



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 10:44 AM UTC

PDB ID : 1GRL / pdb_00001grl
Title : THE CRYSTAL STRUCTURE OF THE BACTERIAL CHAPERONIN
GROEL AT 2.8 ANGSTROMS
Authors : Braig, K.; Otwinowski, Z.; Hegde, R.; Boisvert, D.C.; Joachimiak, A.; Horwich,
A.L.; Sigler, P.B.
Deposited on : 1995-03-07
Resolution : 2.80 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

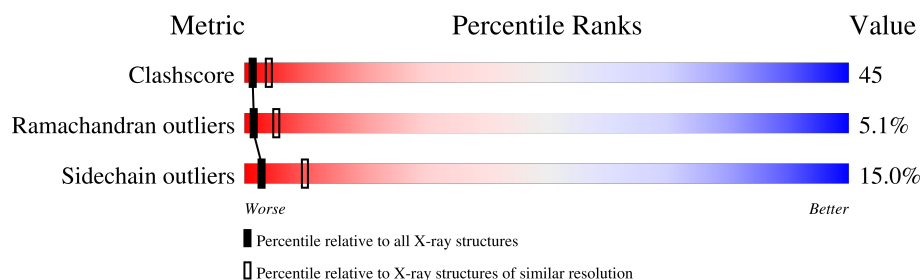
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	
1	G	548	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29274 atoms, of which 5278 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 GROEL (HSP60 CLASS).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	B	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	C	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	D	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	E	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	F	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	G	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	conflict	UNP P06139
A	126	VAL	ALA	conflict	UNP P06139
A	267	MET	ILE	conflict	UNP P06139
B	13	GLY	ARG	conflict	UNP P06139
B	126	VAL	ALA	conflict	UNP P06139
B	267	MET	ILE	conflict	UNP P06139
C	13	GLY	ARG	conflict	UNP P06139
C	126	VAL	ALA	conflict	UNP P06139
C	267	MET	ILE	conflict	UNP P06139
D	13	GLY	ARG	conflict	UNP P06139
D	126	VAL	ALA	conflict	UNP P06139
D	267	MET	ILE	conflict	UNP P06139
E	13	GLY	ARG	conflict	UNP P06139
E	126	VAL	ALA	conflict	UNP P06139
E	267	MET	ILE	conflict	UNP P06139

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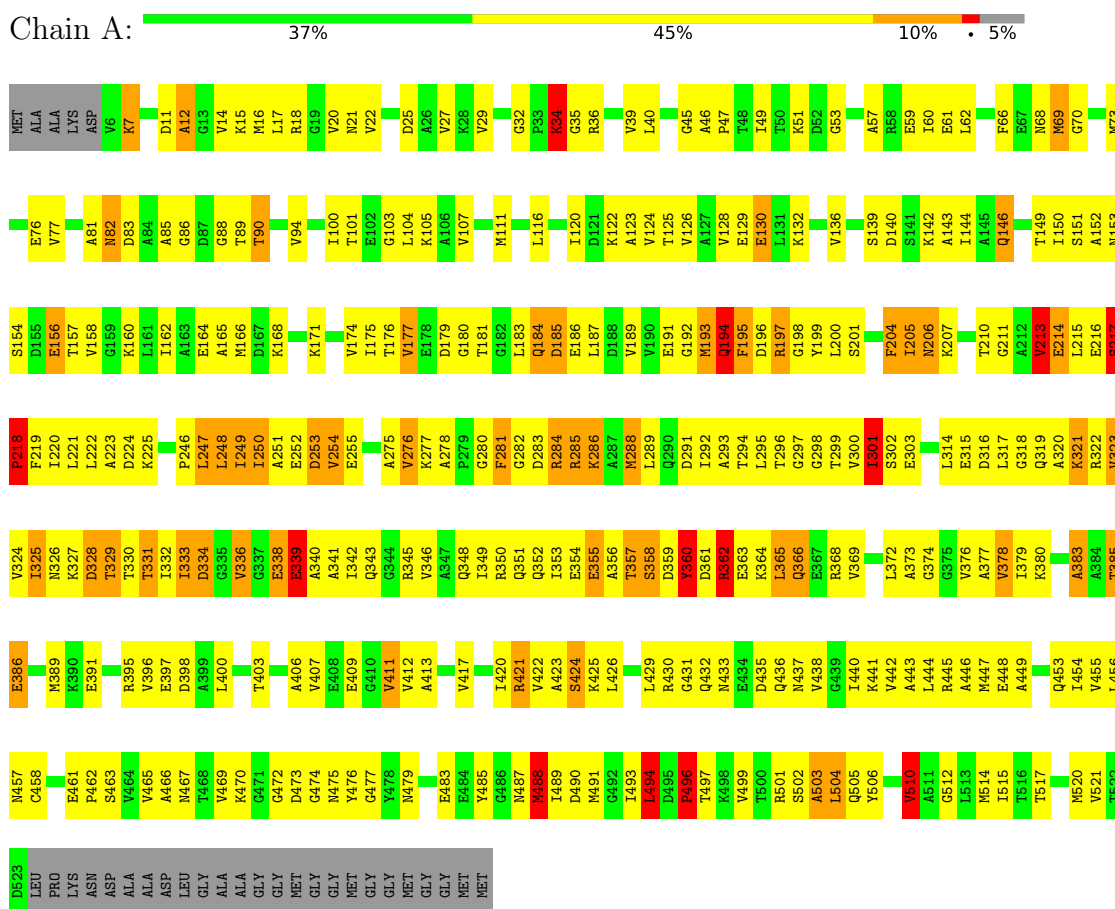
Chain	Residue	Modelled	Actual	Comment	Reference
F	13	GLY	ARG	conflict	UNP P06139
F	126	VAL	ALA	conflict	UNP P06139
F	267	MET	ILE	conflict	UNP P06139
G	13	GLY	ARG	conflict	UNP P06139
G	126	VAL	ALA	conflict	UNP P06139
G	267	MET	ILE	conflict	UNP P06139

3 Residue-property plots

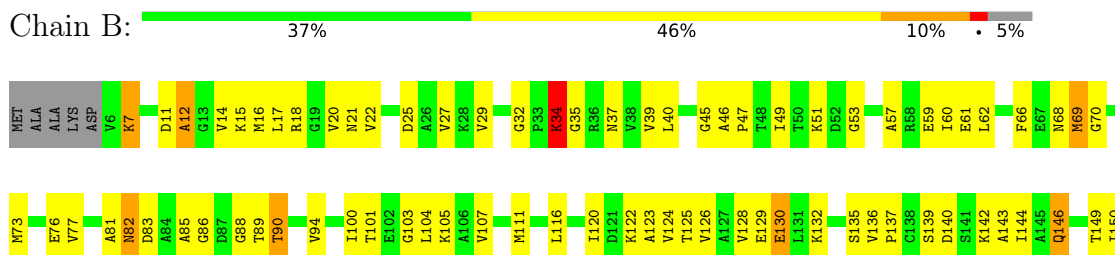
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

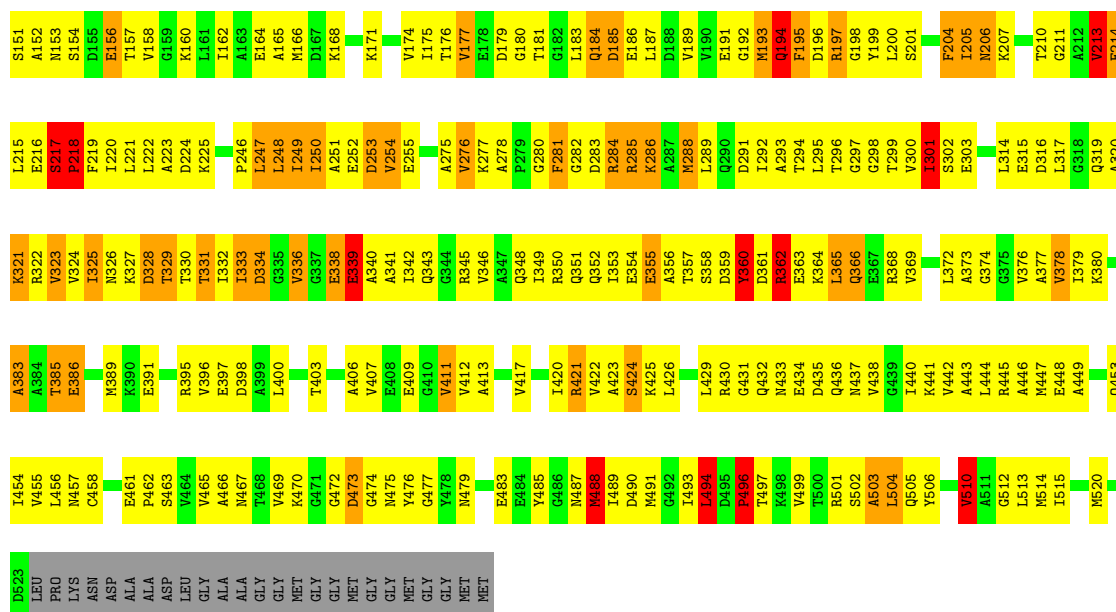
Note EDS was not executed.

- Molecule 1: GROEL (HSP60 CLASS)



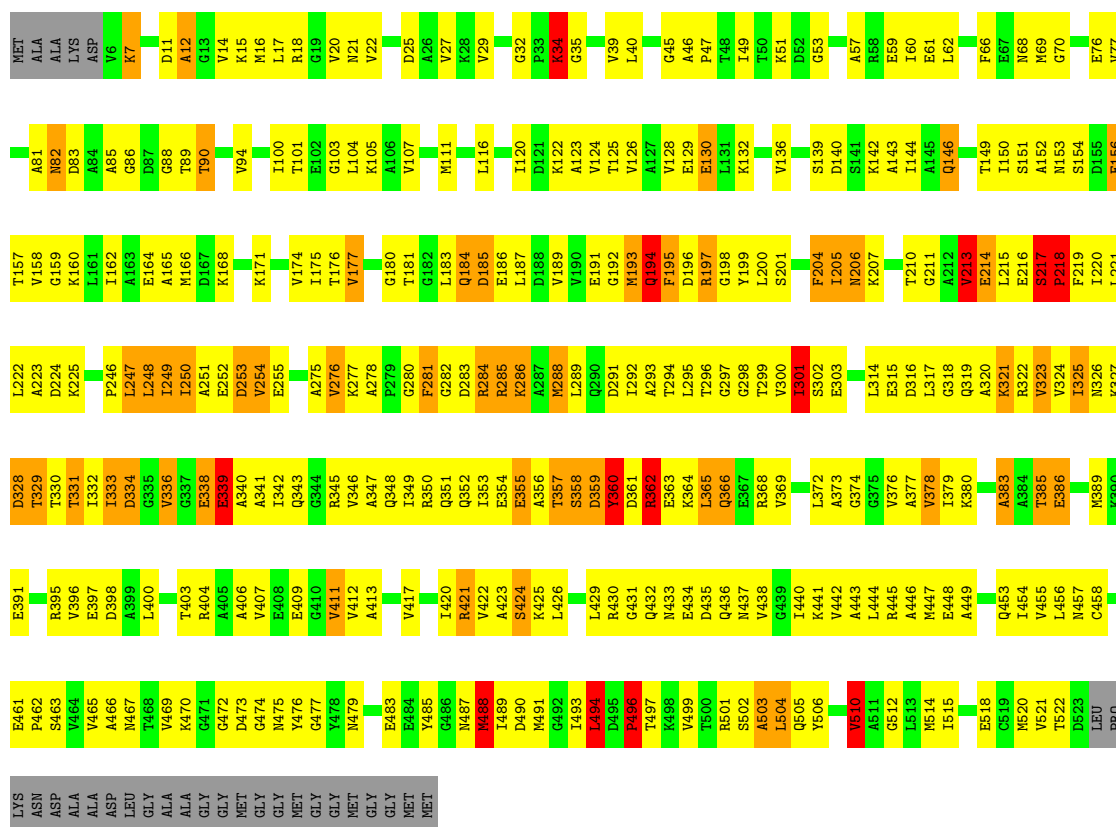
- Molecule 1: GROEL (HSP60 CLASS)





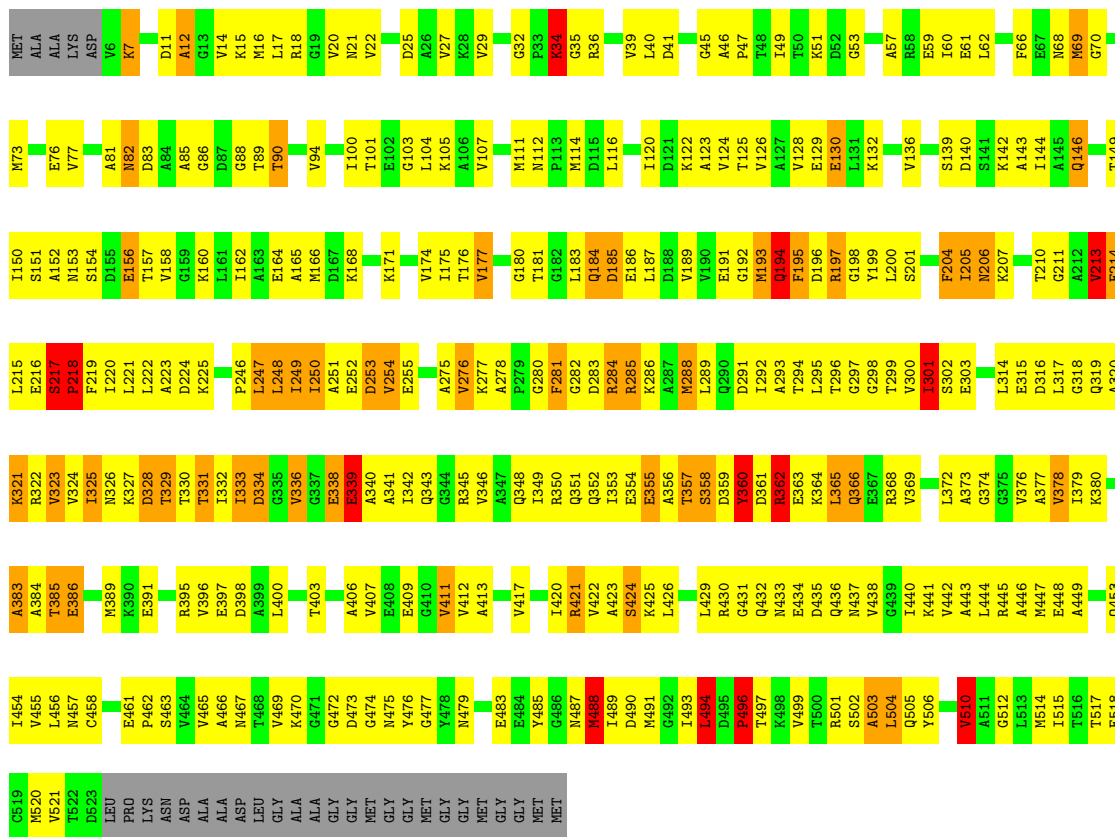
• Molecule 1: GROEL (HSP60 CLASS)

Chain C: 36% 46% 10% 5%

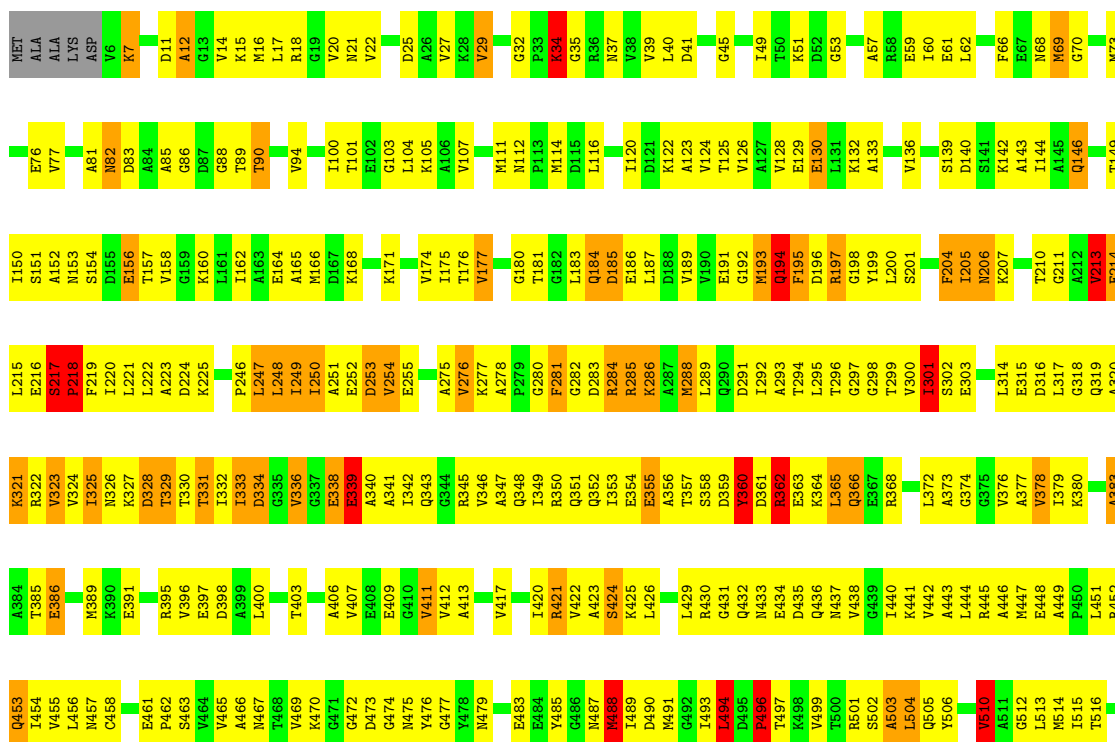


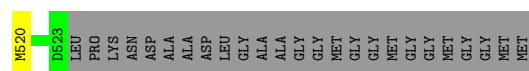
• Molecule 1: GROEL (HSP60 CLASS)

Chain D: 36% 47% 10% 5%



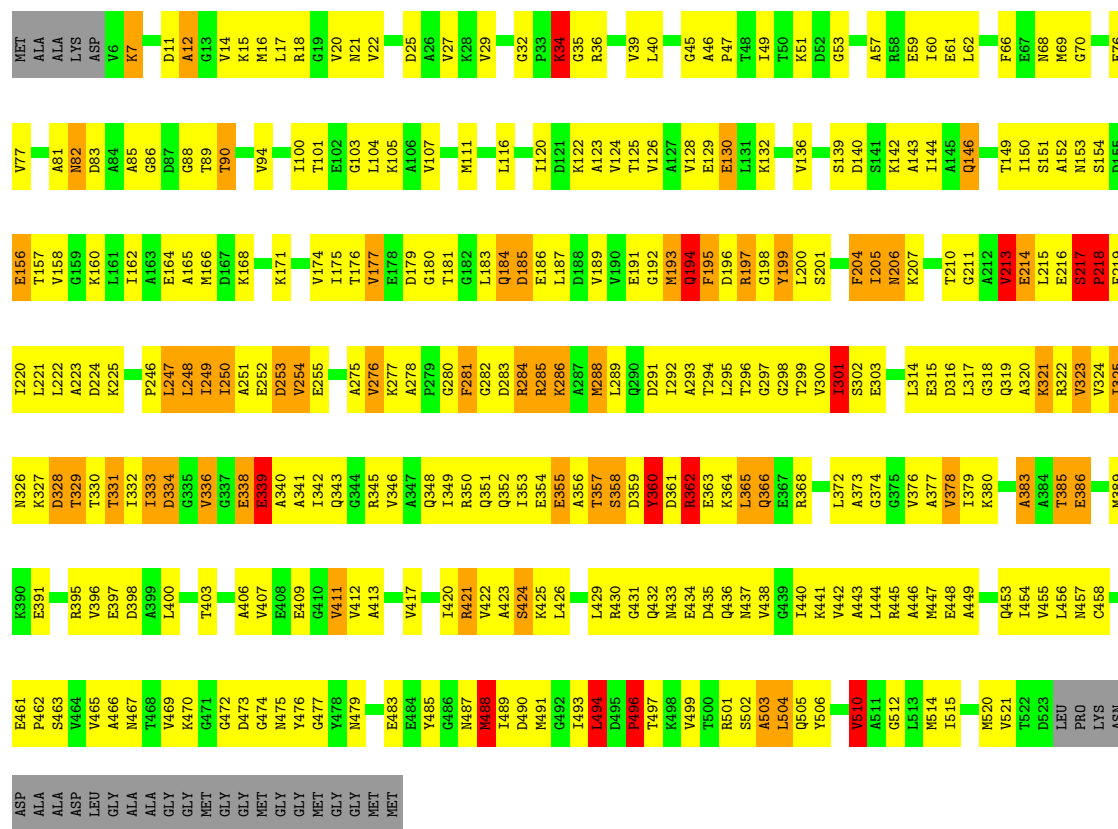
- Molecule 1: GROEL (HSP60 CLASS)





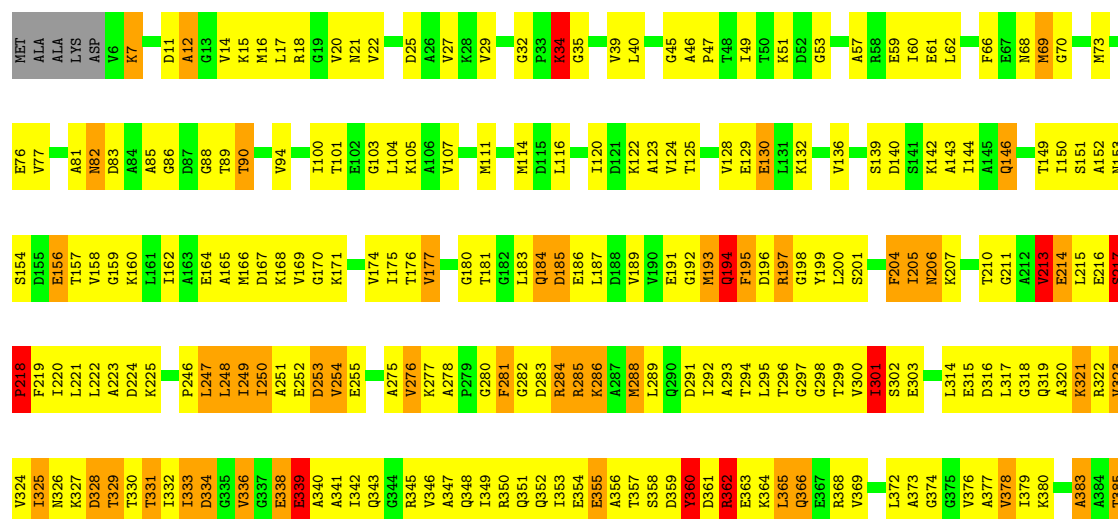
• Molecule 1: GROEL (HSP60 CLASS)

Chain F: 37% 45% 10% 5%



• Molecule 1: GROEL (HSP60 CLASS)

Chain G: 36% 46% 9% 5%



LEU	C458	E386
PRO	E461	K389
LYS	E462	K390
ASN	P463	E391
ASP	P464	
ALA	V465	R395
ASP	V466	V396
LEU	N467	D397
GLY	T468	D398
ALA	V469	K399
ALA	K470	L400
GLY	G471	
GLY	D472	T403
MET	D473	
GLY	G474	A406
GLY	N475	V407
MET	V476	E408
GLY	G477	E409
GLY	V478	G410
MET	N479	V411
GLY		V412
GLY	E483	A413
MET	E484	
MET	Y485	V417
	G486	
	N487	L420
	M488	R421
	L489	V422
	D490	A423
	M491	S424
	G492	K425
	I493	
	L494	L429
	D495	R430
	P496	G431
	T497	Q432
	K498	N433
	V499	E434
	T500	D435
	R501	Q436
	S502	N437
	A503	V438
	L504	G439
	Q505	L440
	Y506	K441
		V442
	V510	A443
	A511	L444
	G512	R445
	L513	A446
	M514	N447
	I515	E448
		A449
	E518	
	C519	Q453
	M520	L454
	V521	V455
	T522	L456
	R523	V457

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	178.00Å 203.00Å 278.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.326 , 0.368	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29274	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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	0.77	1/3389 (0.0%)	1.27	32/4571 (0.7%)
1	B	0.77	1/3389 (0.0%)	1.27	32/4571 (0.7%)
1	C	0.77	0/3389	1.27	33/4571 (0.7%)
1	D	0.77	1/3389 (0.0%)	1.27	32/4571 (0.7%)
1	E	0.77	1/3389 (0.0%)	1.27	33/4571 (0.7%)
1	F	0.77	0/3389	1.27	32/4571 (0.7%)
1	G	0.77	1/3389 (0.0%)	1.27	33/4571 (0.7%)
All	All	0.77	5/23723 (0.0%)	1.27	227/31997 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	MET	SD-CE	-5.02	1.67	1.79
1	E	69	MET	SD-CE	-5.01	1.67	1.79
1	B	69	MET	SD-CE	-5.01	1.67	1.79
1	G	69	MET	SD-CE	-5.01	1.67	1.79
1	A	69	MET	SD-CE	-5.00	1.67	1.79

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	461	GLU	CA-C-N	9.37	129.02	119.56
1	G	461	GLU	C-N-CA	9.37	129.02	119.56
1	C	461	GLU	CA-C-N	9.36	129.02	119.56
1	C	461	GLU	C-N-CA	9.36	129.02	119.56
1	B	461	GLU	CA-C-N	9.36	129.01	119.56
1	B	461	GLU	C-N-CA	9.36	129.01	119.56
1	A	461	GLU	CA-C-N	9.34	128.99	119.56
1	A	461	GLU	C-N-CA	9.34	128.99	119.56
1	E	461	GLU	CA-C-N	9.33	128.98	119.56
1	E	461	GLU	C-N-CA	9.33	128.98	119.56
1	D	461	GLU	CA-C-N	9.31	128.97	119.56
1	D	461	GLU	C-N-CA	9.31	128.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	461	GLU	CA-C-N	9.31	128.96	119.56
1	F	461	GLU	C-N-CA	9.31	128.96	119.56
1	F	333	ILE	N-CA-C	8.36	121.53	111.09
1	G	333	ILE	N-CA-C	8.35	121.52	111.09
1	E	333	ILE	N-CA-C	8.34	121.52	111.09
1	F	360	TYR	N-CA-C	8.34	128.57	110.80
1	C	333	ILE	N-CA-C	8.34	121.51	111.09
1	B	360	TYR	N-CA-C	8.33	128.55	110.80
1	G	360	TYR	N-CA-C	8.33	128.55	110.80
1	A	333	ILE	N-CA-C	8.33	121.50	111.09
1	B	333	ILE	N-CA-C	8.33	121.50	111.09
1	D	360	TYR	N-CA-C	8.32	128.53	110.80
1	E	360	TYR	N-CA-C	8.32	128.52	110.80
1	A	360	TYR	N-CA-C	8.32	128.52	110.80
1	C	360	TYR	N-CA-C	8.32	128.51	110.80
1	D	333	ILE	N-CA-C	8.31	121.48	111.09
1	B	386	GLU	N-CA-C	-7.90	102.67	111.28
1	A	386	GLU	N-CA-C	-7.88	102.69	111.28
1	D	386	GLU	N-CA-C	-7.88	102.69	111.28
1	G	386	GLU	N-CA-C	-7.87	102.70	111.28
1	C	386	GLU	N-CA-C	-7.87	102.70	111.28
1	E	386	GLU	N-CA-C	-7.86	102.72	111.28
1	F	386	GLU	N-CA-C	-7.86	102.72	111.28
1	C	331	THR	N-CA-C	7.60	121.89	107.75
1	D	331	THR	N-CA-C	7.60	121.89	107.75
1	B	331	THR	N-CA-C	7.59	121.88	107.75
1	A	331	THR	N-CA-C	7.58	121.86	107.75
1	F	331	THR	N-CA-C	7.58	121.86	107.75
1	E	331	THR	N-CA-C	7.58	121.84	107.75
1	G	331	THR	N-CA-C	7.57	121.83	107.75
1	C	378	VAL	N-CA-C	7.10	118.27	108.89
1	A	378	VAL	N-CA-C	7.09	118.25	108.89
1	G	378	VAL	N-CA-C	7.08	118.24	108.89
1	D	378	VAL	N-CA-C	7.08	118.24	108.89
1	E	378	VAL	N-CA-C	7.08	118.23	108.89
1	F	378	VAL	N-CA-C	7.07	118.22	108.89
1	B	378	VAL	N-CA-C	7.06	118.21	108.89
1	C	503	ALA	N-CA-C	-7.00	104.37	113.12
1	D	503	ALA	N-CA-C	-6.99	104.39	113.12
1	B	503	ALA	N-CA-C	-6.98	104.39	113.12
1	G	503	ALA	N-CA-C	-6.97	104.41	113.12
1	A	503	ALA	N-CA-C	-6.96	104.42	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	503	ALA	N-CA-C	-6.96	104.42	113.12
1	E	503	ALA	N-CA-C	-6.96	104.42	113.12
1	E	366	GLN	N-CA-C	-6.90	105.39	113.88
1	D	366	GLN	N-CA-C	-6.90	105.40	113.88
1	A	366	GLN	N-CA-C	-6.88	105.42	113.88
1	B	366	GLN	N-CA-C	-6.88	105.42	113.88
1	C	366	GLN	N-CA-C	-6.88	105.42	113.88
1	G	366	GLN	N-CA-C	-6.86	105.44	113.88
1	F	366	GLN	N-CA-C	-6.85	105.45	113.88
1	E	130	GLU	N-CA-C	6.57	118.32	111.03
1	C	130	GLU	N-CA-C	6.57	118.32	111.03
1	B	130	GLU	N-CA-C	6.56	118.32	111.03
1	D	130	GLU	N-CA-C	6.56	118.31	111.03
1	G	130	GLU	N-CA-C	6.56	118.31	111.03
1	A	130	GLU	N-CA-C	6.55	118.30	111.03
1	F	130	GLU	N-CA-C	6.51	118.26	111.03
1	F	195	PHE	N-CA-C	6.35	117.87	108.60
1	C	195	PHE	N-CA-C	6.34	117.86	108.60
1	E	195	PHE	N-CA-C	6.34	117.85	108.60
1	D	195	PHE	N-CA-C	6.33	117.84	108.60
1	A	195	PHE	N-CA-C	6.33	117.84	108.60
1	B	195	PHE	N-CA-C	6.33	117.84	108.60
1	G	195	PHE	N-CA-C	6.30	117.79	108.60
1	D	12	ALA	N-CA-C	-6.20	104.07	111.69
1	A	12	ALA	N-CA-C	-6.19	104.08	111.69
1	C	12	ALA	N-CA-C	-6.18	104.08	111.69
1	F	12	ALA	N-CA-C	-6.18	104.08	111.69
1	B	12	ALA	N-CA-C	-6.18	104.09	111.69
1	E	12	ALA	N-CA-C	-6.17	104.09	111.69
1	G	12	ALA	N-CA-C	-6.15	104.12	111.69
1	C	362	ARG	N-CA-C	-6.11	104.90	112.90
1	D	362	ARG	N-CA-C	-6.10	104.91	112.90
1	E	362	ARG	N-CA-C	-6.09	104.92	112.90
1	B	362	ARG	N-CA-C	-6.08	104.93	112.90
1	A	362	ARG	N-CA-C	-6.08	104.93	112.90
1	C	152	ALA	N-CA-C	-6.07	106.13	112.93
1	F	362	ARG	N-CA-C	-6.07	104.95	112.90
1	G	362	ARG	N-CA-C	-6.06	104.96	112.90
1	F	152	ALA	N-CA-C	-6.05	106.16	112.93
1	A	152	ALA	N-CA-C	-6.04	106.17	112.93
1	B	152	ALA	N-CA-C	-6.02	106.19	112.93
1	D	152	ALA	N-CA-C	-6.02	106.19	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	152	ALA	N-CA-C	-6.02	106.19	112.93
1	E	152	ALA	N-CA-C	-6.01	106.20	112.93
1	F	60	ILE	N-CA-C	5.90	117.11	106.61
1	G	60	ILE	N-CA-C	5.89	117.10	106.61
1	B	60	ILE	N-CA-C	5.89	117.10	106.61
1	C	60	ILE	N-CA-C	5.89	117.09	106.61
1	A	60	ILE	N-CA-C	5.89	117.09	106.61
1	F	281	PHE	N-CA-C	5.88	116.33	108.38
1	D	60	ILE	N-CA-C	5.87	117.06	106.61
1	E	281	PHE	N-CA-C	5.87	116.30	108.38
1	E	60	ILE	N-CA-C	5.85	117.03	106.61
1	B	281	PHE	N-CA-C	5.85	116.28	108.38
1	A	281	PHE	N-CA-C	5.85	116.27	108.38
1	C	281	PHE	N-CA-C	5.85	116.28	108.38
1	G	281	PHE	N-CA-C	5.84	116.27	108.38
1	D	281	PHE	N-CA-C	5.84	116.26	108.38
1	E	88	GLY	N-CA-C	5.78	121.65	114.37
1	D	88	GLY	N-CA-C	5.76	121.63	114.37
1	A	88	GLY	N-CA-C	5.75	121.62	114.37
1	F	88	GLY	N-CA-C	5.75	121.62	114.37
1	G	88	GLY	N-CA-C	5.75	121.62	114.37
1	C	88	GLY	N-CA-C	5.74	121.60	114.37
1	B	88	GLY	N-CA-C	5.73	121.59	114.37
1	E	424	SER	N-CA-C	-5.70	106.67	113.97
1	D	424	SER	N-CA-C	-5.69	106.68	113.97
1	F	424	SER	N-CA-C	-5.69	106.69	113.97
1	A	424	SER	N-CA-C	-5.68	106.70	113.97
1	C	424	SER	N-CA-C	-5.67	106.72	113.97
1	B	424	SER	N-CA-C	-5.66	106.72	113.97
1	G	424	SER	N-CA-C	-5.64	106.74	113.97
1	F	494	LEU	N-CA-C	5.61	115.69	108.34
1	C	494	LEU	N-CA-C	5.60	115.68	108.34
1	D	180	GLY	N-CA-C	5.60	121.70	112.30
1	E	180	GLY	N-CA-C	5.59	121.69	112.30
1	B	180	GLY	N-CA-C	5.59	121.69	112.30
1	E	494	LEU	N-CA-C	5.59	115.66	108.34
1	A	180	GLY	N-CA-C	5.58	121.68	112.30
1	G	494	LEU	N-CA-C	5.58	115.65	108.34
1	A	494	LEU	N-CA-C	5.57	115.64	108.34
1	G	180	GLY	N-CA-C	5.57	121.66	112.30
1	F	180	GLY	N-CA-C	5.56	121.65	112.30
1	B	494	LEU	N-CA-C	5.56	115.63	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	GLY	N-CA-C	5.56	121.64	112.30
1	D	494	LEU	N-CA-C	5.53	115.59	108.34
1	E	34	LYS	N-CA-C	-5.48	103.47	111.30
1	G	329	THR	N-CA-C	5.46	116.94	109.18
1	G	34	LYS	N-CA-C	-5.46	103.49	111.30
1	C	34	LYS	N-CA-C	-5.46	103.49	111.30
1	F	329	THR	N-CA-C	5.46	116.93	109.18
1	B	329	THR	N-CA-C	5.45	116.92	109.18
1	F	34	LYS	N-CA-C	-5.45	103.51	111.30
1	A	34	LYS	N-CA-C	-5.45	103.51	111.30
1	D	34	LYS	N-CA-C	-5.45	103.51	111.30
1	E	329	THR	N-CA-C	5.45	116.91	109.18
1	B	34	LYS	N-CA-C	-5.44	103.52	111.30
1	D	329	THR	N-CA-C	5.44	116.91	109.18
1	A	329	THR	N-CA-C	5.44	116.91	109.18
1	C	329	THR	N-CA-C	5.42	116.87	109.18
1	A	249	ILE	N-CA-C	-5.38	100.58	108.11
1	G	249	ILE	N-CA-C	-5.38	100.58	108.11
1	C	249	ILE	N-CA-C	-5.37	100.59	108.11
1	D	249	ILE	N-CA-C	-5.37	100.59	108.11
1	F	249	ILE	N-CA-C	-5.36	100.60	108.11
1	E	249	ILE	N-CA-C	-5.35	100.61	108.11
1	B	249	ILE	N-CA-C	-5.35	100.62	108.11
1	D	510	VAL	CB-CA-C	-5.20	105.31	111.81
1	E	411	VAL	N-CA-C	5.20	116.17	107.18
1	F	411	VAL	N-CA-C	5.17	116.13	107.18
1	F	510	VAL	CB-CA-C	-5.17	105.35	111.81
1	C	323	VAL	N-CA-C	-5.17	100.44	108.86
1	C	462	PRO	N-CA-C	5.17	120.32	113.86
1	A	411	VAL	N-CA-C	5.16	116.11	107.18
1	A	510	VAL	CB-CA-C	-5.16	105.36	111.81
1	C	217	SER	CA-C-N	5.16	126.29	119.84
1	C	217	SER	C-N-CA	5.16	126.29	119.84
1	E	510	VAL	CB-CA-C	-5.16	105.35	111.81
1	C	411	VAL	N-CA-C	5.16	116.10	107.18
1	D	411	VAL	N-CA-C	5.16	116.10	107.18
1	E	217	SER	CA-C-N	5.16	126.29	119.84
1	E	217	SER	C-N-CA	5.16	126.29	119.84
1	C	510	VAL	CB-CA-C	-5.16	105.36	111.81
1	D	462	PRO	N-CA-C	5.16	120.30	113.86
1	G	510	VAL	CB-CA-C	-5.15	105.37	111.81
1	E	462	PRO	N-CA-C	5.15	120.30	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	VAL	CB-CA-C	-5.15	105.37	111.81
1	G	323	VAL	N-CA-C	-5.15	100.46	108.86
1	F	512	GLY	N-CA-C	-5.15	106.26	112.49
1	G	411	VAL	N-CA-C	5.15	116.08	107.18
1	B	411	VAL	N-CA-C	5.14	116.08	107.18
1	A	323	VAL	N-CA-C	-5.14	100.48	108.86
1	D	217	SER	CA-C-N	5.14	126.27	119.84
1	D	217	SER	C-N-CA	5.14	126.27	119.84
1	G	462	PRO	N-CA-C	5.14	120.29	113.86
1	E	512	GLY	N-CA-C	-5.14	106.27	112.49
1	F	323	VAL	N-CA-C	-5.14	100.48	108.86
1	A	462	PRO	N-CA-C	5.14	120.28	113.86
1	B	217	SER	CA-C-N	5.14	126.26	119.84
1	B	217	SER	C-N-CA	5.14	126.26	119.84
1	C	512	GLY	N-CA-C	-5.13	106.28	112.49
1	D	323	VAL	N-CA-C	-5.13	100.49	108.86
1	F	462	PRO	N-CA-C	5.13	120.27	113.86
1	E	323	VAL	N-CA-C	-5.13	100.50	108.86
1	B	323	VAL	N-CA-C	-5.12	100.51	108.86
1	F	217	SER	CA-C-N	5.12	126.24	119.84
1	F	217	SER	C-N-CA	5.12	126.24	119.84
1	G	512	GLY	N-CA-C	-5.12	106.29	112.49
1	A	217	SER	CA-C-N	5.12	126.24	119.84
1	A	217	SER	C-N-CA	5.12	126.24	119.84
1	A	512	GLY	N-CA-C	-5.12	106.30	112.49
1	B	512	GLY	N-CA-C	-5.12	106.30	112.49
1	C	488	MET	N-CA-C	5.11	117.52	111.33
1	B	462	PRO	N-CA-C	5.11	120.25	113.86
1	G	217	SER	CA-C-N	5.10	126.22	119.84
1	G	217	SER	C-N-CA	5.10	126.22	119.84
1	D	488	MET	N-CA-C	5.10	117.50	111.33
1	A	488	MET	N-CA-C	5.10	117.50	111.33
1	D	512	GLY	N-CA-C	-5.10	106.32	112.49
1	G	488	MET	N-CA-C	5.10	117.50	111.33
1	B	136	VAL	N-CA-C	-5.09	101.93	107.73
1	B	488	MET	N-CA-C	5.08	117.48	111.33
1	E	136	VAL	N-CA-C	-5.08	101.94	107.73
1	E	488	MET	N-CA-C	5.08	117.47	111.33
1	F	488	MET	N-CA-C	5.07	117.47	111.33
1	A	136	VAL	N-CA-C	-5.07	101.95	107.73
1	C	136	VAL	N-CA-C	-5.07	101.96	107.73
1	G	136	VAL	N-CA-C	-5.07	101.95	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	VAL	N-CA-C	-5.06	101.96	107.73
1	F	136	VAL	N-CA-C	-5.03	101.99	107.73
1	C	159	GLY	N-CA-C	-5.03	106.55	112.64
1	E	453	GLN	N-CA-C	-5.00	104.79	111.24
1	G	159	GLY	N-CA-C	-5.00	106.59	112.64

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	3428	754	3441	328	1
1	B	3428	754	3441	337	9
1	C	3428	754	3440	347	54
1	D	3428	754	3441	337	0
1	E	3428	754	3441	343	18
1	F	3428	754	3440	337	1
1	G	3428	754	3441	327	55
All	All	23996	5278	24085	2180	75

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 45.

All (2180) 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:181:THR:O	1:G:282:GLY:CA	1.65	1.39
1:D:282:GLY:CA	1:E:181:THR:O	1.69	1.37
1:F:282:GLY:CA	1:G:181:THR:O	1.72	1.36
1:A:282:GLY:HA3	1:B:181:THR:O	1.28	1.30
1:C:281:PHE:HE2	1:D:385:THR:C	1.41	1.26
1:A:386:GLU:OE2	1:G:285:ARG:NH2	1.71	1.23
1:A:181:THR:O	1:G:282:GLY:HA3	1.08	1.23
1:C:281:PHE:CE2	1:D:385:THR:C	2.18	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLY:CA	1:B:181:THR:O	1.97	1.12
1:F:282:GLY:HA3	1:G:181:THR:O	1.34	1.12
1:F:281:PHE:HE2	1:G:385:THR:C	1.61	1.09
1:F:282:GLY:HA2	1:G:181:THR:O	1.47	1.08
1:A:285:ARG:NH2	1:B:386:GLU:OE2	1.87	1.06
1:B:285:ARG:NH2	1:C:386:GLU:OE2	1.90	1.04
1:B:214:GLU:HG2	1:B:324:VAL:HG13	1.41	1.03
1:C:214:GLU:HG2	1:C:324:VAL:HG13	1.41	1.03
1:D:282:GLY:HA3	1:E:181:THR:O	0.86	1.03
1:A:214:GLU:HG2	1:A:324:VAL:HG13	1.41	1.02
1:D:214:GLU:HG2	1:D:324:VAL:HG13	1.41	1.02
1:G:214:GLU:HG2	1:G:324:VAL:HG13	1.41	1.02
1:E:214:GLU:HG2	1:E:324:VAL:HG13	1.41	1.02
1:F:214:GLU:HG2	1:F:324:VAL:HG13	1.41	1.02
1:C:281:PHE:HE2	1:D:385:THR:CA	1.75	0.99
1:A:181:THR:O	1:G:282:GLY:HA2	1.62	0.99
1:E:285:ARG:NH2	1:F:386:GLU:OE2	1.95	0.99
1:B:281:PHE:CZ	1:C:389:MET:HB2	1.97	0.98
1:F:302:SER:C	1:F:303:GLU:CA	2.36	0.98
1:E:302:SER:C	1:E:303:GLU:CA	2.36	0.98
1:G:302:SER:C	1:G:303:GLU:CA	2.36	0.97
1:A:302:SER:C	1:A:303:GLU:CA	2.36	0.97
1:B:302:SER:C	1:B:303:GLU:CA	2.36	0.97
1:C:302:SER:C	1:C:303:GLU:CA	2.36	0.97
1:D:302:SER:C	1:D:303:GLU:CA	2.36	0.97
1:C:281:PHE:CE2	1:D:384:ALA:O	2.18	0.97
1:B:281:PHE:CD2	1:C:386:GLU:HA	1.99	0.96
1:C:281:PHE:CE2	1:D:386:GLU:N	2.36	0.94
1:E:360:TYR:CE1	1:F:183:LEU:HD22	2.02	0.93
1:B:360:TYR:CE1	1:C:183:LEU:HD22	2.03	0.93
1:D:288:MET:HG3	1:D:368:ARG:HD2	1.50	0.93
1:A:288:MET:HG3	1:A:368:ARG:HD2	1.50	0.92
1:B:288:MET:HG3	1:B:368:ARG:HD2	1.50	0.92
1:B:360:TYR:OH	1:C:183:LEU:HD13	1.68	0.92
1:B:281:PHE:HA	1:B:285:ARG:HG2	1.52	0.92
1:E:288:MET:HG3	1:E:368:ARG:HD2	1.50	0.92
1:E:360:TYR:OH	1:F:183:LEU:HD13	1.69	0.92
1:A:82:ASN:HD21	1:A:89:THR:H	1.16	0.92
1:C:69:MET:HE2	1:D:39:VAL:HG12	1.52	0.92
1:C:82:ASN:HD21	1:C:89:THR:H	1.16	0.92
1:C:281:PHE:HA	1:C:285:ARG:HG2	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:MET:HG3	1:C:368:ARG:HD2	1.50	0.92
1:G:82:ASN:HD21	1:G:89:THR:H	1.16	0.92
1:G:288:MET:HG3	1:G:368:ARG:HD2	1.50	0.92
1:A:281:PHE:HA	1:A:285:ARG:HG2	1.52	0.91
1:B:281:PHE:CE2	1:C:386:GLU:HA	2.05	0.91
1:D:82:ASN:HD21	1:D:89:THR:H	1.16	0.91
1:F:288:MET:HG3	1:F:368:ARG:HD2	1.50	0.91
1:D:281:PHE:HA	1:D:285:ARG:HG2	1.52	0.91
1:E:300:VAL:HG21	1:E:317:LEU:HD23	1.52	0.90
1:G:281:PHE:HA	1:G:285:ARG:HG2	1.52	0.90
1:F:300:VAL:HG21	1:F:317:LEU:HD23	1.51	0.90
1:E:281:PHE:HA	1:E:285:ARG:HG2	1.52	0.90
1:C:281:PHE:CZ	1:D:384:ALA:C	2.50	0.90
1:A:300:VAL:HG21	1:A:317:LEU:HD23	1.51	0.90
1:E:281:PHE:CE2	1:F:386:GLU:HA	2.06	0.90
1:E:281:PHE:CZ	1:F:389:MET:HB2	2.07	0.89
1:G:300:VAL:HG21	1:G:317:LEU:HD23	1.52	0.89
1:B:300:VAL:HG21	1:B:317:LEU:HD23	1.51	0.89
1:D:300:VAL:HG21	1:D:317:LEU:HD23	1.52	0.89
1:A:254:VAL:C	1:A:255:GLU:CA	2.46	0.89
1:E:281:PHE:CD2	1:F:386:GLU:HA	2.07	0.89
1:E:254:VAL:C	1:E:255:GLU:CA	2.46	0.89
1:F:281:PHE:HA	1:F:285:ARG:HG2	1.52	0.89
1:C:281:PHE:CZ	1:D:384:ALA:O	2.26	0.89
1:D:254:VAL:C	1:D:255:GLU:CA	2.46	0.89
1:G:254:VAL:C	1:G:255:GLU:CA	2.46	0.89
1:C:300:VAL:HG21	1:C:317:LEU:HD23	1.51	0.89
1:D:282:GLY:HA3	1:E:181:THR:C	1.98	0.89
1:B:254:VAL:C	1:B:255:GLU:CA	2.46	0.89
1:B:82:ASN:HD21	1:B:89:THR:H	1.16	0.88
1:F:82:ASN:HD21	1:F:89:THR:H	1.16	0.88
1:F:254:VAL:C	1:F:255:GLU:CA	2.46	0.88
1:C:254:VAL:C	1:C:255:GLU:CA	2.46	0.88
1:F:281:PHE:CE2	1:G:385:THR:C	2.52	0.88
1:A:39:VAL:HG12	1:G:69:MET:HE2	1.54	0.88
1:E:82:ASN:HD21	1:E:89:THR:H	1.16	0.88
1:D:315:GLU:O	1:D:317:LEU:HG	1.75	0.86
1:C:206:ASN:C	1:C:207:LYS:CA	2.49	0.86
1:F:206:ASN:C	1:F:207:LYS:CA	2.49	0.86
1:G:224:ASP:C	1:G:225:LYS:CA	2.48	0.86
1:A:315:GLU:O	1:A:317:LEU:HG	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:ASP:C	1:E:225:LYS:CA	2.48	0.86
1:D:206:ASN:C	1:D:207:LYS:CA	2.49	0.86
1:G:206:ASN:C	1:G:207:LYS:CA	2.49	0.86
1:G:315:GLU:O	1:G:317:LEU:HG	1.76	0.86
1:B:206:ASN:C	1:B:207:LYS:CA	2.49	0.86
1:C:224:ASP:C	1:C:225:LYS:CA	2.48	0.86
1:C:282:GLY:HA2	1:D:181:THR:O	1.75	0.86
1:E:364:LYS:HZ3	1:E:365:LEU:HD13	1.41	0.86
1:B:224:ASP:C	1:B:225:LYS:CA	2.48	0.86
1:B:364:LYS:HZ3	1:B:365:LEU:HD13	1.41	0.85
1:C:315:GLU:O	1:C:317:LEU:HG	1.76	0.85
1:C:364:LYS:HZ3	1:C:365:LEU:HD13	1.41	0.85
1:D:364:LYS:HZ3	1:D:365:LEU:HD13	1.41	0.85
1:D:224:ASP:C	1:D:225:LYS:CA	2.48	0.85
1:A:224:ASP:C	1:A:225:LYS:CA	2.48	0.85
1:E:315:GLU:O	1:E:317:LEU:HG	1.76	0.85
1:F:364:LYS:HZ3	1:F:365:LEU:HD13	1.41	0.85
1:G:364:LYS:HZ3	1:G:365:LEU:HD13	1.41	0.85
1:A:206:ASN:C	1:A:207:LYS:CA	2.49	0.85
1:F:224:ASP:C	1:F:225:LYS:CA	2.48	0.85
1:F:315:GLU:O	1:F:317:LEU:HG	1.76	0.85
1:B:315:GLU:O	1:B:317:LEU:HG	1.76	0.85
1:E:206:ASN:C	1:E:207:LYS:CA	2.49	0.85
1:G:275:ALA:CA	1:G:276:VAL:N	2.40	0.85
1:A:275:ALA:CA	1:A:276:VAL:N	2.40	0.84
1:C:275:ALA:CA	1:C:276:VAL:N	2.40	0.84
1:G:210:THR:CA	1:G:211:GLY:N	2.41	0.84
1:A:210:THR:CA	1:A:211:GLY:N	2.41	0.84
1:B:275:ALA:CA	1:B:276:VAL:N	2.40	0.84
1:E:210:THR:CA	1:E:211:GLY:N	2.41	0.84
1:F:275:ALA:CA	1:F:276:VAL:N	2.40	0.84
1:C:210:THR:CA	1:C:211:GLY:N	2.41	0.84
1:B:210:THR:CA	1:B:211:GLY:N	2.41	0.84
1:C:206:ASN:HB3	1:C:213:VAL:HA	1.59	0.84
1:D:206:ASN:HB3	1:D:213:VAL:HA	1.59	0.84
1:F:363:GLU:HA	1:F:366:GLN:HE21	1.43	0.84
1:A:206:ASN:HB3	1:A:213:VAL:HA	1.59	0.84
1:D:275:ALA:CA	1:D:276:VAL:N	2.40	0.84
1:E:275:ALA:CA	1:E:276:VAL:N	2.40	0.84
1:B:206:ASN:HB3	1:B:213:VAL:HA	1.59	0.84
1:D:285:ARG:NH2	1:E:386:GLU:OE2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:THR:CA	1:F:211:GLY:N	2.41	0.84
1:B:363:GLU:HA	1:B:366:GLN:HE21	1.43	0.84
1:D:363:GLU:HA	1:D:366:GLN:HE21	1.43	0.84
1:A:364:LYS:HZ3	1:A:365:LEU:HD13	1.43	0.83
1:C:421:ARG:HD2	1:C:474:GLY:O	1.79	0.83
1:G:363:GLU:HA	1:G:366:GLN:HE21	1.43	0.83
1:E:421:ARG:HD2	1:E:474:GLY:O	1.79	0.83
1:A:363:GLU:HA	1:A:366:GLN:HE21	1.43	0.83
1:D:210:THR:CA	1:D:211:GLY:N	2.41	0.83
1:A:421:ARG:HD2	1:A:474:GLY:O	1.79	0.83
1:E:206:ASN:HB3	1:E:213:VAL:HA	1.59	0.83
1:G:206:ASN:HB3	1:G:213:VAL:HA	1.59	0.83
1:E:218:PRO:HD2	1:E:320:ALA:O	1.79	0.83
1:F:206:ASN:HB3	1:F:213:VAL:HA	1.59	0.83
1:D:218:PRO:HD2	1:D:320:ALA:O	1.79	0.83
1:A:246:PRO:CA	1:A:247:LEU:N	2.42	0.82
1:C:246:PRO:CA	1:C:247:LEU:N	2.42	0.82
1:F:218:PRO:HD2	1:F:320:ALA:O	1.79	0.82
1:F:246:PRO:CA	1:F:247:LEU:N	2.42	0.82
1:B:246:PRO:CA	1:B:247:LEU:N	2.42	0.82
1:G:218:PRO:HD2	1:G:320:ALA:O	1.79	0.82
1:G:421:ARG:HD2	1:G:474:GLY:O	1.79	0.82
1:A:385:THR:C	1:G:281:PHE:HE2	1.87	0.82
1:F:421:ARG:HD2	1:F:474:GLY:O	1.79	0.82
1:G:246:PRO:CA	1:G:247:LEU:N	2.42	0.82
1:B:421:ARG:HD2	1:B:474:GLY:O	1.79	0.82
1:C:218:PRO:HD2	1:C:320:ALA:O	1.79	0.82
1:C:363:GLU:HA	1:C:366:GLN:HE21	1.43	0.82
1:E:246:PRO:CA	1:E:247:LEU:N	2.42	0.82
1:A:314:LEU:CA	1:A:315:GLU:N	2.43	0.82
1:D:221:LEU:HD12	1:D:300:VAL:HG11	1.61	0.82
1:G:314:LEU:CA	1:G:315:GLU:N	2.43	0.82
1:A:218:PRO:HD2	1:A:320:ALA:O	1.79	0.81
1:D:246:PRO:CA	1:D:247:LEU:N	2.42	0.81
1:E:363:GLU:HA	1:E:366:GLN:HE21	1.43	0.81
1:B:221:LEU:HD12	1:B:300:VAL:HG11	1.61	0.81
1:C:221:LEU:HD12	1:C:300:VAL:HG11	1.61	0.81
1:C:281:PHE:CD2	1:D:386:GLU:N	2.47	0.81
1:D:421:ARG:HD2	1:D:474:GLY:O	1.79	0.81
1:F:314:LEU:CA	1:F:315:GLU:N	2.43	0.81
1:B:314:LEU:CA	1:B:315:GLU:N	2.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LEU:CA	1:D:315:GLU:N	2.43	0.81
1:B:218:PRO:HD2	1:B:320:ALA:O	1.79	0.81
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.63	0.81
1:E:314:LEU:CA	1:E:315:GLU:N	2.43	0.81
1:B:177:VAL:HG21	1:B:397:GLU:HG3	1.63	0.81
1:A:221:LEU:HD12	1:A:300:VAL:HG11	1.61	0.81
1:E:221:LEU:HD12	1:E:300:VAL:HG11	1.61	0.81
1:F:221:LEU:HD12	1:F:300:VAL:HG11	1.61	0.81
1:G:221:LEU:HD12	1:G:300:VAL:HG11	1.61	0.81
1:C:314:LEU:CA	1:C:315:GLU:N	2.43	0.81
1:E:166:MET:HG3	1:E:171:LYS:HA	1.62	0.80
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.63	0.80
1:C:281:PHE:CE2	1:D:384:ALA:C	2.59	0.80
1:D:166:MET:HG3	1:D:171:LYS:HA	1.62	0.80
1:D:177:VAL:HG21	1:D:397:GLU:HG3	1.63	0.80
1:F:166:MET:HG3	1:F:171:LYS:HA	1.62	0.80
1:D:111:MET:SD	1:D:438:VAL:HG11	2.22	0.80
1:A:166:MET:HG3	1:A:171:LYS:HA	1.62	0.80
1:B:166:MET:HG3	1:B:171:LYS:HA	1.62	0.80
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.63	0.80
1:C:111:MET:SD	1:C:438:VAL:HG11	2.22	0.79
1:C:166:MET:HG3	1:C:171:LYS:HA	1.62	0.79
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.63	0.79
1:E:111:MET:SD	1:E:438:VAL:HG11	2.22	0.79
1:G:166:MET:HG3	1:G:171:LYS:HA	1.62	0.79
1:D:82:ASN:ND2	1:D:89:THR:H	1.80	0.79
1:E:82:ASN:ND2	1:E:89:THR:H	1.80	0.79
1:B:111:MET:SD	1:B:438:VAL:HG11	2.22	0.79
1:A:111:MET:SD	1:A:438:VAL:HG11	2.22	0.79
1:B:281:PHE:CE2	1:C:389:MET:HB2	2.18	0.79
1:F:69:MET:HE2	1:G:39:VAL:HG12	1.63	0.79
1:G:111:MET:SD	1:G:438:VAL:HG11	2.22	0.79
1:F:177:VAL:HG21	1:F:397:GLU:HG3	1.63	0.79
1:A:82:ASN:ND2	1:A:89:THR:H	1.80	0.79
1:D:363:GLU:HA	1:D:366:GLN:NE2	1.97	0.79
1:F:111:MET:SD	1:F:438:VAL:HG11	2.22	0.79
1:F:82:ASN:ND2	1:F:89:THR:H	1.80	0.79
1:G:82:ASN:ND2	1:G:89:THR:H	1.80	0.79
1:B:363:GLU:HA	1:B:366:GLN:NE2	1.97	0.78
1:C:82:ASN:ND2	1:C:89:THR:H	1.80	0.78
1:A:363:GLU:HA	1:A:366:GLN:NE2	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASN:ND2	1:B:89:THR:H	1.80	0.78
1:C:128:VAL:O	1:C:132:LYS:HG2	1.84	0.78
1:C:363:GLU:HA	1:C:366:GLN:NE2	1.97	0.78
1:E:294:THR:HG21	1:E:345:ARG:HD2	1.66	0.78
1:G:363:GLU:HA	1:G:366:GLN:NE2	1.97	0.78
1:A:294:THR:HG21	1:A:345:ARG:HD2	1.66	0.78
1:B:294:THR:HG21	1:B:345:ARG:HD2	1.66	0.78
1:F:194:GLN:NE2	1:F:331:THR:HG22	1.99	0.78
1:E:363:GLU:HA	1:E:366:GLN:NE2	1.97	0.78
1:G:128:VAL:O	1:G:132:LYS:HG2	1.84	0.78
1:C:69:MET:HE2	1:D:39:VAL:CG1	2.14	0.78
1:C:194:GLN:NE2	1:C:331:THR:HG22	1.99	0.78
1:D:294:THR:HG21	1:D:345:ARG:HD2	1.66	0.78
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.66	0.78
1:F:294:THR:HG21	1:F:345:ARG:HD2	1.66	0.78
1:F:363:GLU:HA	1:F:366:GLN:NE2	1.97	0.78
1:B:194:GLN:NE2	1:B:331:THR:HG22	1.99	0.78
1:G:174:VAL:HG13	1:G:376:VAL:HA	1.65	0.78
1:G:194:GLN:NE2	1:G:331:THR:HG22	1.99	0.78
1:G:294:THR:HG21	1:G:345:ARG:HD2	1.66	0.78
1:A:174:VAL:HG13	1:A:376:VAL:HA	1.65	0.77
1:D:128:VAL:O	1:D:132:LYS:HG2	1.84	0.77
1:E:466:ALA:O	1:E:470:LYS:HB2	1.84	0.77
1:A:194:GLN:NE2	1:A:331:THR:HG22	1.99	0.77
1:C:294:THR:HG21	1:C:345:ARG:HD2	1.66	0.77
1:E:194:GLN:NE2	1:E:331:THR:HG22	1.99	0.77
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.66	0.77
1:F:128:VAL:O	1:F:132:LYS:HG2	1.84	0.77
1:F:174:VAL:HG13	1:F:376:VAL:HA	1.65	0.77
1:F:466:ALA:O	1:F:470:LYS:HB2	1.84	0.77
1:B:128:VAL:O	1:B:132:LYS:HG2	1.84	0.77
1:D:466:ALA:O	1:D:470:LYS:HB2	1.84	0.77
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.66	0.77
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.66	0.77
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.66	0.77
1:C:466:ALA:O	1:C:470:LYS:HB2	1.84	0.77
1:D:194:GLN:NE2	1:D:331:THR:HG22	1.99	0.77
1:B:174:VAL:HG13	1:B:376:VAL:HA	1.65	0.77
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.66	0.77
1:A:128:VAL:O	1:A:132:LYS:HG2	1.84	0.76
1:C:411:VAL:HG21	1:C:494:LEU:HG	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:VAL:HG21	1:D:494:LEU:HG	1.68	0.76
1:E:128:VAL:O	1:E:132:LYS:HG2	1.84	0.76
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.66	0.76
1:F:411:VAL:HG21	1:F:494:LEU:HG	1.68	0.76
1:G:466:ALA:O	1:G:470:LYS:HB2	1.84	0.76
1:B:411:VAL:HG21	1:B:494:LEU:HG	1.68	0.76
1:D:174:VAL:HG13	1:D:376:VAL:HA	1.65	0.76
1:E:411:VAL:HG21	1:E:494:LEU:HG	1.68	0.76
1:A:411:VAL:HG21	1:A:494:LEU:HG	1.68	0.76
1:B:438:VAL:O	1:B:442:VAL:HG23	1.86	0.76
1:C:69:MET:CE	1:D:39:VAL:HG12	2.15	0.76
1:C:438:VAL:O	1:C:442:VAL:HG23	1.86	0.76
1:D:73:MET:HG2	1:E:49:ILE:HD11	1.66	0.76
1:G:411:VAL:HG21	1:G:494:LEU:HG	1.68	0.76
1:C:174:VAL:HG13	1:C:376:VAL:HA	1.65	0.76
1:B:466:ALA:O	1:B:470:LYS:HB2	1.84	0.76
1:E:174:VAL:HG13	1:E:376:VAL:HA	1.65	0.76
1:A:438:VAL:O	1:A:442:VAL:HG23	1.86	0.76
1:D:438:VAL:O	1:D:442:VAL:HG23	1.86	0.76
1:B:281:PHE:CE2	1:C:389:MET:CB	2.69	0.75
1:G:438:VAL:O	1:G:442:VAL:HG23	1.86	0.75
1:A:466:ALA:O	1:A:470:LYS:HB2	1.84	0.75
1:B:281:PHE:CZ	1:C:389:MET:CB	2.68	0.75
1:F:295:LEU:HD23	1:F:372:LEU:HD23	1.69	0.75
1:C:220:ILE:HA	1:C:248:LEU:HB3	1.69	0.75
1:E:295:LEU:HD23	1:E:372:LEU:HD23	1.69	0.75
1:B:220:ILE:HA	1:B:248:LEU:HB3	1.69	0.75
1:B:285:ARG:CZ	1:C:386:GLU:OE2	2.34	0.75
1:F:438:VAL:O	1:F:442:VAL:HG23	1.86	0.75
1:E:438:VAL:O	1:E:442:VAL:HG23	1.86	0.74
1:G:295:LEU:HD23	1:G:372:LEU:HD23	1.69	0.74
1:C:295:LEU:HD23	1:C:372:LEU:HD23	1.69	0.74
1:B:295:LEU:HD23	1:B:372:LEU:HD23	1.69	0.74
1:D:112:ASN:ND2	1:E:458:CYS:O	2.19	0.74
1:D:295:LEU:HD23	1:D:372:LEU:HD23	1.69	0.74
1:B:292:ILE:O	1:B:296:THR:HG22	1.88	0.74
1:C:292:ILE:O	1:C:296:THR:HG22	1.88	0.74
1:D:220:ILE:HA	1:D:248:LEU:HB3	1.69	0.74
1:E:292:ILE:O	1:E:296:THR:HG22	1.88	0.74
1:F:220:ILE:HA	1:F:248:LEU:HB3	1.69	0.74
1:F:292:ILE:O	1:F:296:THR:HG22	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:ALA:HA	1:F:343:GLN:HG3	1.68	0.74
1:G:340:ALA:HA	1:G:343:GLN:HG3	1.69	0.74
1:D:292:ILE:O	1:D:296:THR:HG22	1.88	0.74
1:G:292:ILE:O	1:G:296:THR:HG22	1.88	0.74
1:A:292:ILE:O	1:A:296:THR:HG22	1.88	0.74
1:C:340:ALA:HA	1:C:343:GLN:HG3	1.69	0.74
1:A:295:LEU:HD23	1:A:372:LEU:HD23	1.69	0.73
1:B:501:ARG:HH11	1:B:505:GLN:HE22	1.35	0.73
1:D:501:ARG:HH11	1:D:505:GLN:HE22	1.35	0.73
1:E:501:ARG:HH11	1:E:505:GLN:HE22	1.36	0.73
1:C:501:ARG:HH11	1:C:505:GLN:HE22	1.36	0.73
1:G:220:ILE:HA	1:G:248:LEU:HB3	1.69	0.73
1:D:340:ALA:HA	1:D:343:GLN:HG3	1.69	0.73
1:F:501:ARG:HH11	1:F:505:GLN:HE22	1.35	0.73
1:E:340:ALA:HA	1:E:343:GLN:HG3	1.69	0.73
1:B:340:ALA:HA	1:B:343:GLN:HG3	1.69	0.73
1:G:501:ARG:HH11	1:G:505:GLN:HE22	1.35	0.73
1:A:197:ARG:HG2	1:A:197:ARG:HH11	1.54	0.73
1:A:220:ILE:HA	1:A:248:LEU:HB3	1.69	0.73
1:A:501:ARG:HH11	1:A:505:GLN:HE22	1.36	0.73
1:D:197:ARG:HG2	1:D:197:ARG:HH11	1.54	0.73
1:A:340:ALA:HA	1:A:343:GLN:HG3	1.69	0.73
1:E:197:ARG:HH11	1:E:197:ARG:HG2	1.54	0.73
1:A:363:GLU:O	1:A:366:GLN:HG2	1.88	0.73
1:B:363:GLU:O	1:B:366:GLN:HG2	1.88	0.73
1:E:220:ILE:HA	1:E:248:LEU:HB3	1.69	0.73
1:F:281:PHE:CE2	1:G:386:GLU:N	2.57	0.73
1:G:363:GLU:O	1:G:366:GLN:HG2	1.88	0.72
1:C:363:GLU:O	1:C:366:GLN:HG2	1.88	0.72
1:B:197:ARG:HG2	1:B:197:ARG:HH11	1.54	0.72
1:G:197:ARG:HG2	1:G:197:ARG:HH11	1.54	0.72
1:D:363:GLU:O	1:D:366:GLN:HG2	1.88	0.72
1:A:411:VAL:CG2	1:A:494:LEU:HG	2.20	0.72
1:E:363:GLU:O	1:E:366:GLN:HG2	1.88	0.72
1:F:363:GLU:O	1:F:366:GLN:HG2	1.88	0.72
1:C:282:GLY:CA	1:D:181:THR:O	2.38	0.72
1:E:192:GLY:HA3	1:E:376:VAL:HG23	1.72	0.72
1:F:192:GLY:HA3	1:F:376:VAL:HG23	1.72	0.72
1:D:192:GLY:HA3	1:D:376:VAL:HG23	1.72	0.72
1:D:411:VAL:CG2	1:D:494:LEU:HG	2.20	0.72
1:F:197:ARG:HG2	1:F:197:ARG:HH11	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:GLY:HA3	1:G:376:VAL:HG23	1.72	0.72
1:A:192:GLY:HA3	1:A:376:VAL:HG23	1.72	0.71
1:B:281:PHE:CD2	1:C:386:GLU:CA	2.73	0.71
1:C:192:GLY:HA3	1:C:376:VAL:HG23	1.72	0.71
1:E:411:VAL:CG2	1:E:494:LEU:HG	2.20	0.71
1:G:411:VAL:CG2	1:G:494:LEU:HG	2.20	0.71
1:C:197:ARG:HG2	1:C:197:ARG:HH11	1.54	0.71
1:B:192:GLY:HA3	1:B:376:VAL:HG23	1.72	0.71
1:E:198:GLY:HA2	1:E:326:ASN:O	1.91	0.71
1:B:197:ARG:HG2	1:B:197:ARG:NH1	2.06	0.71
1:C:197:ARG:HG2	1:C:197:ARG:NH1	2.06	0.71
1:D:198:GLY:HA2	1:D:326:ASN:O	1.91	0.71
1:F:166:MET:CG	1:F:171:LYS:HA	2.21	0.71
1:G:166:MET:CG	1:G:171:LYS:HA	2.21	0.71
1:B:198:GLY:HA2	1:B:326:ASN:O	1.91	0.71
1:C:198:GLY:HA2	1:C:326:ASN:O	1.91	0.71
1:C:411:VAL:CG2	1:C:494:LEU:HG	2.20	0.71
1:D:69:MET:HE2	1:E:39:VAL:HG12	1.73	0.71
1:D:73:MET:HE3	1:E:49:ILE:HG12	1.72	0.71
1:D:166:MET:CG	1:D:171:LYS:HA	2.21	0.71
1:E:166:MET:CG	1:E:171:LYS:HA	2.21	0.71
1:D:197:ARG:HG2	1:D:197:ARG:NH1	2.06	0.71
1:F:198:GLY:HA2	1:F:326:ASN:O	1.91	0.71
1:A:198:GLY:HA2	1:A:326:ASN:O	1.91	0.70
1:B:411:VAL:CG2	1:B:494:LEU:HG	2.20	0.70
1:G:198:GLY:HA2	1:G:326:ASN:O	1.91	0.70
1:A:166:MET:CG	1:A:171:LYS:HA	2.21	0.70
1:A:197:ARG:HG2	1:A:197:ARG:NH1	2.06	0.70
1:F:411:VAL:CG2	1:F:494:LEU:HG	2.20	0.70
1:C:166:MET:CG	1:C:171:LYS:HA	2.21	0.70
1:E:197:ARG:HG2	1:E:197:ARG:NH1	2.06	0.70
1:B:166:MET:CG	1:B:171:LYS:HA	2.21	0.70
1:F:197:ARG:HG2	1:F:197:ARG:NH1	2.06	0.69
1:G:197:ARG:HG2	1:G:197:ARG:NH1	2.06	0.69
1:D:360:TYR:CE1	1:E:183:LEU:HD22	2.27	0.69
1:C:521:VAL:HB	1:D:40:LEU:HD23	1.75	0.69
1:E:325:ILE:HG22	1:E:326:ASN:N	2.08	0.69
1:F:325:ILE:HG22	1:F:326:ASN:N	2.08	0.69
1:D:325:ILE:HG22	1:D:326:ASN:N	2.08	0.69
1:A:281:PHE:HE2	1:B:385:THR:C	2.00	0.69
1:D:73:MET:HE3	1:E:49:ILE:CG1	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:PHE:CE2	1:F:389:MET:HB2	2.27	0.69
1:C:325:ILE:HG22	1:C:326:ASN:N	2.08	0.69
1:A:216:GLU:HA	1:A:322:ARG:HG2	1.75	0.68
1:C:281:PHE:CE2	1:D:385:THR:CA	2.66	0.68
1:D:216:GLU:HA	1:D:322:ARG:HG2	1.75	0.68
1:E:281:PHE:CE2	1:F:389:MET:CB	2.76	0.68
1:B:216:GLU:HA	1:B:322:ARG:HG2	1.75	0.68
1:D:125:THR:O	1:D:129:GLU:HG3	1.93	0.68
1:G:216:GLU:HA	1:G:322:ARG:HG2	1.75	0.68
1:A:125:THR:O	1:A:129:GLU:HG3	1.93	0.68
1:B:325:ILE:HG22	1:B:326:ASN:N	2.08	0.68
1:C:216:GLU:HA	1:C:322:ARG:HG2	1.75	0.68
1:E:281:PHE:CZ	1:F:389:MET:CB	2.76	0.68
1:F:125:THR:O	1:F:129:GLU:HG3	1.93	0.68
1:E:216:GLU:HA	1:E:322:ARG:HG2	1.75	0.68
1:B:125:THR:O	1:B:129:GLU:HG3	1.93	0.68
1:B:324:VAL:O	1:B:324:VAL:HG12	1.94	0.68
1:E:125:THR:O	1:E:129:GLU:HG3	1.93	0.68
1:F:216:GLU:HA	1:F:322:ARG:HG2	1.75	0.68
1:C:125:THR:O	1:C:129:GLU:HG3	1.93	0.68
1:A:324:VAL:O	1:A:324:VAL:HG12	1.94	0.67
1:A:325:ILE:HG22	1:A:326:ASN:N	2.08	0.67
1:A:351:GLN:O	1:A:354:GLU:HB3	1.95	0.67
1:C:324:VAL:HG12	1:C:324:VAL:O	1.94	0.67
1:G:351:GLN:O	1:G:354:GLU:HB3	1.95	0.67
1:G:125:THR:O	1:G:129:GLU:HG3	1.93	0.67
1:G:324:VAL:O	1:G:324:VAL:HG12	1.94	0.67
1:C:444:LEU:HA	1:C:447:MET:HE3	1.77	0.67
1:G:325:ILE:HG22	1:G:326:ASN:N	2.08	0.67
1:B:351:GLN:O	1:B:354:GLU:HB3	1.95	0.67
1:F:444:LEU:HA	1:F:447:MET:HE3	1.77	0.67
1:G:444:LEU:HA	1:G:447:MET:HE3	1.77	0.67
1:B:281:PHE:CZ	1:C:389:MET:HG3	2.30	0.67
1:F:351:GLN:O	1:F:354:GLU:HB3	1.95	0.67
1:G:501:ARG:HH11	1:G:505:GLN:NE2	1.93	0.67
1:D:247:LEU:HG	1:D:248:LEU:N	2.10	0.67
1:D:444:LEU:HA	1:D:447:MET:HE3	1.77	0.67
1:E:324:VAL:O	1:E:324:VAL:HG12	1.94	0.67
1:E:351:GLN:O	1:E:354:GLU:HB3	1.95	0.67
1:B:501:ARG:HH11	1:B:505:GLN:NE2	1.93	0.67
1:A:247:LEU:HG	1:A:248:LEU:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:VAL:O	1:D:324:VAL:HG12	1.94	0.67
1:E:247:LEU:HG	1:E:248:LEU:N	2.10	0.67
1:E:501:ARG:HH11	1:E:505:GLN:NE2	1.93	0.67
1:C:501:ARG:HH11	1:C:505:GLN:NE2	1.93	0.66
1:F:220:ILE:HD12	1:F:248:LEU:HG	1.77	0.66
1:F:324:VAL:O	1:F:324:VAL:HG12	1.94	0.66
1:G:201:SER:O	1:G:204:PHE:HB2	1.95	0.66
1:B:247:LEU:HG	1:B:248:LEU:N	2.10	0.66
1:B:444:LEU:HA	1:B:447:MET:HE3	1.77	0.66
1:C:201:SER:O	1:C:204:PHE:HB2	1.96	0.66
1:D:351:GLN:O	1:D:354:GLU:HB3	1.95	0.66
1:D:501:ARG:HH11	1:D:505:GLN:NE2	1.93	0.66
1:E:201:SER:O	1:E:204:PHE:HB2	1.96	0.66
1:F:281:PHE:CD2	1:G:386:GLU:CA	2.78	0.66
1:A:69:MET:HE2	1:B:39:VAL:HG12	1.77	0.66
1:C:351:GLN:O	1:C:354:GLU:HB3	1.95	0.66
1:E:285:ARG:CZ	1:F:386:GLU:OE2	2.44	0.66
1:A:220:ILE:HD12	1:A:248:LEU:HG	1.77	0.66
1:B:476:TYR:HE1	1:B:485:TYR:HB3	1.61	0.66
1:G:220:ILE:HD12	1:G:248:LEU:HG	1.77	0.66
1:B:201:SER:O	1:B:204:PHE:HB2	1.95	0.66
1:D:476:TYR:HE1	1:D:485:TYR:HB3	1.61	0.66
1:A:501:ARG:HH11	1:A:505:GLN:NE2	1.93	0.66
1:F:501:ARG:HH11	1:F:505:GLN:NE2	1.93	0.66
1:E:220:ILE:HD12	1:E:248:LEU:HG	1.77	0.66
1:A:201:SER:O	1:A:204:PHE:HB2	1.96	0.66
1:B:7:LYS:HZ1	1:B:15:LYS:HE3	1.61	0.66
1:B:220:ILE:HD12	1:B:248:LEU:HG	1.77	0.66
1:C:220:ILE:HD12	1:C:248:LEU:HG	1.77	0.66
1:B:432:GLN:HB2	1:B:436:GLN:NE2	2.11	0.66
1:C:432:GLN:HB2	1:C:436:GLN:NE2	2.11	0.66
1:E:444:LEU:HA	1:E:447:MET:HE3	1.77	0.66
1:F:476:TYR:HE1	1:F:485:TYR:HB3	1.61	0.66
1:G:247:LEU:HG	1:G:248:LEU:N	2.10	0.66
1:A:432:GLN:HB2	1:A:436:GLN:NE2	2.11	0.65
1:A:444:LEU:HA	1:A:447:MET:HE3	1.77	0.65
1:D:201:SER:O	1:D:204:PHE:HB2	1.96	0.65
1:D:429:LEU:C	1:D:430:ARG:HD2	2.21	0.65
1:D:517:THR:HG21	1:E:39:VAL:HG23	1.77	0.65
1:G:429:LEU:C	1:G:430:ARG:HD2	2.21	0.65
1:C:429:LEU:C	1:C:430:ARG:HD2	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:C	1:A:430:ARG:HD2	2.21	0.65
1:B:429:LEU:C	1:B:430:ARG:HD2	2.21	0.65
1:A:476:TYR:HE1	1:A:485:TYR:HB3	1.61	0.65
1:B:123:ALA:HB2	1:B:440:ILE:HG23	1.78	0.65
1:F:247:LEU:HG	1:F:248:LEU:N	2.10	0.65
1:G:432:GLN:HB2	1:G:436:GLN:NE2	2.11	0.65
1:F:281:PHE:CD2	1:G:386:GLU:HA	2.31	0.65
1:G:476:TYR:HE1	1:G:485:TYR:HB3	1.61	0.65
1:A:281:PHE:CE2	1:B:386:GLU:HA	2.31	0.65
1:C:247:LEU:HG	1:C:248:LEU:N	2.10	0.65
1:D:220:ILE:HD12	1:D:248:LEU:HG	1.77	0.65
1:E:429:LEU:C	1:E:430:ARG:HD2	2.21	0.65
1:F:201:SER:O	1:F:204:PHE:HB2	1.96	0.65
1:A:123:ALA:HB2	1:A:440:ILE:HG23	1.78	0.65
1:E:281:PHE:CZ	1:F:389:MET:HG3	2.32	0.65
1:F:123:ALA:HB2	1:F:440:ILE:HG23	1.78	0.65
1:F:432:GLN:HB2	1:F:436:GLN:NE2	2.11	0.65
1:D:432:GLN:HB2	1:D:436:GLN:NE2	2.11	0.65
1:E:432:GLN:HB2	1:E:436:GLN:NE2	2.11	0.65
1:A:22:VAL:HG11	1:A:62:LEU:HD21	1.78	0.65
1:F:429:LEU:C	1:F:430:ARG:HD2	2.21	0.65
1:C:123:ALA:HB2	1:C:440:ILE:HG23	1.78	0.65
1:F:22:VAL:HG11	1:F:62:LEU:HD21	1.78	0.65
1:E:476:TYR:HE1	1:E:485:TYR:HB3	1.61	0.64
1:E:7:LYS:HZ1	1:E:15:LYS:HE3	1.62	0.64
1:E:123:ALA:HB2	1:E:440:ILE:HG23	1.78	0.64
1:G:22:VAL:HG11	1:G:62:LEU:HD21	1.78	0.64
1:B:22:VAL:HG11	1:B:62:LEU:HD21	1.78	0.64
1:C:22:VAL:HG11	1:C:62:LEU:HD21	1.78	0.64
1:C:476:TYR:HE1	1:C:485:TYR:HB3	1.61	0.64
1:D:123:ALA:HB2	1:D:440:ILE:HG23	1.78	0.64
1:G:123:ALA:HB2	1:G:440:ILE:HG23	1.78	0.64
1:A:386:GLU:HA	1:G:281:PHE:CD2	2.33	0.64
1:A:517:THR:HG21	1:B:39:VAL:HG23	1.79	0.64
1:D:281:PHE:CE2	1:E:386:GLU:HA	2.33	0.64
1:E:22:VAL:HG11	1:E:62:LEU:HD21	1.78	0.64
1:D:22:VAL:HG11	1:D:62:LEU:HD21	1.78	0.64
1:E:281:PHE:CD2	1:F:386:GLU:CA	2.80	0.64
1:A:77:VAL:HG11	1:A:510:VAL:HG22	1.81	0.63
1:G:7:LYS:HZ1	1:G:15:LYS:HE3	1.62	0.63
1:B:281:PHE:CE1	1:C:389:MET:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:HG11	1:B:510:VAL:HG22	1.81	0.63
1:E:77:VAL:HG11	1:E:510:VAL:HG22	1.81	0.63
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.80	0.63
1:F:171:LYS:HB3	1:F:407:VAL:HG11	1.80	0.63
1:D:171:LYS:HB3	1:D:407:VAL:HG11	1.80	0.62
1:G:171:LYS:HB3	1:G:407:VAL:HG11	1.80	0.62
1:D:7:LYS:HZ1	1:D:15:LYS:HE3	1.64	0.62
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.80	0.62
1:D:346:VAL:HG11	1:D:373:ALA:HB2	1.81	0.62
1:E:247:LEU:HD21	1:E:249:ILE:HG13	1.81	0.62
1:F:281:PHE:HE2	1:G:386:GLU:N	1.95	0.62
1:B:476:TYR:CE1	1:B:485:TYR:HB3	2.35	0.62
1:D:476:TYR:CE1	1:D:485:TYR:HB3	2.35	0.62
1:E:144:ILE:HG23	1:E:403:THR:HG21	1.80	0.62
1:E:476:TYR:CE1	1:E:485:TYR:HB3	2.35	0.62
1:A:171:LYS:HB3	1:A:407:VAL:HG11	1.80	0.62
1:A:346:VAL:HG11	1:A:373:ALA:HB2	1.81	0.62
1:B:346:VAL:HG11	1:B:373:ALA:HB2	1.81	0.62
1:C:144:ILE:HG23	1:C:403:THR:HG21	1.80	0.62
1:C:476:TYR:CE1	1:C:485:TYR:HB3	2.35	0.62
1:D:77:VAL:HG11	1:D:510:VAL:HG22	1.81	0.62
1:F:247:LEU:HD21	1:F:249:ILE:HG13	1.81	0.62
1:G:77:VAL:HG11	1:G:510:VAL:HG22	1.81	0.62
1:G:476:TYR:CE1	1:G:485:TYR:HB3	2.35	0.62
1:A:386:GLU:HA	1:G:281:PHE:CE2	2.34	0.62
1:A:476:TYR:CE1	1:A:485:TYR:HB3	2.35	0.62
1:C:144:ILE:HD13	1:C:166:MET:SD	2.40	0.62
1:F:144:ILE:HG23	1:F:403:THR:HG21	1.80	0.62
1:F:476:TYR:CE1	1:F:485:TYR:HB3	2.35	0.62
1:B:144:ILE:HD13	1:B:166:MET:SD	2.40	0.62
1:D:144:ILE:HD13	1:D:166:MET:SD	2.39	0.62
1:F:77:VAL:HG11	1:F:510:VAL:HG22	1.81	0.62
1:G:346:VAL:HG11	1:G:373:ALA:HB2	1.81	0.62
1:A:144:ILE:HG23	1:A:403:THR:HG21	1.80	0.62
1:B:281:PHE:CG	1:C:389:MET:HE3	2.34	0.62
1:C:171:LYS:HB3	1:C:407:VAL:HG11	1.80	0.62
1:C:346:VAL:HG11	1:C:373:ALA:HB2	1.81	0.62
1:D:247:LEU:HD21	1:D:249:ILE:HG13	1.81	0.62
1:E:346:VAL:HG11	1:E:373:ALA:HB2	1.81	0.62
1:A:391:GLU:O	1:A:395:ARG:HG3	2.00	0.62
1:D:391:GLU:O	1:D:395:ARG:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:VAL:HG11	1:F:373:ALA:HB2	1.81	0.62
1:A:7:LYS:HZ1	1:A:15:LYS:HE3	1.65	0.62
1:A:40:LEU:HD23	1:G:521:VAL:HB	1.82	0.62
1:B:247:LEU:HD21	1:B:249:ILE:HG13	1.81	0.62
1:B:436:GLN:O	1:B:440:ILE:HG13	2.00	0.62
1:D:436:GLN:O	1:D:440:ILE:HG13	2.00	0.62
1:E:171:LYS:HB3	1:E:407:VAL:HG11	1.80	0.62
1:E:391:GLU:O	1:E:395:ARG:HG3	2.00	0.62
1:G:144:ILE:HD13	1:G:166:MET:SD	2.40	0.62
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.80	0.62
1:G:281:PHE:HA	1:G:285:ARG:CG	2.29	0.62
1:A:144:ILE:HD13	1:A:166:MET:SD	2.40	0.61
1:C:247:LEU:HD21	1:C:249:ILE:HG13	1.81	0.61
1:G:436:GLN:O	1:G:440:ILE:HG13	2.00	0.61
1:B:281:PHE:HA	1:B:285:ARG:CG	2.29	0.61
1:C:77:VAL:HG11	1:C:510:VAL:HG22	1.81	0.61
1:C:281:PHE:HA	1:C:285:ARG:CG	2.29	0.61
1:E:184:GLN:O	1:E:185:ASP:HB2	2.00	0.61
1:E:436:GLN:O	1:E:440:ILE:HG13	2.00	0.61
1:G:391:GLU:O	1:G:395:ARG:HG3	2.00	0.61
1:A:247:LEU:HD21	1:A:249:ILE:HG13	1.81	0.61
1:B:171:LYS:HB3	1:B:407:VAL:HG11	1.80	0.61
1:C:436:GLN:O	1:C:440:ILE:HG13	2.00	0.61
1:G:247:LEU:HD21	1:G:249:ILE:HG13	1.81	0.61
1:B:391:GLU:O	1:B:395:ARG:HG3	2.00	0.61
1:F:144:ILE:HD13	1:F:166:MET:SD	2.40	0.61
1:C:391:GLU:O	1:C:395:ARG:HG3	2.00	0.61
1:E:144:ILE:HD13	1:E:166:MET:SD	2.40	0.61
1:A:436:GLN:O	1:A:440:ILE:HG13	2.00	0.61
1:C:501:ARG:NH1	1:C:505:GLN:HE22	1.99	0.61
1:E:501:ARG:NH1	1:E:505:GLN:HE22	1.99	0.61
1:F:436:GLN:O	1:F:440:ILE:HG13	2.00	0.61
1:A:501:ARG:NH1	1:A:505:GLN:HE22	1.99	0.61
1:E:281:PHE:HA	1:E:285:ARG:CG	2.29	0.61
1:A:362:ARG:HD2	1:A:366:GLN:HB3	1.83	0.61
1:B:281:PHE:CE2	1:C:386:GLU:CA	2.81	0.61
1:B:362:ARG:HD2	1:B:366:GLN:HB3	1.83	0.61
1:D:114:MET:HG3	1:E:34:LYS:HG3	1.83	0.61
1:D:184:GLN:O	1:D:185:ASP:HB2	2.00	0.61
1:D:281:PHE:HA	1:D:285:ARG:CG	2.29	0.61
1:A:281:PHE:HA	1:A:285:ARG:CG	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ARG:HD2	1:C:366:GLN:HB3	1.83	0.61
1:F:362:ARG:HD2	1:F:366:GLN:HB3	1.83	0.61
1:G:362:ARG:HD2	1:G:366:GLN:HB3	1.83	0.61
1:G:501:ARG:NH1	1:G:505:GLN:HE22	1.99	0.61
1:E:100:ILE:HD13	1:E:514:MET:SD	2.41	0.60
1:F:281:PHE:HA	1:F:285:ARG:CG	2.29	0.60
1:F:391:GLU:O	1:F:395:ARG:HG3	2.00	0.60
1:F:501:ARG:NH1	1:F:505:GLN:HE22	1.99	0.60
1:A:100:ILE:HD13	1:A:514:MET:SD	2.41	0.60
1:A:184:GLN:O	1:A:185:ASP:HB2	2.00	0.60
1:A:517:THR:CG2	1:B:39:VAL:HG23	2.30	0.60
1:C:100:ILE:HD13	1:C:514:MET:SD	2.41	0.60
1:D:298:GLY:C	1:D:300:VAL:H	2.10	0.60
1:E:288:MET:HG3	1:E:368:ARG:CD	2.29	0.60
1:G:100:ILE:HD13	1:G:514:MET:SD	2.41	0.60
1:C:281:PHE:HZ	1:D:384:ALA:C	2.09	0.60
1:D:362:ARG:HD2	1:D:366:GLN:HB3	1.83	0.60
1:E:362:ARG:HD2	1:E:366:GLN:HB3	1.83	0.60
1:F:200:LEU:HD13	1:F:276:VAL:HA	1.82	0.60
1:A:281:PHE:HE2	1:B:386:GLU:N	2.00	0.60
1:B:100:ILE:HD13	1:B:514:MET:SD	2.41	0.60
1:B:184:GLN:O	1:B:185:ASP:HB2	2.00	0.60
1:B:200:LEU:HD13	1:B:276:VAL:HA	1.82	0.60
1:C:487:ASN:O	1:C:491:MET:HG3	2.01	0.60
1:E:281:PHE:CE2	1:F:386:GLU:CA	2.83	0.60
1:E:298:GLY:C	1:E:300:VAL:H	2.10	0.60
1:F:100:ILE:HD13	1:F:514:MET:SD	2.41	0.60
1:G:200:LEU:HD13	1:G:276:VAL:HA	1.82	0.60
1:B:487:ASN:O	1:B:491:MET:HG3	2.01	0.60
1:C:184:GLN:O	1:C:185:ASP:HB2	2.00	0.60
1:C:222:LEU:H	1:C:300:VAL:HG11	1.67	0.60
1:D:487:ASN:O	1:D:491:MET:HG3	2.01	0.60
1:A:200:LEU:HD13	1:A:276:VAL:HA	1.82	0.60
1:B:222:LEU:H	1:B:300:VAL:HG11	1.67	0.60
1:C:200:LEU:HD13	1:C:276:VAL:HA	1.82	0.60
1:D:501:ARG:NH1	1:D:505:GLN:HE22	1.99	0.60
1:F:298:GLY:C	1:F:300:VAL:H	2.10	0.60
1:B:298:GLY:C	1:B:300:VAL:H	2.10	0.60
1:E:487:ASN:O	1:E:491:MET:HG3	2.01	0.60
1:C:214:GLU:CG	1:C:324:VAL:HG13	2.26	0.60
1:D:222:LEU:H	1:D:300:VAL:HG11	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:HD13	1:E:276:VAL:HA	1.82	0.60
1:G:184:GLN:O	1:G:185:ASP:HB2	2.00	0.60
1:A:298:GLY:C	1:A:300:VAL:H	2.10	0.60
1:D:100:ILE:HD13	1:D:514:MET:SD	2.41	0.60
1:D:101:THR:O	1:D:105:LYS:HG3	2.02	0.60
1:F:184:GLN:O	1:F:185:ASP:HB2	2.00	0.60
1:B:501:ARG:NH1	1:B:505:GLN:HE22	1.99	0.60
1:A:487:ASN:O	1:A:491:MET:HG3	2.01	0.59
1:D:200:LEU:HD13	1:D:276:VAL:HA	1.82	0.59
1:E:101:THR:O	1:E:105:LYS:HG3	2.02	0.59
1:F:487:ASN:O	1:F:491:MET:HG3	2.01	0.59
1:B:160:LYS:O	1:B:164:GLU:HG3	2.02	0.59
1:B:214:GLU:CG	1:B:324:VAL:HG13	2.26	0.59
1:C:101:THR:O	1:C:105:LYS:HG3	2.02	0.59
1:C:298:GLY:C	1:C:300:VAL:H	2.10	0.59
1:D:214:GLU:CG	1:D:324:VAL:HG13	2.26	0.59
1:B:300:VAL:CG2	1:B:317:LEU:HA	2.32	0.59
1:F:160:LYS:O	1:F:164:GLU:HG3	2.02	0.59
1:A:214:GLU:CG	1:A:324:VAL:HG13	2.26	0.59
1:A:222:LEU:H	1:A:300:VAL:HG11	1.67	0.59
1:D:288:MET:HG3	1:D:368:ARG:CD	2.29	0.59
1:D:360:TYR:CD1	1:D:360:TYR:C	2.80	0.59
1:D:360:TYR:OH	1:E:183:LEU:HD13	2.03	0.59
1:G:298:GLY:C	1:G:300:VAL:H	2.10	0.59
1:G:487:ASN:O	1:G:491:MET:HG3	2.01	0.59
1:C:300:VAL:CG2	1:C:317:LEU:HA	2.33	0.59
1:G:160:LYS:O	1:G:164:GLU:HG3	2.03	0.59
1:F:360:TYR:CD1	1:F:360:TYR:C	2.80	0.59
1:B:101:THR:O	1:B:105:LYS:HG3	2.02	0.59
1:A:300:VAL:CG2	1:A:317:LEU:HA	2.33	0.59
1:A:340:ALA:CA	1:A:343:GLN:HG3	2.33	0.59
1:B:14:VAL:O	1:B:18:ARG:HD3	2.03	0.59
1:D:340:ALA:CA	1:D:343:GLN:HG3	2.33	0.59
1:E:160:LYS:O	1:E:164:GLU:HG3	2.02	0.59
1:G:360:TYR:CD1	1:G:360:TYR:C	2.80	0.59
1:A:160:LYS:O	1:A:164:GLU:HG3	2.02	0.59
1:D:300:VAL:CG2	1:D:317:LEU:HA	2.33	0.59
1:E:360:TYR:C	1:E:360:TYR:CD1	2.80	0.59
1:F:300:VAL:CG2	1:F:317:LEU:HD23	2.31	0.59
1:C:360:TYR:C	1:C:360:TYR:CD1	2.80	0.59
1:D:160:LYS:O	1:D:164:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:LEU:H	1:E:300:VAL:HG11	1.67	0.59
1:G:340:ALA:CA	1:G:343:GLN:HG3	2.33	0.59
1:A:360:TYR:CD1	1:A:360:TYR:C	2.80	0.58
1:B:281:PHE:CD2	1:C:389:MET:HE3	2.38	0.58
1:F:101:THR:O	1:F:105:LYS:HG3	2.02	0.58
1:G:14:VAL:O	1:G:18:ARG:HD3	2.03	0.58
1:B:360:TYR:CE1	1:C:183:LEU:CD2	2.85	0.58
1:C:160:LYS:O	1:C:164:GLU:HG3	2.03	0.58
1:C:340:ALA:CA	1:C:343:GLN:HG3	2.33	0.58
1:D:14:VAL:O	1:D:18:ARG:HD3	2.03	0.58
1:E:281:PHE:CD2	1:F:389:MET:HE3	2.38	0.58
1:E:300:VAL:CG2	1:E:317:LEU:HA	2.33	0.58
1:G:222:LEU:H	1:G:300:VAL:HG11	1.67	0.58
1:G:300:VAL:CG2	1:G:317:LEU:HA	2.33	0.58
1:C:82:ASN:ND2	1:C:89:THR:N	2.52	0.58
1:F:222:LEU:H	1:F:300:VAL:HG11	1.67	0.58
1:G:281:PHE:CA	1:G:285:ARG:HG2	2.32	0.58
1:A:342:ILE:HG23	1:A:372:LEU:HD22	1.85	0.58
1:B:342:ILE:HG23	1:B:372:LEU:HD22	1.85	0.58
1:G:342:ILE:HG23	1:G:372:LEU:HD22	1.85	0.58
1:B:360:TYR:CD1	1:B:360:TYR:C	2.80	0.58
1:E:14:VAL:O	1:E:18:ARG:HD3	2.03	0.58
1:E:214:GLU:CG	1:E:324:VAL:HG13	2.26	0.58
1:F:342:ILE:HG23	1:F:372:LEU:HD22	1.85	0.58
1:E:340:ALA:CA	1:E:343:GLN:HG3	2.33	0.58
1:G:101:THR:O	1:G:105:LYS:HG3	2.02	0.58
1:C:281:PHE:CA	1:C:285:ARG:HG2	2.32	0.58
1:D:16:MET:HA	1:D:70:GLY:HA3	1.86	0.58
1:F:14:VAL:O	1:F:18:ARG:HD3	2.03	0.58
1:A:101:THR:O	1:A:105:LYS:HG3	2.02	0.58
1:A:282:GLY:HA2	1:B:181:THR:O	1.95	0.58
1:C:342:ILE:HG23	1:C:372:LEU:HD22	1.85	0.58
1:F:300:VAL:CG2	1:F:317:LEU:HA	2.32	0.58
1:G:214:GLU:CG	1:G:324:VAL:HG13	2.26	0.58
1:B:340:ALA:CA	1:B:343:GLN:HG3	2.33	0.58
1:D:82:ASN:ND2	1:D:89:THR:N	2.52	0.58
1:E:16:MET:HA	1:E:70:GLY:HA3	1.86	0.58
1:F:157:THR:O	1:F:160:LYS:HB2	2.04	0.58
1:A:213:VAL:HG22	1:A:325:ILE:HB	1.85	0.58
1:C:16:MET:HA	1:C:70:GLY:HA3	1.86	0.58
1:C:219:PHE:HD2	1:C:317:LEU:HD12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:ILE:HG23	1:E:372:LEU:HD22	1.85	0.58
1:F:340:ALA:CA	1:F:343:GLN:HG3	2.33	0.58
1:A:219:PHE:HD2	1:A:317:LEU:HD12	1.69	0.57
1:C:288:MET:HG3	1:C:368:ARG:CD	2.29	0.57
1:E:82:ASN:ND2	1:E:89:THR:N	2.51	0.57
1:F:281:PHE:CA	1:F:285:ARG:HG2	2.32	0.57
1:G:219:PHE:HD2	1:G:317:LEU:HD12	1.69	0.57
1:A:14:VAL:O	1:A:18:ARG:HD3	2.03	0.57
1:F:82:ASN:ND2	1:F:89:THR:N	2.51	0.57
1:G:213:VAL:HG22	1:G:325:ILE:HB	1.85	0.57
1:A:157:THR:O	1:A:160:LYS:HB2	2.04	0.57
1:C:14:VAL:O	1:C:18:ARG:HD3	2.03	0.57
1:D:157:THR:O	1:D:160:LYS:HB2	2.04	0.57
1:E:219:PHE:HD2	1:E:317:LEU:HD12	1.69	0.57
1:E:281:PHE:CA	1:E:285:ARG:HG2	2.32	0.57
1:B:213:VAL:HG22	1:B:325:ILE:HB	1.85	0.57
1:B:16:MET:HA	1:B:70:GLY:HA3	1.86	0.57
1:C:213:VAL:HG22	1:C:325:ILE:HB	1.85	0.57
1:D:213:VAL:HG22	1:D:325:ILE:HB	1.85	0.57
1:F:213:VAL:HG22	1:F:325:ILE:HB	1.85	0.57
1:A:281:PHE:CA	1:A:285:ARG:HG2	2.32	0.57
1:B:157:THR:O	1:B:160:LYS:HB2	2.04	0.57
1:C:288:MET:O	1:C:292:ILE:HG13	2.05	0.57
1:D:342:ILE:HG23	1:D:372:LEU:HD22	1.85	0.57
1:A:288:MET:O	1:A:292:ILE:HG13	2.05	0.57
1:E:213:VAL:HG22	1:E:325:ILE:HB	1.85	0.57
1:F:16:MET:HA	1:F:70:GLY:HA3	1.86	0.57
1:D:206:ASN:HB3	1:D:213:VAL:CA	2.32	0.57
1:F:219:PHE:HD2	1:F:317:LEU:HD12	1.69	0.57
1:C:157:THR:O	1:C:160:LYS:HB2	2.04	0.57
1:C:206:ASN:HB3	1:C:213:VAL:CA	2.32	0.57
1:E:281:PHE:CG	1:F:389:MET:HE3	2.40	0.57
1:F:281:PHE:HE2	1:G:385:THR:O	1.88	0.57
1:B:219:PHE:HD2	1:B:317:LEU:HD12	1.69	0.57
1:F:433:ASN:ND2	1:F:436:GLN:HG3	2.20	0.57
1:A:386:GLU:CA	1:G:281:PHE:CD2	2.87	0.56
1:B:281:PHE:HD2	1:C:386:GLU:CA	2.18	0.56
1:E:288:MET:O	1:E:292:ILE:HG13	2.05	0.56
1:F:288:MET:O	1:F:292:ILE:HG13	2.05	0.56
1:G:288:MET:O	1:G:292:ILE:HG13	2.05	0.56
1:B:433:ASN:ND2	1:B:436:GLN:HG3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:ASN:ND2	1:C:436:GLN:HG3	2.20	0.56
1:D:433:ASN:ND2	1:D:436:GLN:HG3	2.20	0.56
1:E:73:MET:HG2	1:F:49:ILE:HD11	1.87	0.56
1:E:157:THR:O	1:E:160:LYS:HB2	2.04	0.56
1:G:157:THR:O	1:G:160:LYS:HB2	2.04	0.56
1:G:433:ASN:ND2	1:G:436:GLN:HG3	2.20	0.56
1:A:281:PHE:CE2	1:B:386:GLU:CA	2.89	0.56
1:A:433:ASN:ND2	1:A:436:GLN:HG3	2.20	0.56
1:B:206:ASN:HB3	1:B:213:VAL:CA	2.32	0.56
1:B:288:MET:HG3	1:B:368:ARG:CD	2.29	0.56
1:E:433:ASN:ND2	1:E:436:GLN:HG3	2.20	0.56
1:D:219:PHE:HD2	1:D:317:LEU:HD12	1.69	0.56
1:D:327:LYS:HG3	1:D:327:LYS:O	2.06	0.56
1:F:281:PHE:CE2	1:G:386:GLU:HA	2.41	0.56
1:G:82:ASN:ND2	1:G:89:THR:N	2.52	0.56
1:A:327:LYS:HG3	1:A:327:LYS:O	2.06	0.56
1:F:252:GLU:O	1:F:254:VAL:N	2.39	0.56
1:G:206:ASN:HB3	1:G:213:VAL:CA	2.32	0.56
1:G:252:GLU:O	1:G:254:VAL:N	2.39	0.56
1:A:16:MET:HA	1:A:70:GLY:HA3	1.86	0.56
1:A:206:ASN:HB3	1:A:213:VAL:CA	2.32	0.56
1:A:502:SER:O	1:A:506:TYR:HD2	1.88	0.56
1:B:69:MET:HE2	1:C:39:VAL:HG12	1.87	0.56
1:B:288:MET:O	1:B:292:ILE:HG13	2.05	0.56
1:B:300:VAL:HG23	1:B:317:LEU:H	1.71	0.56
1:D:502:SER:O	1:D:506:TYR:HD2	1.88	0.56
1:E:206:ASN:HB3	1:E:213:VAL:CA	2.32	0.56
1:E:300:VAL:HG23	1:E:317:LEU:H	1.71	0.56
1:F:320:ALA:HA	1:F:334:ASP:O	2.06	0.56
1:G:16:MET:HA	1:G:70:GLY:HA3	1.86	0.56
1:G:300:VAL:HG23	1:G:317:LEU:H	1.71	0.56
1:C:502:SER:O	1:C:506:TYR:HD2	1.88	0.56
1:E:281:PHE:CE1	1:F:389:MET:HG3	2.41	0.56
1:F:214:GLU:CG	1:F:324:VAL:HG13	2.26	0.56
1:G:193:MET:SD	1:G:292:ILE:HG12	2.46	0.56
1:G:421:ARG:NH2	1:G:470:LYS:O	2.39	0.56
1:A:193:MET:SD	1:A:292:ILE:HG12	2.46	0.56
1:A:252:GLU:O	1:A:254:VAL:N	2.39	0.56
1:B:327:LYS:HG3	1:B:327:LYS:O	2.06	0.56
1:C:320:ALA:HA	1:C:334:ASP:O	2.06	0.56
1:D:193:MET:SD	1:D:292:ILE:HG12	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ALA:HB3	1:D:251:ALA:HB2	1.88	0.56
1:E:252:GLU:O	1:E:254:VAL:N	2.39	0.56
1:E:327:LYS:HG3	1:E:327:LYS:O	2.06	0.56
1:F:206:ASN:HB3	1:F:213:VAL:CA	2.32	0.56
1:F:502:SER:O	1:F:506:TYR:HD2	1.88	0.56
1:C:421:ARG:NH2	1:C:470:LYS:O	2.39	0.56
1:D:288:MET:O	1:D:292:ILE:HG13	2.05	0.56
1:D:300:VAL:HG23	1:D:317:LEU:H	1.71	0.56
1:D:421:ARG:NH2	1:D:470:LYS:O	2.39	0.56
1:G:320:ALA:HA	1:G:334:ASP:O	2.06	0.56
1:D:281:PHE:CA	1:D:285:ARG:HG2	2.32	0.56
1:D:338:GLU:O	1:D:341:ALA:N	2.39	0.56
1:E:320:ALA:HA	1:E:334:ASP:O	2.06	0.56
1:E:421:ARG:NH2	1:E:470:LYS:O	2.39	0.56
1:G:502:SER:O	1:G:506:TYR:HD2	1.88	0.56
1:A:421:ARG:NH2	1:A:470:LYS:O	2.39	0.55
1:B:193:MET:SD	1:B:292:ILE:HG12	2.46	0.55
1:E:186:GLU:HB2	1:E:380:LYS:HB2	1.89	0.55
1:E:193:MET:SD	1:E:292:ILE:HG12	2.46	0.55
1:F:193:MET:SD	1:F:292:ILE:HG12	2.46	0.55
1:G:338:GLU:O	1:G:341:ALA:N	2.39	0.55
1:A:223:ALA:HB3	1:A:251:ALA:HB2	1.88	0.55
1:A:320:ALA:HA	1:A:334:ASP:O	2.06	0.55
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.89	0.55
1:C:193:MET:SD	1:C:292:ILE:HG12	2.46	0.55
1:D:186:GLU:HB2	1:D:380:LYS:HB2	1.89	0.55
1:E:223:ALA:HB3	1:E:251:ALA:HB2	1.88	0.55
1:B:252:GLU:O	1:B:254:VAL:N	2.39	0.55
1:B:320:ALA:HA	1:B:334:ASP:O	2.06	0.55
1:B:502:SER:O	1:B:506:TYR:HD2	1.88	0.55
1:C:338:GLU:O	1:C:341:ALA:N	2.39	0.55
1:D:114:MET:HE2	1:E:34:LYS:C	2.31	0.55
1:D:252:GLU:O	1:D:254:VAL:N	2.39	0.55
1:E:502:SER:O	1:E:506:TYR:HD2	1.88	0.55
1:B:186:GLU:HB2	1:B:380:LYS:HB2	1.89	0.55
1:C:252:GLU:O	1:C:254:VAL:N	2.39	0.55
1:D:320:ALA:HA	1:D:334:ASP:O	2.06	0.55
1:G:223:ALA:HB3	1:G:251:ALA:HB2	1.88	0.55
1:G:327:LYS:HG3	1:G:327:LYS:O	2.06	0.55
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.89	0.55
1:B:223:ALA:HB3	1:B:251:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:GLU:O	1:E:341:ALA:N	2.39	0.55
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.89	0.55
1:F:281:PHE:CE2	1:G:386:GLU:CA	2.89	0.55
1:F:281:PHE:CD2	1:G:386:GLU:N	2.74	0.55
1:F:338:GLU:O	1:F:341:ALA:N	2.39	0.55
1:A:338:GLU:O	1:A:341:ALA:N	2.39	0.55
1:E:362:ARG:HD2	1:E:362:ARG:O	2.07	0.55
1:A:362:ARG:HD2	1:A:362:ARG:O	2.07	0.55
1:A:465:VAL:O	1:A:469:VAL:HG23	2.07	0.55
1:D:213:VAL:O	1:D:213:VAL:HG23	2.06	0.55
1:E:213:VAL:HG23	1:E:213:VAL:O	2.06	0.55
1:E:465:VAL:O	1:E:469:VAL:HG23	2.07	0.55
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.89	0.55
1:G:362:ARG:HD2	1:G:362:ARG:O	2.07	0.55
1:A:288:MET:HG3	1:A:368:ARG:CD	2.29	0.55
1:G:82:ASN:HD22	1:G:82:ASN:H	1.54	0.55
1:B:362:ARG:HD2	1:B:362:ARG:O	2.06	0.55
1:C:300:VAL:HG23	1:C:317:LEU:H	1.71	0.55
1:C:327:LYS:O	1:C:327:LYS:HG3	2.06	0.55
1:C:362:ARG:HD2	1:C:362:ARG:O	2.07	0.55
1:D:362:ARG:HD2	1:D:362:ARG:O	2.06	0.55
1:E:12:ALA:HB1	1:E:520:MET:HG3	1.89	0.55
1:F:300:VAL:HG23	1:F:317:LEU:H	1.71	0.55
1:F:362:ARG:HD2	1:F:362:ARG:O	2.06	0.55
1:F:421:ARG:NH2	1:F:470:LYS:O	2.39	0.55
1:A:12:ALA:HB1	1:A:520:MET:HG3	1.89	0.55
1:A:66:PHE:HD1	1:A:520:MET:HE3	1.72	0.55
1:A:82:ASN:ND2	1:A:89:THR:N	2.51	0.55
1:A:82:ASN:HD22	1:A:82:ASN:H	1.55	0.55
1:A:191:GLU:O	1:A:334:ASP:HA	2.07	0.55
1:A:300:VAL:HG23	1:A:317:LEU:H	1.71	0.55
1:B:465:VAL:O	1:B:469:VAL:HG23	2.07	0.55
1:C:82:ASN:H	1:C:82:ASN:HD22	1.54	0.55
1:C:223:ALA:HB3	1:C:251:ALA:HB2	1.88	0.55
1:D:7:LYS:NZ	1:D:15:LYS:HE3	2.22	0.55
1:B:191:GLU:O	1:B:334:ASP:HA	2.07	0.54
1:B:421:ARG:NH2	1:B:470:LYS:O	2.39	0.54
1:F:82:ASN:H	1:F:82:ASN:HD22	1.55	0.54
1:F:223:ALA:HB3	1:F:251:ALA:HB2	1.88	0.54
1:F:327:LYS:O	1:F:327:LYS:HG3	2.06	0.54
1:A:281:PHE:CE2	1:B:386:GLU:N	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:PHE:HD1	1:C:520:MET:HE3	1.72	0.54
1:C:191:GLU:O	1:C:334:ASP:HA	2.07	0.54
1:D:465:VAL:O	1:D:469:VAL:HG23	2.07	0.54
1:E:7:LYS:NZ	1:E:15:LYS:HE3	2.22	0.54
1:F:66:PHE:HD1	1:F:520:MET:HE3	1.72	0.54
1:B:82:ASN:HD22	1:B:82:ASN:H	1.55	0.54
1:B:281:PHE:CA	1:B:285:ARG:HG2	2.32	0.54
1:C:213:VAL:HG23	1:C:213:VAL:O	2.06	0.54
1:E:140:ASP:OD1	1:E:143:ALA:HB2	2.07	0.54
1:A:517:THR:HA	1:B:37:ASN:HB2	1.89	0.54
1:C:7:LYS:NZ	1:C:15:LYS:HE3	2.22	0.54
1:F:140:ASP:OD1	1:F:143:ALA:HB2	2.07	0.54
1:F:213:VAL:HG23	1:F:213:VAL:O	2.06	0.54
1:F:300:VAL:HG21	1:F:317:LEU:HA	1.90	0.54
1:F:465:VAL:O	1:F:469:VAL:HG23	2.07	0.54
1:B:12:ALA:HB1	1:B:520:MET:HG3	1.89	0.54
1:C:300:VAL:HG21	1:C:317:LEU:HA	1.90	0.54
1:D:12:ALA:HB1	1:D:520:MET:HG3	1.89	0.54
1:D:66:PHE:HD1	1:D:520:MET:HE3	1.73	0.54
1:G:191:GLU:O	1:G:334:ASP:HA	2.07	0.54
1:G:300:VAL:HG21	1:G:317:LEU:HA	1.90	0.54
1:B:7:LYS:NZ	1:B:15:LYS:HE3	2.22	0.54
1:B:140:ASP:OD1	1:B:143:ALA:HB2	2.07	0.54
1:B:281:PHE:CG	1:C:389:MET:CE	2.91	0.54
1:B:300:VAL:HG21	1:B:317:LEU:HA	1.90	0.54
1:B:338:GLU:O	1:B:341:ALA:N	2.40	0.54
1:C:140:ASP:OD1	1:C:143:ALA:HB2	2.07	0.54
1:D:82:ASN:HD22	1:D:82:ASN:H	1.55	0.54
1:D:140:ASP:OD1	1:D:143:ALA:HB2	2.07	0.54
1:E:191:GLU:O	1:E:334:ASP:HA	2.07	0.54
1:E:360:TYR:CE1	1:F:183:LEU:CD2	2.85	0.54
1:G:213:VAL:O	1:G:213:VAL:HG23	2.06	0.54
1:G:465:VAL:O	1:G:469:VAL:HG23	2.07	0.54
1:A:386:GLU:N	1:G:281:PHE:CE2	2.76	0.54
1:D:82:ASN:HD21	1:D:89:THR:N	1.97	0.54
1:E:82:ASN:H	1:E:82:ASN:HD22	1.55	0.54
1:E:300:VAL:HG21	1:E:317:LEU:HA	1.90	0.54
1:F:12:ALA:HB1	1:F:520:MET:HG3	1.89	0.54
1:F:176:THR:HG21	1:F:333:ILE:HD11	1.90	0.54
1:G:140:ASP:OD1	1:G:143:ALA:HB2	2.07	0.54
1:B:213:VAL:HG23	1:B:213:VAL:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:THR:HG21	1:G:333:ILE:HD11	1.90	0.54
1:A:140:ASP:OD1	1:A:143:ALA:HB2	2.07	0.54
1:A:176:THR:HG21	1:A:333:ILE:HD11	1.90	0.54
1:A:300:VAL:HG21	1:A:317:LEU:HA	1.90	0.54
1:E:66:PHE:HD1	1:E:520:MET:HE3	1.72	0.54
1:E:132:LYS:HE3	1:E:409:GLU:HB3	1.90	0.54
1:F:7:LYS:NZ	1:F:15:LYS:HE3	2.22	0.54
1:G:12:ALA:HB1	1:G:520:MET:HG3	1.89	0.54
1:B:66:PHE:HD1	1:B:520:MET:HE3	1.72	0.54
1:B:82:ASN:ND2	1:B:89:THR:N	2.51	0.54
1:B:281:PHE:HE2	1:C:385:THR:C	2.16	0.54
1:D:132:LYS:HE3	1:D:409:GLU:HB3	1.90	0.54
1:D:191:GLU:O	1:D:334:ASP:HA	2.07	0.54
1:F:132:LYS:HE3	1:F:409:GLU:HB3	1.90	0.54
1:B:176:THR:HG21	1:B:333:ILE:HD11	1.90	0.53
1:C:66:PHE:CD1	1:C:520:MET:HE3	2.43	0.53
1:C:176:THR:HG21	1:C:333:ILE:HD11	1.90	0.53
1:D:300:VAL:HG21	1:D:317:LEU:HA	1.90	0.53
1:E:176:THR:HG21	1:E:333:ILE:HD11	1.90	0.53
1:A:378:VAL:HG12	1:A:380:LYS:HD2	1.90	0.53
1:B:66:PHE:CD1	1:B:520:MET:HE3	2.43	0.53
1:D:66:PHE:CD1	1:D:520:MET:HE3	2.44	0.53
1:F:66:PHE:CD1	1:F:520:MET:HE3	2.43	0.53
1:A:213:VAL:HG23	1:A:213:VAL:O	2.06	0.53
1:A:360:TYR:HD1	1:A:361:ASP:N	2.07	0.53
1:C:465:VAL:O	1:C:469:VAL:HG23	2.07	0.53
1:C:521:VAL:N	1:D:39:VAL:O	2.25	0.53
1:F:191:GLU:O	1:F:334:ASP:HA	2.07	0.53
1:F:360:TYR:HD1	1:F:361:ASP:N	2.07	0.53
1:G:66:PHE:CD1	1:G:520:MET:HE3	2.43	0.53
1:G:378:VAL:HG12	1:G:380:LYS:HD2	1.90	0.53
1:A:7:LYS:NZ	1:A:15:LYS:HE3	2.22	0.53
1:A:517:THR:HG21	1:B:39:VAL:CG2	2.38	0.53
1:B:360:TYR:HD1	1:B:361:ASP:N	2.07	0.53
1:C:360:TYR:HD1	1:C:361:ASP:N	2.07	0.53
1:C:378:VAL:HG12	1:C:380:LYS:HD2	1.90	0.53
1:D:176:THR:HG21	1:D:333:ILE:HD11	1.90	0.53
1:D:360:TYR:HD1	1:D:361:ASP:N	2.07	0.53
1:E:66:PHE:CD1	1:E:520:MET:HE3	2.43	0.53
1:E:360:TYR:HD1	1:E:361:ASP:N	2.07	0.53
1:E:463:SER:O	1:E:467:ASN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:LYS:O	1:F:457:ASN:HB3	2.09	0.53
1:G:132:LYS:HE3	1:G:409:GLU:HB3	1.90	0.53
1:G:360:TYR:HD1	1:G:361:ASP:N	2.07	0.53
1:A:66:PHE:CD1	1:A:520:MET:HE3	2.43	0.53
1:A:386:GLU:N	1:G:281:PHE:HE2	2.07	0.53
1:C:132:LYS:HE3	1:C:409:GLU:HB3	1.90	0.53
1:G:34:LYS:O	1:G:457:ASN:HB3	2.09	0.53
1:G:288:MET:HG3	1:G:368:ARG:CD	2.29	0.53
1:A:385:THR:C	1:G:281:PHE:CE2	2.79	0.53
1:A:386:GLU:CA	1:G:281:PHE:CE2	2.92	0.53
1:A:39:VAL:CG1	1:G:69:MET:HE2	2.33	0.53
1:F:463:SER:O	1:F:467:ASN:HB2	2.09	0.53
1:G:7:LYS:NZ	1:G:15:LYS:HE3	2.22	0.53
1:A:300:VAL:CG2	1:A:317:LEU:HD23	2.31	0.53
1:C:518:GLU:HG3	1:D:36:ARG:HG3	1.89	0.53
1:E:34:LYS:O	1:E:457:ASN:HB3	2.09	0.53
1:F:378:VAL:HG12	1:F:380:LYS:HD2	1.90	0.53
1:A:34:LYS:O	1:A:457:ASN:HB3	2.09	0.53
1:A:132:LYS:HE3	1:A:409:GLU:HB3	1.90	0.53
1:B:378:VAL:HG12	1:B:380:LYS:HD2	1.90	0.53
1:C:12:ALA:HB1	1:C:520:MET:HG3	1.89	0.53
1:D:34:LYS:O	1:D:457:ASN:HB3	2.09	0.53
1:D:378:VAL:HG12	1:D:380:LYS:HD2	1.90	0.53
1:D:463:SER:O	1:D:467:ASN:HB2	2.09	0.53
1:F:288:MET:HG3	1:F:368:ARG:CD	2.29	0.53
1:C:463:SER:O	1:C:467:ASN:HB2	2.09	0.52
1:G:66:PHE:HD1	1:G:520:MET:HE3	1.72	0.52
1:B:132:LYS:HE3	1:B:409:GLU:HB3	1.90	0.52
1:B:281:PHE:CZ	1:C:389:MET:CG	2.92	0.52
1:A:36:ARG:HG3	1:G:518:GLU:HG3	1.91	0.52
1:A:82:ASN:HD21	1:A:89:THR:N	1.97	0.52
1:A:362:ARG:CZ	1:A:366:GLN:NE2	2.72	0.52
1:B:362:ARG:CZ	1:B:366:GLN:NE2	2.72	0.52
1:C:300:VAL:CG2	1:C:317:LEU:HD23	2.31	0.52
1:E:378:VAL:HG12	1:E:380:LYS:HD2	1.90	0.52
1:F:325:ILE:HG22	1:F:326:ASN:H	1.74	0.52
1:G:321:LYS:HA	1:G:321:LYS:HE3	1.91	0.52
1:A:288:MET:HA	1:A:291:ASP:OD2	2.10	0.52
1:B:300:VAL:CG2	1:B:317:LEU:HD23	2.31	0.52
1:B:321:LYS:HE3	1:B:321:LYS:HA	1.91	0.52
1:D:69:MET:HE3	1:E:41:ASP:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:MET:HA	1:F:291:ASP:OD2	2.10	0.52
1:F:321:LYS:HA	1:F:321:LYS:HE3	1.91	0.52
1:G:463:SER:O	1:G:467:ASN:HB2	2.09	0.52
1:A:501:ARG:NH1	1:A:505:GLN:OE1	2.43	0.52
1:D:183:LEU:HD12	1:D:383:ALA:O	2.10	0.52
1:D:300:VAL:CG2	1:D:317:LEU:HD23	2.31	0.52
1:D:386:GLU:HG3	1:D:389:MET:HE3	1.91	0.52
1:A:321:LYS:HA	1:A:321:LYS:HE3	1.92	0.52
1:C:34:LYS:O	1:C:457:ASN:HB3	2.09	0.52
1:C:362:ARG:CZ	1:C:366:GLN:NE2	2.73	0.52
1:D:288:MET:HA	1:D:291:ASP:OD2	2.10	0.52
1:E:362:ARG:CZ	1:E:366:GLN:NE2	2.73	0.52
1:E:501:ARG:NH1	1:E:505:GLN:NE2	2.58	0.52
1:B:288:MET:HA	1:B:291:ASP:OD2	2.10	0.52
1:C:501:ARG:NH1	1:C:505:GLN:OE1	2.43	0.52
1:D:362:ARG:CZ	1:D:366:GLN:NE2	2.72	0.52
1:D:517:THR:HA	1:E:37:ASN:HB2	1.91	0.52
1:G:501:ARG:NH1	1:G:505:GLN:OE1	2.43	0.52
1:B:386:GLU:HG3	1:B:389:MET:HE3	1.91	0.52
1:B:463:SER:O	1:B:467:ASN:HB2	2.09	0.52
1:C:183:LEU:HD12	1:C:383:ALA:O	2.10	0.52
1:C:288:MET:HA	1:C:291:ASP:OD2	2.10	0.52
1:E:321:LYS:HA	1:E:321:LYS:HE3	1.92	0.52
1:E:325:ILE:HG22	1:E:326:ASN:H	1.74	0.52
1:F:521:VAL:HB	1:G:40:LEU:HD23	1.90	0.52
1:A:386:GLU:HG3	1:A:389:MET:HE3	1.91	0.52
1:B:34:LYS:O	1:B:457:ASN:HB3	2.09	0.52
1:C:386:GLU:HG3	1:C:389:MET:HE3	1.91	0.52
1:B:183:LEU:HD12	1:B:383:ALA:O	2.10	0.52
1:C:321:LYS:HA	1:C:321:LYS:HE3	1.91	0.52
1:E:288:MET:HA	1:E:291:ASP:OD2	2.10	0.52
1:E:386:GLU:HG3	1:E:389:MET:HE3	1.91	0.52
1:E:501:ARG:NH1	1:E:505:GLN:OE1	2.43	0.52
1:A:183:LEU:HD12	1:A:383:ALA:O	2.10	0.51
1:B:281:PHE:CE2	1:C:389:MET:HB3	2.43	0.51
1:B:501:ARG:NH1	1:B:505:GLN:OE1	2.43	0.51
1:D:501:ARG:NH1	1:D:505:GLN:OE1	2.43	0.51
1:F:501:ARG:NH1	1:F:505:GLN:OE1	2.43	0.51
1:G:362:ARG:CZ	1:G:366:GLN:NE2	2.72	0.51
1:G:386:GLU:HG3	1:G:389:MET:HE3	1.91	0.51
1:E:183:LEU:HD12	1:E:383:ALA:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:501:ARG:NH1	1:G:505:GLN:NE2	2.58	0.51
1:B:501:ARG:NH1	1:B:505:GLN:NE2	2.58	0.51
1:G:183:LEU:HD12	1:G:383:ALA:O	2.10	0.51
1:G:288:MET:HA	1:G:291:ASP:OD2	2.10	0.51
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.93	0.51
1:D:453:GLN:O	1:D:456:LEU:N	2.44	0.51
1:F:362:ARG:CZ	1:F:366:GLN:NE2	2.73	0.51
1:F:386:GLU:HG3	1:F:389:MET:HE3	1.91	0.51
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.93	0.51
1:D:325:ILE:HG22	1:D:326:ASN:H	1.74	0.51
1:E:69:MET:HE2	1:F:39:VAL:HG12	1.92	0.51
1:E:453:GLN:O	1:E:456:LEU:N	2.44	0.51
1:A:107:VAL:HG21	1:A:515:ILE:HG23	1.93	0.51
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.93	0.51
1:A:463:SER:O	1:A:467:ASN:HB2	2.09	0.51
1:E:107:VAL:HG21	1:E:515:ILE:HG23	1.93	0.51
1:A:453:GLN:O	1:A:456:LEU:N	2.44	0.51
1:B:107:VAL:HG21	1:B:515:ILE:HG23	1.93	0.51
1:C:107:VAL:HG21	1:C:515:ILE:HG23	1.93	0.51
1:D:16:MET:O	1:D:20:VAL:HG23	2.11	0.51
1:D:107:VAL:HG21	1:D:515:ILE:HG23	1.93	0.51
1:E:16:MET:O	1:E:20:VAL:HG23	2.11	0.51
1:E:82:ASN:HD21	1:E:89:THR:N	1.97	0.51
1:E:146:GLN:HA	1:E:146:GLN:HE21	1.75	0.51
1:E:432:GLN:HB2	1:E:436:GLN:CD	2.36	0.51
1:F:183:LEU:HD12	1:F:383:ALA:O	2.10	0.51
1:G:107:VAL:HG21	1:G:515:ILE:HG23	1.93	0.51
1:G:124:VAL:HG13	1:G:504:LEU:HD13	1.93	0.51
1:G:146:GLN:HA	1:G:146:GLN:HE21	1.75	0.51
1:G:300:VAL:CG2	1:G:317:LEU:HD23	2.31	0.51
1:D:327:LYS:O	1:D:328:ASP:HB2	2.11	0.51
1:F:453:GLN:O	1:F:456:LEU:N	2.44	0.51
1:G:453:GLN:O	1:G:456:LEU:N	2.44	0.51
1:A:146:GLN:HA	1:A:146:GLN:HE21	1.75	0.51
1:C:146:GLN:HE21	1:C:146:GLN:HA	1.75	0.51
1:D:321:LYS:HA	1:D:321:LYS:HE3	1.91	0.51
1:F:124:VAL:HG13	1:F:504:LEU:HD13	1.93	0.51
1:G:16:MET:O	1:G:20:VAL:HG23	2.11	0.51
1:A:103:GLY:O	1:A:107:VAL:HG23	2.11	0.51
1:C:124:VAL:HG13	1:C:504:LEU:HD13	1.93	0.51
1:C:327:LYS:O	1:C:328:ASP:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:MET:O	1:F:20:VAL:HG23	2.11	0.51
1:F:432:GLN:HB2	1:F:436:GLN:CD	2.36	0.51
1:A:16:MET:O	1:A:20:VAL:HG23	2.11	0.50
1:A:197:ARG:HH11	1:A:197:ARG:CG	2.23	0.50
1:A:432:GLN:HB2	1:A:436:GLN:CD	2.36	0.50
1:B:73:MET:HG2	1:C:49:ILE:HD11	1.93	0.50
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.93	0.50
1:C:196:ASP:HA	1:C:328:ASP:O	2.12	0.50
1:C:453:GLN:O	1:C:456:LEU:N	2.44	0.50
1:D:432:GLN:HB2	1:D:436:GLN:CD	2.36	0.50
1:D:501:ARG:NH1	1:D:505:GLN:NE2	2.58	0.50
1:E:327:LYS:O	1:E:328:ASP:HB2	2.11	0.50
1:E:349:ILE:HG23	1:E:365:LEU:HG	1.93	0.50
1:F:107:VAL:HG21	1:F:515:ILE:HG23	1.93	0.50
1:F:364:LYS:NZ	1:F:365:LEU:HD13	2.22	0.50
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.93	0.50
1:B:453:GLN:O	1:B:456:LEU:N	2.44	0.50
1:C:140:ASP:OD2	1:C:142:LYS:HB2	2.11	0.50
1:C:197:ARG:HH11	1:C:197:ARG:CG	2.23	0.50
1:D:197:ARG:HH11	1:D:197:ARG:CG	2.23	0.50
1:F:146:GLN:HE21	1:F:146:GLN:HA	1.75	0.50
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.94	0.50
1:G:103:GLY:O	1:G:107:VAL:HG23	2.10	0.50
1:G:196:ASP:HA	1:G:328:ASP:O	2.12	0.50
1:A:124:VAL:HG13	1:A:504:LEU:HD13	1.93	0.50
1:B:16:MET:O	1:B:20:VAL:HG23	2.11	0.50
1:B:35:GLY:O	1:B:51:LYS:HE2	2.12	0.50
1:B:140:ASP:OD2	1:B:142:LYS:HB2	2.11	0.50
1:B:197:ARG:HH11	1:B:197:ARG:CG	2.23	0.50
1:C:325:ILE:HG22	1:C:326:ASN:H	1.74	0.50
1:D:35:GLY:O	1:D:51:LYS:HE2	2.11	0.50
1:D:251:ALA:O	1:D:277:LYS:HA	2.12	0.50
1:F:35:GLY:O	1:F:51:LYS:HE2	2.11	0.50
1:F:196:ASP:HA	1:F:328:ASP:O	2.12	0.50
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.94	0.50
1:A:140:ASP:OD2	1:A:142:LYS:HB2	2.11	0.50
1:B:103:GLY:O	1:B:107:VAL:HG23	2.11	0.50
1:C:16:MET:O	1:C:20:VAL:HG23	2.11	0.50
1:C:103:GLY:O	1:C:107:VAL:HG23	2.10	0.50
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.93	0.50
1:E:124:VAL:HG13	1:E:504:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ALA:O	1:E:277:LYS:HA	2.12	0.50
1:F:327:LYS:O	1:F:328:ASP:HB2	2.11	0.50
1:F:413:ALA:HB2	1:F:475:ASN:HB3	1.93	0.50
1:G:197:ARG:HH11	1:G:197:ARG:CG	2.23	0.50
1:G:432:GLN:HB2	1:G:436:GLN:CD	2.36	0.50
1:B:82:ASN:HD22	1:B:82:ASN:N	2.09	0.50
1:B:327:LYS:O	1:B:328:ASP:HB2	2.12	0.50
1:D:124:VAL:HG13	1:D:504:LEU:HD13	1.93	0.50
1:D:205:ILE:HD11	1:D:211:GLY:C	2.37	0.50
1:D:349:ILE:HG23	1:D:365:LEU:HG	1.93	0.50
1:E:221:LEU:HD12	1:E:300:VAL:CG1	2.39	0.50
1:G:35:GLY:O	1:G:51:LYS:HE2	2.11	0.50
1:B:146:GLN:HA	1:B:146:GLN:HE21	1.75	0.50
1:C:251:ALA:O	1:C:277:LYS:HA	2.12	0.50
1:C:432:GLN:HB2	1:C:436:GLN:CD	2.36	0.50
1:D:146:GLN:HA	1:D:146:GLN:HE21	1.75	0.50
1:D:281:PHE:CD2	1:E:386:GLU:HA	2.47	0.50
1:E:35:GLY:O	1:E:51:LYS:HE2	2.11	0.50
1:G:413:ALA:HB2	1:G:475:ASN:HB3	1.93	0.50
1:A:413:ALA:HB2	1:A:475:ASN:HB3	1.93	0.50
1:C:82:ASN:HD22	1:C:82:ASN:N	2.09	0.50
1:D:82:ASN:O	1:D:86:GLY:N	2.43	0.50
1:D:140:ASP:OD2	1:D:142:LYS:HB2	2.11	0.50
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.94	0.50
1:E:513:LEU:HD22	1:F:49:ILE:HG21	1.94	0.50
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.93	0.50
1:B:196:ASP:HA	1:B:328:ASP:O	2.12	0.50
1:B:300:VAL:HG21	1:B:317:LEU:CD2	2.34	0.50
1:D:103:GLY:O	1:D:107:VAL:HG23	2.10	0.50
1:E:194:GLN:CD	1:E:331:THR:HG22	2.37	0.50
1:E:196:ASP:HA	1:E:328:ASP:O	2.12	0.50
1:E:197:ARG:HH11	1:E:197:ARG:CG	2.23	0.50
1:E:413:ALA:HB2	1:E:475:ASN:HB3	1.93	0.50
1:F:82:ASN:HD22	1:F:82:ASN:N	2.09	0.50
1:F:176:THR:HG21	1:F:333:ILE:CD1	2.42	0.50
1:G:140:ASP:OD2	1:G:142:LYS:HB2	2.11	0.50
1:A:35:GLY:O	1:A:51:LYS:HE2	2.12	0.50
1:A:349:ILE:HG23	1:A:365:LEU:HG	1.93	0.50
1:B:349:ILE:HG23	1:B:365:LEU:HG	1.92	0.50
1:E:300:VAL:CG2	1:E:317:LEU:HD23	2.31	0.50
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:GLN:CD	1:F:331:THR:HG22	2.37	0.50
1:F:197:ARG:HH11	1:F:197:ARG:CG	2.23	0.50
1:F:349:ILE:HG23	1:F:365:LEU:HG	1.93	0.50
1:A:348:GLN:O	1:A:352:GLN:HG3	2.12	0.49
1:A:361:ASP:O	1:A:365:LEU:HB2	2.12	0.49
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.94	0.49
1:B:194:GLN:CD	1:B:331:THR:HG22	2.36	0.49
1:B:222:LEU:HD22	1:B:289:LEU:O	2.12	0.49
1:B:413:ALA:HB2	1:B:475:ASN:HB3	1.93	0.49
1:C:194:GLN:CD	1:C:331:THR:HG22	2.36	0.49
1:C:205:ILE:HD11	1:C:211:GLY:C	2.37	0.49
1:C:349:ILE:HG23	1:C:365:LEU:HG	1.93	0.49
1:C:413:ALA:HB2	1:C:475:ASN:HB3	1.93	0.49
1:D:194:GLN:CD	1:D:331:THR:HG22	2.36	0.49
1:D:298:GLY:C	1:D:300:VAL:N	2.70	0.49
1:D:517:THR:CG2	1:E:39:VAL:HG23	2.42	0.49
1:E:82:ASN:HD22	1:E:82:ASN:N	2.09	0.49
1:F:103:GLY:O	1:F:107:VAL:HG23	2.11	0.49
1:G:205:ILE:HD11	1:G:211:GLY:C	2.37	0.49
1:G:327:LYS:O	1:G:328:ASP:HB2	2.12	0.49
1:G:348:GLN:O	1:G:352:GLN:HG3	2.12	0.49
1:A:205:ILE:HD11	1:A:211:GLY:C	2.37	0.49
1:A:327:LYS:O	1:A:328:ASP:HB2	2.11	0.49
1:B:176:THR:HG21	1:B:333:ILE:CD1	2.42	0.49
1:B:251:ALA:O	1:B:277:LYS:HA	2.12	0.49
1:B:432:GLN:HB2	1:B:436:GLN:CD	2.36	0.49
1:C:35:GLY:O	1:C:51:LYS:HE2	2.11	0.49
1:C:298:GLY:C	1:C:300:VAL:N	2.70	0.49
1:C:348:GLN:O	1:C:352:GLN:HG3	2.12	0.49
1:C:361:ASP:O	1:C:365:LEU:HB2	2.12	0.49
1:C:455:VAL:O	1:C:458:CYS:HB2	2.13	0.49
1:D:348:GLN:O	1:D:352:GLN:HG3	2.12	0.49
1:F:251:ALA:O	1:F:277:LYS:HA	2.12	0.49
1:G:194:GLN:CD	1:G:331:THR:HG22	2.37	0.49
1:G:349:ILE:HG23	1:G:365:LEU:HG	1.93	0.49
1:G:361:ASP:O	1:G:365:LEU:HB2	2.12	0.49
1:A:196:ASP:HA	1:A:328:ASP:O	2.12	0.49
1:A:386:GLU:OE2	1:G:285:ARG:CZ	2.51	0.49
1:C:222:LEU:HD22	1:C:289:LEU:O	2.12	0.49
1:D:196:ASP:HA	1:D:328:ASP:O	2.12	0.49
1:D:222:LEU:HD22	1:D:289:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.94	0.49
1:E:455:VAL:O	1:E:458:CYS:HB2	2.13	0.49
1:F:348:GLN:O	1:F:352:GLN:HG3	2.12	0.49
1:G:82:ASN:HD22	1:G:82:ASN:N	2.09	0.49
1:G:455:VAL:O	1:G:458:CYS:HB2	2.12	0.49
1:A:194:GLN:CD	1:A:331:THR:HG22	2.36	0.49
1:A:222:LEU:HD22	1:A:289:LEU:O	2.12	0.49
1:A:364:LYS:NZ	1:A:365:LEU:HD13	2.22	0.49
1:B:348:GLN:O	1:B:352:GLN:HG3	2.12	0.49
1:D:82:ASN:HD22	1:D:82:ASN:N	2.09	0.49
1:D:162:ILE:O	1:D:166:MET:HB2	2.13	0.49
1:D:176:THR:HG21	1:D:333:ILE:CD1	2.42	0.49
1:D:413:ALA:HB2	1:D:475:ASN:HB3	1.93	0.49
1:E:348:GLN:O	1:E:352:GLN:HG3	2.12	0.49
1:G:176:THR:HG21	1:G:333:ILE:CD1	2.42	0.49
1:G:251:ALA:O	1:G:277:LYS:HA	2.12	0.49
1:A:132:LYS:HD2	1:A:497:THR:HG21	1.95	0.49
1:B:325:ILE:HG22	1:B:326:ASN:H	1.74	0.49
1:C:82:ASN:O	1:C:86:GLY:N	2.43	0.49
1:C:162:ILE:O	1:C:166:MET:HB2	2.13	0.49
1:D:132:LYS:HD2	1:D:497:THR:HG21	1.95	0.49
1:D:441:LYS:HE3	1:D:445:ARG:NH1	2.28	0.49
1:E:82:ASN:O	1:E:86:GLY:N	2.43	0.49
1:E:140:ASP:OD2	1:E:142:LYS:HB2	2.11	0.49
1:E:205:ILE:HD11	1:E:211:GLY:C	2.37	0.49
1:E:361:ASP:O	1:E:365:LEU:HB2	2.12	0.49
1:G:132:LYS:HD2	1:G:497:THR:HG21	1.95	0.49
1:G:300:VAL:HG21	1:G:317:LEU:CD2	2.34	0.49
1:A:82:ASN:HD22	1:A:82:ASN:N	2.09	0.49
1:A:455:VAL:O	1:A:458:CYS:HB2	2.13	0.49
1:C:132:LYS:HD2	1:C:497:THR:HG21	1.95	0.49
1:C:349:ILE:O	1:C:353:ILE:HG13	2.13	0.49
1:D:300:VAL:HG21	1:D:317:LEU:CD2	2.34	0.49
1:E:103:GLY:O	1:E:107:VAL:HG23	2.10	0.49
1:E:132:LYS:HD2	1:E:497:THR:HG21	1.95	0.49
1:E:281:PHE:CZ	1:F:389:MET:CG	2.96	0.49
1:A:349:ILE:O	1:A:353:ILE:HG13	2.13	0.49
1:B:162:ILE:O	1:B:166:MET:HB2	2.13	0.49
1:B:298:GLY:C	1:B:300:VAL:N	2.70	0.49
1:E:349:ILE:O	1:E:353:ILE:HG13	2.13	0.49
1:F:132:LYS:HD2	1:F:497:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:361:ASP:O	1:F:365:LEU:HB2	2.12	0.49
1:F:441:LYS:HE3	1:F:445:ARG:NH1	2.28	0.49
1:G:353:ILE:O	1:G:356:ALA:HB3	2.13	0.49
1:A:176:THR:HG21	1:A:333:ILE:CD1	2.42	0.49
1:B:132:LYS:HD2	1:B:497:THR:HG21	1.95	0.49
1:B:353:ILE:O	1:B:356:ALA:HB3	2.13	0.49
1:B:441:LYS:HE3	1:B:445:ARG:NH1	2.28	0.49
1:C:281:PHE:CD2	1:D:386:GLU:CA	2.96	0.49
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.94	0.49
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.94	0.49
1:F:298:GLY:C	1:F:300:VAL:N	2.70	0.49
1:A:300:VAL:HG21	1:A:317:LEU:CD2	2.34	0.49
1:A:389:MET:HB2	1:G:281:PHE:CZ	2.48	0.49
1:B:82:ASN:O	1:B:86:GLY:N	2.43	0.49
1:B:361:ASP:O	1:B:365:LEU:HB2	2.12	0.49
1:B:455:VAL:O	1:B:458:CYS:HB2	2.13	0.49
1:E:162:ILE:O	1:E:166:MET:HB2	2.13	0.49
1:E:222:LEU:HD22	1:E:289:LEU:O	2.12	0.49
1:E:281:PHE:CG	1:F:389:MET:CE	2.96	0.49
1:E:353:ILE:O	1:E:356:ALA:HB3	2.13	0.49
1:F:140:ASP:OD2	1:F:142:LYS:HB2	2.11	0.49
1:F:165:ALA:HB2	1:F:379:ILE:HD11	1.94	0.49
1:G:298:GLY:C	1:G:300:VAL:N	2.70	0.49
1:C:300:VAL:HG21	1:C:317:LEU:CD2	2.34	0.49
1:D:353:ILE:O	1:D:356:ALA:HB3	2.13	0.49
1:F:205:ILE:HD11	1:F:211:GLY:C	2.37	0.49
1:G:222:LEU:HD22	1:G:289:LEU:O	2.12	0.49
1:G:349:ILE:O	1:G:353:ILE:HG13	2.13	0.49
1:G:441:LYS:HE3	1:G:445:ARG:NH1	2.28	0.49
1:A:441:LYS:HE3	1:A:445:ARG:NH1	2.28	0.48
1:B:284:ARG:NH2	1:B:360:TYR:HH	2.11	0.48
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.94	0.48
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.94	0.48
1:E:165:ALA:HB2	1:E:379:ILE:HD11	1.95	0.48
1:E:298:GLY:C	1:E:300:VAL:N	2.70	0.48
1:F:27:VAL:HG21	1:F:57:ALA:HB2	1.95	0.48
1:F:222:LEU:HD22	1:F:289:LEU:O	2.12	0.48
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.94	0.48
1:A:298:GLY:C	1:A:300:VAL:N	2.70	0.48
1:A:325:ILE:HG22	1:A:326:ASN:H	1.74	0.48
1:A:353:ILE:O	1:A:356:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.94	0.48
1:B:349:ILE:O	1:B:353:ILE:HG13	2.13	0.48
1:C:27:VAL:HG21	1:C:57:ALA:HB2	1.96	0.48
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.94	0.48
1:C:353:ILE:O	1:C:356:ALA:HB3	2.13	0.48
1:D:282:GLY:HA2	1:E:181:THR:O	1.94	0.48
1:F:162:ILE:O	1:F:166:MET:HB2	2.13	0.48
1:G:130:GLU:OE2	1:G:425:LYS:HD3	2.13	0.48
1:A:251:ALA:O	1:A:277:LYS:HA	2.12	0.48
1:A:501:ARG:NH1	1:A:505:GLN:NE2	2.58	0.48
1:B:27:VAL:HG21	1:B:57:ALA:HB2	1.96	0.48
1:B:205:ILE:HD11	1:B:211:GLY:C	2.37	0.48
1:C:522:THR:HA	1:D:41:ASP:HB2	1.96	0.48
1:E:27:VAL:HG21	1:E:57:ALA:HB2	1.95	0.48
1:E:281:PHE:HD2	1:F:386:GLU:CA	2.26	0.48
1:F:455:VAL:O	1:F:458:CYS:HB2	2.12	0.48
1:F:501:ARG:NH1	1:F:505:GLN:NE2	2.58	0.48
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.94	0.48
1:A:162:ILE:O	1:A:166:MET:HB2	2.13	0.48
1:A:324:VAL:O	1:A:324:VAL:CG1	2.62	0.48
1:B:130:GLU:OE2	1:B:425:LYS:HD3	2.14	0.48
1:D:455:VAL:O	1:D:458:CYS:HB2	2.13	0.48
1:E:176:THR:HG21	1:E:333:ILE:CD1	2.42	0.48
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.94	0.48
1:F:111:MET:HG2	1:F:435:ASP:OD1	2.13	0.48
1:C:176:THR:HG21	1:C:333:ILE:CD1	2.42	0.48
1:C:221:LEU:HD12	1:C:300:VAL:CG1	2.39	0.48
1:C:441:LYS:HE3	1:C:445:ARG:NH1	2.28	0.48
1:E:146:GLN:O	1:E:150:ILE:HG13	2.14	0.48
1:E:488:MET:HE2	1:E:493:ILE:HB	1.95	0.48
1:G:324:VAL:O	1:G:324:VAL:CG1	2.62	0.48
1:A:82:ASN:O	1:A:86:GLY:N	2.43	0.48
1:A:165:ALA:HB2	1:A:379:ILE:HD11	1.94	0.48
1:B:128:VAL:HG22	1:B:501:ARG:HG3	1.96	0.48
1:C:327:LYS:O	1:C:328:ASP:CB	2.62	0.48
1:C:364:LYS:NZ	1:C:365:LEU:HD13	2.22	0.48
1:D:128:VAL:HG22	1:D:501:ARG:HG3	1.96	0.48
1:D:346:VAL:HG21	1:D:373:ALA:HB2	1.96	0.48
1:E:111:MET:HG2	1:E:435:ASP:OD1	2.13	0.48
1:E:128:VAL:HG22	1:E:501:ARG:HG3	1.96	0.48
1:F:349:ILE:O	1:F:353:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:ILE:O	1:F:356:ALA:HB3	2.13	0.48
1:G:82:ASN:O	1:G:86:GLY:N	2.43	0.48
1:G:111:MET:HG2	1:G:435:ASP:OD1	2.13	0.48
1:A:111:MET:HG2	1:A:435:ASP:OD1	2.13	0.48
1:B:165:ALA:HB2	1:B:379:ILE:HD11	1.95	0.48
1:C:128:VAL:HG22	1:C:501:ARG:HG3	1.96	0.48
1:C:346:VAL:HG21	1:C:373:ALA:HB2	1.96	0.48
1:D:130:GLU:OE2	1:D:425:LYS:HD3	2.13	0.48
1:D:165:ALA:HB2	1:D:379:ILE:HD11	1.95	0.48
1:D:327:LYS:O	1:D:328:ASP:CB	2.62	0.48
1:D:349:ILE:O	1:D:353:ILE:HG13	2.13	0.48
1:D:361:ASP:O	1:D:365:LEU:HB2	2.12	0.48
1:F:82:ASN:O	1:F:86:GLY:N	2.43	0.48
1:F:128:VAL:HG22	1:F:501:ARG:HG3	1.96	0.48
1:F:146:GLN:O	1:F:150:ILE:HG13	2.14	0.48
1:B:327:LYS:O	1:B:328:ASP:CB	2.62	0.48
1:B:346:VAL:HG21	1:B:373:ALA:HB2	1.96	0.48
1:C:165:ALA:HB2	1:C:379:ILE:HD11	1.94	0.48
1:D:32:GLY:HA2	1:D:454:ILE:HG12	1.96	0.48
1:D:146:GLN:O	1:D:150:ILE:HG13	2.14	0.48
1:D:521:VAL:HB	1:E:40:LEU:CD2	2.43	0.48
1:F:413:ALA:HA	1:F:489:ILE:HD11	1.96	0.48
1:G:27:VAL:HG21	1:G:57:ALA:HB2	1.96	0.48
1:G:325:ILE:HG22	1:G:326:ASN:H	1.74	0.48
1:B:111:MET:HG2	1:B:435:ASP:OD1	2.13	0.48
1:C:501:ARG:NH1	1:C:505:GLN:NE2	2.58	0.48
1:D:195:PHE:HZ	1:D:250:ILE:HD11	1.79	0.48
1:E:413:ALA:HA	1:E:489:ILE:HD11	1.96	0.48
1:E:441:LYS:HE3	1:E:445:ARG:NH1	2.28	0.48
1:G:162:ILE:O	1:G:166:MET:HB2	2.13	0.48
1:G:165:ALA:HB2	1:G:379:ILE:HD11	1.95	0.48
1:A:128:VAL:HG22	1:A:501:ARG:HG3	1.96	0.48
1:A:146:GLN:O	1:A:150:ILE:HG13	2.14	0.48
1:B:353:ILE:CG2	1:B:362:ARG:HG2	2.44	0.48
1:C:353:ILE:CG2	1:C:362:ARG:HG2	2.44	0.48
1:E:32:GLY:HA2	1:E:454:ILE:HG12	1.96	0.48
1:E:300:VAL:HG21	1:E:317:LEU:CD2	2.34	0.48
1:F:49:ILE:N	1:F:49:ILE:HD12	2.29	0.48
1:F:300:VAL:HG21	1:F:317:LEU:CD2	2.34	0.48
1:F:324:VAL:O	1:F:324:VAL:CG1	2.62	0.48
1:A:327:LYS:O	1:A:328:ASP:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:VAL:HG21	1:A:373:ALA:HB2	1.96	0.47
1:B:49:ILE:HD12	1:B:49:ILE:N	2.29	0.47
1:B:195:PHE:HZ	1:B:250:ILE:HD11	1.79	0.47
1:B:300:VAL:C	1:B:301:ILE:HG13	2.39	0.47
1:C:32:GLY:HA2	1:C:454:ILE:HG12	1.96	0.47
1:C:49:ILE:N	1:C:49:ILE:HD12	2.29	0.47
1:C:146:GLN:O	1:C:150:ILE:HG13	2.14	0.47
1:C:300:VAL:C	1:C:301:ILE:HG13	2.39	0.47
1:E:195:PHE:CE2	1:E:197:ARG:HB2	2.49	0.47
1:E:346:VAL:HG21	1:E:373:ALA:HB2	1.96	0.47
1:F:32:GLY:HA2	1:F:454:ILE:HG12	1.96	0.47
1:F:195:PHE:HZ	1:F:250:ILE:HD11	1.79	0.47
1:G:49:ILE:HD12	1:G:49:ILE:N	2.29	0.47
1:G:221:LEU:HD12	1:G:300:VAL:CG1	2.39	0.47
1:G:413:ALA:HA	1:G:489:ILE:HD11	1.96	0.47
1:A:49:ILE:HD12	1:A:49:ILE:N	2.29	0.47
1:E:49:ILE:HD12	1:E:49:ILE:N	2.29	0.47
1:E:130:GLU:OE2	1:E:425:LYS:HD3	2.13	0.47
1:E:218:PRO:O	1:E:319:GLN:O	2.32	0.47
1:E:281:PHE:HE2	1:F:385:THR:C	2.21	0.47
1:F:353:ILE:CG2	1:F:362:ARG:HG2	2.44	0.47
1:F:488:MET:HE2	1:F:493:ILE:HB	1.95	0.47
1:G:128:VAL:HG22	1:G:501:ARG:HG3	1.96	0.47
1:G:146:GLN:O	1:G:150:ILE:HG13	2.14	0.47
1:G:346:VAL:HG21	1:G:373:ALA:HB2	1.96	0.47
1:A:195:PHE:CE2	1:A:197:ARG:HB2	2.49	0.47
1:A:300:VAL:C	1:A:301:ILE:HG13	2.39	0.47
1:C:111:MET:HG2	1:C:435:ASP:OD1	2.13	0.47
1:C:130:GLU:OE2	1:C:425:LYS:HD3	2.14	0.47
1:D:49:ILE:HD12	1:D:49:ILE:N	2.29	0.47
1:D:521:VAL:HB	1:E:40:LEU:HD23	1.97	0.47
1:E:195:PHE:HZ	1:E:250:ILE:HD11	1.79	0.47
1:F:130:GLU:OE2	1:F:425:LYS:HD3	2.13	0.47
1:F:195:PHE:CE2	1:F:197:ARG:HB2	2.49	0.47
1:F:346:VAL:HG21	1:F:373:ALA:HB2	1.96	0.47
1:G:32:GLY:HA2	1:G:454:ILE:HG12	1.96	0.47
1:A:195:PHE:HZ	1:A:250:ILE:HD11	1.79	0.47
1:A:488:MET:HE2	1:A:493:ILE:HB	1.95	0.47
1:B:32:GLY:HA2	1:B:454:ILE:HG12	1.96	0.47
1:B:82:ASN:HD21	1:B:89:THR:N	1.97	0.47
1:C:195:PHE:HZ	1:C:250:ILE:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:VAL:HG21	1:D:57:ALA:HB2	1.95	0.47
1:D:488:MET:HE2	1:D:493:ILE:HB	1.95	0.47
1:E:327:LYS:O	1:E:328:ASP:CB	2.62	0.47
1:A:27:VAL:HG21	1:A:57:ALA:HB2	1.95	0.47
1:A:32:GLY:HA2	1:A:454:ILE:HG12	1.96	0.47
1:B:146:GLN:O	1:B:150:ILE:HG13	2.14	0.47
1:B:286:LYS:HE2	1:B:286:LYS:HB3	1.77	0.47
1:B:488:MET:HE2	1:B:493:ILE:HB	1.95	0.47
1:C:195:PHE:CE2	1:C:197:ARG:HB2	2.49	0.47
1:G:195:PHE:CE2	1:G:197:ARG:HB2	2.49	0.47
1:G:218:PRO:O	1:G:319:GLN:O	2.32	0.47
1:G:325:ILE:CG2	1:G:326:ASN:N	2.77	0.47
1:A:130:GLU:OE2	1:A:425:LYS:HD3	2.13	0.47
1:A:353:ILE:CG2	1:A:362:ARG:HG2	2.44	0.47
1:A:376:VAL:HG12	1:A:377:ALA:N	2.29	0.47
1:D:111:MET:HG2	1:D:435:ASP:OD1	2.13	0.47
1:D:300:VAL:C	1:D:301:ILE:HG13	2.39	0.47
1:E:332:ILE:O	1:E:332:ILE:HG22	2.14	0.47
1:F:218:PRO:O	1:F:319:GLN:O	2.32	0.47
1:F:376:VAL:HG12	1:F:377:ALA:N	2.29	0.47
1:A:284:ARG:NH2	1:A:360:TYR:OH	2.48	0.47
1:A:332:ILE:HG22	1:A:332:ILE:O	2.14	0.47
1:A:395:ARG:O	1:A:398:ASP:HB3	2.15	0.47
1:A:413:ALA:HA	1:A:489:ILE:HD11	1.96	0.47
1:B:281:PHE:HE2	1:C:385:THR:O	1.97	0.47
1:B:376:VAL:HG12	1:B:377:ALA:N	2.29	0.47
1:C:218:PRO:O	1:C:319:GLN:O	2.32	0.47
1:C:286:LYS:HE2	1:C:286:LYS:HB3	1.77	0.47
1:D:218:PRO:O	1:D:319:GLN:O	2.32	0.47
1:D:297:GLY:O	1:D:299:THR:HG23	2.15	0.47
1:D:353:ILE:CG2	1:D:362:ARG:HG2	2.44	0.47
1:D:395:ARG:O	1:D:398:ASP:HB3	2.15	0.47
1:D:413:ALA:HA	1:D:489:ILE:HD11	1.96	0.47
1:E:297:GLY:O	1:E:299:THR:HG23	2.15	0.47
1:E:324:VAL:O	1:E:324:VAL:CG1	2.62	0.47
1:F:82:ASN:HD21	1:F:89:THR:N	1.97	0.47
1:F:297:GLY:O	1:F:299:THR:HG23	2.15	0.47
1:F:327:LYS:O	1:F:328:ASP:CB	2.62	0.47
1:F:332:ILE:O	1:F:332:ILE:HG22	2.14	0.47
1:F:395:ARG:O	1:F:398:ASP:HB3	2.15	0.47
1:G:327:LYS:O	1:G:328:ASP:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PRO:O	1:B:319:GLN:O	2.32	0.47
1:B:284:ARG:NH2	1:B:360:TYR:OH	2.48	0.47
1:C:395:ARG:O	1:C:398:ASP:HB3	2.15	0.47
1:G:195:PHE:HZ	1:G:250:ILE:HD11	1.79	0.47
1:G:353:ILE:CG2	1:G:362:ARG:HG2	2.44	0.47
1:A:218:PRO:O	1:A:319:GLN:O	2.32	0.47
1:C:488:MET:HE2	1:C:493:ILE:HB	1.95	0.47
1:D:217:SER:N	1:D:321:LYS:O	2.48	0.47
1:D:332:ILE:O	1:D:332:ILE:HG22	2.14	0.47
1:E:284:ARG:NH2	1:E:360:TYR:OH	2.48	0.47
1:E:353:ILE:CG2	1:E:362:ARG:HG2	2.44	0.47
1:E:376:VAL:HG12	1:E:377:ALA:N	2.29	0.47
1:A:221:LEU:HD12	1:A:300:VAL:CG1	2.39	0.47
1:B:195:PHE:CE2	1:B:197:ARG:HB2	2.49	0.47
1:B:217:SER:N	1:B:321:LYS:O	2.48	0.47
1:B:351:GLN:O	1:B:352:GLN:C	2.58	0.47
1:B:395:ARG:O	1:B:398:ASP:HB3	2.15	0.47
1:C:284:ARG:NH2	1:C:360:TYR:OH	2.48	0.47
1:F:284:ARG:NH2	1:F:360:TYR:OH	2.48	0.47
1:F:300:VAL:C	1:F:301:ILE:HG13	2.39	0.47
1:G:284:ARG:NH2	1:G:360:TYR:OH	2.48	0.47
1:C:319:GLN:HB2	1:C:336:VAL:HG21	1.97	0.46
1:D:319:GLN:HB2	1:D:336:VAL:HG21	1.97	0.46
1:E:217:SER:N	1:E:321:LYS:O	2.48	0.46
1:E:352:GLN:O	1:E:355:GLU:HG2	2.15	0.46
1:E:395:ARG:O	1:E:398:ASP:HB3	2.15	0.46
1:G:297:GLY:O	1:G:299:THR:HG23	2.15	0.46
1:A:319:GLN:HB2	1:A:336:VAL:HG21	1.97	0.46
1:B:174:VAL:HG13	1:B:174:VAL:O	2.16	0.46
1:C:217:SER:N	1:C:321:LYS:O	2.48	0.46
1:C:351:GLN:O	1:C:352:GLN:C	2.58	0.46
1:C:376:VAL:HG12	1:C:377:ALA:N	2.29	0.46
1:C:479:ASN:O	1:C:483:GLU:N	2.49	0.46
1:D:351:GLN:O	1:D:352:GLN:C	2.58	0.46
1:E:300:VAL:C	1:E:301:ILE:HG13	2.39	0.46
1:F:479:ASN:O	1:F:483:GLU:N	2.49	0.46
1:G:300:VAL:C	1:G:301:ILE:HG13	2.39	0.46
1:G:488:MET:HE2	1:G:493:ILE:HB	1.95	0.46
1:A:479:ASN:O	1:A:483:GLU:N	2.49	0.46
1:B:319:GLN:HB2	1:B:336:VAL:HG21	1.97	0.46
1:B:332:ILE:O	1:B:332:ILE:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:VAL:HG13	1:C:174:VAL:O	2.16	0.46
1:C:252:GLU:O	1:C:253:ASP:C	2.58	0.46
1:C:297:GLY:O	1:C:299:THR:HG23	2.15	0.46
1:D:195:PHE:CE2	1:D:197:ARG:HB2	2.49	0.46
1:E:281:PHE:CE2	1:F:389:MET:HB3	2.50	0.46
1:F:100:ILE:CD1	1:F:514:MET:SD	3.03	0.46
1:G:376:VAL:HG12	1:G:377:ALA:N	2.29	0.46
1:A:351:GLN:O	1:A:352:GLN:C	2.58	0.46
1:B:325:ILE:CG2	1:B:326:ASN:N	2.77	0.46
1:C:332:ILE:O	1:C:332:ILE:HG22	2.14	0.46
1:D:100:ILE:CD1	1:D:514:MET:SD	3.03	0.46
1:D:174:VAL:HG13	1:D:174:VAL:O	2.16	0.46
1:E:252:GLU:O	1:E:253:ASP:C	2.58	0.46
1:E:479:ASN:O	1:E:483:GLU:N	2.49	0.46
1:F:217:SER:N	1:F:321:LYS:O	2.48	0.46
1:F:499:VAL:O	1:F:503:ALA:HB2	2.16	0.46
1:G:217:SER:N	1:G:321:LYS:O	2.48	0.46
1:G:319:GLN:HB2	1:G:336:VAL:HG21	1.97	0.46
1:G:499:VAL:O	1:G:503:ALA:HB2	2.16	0.46
1:A:116:LEU:O	1:A:120:ILE:HG13	2.15	0.46
1:A:217:SER:N	1:A:321:LYS:O	2.48	0.46
1:A:297:GLY:O	1:A:299:THR:HG23	2.15	0.46
1:B:252:GLU:O	1:B:253:ASP:C	2.58	0.46
1:B:293:ALA:O	1:B:298:GLY:N	2.49	0.46
1:B:413:ALA:HA	1:B:489:ILE:HD11	1.96	0.46
1:C:293:ALA:O	1:C:298:GLY:N	2.49	0.46
1:D:284:ARG:NH2	1:D:360:TYR:OH	2.48	0.46
1:D:324:VAL:O	1:D:324:VAL:CG1	2.62	0.46
1:D:352:GLN:O	1:D:355:GLU:HG2	2.15	0.46
1:E:499:VAL:O	1:E:503:ALA:HB2	2.16	0.46
1:F:325:ILE:CG2	1:F:326:ASN:N	2.77	0.46
1:G:364:LYS:NZ	1:G:365:LEU:HD13	2.22	0.46
1:A:174:VAL:HG13	1:A:174:VAL:O	2.16	0.46
1:B:499:VAL:O	1:B:503:ALA:HB2	2.16	0.46
1:C:100:ILE:CD1	1:C:514:MET:SD	3.03	0.46
1:D:376:VAL:HG12	1:D:377:ALA:N	2.29	0.46
1:F:221:LEU:HD12	1:F:300:VAL:CG1	2.39	0.46
1:F:281:PHE:CZ	1:G:389:MET:HB2	2.50	0.46
1:G:252:GLU:O	1:G:253:ASP:C	2.58	0.46
1:B:352:GLN:O	1:B:355:GLU:HG2	2.15	0.46
1:C:413:ALA:HA	1:C:489:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LEU:H	1:D:300:VAL:CG1	2.29	0.46
1:D:293:ALA:O	1:D:298:GLY:N	2.49	0.46
1:D:479:ASN:O	1:D:483:GLU:N	2.49	0.46
1:E:284:ARG:NH2	1:E:360:TYR:HH	2.14	0.46
1:E:351:GLN:O	1:E:352:GLN:C	2.58	0.46
1:G:116:LEU:O	1:G:120:ILE:HG13	2.15	0.46
1:G:205:ILE:HD13	1:G:205:ILE:HA	1.61	0.46
1:G:395:ARG:O	1:G:398:ASP:HB3	2.15	0.46
1:A:281:PHE:CD2	1:B:386:GLU:HA	2.50	0.46
1:A:352:GLN:O	1:A:355:GLU:HG2	2.15	0.46
1:A:499:VAL:O	1:A:503:ALA:HB2	2.16	0.46
1:B:100:ILE:CD1	1:B:514:MET:SD	3.03	0.46
1:C:222:LEU:H	1:C:300:VAL:CG1	2.29	0.46
1:E:114:MET:HE2	1:F:34:LYS:C	2.40	0.46
1:F:319:GLN:HB2	1:F:336:VAL:HG21	1.97	0.46
1:F:340:ALA:HA	1:F:343:GLN:CG	2.42	0.46
1:F:362:ARG:CZ	1:F:366:GLN:HE22	2.29	0.46
1:G:351:GLN:O	1:G:352:GLN:C	2.58	0.46
1:A:252:GLU:O	1:A:253:ASP:C	2.58	0.46
1:A:293:ALA:O	1:A:298:GLY:N	2.49	0.46
1:B:364:LYS:NZ	1:B:365:LEU:HD13	2.22	0.46
1:B:479:ASN:O	1:B:483:GLU:N	2.49	0.46
1:C:324:VAL:O	1:C:324:VAL:CG1	2.62	0.46
1:E:100:ILE:CD1	1:E:514:MET:SD	3.03	0.46
1:F:286:LYS:HE2	1:F:286:LYS:HB3	1.77	0.46
1:G:174:VAL:HG13	1:G:174:VAL:O	2.16	0.46
1:B:116:LEU:O	1:B:120:ILE:HG13	2.15	0.46
1:B:297:GLY:O	1:B:299:THR:HG23	2.15	0.46
1:C:116:LEU:O	1:C:120:ILE:HG13	2.15	0.46
1:D:116:LEU:O	1:D:120:ILE:HG13	2.15	0.46
1:D:221:LEU:HD12	1:D:300:VAL:CG1	2.39	0.46
1:E:319:GLN:HB2	1:E:336:VAL:HG21	1.97	0.46
1:G:332:ILE:HG22	1:G:332:ILE:O	2.14	0.46
1:A:100:ILE:CD1	1:A:514:MET:SD	3.03	0.45
1:A:286:LYS:HE2	1:A:286:LYS:HB3	1.77	0.45
1:B:362:ARG:CZ	1:B:366:GLN:HE22	2.29	0.45
1:C:499:VAL:O	1:C:503:ALA:HB2	2.16	0.45
1:F:174:VAL:HG13	1:F:174:VAL:O	2.16	0.45
1:G:352:GLN:O	1:G:355:GLU:HG2	2.15	0.45
1:G:362:ARG:CZ	1:G:366:GLN:HE22	2.29	0.45
1:G:479:ASN:O	1:G:483:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:H	1:B:300:VAL:CG1	2.29	0.45
1:D:362:ARG:CZ	1:D:366:GLN:HE22	2.29	0.45
1:D:499:VAL:O	1:D:503:ALA:HB2	2.16	0.45
1:E:116:LEU:O	1:E:120:ILE:HG13	2.15	0.45
1:E:350:ARG:HA	1:E:353:ILE:HD12	1.98	0.45
1:F:116:LEU:O	1:F:120:ILE:HG13	2.15	0.45
1:G:195:PHE:O	1:G:330:THR:HG22	2.17	0.45
1:G:286:LYS:HE2	1:G:286:LYS:HB3	1.77	0.45
1:D:325:ILE:CG2	1:D:326:ASN:N	2.77	0.45
1:D:360:TYR:CZ	1:E:183:LEU:HD22	2.51	0.45
1:E:293:ALA:O	1:E:298:GLY:N	2.49	0.45
1:F:77:VAL:CG1	1:F:510:VAL:HG22	2.46	0.45
1:G:293:ALA:O	1:G:298:GLY:N	2.49	0.45
1:A:73:MET:HE3	1:B:49:ILE:HG12	1.97	0.45
1:D:114:MET:HG3	1:E:34:LYS:HB3	1.99	0.45
1:D:252:GLU:O	1:D:253:ASP:C	2.58	0.45
1:D:420:ILE:HG13	1:D:448:GLU:HG2	1.99	0.45
1:D:423:ALA:HB2	1:D:447:MET:SD	2.56	0.45
1:E:77:VAL:CG1	1:E:510:VAL:HG22	2.46	0.45
1:E:174:VAL:HG13	1:E:174:VAL:O	2.16	0.45
1:E:195:PHE:O	1:E:330:THR:HG22	2.17	0.45
1:F:350:ARG:HA	1:F:353:ILE:HD12	1.98	0.45
1:A:222:LEU:H	1:A:300:VAL:CG1	2.29	0.45
1:A:423:ALA:HB2	1:A:447:MET:SD	2.56	0.45
1:B:195:PHE:O	1:B:330:THR:HG22	2.17	0.45
1:C:195:PHE:O	1:C:330:THR:HG22	2.17	0.45
1:C:352:GLN:O	1:C:355:GLU:HG2	2.15	0.45
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.99	0.45
1:D:165:ALA:HB1	1:D:175:ILE:CG2	2.47	0.45
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.99	0.45
1:E:423:ALA:HB2	1:E:447:MET:SD	2.56	0.45
1:A:49:ILE:HG12	1:G:73:MET:HE3	1.99	0.45
1:A:168:LYS:HD3	1:A:189:VAL:HG23	1.98	0.45
1:A:281:PHE:CD2	1:B:386:GLU:CA	3.00	0.45
1:A:362:ARG:CZ	1:A:366:GLN:HE22	2.29	0.45
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.99	0.45
1:C:165:ALA:HB1	1:C:175:ILE:CG2	2.47	0.45
1:C:423:ALA:HB2	1:C:447:MET:SD	2.56	0.45
1:D:77:VAL:CG1	1:D:510:VAL:HG22	2.47	0.45
1:E:165:ALA:HB1	1:E:175:ILE:CG2	2.47	0.45
1:F:165:ALA:HB1	1:F:175:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:LYS:HD3	1:F:189:VAL:HG23	1.98	0.45
1:F:352:GLN:O	1:F:355:GLU:HG2	2.15	0.45
1:F:423:ALA:HB2	1:F:447:MET:SD	2.56	0.45
1:G:165:ALA:HB1	1:G:175:ILE:CG2	2.47	0.45
1:G:168:LYS:HD3	1:G:189:VAL:HG23	1.98	0.45
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.99	0.45
1:G:423:ALA:HB2	1:G:447:MET:SD	2.56	0.45
1:A:346:VAL:HG11	1:A:373:ALA:CB	2.46	0.45
1:D:350:ARG:HA	1:D:353:ILE:HD12	1.99	0.45
1:E:362:ARG:CZ	1:E:366:GLN:HE22	2.29	0.45
1:E:364:LYS:NZ	1:E:365:LEU:HD13	2.22	0.45
1:F:252:GLU:O	1:F:253:ASP:C	2.58	0.45
1:F:293:ALA:O	1:F:298:GLY:N	2.49	0.45
1:F:351:GLN:O	1:F:352:GLN:C	2.58	0.45
1:B:168:LYS:HD3	1:B:189:VAL:HG23	1.98	0.45
1:C:168:LYS:HD3	1:C:189:VAL:HG23	1.99	0.45
1:E:321:LYS:HB3	1:E:334:ASP:HB3	1.99	0.45
1:F:7:LYS:HZ1	1:F:15:LYS:HE3	1.81	0.45
1:F:420:ILE:HG13	1:F:448:GLU:HG2	1.99	0.45
1:A:420:ILE:HG13	1:A:448:GLU:HG2	1.99	0.45
1:B:423:ALA:HB2	1:B:447:MET:SD	2.56	0.45
1:D:319:GLN:O	1:D:320:ALA:HB3	2.17	0.45
1:D:364:LYS:NZ	1:D:365:LEU:HD13	2.22	0.45
1:E:197:ARG:NH2	1:E:280:GLY:H	2.15	0.45
1:F:321:LYS:HB3	1:F:334:ASP:HB3	1.99	0.45
1:G:350:ARG:HA	1:G:353:ILE:HD12	1.98	0.45
1:A:165:ALA:HB1	1:A:175:ILE:CG2	2.47	0.45
1:B:165:ALA:HB1	1:B:175:ILE:CG2	2.47	0.45
1:C:350:ARG:HA	1:C:353:ILE:HD12	1.98	0.45
1:D:168:LYS:HD3	1:D:189:VAL:HG23	1.98	0.45
1:A:34:LYS:HG3	1:G:114:MET:HG3	1.98	0.44
1:A:195:PHE:O	1:A:330:THR:HG22	2.17	0.44
1:A:362:ARG:NE	1:A:366:GLN:NE2	2.65	0.44
1:B:324:VAL:O	1:B:324:VAL:CG1	2.62	0.44
1:B:346:VAL:HG11	1:B:373:ALA:CB	2.46	0.44
1:B:362:ARG:NE	1:B:366:GLN:NE2	2.65	0.44
1:C:77:VAL:CG1	1:C:510:VAL:HG22	2.47	0.44
1:D:146:GLN:HE21	1:D:146:GLN:CA	2.31	0.44
1:D:195:PHE:O	1:D:330:THR:HG22	2.17	0.44
1:E:168:LYS:HD3	1:E:189:VAL:HG23	1.98	0.44
1:G:213:VAL:O	1:G:215:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:LEU:H	1:G:300:VAL:CG1	2.29	0.44
1:G:346:VAL:HG11	1:G:373:ALA:CB	2.46	0.44
1:A:213:VAL:O	1:A:215:LEU:N	2.50	0.44
1:A:319:GLN:O	1:A:320:ALA:HB3	2.17	0.44
1:A:325:ILE:CG2	1:A:326:ASN:N	2.77	0.44
1:A:350:ARG:HA	1:A:353:ILE:HD12	1.98	0.44
1:B:146:GLN:HE21	1:B:146:GLN:CA	2.31	0.44
1:C:400:LEU:HD23	1:C:400:LEU:C	2.42	0.44
1:E:146:GLN:HE21	1:E:146:GLN:CA	2.31	0.44
1:E:413:ALA:HA	1:E:489:ILE:CD1	2.48	0.44
1:F:197:ARG:NH2	1:F:280:GLY:H	2.15	0.44
1:G:100:ILE:CD1	1:G:514:MET:SD	3.03	0.44
1:B:350:ARG:HA	1:B:353:ILE:HD12	1.98	0.44
1:C:362:ARG:CZ	1:C:366:GLN:HE22	2.29	0.44
1:C:362:ARG:NE	1:C:366:GLN:NE2	2.65	0.44
1:D:282:GLY:CA	1:E:181:THR:C	2.73	0.44
1:D:362:ARG:NE	1:D:366:GLN:NE2	2.65	0.44
1:D:413:ALA:HA	1:D:489:ILE:CD1	2.48	0.44
1:E:400:LEU:C	1:E:400:LEU:HD23	2.42	0.44
1:F:213:VAL:O	1:F:215:LEU:N	2.50	0.44
1:G:319:GLN:O	1:G:320:ALA:HB3	2.17	0.44
1:G:362:ARG:NE	1:G:366:GLN:NE2	2.65	0.44
1:G:400:LEU:HD23	1:G:400:LEU:C	2.42	0.44
1:B:197:ARG:NH2	1:B:280:GLY:H	2.15	0.44
1:D:213:VAL:O	1:D:215:LEU:N	2.51	0.44
1:D:321:LYS:HB3	1:D:334:ASP:HB3	1.99	0.44
1:F:146:GLN:HE21	1:F:146:GLN:CA	2.31	0.44
1:F:413:ALA:HA	1:F:489:ILE:CD1	2.48	0.44
1:G:197:ARG:NH2	1:G:280:GLY:H	2.15	0.44
1:A:400:LEU:HD23	1:A:400:LEU:C	2.42	0.44
1:B:281:PHE:HD2	1:C:386:GLU:CB	2.30	0.44
1:B:321:LYS:HB3	1:B:334:ASP:HB3	1.99	0.44
1:B:433:ASN:HD21	1:B:436:GLN:HG3	1.82	0.44
1:C:346:VAL:HG11	1:C:373:ALA:CB	2.46	0.44
1:C:413:ALA:HA	1:C:489:ILE:CD1	2.48	0.44
1:C:501:ARG:C	1:C:503:ALA:H	2.26	0.44
1:D:197:ARG:NH2	1:D:280:GLY:H	2.15	0.44
1:E:282:GLY:HA2	1:F:181:THR:HA	1.73	0.44
1:E:319:GLN:O	1:E:320:ALA:HB3	2.17	0.44
1:F:277:LYS:HG2	1:F:278:ALA:N	2.32	0.44
1:F:400:LEU:HD23	1:F:400:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:LYS:HB3	1:G:334:ASP:HB3	1.99	0.44
1:A:321:LYS:HB3	1:A:334:ASP:HB3	1.99	0.44
1:B:213:VAL:O	1:B:215:LEU:N	2.50	0.44
1:C:319:GLN:O	1:C:320:ALA:HB3	2.17	0.44
1:C:321:LYS:HB3	1:C:334:ASP:HB3	1.99	0.44
1:E:16:MET:HG2	1:E:70:GLY:HA2	1.99	0.44
1:G:413:ALA:HA	1:G:489:ILE:CD1	2.48	0.44
1:A:146:GLN:HE21	1:A:146:GLN:CA	2.30	0.44
1:A:501:ARG:C	1:A:503:ALA:H	2.26	0.44
1:B:77:VAL:CG1	1:B:510:VAL:HG22	2.47	0.44
1:B:277:LYS:HG2	1:B:278:ALA:N	2.32	0.44
1:B:319:GLN:O	1:B:320:ALA:HB3	2.17	0.44
1:B:360:TYR:HE1	1:C:183:LEU:HD22	1.72	0.44
1:B:400:LEU:HD23	1:B:400:LEU:C	2.42	0.44
1:C:213:VAL:O	1:C:215:LEU:N	2.50	0.44
1:E:213:VAL:O	1:E:215:LEU:N	2.51	0.44
1:E:277:LYS:HG2	1:E:278:ALA:N	2.32	0.44
1:F:195:PHE:O	1:F:330:THR:HG22	2.17	0.44
1:F:339:GLU:O	1:F:343:GLN:HG3	2.18	0.44
1:F:362:ARG:NE	1:F:366:GLN:NE2	2.65	0.44
1:F:433:ASN:HD21	1:F:436:GLN:HG3	1.82	0.44
1:G:146:GLN:HE21	1:G:146:GLN:CA	2.30	0.44
1:G:277:LYS:HG2	1:G:278:ALA:N	2.32	0.44
1:G:339:GLU:O	1:G:343:GLN:HG3	2.18	0.44
1:A:433:ASN:HD21	1:A:436:GLN:HG3	1.82	0.44
1:B:340:ALA:O	1:B:343:GLN:HB2	2.18	0.44
1:C:197:ARG:NH2	1:C:280:GLY:H	2.15	0.44
1:D:16:MET:HG2	1:D:70:GLY:HA2	2.00	0.44
1:E:346:VAL:HG11	1:E:373:ALA:CB	2.46	0.44
1:A:339:GLU:O	1:A:343:GLN:HG3	2.18	0.44
1:C:340:ALA:O	1:C:343:GLN:HB2	2.18	0.44
1:D:277:LYS:HG2	1:D:278:ALA:N	2.32	0.44
1:D:357:THR:OG1	1:D:358:SER:N	2.50	0.44
1:F:319:GLN:O	1:F:320:ALA:HB3	2.17	0.44
1:A:105:LYS:HB3	1:A:105:LYS:HE2	1.80	0.43
1:C:281:PHE:CE2	1:D:385:THR:N	2.85	0.43
1:D:149:THR:HG22	1:D:156:GLU:HA	2.00	0.43
1:D:494:LEU:C	1:D:494:LEU:CD2	2.91	0.43
1:E:339:GLU:O	1:E:343:GLN:HG3	2.18	0.43
1:E:362:ARG:NE	1:E:366:GLN:NE2	2.65	0.43
1:A:277:LYS:HG2	1:A:278:ALA:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ALA:O	1:A:343:GLN:HB2	2.18	0.43
1:A:413:ALA:HA	1:A:489:ILE:CD1	2.48	0.43
1:A:494:LEU:C	1:A:494:LEU:CD2	2.91	0.43
1:A:521:VAL:HB	1:B:40:LEU:HD23	2.00	0.43
1:B:285:ARG:NH1	1:C:386:GLU:OE2	2.50	0.43
1:B:413:ALA:HA	1:B:489:ILE:CD1	2.48	0.43
1:C:146:GLN:HE21	1:C:146:GLN:CA	2.30	0.43
1:F:222:LEU:H	1:F:300:VAL:CG1	2.29	0.43
1:F:351:GLN:O	1:F:354:GLU:N	2.52	0.43
1:G:433:ASN:HD21	1:G:436:GLN:HG3	1.82	0.43
1:B:16:MET:HG2	1:B:70:GLY:HA2	1.99	0.43
1:B:494:LEU:C	1:B:494:LEU:CD2	2.91	0.43
1:C:494:LEU:C	1:C:494:LEU:CD2	2.91	0.43
1:D:417:VAL:HG21	1:D:488:MET:HG3	2.00	0.43
1:D:518:GLU:HB3	1:E:29:VAL:HG21	2.01	0.43
1:F:16:MET:HG2	1:F:70:GLY:HA2	1.99	0.43
1:F:346:VAL:HG11	1:F:373:ALA:CB	2.46	0.43
1:A:32:GLY:CA	1:A:454:ILE:HG12	2.49	0.43
1:A:197:ARG:NH2	1:A:280:GLY:H	2.15	0.43
1:B:282:GLY:HA2	1:C:181:THR:HA	1.64	0.43
1:B:339:GLU:O	1:B:343:GLN:HG3	2.18	0.43
1:C:7:LYS:HZ2	1:C:15:LYS:HE3	1.83	0.43
1:C:16:MET:HG2	1:C:70:GLY:HA2	1.99	0.43
1:D:340:ALA:O	1:D:343:GLN:HB2	2.18	0.43
1:D:363:GLU:CA	1:D:366:GLN:HE21	2.24	0.43
1:D:400:LEU:HD23	1:D:400:LEU:C	2.42	0.43
1:E:205:ILE:HD13	1:E:205:ILE:HA	1.61	0.43
1:E:302:SER:O	1:E:303:GLU:CA	2.64	0.43
1:E:494:LEU:C	1:E:494:LEU:CD2	2.91	0.43
1:F:69:MET:HE2	1:G:39:VAL:CG1	2.40	0.43
1:F:494:LEU:CD2	1:F:494:LEU:C	2.91	0.43
1:A:351:GLN:O	1:A:354:GLU:N	2.52	0.43
1:C:32:GLY:CA	1:C:454:ILE:HG12	2.49	0.43
1:D:351:GLN:O	1:D:354:GLU:N	2.52	0.43
1:E:149:THR:HG22	1:E:156:GLU:HA	2.00	0.43
1:E:501:ARG:C	1:E:503:ALA:H	2.26	0.43
1:F:501:ARG:C	1:F:503:ALA:H	2.26	0.43
1:G:81:ALA:O	1:G:82:ASN:C	2.62	0.43
1:G:107:VAL:CG2	1:G:515:ILE:HG23	2.49	0.43
1:A:81:ALA:O	1:A:82:ASN:C	2.62	0.43
1:C:277:LYS:HG2	1:C:278:ALA:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:PHE:HE2	1:D:385:THR:N	2.13	0.43
1:C:325:ILE:CG2	1:C:326:ASN:N	2.77	0.43
1:C:351:GLN:O	1:C:354:GLU:N	2.52	0.43
1:D:300:VAL:CG1	1:D:301:ILE:N	2.82	0.43
1:E:183:LEU:HA	1:E:383:ALA:O	2.19	0.43
1:E:300:VAL:CG1	1:E:301:ILE:N	2.82	0.43
1:F:349:ILE:CG2	1:F:365:LEU:HG	2.49	0.43
1:F:353:ILE:HG23	1:F:362:ARG:HG2	2.01	0.43
1:G:16:MET:HG2	1:G:70:GLY:HA2	1.99	0.43
1:G:340:ALA:O	1:G:343:GLN:HB2	2.18	0.43
1:A:352:GLN:HA	1:A:355:GLU:HG2	2.01	0.43
1:B:281:PHE:HZ	1:C:389:MET:HB2	1.71	0.43
1:B:351:GLN:O	1:B:354:GLU:N	2.52	0.43
1:C:107:VAL:CG2	1:C:515:ILE:HG23	2.49	0.43
1:C:149:THR:HG22	1:C:156:GLU:HA	2.00	0.43
1:C:183:LEU:HA	1:C:383:ALA:O	2.19	0.43
1:C:353:ILE:HG23	1:C:362:ARG:HG2	2.01	0.43
1:C:417:VAL:HG21	1:C:488:MET:HG3	2.00	0.43
1:C:433:ASN:HD21	1:C:436:GLN:HG3	1.82	0.43
1:D:27:VAL:HG13	1:D:53:GLY:O	2.19	0.43
1:D:302:SER:O	1:D:303:GLU:CA	2.64	0.43
1:D:339:GLU:O	1:D:343:GLN:HG3	2.18	0.43
1:D:346:VAL:HG11	1:D:373:ALA:CB	2.46	0.43
1:D:349:ILE:CG2	1:D:365:LEU:HG	2.49	0.43
1:E:27:VAL:HG13	1:E:53:GLY:O	2.19	0.43
1:F:81:ALA:O	1:F:82:ASN:C	2.62	0.43
1:F:300:VAL:CG1	1:F:301:ILE:N	2.82	0.43
1:F:357:THR:OG1	1:F:358:SER:N	2.50	0.43
1:F:365:LEU:HD12	1:F:365:LEU:HA	1.86	0.43
1:G:302:SER:O	1:G:303:GLU:CA	2.64	0.43
1:G:494:LEU:C	1:G:494:LEU:CD2	2.91	0.43
1:A:46:ALA:HA	1:A:47:PRO:HD2	1.86	0.43
1:A:77:VAL:CG1	1:A:510:VAL:HG22	2.46	0.43
1:B:149:THR:HG22	1:B:156:GLU:HA	2.00	0.43
1:B:302:SER:O	1:B:303:GLU:CA	2.64	0.43
1:D:12:ALA:HA	1:D:520:MET:HE2	2.00	0.43
1:D:107:VAL:CG2	1:D:515:ILE:HG23	2.49	0.43
1:E:417:VAL:HG21	1:E:488:MET:HG3	2.00	0.43
1:E:433:ASN:HD21	1:E:436:GLN:HG3	1.82	0.43
1:F:32:GLY:CA	1:F:454:ILE:HG12	2.49	0.43
1:F:149:THR:HG22	1:F:156:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:SER:O	1:F:303:GLU:CA	2.64	0.43
1:F:340:ALA:O	1:F:343:GLN:HB2	2.18	0.43
1:G:149:THR:HG22	1:G:156:GLU:HA	2.00	0.43
1:G:183:LEU:HA	1:G:383:ALA:O	2.19	0.43
1:G:501:ARG:C	1:G:503:ALA:H	2.26	0.43
1:A:16:MET:HG2	1:A:70:GLY:HA2	1.99	0.43
1:A:16:MET:HG2	1:A:70:GLY:CA	2.49	0.43
1:A:349:ILE:CG2	1:A:365:LEU:HG	2.49	0.43
1:B:353:ILE:HG23	1:B:362:ARG:HG2	2.01	0.43
1:B:417:VAL:HG21	1:B:488:MET:HG3	2.00	0.43
1:C:164:GLU:O	1:C:168:LYS:HB2	2.19	0.43
1:C:345:ARG:O	1:C:348:GLN:HB3	2.19	0.43
1:C:349:ILE:CG2	1:C:365:LEU:HG	2.49	0.43
1:D:151:SER:C	1:D:153:ASN:H	2.26	0.43
1:D:406:ALA:HB2	1:D:496:PRO:HG3	2.01	0.43
1:E:40:LEU:HD13	1:E:59:GLU:HG3	2.01	0.43
1:E:112:ASN:ND2	1:F:458:CYS:O	2.45	0.43
1:E:151:SER:C	1:E:153:ASN:H	2.26	0.43
1:F:40:LEU:HD13	1:F:59:GLU:HG3	2.01	0.43
1:F:164:GLU:O	1:F:168:LYS:HB2	2.19	0.43
1:G:345:ARG:O	1:G:348:GLN:HB3	2.19	0.43
1:G:351:GLN:O	1:G:354:GLU:N	2.52	0.43
1:A:302:SER:O	1:A:303:GLU:CA	2.64	0.43
1:A:406:ALA:HB2	1:A:496:PRO:HG3	2.01	0.43
1:B:40:LEU:HD13	1:B:59:GLU:HG3	2.01	0.43
1:B:81:ALA:O	1:B:82:ASN:C	2.62	0.43
1:B:352:GLN:HA	1:B:355:GLU:HG2	2.01	0.43
1:C:16:MET:HG2	1:C:70:GLY:CA	2.49	0.43
1:C:40:LEU:HD13	1:C:59:GLU:HG3	2.01	0.43
1:C:300:VAL:CG1	1:C:301:ILE:N	2.82	0.43
1:D:32:GLY:CA	1:D:454:ILE:HG12	2.49	0.43
1:D:324:VAL:HB	1:D:331:THR:OG1	2.19	0.43
1:D:352:GLN:HA	1:D:355:GLU:HG2	2.01	0.43
1:E:12:ALA:HA	1:E:520:MET:HE2	2.00	0.43
1:E:81:ALA:O	1:E:82:ASN:C	2.62	0.43
1:E:107:VAL:CG2	1:E:515:ILE:HG23	2.49	0.43
1:E:406:ALA:HB2	1:E:496:PRO:HG3	2.01	0.43
1:F:27:VAL:HG13	1:F:53:GLY:O	2.19	0.43
1:G:40:LEU:HD13	1:G:59:GLU:HG3	2.01	0.43
1:A:149:THR:HG22	1:A:156:GLU:HA	2.00	0.42
1:A:340:ALA:HA	1:A:343:GLN:CG	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:CA	1:A:366:GLN:HE21	2.24	0.42
1:B:324:VAL:HB	1:B:331:THR:OG1	2.19	0.42
1:B:406:ALA:HB2	1:B:496:PRO:HG3	2.01	0.42
1:C:17:LEU:HD13	1:C:104:LEU:HD12	2.01	0.42
1:C:27:VAL:HG13	1:C:53:GLY:O	2.19	0.42
1:C:281:PHE:CE2	1:D:385:THR:O	2.66	0.42
1:C:339:GLU:O	1:C:343:GLN:HG3	2.18	0.42
1:D:40:LEU:HD13	1:D:59:GLU:HG3	2.01	0.42
1:D:281:PHE:O	1:D:284:ARG:HB2	2.19	0.42
1:E:340:ALA:O	1:E:343:GLN:HB2	2.18	0.42
1:E:351:GLN:O	1:E:354:GLU:N	2.52	0.42
1:F:406:ALA:HB2	1:F:496:PRO:HG3	2.01	0.42
1:G:27:VAL:HG13	1:G:53:GLY:O	2.19	0.42
1:G:197:ARG:HA	1:G:197:ARG:HD3	1.80	0.42
1:G:353:ILE:HG23	1:G:362:ARG:HG2	2.01	0.42
1:G:364:LYS:HG3	1:G:365:LEU:N	2.34	0.42
1:G:406:ALA:HB2	1:G:496:PRO:HG3	2.01	0.42
1:A:183:LEU:HA	1:A:383:ALA:O	2.19	0.42
1:A:218:PRO:HG3	1:A:323:VAL:HG23	2.02	0.42
1:A:357:THR:OG1	1:A:358:SER:N	2.50	0.42
1:A:417:VAL:HG21	1:A:488:MET:HG3	2.00	0.42
1:B:164:GLU:O	1:B:168:LYS:HB2	2.19	0.42
1:B:218:PRO:HG3	1:B:323:VAL:HG23	2.01	0.42
1:B:349:ILE:CG2	1:B:365:LEU:HG	2.49	0.42
1:C:82:ASN:HD21	1:C:89:THR:N	1.97	0.42
1:C:352:GLN:HA	1:C:355:GLU:HG2	2.01	0.42
1:C:406:ALA:HB2	1:C:496:PRO:HG3	2.01	0.42
1:E:17:LEU:HD13	1:E:104:LEU:HD12	2.01	0.42
1:E:164:GLU:O	1:E:168:LYS:HB2	2.19	0.42
1:E:349:ILE:CG2	1:E:365:LEU:HG	2.49	0.42
1:F:17:LEU:HD13	1:F:104:LEU:HD12	2.01	0.42
1:G:164:GLU:O	1:G:168:LYS:HB2	2.19	0.42
1:G:218:PRO:HG3	1:G:323:VAL:HG23	2.02	0.42
1:G:324:VAL:HB	1:G:331:THR:OG1	2.19	0.42
1:G:352:GLN:HA	1:G:355:GLU:HG2	2.01	0.42
1:A:27:VAL:HG13	1:A:53:GLY:O	2.19	0.42
1:A:40:LEU:HD13	1:A:59:GLU:HG3	2.01	0.42
1:A:94:VAL:HG12	1:A:449:ALA:HB1	2.01	0.42
1:A:107:VAL:CG2	1:A:515:ILE:HG23	2.49	0.42
1:B:17:LEU:HD13	1:B:104:LEU:HD12	2.01	0.42
1:B:501:ARG:C	1:B:503:ALA:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:PHE:O	1:C:284:ARG:HB2	2.19	0.42
1:E:286:LYS:HE2	1:E:286:LYS:HB3	1.77	0.42
1:E:353:ILE:HG23	1:E:362:ARG:HG2	2.01	0.42
1:G:32:GLY:CA	1:G:454:ILE:HG12	2.49	0.42
1:G:300:VAL:CG1	1:G:301:ILE:N	2.82	0.42
1:G:349:ILE:CG2	1:G:365:LEU:HG	2.49	0.42
1:G:417:VAL:HG21	1:G:488:MET:HG3	2.00	0.42
1:A:151:SER:C	1:A:153:ASN:H	2.26	0.42
1:A:364:LYS:HG3	1:A:365:LEU:N	2.34	0.42
1:B:340:ALA:HA	1:B:343:GLN:CG	2.42	0.42
1:B:360:TYR:CZ	1:C:183:LEU:HD13	2.52	0.42
1:C:338:GLU:O	1:C:339:GLU:C	2.62	0.42
1:D:94:VAL:HG12	1:D:449:ALA:HB1	2.01	0.42
1:D:340:ALA:HA	1:D:343:GLN:CG	2.42	0.42
1:D:345:ARG:O	1:D:348:GLN:HB3	2.19	0.42
1:E:32:GLY:CA	1:E:454:ILE:HG12	2.49	0.42
1:E:325:ILE:CG2	1:E:326:ASN:N	2.77	0.42
1:E:352:GLN:HA	1:E:355:GLU:HG2	2.01	0.42
1:F:16:MET:HG2	1:F:70:GLY:CA	2.49	0.42
1:F:205:ILE:HD13	1:F:205:ILE:HA	1.61	0.42
1:F:417:VAL:HG21	1:F:488:MET:HG3	2.00	0.42
1:G:16:MET:HG2	1:G:70:GLY:CA	2.49	0.42
1:G:17:LEU:HD13	1:G:104:LEU:HD12	2.01	0.42
1:G:46:ALA:HA	1:G:47:PRO:HD2	1.86	0.42
1:A:61:GLU:HA	1:A:68:ASN:ND2	2.35	0.42
1:A:345:ARG:O	1:A:348:GLN:HB3	2.19	0.42
1:B:32:GLY:CA	1:B:454:ILE:HG12	2.49	0.42
1:B:94:VAL:HG12	1:B:449:ALA:HB1	2.01	0.42
1:B:107:VAL:CG2	1:B:515:ILE:HG23	2.49	0.42
1:B:183:LEU:HA	1:B:383:ALA:O	2.19	0.42
1:C:61:GLU:HA	1:C:68:ASN:ND2	2.35	0.42
1:C:81:ALA:O	1:C:82:ASN:C	2.62	0.42
1:D:17:LEU:HD13	1:D:104:LEU:HD12	2.01	0.42
1:D:81:ALA:O	1:D:82:ASN:C	2.62	0.42
1:E:16:MET:HG2	1:E:70:GLY:CA	2.49	0.42
1:F:107:VAL:CG2	1:F:515:ILE:HG23	2.49	0.42
1:F:218:PRO:HG3	1:F:323:VAL:HG23	2.01	0.42
1:F:324:VAL:HB	1:F:331:THR:OG1	2.19	0.42
1:F:352:GLN:HA	1:F:355:GLU:HG2	2.01	0.42
1:G:94:VAL:HG12	1:G:449:ALA:HB1	2.01	0.42
1:A:12:ALA:HA	1:A:520:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD13	1:A:104:LEU:HD12	2.01	0.42
1:B:61:GLU:HA	1:B:68:ASN:ND2	2.35	0.42
1:B:281:PHE:O	1:B:284:ARG:HB2	2.19	0.42
1:C:94:VAL:HG12	1:C:449:ALA:HB1	2.01	0.42
1:C:340:ALA:HA	1:C:343:GLN:CG	2.42	0.42
1:C:364:LYS:HG3	1:C:365:LEU:N	2.34	0.42
1:D:281:PHE:CZ	1:E:389:MET:HB2	2.55	0.42
1:D:487:ASN:HB3	1:D:490:ASP:HB2	2.02	0.42
1:E:222:LEU:H	1:E:300:VAL:CG1	2.29	0.42
1:E:434:GLU:O	1:E:437:ASN:N	2.50	0.42
1:F:183:LEU:HA	1:F:383:ALA:O	2.19	0.42
1:G:293:ALA:HB1	1:G:298:GLY:HA3	2.02	0.42
1:A:281:PHE:O	1:A:284:ARG:HB2	2.19	0.42
1:B:27:VAL:HG13	1:B:53:GLY:O	2.19	0.42
1:B:221:LEU:HD12	1:B:300:VAL:CG1	2.39	0.42
1:C:46:ALA:HA	1:C:47:PRO:HD2	1.86	0.42
1:D:21:ASN:O	1:D:25:ASP:HB2	2.20	0.42
1:D:183:LEU:HA	1:D:383:ALA:O	2.19	0.42
1:D:501:ARG:C	1:D:503:ALA:H	2.26	0.42
1:E:94:VAL:HG12	1:E:449:ALA:HB1	2.01	0.42
1:E:281:PHE:HD2	1:F:386:GLU:CB	2.32	0.42
1:E:293:ALA:HB1	1:E:298:GLY:HA3	2.02	0.42
1:E:487:ASN:HB3	1:E:490:ASP:HB2	2.02	0.42
1:F:151:SER:C	1:F:153:ASN:H	2.26	0.42
1:F:214:GLU:HA	1:F:324:VAL:HA	2.01	0.42
1:F:293:ALA:HB1	1:F:298:GLY:HA3	2.02	0.42
1:F:487:ASN:HB3	1:F:490:ASP:HB2	2.02	0.42
1:G:281:PHE:O	1:G:284:ARG:HB2	2.19	0.42
1:A:21:ASN:O	1:A:25:ASP:HB2	2.20	0.42
1:A:338:GLU:O	1:A:339:GLU:C	2.62	0.42
1:B:21:ASN:O	1:B:25:ASP:HB2	2.20	0.42
1:B:345:ARG:O	1:B:348:GLN:HB3	2.19	0.42
1:C:21:ASN:O	1:C:25:ASP:HB2	2.20	0.42
1:C:218:PRO:HG3	1:C:323:VAL:HG23	2.02	0.42
1:C:487:ASN:HB3	1:C:490:ASP:HB2	2.02	0.42
1:D:164:GLU:O	1:D:168:LYS:HB2	2.19	0.42
1:D:433:ASN:HD21	1:D:436:GLN:HG3	1.82	0.42
1:E:214:GLU:HA	1:E:324:VAL:HA	2.01	0.42
1:E:281:PHE:O	1:E:284:ARG:HB2	2.19	0.42
1:E:324:VAL:HB	1:E:331:THR:OG1	2.19	0.42
1:E:338:GLU:O	1:E:339:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:345:ARG:O	1:F:348:GLN:HB3	2.19	0.42
1:G:430:ARG:HD2	1:G:430:ARG:N	2.35	0.42
1:A:353:ILE:HG23	1:A:362:ARG:HG2	2.01	0.42
1:A:422:VAL:C	1:A:424:SER:H	2.28	0.42
1:B:16:MET:HG2	1:B:70:GLY:CA	2.49	0.42
1:C:151:SER:C	1:C:153:ASN:H	2.26	0.42
1:D:16:MET:HG2	1:D:70:GLY:CA	2.49	0.42
1:D:293:ALA:HB1	1:D:298:GLY:HA3	2.02	0.42
1:D:353:ILE:HG23	1:D:362:ARG:HG2	2.01	0.42
1:F:94:VAL:HG12	1:F:449:ALA:HB1	2.01	0.42
1:G:12:ALA:HA	1:G:520:MET:HE2	2.00	0.42
1:A:293:ALA:HB1	1:A:298:GLY:HA3	2.02	0.42
1:C:12:ALA:HA	1:C:520:MET:HE2	2.00	0.42
1:C:293:ALA:HB1	1:C:298:GLY:HA3	2.02	0.42
1:C:300:VAL:HG23	1:C:317:LEU:HA	2.02	0.42
1:C:324:VAL:HB	1:C:331:THR:OG1	2.19	0.42
1:D:364:LYS:HG3	1:D:365:LEU:N	2.34	0.42
1:E:300:VAL:HG23	1:E:317:LEU:HA	2.02	0.42
1:F:281:PHE:O	1:F:284:ARG:HB2	2.19	0.42
1:F:364:LYS:HG3	1:F:365:LEU:N	2.34	0.42
1:G:338:GLU:O	1:G:339:GLU:C	2.62	0.42
1:G:422:VAL:C	1:G:424:SER:H	2.28	0.42
1:A:324:VAL:HB	1:A:331:THR:OG1	2.19	0.41
1:B:151:SER:C	1:B:153:ASN:H	2.26	0.41
1:B:293:ALA:HB1	1:B:298:GLY:HA3	2.02	0.41
1:B:338:GLU:O	1:B:339:GLU:C	2.62	0.41
1:B:487:ASN:HB3	1:B:490:ASP:HB2	2.02	0.41
1:C:105:LYS:HB3	1:C:105:LYS:HE2	1.80	0.41
1:C:214:GLU:HA	1:C:324:VAL:HA	2.01	0.41
1:C:302:SER:O	1:C:303:GLU:CA	2.64	0.41
1:C:430:ARG:HD2	1:C:430:ARG:N	2.35	0.41
1:D:61:GLU:HA	1:D:68:ASN:ND2	2.35	0.41
1:E:21:ASN:O	1:E:25:ASP:HB2	2.20	0.41
1:E:430:ARG:HD2	1:E:430:ARG:N	2.35	0.41
1:F:434:GLU:O	1:F:437:ASN:N	2.50	0.41
1:G:21:ASN:O	1:G:25:ASP:HB2	2.20	0.41
1:G:434:GLU:O	1:G:437:ASN:N	2.50	0.41
1:A:164:GLU:O	1:A:168:LYS:HB2	2.19	0.41
1:A:300:VAL:CG1	1:A:301:ILE:N	2.82	0.41
1:B:214:GLU:HA	1:B:324:VAL:HA	2.01	0.41
1:B:430:ARG:HD2	1:B:430:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:GLU:HA	1:D:324:VAL:HA	2.01	0.41
1:E:218:PRO:HG3	1:E:323:VAL:HG23	2.01	0.41
1:F:300:VAL:HG12	1:F:301:ILE:N	2.35	0.41
1:G:61:GLU:HA	1:G:68:ASN:ND2	2.35	0.41
1:G:214:GLU:HA	1:G:324:VAL:HA	2.01	0.41
1:G:300:VAL:HG23	1:G:317:LEU:HA	2.02	0.41
1:D:300:VAL:HG12	1:D:301:ILE:N	2.35	0.41
1:D:422:VAL:C	1:D:424:SER:H	2.28	0.41
1:E:345:ARG:O	1:E:348:GLN:HB3	2.19	0.41
1:F:61:GLU:HA	1:F:68:ASN:ND2	2.35	0.41
1:G:151:SER:C	1:G:153:ASN:H	2.26	0.41
1:A:158:VAL:HG13	1:A:396:VAL:HG22	2.02	0.41
1:A:300:VAL:HG12	1:A:301:ILE:N	2.35	0.41
1:B:46:ALA:HA	1:B:47:PRO:HD2	1.86	0.41
1:B:300:VAL:HG12	1:B:301:ILE:N	2.35	0.41
1:D:338:GLU:O	1:D:339:GLU:C	2.62	0.41
1:F:12:ALA:HA	1:F:520:MET:HE2	2.01	0.41
1:F:338:GLU:O	1:F:339:GLU:C	2.62	0.41
1:F:430:ARG:HD2	1:F:430:ARG:N	2.35	0.41
1:G:77:VAL:CG1	1:G:510:VAL:HG22	2.46	0.41
1:A:214:GLU:HA	1:A:324:VAL:HA	2.01	0.41
1:B:12:ALA:HA	1:B:520:MET:HE2	2.01	0.41
1:B:250:ILE:O	1:B:250:ILE:HG22	2.21	0.41
1:C:158:VAL:HG13	1:C:396:VAL:HG22	2.02	0.41
1:D:430:ARG:HD2	1:D:430:ARG:N	2.35	0.41
1:E:360:TYR:CZ	1:F:183:LEU:HD22	2.53	0.41
1:E:364:LYS:HG3	1:E:365:LEU:N	2.34	0.41
1:E:516:THR:O	1:F:36:ARG:HB3	2.20	0.41
1:F:21:ASN:O	1:F:25:ASP:HB2	2.20	0.41
1:F:431:GLY:H	1:F:437:ASN:ND2	2.19	0.41
1:G:82:ASN:HD21	1:G:89:THR:N	1.97	0.41
1:G:340:ALA:HA	1:G:343:GLN:CG	2.42	0.41
1:G:487:ASN:HB3	1:G:490:ASP:HB2	2.02	0.41
1:A:250:ILE:O	1:A:250:ILE:HG22	2.21	0.41
1:C:363:GLU:CA	1:C:366:GLN:HE21	2.24	0.41
1:D:158:VAL:HG13	1:D:396:VAL:HG22	2.03	0.41
1:D:218:PRO:HG3	1:D:323:VAL:HG23	2.02	0.41
1:E:61:GLU:HA	1:E:68:ASN:ND2	2.35	0.41
1:G:250:ILE:O	1:G:250:ILE:HG22	2.21	0.41
1:G:365:LEU:HD12	1:G:365:LEU:HA	1.86	0.41
1:G:431:GLY:H	1:G:437:ASN:ND2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG13	1:B:396:VAL:HG22	2.03	0.41
1:B:300:VAL:HG23	1:B:317:LEU:HA	2.02	0.41
1:C:126:VAL:HG11	1:C:426:LEU:HD22	2.03	0.41
1:D:126:VAL:HG11	1:D:426:LEU:HD22	2.03	0.41
1:E:187:LEU:HD13	1:E:379:ILE:HG12	2.03	0.41
1:F:422:VAL:C	1:F:424:SER:H	2.28	0.41
1:G:300:VAL:HG12	1:G:301:ILE:N	2.35	0.41
1:A:413:ALA:HB2	1:A:475:ASN:CB	2.51	0.41
1:A:430:ARG:HD2	1:A:430:ARG:N	2.35	0.41
1:A:431:GLY:H	1:A:437:ASN:ND2	2.19	0.41
1:B:281:PHE:CD1	1:C:389:MET:HE2	2.55	0.41
1:B:300:VAL:CG1	1:B:301:ILE:N	2.82	0.41
1:B:422:VAL:C	1:B:424:SER:H	2.28	0.41
1:B:431:GLY:H	1:B:437:ASN:ND2	2.19	0.41
1:B:434:GLU:O	1:B:437:ASN:N	2.50	0.41
1:C:250:ILE:HG22	1:C:250:ILE:O	2.21	0.41
1:D:413:ALA:HB2	1:D:475:ASN:CB	2.51	0.41
1:E:158:VAL:HG13	1:E:396:VAL:HG22	2.02	0.41
1:E:443:ALA:O	1:E:446:ALA:HB3	2.20	0.41
1:F:281:PHE:CE2	1:G:385:THR:O	2.67	0.41
1:G:443:ALA:O	1:G:446:ALA:HB3	2.20	0.41
1:A:49:ILE:HD11	1:G:73:MET:HG2	2.03	0.41
1:A:187:LEU:HD13	1:A:379:ILE:HG12	2.03	0.41
1:A:205:ILE:HD11	1:A:211:GLY:HA2	2.03	0.41
1:A:443:ALA:O	1:A:446:ALA:HB3	2.20	0.41
1:B:126:VAL:HG11	1:B:426:LEU:HD22	2.03	0.41
1:B:187:LEU:HD13	1:B:379:ILE:HG12	2.03	0.41
1:B:205:ILE:HD11	1:B:211:GLY:HA2	2.03	0.41
1:B:205:ILE:HD13	1:B:205:ILE:HA	1.61	0.41
1:B:413:ALA:HB2	1:B:475:ASN:CB	2.51	0.41
1:B:431:GLY:H	1:B:437:ASN:HD21	1.68	0.41
1:B:443:ALA:O	1:B:446:ALA:HB3	2.20	0.41
1:B:513:LEU:HD22	1:C:49:ILE:HG21	2.02	0.41
1:C:187:LEU:HD13	1:C:379:ILE:HG12	2.03	0.41
1:C:205:ILE:HD11	1:C:211:GLY:HA2	2.03	0.41
1:C:300:VAL:HG12	1:C:301:ILE:N	2.36	0.41
1:C:357:THR:OG1	1:C:358:SER:N	2.50	0.41
1:C:422:VAL:C	1:C:424:SER:H	2.28	0.41
1:C:431:GLY:H	1:C:437:ASN:ND2	2.19	0.41
1:C:434:GLU:O	1:C:437:ASN:N	2.50	0.41
1:D:187:LEU:HD13	1:D:379:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ILE:HD11	1:D:211:GLY:HA2	2.03	0.41
1:D:219:PHE:HA	1:D:318:GLY:O	2.21	0.41
1:D:434:GLU:O	1:D:435:ASP:C	2.64	0.41
1:E:126:VAL:HG11	1:E:426:LEU:HD22	2.03	0.41
1:E:219:PHE:HA	1:E:318:GLY:O	2.21	0.41
1:E:413:ALA:HB2	1:E:475:ASN:CB	2.51	0.41
1:E:422:VAL:C	1:E:424:SER:H	2.28	0.41
1:F:205:ILE:HD11	1:F:211:GLY:HA2	2.03	0.41
1:F:250:ILE:HG22	1:F:250:ILE:O	2.21	0.41
1:F:413:ALA:HB2	1:F:475:ASN:CB	2.51	0.41
1:F:443:ALA:O	1:F:446:ALA:HB3	2.20	0.41
1:G:158:VAL:HG13	1:G:396:VAL:HG22	2.03	0.41
1:G:205:ILE:HD11	1:G:211:GLY:HA2	2.03	0.41
1:G:413:ALA:HB2	1:G:475:ASN:CB	2.51	0.41
1:A:281:PHE:HD2	1:B:386:GLU:HB2	1.86	0.41
1:B:364:LYS:HG3	1:B:365:LEU:N	2.34	0.41
1:C:413:ALA:HB2	1:C:475:ASN:CB	2.51	0.41
1:C:431:GLY:H	1:C:437:ASN:HD21	1.69	0.41
1:D:443:ALA:O	1:D:446:ALA:HB3	2.20	0.41
1:E:205:ILE:HD11	1:E:211:GLY:HA2	2.03	0.41
1:E:431:GLY:H	1:E:437:ASN:ND2	2.19	0.41
1:F:126:VAL:HG11	1:F:426:LEU:HD22	2.03	0.41
1:F:158:VAL:HG13	1:F:396:VAL:HG22	2.03	0.41
1:F:187:LEU:HD13	1:F:379:ILE:HG12	2.03	0.41
1:A:40:LEU:CD2	1:G:521:VAL:HB	2.48	0.40
1:C:219:PHE:HA	1:C:318:GLY:O	2.21	0.40
1:C:443:ALA:O	1:C:446:ALA:HB3	2.20	0.40
1:C:520:MET:HA	1:D:39:VAL:HB	2.02	0.40
1:D:46:ALA:HA	1:D:47:PRO:HD2	1.86	0.40
1:D:69:MET:HE3	1:E:41:ASP:HB2	2.02	0.40
1:D:205:ILE:HD13	1:D:205:ILE:HA	1.61	0.40
1:D:431:GLY:H	1:D:437:ASN:ND2	2.19	0.40
1:A:205:ILE:HD13	1:A:205:ILE:HA	1.61	0.40
1:A:487:ASN:HB3	1:A:490:ASP:HB2	2.02	0.40
1:B:349:ILE:HG21	1:B:369:VAL:CG1	2.52	0.40
1:E:176:THR:HB	1:E:378:VAL:HG22	2.03	0.40
1:F:35:GLY:O	1:F:51:LYS:NZ	2.53	0.40
1:F:431:GLY:H	1:F:437:ASN:HD21	1.68	0.40
1:G:187:LEU:HD13	1:G:379:ILE:HG12	2.03	0.40
1:A:514:MET:HE2	1:A:514:MET:HB3	1.88	0.40
1:C:123:ALA:HA	1:C:429:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LEU:O	1:C:184:GLN:C	2.64	0.40
1:C:404:ARG:HA	1:C:404:ARG:HD2	1.91	0.40
1:D:123:ALA:HA	1:D:429:LEU:HD21	2.04	0.40
1:D:183:LEU:O	1:D:184:GLN:C	2.64	0.40
1:E:434:GLU:O	1:E:435:ASP:C	2.64	0.40
1:F:176:THR:HB	1:F:378:VAL:HG22	2.03	0.40
1:F:219:PHE:HA	1:F:318:GLY:O	2.21	0.40
1:F:477:GLY:O	1:F:485:TYR:HA	2.22	0.40
1:G:176:THR:HB	1:G:378:VAL:HG22	2.03	0.40
1:A:35:GLY:O	1:A:51:LYS:NZ	2.53	0.40
1:A:126:VAL:HG11	1:A:426:LEU:HD22	2.03	0.40
1:B:179:ASP:OD1	1:B:389:MET:SD	2.80	0.40
1:C:453:GLN:O	1:C:454:ILE:C	2.65	0.40
1:D:366:GLN:O	1:D:369:VAL:HG22	2.21	0.40
1:E:340:ALA:HA	1:E:343:GLN:CG	2.42	0.40
1:E:347:ALA:O	1:E:350:ARG:HB2	2.22	0.40
1:E:453:GLN:O	1:E:454:ILE:C	2.65	0.40
1:F:179:ASP:OD1	1:F:389:MET:SD	2.80	0.40
1:F:197:ARG:HA	1:F:197:ARG:HD3	1.81	0.40
1:G:183:LEU:O	1:G:184:GLN:C	2.64	0.40
1:G:349:ILE:HG21	1:G:369:VAL:CG1	2.52	0.40
1:G:477:GLY:O	1:G:485:TYR:HA	2.22	0.40
1:A:123:ALA:HA	1:A:429:LEU:HD21	2.04	0.40
1:A:179:ASP:OD1	1:A:389:MET:SD	2.80	0.40
1:A:219:PHE:HA	1:A:318:GLY:O	2.21	0.40
1:A:346:VAL:HG13	1:A:369:VAL:HB	2.03	0.40
1:A:453:GLN:O	1:A:454:ILE:C	2.65	0.40
1:B:123:ALA:HA	1:B:429:LEU:HD21	2.04	0.40
1:B:346:VAL:HG13	1:B:369:VAL:HB	2.03	0.40
1:C:346:VAL:HG13	1:C:369:VAL:HB	2.03	0.40
1:C:347:ALA:O	1:C:350:ARG:HB2	2.22	0.40
1:D:176:THR:HB	1:D:378:VAL:HG22	2.03	0.40
1:D:353:ILE:HA	1:D:356:ALA:HB2	2.03	0.40
1:E:300:VAL:HG12	1:E:301:ILE:N	2.35	0.40
1:E:451:LEU:O	1:E:452:ARG:C	2.64	0.40
1:F:46:ALA:HA	1:F:47:PRO:HD2	1.87	0.40
1:F:199:TYR:HD1	1:F:199:TYR:O	2.04	0.40
1:G:219:PHE:HA	1:G:318:GLY:O	2.21	0.40
1:G:346:VAL:HG13	1:G:369:VAL:HB	2.03	0.40
1:G:347:ALA:O	1:G:350:ARG:HB2	2.22	0.40

All (75) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:SER:OG	1:G:169:VAL:CB[5_455]	0.65	1.55
1:C:358:SER:CB	1:G:169:VAL:CA[5_455]	0.74	1.46
1:C:358:SER:CA	1:G:169:VAL:CA[5_455]	0.89	1.31
1:C:359:ASP:N	1:G:170:GLY:H[5_455]	0.31	1.29
1:C:359:ASP:CB	1:G:167:ASP:CA[5_455]	0.97	1.23
1:E:338:GLU:CD	1:E:338:GLU:CD[3_454]	1.00	1.20
1:C:359:ASP:CG	1:G:167:ASP:N[5_455]	1.02	1.18
1:C:359:ASP:OD2	1:G:166:MET:C[5_455]	1.08	1.12
1:E:338:GLU:CD	1:E:338:GLU:OE1[3_454]	1.14	1.06
1:E:338:GLU:CB	1:E:338:GLU:CB[3_454]	1.15	1.05
1:G:340:ALA:CB	1:G:340:ALA:CB[3_554]	1.15	1.05
1:E:338:GLU:CG	1:E:338:GLU:CG[3_454]	1.20	1.00
1:C:358:SER:CB	1:G:169:VAL:N[5_455]	1.23	0.97
1:C:359:ASP:N	1:G:170:GLY:N[5_455]	1.26	0.94
1:C:359:ASP:CG	1:G:166:MET:C[5_455]	1.26	0.94
1:C:359:ASP:OD2	1:G:166:MET:CA[5_455]	1.27	0.93
1:C:359:ASP:OD2	1:G:167:ASP:N[5_455]	1.29	0.91
1:E:338:GLU:CB	1:E:338:GLU:CG[3_454]	1.32	0.88
1:C:358:SER:OG	1:G:169:VAL:CG1[5_455]	1.35	0.85
1:B:137:PRO:CD	1:E:132:LYS:O[5_555]	1.37	0.83
1:E:338:GLU:CG	1:E:338:GLU:CD[3_454]	1.42	0.78
1:C:359:ASP:CB	1:G:167:ASP:N[5_455]	1.46	0.74
1:C:357:THR:OG1	1:G:168:LYS:O[5_455]	1.49	0.71
1:C:359:ASP:OD1	1:G:165:ALA:O[5_455]	1.49	0.71
1:C:359:ASP:CA	1:G:166:MET:O[5_455]	1.52	0.68
1:C:359:ASP:OD2	1:G:166:MET:N[5_455]	1.55	0.65
1:C:359:ASP:OD1	1:G:168:LYS:N[5_455]	1.55	0.65
1:C:358:SER:N	1:G:168:LYS:O[5_455]	1.59	0.61
1:B:135:SER:O	1:E:133:ALA:CB[5_555]	1.60	0.60
1:E:338:GLU:OE1	1:E:338:GLU:OE1[3_454]	1.61	0.59
1:E:338:GLU:OE1	1:E:338:GLU:OE2[3_454]	1.61	0.59
1:C:357:THR:O	1:G:169:VAL:CG2[5_455]	1.62	0.58
1:C:358:SER:CB	1:G:169:VAL:CB[5_455]	1.62	0.58
1:C:358:SER:CA	1:G:169:VAL:C[5_455]	1.62	0.58
1:B:135:SER:O	1:E:133:ALA:CA[5_555]	1.65	0.55
1:C:358:SER:C	1:G:170:GLY:N[5_455]	1.65	0.55
1:C:358:SER:OG	1:G:169:VAL:CA[5_455]	1.66	0.54
1:C:359:ASP:H	1:G:170:GLY:H[5_455]	1.08	0.52
1:C:359:ASP:CB	1:G:167:ASP:C[5_455]	1.68	0.52
1:C:358:SER:CB	1:G:169:VAL:C[5_455]	1.71	0.49
1:B:473:ASP:O	1:E:425:LYS:O[5_555]	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ASP:OD2	1:E:126:VAL:CG2[5_555]	1.77	0.43
1:C:359:ASP:CB	1:G:166:MET:O[5_455]	1.79	0.41
1:C:358:SER:HG	1:G:169:VAL:CG1[5_455]	1.20	0.40
1:C:358:SER:C	1:G:170:GLY:H[5_455]	1.21	0.39
1:C:359:ASP:CB	1:G:166:MET:C[5_455]	1.81	0.39
1:C:357:THR:CB	1:G:168:LYS:O[5_455]	1.82	0.38
1:C:358:SER:CA	1:G:169:VAL:N[5_455]	1.82	0.38
1:C:358:SER:N	1:G:169:VAL:CA[5_455]	1.88	0.32
1:C:359:ASP:CG	1:G:167:ASP:CA[5_455]	1.88	0.32
1:B:168:LYS:CG	1:E:362:ARG:NH2[5_555]	1.91	0.29
1:C:359:ASP:OD1	1:G:168:LYS:H[5_455]	1.34	0.26
1:E:338:GLU:CA	1:E:338:GLU:CG[3_454]	1.98	0.22
1:B:490:ASP:OD1	1:E:129:GLU:OE2[5_555]	1.99	0.21
1:C:358:SER:H	1:G:168:LYS:O[5_455]	1.41	0.19
1:C:359:ASP:H	1:G:170:GLY:N[5_455]	1.41	0.19
1:C:359:ASP:OD2	1:G:167:ASP:H[5_455]	1.41	0.19
1:A:315:GLU:OE1	1:A:338:GLU:OE2[3_554]	2.02	0.18
1:C:359:ASP:CG	1:G:166:MET:O[5_455]	2.02	0.18
1:E:338:GLU:CG	1:E:338:GLU:OE1[3_454]	2.04	0.16
1:B:137:PRO:CG	1:E:132:LYS:O[5_555]	2.08	0.12
1:B:434:GLU:OE2	1:F:434:GLU:OE2[4_555]	2.08	0.12
1:C:357:THR:C	1:G:168:LYS:O[5_455]	2.11	0.09
1:C:358:SER:C	1:G:169:VAL:C[5_455]	2.11	0.09
1:C:359:ASP:OD2	1:G:165:ALA:C[5_455]	2.12	0.08
1:C:358:SER:N	1:G:168:LYS:C[5_455]	2.14	0.06
1:C:359:ASP:OD1	1:G:167:ASP:C[5_455]	2.14	0.06
1:C:359:ASP:OD1	1:G:167:ASP:N[5_455]	2.14	0.06
1:C:358:SER:HG	1:G:169:VAL:CB[5_455]	1.55	0.05
1:C:359:ASP:CG	1:G:165:ALA:O[5_455]	2.16	0.04
1:C:359:ASP:N	1:G:166:MET:O[5_455]	2.16	0.04
1:C:358:SER:C	1:G:169:VAL:CA[5_455]	2.17	0.03
1:C:358:SER:OG	1:G:169:VAL:CG2[5_455]	2.17	0.03
1:C:359:ASP:CG	1:G:167:ASP:C[5_455]	2.17	0.03
1:C:359:ASP:CA	1:G:170:GLY:H[5_455]	1.60	0.00

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	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	B	449/548 (82%)	359 (80%)	67 (15%)	23 (5%)	1	5
1	C	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	D	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	E	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	F	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
1	G	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	1	5
All	All	3143/3836 (82%)	2507 (80%)	475 (15%)	161 (5%)	1	5

All (161) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	185	ASP
1	A	214	GLU
1	A	253	ASP
1	A	301	ILE
1	A	325	ILE
1	A	359	ASP
1	A	360	TYR
1	B	184	GLN
1	B	185	ASP
1	B	214	GLU
1	B	253	ASP
1	B	301	ILE
1	B	325	ILE
1	B	359	ASP
1	B	360	TYR
1	C	184	GLN
1	C	185	ASP
1	C	214	GLU
1	C	253	ASP
1	C	301	ILE
1	C	325	ILE
1	C	359	ASP
1	C	360	TYR

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Mol	Chain	Res	Type
1	D	184	GLN
1	D	185	ASP
1	D	214	GLU
1	D	253	ASP
1	D	301	ILE
1	D	325	ILE
1	D	359	ASP
1	D	360	TYR
1	E	184	GLN
1	E	185	ASP
1	E	214	GLU
1	E	253	ASP
1	E	301	ILE
1	E	325	ILE
1	E	359	ASP
1	E	360	TYR
1	F	184	GLN
1	F	185	ASP
1	F	214	GLU
1	F	253	ASP
1	F	301	ILE
1	F	325	ILE
1	F	359	ASP
1	F	360	TYR
1	G	184	GLN
1	G	185	ASP
1	G	214	GLU
1	G	253	ASP
1	G	301	ILE
1	G	325	ILE
1	G	359	ASP
1	G	360	TYR
1	A	45	GLY
1	A	316	ASP
1	A	328	ASP
1	A	357	THR
1	B	45	GLY
1	B	316	ASP
1	B	328	ASP
1	B	357	THR
1	C	45	GLY
1	C	316	ASP

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Mol	Chain	Res	Type
1	C	328	ASP
1	C	357	THR
1	D	45	GLY
1	D	316	ASP
1	D	328	ASP
1	D	357	THR
1	E	45	GLY
1	E	316	ASP
1	E	328	ASP
1	E	357	THR
1	F	45	GLY
1	F	316	ASP
1	F	328	ASP
1	F	357	THR
1	G	45	GLY
1	G	316	ASP
1	G	328	ASP
1	G	357	THR
1	A	154	SER
1	A	194	GLN
1	A	358	SER
1	A	374	GLY
1	B	154	SER
1	B	194	GLN
1	B	358	SER
1	B	374	GLY
1	C	154	SER
1	C	194	GLN
1	C	358	SER
1	C	374	GLY
1	D	154	SER
1	D	194	GLN
1	D	358	SER
1	D	374	GLY
1	E	154	SER
1	E	194	GLN
1	E	358	SER
1	E	374	GLY
1	F	154	SER
1	F	194	GLN
1	F	358	SER
1	F	374	GLY

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Mol	Chain	Res	Type
1	G	154	SER
1	G	194	GLN
1	G	358	SER
1	G	374	GLY
1	A	218	PRO
1	A	339	GLU
1	B	218	PRO
1	B	339	GLU
1	B	496	PRO
1	C	218	PRO
1	C	339	GLU
1	D	218	PRO
1	D	339	GLU
1	E	218	PRO
1	E	339	GLU
1	E	496	PRO
1	F	218	PRO
1	F	339	GLU
1	G	218	PRO
1	G	339	GLU
1	A	217	SER
1	A	383	ALA
1	A	496	PRO
1	B	217	SER
1	B	383	ALA
1	C	217	SER
1	C	383	ALA
1	C	496	PRO
1	D	217	SER
1	D	383	ALA
1	D	496	PRO
1	E	217	SER
1	E	383	ALA
1	F	217	SER
1	F	383	ALA
1	F	496	PRO
1	G	217	SER
1	G	383	ALA
1	G	496	PRO
1	D	213	VAL
1	E	213	VAL
1	G	213	VAL

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Mol	Chain	Res	Type
1	A	213	VAL
1	B	213	VAL
1	C	213	VAL
1	F	213	VAL
1	E	472	GLY
1	F	472	GLY
1	A	472	GLY
1	B	472	GLY
1	C	472	GLY
1	D	472	GLY
1	G	472	GLY

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	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	B	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	C	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	D	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	E	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	F	353/414 (85%)	300 (85%)	53 (15%)	3	10
1	G	353/414 (85%)	300 (85%)	53 (15%)	3	10
All	All	2471/2898 (85%)	2100 (85%)	371 (15%)	3	10

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	11	ASP
1	A	29	VAL
1	A	34	LYS
1	A	76	GLU
1	A	82	ASN

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Mol	Chain	Res	Type
1	A	83	ASP
1	A	90	THR
1	A	122	LYS
1	A	139	SER
1	A	146	GLN
1	A	156	GLU
1	A	177	VAL
1	A	193	MET
1	A	194	GLN
1	A	197	ARG
1	A	199	TYR
1	A	204	PHE
1	A	205	ILE
1	A	206	ASN
1	A	213	VAL
1	A	217	SER
1	A	218	PRO
1	A	247	LEU
1	A	248	LEU
1	A	250	ILE
1	A	254	VAL
1	A	276	VAL
1	A	283	ASP
1	A	284	ARG
1	A	285	ARG
1	A	286	LYS
1	A	288	MET
1	A	301	ILE
1	A	321	LYS
1	A	329	THR
1	A	334	ASP
1	A	336	VAL
1	A	338	GLU
1	A	339	GLU
1	A	355	GLU
1	A	360	TYR
1	A	362	ARG
1	A	365	LEU
1	A	385	THR
1	A	412	VAL
1	A	421	ARG
1	A	473	ASP

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Mol	Chain	Res	Type
1	A	488	MET
1	A	494	LEU
1	A	496	PRO
1	A	504	LEU
1	A	510	VAL
1	B	7	LYS
1	B	11	ASP
1	B	29	VAL
1	B	34	LYS
1	B	76	GLU
1	B	82	ASN
1	B	83	ASP
1	B	90	THR
1	B	122	LYS
1	B	139	SER
1	B	146	GLN
1	B	156	GLU
1	B	177	VAL
1	B	193	MET
1	B	194	GLN
1	B	197	ARG
1	B	199	TYR
1	B	204	PHE
1	B	205	ILE
1	B	206	ASN
1	B	213	VAL
1	B	217	SER
1	B	218	PRO
1	B	247	LEU
1	B	248	LEU
1	B	250	ILE
1	B	254	VAL
1	B	276	VAL
1	B	283	ASP
1	B	284	ARG
1	B	285	ARG
1	B	286	LYS
1	B	288	MET
1	B	301	ILE
1	B	321	LYS
1	B	329	THR
1	B	334	ASP

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Mol	Chain	Res	Type
1	B	336	VAL
1	B	338	GLU
1	B	339	GLU
1	B	355	GLU
1	B	360	TYR
1	B	362	ARG
1	B	365	LEU
1	B	385	THR
1	B	412	VAL
1	B	421	ARG
1	B	473	ASP
1	B	488	MET
1	B	494	LEU
1	B	496	PRO
1	B	504	LEU
1	B	510	VAL
1	C	7	LYS
1	C	11	ASP
1	C	29	VAL
1	C	34	LYS
1	C	76	GLU
1	C	82	ASN
1	C	83	ASP
1	C	90	THR
1	C	122	LYS
1	C	139	SER
1	C	146	GLN
1	C	156	GLU
1	C	177	VAL
1	C	193	MET
1	C	194	GLN
1	C	197	ARG
1	C	199	TYR
1	C	204	PHE
1	C	205	ILE
1	C	206	ASN
1	C	213	VAL
1	C	217	SER
1	C	218	PRO
1	C	247	LEU
1	C	248	LEU
1	C	250	ILE

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Mol	Chain	Res	Type
1	C	254	VAL
1	C	276	VAL
1	C	283	ASP
1	C	284	ARG
1	C	285	ARG
1	C	286	LYS
1	C	288	MET
1	C	301	ILE
1	C	321	LYS
1	C	329	THR
1	C	334	ASP
1	C	336	VAL
1	C	338	GLU
1	C	339	GLU
1	C	355	GLU
1	C	360	TYR
1	C	362	ARG
1	C	365	LEU
1	C	385	THR
1	C	412	VAL
1	C	421	ARG
1	C	473	ASP
1	C	488	MET
1	C	494	LEU
1	C	496	PRO
1	C	504	LEU
1	C	510	VAL
1	D	7	LYS
1	D	11	ASP
1	D	29	VAL
1	D	34	LYS
1	D	76	GLU
1	D	82	ASN
1	D	83	ASP
1	D	90	THR
1	D	122	LYS
1	D	139	SER
1	D	146	GLN
1	D	156	GLU
1	D	177	VAL
1	D	193	MET
1	D	194	GLN

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Mol	Chain	Res	Type
1	D	197	ARG
1	D	199	TYR
1	D	204	PHE
1	D	205	ILE
1	D	206	ASN
1	D	213	VAL
1	D	217	SER
1	D	218	PRO
1	D	247	LEU
1	D	248	LEU
1	D	250	ILE
1	D	254	VAL
1	D	276	VAL
1	D	283	ASP
1	D	284	ARG
1	D	285	ARG
1	D	286	LYS
1	D	288	MET
1	D	301	ILE
1	D	321	LYS
1	D	329	THR
1	D	334	ASP
1	D	336	VAL
1	D	338	GLU
1	D	339	GLU
1	D	355	GLU
1	D	360	TYR
1	D	362	ARG
1	D	365	LEU
1	D	385	THR
1	D	412	VAL
1	D	421	ARG
1	D	473	ASP
1	D	488	MET
1	D	494	LEU
1	D	496	PRO
1	D	504	LEU
1	D	510	VAL
1	E	7	LYS
1	E	11	ASP
1	E	29	VAL
1	E	34	LYS

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Mol	Chain	Res	Type
1	E	76	GLU
1	E	82	ASN
1	E	83	ASP
1	E	90	THR
1	E	122	LYS
1	E	139	SER
1	E	146	GLN
1	E	156	GLU
1	E	177	VAL
1	E	193	MET
1	E	194	GLN
1	E	197	ARG
1	E	199	TYR
1	E	204	PHE
1	E	205	ILE
1	E	206	ASN
1	E	213	VAL
1	E	217	SER
1	E	218	PRO
1	E	247	LEU
1	E	248	LEU
1	E	250	ILE
1	E	254	VAL
1	E	276	VAL
1	E	283	ASP
1	E	284	ARG
1	E	285	ARG
1	E	286	LYS
1	E	288	MET
1	E	301	ILE
1	E	321	LYS
1	E	329	THR
1	E	334	ASP
1	E	336	VAL
1	E	338	GLU
1	E	339	GLU
1	E	355	GLU
1	E	360	TYR
1	E	362	ARG
1	E	365	LEU
1	E	385	THR
1	E	412	VAL

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Mol	Chain	Res	Type
1	E	421	ARG
1	E	473	ASP
1	E	488	MET
1	E	494	LEU
1	E	496	PRO
1	E	504	LEU
1	E	510	VAL
1	F	7	LYS
1	F	11	ASP
1	F	29	VAL
1	F	34	LYS
1	F	76	GLU
1	F	82	ASN
1	F	83	ASP
1	F	90	THR
1	F	122	LYS
1	F	139	SER
1	F	146	GLN
1	F	156	GLU
1	F	177	VAL
1	F	193	MET
1	F	194	GLN
1	F	197	ARG
1	F	199	TYR
1	F	204	PHE
1	F	205	ILE
1	F	206	ASN
1	F	213	VAL
1	F	217	SER
1	F	218	PRO
1	F	247	LEU
1	F	248	LEU
1	F	250	ILE
1	F	254	VAL
1	F	276	VAL
1	F	283	ASP
1	F	284	ARG
1	F	285	ARG
1	F	286	LYS
1	F	288	MET
1	F	301	ILE
1	F	321	LYS

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Mol	Chain	Res	Type
1	F	329	THR
1	F	334	ASP
1	F	336	VAL
1	F	338	GLU
1	F	339	GLU
1	F	355	GLU
1	F	360	TYR
1	F	362	ARG
1	F	365	LEU
1	F	385	THR
1	F	412	VAL
1	F	421	ARG
1	F	473	ASP
1	F	488	MET
1	F	494	LEU
1	F	496	PRO
1	F	504	LEU
1	F	510	VAL
1	G	7	LYS
1	G	11	ASP
1	G	29	VAL
1	G	34	LYS
1	G	76	GLU
1	G	82	ASN
1	G	83	ASP
1	G	90	THR
1	G	122	LYS
1	G	139	SER
1	G	146	GLN
1	G	156	GLU
1	G	177	VAL
1	G	193	MET
1	G	194	GLN
1	G	197	ARG
1	G	199	TYR
1	G	204	PHE
1	G	205	ILE
1	G	206	ASN
1	G	213	VAL
1	G	217	SER
1	G	218	PRO
1	G	247	LEU

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Mol	Chain	Res	Type
1	G	248	LEU
1	G	250	ILE
1	G	254	VAL
1	G	276	VAL
1	G	283	ASP
1	G	284	ARG
1	G	285	ARG
1	G	286	LYS
1	G	288	MET
1	G	301	ILE
1	G	321	LYS
1	G	329	THR
1	G	334	ASP
1	G	336	VAL
1	G	338	GLU
1	G	339	GLU
1	G	355	GLU
1	G	360	TYR
1	G	362	ARG
1	G	365	LEU
1	G	385	THR
1	G	412	VAL
1	G	421	ARG
1	G	473	ASP
1	G	488	MET
1	G	494	LEU
1	G	496	PRO
1	G	504	LEU
1	G	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	68	ASN
1	A	72	GLN
1	A	82	ASN
1	A	146	GLN
1	A	194	GLN
1	A	366	GLN
1	A	436	GLN
1	A	437	ASN

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Mol	Chain	Res	Type
1	A	453	GLN
1	A	457	ASN
1	B	10	ASN
1	B	68	ASN
1	B	72	GLN
1	B	82	ASN
1	B	146	GLN
1	B	194	GLN
1	B	366	GLN
1	B	436	GLN
1	B	437	ASN
1	B	453	GLN
1	B	457	ASN
1	C	10	ASN
1	C	68	ASN
1	C	72	GLN
1	C	82	ASN
1	C	146	GLN
1	C	194	GLN
1	C	366	GLN
1	C	436	GLN
1	C	437	ASN
1	C	453	GLN
1	C	457	ASN
1	D	10	ASN
1	D	68	ASN
1	D	72	GLN
1	D	82	ASN
1	D	146	GLN
1	D	194	GLN
1	D	366	GLN
1	D	436	GLN
1	D	437	ASN
1	D	453	GLN
1	D	457	ASN
1	E	10	ASN
1	E	37	ASN
1	E	68	ASN
1	E	72	GLN
1	E	82	ASN
1	E	146	GLN
1	E	194	GLN

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Mol	Chain	Res	Type
1	E	366	GLN
1	E	436	GLN
1	E	437	ASN
1	E	453	GLN
1	E	457	ASN
1	F	10	ASN
1	F	68	ASN
1	F	72	GLN
1	F	82	ASN
1	F	146	GLN
1	F	194	GLN
1	F	366	GLN
1	F	436	GLN
1	F	437	ASN
1	F	453	GLN
1	F	457	ASN
1	G	10	ASN
1	G	68	ASN
1	G	72	GLN
1	G	82	ASN
1	G	146	GLN
1	G	194	GLN
1	G	366	GLN
1	G	436	GLN
1	G	437	ASN
1	G	453	GLN
1	G	457	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.