO:HD2	1.97	0.46
1:A:78:THR:O	1:A:79:LEU:C	2.59	0.46
1:A:268:VAL:O	1:A:269:THR:CB	2.60	0.46
1:B:35:ARG:NH1	1:B:59:GLN:OE1	2.49	0.46
1:B:124:ARG:HB3	1:B:158:GLU:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:PHE:HB3	1:C:257:LEU:HD12	1.98	0.46
1:D:393:ARG:O	1:D:397:TYR:HD2	1.99	0.46
1:E:59:GLN:HE21	1:E:139:ASP:CB	2.29	0.46
1:E:247:TYR:O	1:E:248:ASN:HB2	2.15	0.46
1:B:156:MET:HE1	1:B:178:LEU:O	2.16	0.46
1:B:377:ALA:O	1:B:381:VAL:HG23	2.16	0.46
1:E:168:LEU:HD12	1:E:168:LEU:O	2.16	0.46
1:E:248:ASN:OD1	1:E:250:GLU:HB2	2.16	0.46
1:E:407:ALA:O	1:E:411:ARG:HG3	2.16	0.46
1:D:44:ARG:NH1	1:D:44:ARG:HG3	2.30	0.45
1:E:71:ILE:O	1:E:144:ASP:HB3	2.16	0.45
1:E:148:ASN:OD1	1:E:151:VAL:HG23	2.16	0.45
1:E:352:TRP:CZ2	1:E:356:LEU:HD11	2.51	0.45
1:F:361:TRP:CD1	1:F:361:TRP:N	2.83	0.45
1:C:163:VAL:HG12	1:C:165:HIS:H	1.80	0.45
1:D:62:VAL:O	1:D:62:VAL:HG13	2.16	0.45
1:C:247:TYR:O	1:C:248:ASN:HB2	2.15	0.45
1:D:399:LEU:O	1:D:399:LEU:HD12	2.16	0.45
1:F:317:GLY:N	1:F:318:PRO:CD	2.79	0.45
1:A:59:GLN:HE22	1:A:133:ILE:CG2	2.29	0.45
1:A:197:GLY:O	1:A:200:MET:HB2	2.15	0.45
1:B:124:ARG:CB	1:B:158:GLU:HG3	2.45	0.45
1:B:156:MET:HE2	1:B:168:LEU:CB	2.43	0.45
1:D:156:MET:HE1	1:D:178:LEU:O	2.16	0.45
1:E:44:ARG:NH1	1:E:44:ARG:HG3	2.31	0.45
1:E:59:GLN:HE21	1:E:139:ASP:HB2	1.81	0.45
1:F:217:PHE:CD2	1:F:261:LYS:HG3	2.47	0.45
1:A:121:ARG:HE	1:A:121:ARG:HB2	1.62	0.45
1:A:152:ILE:HG23	1:A:174:LYS:HG2	1.98	0.45
1:A:399:LEU:O	1:A:403:ARG:HG3	2.17	0.45
1:C:376:GLY:O	1:C:377:ALA:C	2.59	0.45
1:D:194:VAL:HG11	1:D:374:MET:HB3	1.98	0.45
1:E:152:ILE:HG23	1:E:174:LYS:HG2	1.97	0.45
1:E:296:GLY:O	1:E:297:ALA:C	2.59	0.45
1:F:121:ARG:HE	1:F:121:ARG:HB2	1.64	0.45
1:F:173:GLY:N	1:F:351:GLU:OE1	2.50	0.45
1:A:52:VAL:HG11	1:F:32:ARG:HD3	1.99	0.45
1:A:167:VAL:HG12	1:A:169:GLY:H	1.81	0.45
1:B:71:ILE:O	1:B:144:ASP:HB3	2.16	0.45
1:B:128:ARG:HD3	1:B:162:ASN:HD21	1.82	0.45
1:E:26:LEU:HD22	1:E:409:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:GLU:HB3	1:E:53:PHE:HE1	1.80	0.45
1:A:44:ARG:NH1	1:A:44:ARG:HG3	2.31	0.45
1:A:73:TYR:CD1	1:A:147:THR:HG22	2.52	0.45
1:C:406:TYR:OH	1:C:410:LYS:HE2	2.16	0.45
1:E:198:LEU:HD11	1:E:375:LYS:HA	1.98	0.45
1:B:44:ARG:NH1	1:B:44:ARG:HG3	2.32	0.45
1:E:124:ARG:HB3	1:E:158:GLU:CG	2.47	0.45
1:A:92:LYS:HE2	1:A:342:ALA:HA	1.99	0.45
1:B:148:ASN:OD1	1:B:151:VAL:HG23	2.16	0.45
1:C:35:ARG:NH1	1:C:59:GLN:OE1	2.50	0.45
1:D:74:HIS:O	1:D:108:ARG:HA	2.17	0.45
1:D:350:PHE:CZ	1:D:369:ALA:HB1	2.52	0.45
1:A:74:HIS:O	1:A:108:ARG:HA	2.16	0.45
1:B:203:LEU:HD23	1:B:309:LYS:HB2	1.99	0.45
1:B:393:ARG:CG	1:B:397:TYR:HE2	2.29	0.44
1:D:71:ILE:O	1:D:144:ASP:HB3	2.17	0.44
1:E:121:ARG:HE	1:E:121:ARG:HB2	1.64	0.44
1:E:217:PHE:CD2	1:E:261:LYS:HG3	2.51	0.44
1:F:163:VAL:HG12	1:F:165:HIS:H	1.82	0.44
1:C:59:GLN:NE2	1:C:133:ILE:HG23	2.32	0.44
1:C:247:TYR:CZ	1:C:249:PRO:HD3	2.52	0.44
1:D:40:GLU:HA	1:D:53:PHE:O	2.18	0.44
1:A:36:VAL:HG22	1:A:58:VAL:CG2	2.37	0.44
1:C:202:VAL:HG11	1:C:382:MET:HE2	1.99	0.44
1:E:144:ASP:CG	1:E:145:VAL:H	2.25	0.44
1:F:117:ARG:HA	1:F:117:ARG:HD3	1.73	0.44
1:A:260:TYR:CZ	1:A:270:TYR:HA	2.52	0.44
1:B:258:ILE:O	1:B:262:LYS:HG3	2.17	0.44
1:C:85:LEU:HB3	1:C:104:LYS:HE2	2.00	0.44
1:D:96:MET:HE2	1:D:346:THR:OG1	2.16	0.44
1:E:8:MET:HE2	1:E:8:MET:HB3	1.94	0.44
1:E:399:LEU:HD12	1:E:399:LEU:O	2.16	0.44
1:A:361:TRP:N	1:A:361:TRP:CD1	2.85	0.44
1:B:34:LYS:HD3	1:B:35:ARG:HG3	1.99	0.44
1:C:98:LEU:O	1:C:100:PHE:N	2.40	0.44
1:B:59:GLN:NE2	1:B:139:ASP:HB2	2.32	0.44
1:B:142:ALA:HB1	1:B:143:PRO:HD2	2.00	0.44
1:C:373:MET:HE2	1:C:373:MET:HB3	1.86	0.44
1:D:203:LEU:HD23	1:D:309:LYS:HB2	2.00	0.44
1:E:35:ARG:NH1	1:E:59:GLN:OE1	2.50	0.44
1:F:57:ARG:HD2	1:F:57:ARG:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:GLN:NE2	1:F:133:ILE:HG23	2.33	0.44
1:A:28:GLU:OE2	1:A:28:GLU:HA	2.18	0.44
1:A:57:ARG:HD2	1:A:104:LYS:O	2.18	0.44
1:C:167:VAL:HG12	1:C:169:GLY:H	1.82	0.44
1:E:25:ASP:OD1	1:E:25:ASP:N	2.49	0.44
1:E:317:GLY:N	1:E:318:PRO:CD	2.80	0.44
1:F:26:LEU:O	1:F:29:VAL:HG22	2.18	0.44
1:F:148:ASN:OD1	1:F:151:VAL:HG23	2.17	0.44
1:B:22:LEU:O	1:B:23:GLU:C	2.61	0.44
1:B:197:GLY:HA2	1:B:200:MET:HE3	2.00	0.44
1:C:407:ALA:O	1:C:411:ARG:HG3	2.17	0.44
1:F:124:ARG:HB3	1:F:158:GLU:CG	2.48	0.44
1:D:22:LEU:O	1:D:23:GLU:C	2.61	0.44
1:D:277:THR:HG23	1:D:280:GLU:CB	2.42	0.44
1:E:28:GLU:HA	1:E:28:GLU:OE2	2.18	0.44
1:E:190:ARG:HD2	1:E:370:LEU:HD23	2.00	0.44
1:F:29:VAL:HG23	1:F:30:LEU:HD23	2.00	0.44
1:F:336:PRO:HD3	1:F:392:MET:HB3	2.00	0.44
1:A:124:ARG:HB3	1:A:158:GLU:CG	2.47	0.43
1:B:57:ARG:HD2	1:B:57:ARG:HA	1.77	0.43
1:B:59:GLN:OE1	1:B:133:ILE:HG23	2.18	0.43
1:B:74:HIS:O	1:B:108:ARG:HA	2.18	0.43
1:B:296:GLY:O	1:B:297:ALA:C	2.61	0.43
1:C:57:ARG:HD2	1:C:57:ARG:HA	1.76	0.43
1:C:260:TYR:CD1	1:C:270:TYR:HD1	2.36	0.43
1:D:124:ARG:HB3	1:D:158:GLU:CG	2.48	0.43
1:E:57:ARG:HD2	1:E:57:ARG:HA	1.76	0.43
1:A:168:LEU:HD12	1:A:168:LEU:O	2.18	0.43
1:B:38:ILE:HG23	1:B:56:TYR:CE2	2.52	0.43
1:C:40:GLU:HG3	1:D:32:ARG:HB3	1.99	0.43
1:D:25:ASP:OD1	1:D:25:ASP:N	2.51	0.43
1:D:84:ALA:O	1:D:87:PHE:HB3	2.18	0.43
1:D:163:VAL:HG12	1:D:165:HIS:H	1.83	0.43
1:D:178:LEU:HD12	1:D:178:LEU:HA	1.82	0.43
1:E:298:ILE:HD12	1:E:319:THR:HG22	2.01	0.43
1:D:121:ARG:HE	1:D:121:ARG:HB2	1.58	0.43
1:F:174:LYS:NZ	1:F:355:ASP:OD2	2.50	0.43
1:F:275:ARG:HE	1:F:275:ARG:HB2	1.49	0.43
1:A:117:ARG:HA	1:A:117:ARG:HD3	1.76	0.43
1:C:291:PRO:HB2	1:C:318:PRO:HB3	2.00	0.43
1:A:33:PRO:HA	1:A:60:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:HD11	1:A:257:LEU:HD21	1.99	0.43
1:B:291:PRO:HB2	1:B:318:PRO:HB3	2.01	0.43
1:D:29:VAL:HG23	1:D:30:LEU:HD23	1.99	0.43
1:D:57:ARG:HA	1:D:57:ARG:HD2	1.78	0.43
1:A:202:VAL:HG11	1:A:382:MET:HE2	2.00	0.43
1:C:70:GLY:HA2	1:C:142:ALA:O	2.19	0.43
1:D:128:ARG:HD3	1:D:162:ASN:HD21	1.82	0.43
1:E:38:ILE:HG23	1:E:56:TYR:CD2	2.53	0.43
1:E:202:VAL:HG11	1:E:382:MET:HE2	2.00	0.43
1:E:275:ARG:HE	1:E:275:ARG:HB2	1.50	0.43
1:F:8:MET:HE2	1:F:8:MET:HB3	1.90	0.43
1:F:298:ILE:HG23	1:F:306:ILE:CD1	2.49	0.43
1:A:72:ARG:HG3	1:A:144:ASP:OD1	2.19	0.43
1:A:217:PHE:CD2	1:A:261:LYS:HG3	2.47	0.43
1:C:145:VAL:O	1:C:146:ASN:HB2	2.17	0.43
1:D:88:TRP:CZ3	1:D:397:TYR:HE1	2.34	0.43
1:F:78:THR:O	1:F:79:LEU:C	2.61	0.43
1:F:172:THR:HA	1:F:351:GLU:OE1	2.19	0.43
1:A:161:MET:HB3	1:E:128:ARG:HH11	1.84	0.43
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.84	0.43
1:C:38:ILE:HG23	1:C:56:TYR:CD2	2.53	0.43
1:C:51:GLU:HB3	1:C:53:PHE:HE1	1.83	0.43
1:F:25:ASP:OD1	1:F:25:ASP:N	2.49	0.43
1:F:247:TYR:O	1:F:248:ASN:HB2	2.18	0.43
1:A:200:MET:SD	1:A:207:PRO:HA	2.59	0.43
1:B:337:ASP:OD2	1:B:337:ASP:N	2.50	0.43
1:B:393:ARG:O	1:B:397:TYR:HD2	2.02	0.43
1:C:92:LYS:HE2	1:C:342:ALA:HA	2.01	0.43
1:D:190:ARG:HD2	1:D:370:LEU:HD23	2.01	0.43
1:D:275:ARG:HE	1:D:275:ARG:HB2	1.51	0.43
1:E:243:ARG:HD3	1:E:266:THR:CG2	2.25	0.43
1:F:168:LEU:HD12	1:F:355:ASP:CB	2.48	0.43
1:F:296:GLY:HA2	1:F:320:THR:HG23	2.01	0.43
1:D:32:ARG:HH11	1:D:32:ARG:CG	2.32	0.43
1:E:125:ARG:O	1:E:129:GLU:HG2	2.19	0.43
1:E:145:VAL:O	1:E:146:ASN:HB2	2.19	0.43
1:E:241:ASP:CG	1:E:266:THR:HB	2.44	0.43
1:F:44:ARG:NH1	1:F:44:ARG:HG3	2.33	0.43
1:F:302:ASN:OD1	1:F:302:ASN:N	2.50	0.43
1:A:288:ILE:HG13	1:A:310:ALA:HB3	2.01	0.42
1:C:260:TYR:CZ	1:C:270:TYR:HA	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:GLY:HA2	1:E:142:ALA:O	2.19	0.42
1:E:74:HIS:O	1:E:108:ARG:HA	2.19	0.42
1:E:186:GLU:O	1:E:187:ALA:C	2.62	0.42
1:F:62:VAL:O	1:F:62:VAL:HG13	2.17	0.42
1:A:62:VAL:O	1:A:62:VAL:HG13	2.20	0.42
1:C:73:TYR:CD1	1:C:147:THR:HG22	2.54	0.42
1:C:178:LEU:HD12	1:C:178:LEU:HA	1.73	0.42
1:C:200:MET:HE1	1:C:232:LEU:HD13	2.01	0.42
1:D:361:TRP:CD1	1:D:361:TRP:N	2.86	0.42
1:E:22:LEU:O	1:E:23:GLU:C	2.62	0.42
1:F:40:GLU:OE1	1:F:54:THR:OG1	2.34	0.42
1:F:70:GLY:HA2	1:F:142:ALA:O	2.18	0.42
1:A:59:GLN:NE2	1:A:133:ILE:HG23	2.33	0.42
1:B:69:GLY:HA3	1:B:103:GLY:O	2.18	0.42
1:E:51:GLU:HB3	1:E:53:PHE:CE1	2.54	0.42
1:E:156:MET:HE1	1:E:178:LEU:O	2.20	0.42
1:C:44:ARG:NH1	1:C:44:ARG:HG3	2.35	0.42
1:D:38:ILE:HG23	1:D:56:TYR:CD2	2.54	0.42
1:D:197:GLY:HA2	1:D:200:MET:HE3	2.01	0.42
1:A:302:ASN:O	1:A:303:ALA:C	2.62	0.42
1:B:88:TRP:CZ3	1:B:397:TYR:HE1	2.31	0.42
1:C:124:ARG:HB3	1:C:158:GLU:CG	2.50	0.42
1:C:399:LEU:O	1:C:399:LEU:HD12	2.19	0.42
1:D:327:LEU:CD2	1:D:332:ILE:HD12	2.50	0.42
1:D:382:MET:SD	1:D:392:MET:HE3	2.59	0.42
1:E:72:ARG:HG3	1:E:144:ASP:OD1	2.19	0.42
1:F:34:LYS:HD3	1:F:35:ARG:HG3	2.01	0.42
1:A:298:ILE:HD12	1:A:319:THR:HG22	2.00	0.42
1:E:195:CYS:SG	1:E:374:MET:HE2	2.60	0.42
1:B:138:ASN:N	1:B:138:ASN:HD22	2.18	0.42
1:C:261:LYS:HD3	1:C:261:LYS:O	2.19	0.42
1:E:34:LYS:HD3	1:E:35:ARG:HG3	2.02	0.42
1:E:197:GLY:O	1:E:200:MET:HB2	2.18	0.42
1:E:200:MET:HG3	1:E:288:ILE:HD13	1.96	0.42
1:E:258:ILE:O	1:E:262:LYS:HG3	2.19	0.42
1:F:248:ASN:OD1	1:F:250:GLU:HB2	2.19	0.42
1:A:38:ILE:HG23	1:A:56:TYR:CE2	2.55	0.42
1:A:65:GLY:HA3	1:A:99:PRO:O	2.20	0.42
1:A:316:ASN:C	1:A:318:PRO:HD3	2.45	0.42
1:B:260:TYR:CZ	1:B:270:TYR:HA	2.54	0.42
1:B:350:PHE:CZ	1:B:369:ALA:HB1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LEU:C	1:D:100:PHE:N	2.78	0.42
1:D:145:VAL:O	1:D:146:ASN:HB2	2.20	0.42
1:E:246:ILE:HG13	1:E:252:PHE:CZ	2.55	0.42
1:E:260:TYR:CZ	1:E:270:TYR:HA	2.54	0.42
1:B:260:TYR:CD1	1:B:270:TYR:HD1	2.38	0.42
1:B:78:THR:O	1:B:79:LEU:C	2.63	0.42
1:B:117:ARG:HA	1:B:117:ARG:HD3	1.80	0.42
1:C:5:LEU:HD13	1:C:5:LEU:HA	1.85	0.42
1:C:361:TRP:CD1	1:C:361:TRP:N	2.88	0.42
1:D:202:VAL:HG11	1:D:382:MET:HE2	2.02	0.42
1:F:62:VAL:O	1:F:62:VAL:CG1	2.67	0.42
1:F:186:GLU:O	1:F:187:ALA:C	2.63	0.42
1:A:8:MET:HE2	1:A:8:MET:HB3	1.92	0.41
1:A:203:LEU:HD23	1:A:309:LYS:HB2	2.00	0.41
1:A:260:TYR:CD1	1:A:270:TYR:HD1	2.37	0.41
1:B:144:ASP:CG	1:B:145:VAL:H	2.28	0.41
1:D:327:LEU:HD23	1:D:332:ILE:HD12	2.00	0.41
1:F:203:LEU:HD23	1:F:309:LYS:HB2	2.01	0.41
1:A:145:VAL:O	1:A:146:ASN:HB2	2.20	0.41
1:A:363:LEU:HD12	1:A:363:LEU:HA	1.86	0.41
1:D:70:GLY:HA2	1:D:142:ALA:O	2.20	0.41
1:D:195:CYS:SG	1:D:374:MET:HE2	2.59	0.41
1:E:377:ALA:O	1:E:381:VAL:HG23	2.19	0.41
1:F:152:ILE:CG2	1:F:174:LYS:HG2	2.50	0.41
1:F:156:MET:HE3	1:F:174:LYS:CD	2.38	0.41
1:B:121:ARG:HE	1:B:121:ARG:HB2	1.64	0.41
1:B:252:PHE:HB3	1:B:257:LEU:HD12	2.01	0.41
1:C:25:ASP:N	1:C:25:ASP:OD1	2.53	0.41
1:C:248:ASN:OD1	1:C:250:GLU:HB2	2.20	0.41
1:E:167:VAL:O	1:E:168:LEU:HG	2.20	0.41
1:F:190:ARG:HD2	1:F:370:LEU:HD23	2.00	0.41
1:F:248:ASN:ND2	1:F:272:LYS:HD3	2.35	0.41
1:A:211:THR:OG1	1:A:286:VAL:HG12	2.20	0.41
1:A:296:GLY:HA2	1:A:320:THR:HG23	2.03	0.41
1:B:70:GLY:HA2	1:B:142:ALA:O	2.20	0.41
1:C:59:GLN:OE1	1:C:133:ILE:HG23	2.20	0.41
1:E:124:ARG:CB	1:E:158:GLU:HG3	2.50	0.41
1:E:288:ILE:HG13	1:E:310:ALA:HB3	2.03	0.41
1:B:298:ILE:HB	1:B:319:THR:HG22	2.02	0.41
1:C:32:ARG:HD3	1:D:52:VAL:HG11	2.03	0.41
1:C:253:ASP:OD2	1:C:256:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LEU:O	1:E:29:VAL:HG22	2.20	0.41
1:E:62:VAL:O	1:E:62:VAL:CG1	2.65	0.41
1:E:62:VAL:O	1:E:62:VAL:HG13	2.19	0.41
1:F:212:VAL:HG12	1:F:213:ALA:N	2.35	0.41
1:F:252:PHE:HB3	1:F:257:LEU:HD12	2.01	0.41
1:F:334:VAL:O	1:F:334:VAL:HG12	2.20	0.41
1:B:288:ILE:HG13	1:B:310:ALA:HB3	2.01	0.41
1:D:66:PRO:HD2	1:D:99:PRO:O	2.20	0.41
1:D:78:THR:O	1:D:79:LEU:C	2.63	0.41
1:D:296:GLY:HA2	1:D:320:THR:HG23	2.01	0.41
1:E:337:ASP:O	1:E:338:ILE:C	2.64	0.41
1:F:260:TYR:CZ	1:F:270:TYR:HA	2.55	0.41
1:A:291:PRO:HB2	1:A:318:PRO:HB3	2.03	0.41
1:A:363:LEU:O	1:A:364:ASP:C	2.64	0.41
1:D:373:MET:HE2	1:D:373:MET:HB3	1.87	0.41
1:E:29:VAL:HG23	1:E:30:LEU:HD23	2.01	0.41
1:E:84:ALA:O	1:E:87:PHE:HB3	2.20	0.41
1:E:218:GLY:O	1:E:222:GLN:HG3	2.20	0.41
1:F:198:LEU:HD11	1:F:375:LYS:HA	2.02	0.41
1:B:168:LEU:HD12	1:B:355:ASP:CG	2.46	0.41
1:B:399:LEU:O	1:B:403:ARG:HG3	2.21	0.41
1:D:59:GLN:OE1	1:D:133:ILE:HG23	2.21	0.41
1:D:260:TYR:CZ	1:D:270:TYR:HA	2.55	0.41
1:D:317:GLY:N	1:D:318:PRO:CD	2.83	0.41
1:E:252:PHE:HB3	1:E:257:LEU:HD12	2.03	0.41
1:A:138:ASN:HD22	1:A:138:ASN:N	2.19	0.41
1:A:376:GLY:O	1:A:377:ALA:C	2.64	0.41
1:B:302:ASN:O	1:B:303:ALA:C	2.63	0.41
1:B:337:ASP:O	1:B:338:ILE:C	2.64	0.41
1:C:26:LEU:O	1:C:29:VAL:HG22	2.21	0.41
1:C:78:THR:O	1:C:79:LEU:C	2.64	0.41
1:C:203:LEU:CD2	1:C:309:LYS:HB2	2.51	0.41
1:C:248:ASN:ND2	1:C:272:LYS:HD3	2.36	0.41
1:D:156:MET:HE2	1:D:168:LEU:CB	2.46	0.41
1:D:261:LYS:HE3	1:D:266:THR:HA	2.03	0.41
1:E:248:ASN:ND2	1:E:272:LYS:HD3	2.35	0.41
1:E:260:TYR:CD1	1:E:270:TYR:HD1	2.39	0.41
1:E:336:PRO:HD3	1:E:392:MET:HB3	2.02	0.41
1:F:84:ALA:O	1:F:87:PHE:HB3	2.21	0.41
1:F:337:ASP:OD2	1:F:337:ASP:N	2.53	0.41
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:N	1:A:138:ASN:ND2	2.69	0.41
1:B:29:VAL:HG23	1:B:30:LEU:HD23	2.01	0.41
1:C:29:VAL:HG23	1:C:30:LEU:HD23	2.02	0.41
1:D:8:MET:HE2	1:D:8:MET:HB3	1.90	0.41
1:E:139:ASP:O	1:E:141:PRO:HD3	2.21	0.41
1:E:157:ASP:OD1	1:F:411:ARG:HB3	2.21	0.41
1:E:203:LEU:HD23	1:E:309:LYS:HB2	2.01	0.41
1:E:232:LEU:HA	1:E:232:LEU:HD23	1.85	0.41
1:E:257:LEU:HD22	1:E:267:VAL:HG12	2.02	0.41
1:F:337:ASP:O	1:F:338:ILE:C	2.63	0.41
1:A:380:ASP:HB3	1:A:399:LEU:HD21	2.03	0.40
1:B:89:MET:HE3	1:B:93:THR:HG23	2.03	0.40
1:E:59:GLN:CD	1:E:133:ILE:HG23	2.47	0.40
1:E:298:ILE:HG23	1:E:306:ILE:CD1	2.49	0.40
1:E:302:ASN:O	1:E:303:ALA:C	2.63	0.40
1:F:22:LEU:O	1:F:23:GLU:C	2.64	0.40
1:F:296:GLY:O	1:F:297:ALA:C	2.64	0.40
1:C:89:MET:HE3	1:C:93:THR:HG23	2.03	0.40
1:C:92:LYS:O	1:C:95:VAL:HG13	2.21	0.40
1:D:97:ASN:HD22	1:D:97:ASN:HA	1.68	0.40
1:E:280:GLU:O	1:E:284:LEU:HD23	2.21	0.40
1:E:302:ASN:OD1	1:E:302:ASN:N	2.51	0.40
1:F:71:ILE:CD1	1:F:126:PHE:HE2	2.34	0.40
1:A:144:ASP:CG	1:A:145:VAL:H	2.28	0.40
1:A:258:ILE:O	1:A:262:LYS:HG3	2.22	0.40
1:C:53:PHE:HE2	1:C:109:VAL:CG2	2.34	0.40
1:D:125:ARG:O	1:D:129:GLU:HG2	2.21	0.40
1:F:71:ILE:O	1:F:144:ASP:HB3	2.21	0.40
1:A:247:TYR:O	1:A:248:ASN:HB2	2.20	0.40
1:A:337:ASP:O	1:A:338:ILE:C	2.62	0.40
1:B:145:VAL:O	1:B:146:ASN:HB2	2.21	0.40
1:C:32:ARG:HH11	1:C:32:ARG:CG	2.30	0.40
1:D:218:GLY:O	1:D:222:GLN:HG3	2.21	0.40
1:F:32:ARG:HH11	1:F:32:ARG:CG	2.31	0.40
1:F:376:GLY:O	1:F:377:ALA:C	2.64	0.40
1:A:36:VAL:CG1	1:F:38:ILE:HD12	2.51	0.40
1:B:16:ALA:HB1	1:B:398:ILE:HG13	2.04	0.40
1:B:51:GLU:HB3	1:B:53:PHE:HE1	1.87	0.40
1:B:138:ASN:N	1:B:138:ASN:ND2	2.69	0.40
1:B:382:MET:SD	1:B:392:MET:HE3	2.61	0.40
1:C:59:GLN:NE2	1:C:133:ILE:CG2	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:LEU:HD23	1:D:232:LEU:HA	1.96	0.40
1:D:393:ARG:O	1:D:397:TYR:CD2	2.74	0.40
1:E:44:ARG:HG3	1:E:44:ARG:HH11	1.86	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	406/415 (98%)	363 (89%)	39 (10%)	4 (1%)	12	39
1	B	406/415 (98%)	364 (90%)	36 (9%)	6 (2%)	8	28
1	C	406/415 (98%)	362 (89%)	40 (10%)	4 (1%)	12	39
1	D	406/415 (98%)	371 (91%)	30 (7%)	5 (1%)	10	34
1	E	406/415 (98%)	366 (90%)	35 (9%)	5 (1%)	10	34
1	F	406/415 (98%)	369 (91%)	33 (8%)	4 (1%)	12	39
All	All	2436/2490 (98%)	2195 (90%)	213 (9%)	28 (1%)	11	36

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ALA
1	A	265	GLY
1	B	187	ALA
1	B	265	GLY
1	C	187	ALA
1	C	265	GLY
1	D	187	ALA
1	D	265	GLY
1	E	187	ALA

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Mol	Chain	Res	Type
1	E	265	GLY
1	F	187	ALA
1	F	265	GLY
1	B	358	SER
1	B	248	ASN
1	D	248	ASN
1	D	358	SER
1	E	248	ASN
1	B	141	PRO
1	C	248	ASN
1	D	99	PRO
1	E	99	PRO
1	F	248	ASN
1	A	248	ASN
1	C	99	PRO
1	E	141	PRO
1	F	99	PRO
1	B	99	PRO
1	A	99	PRO

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	332/338 (98%)	262 (79%)	70 (21%)	1	4
1	B	332/338 (98%)	264 (80%)	68 (20%)	1	4
1	C	332/338 (98%)	262 (79%)	70 (21%)	1	4
1	D	332/338 (98%)	261 (79%)	71 (21%)	1	4
1	E	332/338 (98%)	264 (80%)	68 (20%)	1	4
1	F	332/338 (98%)	260 (78%)	72 (22%)	1	3
All	All	1992/2028 (98%)	1573 (79%)	419 (21%)	1	4

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	5	LEU
1	A	12	GLN
1	A	15	ARG
1	A	21	ASP
1	A	29	VAL
1	A	30	LEU
1	A	32	ARG
1	A	36	VAL
1	A	50	VAL
1	A	62	VAL
1	A	68	LYS
1	A	71	ILE
1	A	72	ARG
1	A	77	VAL
1	A	78	THR
1	A	83	LYS
1	A	95	VAL
1	A	97	ASN
1	A	104	LYS
1	A	108	ARG
1	A	113	LYS
1	A	117	ARG
1	A	120	GLU
1	A	121	ARG
1	A	128	ARG
1	A	132	VAL
1	A	133	ILE
1	A	138	ASN
1	A	152	ILE
1	A	156	MET
1	A	158	GLU
1	A	161	MET
1	A	163	VAL
1	A	166	THR
1	A	168	LEU
1	A	172	THR
1	A	178	LEU
1	A	193	LYS
1	A	202	VAL
1	A	209	LYS
1	A	226	LEU
1	A	239	VAL

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Mol	Chain	Res	Type
1	A	240	SER
1	A	241	ASP
1	A	242	SER
1	A	246	ILE
1	A	254	VAL
1	A	258	ILE
1	A	259	ARG
1	A	261	LYS
1	A	266	THR
1	A	267	VAL
1	A	268	VAL
1	A	275	ARG
1	A	277	THR
1	A	279	GLU
1	A	284	LEU
1	A	286	VAL
1	A	288	ILE
1	A	295	GLU
1	A	305	ARG
1	A	309	LYS
1	A	322	GLU
1	A	324	ASP
1	A	339	LEU
1	A	373	MET
1	A	382	MET
1	A	386	GLU
1	A	390	VAL
1	B	4	SER
1	B	5	LEU
1	B	12	GLN
1	B	15	ARG
1	B	21	ASP
1	B	29	VAL
1	B	30	LEU
1	B	32	ARG
1	B	50	VAL
1	B	62	VAL
1	B	68	LYS
1	B	71	ILE
1	B	72	ARG
1	B	77	VAL
1	B	78	THR

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Mol	Chain	Res	Type
1	B	95	VAL
1	B	97	ASN
1	B	104	LYS
1	B	108	ARG
1	B	113	LYS
1	B	117	ARG
1	B	120	GLU
1	B	121	ARG
1	B	128	ARG
1	B	132	VAL
1	B	133	ILE
1	B	138	ASN
1	B	152	ILE
1	B	156	MET
1	B	158	GLU
1	B	161	MET
1	B	163	VAL
1	B	166	THR
1	B	168	LEU
1	B	172	THR
1	B	178	LEU
1	B	193	LYS
1	B	202	VAL
1	B	209	LYS
1	B	226	LEU
1	B	239	VAL
1	B	240	SER
1	B	241	ASP
1	B	242	SER
1	B	246	ILE
1	B	254	VAL
1	B	258	ILE
1	B	259	ARG
1	B	261	LYS
1	B	266	THR
1	B	267	VAL
1	B	268	VAL
1	B	275	ARG
1	B	277	THR
1	B	279	GLU
1	B	284	LEU
1	B	286	VAL

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Mol	Chain	Res	Type
1	B	288	ILE
1	B	295	GLU
1	B	302	ASN
1	B	304	GLU
1	B	305	ARG
1	B	309	LYS
1	B	322	GLU
1	B	324	ASP
1	B	339	LEU
1	B	382	MET
1	B	386	GLU
1	C	4	SER
1	C	5	LEU
1	C	12	GLN
1	C	15	ARG
1	C	21	ASP
1	C	29	VAL
1	C	30	LEU
1	C	32	ARG
1	C	36	VAL
1	C	50	VAL
1	C	59	GLN
1	C	62	VAL
1	C	71	ILE
1	C	72	ARG
1	C	77	VAL
1	C	78	THR
1	C	95	VAL
1	C	97	ASN
1	C	104	LYS
1	C	108	ARG
1	C	113	LYS
1	C	117	ARG
1	C	121	ARG
1	C	128	ARG
1	C	132	VAL
1	C	133	ILE
1	C	138	ASN
1	C	152	ILE
1	C	156	MET
1	C	158	GLU
1	C	161	MET

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Mol	Chain	Res	Type
1	C	163	VAL
1	C	166	THR
1	C	168	LEU
1	C	172	THR
1	C	178	LEU
1	C	193	LYS
1	C	202	VAL
1	C	209	LYS
1	C	226	LEU
1	C	239	VAL
1	C	240	SER
1	C	241	ASP
1	C	242	SER
1	C	246	ILE
1	C	254	VAL
1	C	257	LEU
1	C	258	ILE
1	C	259	ARG
1	C	261	LYS
1	C	266	THR
1	C	267	VAL
1	C	268	VAL
1	C	275	ARG
1	C	277	THR
1	C	284	LEU
1	C	286	VAL
1	C	288	ILE
1	C	295	GLU
1	C	302	ASN
1	C	304	GLU
1	C	305	ARG
1	C	309	LYS
1	C	319	THR
1	C	322	GLU
1	C	324	ASP
1	C	339	LEU
1	C	373	MET
1	C	382	MET
1	C	386	GLU
1	D	4	SER
1	D	5	LEU
1	D	12	GLN

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Mol	Chain	Res	Type
1	D	15	ARG
1	D	21	ASP
1	D	29	VAL
1	D	30	LEU
1	D	32	ARG
1	D	36	VAL
1	D	50	VAL
1	D	59	GLN
1	D	62	VAL
1	D	68	LYS
1	D	71	ILE
1	D	72	ARG
1	D	77	VAL
1	D	78	THR
1	D	83	LYS
1	D	95	VAL
1	D	97	ASN
1	D	104	LYS
1	D	108	ARG
1	D	113	LYS
1	D	117	ARG
1	D	120	GLU
1	D	121	ARG
1	D	132	VAL
1	D	133	ILE
1	D	138	ASN
1	D	152	ILE
1	D	156	MET
1	D	158	GLU
1	D	161	MET
1	D	163	VAL
1	D	166	THR
1	D	168	LEU
1	D	172	THR
1	D	178	LEU
1	D	193	LYS
1	D	202	VAL
1	D	203	LEU
1	D	209	LYS
1	D	226	LEU
1	D	239	VAL
1	D	240	SER

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Mol	Chain	Res	Type
1	D	241	ASP
1	D	242	SER
1	D	246	ILE
1	D	254	VAL
1	D	257	LEU
1	D	258	ILE
1	D	259	ARG
1	D	261	LYS
1	D	263	GLU
1	D	266	THR
1	D	267	VAL
1	D	268	VAL
1	D	275	ARG
1	D	277	THR
1	D	284	LEU
1	D	286	VAL
1	D	288	ILE
1	D	295	GLU
1	D	302	ASN
1	D	305	ARG
1	D	307	LYS
1	D	322	GLU
1	D	324	ASP
1	D	339	LEU
1	D	382	MET
1	D	386	GLU
1	E	4	SER
1	E	5	LEU
1	E	12	GLN
1	E	15	ARG
1	E	21	ASP
1	E	29	VAL
1	E	32	ARG
1	E	50	VAL
1	E	59	GLN
1	E	62	VAL
1	E	68	LYS
1	E	71	ILE
1	E	72	ARG
1	E	77	VAL
1	E	78	THR
1	E	95	VAL

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Mol	Chain	Res	Type
1	E	97	ASN
1	E	104	LYS
1	E	108	ARG
1	E	113	LYS
1	E	117	ARG
1	E	120	GLU
1	E	121	ARG
1	E	132	VAL
1	E	133	ILE
1	E	138	ASN
1	E	152	ILE
1	E	156	MET
1	E	158	GLU
1	E	161	MET
1	E	163	VAL
1	E	166	THR
1	E	168	LEU
1	E	172	THR
1	E	178	LEU
1	E	193	LYS
1	E	202	VAL
1	E	203	LEU
1	E	209	LYS
1	E	226	LEU
1	E	239	VAL
1	E	240	SER
1	E	242	SER
1	E	246	ILE
1	E	254	VAL
1	E	257	LEU
1	E	258	ILE
1	E	259	ARG
1	E	261	LYS
1	E	266	THR
1	E	267	VAL
1	E	268	VAL
1	E	275	ARG
1	E	277	THR
1	E	284	LEU
1	E	286	VAL
1	E	288	ILE
1	E	295	GLU

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Mol	Chain	Res	Type
1	E	304	GLU
1	E	305	ARG
1	E	309	LYS
1	E	319	THR
1	E	322	GLU
1	E	324	ASP
1	E	339	LEU
1	E	373	MET
1	E	382	MET
1	E	386	GLU
1	F	4	SER
1	F	5	LEU
1	F	12	GLN
1	F	15	ARG
1	F	21	ASP
1	F	29	VAL
1	F	30	LEU
1	F	32	ARG
1	F	35	ARG
1	F	36	VAL
1	F	50	VAL
1	F	62	VAL
1	F	68	LYS
1	F	71	ILE
1	F	72	ARG
1	F	77	VAL
1	F	78	THR
1	F	95	VAL
1	F	97	ASN
1	F	104	LYS
1	F	108	ARG
1	F	113	LYS
1	F	117	ARG
1	F	121	ARG
1	F	128	ARG
1	F	132	VAL
1	F	133	ILE
1	F	138	ASN
1	F	152	ILE
1	F	156	MET
1	F	158	GLU
1	F	161	MET

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Mol	Chain	Res	Type
1	F	163	VAL
1	F	166	THR
1	F	168	LEU
1	F	172	THR
1	F	178	LEU
1	F	193	LYS
1	F	202	VAL
1	F	203	LEU
1	F	209	LYS
1	F	226	LEU
1	F	239	VAL
1	F	240	SER
1	F	241	ASP
1	F	242	SER
1	F	246	ILE
1	F	254	VAL
1	F	257	LEU
1	F	258	ILE
1	F	259	ARG
1	F	261	LYS
1	F	263	GLU
1	F	266	THR
1	F	267	VAL
1	F	268	VAL
1	F	275	ARG
1	F	277	THR
1	F	284	LEU
1	F	286	VAL
1	F	288	ILE
1	F	295	GLU
1	F	302	ASN
1	F	304	GLU
1	F	305	ARG
1	F	309	LYS
1	F	319	THR
1	F	322	GLU
1	F	324	ASP
1	F	339	LEU
1	F	382	MET
1	F	386	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	97	ASN
1	A	131	GLN
1	A	162	ASN
1	A	165	HIS
1	A	219	ASN
1	A	278	ASN
1	A	299	HIS
1	A	365	GLN
1	A	368	ASN
1	B	12	GLN
1	B	59	GLN
1	B	97	ASN
1	B	131	GLN
1	B	162	ASN
1	B	165	HIS
1	B	219	ASN
1	B	278	ASN
1	B	299	HIS
1	B	365	GLN
1	C	12	GLN
1	C	97	ASN
1	C	131	GLN
1	C	138	ASN
1	C	162	ASN
1	C	165	HIS
1	C	219	ASN
1	C	230	GLN
1	C	278	ASN
1	C	365	GLN
1	C	368	ASN
1	D	12	GLN
1	D	59	GLN
1	D	97	ASN
1	D	138	ASN
1	D	162	ASN
1	D	165	HIS
1	D	219	ASN
1	D	278	ASN
1	D	357	GLN
1	D	365	GLN
1	E	97	ASN
1	E	131	GLN

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Mol	Chain	Res	Type
1	E	138	ASN
1	E	162	ASN
1	E	165	HIS
1	E	219	ASN
1	E	278	ASN
1	E	299	HIS
1	E	365	GLN
1	E	368	ASN
1	F	12	GLN
1	F	97	ASN
1	F	131	GLN
1	F	162	ASN
1	F	165	HIS
1	F	219	ASN
1	F	230	GLN
1	F	278	ASN
1	F	299	HIS
1	F	357	GLN
1	F	365	GLN
1	F	368	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.