



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:33 PM UTC

PDB ID : 1BVU / pdb_00001bvu
Title : GLUTAMATE DEHYDROGENASE FROM THERMOCOCCUS LITORALIS
Authors : Baker, P.J.; Britton, K.L.; Yip, K.S.; Stillman, T.J.; Rice, D.W.
Deposited on : 1999-07-20
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

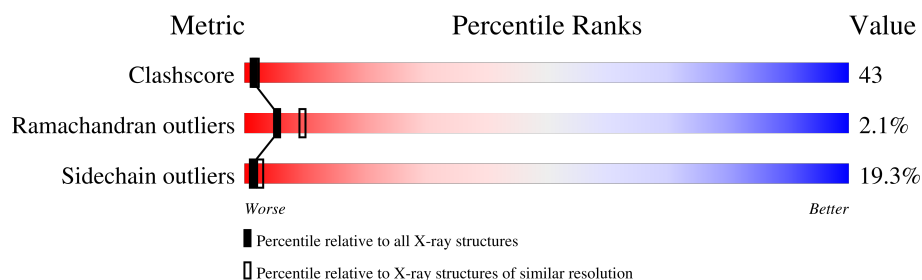
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	418	32% 50% 16% .
1	B	418	38% 50% 11% .
1	C	418	39% 44% 15% .
1	D	418	35% 46% 17% .
1	E	418	37% 49% 12% .
1	F	418	38% 48% 14% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19566 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).

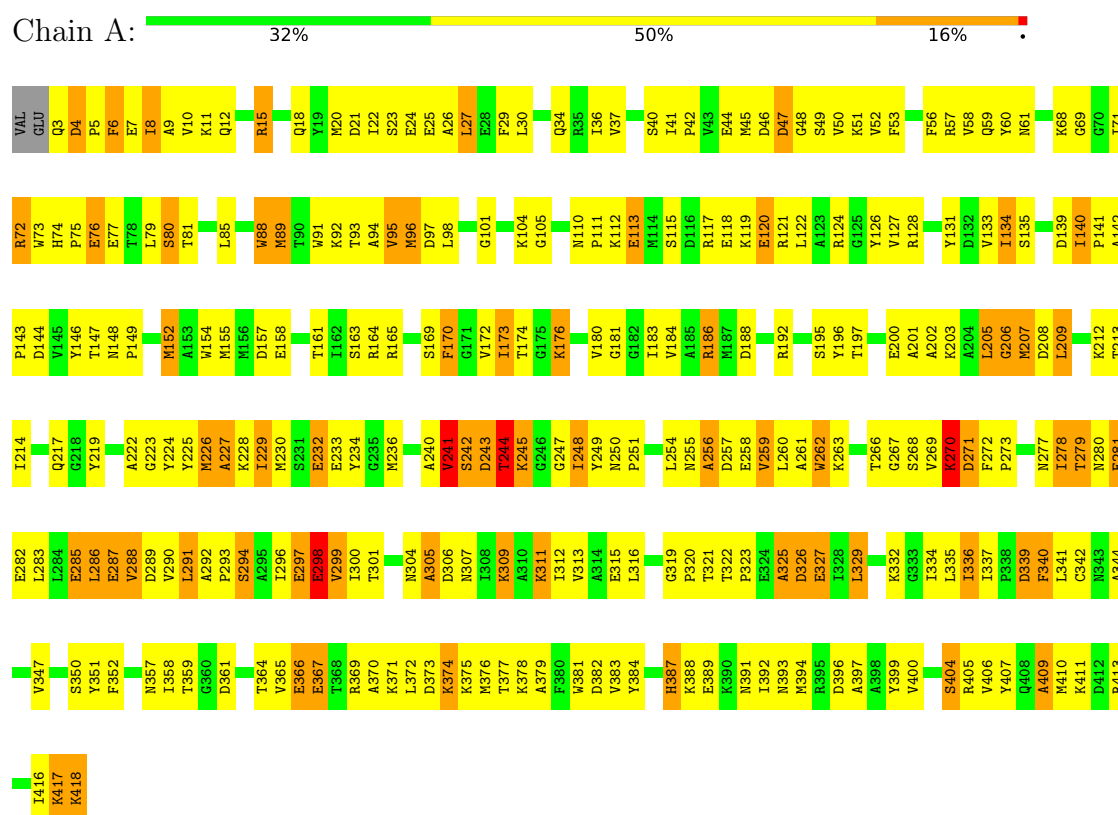
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	B	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	C	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	D	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	E	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	F	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			

3 Residue-property plots

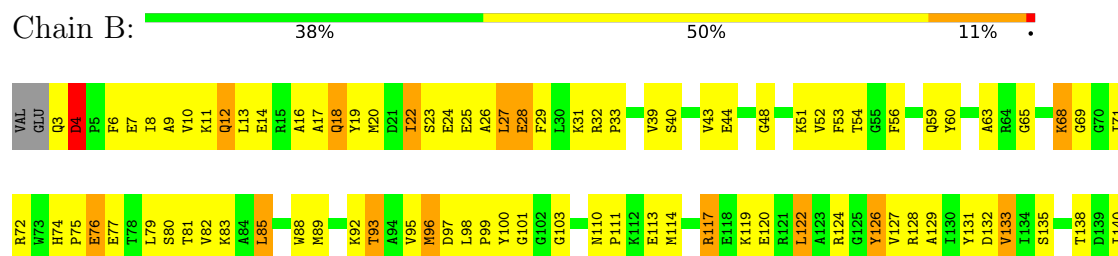
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

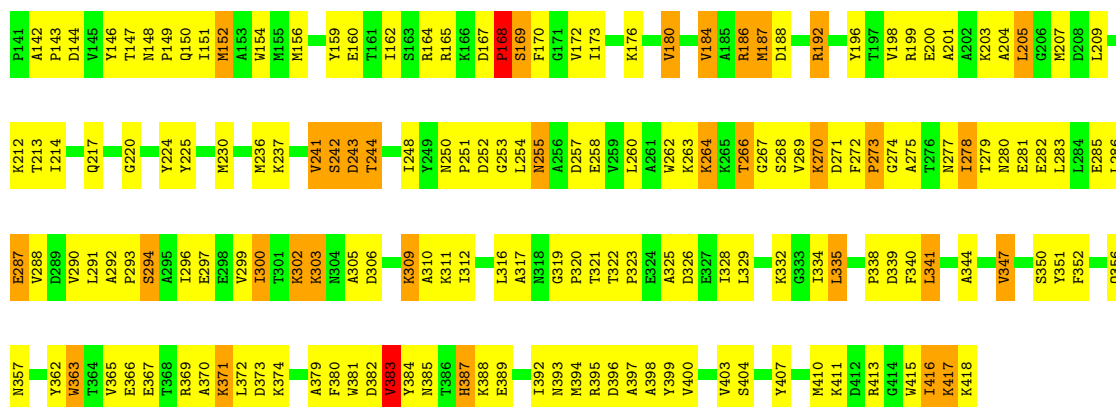
Note EDS was not executed.

• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)



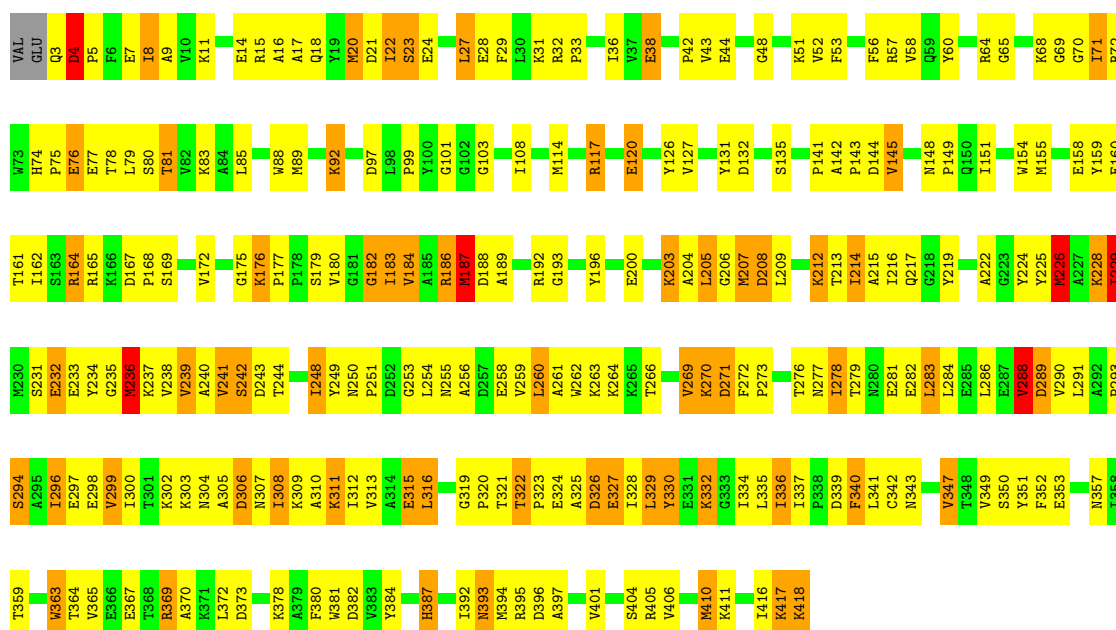
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)





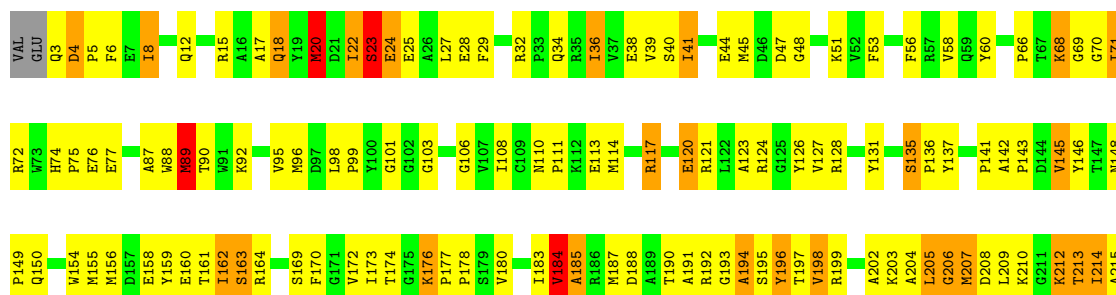
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

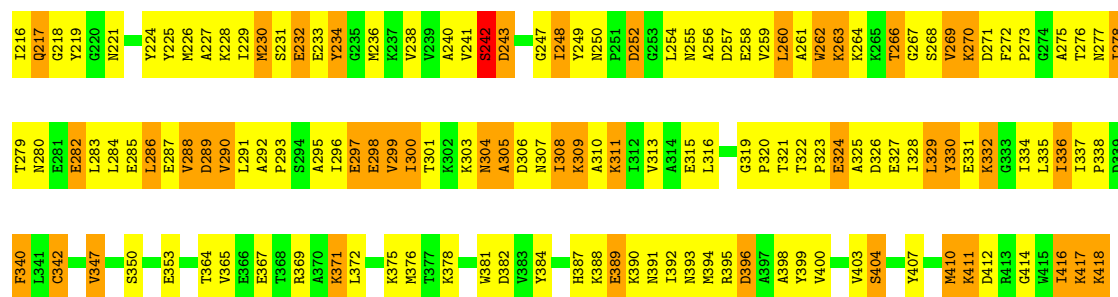
Chain C: 39% 44% 15%



• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

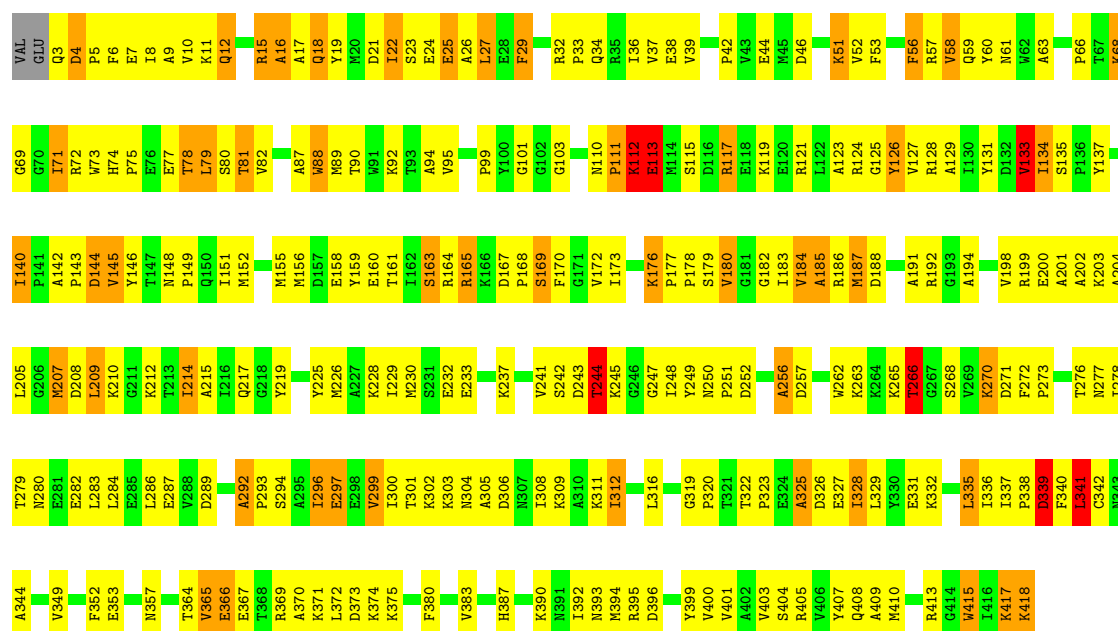
Chain D: 35% 46% 17%





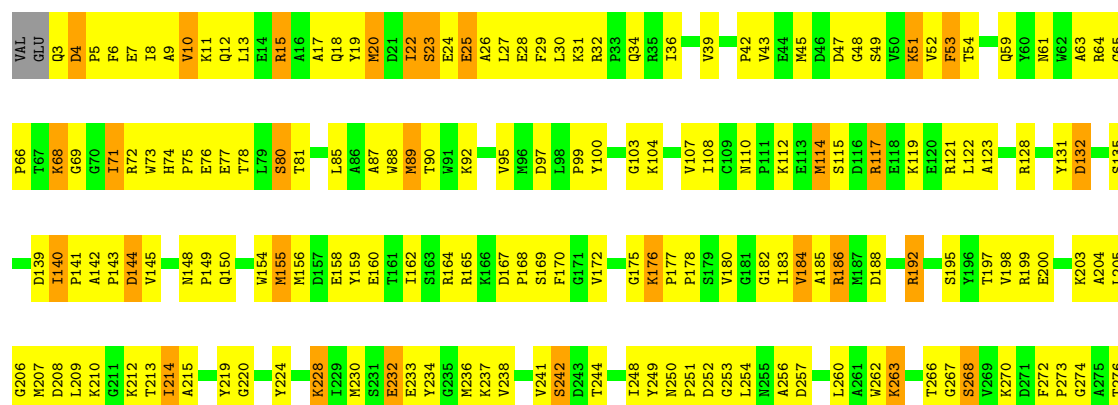
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

Chain E: 37% 49% 12%



• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

Chain F: 38% 48% 14%



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4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.90Å 197.50Å 125.70Å 90.00° 113.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	87.0 (10.00-2.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19566	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

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	0.87	1/3331 (0.0%)	1.29	30/4511 (0.7%)
1	B	0.91	3/3331 (0.1%)	1.25	18/4511 (0.4%)
1	C	0.90	4/3331 (0.1%)	1.27	34/4511 (0.8%)
1	D	0.90	3/3331 (0.1%)	1.25	31/4511 (0.7%)
1	E	0.95	6/3331 (0.2%)	1.32	30/4511 (0.7%)
1	F	0.91	2/3331 (0.1%)	1.28	24/4511 (0.5%)
All	All	0.91	19/19986 (0.1%)	1.28	167/27066 (0.6%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	410	MET	SD-CE	-8.58	1.58	1.79
1	A	410	MET	SD-CE	-7.52	1.60	1.79
1	D	45	MET	SD-CE	-7.24	1.61	1.79
1	C	127	VAL	CA-CB	-6.52	1.47	1.54
1	F	156	MET	SD-CE	-6.19	1.64	1.79
1	E	187	MET	SD-CE	5.90	1.94	1.79
1	E	133	VAL	CA-CB	5.64	1.61	1.54
1	E	244	THR	CA-CB	5.50	1.62	1.53
1	C	187	MET	SD-CE	5.41	1.93	1.79
1	D	20	MET	SD-CE	-5.37	1.66	1.79
1	C	108	ILE	CA-CB	-5.30	1.47	1.53
1	E	10	VAL	CA-CB	-5.28	1.48	1.54
1	F	155	MET	SD-CE	5.22	1.92	1.79
1	B	43	VAL	CA-CB	-5.21	1.48	1.54
1	B	152	MET	SD-CE	-5.20	1.66	1.79
1	E	140	ILE	CA-CB	5.16	1.59	1.54
1	B	347	VAL	CA-CB	-5.12	1.47	1.54
1	D	410	MET	SD-CE	-5.04	1.67	1.79
1	E	308	ILE	CA-CB	-5.02	1.48	1.54

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	25	GLU	N-CA-C	-9.95	100.42	111.07
1	E	299	VAL	N-CA-C	-9.36	104.36	113.53
1	A	325	ALA	N-CA-C	-9.12	101.34	111.28
1	A	241	VAL	N-CA-C	-8.79	98.10	108.82
1	B	341	LEU	N-CA-C	-8.73	101.32	112.93
1	B	126	TYR	N-CA-C	-8.40	101.82	110.97
1	A	351	TYR	N-CA-C	-8.39	101.16	111.40
1	F	341	LEU	N-CA-C	-8.29	103.11	113.55
1	B	25	GLU	N-CA-C	-8.17	102.07	110.97
1	D	41	ILE	CB-CA-C	-8.12	103.36	111.08
1	B	52	VAL	CB-CA-C	-8.05	101.66	111.08
1	C	239	VAL	N-CA-C	-7.98	105.09	112.43
1	F	299	VAL	N-CA-C	-7.95	104.77	113.43
1	A	299	VAL	N-CA-C	-7.79	105.72	113.20
1	A	169	SER	N-CA-C	7.72	121.63	111.75
1	A	140	ILE	N-CA-C	7.63	115.70	108.15
1	A	8	ILE	CB-CA-C	-7.58	102.26	111.97
1	C	127	VAL	N-CA-C	7.58	118.32	110.36
1	E	126	TYR	N-CA-C	-7.46	101.92	111.02
1	A	25	GLU	N-CA-C	-7.43	103.12	111.14
1	C	266	THR	N-CA-C	7.30	118.93	110.97
1	C	184	VAL	N-CA-C	7.28	119.30	111.58
1	A	6	PHE	N-CA-C	-7.25	103.06	110.97
1	C	81	THR	N-CA-C	-7.21	103.50	111.36
1	E	101	GLY	N-CA-C	-7.20	102.30	112.60
1	B	39	VAL	N-CA-C	7.19	119.92	108.85
1	C	70	GLY	N-CA-C	7.13	121.80	112.25
1	C	270	LYS	N-CA-C	7.07	119.11	110.41
1	E	140	ILE	N-CA-C	7.04	115.12	108.15
1	A	229	ILE	CB-CA-C	-7.02	102.82	112.02
1	E	81	THR	N-CA-C	-7.02	103.71	111.36
1	D	184	VAL	N-CA-C	-7.00	98.36	109.20
1	D	234	TYR	N-CA-C	6.83	121.66	113.12
1	B	101	GLY	N-CA-C	-6.83	100.53	112.55
1	C	351	TYR	N-CA-C	-6.82	103.30	111.69
1	D	342	CYS	N-CA-C	6.78	119.51	111.71
1	D	198	VAL	N-CA-C	-6.76	103.74	110.30
1	C	290	VAL	N-CA-C	6.73	117.53	108.11
1	A	377	THR	N-CA-C	6.71	118.25	111.07
1	D	194	ALA	N-CA-C	6.68	118.57	111.28
1	F	89	MET	N-CA-C	-6.68	103.92	111.07
1	C	89	MET	N-CA-C	-6.64	103.96	111.07
1	C	20	MET	N-CA-C	6.64	118.29	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	10	VAL	CB-CA-C	-6.59	103.45	111.88
1	C	52	VAL	CB-CA-C	-6.55	102.79	110.91
1	C	177	PRO	N-CA-C	-6.53	103.59	110.58
1	C	193	GLY	N-CA-C	-6.52	104.94	112.50
1	D	41	ILE	N-CA-C	6.49	114.58	108.15
1	C	229	ILE	N-CA-C	6.44	116.60	110.42
1	F	304	ASN	N-CA-C	6.43	120.33	112.23
1	F	351	TYR	N-CA-C	-6.39	104.40	111.36
1	F	24	GLU	N-CA-C	-6.36	105.68	113.50
1	A	24	GLU	N-CA-C	-6.35	105.35	113.23
1	E	25	GLU	N-CA-C	-6.35	104.44	111.36
1	D	36	ILE	CA-C-N	-6.33	114.85	123.14
1	D	36	ILE	C-N-CA	-6.33	114.85	123.14
1	C	226	MET	N-CA-C	-6.31	104.03	111.03
1	E	209	LEU	N-CA-C	6.30	118.96	111.71
1	C	182	GLY	N-CA-C	-6.30	103.55	112.37
1	D	89	MET	N-CA-C	-6.23	104.49	111.28
1	D	396	ASP	N-CA-C	-6.21	104.43	111.14
1	B	96	MET	N-CA-C	-6.21	105.67	113.18
1	D	96	MET	N-CA-C	-6.18	105.22	112.89
1	F	274	GLY	N-CA-C	-6.17	107.74	115.08
1	A	243	ASP	N-CA-C	6.13	117.20	108.74
1	E	341	LEU	N-CA-C	-6.12	103.75	112.13
1	D	299	VAL	N-CA-C	-6.11	107.03	112.90
1	E	292	ALA	N-CA-C	6.11	121.22	108.39
1	D	297	GLU	N-CA-C	6.09	118.39	110.53
1	E	229	ILE	N-CA-C	6.08	116.20	110.30
1	A	232	GLU	N-CA-C	6.08	119.89	112.23
1	C	24	GLU	N-CA-C	-6.07	104.58	112.23
1	C	342	CYS	N-CA-C	6.01	118.36	111.02
1	F	400	VAL	N-CA-C	-5.97	104.49	111.00
1	D	330	TYR	N-CA-C	-5.96	104.47	110.97
1	E	312	ILE	CB-CA-C	-5.93	101.36	110.50
1	A	120	GLU	N-CA-C	-5.91	104.92	111.36
1	B	383	VAL	N-CA-C	5.90	116.64	110.62
1	D	196	TYR	N-CA-C	-5.90	104.85	111.28
1	A	95	VAL	N-CA-C	-5.89	104.77	110.72
1	D	270	LYS	N-CA-C	5.84	118.83	110.24
1	B	383	VAL	CB-CA-C	-5.84	104.26	112.14
1	E	185	ALA	N-CA-C	-5.82	101.66	113.29
1	D	193	GLY	N-CA-C	-5.78	105.79	112.50
1	A	270	LYS	N-CA-C	5.76	118.12	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	36	ILE	CB-CA-C	-5.76	101.92	110.33
1	D	267	GLY	N-CA-C	-5.75	107.45	114.92
1	A	173	ILE	CB-CA-C	-5.74	103.30	111.40
1	C	330	TYR	N-CA-C	-5.74	104.71	110.97
1	C	288	VAL	CB-CA-C	-5.73	103.34	111.19
1	D	252	ASP	N-CA-C	-5.68	106.70	113.97
1	B	169	SER	N-CA-C	5.67	118.19	111.33
1	B	147	THR	N-CA-C	-5.66	100.75	109.52
1	D	174	THR	N-CA-C	5.66	118.10	109.95
1	A	41	ILE	CB-CA-C	-5.63	104.70	111.18
1	B	213	THR	N-CA-C	5.62	118.89	109.95
1	A	409	ALA	N-CA-C	5.62	117.85	111.11
1	B	168	PRO	CA-C-N	5.62	128.07	120.38
1	B	168	PRO	C-N-CA	5.62	128.07	120.38
1	F	114	MET	N-CA-C	5.61	118.55	109.40
1	D	187	MET	N-CA-C	5.61	117.40	111.28
1	D	24	GLU	N-CA-C	-5.60	105.56	112.90
1	C	203	LYS	N-CA-C	-5.58	105.27	111.36
1	F	140	ILE	N-CA-C	5.56	113.66	108.15
1	D	101	GLY	N-CA-C	-5.55	104.97	112.57
1	C	341	LEU	N-CA-C	-5.54	105.31	112.68
1	F	39	VAL	N-CA-C	5.52	117.86	108.86
1	E	328	ILE	CB-CA-C	-5.51	104.91	111.97
1	E	24	GLU	N-CA-C	-5.50	106.41	113.23
1	F	154	TRP	N-CA-C	-5.49	105.30	111.28
1	F	403	VAL	N-CA-C	5.49	120.76	109.34
1	D	70	GLY	N-CA-C	5.47	120.88	112.51
1	E	29	PHE	N-CA-C	-5.46	105.25	111.14
1	A	181	GLY	N-CA-C	-5.45	107.58	115.27
1	D	416	ILE	N-CA-C	-5.43	100.02	108.86
1	C	208	ASP	N-CA-C	5.40	117.32	108.52
1	E	344	ALA	N-CA-C	5.38	119.46	113.01
1	E	256	ALA	N-CA-C	5.37	118.62	111.75
1	B	184	VAL	N-CA-C	5.37	120.50	109.34
1	A	101	GLY	N-CA-C	-5.33	105.46	112.81
1	E	266	THR	N-CA-C	5.32	117.89	111.40
1	E	338	PRO	N-CA-C	5.32	119.57	111.11
1	C	175	GLY	N-CA-C	-5.32	105.72	114.76
1	D	266	THR	N-CA-C	5.32	117.16	111.36
1	D	290	VAL	N-CA-C	5.30	115.67	107.78
1	E	302	LYS	N-CA-C	-5.29	105.51	111.28
1	C	294	SER	N-CA-C	5.27	116.76	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	39	VAL	CB-CA-C	-5.27	103.31	110.90
1	A	233	GLU	N-CA-C	-5.26	106.88	113.72
1	C	164	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	F	345	GLY	N-CA-C	-5.24	106.38	113.24
1	B	122	LEU	N-CA-C	-5.23	104.51	112.04
1	F	54	THR	CA-C-N	-5.22	117.44	121.82
1	F	54	THR	C-N-CA	-5.22	117.44	121.82
1	B	416	ILE	N-CA-C	-5.21	100.86	108.99
1	C	16	ALA	N-CA-C	-5.20	105.69	111.36
1	F	20	MET	N-CA-C	5.20	116.74	108.79
1	D	232	GLU	N-CA-C	5.19	117.35	111.02
1	D	315	GLU	N-CA-C	5.19	117.54	108.52
1	A	311	LYS	N-CA-C	-5.18	105.70	112.23
1	E	325	ALA	N-CA-C	-5.15	105.84	111.82
1	C	416	ILE	N-CA-C	-5.15	100.47	108.86
1	D	39	VAL	N-CA-C	5.14	117.24	108.86
1	C	370	ALA	N-CA-C	-5.13	105.38	110.97
1	A	170	PHE	N-CA-C	-5.13	105.87	111.82
1	E	112	LYS	N-CA-C	5.13	121.72	110.80
1	A	226	MET	N-CA-C	-5.12	105.59	111.07
1	E	177	PRO	N-CA-C	-5.11	104.46	110.70
1	E	263	LYS	N-CA-C	-5.11	105.79	111.36
1	F	319	GLY	N-CA-C	5.11	122.76	112.34
1	C	4	ASP	N-CA-C	5.10	121.09	109.81
1	A	174	THR	N-CA-C	5.09	118.00	109.96
1	B	243	ASP	N-CA-C	5.09	115.76	108.74
1	A	98	LEU	N-CA-C	-5.09	103.78	110.39
1	E	297	GLU	N-CA-C	5.08	118.00	110.48
1	A	10	VAL	N-CA-C	5.07	115.68	110.36
1	A	312	ILE	N-CA-C	5.06	115.56	108.17
1	E	415	TRP	N-CA-C	-5.05	105.86	111.36
1	F	400	VAL	CB-CA-C	5.05	119.00	112.24
1	C	132	ASP	N-CA-C	5.04	118.92	112.87
1	E	383	VAL	CB-CA-C	-5.04	105.27	112.22
1	C	187	MET	N-CA-C	5.04	117.55	111.40
1	C	101	GLY	N-CA-C	-5.03	103.70	112.55
1	E	16	ALA	N-CA-C	-5.01	105.52	111.69
1	E	184	VAL	N-CA-C	-5.01	102.70	108.82
1	F	88	TRP	N-CA-C	5.01	117.12	111.11
1	F	52	VAL	CB-CA-C	-5.00	104.91	110.96

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	3261	0	3254	336	0
1	B	3261	0	3254	257	0
1	C	3261	0	3254	283	0
1	D	3261	0	3254	322	0
1	E	3261	0	3254	272	0
1	F	3261	0	3254	259	0
All	All	19566	0	19524	1675	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 43.

All (1675) 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:A:329:LEU:HD23	1:A:334:ILE:CD1	1.54	1.36
1:D:255:ASN:O	1:D:259:VAL:HG23	1.25	1.30
1:A:279:THR:HG22	1:A:282:GLU:OE2	1.28	1.27
1:A:329:LEU:CD2	1:A:334:ILE:HD12	1.63	1.27
1:C:384:TYR:HD1	1:C:394:MET:CE	1.49	1.25
1:E:29:PHE:CD1	1:E:410:MET:CE	2.21	1.23
1:B:29:PHE:CD2	1:B:410:MET:HE3	1.73	1.21
1:F:29:PHE:CD2	1:F:410:MET:HE3	1.74	1.21
1:C:225:TYR:O	1:C:229:ILE:HG13	1.35	1.20
1:C:384:TYR:CD1	1:C:394:MET:HE1	1.76	1.18
1:D:283:LEU:HA	1:D:286:LEU:CD1	1.74	1.17
1:E:188:ASP:OD2	1:E:192:ARG:NH1	1.80	1.15
1:A:279:THR:HG23	1:A:282:GLU:HG3	1.18	1.14
1:C:3:GLN:HG2	1:C:4:ASP:H	1.02	1.12
1:D:241:VAL:HG12	1:D:242:SER:H	1.13	1.12
1:C:384:TYR:CD1	1:C:394:MET:CE	2.30	1.11
1:E:29:PHE:CD1	1:E:410:MET:HE1	1.82	1.11
1:A:209:LEU:HA	1:A:212:LYS:HG3	1.20	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:TYR:HD1	1:C:394:MET:HE1	1.03	1.11
1:B:3:GLN:HG2	1:B:4:ASP:H	1.10	1.10
1:D:283:LEU:CA	1:D:286:LEU:HD12	1.82	1.10
1:C:214:ILE:HG22	1:C:236:MET:HE2	1.30	1.10
1:E:226:MET:HE3	1:E:230:MET:CG	1.85	1.07
1:A:110:ASN:ND2	1:A:113:GLU:OE2	1.87	1.06
1:B:74:HIS:ND1	1:B:75:PRO:HD2	1.69	1.06
1:C:329:LEU:HD23	1:C:334:ILE:HD12	1.08	1.06
1:C:329:LEU:HD23	1:C:334:ILE:CD1	1.84	1.05
1:A:321:THR:HG22	1:A:322:THR:H	1.20	1.05
1:E:12:GLN:OE1	1:E:88:TRP:HH2	1.37	1.04
1:A:283:LEU:O	1:A:286:LEU:HB2	1.57	1.03
1:E:88:TRP:CZ2	1:E:399:TYR:OH	2.11	1.03
1:A:279:THR:HG23	1:A:282:GLU:CG	1.87	1.03
1:D:241:VAL:CG1	1:D:242:SER:H	1.72	1.03
1:A:279:THR:CG2	1:A:282:GLU:OE2	2.07	1.02
1:B:325:ALA:O	1:B:329:LEU:HD12	1.59	1.02
1:F:29:PHE:CD2	1:F:410:MET:CE	2.43	1.02
1:C:214:ILE:HG22	1:C:236:MET:CE	1.90	1.01
1:C:213:THR:OG1	1:C:288:VAL:HG12	1.60	1.01
1:F:184:VAL:HG12	1:F:185:ALA:N	1.67	1.01
1:A:287:GLU:HG3	1:A:309:LYS:HD2	1.43	1.00
1:C:51:LYS:HG2	1:C:53:PHE:CE1	1.97	0.98
1:D:241:VAL:HG12	1:D:242:SER:N	1.67	0.98
1:B:294:SER:HB3	1:B:316:LEU:CB	1.92	0.98
1:C:297:GLU:HG3	1:C:298:GLU:HG3	1.45	0.97
1:E:262:TRP:O	1:E:266:THR:HB	1.63	0.97
1:F:184:VAL:CG1	1:F:185:ALA:N	2.27	0.97
1:E:29:PHE:CD1	1:E:410:MET:HE3	1.95	0.97
1:C:3:GLN:CG	1:C:4:ASP:H	1.78	0.96
1:D:279:THR:N	1:D:282:GLU:OE1	1.99	0.95
1:A:170:PHE:O	1:A:176:LYS:NZ	1.99	0.95
1:C:300:ILE:O	1:C:322:THR:HG23	1.67	0.95
1:A:126:TYR:HD2	1:A:155:MET:HE2	1.31	0.95
1:C:208:ASP:O	1:C:212:LYS:NZ	1.98	0.95
1:E:364:THR:OG1	1:E:367:GLU:HG3	1.64	0.95
1:B:29:PHE:CD2	1:B:410:MET:CE	2.50	0.95
1:C:214:ILE:CG2	1:C:236:MET:HE2	1.96	0.94
1:E:323:PRO:O	1:E:326:ASP:HB2	1.68	0.94
1:A:20:MET:CE	1:A:400:VAL:HA	1.98	0.94
1:A:321:THR:HG22	1:A:322:THR:N	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:O	1:B:11:LYS:HG3	1.68	0.94
1:E:12:GLN:OE1	1:E:88:TRP:CH2	2.20	0.94
1:A:248:ILE:HD12	1:A:254:LEU:HD13	1.50	0.93
1:B:279:THR:OG1	1:B:282:GLU:HG3	1.68	0.93
1:C:183:ILE:HD13	1:C:353:GLU:HB2	1.49	0.93
1:D:184:VAL:O	1:D:185:ALA:CB	2.16	0.93
1:B:321:THR:HG22	1:B:322:THR:N	1.82	0.93
1:A:48:GLY:HA2	1:E:117:ARG:NH2	1.84	0.92
1:D:255:ASN:O	1:D:259:VAL:CG2	2.17	0.92
1:E:176:LYS:NZ	1:E:353:GLU:OE2	2.01	0.92
1:C:270:LYS:HG3	1:C:277:ASN:HD21	1.32	0.92
1:F:184:VAL:CG1	1:F:185:ALA:H	1.81	0.92
1:F:208:ASP:O	1:F:212:LYS:NZ	2.01	0.92
1:C:3:GLN:HG2	1:C:4:ASP:N	1.79	0.91
1:C:393:ASN:ND2	1:C:396:ASP:H	1.69	0.91
1:E:226:MET:HE3	1:E:230:MET:HG2	1.50	0.91
1:B:148:ASN:HB2	1:B:149:PRO:HD2	1.51	0.91
1:B:242:SER:HB3	1:B:283:LEU:HD13	1.52	0.91
1:F:323:PRO:O	1:F:326:ASP:HB2	1.71	0.91
1:C:329:LEU:CD2	1:C:334:ILE:HD12	2.00	0.90
1:A:279:THR:CG2	1:A:282:GLU:HG3	1.98	0.90
1:E:4:ASP:O	1:E:8:ILE:HG13	1.72	0.90
1:F:3:GLN:NE2	1:F:80:SER:OG	2.03	0.90
1:A:335:LEU:HD11	1:A:394:MET:HE2	1.53	0.90
1:A:209:LEU:HA	1:A:212:LYS:CG	2.02	0.90
1:C:5:PRO:HA	1:C:8:ILE:HD12	1.53	0.89
1:C:243:ASP:OD2	1:C:269:VAL:HG22	1.72	0.89
1:C:188:ASP:OD2	1:C:192:ARG:NH1	2.05	0.89
1:D:170:PHE:O	1:D:176:LYS:HE3	1.73	0.89
1:C:148:ASN:HB2	1:C:149:PRO:HD2	1.54	0.89
1:D:3:GLN:C	1:D:5:PRO:HD2	1.97	0.89
1:F:188:ASP:OD2	1:F:192:ARG:NH1	2.06	0.89
1:A:48:GLY:HA2	1:E:117:ARG:HH22	1.38	0.88
1:D:3:GLN:HG2	1:D:4:ASP:H	1.38	0.88
1:B:3:GLN:HG2	1:B:4:ASP:N	1.86	0.88
1:B:63:ALA:HB2	1:B:415:TRP:CZ3	2.08	0.88
1:C:120:GLU:HA	1:C:154:TRP:CE3	2.09	0.88
1:C:29:PHE:CD2	1:C:410:MET:CE	2.56	0.88
1:A:315:GLU:OE2	1:A:336:ILE:CD1	2.22	0.87
1:C:241:VAL:HG12	1:C:242:SER:N	1.87	0.87
1:A:51:LYS:HG2	1:A:53:PHE:CE1	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:O	1:A:192:ARG:HB3	1.73	0.87
1:B:294:SER:HB3	1:B:316:LEU:HB3	1.57	0.87
1:E:219:TYR:CD1	1:E:241:VAL:HG11	2.10	0.87
1:C:48:GLY:C	1:F:117:ARG:HH22	1.82	0.87
1:A:20:MET:HE1	1:A:400:VAL:HA	1.57	0.86
1:D:322:THR:HB	1:D:323:PRO:HD2	1.55	0.86
1:E:167:ASP:HB2	1:E:168:PRO:HD2	1.55	0.86
1:E:29:PHE:CG	1:E:410:MET:HE1	2.10	0.86
1:D:214:ILE:HD12	1:D:290:VAL:CG1	2.06	0.86
1:E:68:LYS:HD3	1:E:140:ILE:HB	1.56	0.86
1:A:400:VAL:O	1:A:404:SER:HB3	1.76	0.86
1:E:322:THR:HB	1:E:323:PRO:HD2	1.58	0.85
1:E:270:LYS:HG2	1:E:277:ASN:HD21	1.41	0.85
1:C:335:LEU:HD23	1:C:336:ILE:N	1.90	0.85
1:D:262:TRP:CH2	1:D:273:PRO:HD3	2.10	0.85
1:C:224:TYR:CD1	1:C:260:LEU:CD2	2.59	0.85
1:C:323:PRO:O	1:C:326:ASP:HB2	1.77	0.85
1:F:392:ILE:HD12	1:F:396:ASP:HB3	1.56	0.85
1:C:4:ASP:HB3	1:C:5:PRO:HD3	1.58	0.84
1:B:22:ILE:HG12	1:B:23:SER:N	1.92	0.84
1:C:397:ALA:O	1:C:401:VAL:HG23	1.78	0.84
1:A:322:THR:O	1:A:326:ASP:N	2.10	0.84
1:C:15:ARG:HG3	1:C:18:GLN:NE2	1.92	0.84
1:B:3:GLN:CG	1:B:4:ASP:H	1.90	0.84
1:C:207:MET:HE1	1:C:311:LYS:CD	2.07	0.84
1:E:3:GLN:NE2	1:E:80:SER:OG	2.10	0.84
1:F:3:GLN:O	1:F:5:PRO:HD2	1.76	0.83
1:D:214:ILE:HD12	1:D:290:VAL:HG12	1.59	0.83
1:D:279:THR:HG22	1:D:282:GLU:OE1	1.79	0.83
1:A:249:TYR:CE2	1:A:251:PRO:HG3	2.13	0.83
1:A:3:GLN:O	1:A:4:ASP:C	2.20	0.83
1:C:214:ILE:HB	1:C:236:MET:HE1	1.61	0.82
1:E:3:GLN:C	1:E:7:GLU:HG3	2.04	0.82
1:C:214:ILE:CG2	1:C:236:MET:CE	2.53	0.82
1:A:321:THR:CG2	1:A:322:THR:H	1.91	0.82
1:D:283:LEU:HA	1:D:286:LEU:HD12	0.89	0.82
1:B:241:VAL:CG1	1:B:242:SER:N	2.42	0.82
1:F:142:ALA:HB1	1:F:143:PRO:HD2	1.61	0.82
1:C:29:PHE:CD2	1:C:410:MET:HE1	2.13	0.82
1:C:224:TYR:CD1	1:C:260:LEU:HD22	2.13	0.82
1:F:142:ALA:HB1	1:F:143:PRO:CD	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:SER:HB3	1:B:316:LEU:HB2	1.61	0.82
1:A:89:MET:HE3	1:A:89:MET:HA	1.62	0.81
1:E:296:ILE:HD12	1:E:299:VAL:CG1	2.09	0.81
1:E:167:ASP:HB2	1:E:168:PRO:CD	2.10	0.81
1:B:69:GLY:HA3	1:B:103:GLY:O	1.79	0.81
1:C:186:ARG:HG2	1:C:186:ARG:HH11	1.43	0.81
1:E:184:VAL:HG12	1:E:185:ALA:N	1.96	0.81
1:E:51:LYS:HG2	1:E:53:PHE:CE1	2.15	0.81
1:A:329:LEU:HD22	1:A:334:ILE:HG21	1.63	0.80
1:C:186:ARG:HH11	1:C:186:ARG:CG	1.94	0.80
1:F:379:ALA:O	1:F:383:VAL:HG23	1.81	0.80
1:A:291:LEU:HD22	1:A:293:PRO:HD3	1.63	0.80
1:E:172:VAL:HG22	1:E:172:VAL:O	1.81	0.80
1:B:29:PHE:HD2	1:B:410:MET:HE3	1.39	0.80
1:A:249:TYR:CZ	1:A:251:PRO:HG3	2.16	0.80
1:C:142:ALA:HB1	1:C:143:PRO:HD2	1.62	0.80
1:E:3:GLN:HG2	1:E:5:PRO:HD3	1.61	0.80
1:D:184:VAL:O	1:D:185:ALA:HB3	1.81	0.80
1:A:329:LEU:CD2	1:A:334:ILE:CD1	2.37	0.80
1:D:188:ASP:OD2	1:D:192:ARG:NH1	2.15	0.80
1:A:126:TYR:CD2	1:A:155:MET:HE2	2.15	0.80
1:D:120:GLU:HB2	1:D:154:TRP:CE3	2.17	0.80
1:E:184:VAL:O	1:E:185:ALA:HB3	1.81	0.80
1:E:242:SER:HB3	1:E:283:LEU:HD13	1.62	0.80
1:B:328:ILE:O	1:B:332:LYS:HB2	1.82	0.79
1:A:30:LEU:HD22	1:A:91:TRP:HH2	1.47	0.79
1:E:74:HIS:ND1	1:E:75:PRO:HD2	1.96	0.79
1:A:407:TYR:OH	1:A:418:LYS:O	1.99	0.79
1:E:110:ASN:O	1:E:111:PRO:C	2.25	0.79
1:A:228:LYS:O	1:A:232:GLU:HB2	1.82	0.79
1:C:237:LYS:O	1:C:239:VAL:HG13	1.83	0.78
1:D:4:ASP:O	1:D:8:ILE:HG13	1.84	0.78
1:C:225:TYR:O	1:C:229:ILE:CG1	2.27	0.78
1:C:255:ASN:O	1:C:259:VAL:HG23	1.82	0.78
1:B:74:HIS:ND1	1:B:75:PRO:CD	2.46	0.78
1:D:3:GLN:HG2	1:D:4:ASP:N	1.95	0.78
1:C:384:TYR:HA	1:C:394:MET:HE1	1.66	0.78
1:B:148:ASN:HB2	1:B:149:PRO:CD	2.14	0.78
1:E:123:ALA:HA	1:E:155:MET:HE3	1.66	0.78
1:A:364:THR:HG23	1:A:367:GLU:OE1	1.83	0.78
1:F:184:VAL:C	1:F:186:ARG:H	1.91	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LYS:HG2	1:C:117:ARG:NH2	1.98	0.77
1:B:29:PHE:HE1	1:E:42:PRO:HG3	1.49	0.77
1:D:194:ALA:O	1:D:197:THR:OG1	2.02	0.77
1:E:22:ILE:HD11	1:E:26:ALA:HB3	1.64	0.77
1:E:29:PHE:CE1	1:E:410:MET:HE3	2.20	0.77
1:D:262:TRP:CZ3	1:D:273:PRO:CD	2.67	0.77
1:E:3:GLN:NE2	1:E:80:SER:CB	2.46	0.77
1:B:323:PRO:O	1:B:326:ASP:HB2	1.83	0.77
1:B:321:THR:CG2	1:B:322:THR:N	2.47	0.77
1:A:200:GLU:OE2	1:A:203:LYS:NZ	2.18	0.77
1:E:117:ARG:O	1:E:121:ARG:HG3	1.85	0.77
1:A:5:PRO:HA	1:A:8:ILE:HD12	1.67	0.77
1:F:184:VAL:O	1:F:185:ALA:HB3	1.84	0.76
1:A:120:GLU:HG3	1:A:154:TRP:CD2	2.19	0.76
1:A:117:ARG:NH1	1:B:417:LYS:HG2	2.00	0.76
1:A:417:LYS:HG2	1:C:117:ARG:CZ	2.15	0.76
1:D:322:THR:HB	1:D:323:PRO:CD	2.15	0.76
1:F:393:ASN:ND2	1:F:396:ASP:H	1.83	0.76
1:D:120:GLU:HB2	1:D:154:TRP:CD2	2.20	0.76
1:A:44:GLU:CG	1:E:117:ARG:HH21	1.97	0.76
1:B:172:VAL:O	1:B:172:VAL:HG22	1.86	0.76
1:C:48:GLY:O	1:F:117:ARG:NH2	2.12	0.76
1:C:324:GLU:O	1:C:328:ILE:HG13	1.86	0.76
1:E:3:GLN:HE21	1:E:80:SER:CB	1.98	0.76
1:D:399:TYR:O	1:D:403:VAL:HG23	1.85	0.76
1:E:322:THR:HB	1:E:323:PRO:CD	2.15	0.76
1:A:225:TYR:O	1:A:229:ILE:HG13	1.85	0.75
1:E:170:PHE:O	1:E:176:LYS:HE2	1.86	0.75
1:C:393:ASN:HD22	1:C:396:ASP:H	1.30	0.75
1:D:307:ASN:O	1:D:309:LYS:HG2	1.86	0.75
1:E:22:ILE:HD11	1:E:26:ALA:CB	2.16	0.75
1:B:236:MET:HE1	1:B:290:VAL:CG2	2.17	0.75
1:F:322:THR:HB	1:F:323:PRO:HD2	1.68	0.75
1:C:241:VAL:HG12	1:C:242:SER:H	1.50	0.75
1:C:214:ILE:CB	1:C:236:MET:HE1	2.17	0.75
1:C:384:TYR:HD1	1:C:394:MET:HE3	1.48	0.75
1:A:209:LEU:CA	1:A:212:LYS:HG3	2.11	0.74
1:E:270:LYS:O	1:E:271:ASP:HB2	1.85	0.74
1:A:30:LEU:HD22	1:A:91:TRP:CH2	2.22	0.74
1:D:229:ILE:HG23	1:D:233:GLU:CD	2.11	0.74
1:C:214:ILE:HG13	1:C:215:ALA:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:PHE:CD1	1:D:410:MET:CE	2.71	0.74
1:D:276:THR:HG22	1:D:277:ASN:N	2.02	0.74
1:A:262:TRP:O	1:A:266:THR:N	2.16	0.74
1:D:213:THR:HB	1:D:288:VAL:CG1	2.17	0.74
1:F:3:GLN:C	1:F:5:PRO:HD2	2.12	0.74
1:F:63:ALA:HB2	1:F:415:TRP:CZ3	2.22	0.74
1:E:22:ILE:HD13	1:E:27:LEU:HD23	1.70	0.74
1:A:152:MET:HE2	1:A:152:MET:HA	1.71	0.73
1:A:48:GLY:CA	1:E:117:ARG:HH22	2.00	0.73
1:B:111:PRO:HG2	1:B:146:TYR:CD2	2.23	0.73
1:E:3:GLN:NE2	1:E:80:SER:HB2	2.02	0.73
1:B:270:LYS:HG2	1:B:277:ASN:ND2	2.03	0.73
1:B:371:LYS:HB3	1:B:371:LYS:HZ3	1.54	0.73
1:A:94:ALA:O	1:A:405:ARG:NH1	2.21	0.73
1:B:131:TYR:HE1	1:B:159:TYR:CE1	2.07	0.73
1:E:12:GLN:CD	1:E:88:TRP:HH2	1.95	0.73
1:C:226:MET:HE2	1:C:316:LEU:HD11	1.69	0.73
1:D:51:LYS:HD3	1:D:53:PHE:CZ	2.23	0.73
1:D:248:ILE:HD13	1:D:269:VAL:HG23	1.71	0.73
1:F:34:GLN:OE1	1:F:61:ASN:HA	1.89	0.73
1:F:228:LYS:O	1:F:232:GLU:HB2	1.89	0.72
1:A:176:LYS:NZ	1:A:357:ASN:OD1	2.18	0.72
1:D:3:GLN:O	1:D:4:ASP:C	2.32	0.72
1:B:371:LYS:HB3	1:B:371:LYS:NZ	2.02	0.72
1:C:241:VAL:CG1	1:C:242:SER:N	2.51	0.72
1:D:393:ASN:ND2	1:D:396:ASP:OD2	2.22	0.72
1:A:74:HIS:ND1	1:A:75:PRO:HD2	2.04	0.72
1:F:184:VAL:HG12	1:F:185:ALA:H	1.44	0.72
1:E:156:MET:SD	1:E:156:MET:C	2.72	0.71
1:D:226:MET:HE3	1:D:230:MET:CG	2.20	0.71
1:E:3:GLN:HG2	1:E:5:PRO:CD	2.19	0.71
1:B:344:ALA:O	1:B:347:VAL:HG12	1.90	0.71
1:C:167:ASP:HB2	1:C:168:PRO:CD	2.19	0.71
1:D:3:GLN:CG	1:D:4:ASP:H	2.04	0.71
1:E:92:LYS:O	1:E:95:VAL:HG12	1.90	0.71
1:F:186:ARG:O	1:F:186:ARG:HG3	1.88	0.71
1:A:279:THR:OG1	1:A:281:GLU:HG2	1.89	0.71
1:B:117:ARG:NH1	1:C:417:LYS:HG2	2.05	0.71
1:C:291:LEU:HG	1:C:293:PRO:HD3	1.72	0.71
1:C:384:TYR:O	1:C:387:HIS:HD2	1.74	0.71
1:E:179:SER:O	1:E:180:VAL:HG13	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ASN:OD1	1:F:251:PRO:HD2	1.90	0.71
1:A:226:MET:HG2	1:A:316:LEU:HD11	1.72	0.71
1:D:213:THR:HB	1:D:288:VAL:HG13	1.71	0.71
1:F:51:LYS:HG2	1:F:53:PHE:CE1	2.26	0.71
1:C:241:VAL:CG1	1:C:242:SER:H	2.03	0.71
1:D:313:VAL:HB	1:D:336:ILE:HG12	1.73	0.71
1:B:3:GLN:O	1:B:7:GLU:N	2.23	0.70
1:C:15:ARG:HG3	1:C:18:GLN:HE22	1.55	0.70
1:C:183:ILE:HD13	1:C:353:GLU:CB	2.20	0.70
1:D:278:ILE:HB	1:D:282:GLU:CD	2.15	0.70
1:E:323:PRO:C	1:E:326:ASP:HB2	2.16	0.70
1:A:126:TYR:CD2	1:A:155:MET:CE	2.74	0.70
1:C:176:LYS:O	1:C:182:GLY:HA3	1.92	0.70
1:E:66:PRO:HB3	1:E:137:TYR:O	1.92	0.70
1:E:219:TYR:HD1	1:E:241:VAL:HG11	1.56	0.70
1:A:96:MET:HE1	1:A:376:MET:SD	2.31	0.70
1:B:379:ALA:O	1:B:383:VAL:HG23	1.90	0.70
1:B:142:ALA:HB1	1:B:143:PRO:HD2	1.72	0.70
1:C:148:ASN:HB2	1:C:149:PRO:CD	2.18	0.70
1:E:22:ILE:CD1	1:E:26:ALA:HB3	2.21	0.70
1:C:365:VAL:O	1:C:369:ARG:HG3	1.91	0.70
1:A:44:GLU:HG3	1:E:117:ARG:HH21	1.56	0.70
1:A:144:ASP:N	1:A:147:THR:OG1	2.21	0.70
1:A:3:GLN:HB3	1:A:80:SER:HB3	1.74	0.70
1:C:248:ILE:HD13	1:C:269:VAL:O	1.92	0.70
1:D:126:TYR:HD2	1:D:155:MET:HE2	1.57	0.70
1:F:337:ILE:HG22	1:F:342:CYS:HB2	1.74	0.70
1:B:384:TYR:O	1:B:387:HIS:HD2	1.74	0.70
1:D:213:THR:CG2	1:D:288:VAL:HG13	2.21	0.70
1:D:156:MET:SD	1:D:156:MET:C	2.75	0.69
1:A:44:GLU:CD	1:E:117:ARG:HE	1.99	0.69
1:D:226:MET:HE3	1:D:230:MET:HG2	1.74	0.69
1:E:270:LYS:HG2	1:E:277:ASN:ND2	2.06	0.69
1:A:315:GLU:OE2	1:A:336:ILE:HD12	1.91	0.69
1:B:288:VAL:O	1:B:310:ALA:HA	1.92	0.69
1:C:335:LEU:HD23	1:C:336:ILE:H	1.54	0.69
1:D:288:VAL:O	1:D:310:ALA:HA	1.93	0.69
1:A:12:GLN:NE2	1:A:88:TRP:HH2	1.90	0.69
1:C:27:LEU:HD13	1:C:31:LYS:HE3	1.72	0.69
1:A:50:VAL:CG2	1:F:417:LYS:HG2	2.22	0.69
1:A:148:ASN:HB2	1:A:149:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASN:HB3	1:A:254:LEU:CD2	2.23	0.69
1:A:296:ILE:HD11	1:A:299:VAL:HG12	1.72	0.69
1:A:358:ILE:HD11	1:C:359:THR:O	1.92	0.69
1:B:262:TRP:O	1:B:266:THR:HB	1.92	0.69
1:C:339:ASP:OD1	1:C:339:ASP:N	2.21	0.69
1:D:213:THR:O	1:D:288:VAL:HG12	1.93	0.69
1:D:160:GLU:HG2	1:D:169:SER:HB3	1.75	0.69
1:D:411:LYS:O	1:D:414:GLY:N	2.23	0.69
1:D:230:MET:O	1:D:234:TYR:HB2	1.91	0.69
1:D:242:SER:HA	1:D:247:GLY:HA2	1.75	0.68
1:F:399:TYR:O	1:F:403:VAL:HG23	1.93	0.68
1:B:236:MET:HE1	1:B:290:VAL:HG21	1.73	0.68
1:D:304:ASN:O	1:D:307:ASN:N	2.20	0.68
1:B:321:THR:HG22	1:B:322:THR:O	1.93	0.68
1:C:69:GLY:HA3	1:C:103:GLY:O	1.94	0.68
1:D:400:VAL:O	1:D:404:SER:OG	2.10	0.68
1:E:184:VAL:CG1	1:E:185:ALA:N	2.56	0.68
1:A:89:MET:HE3	1:A:89:MET:CA	2.20	0.68
1:A:144:ASP:H	1:A:147:THR:HG1	1.39	0.68
1:C:33:PRO:HB3	1:C:60:TYR:CD1	2.29	0.68
1:F:29:PHE:HB3	1:F:410:MET:HE1	1.74	0.68
1:E:88:TRP:CH2	1:E:399:TYR:OH	2.47	0.68
1:F:160:GLU:HG2	1:F:169:SER:CB	2.24	0.68
1:F:250:ASN:OD1	1:F:252:ASP:N	2.26	0.68
1:D:279:THR:O	1:D:282:GLU:HB2	1.94	0.68
1:F:3:GLN:O	1:F:5:PRO:CD	2.42	0.68
1:F:20:MET:HE2	1:F:22:ILE:HG21	1.75	0.68
1:A:3:GLN:HG2	1:A:4:ASP:N	2.09	0.67
1:C:29:PHE:HD2	1:C:410:MET:HE1	1.57	0.67
1:A:3:GLN:C	1:A:5:PRO:HD2	2.19	0.67
1:C:192:ARG:NH2	1:C:233:GLU:OE2	2.28	0.67
1:D:41:ILE:O	1:D:41:ILE:HG22	1.94	0.67
1:A:172:VAL:HG22	1:A:172:VAL:O	1.94	0.67
1:B:241:VAL:HG12	1:B:242:SER:N	2.07	0.67
1:F:160:GLU:HG2	1:F:169:SER:HB3	1.76	0.67
1:A:323:PRO:O	1:A:326:ASP:HB2	1.94	0.67
1:E:401:VAL:O	1:E:405:ARG:HG3	1.94	0.67
1:F:29:PHE:HD2	1:F:410:MET:HE3	1.54	0.67
1:B:242:SER:OG	1:B:280:ASN:ND2	2.27	0.67
1:E:3:GLN:C	1:E:5:PRO:HD2	2.20	0.67
1:A:205:LEU:O	1:A:206:GLY:C	2.37	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:GLU:O	1:B:370:ALA:HB3	1.95	0.67
1:D:29:PHE:CD1	1:D:410:MET:HE3	2.28	0.67
1:E:212:LYS:HB3	1:E:289:ASP:OD2	1.95	0.67
1:A:240:ALA:HA	1:A:248:ILE:O	1.95	0.67
1:B:117:ARG:CZ	1:C:417:LYS:HG2	2.25	0.67
1:C:5:PRO:CA	1:C:8:ILE:HD12	2.24	0.67
1:C:387:HIS:CD2	1:C:394:MET:HE2	2.30	0.67
1:C:158:GLU:O	1:C:162:ILE:HG13	1.94	0.67
1:D:163:SER:O	1:D:164:ARG:HB2	1.94	0.67
1:A:249:TYR:CE2	1:A:251:PRO:HD3	2.31	0.66
1:E:29:PHE:CG	1:E:410:MET:CE	2.72	0.66
1:F:228:LYS:HE3	1:F:232:GLU:OE1	1.95	0.66
1:B:273:PRO:C	1:B:275:ALA:H	2.03	0.66
1:C:142:ALA:HB1	1:C:143:PRO:CD	2.24	0.66
1:D:203:LYS:O	1:D:206:GLY:N	2.24	0.66
1:E:59:GLN:HE22	1:E:133:VAL:HG23	1.61	0.66
1:A:131:TYR:CD2	1:E:164:ARG:HD3	2.30	0.66
1:A:270:LYS:HG2	1:A:277:ASN:HD21	1.61	0.66
1:A:279:THR:CG2	1:A:282:GLU:CG	2.66	0.66
1:F:5:PRO:HG2	1:F:80:SER:HB2	1.76	0.66
1:B:287:GLU:HG3	1:B:309:LYS:HD2	1.77	0.66
1:D:74:HIS:ND1	1:D:75:PRO:HD2	2.10	0.66
1:E:242:SER:HB3	1:E:283:LEU:CD1	2.25	0.66
1:C:315:GLU:HB3	1:C:320:PRO:HG3	1.78	0.66
1:E:192:ARG:NH2	1:E:233:GLU:OE2	2.28	0.66
1:F:78:THR:HG1	1:F:81:THR:HG1	1.25	0.66
1:B:339:ASP:OD1	1:B:340:PHE:N	2.24	0.66
1:C:186:ARG:CG	1:C:186:ARG:NH1	2.54	0.66
1:D:248:ILE:HG13	1:D:254:LEU:HD21	1.78	0.66
1:E:46:ASP:OD2	1:E:115:SER:OG	2.07	0.66
1:E:184:VAL:HG12	1:E:185:ALA:H	1.60	0.66
1:F:242:SER:OG	1:F:280:ASN:ND2	2.29	0.66
1:A:250:ASN:HB3	1:A:254:LEU:HD23	1.78	0.66
1:D:224:TYR:OH	1:D:257:ASP:OD1	2.13	0.66
1:A:96:MET:CE	1:A:376:MET:SD	2.84	0.66
1:A:110:ASN:HD22	1:A:113:GLU:CD	1.96	0.66
1:A:315:GLU:O	1:A:342:CYS:HB3	1.95	0.66
1:B:255:ASN:C	1:B:255:ASN:OD1	2.38	0.66
1:C:297:GLU:O	1:C:299:VAL:HG13	1.96	0.66
1:D:257:ASP:O	1:D:260:LEU:HB3	1.95	0.66
1:A:34:GLN:HG3	1:A:60:TYR:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LYS:O	1:A:271:ASP:HB2	1.96	0.66
1:C:176:LYS:NZ	1:C:357:ASN:OD1	2.19	0.66
1:B:176:LYS:NZ	1:B:357:ASN:HD21	1.94	0.65
1:D:323:PRO:O	1:D:326:ASP:HB2	1.96	0.65
1:C:228:LYS:NZ	1:C:232:GLU:OE2	2.29	0.65
1:C:393:ASN:ND2	1:C:395:ARG:HB3	2.12	0.65
1:D:249:TYR:HB2	1:D:278:ILE:CD1	2.26	0.65
1:D:297:GLU:HG3	1:D:298:GLU:HG3	1.78	0.65
1:E:16:ALA:O	1:E:17:ALA:C	2.39	0.65
1:B:29:PHE:HD2	1:B:410:MET:CE	2.00	0.65
1:D:384:TYR:CE2	1:D:388:LYS:NZ	2.65	0.65
1:E:323:PRO:O	1:E:326:ASP:CB	2.44	0.65
1:B:270:LYS:HG2	1:B:277:ASN:HD21	1.61	0.65
1:F:176:LYS:HB2	1:F:176:LYS:NZ	2.11	0.65
1:B:88:TRP:CZ2	1:B:399:TYR:OH	2.49	0.65
1:A:4:ASP:HB3	1:A:5:PRO:HD3	1.79	0.65
1:B:242:SER:HB3	1:B:283:LEU:CD1	2.26	0.65
1:C:186:ARG:O	1:C:186:ARG:HG3	1.97	0.65
1:E:17:ALA:O	1:E:19:TYR:N	2.30	0.65
1:E:124:ARG:O	1:E:128:ARG:HG3	1.96	0.65
1:C:258:GLU:O	1:C:261:ALA:HB3	1.96	0.65
1:D:213:THR:CB	1:D:288:VAL:HG13	2.26	0.65
1:E:156:MET:HE2	1:E:170:PHE:CD1	2.32	0.65
1:E:184:VAL:CG1	1:E:185:ALA:H	2.08	0.65
1:E:228:LYS:O	1:E:232:GLU:HB2	1.97	0.65
1:F:407:TYR:OH	1:F:418:LYS:O	2.12	0.65
1:A:249:TYR:OH	1:A:251:PRO:HG3	1.96	0.65
1:A:301:THR:O	1:A:305:ALA:HB2	1.97	0.65
1:D:271:ASP:O	1:D:272:PHE:C	2.39	0.65
1:F:250:ASN:OD1	1:F:250:ASN:C	2.38	0.65
1:C:208:ASP:O	1:C:212:LYS:CE	2.44	0.64
1:E:176:LYS:NZ	1:E:357:ASN:HD21	1.94	0.64
1:E:228:LYS:HE2	1:E:257:ASP:OD1	1.97	0.64
1:E:283:LEU:O	1:E:286:LEU:HB2	1.97	0.64
1:C:384:TYR:CD1	1:C:394:MET:HE3	2.27	0.64
1:D:158:GLU:O	1:D:162:ILE:HG13	1.97	0.64
1:B:6:PHE:O	1:B:9:ALA:HB3	1.97	0.64
1:D:17:ALA:HA	1:D:20:MET:HE2	1.78	0.64
1:E:9:ALA:O	1:E:12:GLN:HB2	1.97	0.64
1:F:29:PHE:CG	1:F:410:MET:CE	2.79	0.64
1:D:208:ASP:O	1:D:212:LYS:HE3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LYS:NZ	1:B:371:LYS:CB	2.58	0.64
1:E:71:ILE:HD13	1:E:126:TYR:CE2	2.33	0.64
1:F:209:LEU:O	1:F:210:LYS:C	2.40	0.64
1:D:249:TYR:HB2	1:D:278:ILE:HD13	1.78	0.64
1:F:4:ASP:O	1:F:8:ILE:HG13	1.97	0.64
1:A:322:THR:OG1	1:A:325:ALA:CB	2.46	0.64
1:B:217:GLN:HE22	1:B:299:VAL:HG11	1.62	0.64
1:D:296:ILE:CD1	1:D:299:VAL:CG1	2.76	0.64
1:D:98:LEU:HD23	1:D:375:LYS:NZ	2.12	0.64
1:E:3:GLN:C	1:E:5:PRO:CD	2.71	0.64
1:F:29:PHE:O	1:F:31:LYS:N	2.31	0.64
1:A:322:THR:HB	1:A:323:PRO:HD2	1.80	0.64
1:B:72:ARG:NE	1:B:77:GLU:OE2	2.19	0.64
1:C:23:SER:OG	1:C:418:LYS:OXT	2.16	0.64
1:C:278:ILE:HB	1:C:282:GLU:OE1	1.98	0.64
1:C:378:LYS:NZ	1:C:382:ASP:OD2	2.21	0.64
1:F:184:VAL:HG13	1:F:185:ALA:H	1.59	0.64
1:E:152:MET:HE2	1:E:152:MET:HA	1.80	0.63
1:D:4:ASP:C	1:D:8:ILE:HG13	2.23	0.63
1:F:339:ASP:N	1:F:339:ASP:OD1	2.29	0.63
1:B:131:TYR:CE1	1:B:159:TYR:CE1	2.86	0.63
1:B:335:LEU:HD11	1:B:394:MET:HE2	1.81	0.63
1:F:192:ARG:NH2	1:F:233:GLU:OE2	2.31	0.63
1:A:214:ILE:HA	1:A:288:VAL:HG21	1.81	0.63
1:A:228:LYS:NZ	1:A:257:ASP:OD2	2.31	0.63
1:C:259:VAL:HG12	1:C:269:VAL:HG12	1.81	0.63
1:C:329:LEU:CD2	1:C:334:ILE:CD1	2.69	0.63
1:D:29:PHE:CD1	1:D:410:MET:HE1	2.34	0.63
1:A:3:GLN:HG2	1:A:4:ASP:H	1.64	0.63
1:A:207:MET:HG3	1:A:208:ASP:N	2.13	0.63
1:C:219:TYR:CD1	1:C:241:VAL:HG11	2.34	0.63
1:E:3:GLN:O	1:E:4:ASP:C	2.41	0.63
1:C:48:GLY:C	1:F:117:ARG:NH2	2.55	0.63
1:D:18:GLN:O	1:D:18:GLN:HG3	1.99	0.63
1:E:79:LEU:HD12	1:E:79:LEU:O	1.98	0.63
1:F:348:THR:HG21	1:F:372:LEU:HD12	1.80	0.63
1:A:72:ARG:HG2	1:A:144:ASP:HB3	1.80	0.62
1:A:92:LYS:O	1:A:95:VAL:HG12	1.98	0.62
1:A:214:ILE:CA	1:A:288:VAL:HG21	2.29	0.62
1:A:261:ALA:O	1:A:262:TRP:C	2.42	0.62
1:B:367:GLU:O	1:B:371:LYS:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:THR:HG23	1:D:282:GLU:H	1.64	0.62
1:F:328:ILE:O	1:F:332:LYS:HG3	1.99	0.62
1:B:180:VAL:HG23	1:B:180:VAL:O	1.98	0.62
1:D:3:GLN:CG	1:D:4:ASP:N	2.62	0.62
1:E:3:GLN:O	1:E:6:PHE:N	2.31	0.62
1:A:81:THR:HG22	1:A:85:LEU:HD11	1.80	0.62
1:A:279:THR:CG2	1:A:282:GLU:CD	2.72	0.62
1:A:288:VAL:HG22	1:A:290:VAL:H	1.64	0.62
1:E:173:ILE:O	1:E:176:LYS:HE3	1.98	0.62
1:E:296:ILE:HD12	1:E:299:VAL:HG11	1.79	0.62
1:F:176:LYS:HB2	1:F:176:LYS:HZ3	1.64	0.62
1:A:4:ASP:HB3	1:A:5:PRO:CD	2.29	0.62
1:A:296:ILE:CD1	1:A:299:VAL:HG12	2.29	0.62
1:E:127:VAL:HG23	1:E:155:MET:HG2	1.80	0.62
1:E:159:TYR:O	1:E:163:SER:HB3	1.99	0.62
1:A:20:MET:HE2	1:A:400:VAL:HA	1.80	0.62
1:A:230:MET:O	1:A:234:TYR:HB2	2.00	0.62
1:C:207:MET:HE1	1:C:311:LYS:CG	2.29	0.62
1:E:72:ARG:HG3	1:E:144:ASP:HB3	1.81	0.62
1:A:329:LEU:HD23	1:A:334:ILE:HD12	0.71	0.62
1:A:248:ILE:HD12	1:A:254:LEU:CD1	2.27	0.62
1:D:184:VAL:O	1:D:185:ALA:HB2	1.99	0.62
1:A:249:TYR:CE2	1:A:251:PRO:CG	2.82	0.61
1:B:250:ASN:C	1:B:250:ASN:OD1	2.42	0.61
1:D:262:TRP:CE3	1:D:273:PRO:HD2	2.35	0.61
1:E:78:THR:OG1	1:E:81:THR:OG1	2.17	0.61
1:A:157:ASP:OD2	1:B:413:ARG:HD3	2.00	0.61
1:A:208:ASP:O	1:A:212:LYS:NZ	2.32	0.61
1:A:278:ILE:HG13	1:A:279:THR:N	2.15	0.61
1:D:209:LEU:HA	1:D:212:LYS:HG2	1.82	0.61
1:A:329:LEU:CD2	1:A:334:ILE:HG21	2.30	0.61
1:A:255:ASN:HB3	1:A:258:GLU:HG3	1.82	0.61
1:D:262:TRP:CZ3	1:D:273:PRO:CG	2.84	0.61
1:B:4:ASP:O	1:B:8:ILE:HG13	2.00	0.61
1:C:297:GLU:O	1:C:299:VAL:CG1	2.48	0.61
1:D:304:ASN:O	1:D:306:ASP:N	2.33	0.61
1:C:213:THR:CB	1:C:288:VAL:HG12	2.30	0.61
1:C:219:TYR:CD1	1:C:241:VAL:CG1	2.84	0.61
1:F:416:ILE:HD12	1:F:416:ILE:O	2.00	0.61
1:C:270:LYS:C	1:C:272:PHE:H	2.07	0.61
1:D:296:ILE:HD12	1:D:299:VAL:CG1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:CG2	1:A:155:MET:HG2	2.31	0.61
1:A:392:ILE:HD11	1:A:397:ALA:CA	2.31	0.61
1:A:392:ILE:HD11	1:A:397:ALA:HA	1.83	0.61
1:F:3:GLN:O	1:F:4:ASP:C	2.44	0.61
1:B:291:LEU:O	1:B:293:PRO:HD2	2.01	0.61
1:B:410:MET:HG2	1:B:415:TRP:CE3	2.35	0.61
1:E:179:SER:O	1:E:180:VAL:CG1	2.49	0.61
1:C:126:TYR:HD2	1:C:155:MET:HE2	1.66	0.60
1:C:214:ILE:CG2	1:C:236:MET:HE1	2.30	0.60
1:D:98:LEU:HB3	1:D:99:PRO:HD2	1.83	0.60
1:A:47:ASP:OD1	1:A:47:ASP:C	2.43	0.60
1:C:224:TYR:CE1	1:C:260:LEU:HD23	2.36	0.60
1:D:301:THR:O	1:D:305:ALA:HB2	2.02	0.60
1:E:127:VAL:CG2	1:E:155:MET:HG2	2.31	0.60
1:A:127:VAL:HG23	1:A:155:MET:HG2	1.83	0.60
1:C:288:VAL:O	1:C:310:ALA:HA	2.01	0.60
1:D:236:MET:HE1	1:D:290:VAL:HG21	1.82	0.60
1:E:226:MET:HE3	1:E:230:MET:SD	2.40	0.60
1:C:328:ILE:O	1:C:332:LYS:HB2	2.02	0.60
1:F:205:LEU:O	1:F:206:GLY:C	2.44	0.60
1:A:46:ASP:OD1	1:A:118:GLU:HG3	2.01	0.60
1:C:406:VAL:O	1:C:410:MET:HG3	2.01	0.60
1:D:34:GLN:HG3	1:D:60:TYR:O	2.02	0.60
1:D:250:ASN:OD1	1:D:252:ASP:HB2	2.01	0.60
1:E:305:ALA:HB3	1:E:328:ILE:HD13	1.83	0.60
1:F:3:GLN:HB3	1:F:80:SER:HB3	1.83	0.60
1:A:322:THR:OG1	1:A:325:ALA:HB2	2.02	0.60
1:F:337:ILE:O	1:F:338:PRO:C	2.45	0.60
1:A:304:ASN:O	1:A:305:ALA:C	2.45	0.60
1:B:74:HIS:CG	1:B:75:PRO:CD	2.85	0.60
1:B:291:LEU:HG	1:B:293:PRO:HD3	1.83	0.60
1:C:213:THR:OG1	1:C:288:VAL:CG1	2.44	0.60
1:D:242:SER:HA	1:D:247:GLY:CA	2.31	0.60
1:B:9:ALA:O	1:B:12:GLN:HB2	2.01	0.59
1:B:321:THR:CG2	1:B:322:THR:H	2.14	0.59
1:B:241:VAL:HG13	1:B:242:SER:N	2.16	0.59
1:D:3:GLN:O	1:D:5:PRO:HD2	2.02	0.59
1:A:26:ALA:HB2	1:A:407:TYR:CE1	2.37	0.59
1:A:142:ALA:HB1	1:A:143:PRO:HD2	1.84	0.59
1:A:164:ARG:NH2	1:E:131:TYR:HB3	2.16	0.59
1:C:79:LEU:HG	1:C:83:LYS:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TYR:CE1	1:F:168:PRO:HG3	2.38	0.59
1:F:400:VAL:O	1:F:404:SER:OG	2.19	0.59
1:C:262:TRP:NE1	1:C:270:LYS:O	2.34	0.59
1:E:72:ARG:NE	1:E:77:GLU:OE2	2.32	0.59
1:F:3:GLN:HB3	1:F:80:SER:CB	2.32	0.59
1:D:213:THR:C	1:D:288:VAL:CG1	2.75	0.59
1:D:313:VAL:HG23	1:D:334:ILE:CG2	2.33	0.59
1:E:250:ASN:C	1:E:250:ASN:OD1	2.46	0.59
1:F:6:PHE:O	1:F:9:ALA:N	2.35	0.59
1:F:230:MET:HE3	1:F:234:TYR:HB2	1.84	0.59
1:B:120:GLU:HA	1:B:154:TRP:CE3	2.38	0.59
1:C:224:TYR:CD1	1:C:260:LEU:HD23	2.36	0.59
1:A:117:ARG:O	1:A:121:ARG:HG3	2.03	0.59
1:C:381:TRP:O	1:C:382:ASP:C	2.46	0.59
1:A:242:SER:OG	1:A:280:ASN:ND2	2.36	0.59
1:A:297:GLU:O	1:A:299:VAL:HG13	2.01	0.59
1:B:65:GLY:HA3	1:B:99:PRO:O	2.03	0.59
1:C:207:MET:HE1	1:C:311:LYS:HD2	1.83	0.59
1:D:23:SER:OG	1:D:418:LYS:OXT	2.19	0.59
1:E:77:GLU:OE1	1:E:77:GLU:HA	2.03	0.59
1:E:184:VAL:C	1:E:186:ARG:H	2.08	0.59
1:E:279:THR:OG1	1:E:282:GLU:HG3	2.03	0.59
1:C:167:ASP:HB2	1:C:168:PRO:HD2	1.85	0.58
1:B:201:ALA:O	1:B:205:LEU:HD22	2.03	0.58
1:C:74:HIS:ND1	1:C:75:PRO:HD2	2.17	0.58
1:F:281:GLU:O	1:F:285:GLU:HG3	2.03	0.58
1:B:74:HIS:CE1	1:B:75:PRO:HD2	2.37	0.58
1:A:36:ILE:HG12	1:A:58:VAL:HG22	1.85	0.58
1:B:117:ARG:HH21	1:D:44:GLU:CG	2.15	0.58
1:D:126:TYR:CD2	1:D:155:MET:HE2	2.38	0.58
1:D:213:THR:HG22	1:D:288:VAL:HG13	1.84	0.58
1:F:304:ASN:O	1:F:305:ALA:C	2.45	0.58
1:F:283:LEU:HD23	1:F:284:LEU:HD23	1.85	0.58
1:A:71:ILE:HD13	1:A:126:TYR:CE2	2.38	0.58
1:B:29:PHE:CE2	1:B:410:MET:HE3	2.36	0.58
1:C:260:LEU:O	1:C:263:LYS:N	2.36	0.58
1:F:311:LYS:O	1:F:334:ILE:HG23	2.03	0.58
1:C:48:GLY:HA2	1:F:117:ARG:NH2	2.19	0.58
1:F:391:ASN:O	1:F:392:ILE:HG22	2.03	0.58
1:A:242:SER:HA	1:A:247:GLY:HA2	1.86	0.58
1:B:26:ALA:O	1:B:27:LEU:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ILE:O	1:E:144:ASP:CB	2.52	0.58
1:E:194:ALA:O	1:E:198:VAL:HG23	2.03	0.58
1:F:64:ARG:NH2	1:F:97:ASP:HA	2.18	0.58
1:F:416:ILE:HD12	1:F:416:ILE:C	2.28	0.58
1:A:4:ASP:O	1:A:7:GLU:HB2	2.03	0.58
1:A:213:THR:C	1:A:288:VAL:HG23	2.29	0.58
1:E:176:LYS:HZ1	1:E:357:ASN:HD21	1.50	0.58
1:F:278:ILE:HB	1:F:282:GLU:HG2	1.86	0.58
1:A:148:ASN:HB2	1:A:149:PRO:CD	2.33	0.57
1:B:164:ARG:O	1:B:165:ARG:HB2	2.04	0.57
1:D:208:ASP:O	1:D:212:LYS:HG2	2.04	0.57
1:F:176:LYS:NZ	1:F:353:GLU:OE2	2.36	0.57
1:B:22:ILE:HD13	1:B:27:LEU:HD23	1.85	0.57
1:F:263:LYS:HA	1:F:268:SER:O	2.04	0.57
1:A:42:PRO:HG3	1:F:29:PHE:HE1	1.68	0.57
1:A:68:LYS:HD2	1:A:140:ILE:O	2.04	0.57
1:C:325:ALA:HA	1:C:328:ILE:HD12	1.86	0.57
1:B:176:LYS:HZ1	1:B:357:ASN:HD21	1.51	0.57
1:B:399:TYR:O	1:B:403:VAL:HG23	2.03	0.57
1:C:207:MET:CE	1:C:311:LYS:CD	2.82	0.57
1:D:160:GLU:HG2	1:D:169:SER:CB	2.33	0.57
1:D:250:ASN:C	1:D:252:ASP:H	2.12	0.57
1:E:184:VAL:O	1:E:185:ALA:CB	2.47	0.57
1:E:271:ASP:O	1:E:272:PHE:C	2.47	0.57
1:F:262:TRP:O	1:F:266:THR:HB	2.04	0.57
1:B:114:MET:HE1	1:B:122:LEU:HD22	1.87	0.57
1:B:373:ASP:OD1	1:B:373:ASP:C	2.46	0.57
1:B:100:TYR:HE2	1:B:351:TYR:HB2	1.69	0.57
1:C:81:THR:O	1:C:85:LEU:HD12	2.05	0.57
1:C:183:ILE:CD1	1:C:353:GLU:HB2	2.30	0.57
1:D:276:THR:CG2	1:D:277:ASN:N	2.68	0.57
1:F:87:ALA:O	1:F:90:THR:HB	2.04	0.57
1:C:72:ARG:HE	1:C:77:GLU:CD	2.12	0.57
1:D:47:ASP:OD1	1:D:47:ASP:C	2.46	0.57
1:D:319:GLY:N	1:D:320:PRO:CD	2.67	0.57
1:F:291:LEU:HG	1:F:293:PRO:HD3	1.87	0.57
1:B:248:ILE:HG21	1:B:269:VAL:O	2.04	0.57
1:E:3:GLN:O	1:E:5:PRO:HD2	2.04	0.57
1:A:3:GLN:O	1:A:6:PHE:N	2.38	0.57
1:B:10:VAL:O	1:B:13:LEU:HB3	2.05	0.57
1:C:364:THR:HG23	1:C:367:GLU:OE2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:ASN:HD22	1:F:396:ASP:H	1.53	0.57
1:B:110:ASN:ND2	1:B:113:GLU:OE2	2.38	0.56
1:B:283:LEU:HA	1:B:286:LEU:HG	1.87	0.56
1:D:305:ALA:CB	1:D:328:ILE:HD13	2.34	0.56
1:E:123:ALA:CA	1:E:155:MET:HE3	2.33	0.56
1:F:250:ASN:HB3	1:F:254:LEU:HD21	1.87	0.56
1:A:188:ASP:O	1:A:192:ARG:CB	2.49	0.56
1:B:14:GLU:O	1:B:17:ALA:HB3	2.04	0.56
1:D:142:ALA:HB1	1:D:143:PRO:CD	2.35	0.56
1:A:48:GLY:C	1:E:117:ARG:HH22	2.13	0.56
1:B:188:ASP:OD2	1:B:192:ARG:NH1	2.37	0.56
1:D:284:LEU:O	1:D:308:ILE:HD12	2.05	0.56
1:F:68:LYS:HD3	1:F:140:ILE:HB	1.87	0.56
1:A:4:ASP:N	1:A:5:PRO:HD2	2.21	0.56
1:C:3:GLN:CG	1:C:4:ASP:N	2.49	0.56
1:F:51:LYS:HD3	1:F:53:PHE:CZ	2.40	0.56
1:A:184:VAL:C	1:A:186:ARG:H	2.11	0.56
1:B:384:TYR:CE2	1:B:388:LYS:HD3	2.41	0.56
1:D:262:TRP:O	1:D:266:THR:N	2.27	0.56
1:E:112:LYS:C	1:E:113:GLU:HG3	2.30	0.56
1:F:9:ALA:O	1:F:12:GLN:HB2	2.06	0.56
1:B:384:TYR:O	1:B:387:HIS:CD2	2.58	0.56
1:C:276:THR:HG22	1:C:277:ASN:N	2.20	0.56
1:E:156:MET:HE2	1:E:170:PHE:CE1	2.40	0.56
1:A:68:LYS:HD2	1:A:140:ILE:HB	1.88	0.56
1:B:273:PRO:O	1:B:275:ALA:N	2.39	0.56
1:C:214:ILE:HG13	1:C:215:ALA:O	2.04	0.56
1:C:384:TYR:HA	1:C:394:MET:CE	2.35	0.56
1:F:29:PHE:C	1:F:31:LYS:H	2.14	0.56
1:B:117:ARG:HH21	1:D:44:GLU:HG3	1.70	0.56
1:C:92:LYS:HD3	1:C:347:VAL:HG21	1.88	0.56
1:F:220:GLY:O	1:F:224:TYR:HB3	2.05	0.56
1:A:323:PRO:C	1:A:326:ASP:HB2	2.31	0.56
1:B:170:PHE:O	1:B:357:ASN:ND2	2.39	0.56
1:D:279:THR:O	1:D:282:GLU:N	2.38	0.56
1:A:296:ILE:HG13	1:A:299:VAL:CG1	2.36	0.56
1:B:48:GLY:C	1:D:117:ARG:HH22	2.13	0.56
1:C:176:LYS:HE2	1:C:353:GLU:OE2	2.06	0.56
1:D:72:ARG:HE	1:D:77:GLU:CD	2.14	0.56
1:E:57:ARG:NH1	1:E:69:GLY:O	2.36	0.56
1:F:322:THR:O	1:F:326:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PHE:O	1:A:9:ALA:N	2.39	0.55
1:B:305:ALA:HB3	1:B:328:ILE:HD12	1.89	0.55
1:D:126:TYR:CD2	1:D:155:MET:CE	2.89	0.55
1:D:322:THR:CB	1:D:323:PRO:CD	2.79	0.55
1:E:22:ILE:CD1	1:E:27:LEU:CD2	2.85	0.55
1:C:7:GLU:O	1:C:11:LYS:HG3	2.05	0.55
1:D:248:ILE:HD13	1:D:269:VAL:CG2	2.35	0.55
1:F:184:VAL:C	1:F:186:ARG:N	2.59	0.55
1:D:240:ALA:HB1	1:D:283:LEU:HD12	1.89	0.55
1:A:3:GLN:HB3	1:A:80:SER:CB	2.36	0.55
1:A:23:SER:OG	1:A:418:LYS:OXT	2.24	0.55
1:C:71:ILE:HD13	1:C:126:TYR:CE2	2.42	0.55
1:D:217:GLN:OE1	1:D:284:LEU:HD21	2.06	0.55
1:B:88:TRP:CH2	1:B:399:TYR:OH	2.59	0.55
1:B:241:VAL:HG13	1:B:242:SER:H	1.71	0.55
1:C:297:GLU:HA	1:C:320:PRO:HA	1.88	0.55
1:D:248:ILE:CG1	1:D:254:LEU:HD21	2.36	0.55
1:F:18:GLN:NE2	1:F:19:TYR:CE2	2.68	0.55
1:F:115:SER:O	1:F:119:LYS:HG3	2.07	0.55
1:A:409:ALA:O	1:A:413:ARG:HG3	2.07	0.55
1:B:204:ALA:HB1	1:B:384:TYR:CE1	2.42	0.55
1:C:249:TYR:HB2	1:C:278:ILE:HD13	1.89	0.55
1:D:384:TYR:HE2	1:D:388:LYS:NZ	2.03	0.55
1:E:23:SER:CB	1:E:418:LYS:OXT	2.54	0.55
1:E:22:ILE:CD1	1:E:27:LEU:HD23	2.35	0.55
1:A:164:ARG:O	1:A:165:ARG:HB2	2.06	0.55
1:B:68:LYS:HD2	1:B:140:ILE:O	2.06	0.55
1:B:302:LYS:HG3	1:B:303:LYS:N	2.22	0.55
1:B:321:THR:HG22	1:B:322:THR:H	1.66	0.55
1:C:126:TYR:CD2	1:C:155:MET:HE2	2.41	0.55
1:C:349:VAL:O	1:C:352:PHE:HB2	2.07	0.55
1:D:297:GLU:HB2	1:D:319:GLY:O	2.07	0.55
1:F:184:VAL:O	1:F:185:ALA:CB	2.52	0.55
1:A:315:GLU:HG3	1:A:337:ILE:O	2.07	0.55
1:B:410:MET:HG2	1:B:415:TRP:HE3	1.72	0.55
1:C:196:TYR:HE2	1:C:372:LEU:HD23	1.72	0.55
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.22	0.55
1:F:65:GLY:HA3	1:F:99:PRO:O	2.06	0.55
1:F:66:PRO:HD2	1:F:99:PRO:O	2.07	0.55
1:C:297:GLU:C	1:C:299:VAL:HG13	2.32	0.55
1:E:208:ASP:C	1:E:208:ASP:OD1	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:CG1	1:A:96:MET:N	2.70	0.54
1:A:392:ILE:HD12	1:A:396:ASP:CB	2.37	0.54
1:D:289:ASP:OD1	1:D:289:ASP:N	2.39	0.54
1:E:160:GLU:HG2	1:E:169:SER:CB	2.37	0.54
1:B:323:PRO:HA	1:B:326:ASP:OD2	2.07	0.54
1:D:213:THR:HB	1:D:288:VAL:HG12	1.89	0.54
1:E:23:SER:HB3	1:E:418:LYS:OXT	2.08	0.54
1:F:142:ALA:CB	1:F:143:PRO:CD	2.78	0.54
1:A:319:GLY:N	1:A:320:PRO:CD	2.69	0.54
1:D:202:ALA:HB1	1:D:207:MET:CG	2.37	0.54
1:D:304:ASN:O	1:D:305:ALA:C	2.50	0.54
1:E:3:GLN:O	1:E:7:GLU:HG3	2.06	0.54
1:F:69:GLY:HA3	1:F:103:GLY:O	2.08	0.54
1:F:158:GLU:O	1:F:162:ILE:HG13	2.07	0.54
1:F:188:ASP:OD2	1:F:192:ARG:HD2	2.08	0.54
1:A:242:SER:HB3	1:A:283:LEU:HD13	1.89	0.54
1:A:315:GLU:OE2	1:A:336:ILE:HD13	2.06	0.54
1:C:270:LYS:C	1:C:272:PHE:N	2.64	0.54
1:D:71:ILE:HD13	1:D:126:TYR:CE2	2.42	0.54
1:A:373:ASP:O	1:A:374:LYS:C	2.50	0.54
1:B:381:TRP:O	1:B:382:ASP:C	2.49	0.54
1:D:416:ILE:HD12	1:D:418:LYS:OXT	2.07	0.54
1:E:19:TYR:O	1:E:390:LYS:NZ	2.38	0.54
1:E:33:PRO:HB3	1:E:60:TYR:CD1	2.42	0.54
1:E:111:PRO:HG2	1:E:146:TYR:CD2	2.42	0.54
1:A:387:HIS:CD2	1:A:388:LYS:N	2.76	0.54
1:B:142:ALA:HB1	1:B:143:PRO:CD	2.37	0.54
1:C:276:THR:CG2	1:C:277:ASN:N	2.70	0.54
1:E:160:GLU:HG2	1:E:169:SER:HB3	1.90	0.54
1:F:250:ASN:OD1	1:F:251:PRO:CD	2.55	0.54
1:B:167:ASP:O	1:B:169:SER:N	2.39	0.54
1:B:236:MET:HE1	1:B:290:VAL:HG23	1.89	0.54
1:B:291:LEU:O	1:B:293:PRO:CD	2.56	0.54
1:D:3:GLN:C	1:D:5:PRO:CD	2.79	0.54
1:D:75:PRO:HD2	1:D:76:GLU:H	1.73	0.54
1:E:3:GLN:HB3	1:E:80:SER:CB	2.37	0.54
1:E:94:ALA:O	1:E:405:ARG:NH1	2.34	0.54
1:A:281:GLU:O	1:A:285:GLU:HG3	2.08	0.54
1:E:167:ASP:O	1:E:169:SER:N	2.36	0.54
1:E:178:PRO:C	1:E:180:VAL:H	2.16	0.54
1:F:391:ASN:O	1:F:392:ILE:CG2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:O	1:A:226:MET:HB2	2.08	0.54
1:A:285:GLU:O	1:A:309:LYS:HE3	2.07	0.54
1:D:389:GLU:HG3	1:D:390:LYS:N	2.21	0.54
1:F:71:ILE:HD11	1:F:141:PRO:CB	2.38	0.54
1:F:114:MET:HE1	1:F:122:LEU:HD22	1.90	0.54
1:A:372:LEU:O	1:A:373:ASP:C	2.51	0.53
1:D:384:TYR:OH	1:D:388:LYS:NZ	2.31	0.53
1:E:73:TRP:O	1:E:145:VAL:HG12	2.08	0.53
1:A:120:GLU:HG3	1:A:154:TRP:CE2	2.42	0.53
1:D:4:ASP:O	1:D:8:ILE:CG1	2.55	0.53
1:D:313:VAL:HG23	1:D:334:ILE:HG21	1.91	0.53
1:E:399:TYR:O	1:E:403:VAL:HG23	2.08	0.53
1:A:12:GLN:NE2	1:A:88:TRP:CH2	2.75	0.53
1:A:243:ASP:O	1:A:244:THR:C	2.52	0.53
1:A:352:PHE:CZ	1:A:371:LYS:HB3	2.44	0.53
1:B:48:GLY:HA2	1:D:117:ARG:NH2	2.23	0.53
1:C:97:ASP:HB2	1:C:405:ARG:NH1	2.22	0.53
1:D:219:TYR:CD2	1:D:219:TYR:O	2.61	0.53
1:D:228:LYS:NZ	1:D:232:GLU:OE1	2.42	0.53
1:F:29:PHE:HD2	1:F:410:MET:CE	2.14	0.53
1:F:250:ASN:HB3	1:F:254:LEU:CD2	2.38	0.53
1:A:339:ASP:O	1:A:342:CYS:N	2.41	0.53
1:C:283:LEU:O	1:C:286:LEU:HB2	2.08	0.53
1:C:393:ASN:ND2	1:C:396:ASP:N	2.48	0.53
1:D:98:LEU:HD23	1:D:375:LYS:HZ2	1.71	0.53
1:D:172:VAL:O	1:D:172:VAL:HG22	2.08	0.53
1:D:242:SER:OG	1:D:243:ASP:N	2.42	0.53
1:E:323:PRO:CA	1:E:326:ASP:HB2	2.39	0.53
1:B:184:VAL:CG1	1:B:184:VAL:O	2.56	0.53
1:E:170:PHE:O	1:E:357:ASN:ND2	2.42	0.53
1:E:304:ASN:O	1:E:305:ALA:C	2.50	0.53
1:F:3:GLN:C	1:F:5:PRO:CD	2.82	0.53
1:A:365:VAL:O	1:A:366:GLU:C	2.49	0.53
1:B:6:PHE:O	1:B:9:ALA:N	2.41	0.53
1:B:68:LYS:HD3	1:B:140:ILE:HB	1.91	0.53
1:C:278:ILE:HD11	1:C:283:LEU:HD12	1.91	0.53
1:D:127:VAL:HG23	1:D:155:MET:HG2	1.89	0.53
1:F:20:MET:HE2	1:F:22:ILE:CG2	2.38	0.53
1:D:4:ASP:O	1:D:8:ILE:N	2.28	0.53
1:D:124:ARG:O	1:D:128:ARG:HG3	2.09	0.53
1:D:276:THR:HG22	1:D:277:ASN:H	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:THR:O	1:D:280:ASN:C	2.51	0.53
1:D:127:VAL:CG2	1:D:155:MET:HG2	2.38	0.53
1:D:322:THR:O	1:D:326:ASP:N	2.32	0.53
1:F:418:LYS:OXT	1:F:418:LYS:HG3	2.09	0.53
1:A:81:THR:HG22	1:A:85:LEU:CD1	2.39	0.52
1:B:347:VAL:O	1:B:350:SER:OG	2.27	0.52
1:D:209:LEU:HA	1:D:212:LYS:CG	2.38	0.52
1:E:94:ALA:O	1:E:405:ARG:HD2	2.09	0.52
1:E:209:LEU:O	1:E:210:LYS:C	2.45	0.52
1:A:115:SER:O	1:A:119:LYS:HG3	2.10	0.52
1:A:209:LEU:CA	1:A:212:LYS:CG	2.81	0.52
1:B:23:SER:OG	1:B:418:LYS:OXT	2.18	0.52
1:F:220:GLY:O	1:F:224:TYR:CB	2.57	0.52
1:A:279:THR:N	1:A:282:GLU:OE2	2.42	0.52
1:B:72:ARG:HG2	1:B:144:ASP:OD2	2.09	0.52
1:E:3:GLN:O	1:E:5:PRO:CD	2.57	0.52
1:E:172:VAL:O	1:E:172:VAL:CG2	2.53	0.52
1:F:78:THR:OG1	1:F:81:THR:OG1	2.04	0.52
1:F:200:GLU:O	1:F:203:LYS:HB2	2.09	0.52
1:A:92:LYS:HE2	1:A:344:ALA:HA	1.91	0.52
1:A:250:ASN:HB3	1:A:254:LEU:HD21	1.91	0.52
1:B:72:ARG:NH2	1:B:77:GLU:OE1	2.24	0.52
1:C:212:LYS:N	1:C:212:LYS:CD	2.73	0.52
1:C:343:ASN:OD1	1:C:343:ASN:C	2.52	0.52
1:A:45:MET:C	1:A:47:ASP:H	2.15	0.52
1:B:59:GLN:HE22	1:B:133:VAL:HG23	1.75	0.52
1:D:72:ARG:O	1:D:106:GLY:HA2	2.10	0.52
1:D:229:ILE:HG23	1:D:233:GLU:CG	2.40	0.52
1:D:322:THR:O	1:D:325:ALA:HB3	2.08	0.52
1:E:179:SER:C	1:E:180:VAL:HG13	2.34	0.52
1:F:71:ILE:HD11	1:F:141:PRO:HB3	1.91	0.52
1:B:3:GLN:N	1:B:6:PHE:HB3	2.25	0.52
1:C:250:ASN:HB3	1:C:254:LEU:HD21	1.90	0.52
1:E:3:GLN:HB3	1:E:80:SER:HB3	1.90	0.52
1:E:319:GLY:N	1:E:320:PRO:CD	2.72	0.52
1:E:370:ALA:O	1:E:374:LYS:HG3	2.08	0.52
1:D:248:ILE:HG23	1:D:269:VAL:HG23	1.92	0.52
1:E:29:PHE:HB3	1:E:410:MET:HE1	1.92	0.52
1:E:79:LEU:HD12	1:E:79:LEU:C	2.35	0.52
1:E:297:GLU:HB2	1:E:319:GLY:O	2.09	0.52
1:A:34:GLN:OE1	1:A:61:ASN:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ALA:O	1:B:20:MET:N	2.36	0.52
1:B:176:LYS:HE2	1:B:180:VAL:O	2.10	0.52
1:F:297:GLU:O	1:F:298:GLU:C	2.52	0.52
1:A:259:VAL:HG12	1:A:269:VAL:HG23	1.90	0.52
1:E:74:HIS:CE1	1:E:75:PRO:HD2	2.45	0.52
1:E:184:VAL:C	1:E:186:ARG:N	2.66	0.52
1:A:72:ARG:HG2	1:A:144:ASP:OD2	2.10	0.52
1:A:370:ALA:O	1:A:374:LYS:HG3	2.10	0.52
1:A:392:ILE:CD1	1:A:397:ALA:N	2.73	0.52
1:B:209:LEU:HA	1:B:212:LYS:HG2	1.92	0.52
1:D:328:ILE:O	1:D:332:LYS:HB2	2.10	0.52
1:D:336:ILE:O	1:D:338:PRO:HD3	2.09	0.52
1:E:29:PHE:CB	1:E:410:MET:HE1	2.40	0.52
1:E:249:TYR:CE2	1:E:251:PRO:HD3	2.45	0.52
1:F:74:HIS:ND1	1:F:75:PRO:HD2	2.25	0.52
1:F:391:ASN:C	1:F:392:ILE:CG2	2.82	0.52
1:A:110:ASN:ND2	1:A:113:GLU:HG3	2.25	0.51
1:C:321:THR:HG22	1:C:322:THR:N	2.24	0.51
1:C:393:ASN:HD21	1:C:395:ARG:HB3	1.76	0.51
1:D:141:PRO:HB2	1:D:173:ILE:HG13	1.90	0.51
1:E:226:MET:HE3	1:E:230:MET:HG3	1.85	0.51
1:F:248:ILE:C	1:F:278:ILE:HD13	2.35	0.51
1:F:291:LEU:O	1:F:293:PRO:HD2	2.09	0.51
1:B:72:ARG:HH21	1:B:77:GLU:CD	2.15	0.51
1:E:29:PHE:HD1	1:E:410:MET:CE	2.11	0.51
1:F:192:ARG:O	1:F:195:SER:OG	2.23	0.51
1:F:337:ILE:O	1:F:338:PRO:O	2.28	0.51
1:D:74:HIS:ND1	1:D:75:PRO:CD	2.73	0.51
1:F:205:LEU:HD11	1:F:335:LEU:HD23	1.92	0.51
1:F:344:ALA:O	1:F:347:VAL:HG12	2.10	0.51
1:A:214:ILE:HG22	1:A:236:MET:HE2	1.91	0.51
1:B:172:VAL:O	1:B:172:VAL:CG2	2.56	0.51
1:B:294:SER:CB	1:B:316:LEU:HB2	2.36	0.51
1:E:339:ASP:O	1:E:341:LEU:N	2.43	0.51
1:F:29:PHE:HB3	1:F:410:MET:CE	2.41	0.51
1:A:268:SER:C	1:A:270:LYS:H	2.17	0.51
1:B:11:LYS:O	1:B:12:GLN:C	2.53	0.51
1:D:213:THR:C	1:D:288:VAL:HG12	2.34	0.51
1:E:148:ASN:HB2	1:E:149:PRO:HD2	1.93	0.51
1:E:294:SER:HB3	1:E:316:LEU:HB2	1.91	0.51
1:A:217:GLN:HB3	1:A:293:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:HG3	1:B:186:ARG:O	2.09	0.51
1:C:322:THR:HB	1:C:323:PRO:CD	2.41	0.51
1:D:364:THR:HG23	1:D:367:GLU:OE1	2.11	0.51
1:E:126:TYR:HB3	1:E:155:MET:HE2	1.93	0.51
1:E:176:LYS:HB2	1:E:176:LYS:HZ2	1.75	0.51
1:F:366:GLU:CD	1:F:366:GLU:H	2.18	0.51
1:A:131:TYR:O	1:A:134:ILE:HG13	2.10	0.51
1:B:18:GLN:NE2	1:B:19:TYR:CE2	2.78	0.51
1:B:81:THR:HG22	1:B:85:LEU:HD11	1.93	0.51
1:B:214:ILE:HA	1:B:290:VAL:O	2.10	0.51
1:C:48:GLY:CA	1:F:117:ARG:NH2	2.73	0.51
1:B:3:GLN:O	1:B:6:PHE:N	2.44	0.51
1:B:270:LYS:O	1:B:271:ASP:HB2	2.10	0.51
1:D:321:THR:CG2	1:D:322:THR:N	2.74	0.51
1:D:325:ALA:HA	1:D:328:ILE:HD12	1.92	0.51
1:F:391:ASN:C	1:F:392:ILE:HG23	2.35	0.51
1:F:411:LYS:O	1:F:414:GLY:N	2.43	0.51
1:A:3:GLN:O	1:A:4:ASP:O	2.29	0.51
1:A:45:MET:C	1:A:47:ASP:N	2.68	0.51
1:A:329:LEU:HD22	1:A:334:ILE:CG2	2.36	0.51
1:B:111:PRO:HG2	1:B:146:TYR:HD2	1.72	0.51
1:C:164:ARG:O	1:C:165:ARG:HB2	2.11	0.51
1:A:249:TYR:CE2	1:A:251:PRO:CD	2.93	0.51
1:B:297:GLU:CB	1:B:319:GLY:O	2.59	0.51
1:B:322:THR:HB	1:B:323:PRO:CD	2.40	0.51
1:C:270:LYS:O	1:C:272:PHE:N	2.44	0.51
1:D:321:THR:HG22	1:D:322:THR:N	2.25	0.51
1:E:69:GLY:HA3	1:E:103:GLY:O	2.11	0.51
1:A:241:VAL:CG1	1:A:242:SER:N	2.73	0.50
1:B:93:THR:HG21	1:B:100:TYR:HB2	1.93	0.50
1:D:110:ASN:ND2	1:D:113:GLU:HG3	2.26	0.50
1:E:228:LYS:NZ	1:E:232:GLU:OE2	2.43	0.50
1:D:262:TRP:CZ3	1:D:273:PRO:HG3	2.46	0.50
1:F:66:PRO:HG2	1:F:100:TYR:HD1	1.76	0.50
1:B:124:ARG:O	1:B:128:ARG:HG3	2.11	0.50
1:B:356:GLN:OE1	1:B:362:TYR:HA	2.12	0.50
1:D:22:ILE:HA	1:D:407:TYR:CE2	2.47	0.50
1:D:249:TYR:O	1:D:275:ALA:HB1	2.11	0.50
1:D:262:TRP:O	1:D:263:LYS:C	2.54	0.50
1:F:170:PHE:O	1:F:176:LYS:CE	2.59	0.50
1:B:24:GLU:O	1:B:28:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ILE:HA	1:B:335:LEU:O	2.12	0.50
1:C:323:PRO:HA	1:C:326:ASP:HB2	1.94	0.50
1:D:242:SER:OG	1:D:280:ASN:ND2	2.45	0.50
1:D:284:LEU:HB3	1:D:308:ILE:HD11	1.93	0.50
1:A:72:ARG:HG2	1:A:144:ASP:CB	2.40	0.50
1:A:248:ILE:HG12	1:A:269:VAL:HG22	1.92	0.50
1:D:225:TYR:O	1:D:226:MET:C	2.53	0.50
1:F:299:VAL:HG23	1:F:300:ILE:HG13	1.92	0.50
1:D:262:TRP:CH2	1:D:273:PRO:CD	2.83	0.50
1:D:296:ILE:HD11	1:D:299:VAL:HG12	1.94	0.50
1:E:34:GLN:HG3	1:E:60:TYR:O	2.12	0.50
1:F:172:VAL:HG22	1:F:172:VAL:O	2.10	0.50
1:A:245:LYS:CD	1:A:268:SER:HB2	2.42	0.50
1:C:38:GLU:HG2	1:D:36:ILE:HD12	1.93	0.50
1:C:205:LEU:HD23	1:C:207:MET:CE	2.41	0.50
1:F:25:GLU:OE1	1:F:418:LYS:HG2	2.12	0.50
1:F:89:MET:O	1:F:92:LYS:HB3	2.12	0.50
1:F:117:ARG:O	1:F:121:ARG:HG3	2.12	0.50
1:F:160:GLU:HG2	1:F:169:SER:OG	2.11	0.50
1:F:238:VAL:O	1:F:254:LEU:N	2.32	0.50
1:A:120:GLU:HG3	1:A:154:TRP:CG	2.47	0.50
1:B:167:ASP:HB2	1:B:168:PRO:HD2	1.93	0.50
1:C:20:MET:HG3	1:C:22:ILE:HG22	1.94	0.50
1:A:30:LEU:HD21	1:A:406:VAL:HG11	1.93	0.50
1:B:114:MET:HB3	1:B:119:LYS:HG3	1.93	0.50
1:B:263:LYS:O	1:B:267:GLY:N	2.42	0.50
1:C:207:MET:CE	1:C:311:LYS:HD2	2.41	0.50
1:D:117:ARG:O	1:D:121:ARG:HG3	2.12	0.50
1:A:417:LYS:HD2	1:A:417:LYS:N	2.26	0.49
1:D:4:ASP:N	1:D:5:PRO:HD2	2.27	0.49
1:D:229:ILE:HG23	1:D:233:GLU:HG3	1.94	0.49
1:F:3:GLN:O	1:F:5:PRO:N	2.45	0.49
1:F:72:ARG:NH2	1:F:77:GLU:OE1	2.39	0.49
1:A:96:MET:O	1:A:97:ASP:CB	2.60	0.49
1:B:29:PHE:HB3	1:B:410:MET:HE1	1.93	0.49
1:C:200:GLU:HB3	1:C:380:PHE:CD2	2.46	0.49
1:C:260:LEU:O	1:C:263:LYS:HB3	2.12	0.49
1:C:384:TYR:O	1:C:387:HIS:CD2	2.59	0.49
1:E:71:ILE:O	1:E:144:ASP:HB3	2.11	0.49
1:E:312:ILE:HA	1:E:335:LEU:O	2.12	0.49
1:C:373:ASP:C	1:C:373:ASP:OD1	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:GLU:HA	1:D:320:PRO:HA	1.94	0.49
1:E:29:PHE:HD1	1:E:410:MET:HE1	1.63	0.49
1:A:263:LYS:HD2	1:A:268:SER:HA	1.94	0.49
1:D:142:ALA:HB1	1:D:143:PRO:HD2	1.95	0.49
1:D:214:ILE:HG13	1:D:215:ALA:N	2.27	0.49
1:D:300:ILE:HA	1:D:304:ASN:ND2	2.28	0.49
1:D:305:ALA:HB3	1:D:328:ILE:HD13	1.93	0.49
1:E:68:LYS:CD	1:E:140:ILE:O	2.61	0.49
1:E:325:ALA:O	1:E:329:LEU:HD12	2.13	0.49
1:F:164:ARG:O	1:F:165:ARG:HB2	2.13	0.49
1:F:324:GLU:O	1:F:328:ILE:HG13	2.13	0.49
1:F:329:LEU:HD13	1:F:336:ILE:HD11	1.94	0.49
1:A:3:GLN:CG	1:A:4:ASP:N	2.75	0.49
1:A:339:ASP:O	1:A:341:LEU:N	2.45	0.49
1:B:262:TRP:O	1:B:266:THR:N	2.40	0.49
1:D:258:GLU:O	1:D:261:ALA:HB3	2.11	0.49
1:E:201:ALA:O	1:E:202:ALA:C	2.53	0.49
1:E:352:PHE:CZ	1:E:371:LYS:HB3	2.47	0.49
1:F:17:ALA:O	1:F:20:MET:N	2.36	0.49
1:A:111:PRO:HG3	1:A:146:TYR:CD2	2.48	0.49
1:A:117:ARG:HE	1:A:117:ARG:HA	1.78	0.49
1:A:224:TYR:O	1:A:227:ALA:HB3	2.13	0.49
1:B:81:THR:O	1:B:85:LEU:HD12	2.12	0.49
1:B:184:VAL:C	1:B:186:ARG:H	2.20	0.49
1:B:393:ASN:O	1:B:394:MET:C	2.55	0.49
1:C:4:ASP:O	1:C:8:ILE:HD12	2.13	0.49
1:C:43:VAL:HG12	1:C:44:GLU:N	2.26	0.49
1:C:74:HIS:CG	1:C:75:PRO:HD2	2.48	0.49
1:C:77:GLU:HG3	1:C:78:THR:N	2.28	0.49
1:F:10:VAL:O	1:F:13:LEU:HB3	2.13	0.49
1:B:278:ILE:HG13	1:B:279:THR:O	2.13	0.49
1:C:71:ILE:CD1	1:C:126:TYR:CE2	2.96	0.49
1:D:12:GLN:CD	1:D:88:TRP:HH2	2.21	0.49
1:D:216:ILE:HG12	1:D:292:ALA:HB3	1.93	0.49
1:E:279:THR:HG23	1:E:282:GLU:OE2	2.12	0.49
1:E:323:PRO:HA	1:E:326:ASP:HB2	1.95	0.49
1:C:14:GLU:O	1:C:17:ALA:HB3	2.13	0.49
1:C:131:TYR:CE1	1:C:159:TYR:CE1	3.00	0.49
1:C:161:THR:HG21	1:F:128:ARG:CZ	2.43	0.49
1:D:202:ALA:HB1	1:D:207:MET:HG2	1.95	0.49
1:E:3:GLN:O	1:E:5:PRO:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLU:HB3	1:E:380:PHE:CD2	2.48	0.49
1:F:238:VAL:O	1:F:253:GLY:HA2	2.13	0.49
1:F:341:LEU:HD22	1:F:383:VAL:HG21	1.95	0.49
1:A:201:ALA:O	1:A:202:ALA:C	2.56	0.49
1:B:81:THR:O	1:B:85:LEU:CD1	2.61	0.49
1:B:131:TYR:CZ	1:B:162:ILE:HG22	2.47	0.49
1:B:322:THR:HB	1:B:323:PRO:HD2	1.94	0.49
1:C:324:GLU:O	1:C:328:ILE:CG1	2.59	0.49
1:F:169:SER:O	1:F:172:VAL:HG12	2.13	0.49
1:F:224:TYR:CE1	1:F:260:LEU:HD22	2.47	0.49
1:B:352:PHE:O	1:B:356:GLN:HG3	2.13	0.49
1:C:219:TYR:CG	1:C:241:VAL:HG11	2.48	0.49
1:C:219:TYR:OH	1:C:256:ALA:HA	2.12	0.49
1:C:289:ASP:N	1:C:289:ASP:OD1	2.39	0.49
1:D:4:ASP:HB3	1:D:5:PRO:HD3	1.95	0.49
1:D:205:LEU:O	1:D:206:GLY:O	2.30	0.49
1:D:304:ASN:OD1	1:D:304:ASN:N	2.24	0.49
1:E:365:VAL:CG2	1:E:366:GLU:N	2.75	0.49
1:F:365:VAL:CG2	1:F:366:GLU:OE2	2.60	0.49
1:A:384:TYR:O	1:A:387:HIS:HD2	1.95	0.48
1:B:207:MET:HE1	1:B:311:LYS:HG2	1.95	0.48
1:B:250:ASN:O	1:B:253:GLY:N	2.35	0.48
1:C:315:GLU:HB3	1:C:320:PRO:CG	2.42	0.48
1:D:337:ILE:HG22	1:D:342:CYS:HB2	1.94	0.48
1:E:23:SER:OG	1:E:26:ALA:N	2.35	0.48
1:C:212:LYS:N	1:C:212:LYS:HD3	2.28	0.48
1:D:4:ASP:N	1:D:5:PRO:CD	2.76	0.48
1:F:296:ILE:HD12	1:F:299:VAL:CG1	2.43	0.48
1:F:323:PRO:O	1:F:326:ASP:CB	2.53	0.48
1:B:3:GLN:O	1:B:4:ASP:C	2.56	0.48
1:B:319:GLY:N	1:B:320:PRO:CD	2.76	0.48
1:D:209:LEU:O	1:D:212:LYS:HB2	2.13	0.48
1:D:219:TYR:HB2	1:D:241:VAL:HG13	1.94	0.48
1:D:416:ILE:O	1:D:416:ILE:HG13	2.10	0.48
1:F:263:LYS:O	1:F:267:GLY:N	2.44	0.48
1:A:161:THR:HG21	1:E:128:ARG:NH2	2.29	0.48
1:B:71:ILE:HD13	1:B:126:TYR:CE2	2.48	0.48
1:C:164:ARG:NE	1:F:131:TYR:HD2	2.11	0.48
1:C:321:THR:CG2	1:C:322:THR:N	2.76	0.48
1:D:324:GLU:O	1:D:325:ALA:C	2.56	0.48
1:B:198:VAL:HG11	1:B:230:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:VAL:CG1	1:D:242:SER:N	2.34	0.48
1:D:296:ILE:HD11	1:D:299:VAL:CG1	2.43	0.48
1:E:117:ARG:O	1:E:121:ARG:CG	2.60	0.48
1:F:263:LYS:O	1:F:267:GLY:CA	2.62	0.48
1:A:296:ILE:HG13	1:A:299:VAL:HG11	1.94	0.48
1:B:393:ASN:O	1:B:396:ASP:N	2.46	0.48
1:E:142:ALA:HB1	1:E:143:PRO:HD2	1.94	0.48
1:A:208:ASP:O	1:A:212:LYS:CG	2.61	0.48
1:A:213:THR:OG1	1:A:288:VAL:HG23	2.14	0.48
1:B:17:ALA:O	1:B:19:TYR:N	2.47	0.48
1:B:167:ASP:HB2	1:B:168:PRO:CD	2.44	0.48
1:B:200:GLU:HB3	1:B:380:PHE:CD2	2.48	0.48
1:D:224:TYR:O	1:D:227:ALA:HB3	2.13	0.48
1:D:262:TRP:CD1	1:D:268:SER:O	2.67	0.48
1:E:22:ILE:HD13	1:E:27:LEU:CD2	2.43	0.48
1:E:36:ILE:HG12	1:E:58:VAL:HG22	1.94	0.48
1:F:249:TYR:N	1:F:276:THR:O	2.38	0.48
1:F:294:SER:HB3	1:F:316:LEU:HB2	1.95	0.48
1:A:74:HIS:CG	1:A:75:PRO:HD2	2.48	0.48
1:B:152:MET:HA	1:B:152:MET:HE2	1.95	0.48
1:F:47:ASP:OD1	1:F:49:SER:HB3	2.14	0.48
1:A:269:VAL:O	1:A:269:VAL:HG13	2.14	0.48
1:B:74:HIS:CG	1:B:75:PRO:HD3	2.48	0.48
1:C:217:GLN:HE22	1:C:299:VAL:HG21	1.78	0.48
1:D:262:TRP:CE3	1:D:273:PRO:CD	2.96	0.48
1:E:68:LYS:HD2	1:E:140:ILE:O	2.13	0.48
1:E:72:ARG:HG2	1:E:145:VAL:HB	1.95	0.48
1:A:209:LEU:C	1:A:212:LYS:HG2	2.38	0.48
1:B:51:LYS:HD3	1:B:53:PHE:CZ	2.49	0.48
1:D:29:PHE:CG	1:D:410:MET:HE1	2.48	0.48
1:D:411:LYS:O	1:D:412:ASP:C	2.57	0.48
1:E:22:ILE:HD11	1:E:26:ALA:HB1	1.96	0.48
1:E:241:VAL:HG12	1:E:242:SER:H	1.78	0.48
1:A:249:TYR:CD2	1:A:251:PRO:HD3	2.49	0.47
1:B:322:THR:CB	1:B:323:PRO:CD	2.92	0.47
1:C:27:LEU:CD1	1:C:31:LYS:HE3	2.40	0.47
1:C:33:PRO:HB3	1:C:60:TYR:HD1	1.76	0.47
1:D:3:GLN:O	1:D:6:PHE:N	2.47	0.47
1:D:276:THR:CG2	1:D:277:ASN:H	2.27	0.47
1:E:29:PHE:CE1	1:E:410:MET:CE	2.82	0.47
1:F:11:LYS:O	1:F:12:GLN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:CB	1:B:149:PRO:CD	2.85	0.47
1:B:156:MET:C	1:B:156:MET:SD	2.97	0.47
1:B:262:TRP:CD1	1:B:268:SER:O	2.68	0.47
1:C:164:ARG:HH21	1:F:132:ASP:CG	2.22	0.47
1:D:89:MET:HE1	1:D:347:VAL:HG11	1.96	0.47
1:E:160:GLU:CG	1:E:169:SER:HB3	2.44	0.47
1:F:25:GLU:OE1	1:F:418:LYS:CG	2.63	0.47
1:F:160:GLU:CG	1:F:169:SER:HB3	2.42	0.47
1:A:241:VAL:HG12	1:A:242:SER:N	2.29	0.47
1:B:352:PHE:CZ	1:B:371:LYS:HB2	2.49	0.47
1:C:120:GLU:HA	1:C:154:TRP:CZ3	2.49	0.47
1:D:176:LYS:HB2	1:D:176:LYS:HZ2	1.80	0.47
1:D:197:THR:O	1:D:198:VAL:C	2.57	0.47
1:D:311:LYS:O	1:D:334:ILE:HG23	2.14	0.47
1:E:409:ALA:O	1:E:413:ARG:HG3	2.15	0.47
1:E:219:TYR:OH	1:E:256:ALA:HB1	2.15	0.47
1:E:237:LYS:HD3	1:E:252:ASP:O	2.14	0.47
1:E:366:GLU:CD	1:E:366:GLU:H	2.23	0.47
1:F:329:LEU:HD23	1:F:334:ILE:HD12	1.97	0.47
1:B:196:TYR:O	1:B:199:ARG:HB3	2.15	0.47
1:B:300:ILE:O	1:B:322:THR:HG23	2.15	0.47
1:D:25:GLU:OE2	1:D:417:LYS:N	2.47	0.47
1:D:148:ASN:OD1	1:D:148:ASN:C	2.57	0.47
1:D:296:ILE:HD12	1:D:299:VAL:HG13	1.95	0.47
1:E:22:ILE:HD12	1:E:27:LEU:CD2	2.44	0.47
1:A:3:GLN:CG	1:A:4:ASP:H	2.27	0.47
1:A:74:HIS:CE1	1:A:75:PRO:HD2	2.49	0.47
1:B:93:THR:HG22	1:B:98:LEU:HD12	1.96	0.47
1:B:273:PRO:C	1:B:275:ALA:N	2.71	0.47
1:C:72:ARG:NH2	1:C:77:GLU:OE1	2.38	0.47
1:C:238:VAL:O	1:C:253:GLY:HA2	2.14	0.47
1:C:260:LEU:O	1:C:261:ALA:C	2.57	0.47
1:C:262:TRP:CZ3	1:C:273:PRO:CD	2.97	0.47
1:C:277:ASN:C	1:C:278:ILE:CG2	2.87	0.47
1:E:72:ARG:HH21	1:E:77:GLU:CD	2.22	0.47
1:E:248:ILE:HA	1:E:276:THR:O	2.14	0.47
1:E:280:ASN:O	1:E:283:LEU:HB3	2.15	0.47
1:F:339:ASP:O	1:F:342:CYS:N	2.46	0.47
1:A:74:HIS:ND1	1:A:75:PRO:CD	2.74	0.47
1:A:323:PRO:O	1:A:326:ASP:CB	2.62	0.47
1:A:417:LYS:CG	1:C:117:ARG:CZ	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLN:CD	1:B:88:TRP:HH2	2.23	0.47
1:C:237:LYS:O	1:C:238:VAL:C	2.58	0.47
1:C:270:LYS:CG	1:C:271:ASP:N	2.78	0.47
1:D:296:ILE:HD12	1:D:297:GLU:O	2.15	0.47
1:A:164:ARG:CZ	1:E:131:TYR:HB3	2.45	0.47
1:A:219:TYR:OH	1:A:256:ALA:CB	2.63	0.47
1:B:29:PHE:HD1	1:E:52:VAL:HG21	1.79	0.47
1:C:243:ASP:C	1:C:243:ASP:OD1	2.58	0.47
1:F:279:THR:O	1:F:282:GLU:HB3	2.14	0.47
1:F:343:ASN:OD1	1:F:343:ASN:O	2.33	0.47
1:A:250:ASN:CB	1:A:254:LEU:HD21	2.45	0.47
1:A:288:VAL:CG2	1:A:289:ASP:N	2.77	0.47
1:A:392:ILE:HD12	1:A:396:ASP:HB2	1.96	0.47
1:D:192:ARG:NH2	1:D:233:GLU:OE2	2.48	0.47
1:D:285:GLU:OE1	1:D:307:ASN:CB	2.63	0.47
1:D:347:VAL:HA	1:D:350:SER:OG	2.15	0.47
1:F:17:ALA:C	1:F:19:TYR:N	2.71	0.47
1:F:45:MET:HG2	1:F:49:SER:O	2.15	0.47
1:A:292:ALA:HB1	1:A:316:LEU:HD12	1.97	0.46
1:C:240:ALA:O	1:C:241:VAL:HG23	2.15	0.46
1:D:238:VAL:O	1:D:254:LEU:HD12	2.15	0.46
1:D:297:GLU:O	1:D:299:VAL:HG13	2.15	0.46
1:E:176:LYS:NZ	1:E:176:LYS:HB2	2.30	0.46
1:A:279:THR:HG23	1:A:282:GLU:CD	2.35	0.46
1:A:300:ILE:HA	1:A:304:ASN:HD21	1.80	0.46
1:A:322:THR:OG1	1:A:325:ALA:HB3	2.15	0.46
1:A:392:ILE:HD12	1:A:397:ALA:N	2.30	0.46
1:C:219:TYR:CD1	1:C:241:VAL:HG13	2.50	0.46
1:C:327:GLU:O	1:C:330:TYR:HB3	2.15	0.46
1:D:240:ALA:CB	1:D:283:LEU:HD12	2.45	0.46
1:E:111:PRO:O	1:E:113:GLU:N	2.45	0.46
1:F:248:ILE:HG13	1:F:248:ILE:O	2.14	0.46
1:A:131:TYR:HA	1:A:134:ILE:HD11	1.97	0.46
1:B:220:GLY:O	1:B:224:TYR:HB3	2.15	0.46
1:B:383:VAL:HG12	1:B:397:ALA:HB3	1.97	0.46
1:C:216:ILE:O	1:C:241:VAL:HA	2.14	0.46
1:D:176:LYS:NZ	1:D:353:GLU:OE2	2.49	0.46
1:F:297:GLU:HA	1:F:320:PRO:HA	1.97	0.46
1:A:339:ASP:C	1:A:341:LEU:N	2.73	0.46
1:D:203:LYS:O	1:D:204:ALA:C	2.57	0.46
1:D:288:VAL:HG12	1:D:289:ASP:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG13	1:A:96:MET:N	2.30	0.46
1:A:270:LYS:O	1:A:271:ASP:CB	2.62	0.46
1:B:280:ASN:O	1:B:281:GLU:C	2.58	0.46
1:C:296:ILE:H	1:C:296:ILE:HG13	1.58	0.46
1:C:363:TRP:CD1	1:C:363:TRP:N	2.84	0.46
1:D:270:LYS:O	1:D:271:ASP:HB2	2.16	0.46
1:D:285:GLU:O	1:D:309:LYS:HE2	2.15	0.46
1:E:63:ALA:HB2	1:E:415:TRP:CZ3	2.50	0.46
1:E:249:TYR:OH	1:E:251:PRO:HG3	2.15	0.46
1:F:170:PHE:O	1:F:176:LYS:HE2	2.15	0.46
1:C:9:ALA:CB	1:C:88:TRP:HZ3	2.28	0.46
1:C:322:THR:CB	1:C:323:PRO:CD	2.93	0.46
1:C:384:TYR:CG	1:C:394:MET:HE1	2.44	0.46
1:D:148:ASN:HB2	1:D:149:PRO:HD2	1.98	0.46
1:E:337:ILE:HG22	1:E:342:CYS:HB2	1.97	0.46
1:F:176:LYS:HD2	1:F:180:VAL:O	2.16	0.46
1:A:186:ARG:O	1:A:186:ARG:HG3	2.15	0.46
1:A:250:ASN:CB	1:A:254:LEU:CD2	2.92	0.46
1:A:384:TYR:HD1	1:A:394:MET:HE1	1.81	0.46
1:C:57:ARG:NH2	1:C:69:GLY:O	2.43	0.46
1:D:88:TRP:CH2	1:D:399:TYR:OH	2.69	0.46
1:D:329:LEU:H	1:D:329:LEU:HG	1.59	0.46
1:E:243:ASP:O	1:E:244:THR:C	2.58	0.46
1:F:53:PHE:N	1:F:53:PHE:CD1	2.83	0.46
1:A:184:VAL:C	1:A:186:ARG:N	2.73	0.46
1:B:75:PRO:HD2	1:B:76:GLU:H	1.80	0.46
1:D:263:LYS:HD2	1:D:268:SER:HA	1.98	0.46
1:D:292:ALA:O	1:D:293:PRO:C	2.58	0.46
1:D:372:LEU:O	1:D:376:MET:HG2	2.16	0.46
1:E:199:ARG:O	1:E:202:ALA:HB3	2.16	0.46
1:F:167:ASP:HB2	1:F:168:PRO:CD	2.46	0.46
1:A:47:ASP:OD1	1:A:47:ASP:O	2.34	0.46
1:C:65:GLY:HA3	1:C:99:PRO:O	2.15	0.46
1:D:29:PHE:HB3	1:D:410:MET:HE1	1.98	0.46
1:F:22:ILE:O	1:F:23:SER:O	2.34	0.46
1:F:313:VAL:O	1:F:313:VAL:HG12	2.15	0.46
1:A:73:TRP:CH2	1:A:122:LEU:HD23	2.51	0.46
1:A:96:MET:HE2	1:A:376:MET:SD	2.56	0.46
1:A:124:ARG:O	1:A:128:ARG:HG3	2.16	0.46
1:D:87:ALA:O	1:D:90:THR:HB	2.15	0.46
1:D:259:VAL:HA	1:D:272:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:ILE:HD13	1:D:308:ILE:HG13	1.98	0.46
1:E:217:GLN:HB3	1:E:293:PRO:HA	1.98	0.46
1:E:243:ASP:O	1:E:245:LYS:N	2.49	0.46
1:F:73:TRP:CD1	1:F:107:VAL:HG23	2.51	0.46
1:F:329:LEU:HD23	1:F:334:ILE:CD1	2.45	0.46
1:A:72:ARG:HG2	1:A:144:ASP:CG	2.40	0.45
1:B:142:ALA:C	1:B:152:MET:SD	3.00	0.45
1:B:329:LEU:HD23	1:B:334:ILE:HD13	1.97	0.45
1:C:222:ALA:O	1:C:226:MET:HB2	2.15	0.45
1:D:120:GLU:HB2	1:D:154:TRP:CZ3	2.49	0.45
1:D:219:TYR:OH	1:D:256:ALA:HA	2.16	0.45
1:E:56:PHE:O	1:E:126:TYR:OH	2.29	0.45
1:F:110:ASN:OD1	1:F:112:LYS:HB2	2.16	0.45
1:F:149:PRO:O	1:F:150:GLN:C	2.59	0.45
1:A:72:ARG:NH2	1:A:77:GLU:OE1	2.24	0.45
1:B:13:LEU:O	1:B:14:GLU:C	2.57	0.45
1:D:248:ILE:HD11	1:D:254:LEU:CD2	2.46	0.45
1:E:393:ASN:O	1:E:394:MET:C	2.58	0.45
1:F:26:ALA:HB2	1:F:407:TYR:CE1	2.52	0.45
1:F:43:VAL:HB	1:F:53:PHE:HE1	1.81	0.45
1:F:72:ARG:HG2	1:F:144:ASP:HB3	1.98	0.45
1:A:3:GLN:N	1:A:6:PHE:HB3	2.31	0.45
1:A:117:ARG:HA	1:A:117:ARG:NE	2.31	0.45
1:D:301:THR:HA	1:D:325:ALA:HB2	1.98	0.45
1:E:74:HIS:ND1	1:E:75:PRO:CD	2.72	0.45
1:E:110:ASN:HB3	1:E:113:GLU:OE2	2.16	0.45
1:F:220:GLY:O	1:F:224:TYR:N	2.43	0.45
1:F:365:VAL:HG23	1:F:366:GLU:N	2.32	0.45
1:A:322:THR:O	1:A:325:ALA:HB3	2.16	0.45
1:B:294:SER:HA	1:B:317:ALA:HB2	1.97	0.45
1:C:417:LYS:HD2	1:C:417:LYS:N	2.31	0.45
1:F:176:LYS:O	1:F:182:GLY:HA3	2.16	0.45
1:F:203:LYS:O	1:F:204:ALA:C	2.58	0.45
1:F:209:LEU:O	1:F:212:LYS:HG2	2.17	0.45
1:A:30:LEU:HD21	1:A:406:VAL:CG1	2.46	0.45
1:A:296:ILE:CD1	1:A:299:VAL:CG1	2.94	0.45
1:B:160:GLU:HG2	1:B:169:SER:HB3	1.99	0.45
1:C:224:TYR:CG	1:C:260:LEU:CD2	3.00	0.45
1:C:306:ASP:C	1:C:332:LYS:HZ1	2.25	0.45
1:E:301:THR:OG1	1:E:303:LYS:HB2	2.15	0.45
1:F:324:GLU:H	1:F:324:GLU:HG2	1.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TRP:CH2	1:A:273:PRO:HD3	2.51	0.45
1:A:329:LEU:CD2	1:A:334:ILE:HD13	2.39	0.45
1:C:64:ARG:NH2	1:C:97:ASP:HA	2.31	0.45
1:C:117:ARG:NH2	1:F:48:GLY:O	2.46	0.45
1:E:34:GLN:OE1	1:E:61:ASN:HA	2.17	0.45
1:A:208:ASP:O	1:A:212:LYS:CE	2.65	0.45
1:B:184:VAL:O	1:B:184:VAL:HG12	2.17	0.45
1:C:71:ILE:CD1	1:C:126:TYR:HE2	2.30	0.45
1:D:58:VAL:O	1:D:103:GLY:HA2	2.17	0.45
1:E:87:ALA:O	1:E:90:THR:HB	2.17	0.45
1:F:313:VAL:HB	1:F:336:ILE:HG12	1.99	0.45
1:A:213:THR:C	1:A:288:VAL:CG2	2.90	0.45
1:E:142:ALA:HB1	1:E:143:PRO:CD	2.47	0.45
1:B:209:LEU:HA	1:B:212:LYS:CG	2.46	0.45
1:D:217:GLN:O	1:D:217:GLN:CG	2.64	0.45
1:D:283:LEU:O	1:D:284:LEU:C	2.60	0.45
1:E:111:PRO:HG2	1:E:146:TYR:HD2	1.81	0.45
1:E:170:PHE:O	1:E:176:LYS:CE	2.62	0.45
1:E:266:THR:HG22	1:E:268:SER:H	1.82	0.45
1:E:339:ASP:OD1	1:E:339:ASP:N	2.50	0.45
1:E:364:THR:HG1	1:E:367:GLU:HG3	1.73	0.45
1:E:393:ASN:O	1:E:396:ASP:N	2.50	0.45
1:F:170:PHE:O	1:F:176:LYS:HE3	2.17	0.45
1:B:16:ALA:O	1:B:17:ALA:C	2.59	0.45
1:B:149:PRO:O	1:B:150:GLN:C	2.56	0.45
1:B:186:ARG:O	1:B:186:ARG:CG	2.64	0.45
1:B:325:ALA:C	1:B:329:LEU:HD12	2.35	0.45
1:B:329:LEU:HD23	1:B:334:ILE:CD1	2.47	0.45
1:C:29:PHE:CD2	1:C:410:MET:HE3	2.46	0.45
1:C:205:LEU:HD12	1:C:205:LEU:HA	1.66	0.45
1:C:277:ASN:O	1:C:278:ILE:HG22	2.17	0.45
1:C:323:PRO:C	1:C:326:ASP:HB2	2.40	0.45
1:E:26:ALA:HB2	1:E:407:TYR:CE1	2.52	0.45
1:C:43:VAL:CG1	1:C:44:GLU:N	2.80	0.44
1:E:51:LYS:HG2	1:E:53:PHE:HE1	1.78	0.44
1:A:69:GLY:O	1:A:141:PRO:HA	2.17	0.44
1:B:79:LEU:O	1:B:82:VAL:HB	2.18	0.44
1:B:397:ALA:O	1:B:398:ALA:C	2.60	0.44
1:C:4:ASP:O	1:C:8:ILE:CD1	2.65	0.44
1:C:304:ASN:N	1:C:304:ASN:OD1	2.51	0.44
1:D:68:LYS:HD2	1:D:68:LYS:HA	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:TYR:CD1	1:D:224:TYR:C	2.93	0.44
1:D:340:PHE:HE1	1:D:398:ALA:HB1	1.81	0.44
1:E:59:GLN:HE22	1:E:133:VAL:CG2	2.26	0.44
1:E:249:TYR:CE2	1:E:251:PRO:HG3	2.52	0.44
1:A:209:LEU:C	1:A:212:LYS:CG	2.89	0.44
1:B:250:ASN:OD1	1:B:251:PRO:HD2	2.16	0.44
1:B:266:THR:O	1:B:266:THR:CG2	2.66	0.44
1:D:38:GLU:HG3	1:D:56:PHE:CD1	2.53	0.44
1:F:59:GLN:HE21	1:F:139:ASP:CG	2.25	0.44
1:A:128:ARG:HD2	1:A:158:GLU:OE2	2.17	0.44
1:A:364:THR:O	1:A:365:VAL:C	2.60	0.44
1:C:131:TYR:HE1	1:C:159:TYR:CE1	2.35	0.44
1:C:319:GLY:N	1:C:320:PRO:CD	2.81	0.44
1:D:272:PHE:HA	1:D:273:PRO:HD2	1.85	0.44
1:E:148:ASN:HB2	1:E:149:PRO:CD	2.47	0.44
1:F:72:ARG:HG2	1:F:144:ASP:OD2	2.17	0.44
1:F:89:MET:O	1:F:92:LYS:N	2.51	0.44
1:F:297:GLU:H	1:F:297:GLU:HG3	1.12	0.44
1:A:270:LYS:HE2	1:A:277:ASN:ND2	2.33	0.44
1:B:257:ASP:O	1:B:260:LEU:N	2.50	0.44
1:C:3:GLN:O	1:C:4:ASP:C	2.60	0.44
1:C:384:TYR:CA	1:C:394:MET:HE1	2.42	0.44
1:D:248:ILE:HG23	1:D:269:VAL:CG2	2.47	0.44
1:E:207:MET:HE3	1:E:207:MET:HB3	1.64	0.44
1:F:394:MET:HE3	1:F:394:MET:HB3	1.60	0.44
1:A:219:TYR:OH	1:A:256:ALA:HA	2.18	0.44
1:B:131:TYR:CE1	1:B:159:TYR:HE1	2.33	0.44
1:B:257:ASP:O	1:B:258:GLU:C	2.61	0.44
1:C:74:HIS:CE1	1:C:76:GLU:HB2	2.52	0.44
1:D:160:GLU:CG	1:D:169:SER:HB3	2.46	0.44
1:D:269:VAL:O	1:D:272:PHE:HB2	2.18	0.44
1:D:329:LEU:O	1:D:330:TYR:C	2.60	0.44
1:F:3:GLN:NE2	1:F:80:SER:HG	2.10	0.44
1:A:93:THR:O	1:A:97:ASP:N	2.51	0.44
1:B:279:THR:HG1	1:B:282:GLU:HG3	1.80	0.44
1:B:338:PRO:HD3	1:B:394:MET:HB3	1.99	0.44
1:D:150:GLN:OE1	1:D:154:TRP:NE1	2.50	0.44
1:D:319:GLY:N	1:D:320:PRO:HD2	2.32	0.44
1:E:71:ILE:HD13	1:E:126:TYR:HE2	1.81	0.44
1:E:74:HIS:CG	1:E:75:PRO:CD	3.01	0.44
1:E:201:ALA:O	1:E:204:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:MET:HE2	1:F:236:MET:SD	2.58	0.44
1:A:209:LEU:O	1:A:236:MET:HG2	2.18	0.44
1:C:15:ARG:O	1:C:18:GLN:CD	2.61	0.44
1:C:158:GLU:O	1:C:158:GLU:HG3	2.18	0.44
1:C:270:LYS:HG3	1:C:277:ASN:ND2	2.14	0.44
1:D:249:TYR:CB	1:D:278:ILE:HD13	2.46	0.44
1:E:176:LYS:O	1:E:182:GLY:HA3	2.17	0.44
1:B:44:GLU:CD	1:D:117:ARG:HE	2.26	0.44
1:C:304:ASN:O	1:C:305:ALA:C	2.61	0.44
1:D:198:VAL:O	1:D:199:ARG:C	2.61	0.44
1:D:328:ILE:O	1:D:331:GLU:HB2	2.18	0.44
1:E:110:ASN:HD22	1:E:113:GLU:CG	2.31	0.44
1:A:197:THR:O	1:A:201:ALA:N	2.50	0.43
1:A:259:VAL:CG1	1:A:269:VAL:HG23	2.48	0.43
1:A:323:PRO:O	1:A:327:GLU:OE2	2.36	0.43
1:B:29:PHE:CD1	1:E:52:VAL:HG21	2.52	0.43
1:C:164:ARG:CZ	1:F:131:TYR:HB3	2.48	0.43
1:C:179:SER:C	1:C:180:VAL:HG13	2.43	0.43
1:C:207:MET:HE1	1:C:311:LYS:HD3	1.97	0.43
1:C:322:THR:HB	1:C:323:PRO:HD2	2.00	0.43
1:D:135:SER:OG	1:D:136:PRO:N	2.51	0.43
1:D:262:TRP:O	1:D:264:LYS:N	2.51	0.43
1:E:126:TYR:O	1:E:129:ALA:HB3	2.18	0.43
1:F:3:GLN:HB3	1:F:80:SER:OG	2.18	0.43
1:F:22:ILE:C	1:F:23:SER:O	2.59	0.43
1:F:302:LYS:O	1:F:303:LYS:C	2.58	0.43
1:A:3:GLN:O	1:A:7:GLU:N	2.49	0.43
1:A:74:HIS:CE1	1:A:76:GLU:HB2	2.53	0.43
1:D:195:SER:HB2	1:D:234:TYR:HE2	1.83	0.43
1:D:202:ALA:HB1	1:D:207:MET:HG3	1.99	0.43
1:F:74:HIS:CG	1:F:75:PRO:HD2	2.53	0.43
1:F:323:PRO:C	1:F:326:ASP:HB2	2.39	0.43
1:A:30:LEU:CD2	1:A:91:TRP:HH2	2.22	0.43
1:A:245:LYS:HD3	1:A:268:SER:HB2	2.00	0.43
1:B:164:ARG:HA	1:B:164:ARG:HD2	1.74	0.43
1:C:15:ARG:HG3	1:C:15:ARG:O	2.18	0.43
1:C:250:ASN:HA	1:C:251:PRO:HD3	1.80	0.43
1:C:328:ILE:O	1:C:332:LYS:N	2.51	0.43
1:D:212:LYS:HA	1:D:212:LYS:HD3	1.36	0.43
1:A:223:GLY:O	1:A:224:TYR:C	2.59	0.43
1:A:291:LEU:O	1:A:293:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:O	1:A:298:GLU:C	2.61	0.43
1:D:296:ILE:CD1	1:D:299:VAL:HG12	2.48	0.43
1:D:384:TYR:HE2	1:D:388:LYS:HZ3	1.65	0.43
1:E:226:MET:CE	1:E:230:MET:SD	3.06	0.43
1:E:322:THR:O	1:E:326:ASP:N	2.51	0.43
1:F:219:TYR:OH	1:F:256:ALA:HB1	2.18	0.43
1:F:279:THR:OG1	1:F:282:GLU:HB2	2.17	0.43
1:B:127:VAL:C	1:B:129:ALA:N	2.75	0.43
1:C:184:VAL:C	1:C:186:ARG:N	2.76	0.43
1:A:50:VAL:HG23	1:F:417:LYS:HG2	1.99	0.43
1:A:57:ARG:NE	1:A:139:ASP:OD2	2.44	0.43
1:A:128:ARG:CZ	1:E:161:THR:HG21	2.48	0.43
1:B:392:ILE:HG21	1:B:392:ILE:HD13	1.74	0.43
1:B:404:SER:O	1:B:407:TYR:HB3	2.18	0.43
1:C:279:THR:H	1:C:282:GLU:HG3	1.83	0.43
1:D:214:ILE:HA	1:D:288:VAL:HG11	2.01	0.43
1:E:112:LYS:C	1:E:113:GLU:CG	2.91	0.43
1:E:207:MET:CG	1:E:208:ASP:N	2.80	0.43
1:B:48:GLY:CA	1:D:117:ARG:HH22	2.32	0.43
1:B:51:LYS:HG2	1:B:53:PHE:CE1	2.53	0.43
1:B:250:ASN:HA	1:B:251:PRO:HD3	1.48	0.43
1:C:270:LYS:HG2	1:C:271:ASP:N	2.34	0.43
1:D:74:HIS:O	1:D:108:ILE:HA	2.19	0.43
1:D:192:ARG:HG2	1:D:372:LEU:HD23	2.01	0.43
1:E:182:GLY:C	1:E:183:ILE:HG23	2.43	0.43
1:A:366:GLU:HG3	1:A:367:GLU:N	2.34	0.43
1:B:48:GLY:HA2	1:D:117:ARG:HH22	1.83	0.43
1:B:173:ILE:O	1:B:173:ILE:CG2	2.65	0.43
1:C:92:LYS:HG3	1:C:340:PHE:O	2.19	0.43
1:C:208:ASP:O	1:C:212:LYS:CD	2.66	0.43
1:C:319:GLY:N	1:C:320:PRO:HD3	2.34	0.43
1:D:145:VAL:O	1:D:145:VAL:HG12	2.18	0.43
1:E:203:LYS:O	1:E:204:ALA:C	2.59	0.43
1:E:208:ASP:O	1:E:212:LYS:HE2	2.18	0.43
1:E:296:ILE:CD1	1:E:299:VAL:CG1	2.91	0.43
1:E:373:ASP:O	1:E:374:LYS:C	2.60	0.43
1:F:213:THR:OG1	1:F:288:VAL:HA	2.19	0.43
1:F:416:ILE:HD13	1:F:418:LYS:C	2.44	0.43
1:A:89:MET:CA	1:A:89:MET:CE	2.94	0.43
1:A:104:LYS:HG3	1:A:105:GLY:H	1.84	0.43
1:A:111:PRO:CG	1:A:146:TYR:CD2	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:VAL:O	1:B:83:LYS:C	2.62	0.43
1:F:77:GLU:HB3	1:F:108:ILE:HG12	2.01	0.43
1:A:340:PHE:O	1:A:344:ALA:HB2	2.18	0.43
1:B:33:PRO:HB3	1:B:60:TYR:CD1	2.54	0.43
1:C:144:ASP:O	1:C:145:VAL:C	2.60	0.43
1:C:284:LEU:HD13	1:C:299:VAL:O	2.19	0.43
1:D:72:ARG:NE	1:D:77:GLU:OE2	2.38	0.43
1:D:394:MET:HB3	1:D:394:MET:HE3	1.83	0.43
1:E:27:LEU:HD22	1:E:27:LEU:HA	1.74	0.43
1:E:192:ARG:HD3	1:E:369:ARG:HG2	2.01	0.43
1:E:214:ILE:HG12	1:E:215:ALA:N	2.33	0.43
1:F:284:LEU:HD23	1:F:284:LEU:N	2.32	0.43
1:F:319:GLY:N	1:F:320:PRO:CD	2.81	0.43
1:F:322:THR:O	1:F:325:ALA:N	2.52	0.43
1:A:96:MET:O	1:A:97:ASP:HB3	2.19	0.42
1:C:184:VAL:C	1:C:186:ARG:H	2.27	0.42
1:D:205:LEU:HA	1:D:205:LEU:HD12	1.64	0.42
1:E:33:PRO:HB3	1:E:60:TYR:HD1	1.81	0.42
1:F:123:ALA:HB1	1:F:155:MET:HG3	2.01	0.42
1:A:304:ASN:HA	1:A:307:ASN:ND2	2.34	0.42
1:B:150:GLN:OE1	1:B:154:TRP:NE1	2.52	0.42
1:B:285:GLU:O	1:B:286:LEU:C	2.61	0.42
1:B:385:ASN:HD22	1:B:388:LYS:HE2	1.83	0.42
1:D:284:LEU:HD13	1:D:299:VAL:O	2.18	0.42
1:E:15:ARG:O	1:E:15:ARG:HG3	2.15	0.42
1:F:66:PRO:HG2	1:F:100:TYR:CD1	2.53	0.42
1:F:198:VAL:O	1:F:199:ARG:C	2.61	0.42
1:A:68:LYS:NZ	1:A:141:PRO:O	2.52	0.42
1:B:26:ALA:HB2	1:B:416:ILE:HD13	2.00	0.42
1:B:184:VAL:C	1:B:186:ARG:N	2.76	0.42
1:C:79:LEU:O	1:C:83:LYS:HG3	2.19	0.42
1:D:236:MET:HE1	1:D:290:VAL:CG2	2.46	0.42
1:E:270:LYS:HE2	1:E:270:LYS:HB3	1.26	0.42
1:F:27:LEU:HD23	1:F:27:LEU:HA	1.80	0.42
1:F:183:ILE:HG12	1:F:353:GLU:HB2	2.02	0.42
1:A:196:TYR:O	1:A:200:GLU:HG2	2.20	0.42
1:B:117:ARG:HH22	1:D:48:GLY:C	2.24	0.42
1:B:203:LYS:O	1:B:204:ALA:C	2.61	0.42
1:C:42:PRO:HB3	1:D:29:PHE:HE2	1.85	0.42
1:C:161:THR:HG21	1:F:128:ARG:NH2	2.34	0.42
1:D:288:VAL:HG12	1:D:289:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:GLU:OE1	1:E:418:LYS:HG3	2.20	0.42
1:E:417:LYS:HA	1:E:417:LYS:HD2	1.63	0.42
1:A:59:GLN:HE22	1:A:133:VAL:HB	1.83	0.42
1:B:243:ASP:O	1:B:244:THR:C	2.63	0.42
1:C:308:ILE:H	1:C:308:ILE:HG12	1.53	0.42
1:D:126:TYR:HD2	1:D:155:MET:CE	2.25	0.42
1:D:224:TYR:CE1	1:D:256:ALA:HB1	2.54	0.42
1:D:407:TYR:OH	1:D:418:LYS:O	2.24	0.42
1:E:404:SER:O	1:E:407:TYR:HB3	2.19	0.42
1:F:197:THR:O	1:F:200:GLU:HB2	2.20	0.42
1:A:196:TYR:CD2	1:A:373:ASP:HA	2.55	0.42
1:B:63:ALA:HB2	1:B:415:TRP:CH2	2.53	0.42
1:C:323:PRO:O	1:C:326:ASP:CB	2.58	0.42
1:D:120:GLU:HA	1:D:154:TRP:CE3	2.54	0.42
1:D:145:VAL:O	1:D:146:TYR:HB2	2.20	0.42
1:D:214:ILE:CA	1:D:288:VAL:HG11	2.50	0.42
1:D:285:GLU:CD	1:D:307:ASN:HB2	2.45	0.42
1:F:17:ALA:O	1:F:18:GLN:C	2.59	0.42
1:F:403:VAL:O	1:F:403:VAL:HG12	2.19	0.42
1:A:170:PHE:C	1:A:176:LYS:NZ	2.75	0.42
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.70	0.42
1:A:359:THR:C	1:A:361:ASP:H	2.27	0.42
1:B:292:ALA:HA	1:B:293:PRO:HD2	1.89	0.42
1:B:365:VAL:H	1:B:365:VAL:HG22	1.61	0.42
1:C:36:ILE:HG12	1:C:58:VAL:HG22	2.02	0.42
1:C:176:LYS:HE2	1:C:176:LYS:HB2	1.64	0.42
1:C:262:TRP:CH2	1:C:273:PRO:HD3	2.55	0.42
1:C:313:VAL:O	1:C:313:VAL:HG12	2.20	0.42
1:C:365:VAL:O	1:C:369:ARG:CG	2.64	0.42
1:D:66:PRO:HD2	1:D:99:PRO:O	2.19	0.42
1:D:69:GLY:HA3	1:D:103:GLY:O	2.20	0.42
1:D:131:TYR:CE1	1:D:159:TYR:CE1	3.08	0.42
1:E:125:GLY:O	1:E:126:TYR:C	2.59	0.42
1:F:177:PRO:HA	1:F:178:PRO:HD3	1.79	0.42
1:F:365:VAL:HG22	1:F:366:GLU:OE2	2.19	0.42
1:A:29:PHE:CE2	1:F:42:PRO:HG3	2.54	0.42
1:A:364:THR:O	1:A:367:GLU:HB2	2.20	0.42
1:B:17:ALA:C	1:B:19:TYR:N	2.76	0.42
1:B:192:ARG:HG2	1:B:372:LEU:HD21	2.02	0.42
1:B:204:ALA:HB1	1:B:384:TYR:CZ	2.55	0.42
1:B:363:TRP:CD1	1:B:363:TRP:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:VAL:HG22	1:C:172:VAL:O	2.19	0.42
1:C:250:ASN:HB3	1:C:254:LEU:CD2	2.50	0.42
1:C:299:VAL:O	1:C:299:VAL:HG23	2.19	0.42
1:C:387:HIS:NE2	1:C:394:MET:HE2	2.34	0.42
1:D:123:ALA:HB1	1:D:155:MET:HG3	2.01	0.42
1:D:262:TRP:CZ2	1:D:273:PRO:HD3	2.53	0.42
1:D:292:ALA:HA	1:D:293:PRO:HD2	1.68	0.42
1:F:15:ARG:O	1:F:18:GLN:HG2	2.19	0.42
1:F:131:TYR:CE1	1:F:159:TYR:CE1	3.08	0.42
1:F:219:TYR:OH	1:F:256:ALA:HA	2.20	0.42
1:A:224:TYR:CZ	1:A:228:LYS:HD2	2.54	0.42
1:A:313:VAL:HB	1:A:336:ILE:HG12	2.02	0.42
1:B:250:ASN:OD1	1:B:252:ASP:N	2.53	0.42
1:D:217:GLN:HB2	1:D:283:LEU:CD2	2.50	0.42
1:D:291:LEU:HG	1:D:293:PRO:HD3	2.02	0.42
1:E:78:THR:O	1:E:82:VAL:HG23	2.20	0.42
1:F:176:LYS:NZ	1:F:176:LYS:CB	2.83	0.42
1:F:392:ILE:HG21	1:F:392:ILE:HD13	1.84	0.42
1:B:214:ILE:HD12	1:B:290:VAL:CG1	2.50	0.42
1:C:148:ASN:CB	1:C:149:PRO:CD	2.84	0.42
1:D:196:TYR:O	1:D:199:ARG:HB3	2.20	0.42
1:D:205:LEU:HD13	1:D:205:LEU:N	2.35	0.42
1:D:209:LEU:O	1:D:236:MET:HG2	2.20	0.42
1:D:283:LEU:O	1:D:286:LEU:HB2	2.19	0.42
1:A:255:ASN:O	1:A:258:GLU:N	2.52	0.41
1:B:260:LEU:O	1:B:264:LYS:HG2	2.18	0.41
1:D:110:ASN:HA	1:D:111:PRO:HD2	1.92	0.41
1:D:177:PRO:HA	1:D:178:PRO:HD3	1.87	0.41
1:F:47:ASP:OD1	1:F:47:ASP:C	2.63	0.41
1:F:214:ILE:HG13	1:F:215:ALA:N	2.34	0.41
1:F:242:SER:HB3	1:F:283:LEU:HD13	2.01	0.41
1:A:45:MET:N	1:A:49:SER:O	2.35	0.41
1:A:241:VAL:HG12	1:A:269:VAL:HG21	2.02	0.41
1:D:110:ASN:O	1:D:114:MET:HG3	2.20	0.41
1:D:260:LEU:HD12	1:D:260:LEU:O	2.21	0.41
1:D:285:GLU:OE1	1:D:307:ASN:HB2	2.20	0.41
1:D:381:TRP:O	1:D:382:ASP:C	2.63	0.41
1:E:11:LYS:O	1:E:12:GLN:C	2.63	0.41
1:E:365:VAL:HG22	1:E:366:GLU:N	2.34	0.41
1:F:73:TRP:NE1	1:F:107:VAL:CG2	2.84	0.41
1:F:224:TYR:OH	1:F:257:ASP:OD1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:VAL:HG23	1:F:366:GLU:OE2	2.20	0.41
1:A:40:SER:HB2	1:A:52:VAL:CG1	2.50	0.41
1:F:272:PHE:HA	1:F:273:PRO:HD2	1.77	0.41
1:A:15:ARG:O	1:A:18:GLN:HG3	2.21	0.41
1:A:340:PHE:CE1	1:A:399:TYR:CE1	3.09	0.41
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.63	0.41
1:C:209:LEU:HD22	1:C:236:MET:SD	2.61	0.41
1:D:137:TYR:CZ	1:F:168:PRO:HG3	2.55	0.41
1:D:190:THR:HG22	1:D:191:ALA:N	2.35	0.41
1:D:218:GLY:HA3	1:D:295:ALA:HB2	2.03	0.41
1:D:271:ASP:O	1:D:272:PHE:O	2.39	0.41
1:E:59:GLN:NE2	1:E:133:VAL:HG23	2.32	0.41
1:E:186:ARG:HA	1:E:349:VAL:HG11	2.01	0.41
1:F:213:THR:OG1	1:F:288:VAL:HG12	2.20	0.41
1:A:263:LYS:O	1:A:267:GLY:N	2.41	0.41
1:B:287:GLU:HA	1:B:309:LYS:HB2	2.02	0.41
1:B:371:LYS:HG2	1:B:371:LYS:H	1.30	0.41
1:C:4:ASP:C	1:C:8:ILE:HD12	2.46	0.41
1:C:15:ARG:O	1:C:18:GLN:NE2	2.53	0.41
1:C:204:ALA:C	1:C:206:GLY:H	2.29	0.41
1:D:271:ASP:C	1:D:272:PHE:O	2.61	0.41
1:E:164:ARG:O	1:E:165:ARG:HB2	2.19	0.41
1:F:178:PRO:C	1:F:180:VAL:N	2.77	0.41
1:A:173:ILE:O	1:A:173:ILE:CG2	2.64	0.41
1:A:323:PRO:HA	1:A:326:ASP:HB2	2.02	0.41
1:A:335:LEU:HD12	1:A:336:ILE:N	2.35	0.41
1:B:12:GLN:HE21	1:B:12:GLN:HB3	1.56	0.41
1:B:187:MET:HE3	1:B:225:TYR:OH	2.20	0.41
1:B:271:ASP:O	1:B:272:PHE:C	2.63	0.41
1:C:343:ASN:OD1	1:C:343:ASN:O	2.39	0.41
1:D:120:GLU:CB	1:D:154:TRP:CE3	2.98	0.41
1:D:250:ASN:C	1:D:252:ASP:N	2.78	0.41
1:E:128:ARG:HD2	1:E:158:GLU:OE2	2.20	0.41
1:E:178:PRO:C	1:E:180:VAL:N	2.73	0.41
1:F:280:ASN:O	1:F:283:LEU:HB3	2.20	0.41
1:F:387:HIS:HB2	1:F:392:ILE:O	2.20	0.41
1:A:205:LEU:HA	1:A:205:LEU:HD12	1.77	0.41
1:A:397:ALA:O	1:A:400:VAL:HB	2.19	0.41
1:B:27:LEU:HD12	1:B:31:LYS:HE3	2.02	0.41
1:B:128:ARG:CZ	1:D:161:THR:HG21	2.51	0.41
1:B:299:VAL:HG23	1:B:300:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LYS:HZ3	1:B:371:LYS:CB	2.22	0.41
1:C:4:ASP:HB3	1:C:5:PRO:CD	2.40	0.41
1:F:85:LEU:HD23	1:F:85:LEU:HA	1.89	0.41
1:F:366:GLU:O	1:F:367:GLU:C	2.63	0.41
1:A:172:VAL:O	1:A:172:VAL:CG2	2.64	0.41
1:A:372:LEU:O	1:A:375:LYS:N	2.54	0.41
1:C:120:GLU:CA	1:C:154:TRP:CE3	2.93	0.41
1:C:294:SER:HB3	1:C:316:LEU:HB2	2.03	0.41
1:F:373:ASP:OD1	1:F:373:ASP:C	2.62	0.41
1:A:44:GLU:HG3	1:E:117:ARG:NH2	2.31	0.41
1:A:248:ILE:CD1	1:A:254:LEU:HD13	2.36	0.41
1:A:283:LEU:HA	1:A:286:LEU:HG	2.03	0.41
1:A:294:SER:HB3	1:A:316:LEU:HB2	2.03	0.41
1:A:336:ILE:HD13	1:A:336:ILE:HG23	1.81	0.41
1:A:340:PHE:HE1	1:A:399:TYR:CE1	2.39	0.41
1:B:282:GLU:O	1:B:283:LEU:C	2.64	0.41
1:C:160:GLU:HG2	1:C:169:SER:HB3	2.03	0.41
1:C:241:VAL:O	1:C:242:SER:HB3	2.20	0.41
1:C:304:ASN:HA	1:C:307:ASN:HD22	1.85	0.41
1:C:307:ASN:O	1:C:309:LYS:HG3	2.21	0.41
1:D:98:LEU:HD23	1:D:375:LYS:HZ3	1.83	0.41
1:D:141:PRO:HD2	1:D:172:VAL:O	2.21	0.41
1:D:260:LEU:HD12	1:D:260:LEU:C	2.45	0.41
1:D:261:ALA:O	1:D:262:TRP:C	2.63	0.41
1:D:276:THR:HG22	1:D:277:ASN:O	2.21	0.41
1:F:3:GLN:O	1:F:6:PHE:N	2.53	0.41
1:F:85:LEU:HB3	1:F:104:LYS:HD3	2.02	0.41
1:F:208:ASP:OD1	1:F:208:ASP:C	2.63	0.41
1:F:416:ILE:HD13	1:F:418:LYS:OXT	2.21	0.41
1:A:8:ILE:O	1:A:12:GLN:HG3	2.21	0.41
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.77	0.41
1:A:224:TYR:OH	1:A:228:LYS:HD2	2.21	0.41
1:B:89:MET:HE3	1:B:89:MET:O	2.21	0.41
1:B:394:MET:H	1:B:394:MET:HG2	1.58	0.41
1:C:401:VAL:HG23	1:C:401:VAL:H	1.66	0.41
1:D:92:LYS:O	1:D:95:VAL:HG12	2.20	0.41
1:D:163:SER:O	1:D:164:ARG:CB	2.62	0.41
1:E:265:LYS:HD2	1:E:265:LYS:HA	1.83	0.41
1:A:4:ASP:O	1:A:5:PRO:C	2.65	0.40
1:A:73:TRP:O	1:A:146:TYR:HB2	2.21	0.40
1:A:381:TRP:O	1:A:382:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LYS:O	1:B:95:VAL:HG12	2.20	0.40
1:B:299:VAL:HG23	1:B:300:ILE:CG1	2.51	0.40
1:D:304:ASN:C	1:D:306:ASP:N	2.80	0.40
1:E:272:PHE:HA	1:E:273:PRO:HD2	1.88	0.40
1:F:29:PHE:CE2	1:F:410:MET:HE3	2.43	0.40
1:F:208:ASP:OD1	1:F:209:LEU:N	2.54	0.40
1:A:164:ARG:HD2	1:A:164:ARG:HA	1.76	0.40
1:A:170:PHE:HB3	1:A:176:LYS:HZ2	1.86	0.40
1:A:184:VAL:O	1:A:184:VAL:CG1	2.68	0.40
1:A:202:ALA:HB2	1:A:209:LEU:HD21	2.03	0.40
1:A:272:PHE:HA	1:A:273:PRO:HD2	1.94	0.40
1:A:322:THR:HB	1:A:323:PRO:CD	2.49	0.40
1:A:358:ILE:HD11	1:C:359:THR:C	2.45	0.40
1:A:378:LYS:HE2	1:A:382:ASP:OD1	2.21	0.40
1:A:379:ALA:O	1:A:383:VAL:HG23	2.21	0.40
1:C:53:PHE:CE2	1:C:114:MET:HE1	2.55	0.40
1:C:234:TYR:O	1:C:235:GLY:C	2.65	0.40
1:E:192:ARG:HG2	1:E:372:LEU:HD23	2.02	0.40
1:E:292:ALA:HB1	1:E:316:LEU:HD12	2.03	0.40
1:F:26:ALA:O	1:F:27:LEU:C	2.62	0.40
1:F:73:TRP:NE1	1:F:107:VAL:HG21	2.35	0.40
1:F:141:PRO:O	1:F:142:ALA:HB2	2.20	0.40
1:F:224:TYR:CZ	1:F:260:LEU:HD22	2.56	0.40
1:A:226:MET:HG2	1:A:316:LEU:CD1	2.47	0.40
1:A:240:ALA:CA	1:A:248:ILE:O	2.65	0.40
1:A:259:VAL:O	1:A:260:LEU:C	2.64	0.40
1:A:279:THR:O	1:A:282:GLU:HB2	2.20	0.40
1:B:93:THR:O	1:B:97:ASP:N	2.54	0.40
1:B:127:VAL:C	1:B:129:ALA:H	2.29	0.40
1:C:141:PRO:HD2	1:C:172:VAL:O	2.21	0.40
1:D:308:ILE:C	1:D:309:LYS:HG2	2.46	0.40
1:E:134:ILE:HD12	1:E:159:TYR:CE1	2.56	0.40
1:F:208:ASP:O	1:F:212:LYS:HG2	2.21	0.40
1:F:249:TYR:HB2	1:F:278:ILE:HD12	2.03	0.40
1:A:4:ASP:O	1:A:8:ILE:N	2.42	0.40
1:A:344:ALA:O	1:A:347:VAL:HG12	2.22	0.40
1:C:187:MET:HE2	1:C:187:MET:HB2	1.45	0.40
1:C:207:MET:HE1	1:C:311:LYS:HG3	1.99	0.40
1:C:261:ALA:O	1:C:264:LYS:HB2	2.21	0.40
1:D:205:LEU:O	1:D:206:GLY:C	2.62	0.40
1:D:209:LEU:CA	1:D:212:LYS:HG2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:PRO:O	1:E:180:VAL:N	2.54	0.40
1:E:247:GLY:O	1:E:248:ILE:HG23	2.22	0.40
1:F:337:ILE:CG2	1:F:342:CYS:HB2	2.45	0.40
1:A:131:TYR:CE2	1:E:164:ARG:HD3	2.56	0.40
1:A:277:ASN:O	1:A:278:ILE:HG22	2.21	0.40
1:B:192:ARG:HG2	1:B:372:LEU:CD2	2.52	0.40
1:C:17:ALA:HB2	1:C:27:LEU:HD21	2.02	0.40
1:C:228:LYS:NZ	1:C:232:GLU:CD	2.78	0.40
1:C:236:MET:HE2	1:C:236:MET:HB3	1.62	0.40
1:D:131:TYR:HE1	1:D:159:TYR:CE1	2.39	0.40
1:D:240:ALA:HB1	1:D:283:LEU:CD1	2.52	0.40
1:D:367:GLU:O	1:D:371:LYS:HG3	2.22	0.40
1:E:66:PRO:HD2	1:E:99:PRO:O	2.22	0.40
1:E:176:LYS:CE	1:E:357:ASN:HD21	2.34	0.40
1:E:191:ALA:HB3	1:E:225:TYR:HB3	2.03	0.40
1:F:29:PHE:CB	1:F:410:MET:CE	3.00	0.40
1:F:149:PRO:HA	1:F:175:GLY:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	414/418 (99%)	355 (86%)	48 (12%)	11 (3%)	4	6
1	B	414/418 (99%)	370 (89%)	39 (9%)	5 (1%)	10	20
1	C	414/418 (99%)	355 (86%)	53 (13%)	6 (1%)	9	17
1	D	414/418 (99%)	356 (86%)	49 (12%)	9 (2%)	5	9
1	E	414/418 (99%)	366 (88%)	38 (9%)	10 (2%)	4	8
1	F	414/418 (99%)	359 (87%)	45 (11%)	10 (2%)	4	8
All	All	2484/2508 (99%)	2161 (87%)	272 (11%)	51 (2%)	5	9

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	B	4	ASP
1	C	4	ASP
1	D	4	ASP
1	D	305	ALA
1	E	18	GLN
1	E	112	LYS
1	E	340	PHE
1	F	4	ASP
1	F	23	SER
1	F	30	LEU
1	A	244	THR
1	A	298	GLU
1	A	340	PHE
1	B	18	GLN
1	C	236	MET
1	D	23	SER
1	D	185	ALA
1	D	206	GLY
1	D	262	TRP
1	E	180	VAL
1	E	244	THR
1	E	339	ASP
1	F	388	LYS
1	A	256	ALA
1	A	339	ASP
1	C	271	ASP
1	E	113	GLU
1	F	7	GLU
1	F	389	GLU
1	B	274	GLY
1	C	241	VAL
1	D	242	SER
1	D	263	LYS
1	E	4	ASP
1	F	402	ALA
1	A	262	TRP
1	A	271	ASP
1	B	168	PRO
1	D	180	VAL
1	E	169	SER
1	F	338	PRO

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Mol	Chain	Res	Type
1	A	206	GLY
1	A	227	ALA
1	A	305	ALA
1	C	189	ALA
1	E	111	PRO
1	F	184	VAL
1	F	303	LYS
1	B	180	VAL
1	C	145	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	342/344 (99%)	273 (80%)	69 (20%)	1	2
1	B	342/344 (99%)	284 (83%)	58 (17%)	2	4
1	C	342/344 (99%)	270 (79%)	72 (21%)	1	2
1	D	342/344 (99%)	269 (79%)	73 (21%)	1	2
1	E	342/344 (99%)	279 (82%)	63 (18%)	1	3
1	F	342/344 (99%)	280 (82%)	62 (18%)	2	3
All	All	2052/2064 (99%)	1655 (81%)	397 (19%)	1	2

All (397) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	15	ARG
1	A	21	ASP
1	A	22	ILE
1	A	27	LEU
1	A	37	VAL
1	A	47	ASP
1	A	56	PHE
1	A	72	ARG

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Mol	Chain	Res	Type
1	A	76	GLU
1	A	79	LEU
1	A	80	SER
1	A	88	TRP
1	A	89	MET
1	A	96	MET
1	A	112	LYS
1	A	113	GLU
1	A	134	ILE
1	A	135	SER
1	A	152	MET
1	A	163	SER
1	A	176	LYS
1	A	180	VAL
1	A	183	ILE
1	A	186	ARG
1	A	195	SER
1	A	205	LEU
1	A	207	MET
1	A	209	LEU
1	A	241	VAL
1	A	242	SER
1	A	244	THR
1	A	245	LYS
1	A	248	ILE
1	A	259	VAL
1	A	270	LYS
1	A	278	ILE
1	A	279	THR
1	A	281	GLU
1	A	285	GLU
1	A	286	LEU
1	A	287	GLU
1	A	288	VAL
1	A	291	LEU
1	A	294	SER
1	A	297	GLU
1	A	298	GLU
1	A	306	ASP
1	A	309	LYS
1	A	311	LYS
1	A	326	ASP

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Mol	Chain	Res	Type
1	A	327	GLU
1	A	329	LEU
1	A	332	LYS
1	A	336	ILE
1	A	350	SER
1	A	366	GLU
1	A	367	GLU
1	A	369	ARG
1	A	374	LYS
1	A	387	HIS
1	A	389	GLU
1	A	391	ASN
1	A	393	ASN
1	A	404	SER
1	A	411	LYS
1	A	416	ILE
1	A	417	LYS
1	A	418	LYS
1	B	4	ASP
1	B	12	GLN
1	B	22	ILE
1	B	27	LEU
1	B	28	GLU
1	B	32	ARG
1	B	40	SER
1	B	54	THR
1	B	56	PHE
1	B	68	LYS
1	B	76	GLU
1	B	80	SER
1	B	85	LEU
1	B	93	THR
1	B	96	MET
1	B	117	ARG
1	B	132	ASP
1	B	133	VAL
1	B	135	SER
1	B	138	THR
1	B	151	ILE
1	B	186	ARG
1	B	187	MET
1	B	192	ARG

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Mol	Chain	Res	Type
1	B	205	LEU
1	B	237	LYS
1	B	241	VAL
1	B	242	SER
1	B	244	THR
1	B	254	LEU
1	B	255	ASN
1	B	264	LYS
1	B	266	THR
1	B	270	LYS
1	B	273	PRO
1	B	278	ILE
1	B	287	GLU
1	B	294	SER
1	B	296	ILE
1	B	300	ILE
1	B	302	LYS
1	B	303	LYS
1	B	306	ASP
1	B	309	LYS
1	B	335	LEU
1	B	341	LEU
1	B	363	TRP
1	B	366	GLU
1	B	369	ARG
1	B	371	LYS
1	B	374	LYS
1	B	383	VAL
1	B	387	HIS
1	B	389	GLU
1	B	395	ARG
1	B	400	VAL
1	B	411	LYS
1	B	417	LYS
1	C	8	ILE
1	C	21	ASP
1	C	22	ILE
1	C	23	SER
1	C	27	LEU
1	C	28	GLU
1	C	32	ARG
1	C	38	GLU

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Mol	Chain	Res	Type
1	C	56	PHE
1	C	68	LYS
1	C	71	ILE
1	C	76	GLU
1	C	80	SER
1	C	92	LYS
1	C	117	ARG
1	C	120	GLU
1	C	135	SER
1	C	151	ILE
1	C	176	LYS
1	C	183	ILE
1	C	186	ARG
1	C	187	MET
1	C	203	LYS
1	C	205	LEU
1	C	207	MET
1	C	212	LYS
1	C	214	ILE
1	C	226	MET
1	C	228	LYS
1	C	229	ILE
1	C	231	SER
1	C	232	GLU
1	C	236	MET
1	C	242	SER
1	C	244	THR
1	C	248	ILE
1	C	260	LEU
1	C	269	VAL
1	C	278	ILE
1	C	281	GLU
1	C	283	LEU
1	C	288	VAL
1	C	289	ASP
1	C	296	ILE
1	C	299	VAL
1	C	302	LYS
1	C	303	LYS
1	C	306	ASP
1	C	308	ILE
1	C	311	LYS

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Mol	Chain	Res	Type
1	C	312	ILE
1	C	315	GLU
1	C	316	LEU
1	C	322	THR
1	C	326	ASP
1	C	327	GLU
1	C	329	LEU
1	C	332	LYS
1	C	336	ILE
1	C	337	ILE
1	C	340	PHE
1	C	347	VAL
1	C	350	SER
1	C	363	TRP
1	C	369	ARG
1	C	387	HIS
1	C	392	ILE
1	C	393	ASN
1	C	404	SER
1	C	411	LYS
1	C	417	LYS
1	C	418	LYS
1	D	8	ILE
1	D	15	ARG
1	D	18	GLN
1	D	20	MET
1	D	22	ILE
1	D	23	SER
1	D	24	GLU
1	D	27	LEU
1	D	28	GLU
1	D	32	ARG
1	D	40	SER
1	D	68	LYS
1	D	71	ILE
1	D	89	MET
1	D	117	ARG
1	D	120	GLU
1	D	135	SER
1	D	145	VAL
1	D	162	ILE
1	D	163	SER

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Mol	Chain	Res	Type
1	D	176	LYS
1	D	183	ILE
1	D	184	VAL
1	D	205	LEU
1	D	207	MET
1	D	210	LYS
1	D	212	LYS
1	D	213	THR
1	D	214	ILE
1	D	217	GLN
1	D	221	ASN
1	D	230	MET
1	D	231	SER
1	D	242	SER
1	D	243	ASP
1	D	248	ILE
1	D	260	LEU
1	D	269	VAL
1	D	278	ILE
1	D	282	GLU
1	D	286	LEU
1	D	287	GLU
1	D	288	VAL
1	D	289	ASP
1	D	298	GLU
1	D	300	ILE
1	D	303	LYS
1	D	304	ASN
1	D	308	ILE
1	D	309	LYS
1	D	311	LYS
1	D	316	LEU
1	D	324	GLU
1	D	327	GLU
1	D	329	LEU
1	D	332	LYS
1	D	335	LEU
1	D	336	ILE
1	D	340	PHE
1	D	347	VAL
1	D	365	VAL
1	D	369	ARG

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Mol	Chain	Res	Type
1	D	371	LYS
1	D	378	LYS
1	D	387	HIS
1	D	389	GLU
1	D	391	ASN
1	D	392	ILE
1	D	395	ARG
1	D	404	SER
1	D	411	LYS
1	D	417	LYS
1	D	418	LYS
1	E	12	GLN
1	E	15	ARG
1	E	18	GLN
1	E	21	ASP
1	E	22	ILE
1	E	27	LEU
1	E	32	ARG
1	E	37	VAL
1	E	38	GLU
1	E	44	GLU
1	E	51	LYS
1	E	56	PHE
1	E	58	VAL
1	E	68	LYS
1	E	71	ILE
1	E	78	THR
1	E	79	LEU
1	E	88	TRP
1	E	89	MET
1	E	113	GLU
1	E	117	ARG
1	E	119	LYS
1	E	133	VAL
1	E	134	ILE
1	E	135	SER
1	E	144	ASP
1	E	145	VAL
1	E	151	ILE
1	E	163	SER
1	E	165	ARG
1	E	176	LYS

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Mol	Chain	Res	Type
1	E	187	MET
1	E	205	LEU
1	E	207	MET
1	E	214	ILE
1	E	244	THR
1	E	266	THR
1	E	270	LYS
1	E	278	ILE
1	E	284	LEU
1	E	287	GLU
1	E	296	ILE
1	E	300	ILE
1	E	306	ASP
1	E	309	LYS
1	E	311	LYS
1	E	327	GLU
1	E	331	GLU
1	E	332	LYS
1	E	335	LEU
1	E	336	ILE
1	E	339	ASP
1	E	341	LEU
1	E	365	VAL
1	E	366	GLU
1	E	375	LYS
1	E	387	HIS
1	E	392	ILE
1	E	395	ARG
1	E	400	VAL
1	E	408	GLN
1	E	417	LYS
1	E	418	LYS
1	F	15	ARG
1	F	22	ILE
1	F	28	GLU
1	F	32	ARG
1	F	51	LYS
1	F	53	PHE
1	F	68	LYS
1	F	71	ILE
1	F	76	GLU
1	F	80	SER

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Mol	Chain	Res	Type
1	F	95	VAL
1	F	117	ARG
1	F	132	ASP
1	F	135	SER
1	F	144	ASP
1	F	145	VAL
1	F	148	ASN
1	F	176	LYS
1	F	186	ARG
1	F	192	ARG
1	F	207	MET
1	F	214	ILE
1	F	228	LYS
1	F	232	GLU
1	F	237	LYS
1	F	241	VAL
1	F	242	SER
1	F	244	THR
1	F	263	LYS
1	F	268	SER
1	F	270	LYS
1	F	278	ILE
1	F	279	THR
1	F	281	GLU
1	F	282	GLU
1	F	287	GLU
1	F	288	VAL
1	F	296	ILE
1	F	297	GLU
1	F	298	GLU
1	F	306	ASP
1	F	309	LYS
1	F	311	LYS
1	F	312	ILE
1	F	324	GLU
1	F	328	ILE
1	F	336	ILE
1	F	339	ASP
1	F	350	SER
1	F	363	TRP
1	F	366	GLU
1	F	369	ARG

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Mol	Chain	Res	Type
1	F	375	LYS
1	F	378	LYS
1	F	387	HIS
1	F	391	ASN
1	F	393	ASN
1	F	394	MET
1	F	400	VAL
1	F	404	SER
1	F	410	MET
1	F	411	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	12	GLN
1	A	18	GLN
1	A	277	ASN
1	A	280	ASN
1	A	307	ASN
1	A	385	ASN
1	B	12	GLN
1	B	59	GLN
1	B	61	ASN
1	B	150	GLN
1	B	217	GLN
1	B	280	ASN
1	B	357	ASN
1	B	385	ASN
1	B	387	HIS
1	C	61	ASN
1	C	150	GLN
1	C	217	GLN
1	C	277	ASN
1	C	280	ASN
1	C	307	ASN
1	C	387	HIS
1	C	393	ASN
1	C	408	GLN
1	D	280	ASN
1	D	385	ASN
1	E	3	GLN

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Mol	Chain	Res	Type
1	E	110	ASN
1	E	150	GLN
1	E	277	ASN
1	E	357	ASN
1	E	385	ASN
1	E	387	HIS
1	E	408	GLN
1	F	3	GLN
1	F	150	GLN
1	F	217	GLN
1	F	280	ASN
1	F	393	ASN

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

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.