



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:03 PM UTC

PDB ID : 5FOA / pdb_00005foa
Title : Crystal Structure of Human Complement C3b in complex with DAF (CCP2-4)
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.
Deposited on : 2015-11-18
Resolution : 4.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

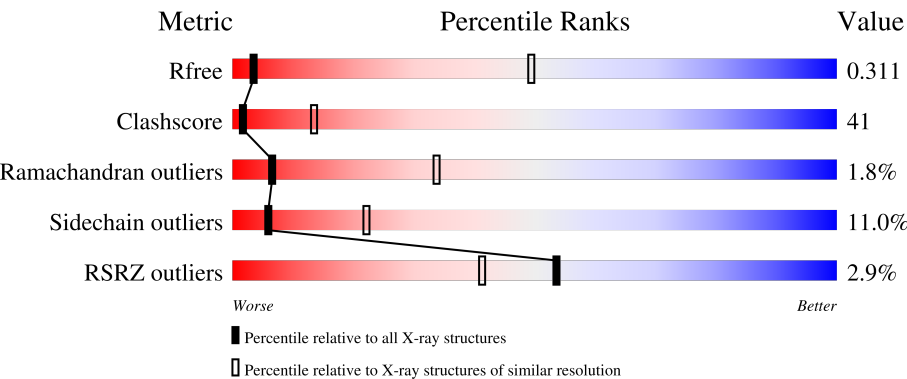
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1026 (4.50-3.86)
Clashscore	190562	1071 (4.50-3.86)
Ramachandran outliers	187476	1014 (4.52-3.84)
Sidechain outliers	187428	1000 (4.52-3.84)
RSRZ outliers	180081	1023 (4.50-3.86)

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

Mol	Chain	Length	Quality of chain
1	A	645	2% 45% 45% 8% .
1	C	645	3% 49% 40% 9% .
2	B	915	2% 40% 45% 11% ..
2	D	915	5% 39% 44% 14% ..
3	E	194	3% 40% 43% 12% ..

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Mol	Chain	Length	Quality of chain
3	F	194	3% 38% 42% 15% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27275 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5002	3185	848	954	15			
1	C	642	Total	C	N	O	S	0	0	0
			5002	3185	848	954	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	902	Total	C	N	O	S	0	0	0
			7177	4550	1205	1384	38			
2	D	902	Total	C	N	O	S	0	0	0
			7164	4543	1204	1380	37			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	SEE REMARK 999	UNP P01024
D	1013	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called DECAY ACCELERATING FACTOR, CD55.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	189	Total	C	N	O	S	0	0	0
			1465	920	249	283	13			
3	F	189	Total	C	N	O	S	0	0	0
			1465	920	249	283	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	GLY	-	expression tag	UNP P08174
E	96	SER	-	expression tag	UNP P08174

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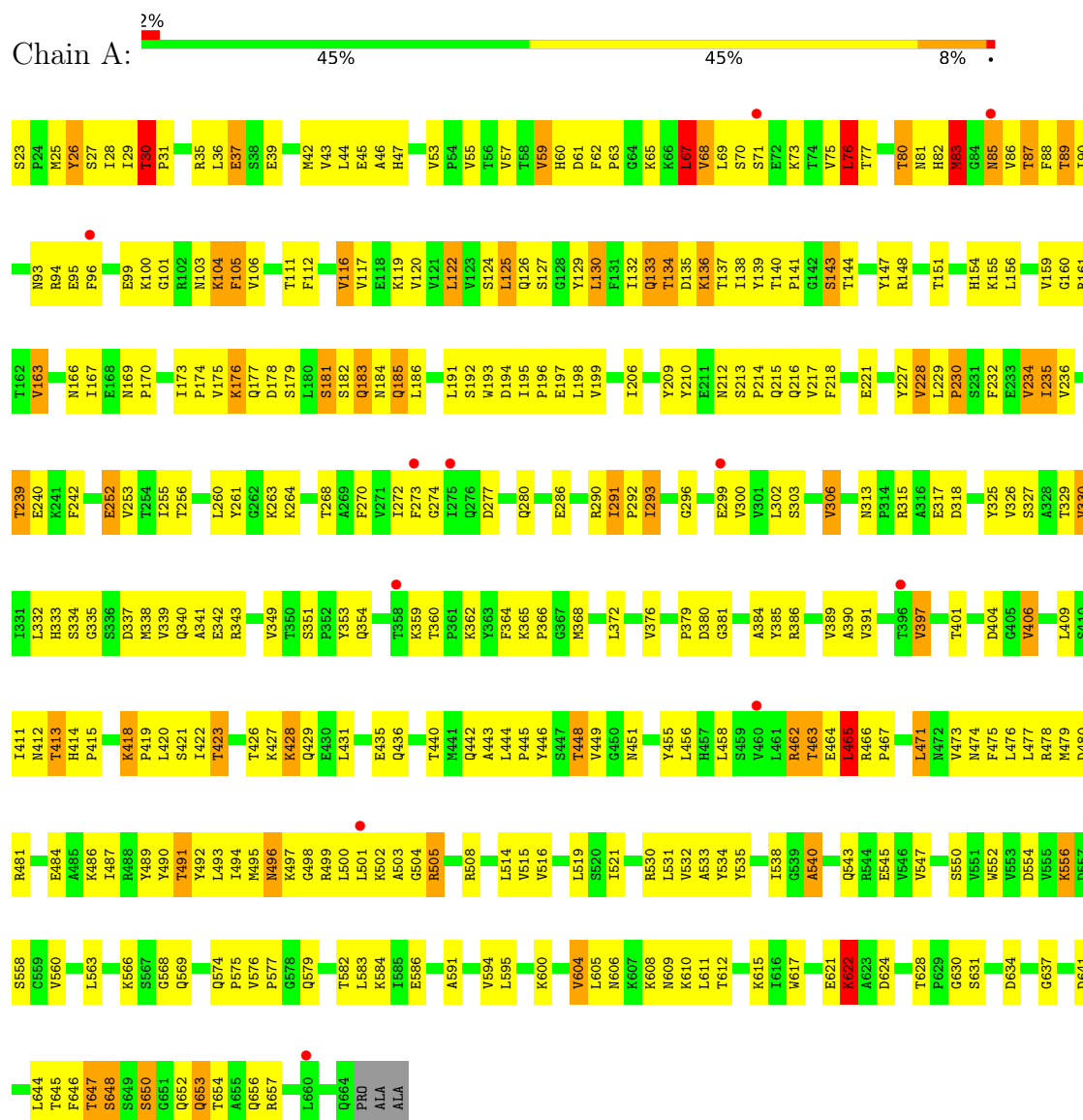
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Chain	Residue	Modelled	Actual	Comment	Reference
E	286	ALA	-	expression tag	UNP P08174
E	287	ALA	-	expression tag	UNP P08174
E	288	ALA	-	expression tag	UNP P08174
F	95	GLY	-	expression tag	UNP P08174
F	96	SER	-	expression tag	UNP P08174
F	286	ALA	-	expression tag	UNP P08174
F	287	ALA	-	expression tag	UNP P08174
F	288	ALA	-	expression tag	UNP P08174

3 Residue-property plots

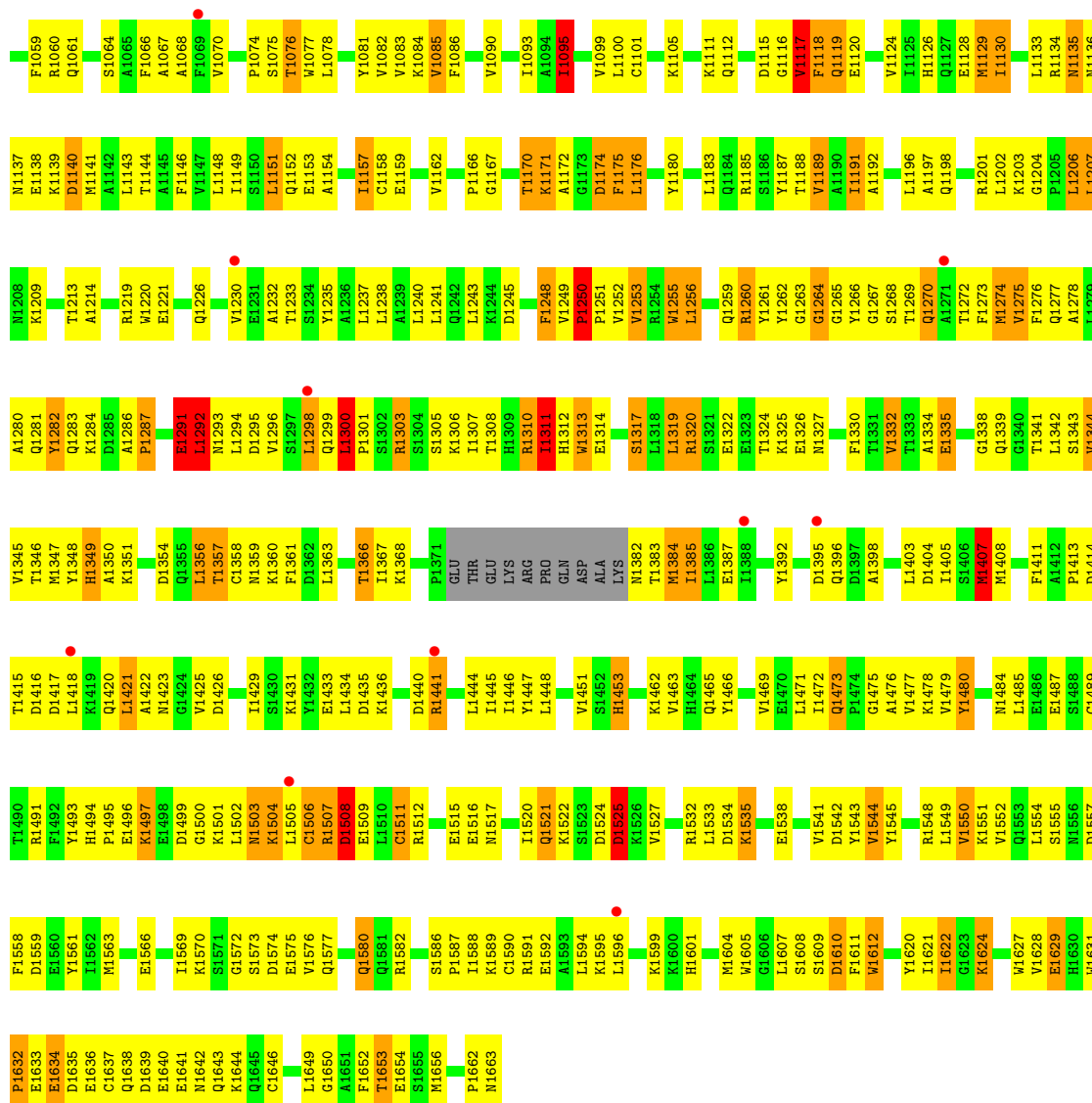
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: COMPLEMENT C3 BETA CHAIN

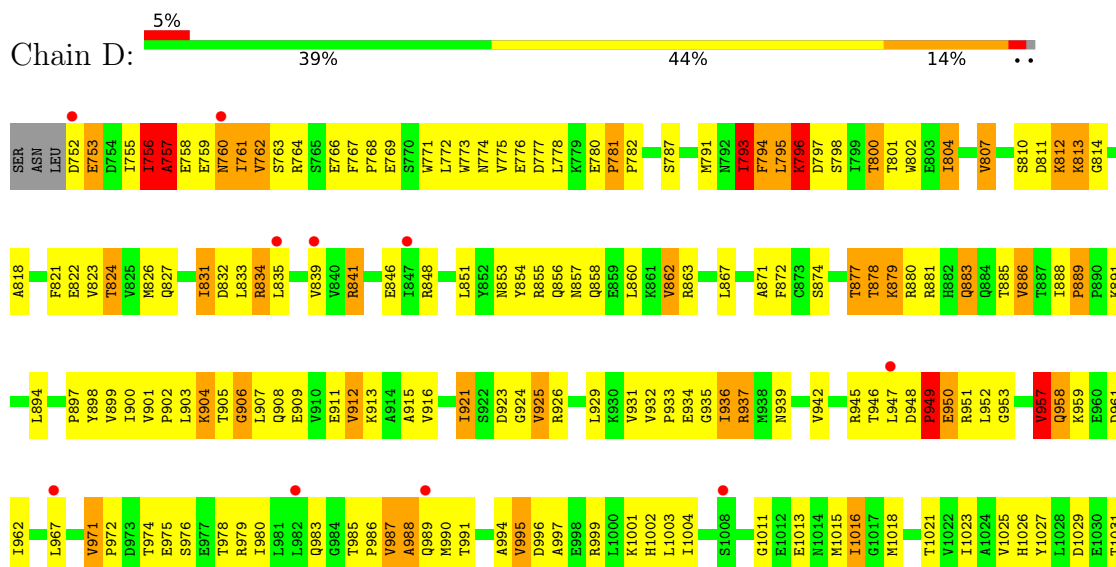


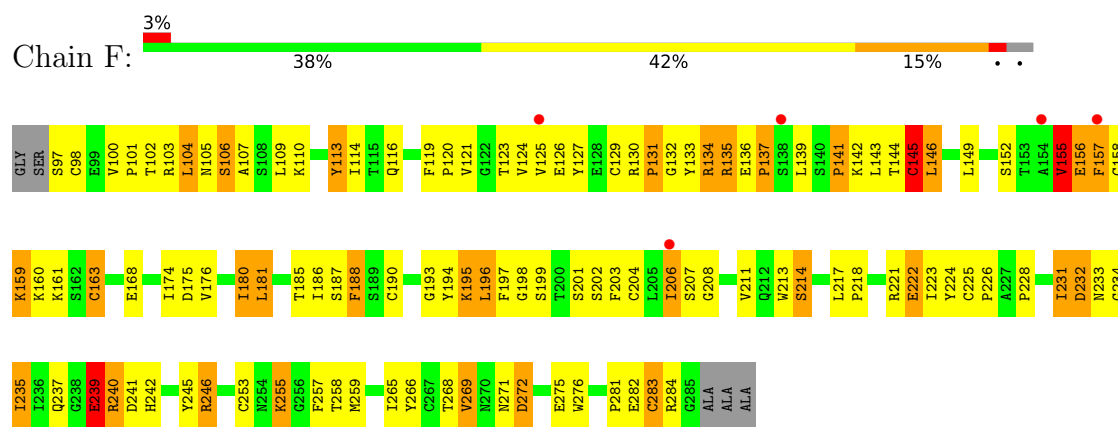
• Molecule 1: COMPLEMENT C3 BETA CHAIN





• Molecule 2: COMPLEMENT C3B ALPHA CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.43Å 142.38Å 323.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.39 – 4.19 110.39 – 4.19	Depositor EDS
% Data completeness (in resolution range)	95.5 (110.39-4.19) 89.5 (110.39-4.19)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 4.15Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.270 , 0.307 0.272 , 0.311	Depositor DCC
R_{free} test set	1955 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	124.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 150.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	27275	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	3/5103 (0.1%)	1.24	42/6934 (0.6%)
1	C	0.80	9/5103 (0.2%)	1.32	55/6934 (0.8%)
2	B	0.86	13/7319 (0.2%)	1.43	111/9912 (1.1%)
2	D	0.87	14/7306 (0.2%)	1.43	118/9896 (1.2%)
3	E	0.89	3/1506 (0.2%)	1.30	18/2048 (0.9%)
3	F	0.81	1/1506 (0.1%)	1.25	11/2048 (0.5%)
All	All	0.83	43/27843 (0.2%)	1.36	355/37772 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	4
2	D	0	4
3	F	0	2
All	All	0	12

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1249	VAL	CA-CB	10.63	1.67	1.54
2	B	1313	TRP	CE3-CZ3	-8.80	1.12	1.38
1	C	90	ILE	CA-CB	8.25	1.62	1.53
3	F	239	GLU	CA-C	7.85	1.63	1.52
2	D	813	LYS	CD-CE	-7.83	1.28	1.52
1	C	67	LEU	CG-CD2	7.80	1.78	1.52
2	D	761	ILE	CA-CB	7.70	1.65	1.54
2	B	1292	LEU	CA-CB	7.45	1.66	1.53
1	C	53	VAL	CA-CB	7.14	1.63	1.54
2	D	756	ILE	CA-CB	-7.04	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	PRO	CA-C	-6.80	1.45	1.52
2	D	1065	ALA	CA-C	-6.73	1.43	1.53
2	D	1554	LEU	CG-CD1	-6.73	1.30	1.52
2	D	841	ARG	CB-CG	-6.50	1.32	1.52
2	B	1119	GLN	C-O	-6.28	1.16	1.24
2	B	962	ILE	CA-CB	6.24	1.59	1.54
2	B	1076	THR	CA-CB	-6.18	1.43	1.53
2	B	1313	TRP	CZ2-CH2	-6.14	1.25	1.37
1	C	569	GLN	CG-CD	-6.11	1.36	1.52
1	C	387	VAL	N-CA	-6.02	1.39	1.46
2	D	1036	LYS	CE-NZ	-5.91	1.31	1.49
2	D	1064	SER	CA-C	-5.70	1.45	1.52
2	D	1218	ASN	CA-C	5.68	1.60	1.52
2	D	1639	ASP	N-CA	-5.68	1.38	1.46
3	E	276	TRP	CB-CG	-5.62	1.32	1.50
2	B	1270	GLN	CA-C	-5.53	1.45	1.52
1	C	69	LEU	N-CA	-5.50	1.39	1.46
2	B	902	PRO	CA-C	-5.47	1.46	1.52
1	C	54	PRO	C-O	-5.45	1.17	1.23
2	B	1580	GLN	CG-CD	-5.37	1.38	1.52
1	C	66	LYS	CD-CE	-5.37	1.36	1.52
2	D	841	ARG	N-CA	-5.36	1.39	1.46
1	A	37	GLU	CG-CD	-5.34	1.38	1.52
1	A	104	LYS	CG-CD	-5.31	1.36	1.52
3	E	143	LEU	CG-CD1	-5.29	1.35	1.52
2	D	781	PRO	CA-C	5.29	1.57	1.52
1	A	76	LEU	N-CA	-5.27	1.39	1.46
2	B	1303	ARG	CB-CG	-5.27	1.36	1.52
2	D	1036	LYS	CD-CE	-5.24	1.36	1.52
3	E	276	TRP	CA-C	-5.20	1.46	1.52
2	B	1035	GLU	CA-C	-5.17	1.46	1.52
2	B	1292	LEU	CA-C	5.13	1.59	1.52
2	B	1300	LEU	CG-CD1	-5.00	1.36	1.52

All (355) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	574	GLN	CA-C-N	-15.84	104.79	120.31
1	C	574	GLN	C-N-CA	-15.84	104.79	120.31
2	B	1292	LEU	CD1-CG-CD2	-15.12	77.54	110.80
2	B	1632	PRO	CA-C-O	-13.12	106.39	121.34
2	B	1291	GLU	N-CA-C	-11.39	86.53	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1250	PRO	CA-C-N	-10.47	106.76	119.84
2	B	1250	PRO	C-N-CA	-10.47	106.76	119.84
2	D	1615	LYS	CA-C-N	-10.40	108.30	120.89
2	D	1615	LYS	C-N-CA	-10.40	108.30	120.89
1	C	30	THR	CA-C-N	-10.37	109.15	120.14
1	C	30	THR	C-N-CA	-10.37	109.15	120.14
2	D	1065	ALA	N-CA-C	-10.30	95.22	110.46
2	B	901	VAL	CA-C-N	10.11	130.52	119.90
2	B	901	VAL	C-N-CA	10.11	130.52	119.90
1	A	80	THR	N-CA-C	-9.61	100.49	112.88
2	D	813	LYS	CB-CG-CD	-9.56	89.31	111.30
1	A	83	MET	CG-SD-CE	-9.29	80.46	100.90
1	C	560	VAL	N-CA-C	-9.23	101.20	110.62
2	B	1119	GLN	CA-C-N	-9.06	110.21	122.72
2	B	1119	GLN	C-N-CA	-9.06	110.21	122.72
2	D	1097	SER	N-CA-C	8.90	122.15	111.82
2	B	1176	LEU	N-CA-C	-8.76	101.74	111.28
1	A	574	GLN	CA-C-N	-8.75	110.86	120.14
1	A	574	GLN	C-N-CA	-8.75	110.86	120.14
2	D	1554	LEU	CD1-CG-CD2	-8.71	91.64	110.80
2	D	1453	HIS	N-CA-C	-8.67	102.07	114.12
2	D	971	VAL	CA-C-N	8.63	128.71	119.90
2	D	971	VAL	C-N-CA	8.63	128.71	119.90
2	B	1248	PHE	N-CA-C	-8.62	102.78	113.38
1	C	123	VAL	N-CA-C	8.61	120.33	107.75
2	D	813	LYS	N-CA-C	8.52	123.67	113.28
1	A	23	SER	CA-C-N	-8.50	110.65	119.83
1	A	23	SER	C-N-CA	-8.50	110.65	119.83
1	C	396	THR	N-CA-C	-8.42	102.06	111.07
2	D	1359	ASN	N-CA-C	8.36	121.97	111.69
2	D	1486	GLU	N-CA-C	8.28	120.30	111.28
2	D	1654	GLU	N-CA-C	-8.17	102.46	111.36
2	B	1035	GLU	N-CA-C	8.08	119.86	111.14
1	C	559	CYS	N-CA-C	-8.04	96.45	109.96
3	F	269	VAL	N-CA-C	8.00	119.31	108.11
2	D	1135	ASN	N-CA-C	7.96	122.69	112.34
1	C	291	ILE	CA-C-N	7.96	128.25	119.90
1	C	291	ILE	C-N-CA	7.96	128.25	119.90
1	C	575	PRO	N-CA-C	7.91	123.59	111.57
2	D	925	VAL	N-CA-C	7.83	119.19	107.75
2	B	1292	LEU	CA-CB-CG	7.72	143.33	116.30
1	A	505	ARG	N-CA-C	7.70	121.77	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ILE	CA-C-N	7.69	127.97	119.90
1	A	291	ILE	C-N-CA	7.69	127.97	119.90
1	A	83	MET	CA-CB-CG	-7.67	98.75	114.10
3	E	170	ARG	CA-C-N	7.64	132.96	122.19
3	E	170	ARG	C-N-CA	7.64	132.96	122.19
3	E	146	LEU	N-CA-C	7.51	120.71	110.35
1	A	465	LEU	N-CA-C	7.50	120.61	109.59
3	E	157	PHE	N-CA-C	7.49	120.40	111.33
1	A	101	GLY	N-CA-C	-7.48	104.25	115.32
2	B	1140	ASP	N-CA-C	-7.48	103.62	112.89
2	B	1294	LEU	N-CA-C	7.47	120.58	108.41
2	D	1282	TYR	N-CA-C	7.47	120.48	111.82
2	B	1117	VAL	N-CA-C	7.44	119.00	108.36
2	D	1204	GLY	CA-C-N	7.43	127.45	119.28
2	D	1204	GLY	C-N-CA	7.43	127.45	119.28
2	D	1259	GLN	N-CA-C	-7.40	103.24	111.82
2	B	1293	ASN	N-CA-C	7.36	122.48	107.69
1	A	75	VAL	CA-C-N	-7.33	111.01	121.50
1	A	75	VAL	C-N-CA	-7.33	111.01	121.50
2	B	1345	VAL	N-CA-C	7.25	118.34	107.75
2	B	1303	ARG	CG-CD-NE	-7.24	96.08	112.00
2	B	971	VAL	CA-C-N	7.19	127.23	119.90
2	B	971	VAL	C-N-CA	7.19	127.23	119.90
2	D	1554	LEU	CB-CG-CD1	-7.17	89.20	110.70
2	B	877	THR	CA-C-N	7.08	129.65	120.44
2	B	877	THR	C-N-CA	7.08	129.65	120.44
2	B	902	PRO	CA-C-O	-7.05	112.99	121.03
2	D	1242	GLN	N-CA-C	-7.04	103.69	111.36
1	C	510	PRO	CA-C-O	-7.00	113.74	121.23
2	B	1332	VAL	N-CA-C	6.96	118.34	107.28
2	D	761	ILE	CB-CA-C	-6.92	103.97	111.59
2	B	1292	LEU	N-CA-C	-6.92	97.34	108.55
2	B	1300	LEU	CD1-CG-CD2	-6.92	95.58	110.80
2	D	1189	VAL	N-CA-C	-6.91	102.41	111.05
1	C	219	SER	N-CA-C	6.91	120.42	109.50
2	B	1504	LYS	CA-C-N	-6.89	113.21	122.72
2	B	1504	LYS	C-N-CA	-6.89	113.21	122.72
2	D	775	VAL	N-CA-C	6.89	118.81	107.24
2	D	796	LYS	CD-CE-NZ	-6.88	89.89	111.90
2	D	1649	LEU	CB-CG-CD2	-6.87	90.09	110.70
2	D	906	GLY	N-CA-C	-6.86	101.95	111.76
2	D	769	GLU	N-CA-C	-6.85	104.73	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	813	LYS	CD-CE-NZ	-6.83	90.04	111.90
2	D	1644	LYS	N-CA-C	6.74	119.46	111.71
1	C	213	SER	CA-C-N	6.74	126.36	119.56
1	C	213	SER	C-N-CA	6.74	126.36	119.56
2	D	1313	TRP	N-CA-C	-6.73	100.50	110.46
2	D	1254	ARG	N-CA-C	-6.72	103.95	111.28
3	E	276	TRP	CA-CB-CG	-6.69	100.89	113.60
1	C	182	SER	N-CA-C	6.67	120.88	113.21
2	B	1292	LEU	CB-CG-CD1	6.63	130.60	110.70
2	B	1119	GLN	O-C-N	-6.63	115.47	123.29
2	B	1303	ARG	NE-CZ-NH1	-6.62	114.88	121.50
2	B	1221	GLU	N-CA-C	6.61	120.24	109.59
2	B	1204	GLY	CA-C-N	6.58	126.52	119.28
2	B	1204	GLY	C-N-CA	6.58	126.52	119.28
2	B	1300	LEU	CB-CG-CD1	-6.57	90.98	110.70
2	B	1014	ASN	N-CA-C	-6.56	104.21	111.82
2	B	1287	PRO	N-CA-CB	6.56	110.13	103.25
2	B	1441	ARG	N-CA-C	6.55	118.95	109.71
1	A	560	VAL	N-CA-C	-6.53	103.96	110.62
2	D	1502	LEU	N-CA-C	-6.53	101.29	110.50
1	C	418	LYS	CA-C-N	6.52	127.99	119.84
1	C	418	LYS	C-N-CA	6.52	127.99	119.84
2	D	1345	VAL	N-CA-C	6.50	117.25	107.75
2	B	1395	ASP	N-CA-C	-6.49	105.66	113.97
2	B	1175	PHE	CA-CB-CG	-6.48	107.32	113.80
2	D	1395	ASP	N-CA-C	-6.43	105.74	113.97
2	B	1076	THR	CA-CB-CG2	-6.42	99.58	110.50
1	C	455	TYR	N-CA-C	6.42	120.10	110.14
2	D	1323	GLU	N-CA-C	6.40	119.94	109.06
2	D	1632	PRO	CA-C-O	-6.40	113.74	121.03
1	C	575	PRO	CA-C-O	-6.39	114.19	122.12
2	D	1250	PRO	N-CA-C	6.39	118.50	110.70
2	B	1282	TYR	N-CA-C	-6.35	104.45	111.82
1	C	581	MET	N-CA-C	6.34	119.52	109.50
2	D	877	THR	CA-C-N	6.34	128.69	120.44
2	D	877	THR	C-N-CA	6.34	128.69	120.44
3	F	141	PRO	N-CA-C	-6.32	107.40	114.92
2	B	761	ILE	N-CA-C	6.31	117.89	108.23
2	D	1243	LEU	N-CA-C	6.29	120.80	113.18
2	D	949	PRO	CA-C-O	-6.29	114.26	121.56
1	A	176	LYS	N-CA-C	6.28	118.61	108.32
2	B	1252	VAL	N-CA-C	-6.25	105.05	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	562	SER	N-CA-C	6.25	118.68	108.55
2	D	796	LYS	N-CA-C	6.24	119.14	109.60
1	A	647	THR	N-CA-C	6.24	119.30	108.76
3	E	146	LEU	CA-CB-CG	6.22	138.09	116.30
2	D	1385	ILE	N-CA-C	6.22	116.88	108.17
2	B	1535	LYS	CB-CG-CD	6.22	125.60	111.30
2	B	906	GLY	N-CA-C	-6.21	102.87	111.76
2	D	1472	ILE	N-CA-C	6.20	117.94	108.71
2	D	1213	THR	N-CA-C	-6.16	105.73	113.18
1	C	238	PRO	CA-C-O	-6.15	113.93	121.31
3	E	172	GLY	N-CA-C	-6.15	98.61	113.18
2	B	1653	THR	N-CA-C	-6.14	104.51	111.14
1	C	510	PRO	CA-C-N	-6.14	112.44	122.20
1	C	510	PRO	C-N-CA	-6.14	112.44	122.20
1	C	388	PRO	CA-C-O	-6.13	114.35	121.34
2	B	1646	CYS	CA-CB-SG	6.13	128.49	114.40
2	B	1580	GLN	CA-CB-CG	-6.09	101.92	114.10
2	D	793	ILE	N-CA-C	6.09	117.53	108.46
2	D	1554	LEU	CB-CG-CD2	6.05	128.85	110.70
2	B	1151	LEU	N-CA-C	6.04	117.94	111.36
3	E	156	GLU	CA-C-N	6.04	128.66	120.38
3	E	156	GLU	C-N-CA	6.04	128.66	120.38
1	A	67	LEU	CA-C-N	6.03	128.69	122.96
1	A	67	LEU	C-N-CA	6.03	128.69	122.96
2	D	1368	LYS	CA-C-N	-6.03	113.76	119.85
2	D	1368	LYS	C-N-CA	-6.03	113.76	119.85
2	D	1258	GLU	CA-CB-CG	6.02	126.15	114.10
2	D	1504	LYS	CA-C-N	-6.02	114.42	122.72
2	D	1504	LYS	C-N-CA	-6.02	114.42	122.72
2	D	1267	GLY	N-CA-C	6.01	124.46	114.48
2	D	1293	ASN	CA-C-N	-6.01	114.29	122.77
2	D	1293	ASN	C-N-CA	-6.01	114.29	122.77
2	B	1335	GLU	N-CA-C	6.00	117.53	108.46
2	B	1119	GLN	N-CA-C	6.00	118.73	109.07
2	D	1511	CYS	CA-CB-SG	5.98	128.15	114.40
1	C	657	ARG	CG-CD-NE	5.97	125.14	112.00
2	B	1344	VAL	N-CA-C	5.97	116.46	107.80
2	D	1060	ARG	CA-CB-CG	5.97	126.04	114.10
1	C	67	LEU	N-CA-C	5.96	116.97	108.74
2	D	1294	LEU	N-CA-C	5.96	118.12	108.34
2	B	1119	GLN	CA-C-O	-5.96	113.88	120.38
1	C	207	ARG	CB-CG-CD	-5.95	97.62	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	937	ARG	N-CA-C	5.94	118.81	109.96
2	D	1151	LEU	N-CA-C	5.91	118.68	111.82
1	A	648	SER	N-CA-C	5.91	118.85	109.81
1	A	185	GLN	N-CA-C	-5.88	105.76	113.17
2	D	1057	LEU	N-CA-C	-5.88	105.94	113.23
3	E	143	LEU	CB-CG-CD1	-5.87	93.09	110.70
2	D	813	LYS	N-CA-CB	-5.85	101.27	110.46
2	B	1646	CYS	N-CA-C	-5.83	104.83	111.07
2	D	1134	ARG	N-CA-C	5.82	118.09	111.11
3	E	143	LEU	CA-CB-CG	5.82	136.65	116.30
2	B	960	GLU	N-CA-C	5.80	118.35	108.02
3	E	145	CYS	N-CA-C	5.80	118.19	108.73
2	B	1525	ASP	N-CA-C	5.79	117.40	111.14
2	D	757	ALA	N-CA-C	5.79	123.12	110.80
2	B	1497	LYS	CD-CE-NZ	-5.78	93.40	111.90
1	C	642	ALA	N-CA-C	-5.78	105.72	112.89
2	D	1421	LEU	CA-C-N	5.77	128.01	120.28
2	D	1421	LEU	C-N-CA	5.77	128.01	120.28
2	D	1416	ASP	N-CA-C	5.76	118.34	111.71
1	C	352	PRO	N-CA-C	-5.76	108.69	114.68
2	D	794	PHE	CA-C-N	5.75	129.97	120.94
2	D	794	PHE	C-N-CA	5.75	129.97	120.94
2	B	1255	TRP	N-CA-C	5.75	117.62	111.36
1	C	304	ARG	CG-CD-NE	-5.74	99.36	112.00
2	D	921	ILE	N-CA-C	5.74	116.56	108.17
1	A	143	SER	N-CA-C	5.73	118.82	110.17
2	D	1173	GLY	N-CA-C	-5.73	105.27	113.86
1	C	229	LEU	CA-CB-CG	5.72	136.33	116.30
2	D	1287	PRO	N-CA-CB	5.72	109.26	103.25
2	B	961	ASP	N-CA-C	5.71	117.98	109.25
2	D	879	LYS	N-CA-C	5.68	120.36	113.38
2	B	873	CYS	CA-CB-SG	-5.67	101.36	114.40
2	B	1500	GLY	N-CA-C	-5.67	105.12	114.76
1	C	231	SER	N-CA-C	5.67	122.34	113.72
2	D	1508	ASP	CA-CB-CG	5.66	118.26	112.60
3	F	181	LEU	CA-CB-CG	-5.66	96.51	116.30
1	A	653	GLN	N-CA-C	5.65	118.89	110.14
1	C	99	GLU	N-CA-C	5.65	122.83	110.80
2	B	1293	ASN	CA-C-N	-5.64	115.05	123.00
2	B	1293	ASN	C-N-CA	-5.64	115.05	123.00
1	C	65	LYS	CA-C-N	5.63	128.59	120.38
1	C	65	LYS	C-N-CA	5.63	128.59	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	VAL	N-CA-C	5.62	116.67	108.53
2	B	949	PRO	CA-C-O	-5.61	114.94	121.34
1	C	54	PRO	CA-C-O	-5.61	114.36	120.92
2	B	1143	LEU	N-CA-C	5.61	117.47	111.36
1	A	30	THR	CA-C-N	-5.60	114.20	120.14
1	A	30	THR	C-N-CA	-5.60	114.20	120.14
2	D	1268	SER	N-CA-C	-5.59	107.04	112.97
2	D	1491	ARG	N-CA-C	-5.58	101.49	110.14
1	A	96	PHE	N-CA-C	5.58	117.44	111.36
2	B	1612	TRP	CA-C-N	-5.57	113.15	122.62
2	B	1612	TRP	C-N-CA	-5.57	113.15	122.62
2	B	1171	LYS	CA-CB-CG	5.57	125.23	114.10
2	D	1332	VAL	N-CA-C	5.54	116.08	107.28
2	D	1473	GLN	N-CA-C	5.54	116.94	109.24
2	D	1650	GLY	N-CA-C	-5.54	105.79	112.49
2	D	848	ARG	CA-CB-CG	-5.53	103.03	114.10
1	C	594	VAL	N-CA-C	5.53	115.83	107.75
2	B	1292	LEU	CA-C-O	-5.52	113.91	120.43
3	E	143	LEU	CB-CG-CD2	5.52	127.27	110.70
2	D	1497	LYS	CA-CB-CG	5.51	125.12	114.10
2	B	1118	PHE	N-CA-C	-5.50	102.14	110.28
1	A	418	LYS	CA-C-N	5.48	126.69	119.84
1	A	418	LYS	C-N-CA	5.48	126.69	119.84
2	B	1219	ARG	N-CA-C	5.48	117.60	108.99
2	D	1493	TYR	N-CA-C	5.48	118.39	108.69
2	B	775	VAL	N-CA-C	5.48	116.44	107.24
2	B	934	GLU	N-CA-C	5.47	117.32	111.36
2	D	1154	ALA	N-CA-C	-5.46	105.84	112.88
2	D	976	SER	CA-C-N	-5.45	115.02	122.93
2	D	976	SER	C-N-CA	-5.45	115.02	122.93
1	A	230	PRO	N-CA-C	5.45	120.67	113.86
1	C	468	GLY	N-CA-C	-5.44	107.51	114.37
2	B	781	PRO	CA-C-N	5.43	125.86	119.99
2	B	781	PRO	C-N-CA	5.43	125.86	119.99
1	A	76	LEU	CD1-CG-CD2	-5.42	98.87	110.80
2	B	1275	VAL	CA-C-N	-5.42	112.54	121.92
2	B	1275	VAL	C-N-CA	-5.42	112.54	121.92
2	D	1657	VAL	N-CA-C	5.42	116.08	110.82
2	D	804	ILE	N-CA-C	5.41	115.38	107.37
2	D	1465	GLN	N-CA-C	5.41	117.12	108.41
2	B	804	ILE	N-CA-C	5.40	115.36	107.37
2	D	1062	PRO	N-CA-C	-5.39	105.99	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	PRO	CA-C-N	-5.39	116.08	123.14
1	C	54	PRO	C-N-CA	-5.39	116.08	123.14
2	D	1148	LEU	CA-CB-CG	5.38	135.15	116.30
1	A	175	VAL	N-CA-C	-5.38	108.04	113.47
1	C	331	ILE	N-CA-C	5.38	115.60	107.75
2	B	769	GLU	N-CA-C	-5.37	106.57	113.23
1	A	622	LYS	CA-C-N	-5.36	114.66	122.86
1	A	622	LYS	C-N-CA	-5.36	114.66	122.86
2	D	1638	GLN	CA-C-O	5.35	126.13	119.97
2	B	1292	LEU	CA-C-N	5.35	131.21	123.13
2	B	1292	LEU	C-N-CA	5.35	131.21	123.13
2	B	1629	GLU	N-CA-C	5.35	118.15	108.69
2	D	1277	GLN	N-CA-C	-5.34	105.62	111.82
1	C	573	ARG	N-CA-C	5.34	117.39	107.99
1	C	205	LYS	N-CA-C	5.33	118.14	109.24
2	B	1497	LYS	CB-CG-CD	-5.32	99.07	111.30
2	D	1106	TRP	CA-CB-CG	-5.32	103.50	113.60
2	D	1328	GLU	CA-CB-CG	5.32	124.73	114.10
2	B	1292	LEU	CB-CA-C	5.31	119.42	109.86
2	D	812	LYS	N-CA-C	-5.29	105.89	112.93
2	D	987	VAL	CA-C-N	5.29	131.65	121.54
2	D	987	VAL	C-N-CA	5.29	131.65	121.54
1	A	228	VAL	CA-C-N	5.29	127.76	120.67
1	A	228	VAL	C-N-CA	5.29	127.76	120.67
2	D	958	GLN	N-CA-C	5.29	118.02	110.24
2	B	972	PRO	N-CA-C	5.29	119.50	111.15
2	B	1280	ALA	N-CA-C	-5.29	105.98	112.90
1	C	501	LEU	N-CA-C	5.28	117.78	111.71
3	F	214	SER	N-CA-C	5.28	117.04	111.28
1	A	73	LYS	N-CA-C	5.28	118.00	109.40
1	A	105	PHE	N-CA-C	5.27	117.39	109.23
1	C	90	ILE	CA-C-N	5.26	125.23	120.03
1	C	90	ILE	C-N-CA	5.26	125.23	120.03
3	E	154	ALA	CA-C-N	-5.24	114.12	122.50
3	E	154	ALA	C-N-CA	-5.24	114.12	122.50
2	B	1095	ILE	N-CA-C	5.22	116.27	108.54
3	E	130	ARG	C-N-CD	-5.21	103.63	125.00
2	D	878	THR	N-CA-C	-5.21	105.50	111.07
2	B	1174	ASP	N-CA-C	-5.20	105.69	111.36
2	B	1575	GLU	CA-CB-CG	-5.20	103.69	114.10
2	D	957	VAL	N-CA-C	5.20	120.16	109.34
2	D	834	ARG	N-CA-C	5.18	117.63	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	VAL	CA-C-N	5.18	125.34	119.90
2	D	901	VAL	C-N-CA	5.18	125.34	119.90
2	D	1418	LEU	N-CA-C	-5.18	105.08	111.40
1	A	500	LEU	N-CA-C	5.17	117.69	107.98
3	F	146	LEU	N-CA-C	5.17	117.48	110.35
2	D	1634	GLU	N-CA-C	-5.16	105.56	111.14
2	D	1644	LYS	CB-CG-CD	5.16	123.17	111.30
1	A	647	THR	OG1-CB-CG2	-5.16	98.98	109.30
2	B	1385	ILE	N-CA-C	5.16	115.28	107.80
2	D	1298	LEU	N-CA-C	5.15	117.30	108.90
3	F	134	ARG	CG-CD-NE	-5.15	100.67	112.00
2	B	1407	MET	CG-SD-CE	-5.15	89.58	100.90
2	B	1506	CYS	CA-CB-SG	5.14	126.21	114.40
2	D	889	PRO	CA-C-N	5.14	125.05	119.76
2	D	889	PRO	C-N-CA	5.14	125.05	119.76
2	D	1505	LEU	CA-CB-CG	-5.13	98.33	116.30
3	F	228	PRO	CA-C-N	5.13	125.04	119.76
3	F	228	PRO	C-N-CA	5.13	125.04	119.76
2	B	1484	ASN	N-CA-C	5.12	116.74	108.34
1	C	595	LEU	N-CA-C	5.11	118.02	110.46
3	F	161	LYS	N-CA-C	5.10	117.83	110.28
2	B	932	VAL	CA-C-N	5.09	125.00	119.85
2	B	932	VAL	C-N-CA	5.09	125.00	119.85
1	C	201	MET	CB-CG-SD	-5.09	97.41	112.70
2	B	1300	LEU	CB-CG-CD2	5.09	125.97	110.70
2	D	1466	TYR	CA-CB-CG	-5.09	104.74	113.90
2	B	1310	ARG	N-CA-C	5.08	116.54	108.67
3	E	246	ARG	CA-C-N	-5.08	114.16	121.42
3	E	246	ARG	C-N-CA	-5.08	114.16	121.42
1	C	182	SER	CA-C-N	5.08	128.06	120.95
1	C	182	SER	C-N-CA	5.08	128.06	120.95
1	C	23	SER	CA-C-N	-5.07	114.35	119.83
1	C	23	SER	C-N-CA	-5.07	114.35	119.83
2	B	842	ASN	CA-CB-CG	5.07	117.67	112.60
2	B	767	PHE	CA-C-N	-5.07	115.01	120.03
2	B	767	PHE	C-N-CA	-5.07	115.01	120.03
2	D	841	ARG	NE-CZ-NH1	-5.06	116.44	121.50
2	D	1501	LYS	N-CA-C	-5.06	102.15	109.59
2	D	781	PRO	CA-C-N	5.05	127.06	120.25
2	D	781	PRO	C-N-CA	5.05	127.06	120.25
1	A	181	SER	N-CA-C	5.04	117.61	108.69
2	D	1061	GLN	CA-C-N	-5.04	113.62	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1061	GLN	C-N-CA	-5.04	113.62	119.47
3	F	145	CYS	N-CA-C	5.04	116.73	108.52
2	D	1221	GLU	N-CA-C	5.04	117.96	109.95
2	B	1010	CYS	CA-CB-SG	5.04	125.98	114.40
2	B	1313	TRP	CA-C-O	-5.04	115.78	121.72
2	B	1129	MET	N-CA-C	-5.03	107.09	113.18
2	B	1542	ASP	N-CA-C	-5.03	105.24	112.13
2	B	1509	GLU	CA-C-N	-5.03	115.78	122.72
2	B	1509	GLU	C-N-CA	-5.03	115.78	122.72
2	B	1473	GLN	N-CA-C	5.03	116.22	109.24
2	B	774	ASN	N-CA-C	5.02	117.92	110.14
1	C	454	ASN	N-CA-C	5.01	116.85	107.99
1	A	428	LYS	N-CA-C	-5.00	102.51	109.96
3	F	130	ARG	C-N-CD	-5.00	104.50	125.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	GLN	Mainchain
1	A	622	LYS	Mainchain
2	B	1292	LEU	Mainchain
2	B	1311	ILE	Mainchain
2	B	1632	PRO	Mainchain
2	B	841	ARG	Mainchain
2	D	1063	SER	Mainchain
2	D	1414	ASP	Mainchain
2	D	1507	ARG	Mainchain
2	D	949	PRO	Mainchain
3	F	232	ASP	Mainchain
3	F	240	ARG	Mainchain

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	5002	0	5058	368	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5002	0	5058	370	1
2	B	7177	0	7086	584	2
2	D	7164	0	7066	697	1
3	E	1465	0	1389	155	1
3	F	1465	0	1389	150	0
All	All	27275	0	27046	2204	4

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 41.

All (2204) 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:C:67:LEU:CD2	1:C:67:LEU:CG	1.78	1.61
1:C:32:ASN:HD21	1:C:657:ARG:HD3	1.11	1.16
1:A:466:ARG:HG3	1:A:556:LYS:HD3	1.28	1.15
1:C:560:VAL:HG22	2:D:813:LYS:HZ1	1.15	1.12
2:D:978:THR:HG22	2:D:1346:THR:HG22	1.31	1.10
3:F:157:PHE:O	3:F:159:LYS:NZ	1.84	1.09
3:F:135:ARG:HH21	3:F:141:PRO:HD3	0.92	1.07
2:D:1559:ASP:OD1	2:D:1591:ARG:NH2	1.87	1.07
2:B:1300:LEU:HD11	2:B:1303:ARG:HG2	1.33	1.06
3:E:246:ARG:NH1	3:E:246:ARG:O	1.87	1.04
2:D:947:LEU:HD11	2:D:1342:LEU:HB3	1.38	1.04
3:F:135:ARG:NH2	3:F:141:PRO:HD3	1.73	1.03
3:E:246:ARG:C	3:E:246:ARG:HH11	1.66	1.03
2:B:1076:THR:HG21	2:B:1111:LYS:HE2	1.09	1.03
1:C:62:PHE:O	1:C:104:LYS:NZ	1.92	1.03
2:D:1140:ASP:O	2:D:1144:THR:OG1	1.78	1.02
2:D:758:GLU:HA	2:D:913:LYS:HZ3	1.21	1.01
2:B:1015:MET:SD	2:B:1056:GLN:NE2	2.34	1.01
2:D:766:GLU:HB3	2:D:796:LYS:HZ1	1.26	1.00
1:A:44:LEU:HD11	1:A:86:VAL:HG22	1.42	1.00
2:B:945:ARG:NH1	2:B:960:GLU:OE2	1.94	1.00
1:C:508:ARG:NH1	1:C:512:GLN:O	1.93	1.00
2:B:1202:LEU:HD13	2:B:1207:LEU:HD11	1.42	1.00
2:B:1517:ASN:ND2	2:B:1521:GLN:OE1	1.95	1.00
1:C:94:ARG:HE	1:C:94:ARG:HA	1.26	0.99
1:A:338:MET:HE1	2:B:1485:LEU:HB2	1.45	0.97
2:B:1202:LEU:HD11	2:B:1243:LEU:HD21	1.46	0.97
2:B:971:VAL:HG22	2:B:1351:LYS:HD2	1.42	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HG11	1:A:462:ARG:HH11	1.30	0.96
1:C:578:GLY:H	2:D:795:LEU:HD11	1.29	0.96
3:E:239:GLU:O	3:E:240:ARG:NH1	1.98	0.96
3:F:180:ILE:HD11	3:F:213:TRP:CZ2	2.00	0.96
1:C:28:ILE:HD11	1:C:42:MET:HG3	1.46	0.96
1:C:138:ILE:HG22	1:C:223:GLU:HB3	1.45	0.95
2:B:1129:MET:O	2:B:1270:GLN:NE2	1.98	0.95
2:D:1577:GLN:H	2:D:1580:GLN:HE21	1.02	0.95
2:D:1105:LYS:HG2	2:D:1106:TRP:CD1	2.01	0.95
2:D:810:SER:HB3	2:D:813:LYS:HB3	1.47	0.94
1:A:181:SER:HB3	3:E:246:ARG:HE	1.30	0.94
2:B:1635:ASP:HA	2:B:1638:GLN:HE22	1.31	0.94
1:C:508:ARG:HG3	1:C:508:ARG:HH11	1.32	0.93
2:D:1369:PRO:HA	2:D:1384:MET:HG2	1.50	0.93
1:A:406:VAL:HG11	1:A:462:ARG:NH1	1.83	0.93
1:C:496:ASN:HB3	1:C:501:LEU:HG	1.47	0.93
1:C:32:ASN:ND2	1:C:657:ARG:HD3	1.81	0.93
2:B:1013:GLU:O	2:B:1016:ILE:HG13	1.68	0.93
2:B:1076:THR:HG21	2:B:1111:LYS:CE	1.99	0.92
2:B:1610:ASP:OD1	2:B:1610:ASP:N	1.99	0.92
2:D:1506:CYS:SG	2:D:1511:CYS:HB2	2.10	0.92
2:D:1149:ILE:HD13	2:D:1194:TYR:HE2	1.33	0.92
1:C:523:THR:HB	1:C:560:VAL:HG23	1.52	0.91
1:C:201:MET:HE1	1:C:225:LYS:HA	1.53	0.91
2:D:757:ALA:O	2:D:913:LYS:NZ	2.04	0.91
2:B:1366:THR:OG1	2:B:1387:GLU:OE2	1.89	0.90
2:D:1101:CYS:SG	2:D:1161:GLN:NE2	2.44	0.90
2:D:1202:LEU:HD11	2:D:1243:LEU:HD21	1.53	0.90
2:B:951:ARG:HH21	2:B:1339:GLN:HG3	1.33	0.90
2:B:1298:LEU:O	2:B:1303:ARG:NH2	2.04	0.90
2:D:1258:GLU:HA	2:D:1260:ARG:NH1	1.87	0.90
1:C:66:LYS:NZ	3:E:145:CYS:O	2.05	0.89
2:D:1202:LEU:HD13	2:D:1207:LEU:HD13	1.54	0.89
3:E:260:ILE:HD12	3:E:284:ARG:HD3	1.55	0.89
2:D:1105:LYS:HE3	2:D:1106:TRP:HE1	1.36	0.89
1:C:349:VAL:HG12	1:C:351:SER:H	1.38	0.88
2:B:1512:ARG:NH1	2:B:1609:SER:O	2.05	0.88
1:A:83:MET:HE3	1:A:505:ARG:HH11	1.38	0.88
2:B:1554:LEU:HD13	2:B:1591:ARG:HH12	1.37	0.88
1:A:418:LYS:HD2	1:A:419:PRO:HD2	1.54	0.88
3:E:170:ARG:HG3	3:E:170:ARG:HH11	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ARG:NH1	1:C:219:SER:OG	2.05	0.88
2:B:841:ARG:NH1	2:B:902:PRO:O	2.06	0.87
1:C:98:SER:O	1:C:101:GLY:N	2.08	0.87
3:F:135:ARG:HH21	3:F:141:PRO:CD	1.83	0.87
2:B:1295:ASP:OD1	2:B:1310:ARG:NE	2.07	0.87
1:C:50:GLN:HE21	1:C:51:GLY:H	1.16	0.86
2:D:1033:GLN:HB3	2:D:1036:LYS:NZ	1.90	0.86
2:D:1298:LEU:HB3	2:D:1332:VAL:HG22	1.55	0.86
1:A:568:GLY:O	3:F:271:ASN:ND2	2.07	0.86
2:B:1136:ASN:HA	2:B:1139:LYS:HZ1	1.41	0.86
1:C:93:ASN:OD1	1:C:94:ARG:N	2.08	0.86
3:E:135:ARG:NH2	3:E:137:PRO:HA	1.90	0.86
1:C:69:LEU:HD21	1:C:91:PRO:HD2	1.58	0.86
2:D:856:GLN:HA	2:D:891:LYS:HE2	1.58	0.86
1:A:103:ASN:ND2	2:B:1035:GLU:OE2	2.08	0.85
2:B:1300:LEU:CD1	2:B:1303:ARG:HG2	2.06	0.85
2:D:764:ARG:NH1	2:D:923:ASP:OD1	2.09	0.85
2:D:867:LEU:HD11	2:D:913:LYS:HE2	1.57	0.85
2:B:1060:ARG:NH2	2:B:1064:SER:OG	2.10	0.84
2:D:1152:GLN:NE2	2:D:1198:GLN:OE1	2.11	0.83
2:D:755:ILE:HG21	2:D:863:ARG:HD3	1.58	0.83
1:A:264:LYS:HB3	1:A:296:GLY:HA3	1.61	0.83
3:F:233:ASN:ND2	3:F:283:CYS:O	2.11	0.83
1:C:594:VAL:HG13	2:D:807:VAL:HG13	1.58	0.83
2:D:832:ASP:OD2	2:D:834:ARG:NH2	2.12	0.83
1:A:181:SER:CB	3:E:246:ARG:HH21	1.91	0.83
2:D:883:GLN:OE1	2:D:883:GLN:N	2.12	0.83
2:D:1106:TRP:CD1	2:D:1106:TRP:N	2.44	0.83
1:A:229:LEU:O	2:B:834:ARG:NH2	2.10	0.83
2:D:1577:GLN:OE1	2:D:1580:GLN:NE2	2.12	0.83
2:D:1190:ALA:HA	2:D:1220:TRP:HZ3	1.42	0.82
2:B:985:THR:OG1	2:B:1339:GLN:O	1.96	0.82
3:F:135:ARG:NH2	3:F:139:LEU:O	2.12	0.82
1:A:349:VAL:HG12	1:A:351:SER:H	1.42	0.82
2:B:1635:ASP:HA	2:B:1638:GLN:NE2	1.95	0.82
1:C:560:VAL:HG22	2:D:813:LYS:NZ	1.93	0.82
3:E:146:LEU:HG	3:E:150:LYS:HB2	1.61	0.82
2:D:1492:PHE:HD1	2:D:1492:PHE:H	1.24	0.82
2:D:755:ILE:HG22	2:D:756:ILE:H	1.44	0.81
2:B:862:VAL:HG12	2:B:916:VAL:HG12	1.61	0.81
2:B:865:GLU:OE1	2:B:883:GLN:NE2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1118:PHE:H	2:B:1144:THR:HG22	1.45	0.81
2:D:871:ALA:O	2:D:903:LEU:N	2.13	0.81
2:D:1105:LYS:HG2	2:D:1106:TRP:HD1	1.42	0.81
1:C:423:THR:HG23	1:C:440:THR:HG22	1.61	0.81
2:D:1106:TRP:N	2:D:1106:TRP:HD1	1.77	0.81
3:E:223:ILE:HD11	3:E:269:VAL:HG22	1.63	0.81
2:B:1572:GLY:O	2:B:1574:ASP:N	2.13	0.81
1:C:535:TYR:CZ	1:C:547:VAL:HG11	2.15	0.81
2:B:1311:ILE:O	2:B:1313:TRP:HZ3	1.64	0.81
2:D:826:MET:HG2	2:D:827:GLN:H	1.46	0.81
1:C:385:TYR:CE1	1:C:386:ARG:HG3	2.15	0.80
2:D:759:GLU:HG2	2:D:760:ASN:H	1.45	0.80
1:A:83:MET:HE1	1:A:491:THR:CG2	2.11	0.80
3:E:109:LEU:HB2	3:E:114:ILE:HG12	1.63	0.80
2:D:1400:MET:HE1	2:D:1447:TYR:HB3	1.63	0.80
1:A:486:LYS:HZ2	1:A:538:ILE:HG12	1.46	0.80
1:C:264:LYS:HB3	1:C:296:GLY:HA3	1.64	0.80
2:B:983:GLN:OE1	2:B:983:GLN:N	2.15	0.80
2:D:1158:CYS:HA	2:D:1161:GLN:NE2	1.95	0.80
2:D:978:THR:OG1	2:D:1324:THR:HG23	1.82	0.80
3:F:136:GLU:HB2	3:F:159:LYS:CE	2.12	0.79
2:D:766:GLU:HB3	2:D:796:LYS:NZ	1.95	0.79
2:B:1300:LEU:HD23	2:B:1324:THR:HG21	1.64	0.79
1:C:168:GLU:HG3	1:C:205:LYS:HB3	1.62	0.79
2:D:1550:VAL:HG21	2:D:1581:GLN:NE2	1.96	0.79
2:B:1313:TRP:N	2:B:1313:TRP:CE3	2.50	0.79
2:D:1397:ASP:HB3	2:D:1450:LYS:HE2	1.64	0.79
2:D:1505:LEU:HD13	2:D:1585:ILE:HD11	1.65	0.79
3:F:136:GLU:HB2	3:F:159:LYS:HE2	1.63	0.78
3:F:223:ILE:HD13	3:F:272:ASP:HA	1.65	0.78
3:F:224:TYR:CE1	3:F:242:HIS:HB3	2.17	0.78
1:A:391:VAL:HG21	1:A:411:ILE:HD11	1.63	0.78
1:A:486:LYS:NZ	1:A:538:ILE:HG12	1.97	0.78
3:E:225:CYS:HB3	3:E:276:TRP:CZ2	2.19	0.78
2:D:1517:ASN:HD21	2:D:1521:GLN:HB2	1.49	0.78
2:D:1577:GLN:H	2:D:1580:GLN:NE2	1.79	0.78
3:F:239:GLU:CD	3:F:240:ARG:H	1.92	0.78
2:B:980:ILE:HD11	2:B:1322:GLU:HB2	1.63	0.78
2:B:1303:ARG:HH12	2:B:1306:LYS:HA	1.48	0.78
1:A:496:ASN:HD22	1:A:501:LEU:HD22	1.47	0.78
1:C:205:LYS:HE2	1:C:207:ARG:HD3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:962:ILE:HG13	2:D:1330:PHE:O	1.82	0.78
2:D:1506:CYS:CB	2:D:1511:CYS:HB2	2.13	0.78
2:D:756:ILE:HD13	2:D:761:ILE:HG13	1.64	0.78
2:B:1240:LEU:HD13	2:B:1249:VAL:HG22	1.66	0.77
1:A:53:VAL:HB	1:A:76:LEU:HD22	1.64	0.77
1:C:59:VAL:HG23	1:C:106:VAL:HG21	1.66	0.77
1:A:28:ILE:HG12	1:A:42:MET:HE3	1.67	0.77
3:E:237:GLN:HB3	3:E:250:THR:HG23	1.65	0.77
3:F:157:PHE:C	3:F:159:LYS:NZ	2.43	0.77
2:B:1238:LEU:HD11	2:B:1277:GLN:HE21	1.47	0.77
1:C:578:GLY:H	2:D:795:LEU:CD1	1.98	0.77
3:F:135:ARG:HH11	3:F:135:ARG:HG3	1.49	0.77
3:F:233:ASN:ND2	3:F:283:CYS:HB3	2.00	0.77
1:A:28:ILE:HG23	1:A:647:THR:OG1	1.85	0.77
2:B:1111:LYS:NZ	2:B:1119:GLN:O	2.16	0.77
1:C:578:GLY:N	2:D:795:LEU:HD11	2.00	0.77
1:A:431:LEU:HD11	1:A:436:GLN:CD	2.09	0.77
1:C:28:ILE:HD11	1:C:42:MET:CG	2.15	0.77
2:B:1146:PHE:O	2:B:1149:ILE:HG13	1.85	0.77
2:B:763:SER:HB2	2:B:926:ARG:HB2	1.67	0.77
3:E:240:ARG:HB2	3:E:243:TYR:CZ	2.20	0.77
2:B:1303:ARG:HH12	2:B:1306:LYS:CA	1.98	0.76
2:D:1104:VAL:HG13	2:D:1151:LEU:HD11	1.66	0.76
1:C:496:ASN:OD1	1:C:497:LYS:HG3	1.85	0.76
1:A:286:GLU:HG3	1:A:306:VAL:HG23	1.65	0.76
1:A:558:SER:O	1:A:617:TRP:NE1	2.17	0.76
2:B:1014:ASN:HB2	2:B:1055:GLN:NE2	1.99	0.76
1:C:312:GLN:OE1	1:C:312:GLN:N	2.17	0.76
1:C:576:VAL:N	1:C:579:GLN:OE1	2.17	0.76
1:C:66:LYS:HG2	3:E:147:GLN:HG3	1.67	0.76
2:D:1551:LYS:HE3	2:D:1562:ILE:CD1	2.16	0.76
2:D:1300:LEU:HD12	2:D:1303:ARG:H	1.49	0.76
1:A:230:PRO:HG3	1:A:604:VAL:HG11	1.67	0.76
1:C:291:ILE:HD13	1:C:300:VAL:HB	1.66	0.76
2:D:1498:GLU:C	2:D:1500:GLY:H	1.94	0.76
2:B:1233:THR:HG21	2:B:1256:LEU:HD11	1.67	0.76
1:C:290:ARG:NH1	2:D:1400:MET:SD	2.59	0.76
1:C:535:TYR:CE1	1:C:547:VAL:HG11	2.21	0.76
1:C:136:LYS:NZ	1:C:138:ILE:O	2.17	0.76
2:B:1494:HIS:HD2	2:B:1495:PRO:HD2	1.50	0.75
2:D:1145:ALA:HA	2:D:1148:LEU:HG	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1303:ARG:NH1	2:B:1307:ILE:HG12	2.01	0.75
1:C:67:LEU:HD13	3:E:144:THR:HG21	1.67	0.75
1:C:207:ARG:HH11	1:C:219:SER:HG	1.33	0.75
2:B:967:LEU:HD22	2:B:1348:TYR:CD2	2.21	0.75
2:B:1303:ARG:NH1	2:B:1305:SER:O	2.20	0.75
1:C:331:ILE:HG12	1:C:338:MET:HB3	1.66	0.75
1:C:214:PRO:HB2	2:D:1316:ALA:HB3	1.68	0.75
1:A:471:LEU:HB3	1:A:521:ILE:HD11	1.68	0.75
2:D:1355:GLN:N	2:D:1356:LEU:HB3	2.02	0.75
3:E:141:PRO:HA	3:E:157:PHE:CD2	2.22	0.75
1:A:44:LEU:HD23	1:A:55:VAL:HG21	1.69	0.74
1:A:291:ILE:HD13	1:A:300:VAL:HB	1.68	0.74
1:A:83:MET:HE3	1:A:505:ARG:HD2	1.69	0.74
1:C:67:LEU:HD12	1:C:68:VAL:H	1.52	0.74
1:A:181:SER:HB3	3:E:246:ARG:NE	2.01	0.74
1:C:69:LEU:HD21	1:C:90:ILE:HA	1.69	0.74
1:A:364:PHE:HE2	1:A:366:PRO:HA	1.52	0.74
1:C:496:ASN:ND2	1:C:524:ASP:O	2.20	0.74
2:D:1597:GLU:HG3	2:D:1600:LYS:HG3	1.67	0.74
1:A:136:LYS:NZ	1:A:138:ILE:O	2.20	0.74
2:B:1311:ILE:O	2:B:1313:TRP:CZ3	2.41	0.74
1:C:69:LEU:CD2	1:C:90:ILE:HA	2.18	0.74
1:C:473:VAL:HG13	1:C:517:LEU:HB3	1.70	0.74
1:A:83:MET:HE1	1:A:491:THR:HG22	1.69	0.74
1:A:650:SER:OG	1:A:652:GLN:NE2	2.20	0.74
2:B:1292:LEU:HD22	2:B:1338:GLY:HA2	1.70	0.74
3:E:143:LEU:C	3:E:143:LEU:HD12	2.13	0.74
2:D:1107:LEU:HD11	2:D:1147:VAL:HG13	1.69	0.73
1:C:67:LEU:CD2	1:C:67:LEU:HG	2.12	0.73
2:D:1284:LYS:NZ	2:D:1285:ASP:OD1	2.20	0.73
2:B:763:SER:OG	2:B:911:GLU:OE2	2.06	0.73
2:B:1136:ASN:HD22	2:B:1139:LYS:NZ	1.87	0.73
2:D:1436:LYS:NZ	2:D:1439:SER:O	2.21	0.73
2:B:1396:GLN:C	2:B:1453:HIS:HD2	1.97	0.73
2:D:1631:TRP:CD1	2:D:1649:LEU:HD21	2.22	0.73
1:A:111:THR:HG22	1:A:116:VAL:HG23	1.70	0.73
2:B:1019:THR:HG1	2:B:1081:TYR:HH	1.34	0.73
1:A:181:SER:HB3	3:E:246:ARG:HH21	1.54	0.73
2:D:1506:CYS:HG	2:D:1511:CYS:CB	2.01	0.73
1:A:134:THR:OG1	1:A:139:TYR:OH	2.07	0.73
2:B:935:GLY:HA3	2:B:1349:HIS:ND1	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1313:TRP:N	2:B:1313:TRP:HE3	1.84	0.73
1:C:508:ARG:NH1	1:C:508:ARG:HG3	2.03	0.73
1:A:37:GLU:OE2	1:A:161:ARG:NH1	2.22	0.73
2:D:1128:GLU:CD	2:D:1267:GLY:HA3	2.14	0.73
2:D:1255:TRP:HA	2:D:1258:GLU:OE2	1.89	0.73
2:B:1240:LEU:CD1	2:B:1249:VAL:HG22	2.19	0.72
1:A:36:LEU:HD12	1:A:37:GLU:HG2	1.70	0.72
2:B:1507:ARG:HB2	2:B:1612:TRP:CZ2	2.24	0.72
1:A:449:VAL:HG21	1:A:545:GLU:HG3	1.71	0.72
1:A:466:ARG:CG	1:A:556:LYS:HD3	2.14	0.72
3:E:135:ARG:HH22	3:E:137:PRO:HA	1.54	0.72
1:A:36:LEU:HD21	1:A:125:LEU:HA	1.72	0.72
1:A:530:ARG:NH1	1:A:624:ASP:OD2	2.21	0.72
2:B:1111:LYS:HE3	2:B:1119:GLN:O	1.89	0.72
2:D:1197:ALA:HB2	2:D:1202:LEU:HD21	1.72	0.72
1:A:313:ASN:OD1	1:A:315:ARG:N	2.22	0.72
1:C:93:ASN:ND2	1:C:95:GLU:OE1	2.21	0.72
1:C:94:ARG:HE	1:C:94:ARG:CA	2.02	0.72
1:C:313:ASN:ND2	1:C:315:ARG:O	2.23	0.72
2:D:1113:LYS:HB2	2:D:1117:VAL:HG22	1.72	0.72
3:F:195:LYS:HD2	3:F:196:LEU:H	1.55	0.72
2:D:1551:LYS:HE3	2:D:1562:ILE:HD11	1.71	0.72
2:B:1407:MET:HE2	2:B:1411:PHE:HB3	1.70	0.72
2:D:937:ARG:HH21	2:D:1349:HIS:HE1	1.37	0.72
2:D:1633:GLU:HB2	2:D:1636:GLU:OE1	1.89	0.72
1:C:561:GLY:HA3	2:D:813:LYS:HE2	1.72	0.72
2:D:1035:GLU:HA	2:D:1039:LEU:CD1	2.19	0.72
2:D:1060:ARG:HD3	2:D:1066:PHE:CZ	2.24	0.72
2:D:1574:ASP:CG	2:D:1582:ARG:HH12	1.98	0.72
2:D:1367:ILE:HD11	2:D:1386:LEU:HD13	1.71	0.72
2:D:1574:ASP:OD2	2:D:1620:TYR:OH	2.05	0.72
1:A:25:MET:SD	1:A:652:GLN:NE2	2.63	0.71
1:A:423:THR:HG22	1:A:440:THR:HG23	1.71	0.71
1:C:422:ILE:HB	1:C:441:MET:HE3	1.72	0.71
2:D:1303:ARG:NH2	3:F:239:GLU:OE1	2.22	0.71
3:E:195:LYS:HE3	3:E:197:PHE:HE1	1.55	0.71
3:E:273:GLU:HG3	3:E:275:GLU:OE2	1.90	0.71
3:F:113:TYR:HA	3:F:116:GLN:HG2	1.72	0.71
1:A:122:LEU:HD11	1:A:657:ARG:HB3	1.72	0.71
2:B:958:GLN:NE2	2:B:1334:ALA:HB3	2.05	0.71
2:B:1298:LEU:HB3	2:B:1332:VAL:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1405:ILE:HG12	2:D:1477:VAL:HG22	1.72	0.71
2:B:1249:VAL:HB	2:B:1250:PRO:HD3	1.72	0.71
2:D:1149:ILE:HD13	2:D:1194:TYR:CE2	2.23	0.71
2:B:780:GLU:OE1	2:B:780:GLU:N	2.24	0.71
2:B:1554:LEU:HD13	2:B:1591:ARG:NH1	2.05	0.71
2:D:1161:GLN:OE1	2:D:1161:GLN:N	2.23	0.71
3:E:224:TYR:CD2	3:E:242:HIS:HB3	2.25	0.71
2:D:1512:ARG:CZ	2:D:1621:ILE:HD13	2.21	0.71
2:B:1117:VAL:HA	2:B:1144:THR:HG21	1.73	0.71
2:B:1174:ASP:HA	2:B:1201:ARG:HH22	1.55	0.71
2:B:1544:VAL:HG22	2:B:1569:ILE:HB	1.73	0.71
3:E:146:LEU:HD13	3:E:148:ASN:H	1.56	0.71
2:D:1249:VAL:CG2	2:D:1250:PRO:HD3	2.19	0.71
3:F:157:PHE:C	3:F:159:LYS:HZ2	1.99	0.71
1:A:652:GLN:OE1	1:A:652:GLN:N	2.22	0.71
2:B:873:CYS:HB3	2:B:901:VAL:HG13	1.72	0.71
2:B:1140:ASP:O	2:B:1144:THR:OG1	2.07	0.71
3:E:170:ARG:HH11	3:E:170:ARG:CG	2.02	0.71
3:E:226:PRO:N	3:E:276:TRP:HH2	1.89	0.71
1:A:26:TYR:HE2	1:A:53:VAL:HG11	1.55	0.70
2:B:1101:CYS:O	2:B:1105:LYS:HG3	1.91	0.70
2:D:1003:LEU:HD11	2:D:1276:PHE:HE2	1.56	0.70
2:D:1067:ALA:HB2	2:D:1074:PRO:HA	1.72	0.70
2:D:1574:ASP:OD2	2:D:1582:ARG:NH1	2.24	0.70
2:B:964:PRO:HB3	2:B:1327:ASN:OD1	1.90	0.70
1:C:29:ILE:HA	1:C:645:THR:O	1.90	0.70
2:D:1507:ARG:HE	2:D:1510:LEU:HD23	1.56	0.70
3:F:246:ARG:HH11	3:F:246:ARG:CG	2.03	0.70
1:C:659:GLU:N	1:C:659:GLU:OE1	2.24	0.70
2:D:758:GLU:HA	2:D:913:LYS:NZ	2.04	0.70
2:D:934:GLU:OE1	2:D:934:GLU:N	2.22	0.70
2:D:1311:ILE:HD11	2:D:1318:LEU:HD23	1.71	0.70
3:E:133:TYR:HB3	3:E:158:CYS:HB3	1.72	0.70
2:D:1508:ASP:CG	2:D:1509:GLU:H	1.98	0.70
2:B:1111:LYS:CE	2:B:1119:GLN:O	2.40	0.70
1:C:99:GLU:CB	1:C:102:ARG:HB2	2.22	0.70
1:A:481:ARG:HA	1:A:484:GLU:OE1	1.92	0.70
2:B:1118:PHE:H	2:B:1144:THR:CG2	2.04	0.70
1:C:390:ALA:HB2	1:C:398:GLN:OE1	1.90	0.69
2:D:776:GLU:HG3	2:D:791:MET:SD	2.31	0.69
2:D:935:GLY:HA2	2:D:1353:LYS:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1485:LEU:HD12	2:D:1486:GLU:H	1.56	0.69
1:A:446:TYR:HE1	1:A:634:ASP:HA	1.57	0.69
1:C:458:LEU:HD11	1:C:533:ALA:HB3	1.73	0.69
2:D:934:GLU:HG2	2:D:1352:ALA:C	2.17	0.69
2:D:987:VAL:HG22	2:D:988:ALA:H	1.57	0.69
2:D:1149:ILE:HA	2:D:1152:GLN:NE2	2.07	0.69
2:D:904:LYS:O	2:D:908:GLN:NE2	2.24	0.69
2:D:1151:LEU:HG	2:D:1165:LEU:HD11	1.74	0.69
2:B:1078:LEU:HD11	2:B:1124:VAL:HG23	1.75	0.69
2:D:768:PRO:HD3	2:D:796:LYS:HZ2	1.56	0.69
2:D:1544:VAL:HG23	2:D:1570:LYS:HD3	1.74	0.69
1:A:125:LEU:HD22	1:A:215:GLN:HE22	1.56	0.69
1:A:647:THR:HG22	1:A:653:GLN:OE1	1.93	0.69
2:B:990:MET:O	2:B:1282:TYR:OH	2.11	0.69
1:C:183:GLN:OE1	1:C:183:GLN:N	2.21	0.69
1:A:141:PRO:HA	1:A:195:ILE:HD12	1.75	0.69
2:B:1050:LYS:O	2:B:1054:THR:HG23	1.92	0.69
2:B:1387:GLU:OE1	2:B:1387:GLU:N	2.25	0.69
2:B:1472:ILE:HD11	2:B:1494:HIS:NE2	2.08	0.69
1:A:647:THR:HG22	1:A:653:GLN:NE2	2.07	0.69
2:B:1497:LYS:HZ3	2:B:1502:LEU:HA	1.57	0.69
2:D:948:ASP:OD2	2:D:951:ARG:NH1	2.26	0.69
2:D:1496:GLU:OE1	2:D:1496:GLU:N	2.23	0.69
2:B:1202:LEU:CD1	2:B:1243:LEU:HD21	2.22	0.69
2:B:1300:LEU:HD12	2:B:1300:LEU:O	1.92	0.69
2:D:1552:VAL:HG12	2:D:1561:TYR:CD1	2.28	0.69
2:B:1202:LEU:HA	2:B:1206:LEU:HD11	1.74	0.68
1:C:646:PHE:H	1:C:654:THR:CG2	2.05	0.68
2:D:1105:LYS:HE3	2:D:1106:TRP:NE1	2.08	0.68
1:A:181:SER:HB2	3:E:246:ARG:HH21	1.58	0.68
1:A:476:LEU:HD13	1:A:514:LEU:HD12	1.75	0.68
2:D:1631:TRP:HD1	2:D:1649:LEU:HD21	1.56	0.68
3:E:106:SER:OG	3:E:156:GLU:HG2	1.92	0.68
3:F:246:ARG:HH11	3:F:246:ARG:HG2	1.58	0.68
1:A:494:ILE:HD13	1:A:531:LEU:HD13	1.74	0.68
2:B:1641:GLU:OE1	2:B:1641:GLU:N	2.27	0.68
1:A:471:LEU:CD1	1:A:519:LEU:HB3	2.23	0.68
2:B:877:THR:HG23	2:B:879:LYS:H	1.57	0.68
2:B:1067:ALA:HB2	2:B:1074:PRO:HA	1.74	0.68
2:B:1544:VAL:HG13	2:B:1570:LYS:HB3	1.73	0.68
1:A:215:GLN:HG2	1:A:216:GLN:N	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1066:PHE:HB2	2:D:1078:LEU:HD11	1.76	0.68
2:B:913:LYS:HD2	2:B:923:ASP:O	1.94	0.68
2:B:1076:THR:CG2	2:B:1111:LYS:HE2	2.04	0.68
2:B:1126:HIS:O	2:B:1129:MET:HG2	1.92	0.68
2:B:1299:GLN:HA	2:B:1303:ARG:NH2	2.09	0.68
2:B:1640:GLU:O	2:B:1643:GLN:HG2	1.93	0.68
1:C:246:TYR:OH	1:C:317:GLU:OE2	2.08	0.68
2:B:1105:LYS:HG2	2:B:1162:VAL:HG22	1.75	0.68
2:B:1494:HIS:ND1	2:B:1497:LYS:HB3	2.09	0.68
2:D:949:PRO:O	2:D:950:GLU:HB2	1.94	0.68
2:B:1174:ASP:OD1	2:B:1175:PHE:N	2.27	0.68
2:D:1035:GLU:HA	2:D:1039:LEU:HD12	1.76	0.68
1:A:234:VAL:HG13	1:A:341:ALA:HB2	1.75	0.68
2:B:1554:LEU:HD12	2:B:1555:SER:N	2.09	0.68
2:B:1586:SER:HB2	2:B:1622:ILE:HG12	1.76	0.68
1:C:94:ARG:HA	1:C:94:ARG:NE	2.04	0.67
2:D:855:ARG:HG2	2:D:858:GLN:HB3	1.76	0.67
2:D:1148:LEU:HD12	2:D:1149:ILE:N	2.09	0.67
1:A:130:LEU:HD11	1:A:151:THR:HG22	1.75	0.67
1:C:231:SER:HB3	2:D:834:ARG:NH2	2.09	0.67
3:F:136:GLU:HB2	3:F:159:LYS:NZ	2.09	0.67
1:C:98:SER:O	1:C:100:LYS:HA	1.95	0.67
3:E:276:TRP:N	3:E:276:TRP:CE3	2.62	0.67
2:D:979:ARG:NH1	2:D:1323:GLU:OE2	2.26	0.67
2:D:1417:ASP:O	2:D:1421:LEU:HG	1.94	0.67
2:D:1492:PHE:HD1	2:D:1492:PHE:N	1.92	0.67
2:B:1263:GLY:HA3	2:B:1272:THR:HG22	1.77	0.67
1:C:28:ILE:HG12	1:C:42:MET:HE3	1.77	0.67
2:D:1015:MET:HE1	2:D:1018:MET:HE2	1.75	0.67
1:A:464:GLU:HB3	1:A:556:LYS:HE3	1.75	0.67
1:A:471:LEU:CD1	1:A:473:VAL:HG23	2.25	0.67
2:B:945:ARG:HD2	2:B:960:GLU:CD	2.20	0.67
2:B:991:THR:HG22	2:B:1282:TYR:HE2	1.59	0.67
2:B:1650:GLY:O	2:B:1653:THR:HG22	1.94	0.67
2:D:1436:LYS:HB3	2:D:1441:ARG:HE	1.60	0.67
1:A:566:LYS:HE3	1:A:584:LYS:HD2	1.75	0.67
1:A:193:TRP:CZ3	1:A:195:ILE:HG22	2.30	0.67
1:C:138:ILE:HD11	1:C:602:VAL:HG13	1.76	0.67
2:D:983:GLN:HB3	2:D:1341:THR:OG1	1.95	0.67
2:D:1659:PHE:HZ	2:D:1662:PRO:HA	1.60	0.67
1:A:141:PRO:HA	1:A:195:ILE:CD1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:229:PRO:HG2	3:E:280:PRO:HG2	1.75	0.66
3:F:107:ALA:HB2	3:F:158:CYS:SG	2.35	0.66
2:B:1202:LEU:CD1	2:B:1207:LEU:HD11	2.24	0.66
2:B:1312:HIS:C	2:B:1313:TRP:CE3	2.73	0.66
1:C:495:MET:HE2	1:C:625:ILE:HD11	1.77	0.66
2:D:906:GLY:O	2:D:931:VAL:HG22	1.95	0.66
2:D:1435:ASP:N	2:D:1435:ASP:OD1	2.25	0.66
3:F:186:ILE:HG13	3:F:188:PHE:HE1	1.60	0.66
2:D:1118:PHE:H	2:D:1144:THR:HG23	1.60	0.66
1:A:160:GLY:C	1:A:161:ARG:HG2	2.19	0.66
2:B:1149:ILE:HA	2:B:1152:GLN:HE22	1.61	0.66
2:D:872:PHE:HD1	2:D:902:PRO:HA	1.60	0.66
2:D:1311:ILE:HD13	2:D:1320:ARG:HH21	1.61	0.66
2:B:867:LEU:HD21	2:B:911:GLU:HB3	1.78	0.66
1:C:201:MET:CE	1:C:225:LYS:HA	2.25	0.66
2:B:1010:CYS:HA	2:B:1059:PHE:CZ	2.30	0.66
2:B:1172:ALA:O	2:B:1176:LEU:HD13	1.95	0.66
2:B:1357:THR:HA	2:B:1359:ASN:N	2.10	0.66
1:C:397:VAL:CG1	1:C:409:LEU:HD22	2.25	0.66
2:D:886:VAL:HG21	2:D:894:LEU:HD23	1.78	0.66
2:D:1225:LYS:HE3	2:D:1227:LEU:HD11	1.78	0.66
1:C:168:GLU:CG	1:C:205:LYS:HB3	2.25	0.66
1:A:317:GLU:H	1:A:317:GLU:CD	2.03	0.66
1:C:59:VAL:HG23	1:C:106:VAL:CG2	2.26	0.66
1:C:97:LYS:HG2	2:D:1314:GLU:HB3	1.78	0.66
1:A:471:LEU:HD11	1:A:519:LEU:HB3	1.76	0.65
1:A:647:THR:HG22	1:A:653:GLN:CD	2.20	0.65
1:C:29:ILE:HB	1:C:43:VAL:CG1	2.26	0.65
2:D:1077:TRP:CZ2	2:D:1130:ILE:HA	2.31	0.65
2:D:1498:GLU:O	2:D:1500:GLY:N	2.29	0.65
1:A:376:VAL:HG13	1:A:384:ALA:HB3	1.78	0.65
2:D:985:THR:CG2	2:D:987:VAL:HG12	2.26	0.65
2:D:1550:VAL:HG21	2:D:1581:GLN:HE22	1.62	0.65
1:A:129:TYR:HA	1:A:218:PHE:HE2	1.61	0.65
2:B:1203:LYS:HA	2:B:1207:LEU:HD22	1.78	0.65
1:C:245:ILE:H	1:C:245:ILE:HD12	1.61	0.65
1:C:488:ARG:NH1	1:C:508:ARG:O	2.29	0.65
1:C:573:ARG:HE	1:C:579:GLN:NE2	1.94	0.65
2:D:1215:LYS:O	2:D:1216:ASP:OD1	2.14	0.65
2:D:1363:LEU:HD21	2:D:1477:VAL:HG12	1.78	0.65
2:B:1604:MET:HA	2:B:1627:TRP:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:GLN:O	3:F:240:ARG:NH2	2.29	0.65
1:C:205:LYS:HE3	1:C:219:SER:HB3	1.77	0.65
1:A:140:THR:HG23	1:A:227:TYR:CE2	2.32	0.65
1:C:404:ASP:OD1	1:C:406:VAL:HG12	1.96	0.65
2:B:1060:ARG:HG3	2:B:1060:ARG:HH11	1.62	0.65
2:B:1525:ASP:OD1	2:B:1525:ASP:N	2.17	0.65
2:D:1506:CYS:SG	2:D:1511:CYS:CB	2.84	0.65
3:E:205:LEU:HD12	3:E:212:GLN:O	1.97	0.65
3:F:246:ARG:HH11	3:F:246:ARG:CB	2.09	0.65
1:A:313:ASN:ND2	1:A:318:ASP:OD2	2.29	0.65
2:D:755:ILE:HG22	2:D:756:ILE:N	2.11	0.65
2:D:1102:GLY:O	2:D:1106:TRP:CD1	2.50	0.65
2:D:756:ILE:HB	3:F:134:ARG:HH22	1.62	0.64
2:D:950:GLU:N	2:D:953:GLY:O	2.27	0.64
3:F:272:ASP:N	3:F:272:ASP:OD1	2.30	0.64
1:A:93:ASN:OD1	1:A:94:ARG:N	2.31	0.64
1:A:196:PRO:HD2	1:A:199:VAL:HG21	1.78	0.64
1:A:446:TYR:CE1	1:A:634:ASP:HA	2.32	0.64
2:B:1607:LEU:HD23	2:B:1608:SER:H	1.60	0.64
1:C:487:ILE:O	1:C:508:ARG:HD3	1.98	0.64
2:D:1326:GLU:OE1	2:D:1328:GLU:HB2	1.98	0.64
3:E:110:LYS:HD3	3:E:128:GLU:HB3	1.78	0.64
3:F:135:ARG:HG3	3:F:135:ARG:NH1	2.12	0.64
1:A:35:ARG:HD3	1:A:154:HIS:NE2	2.11	0.64
2:B:1066:PHE:CE1	2:B:1082:VAL:HG11	2.32	0.64
1:C:25:MET:HE2	1:C:47:HIS:HD2	1.61	0.64
1:A:166:ASN:HD21	1:A:174:PRO:HG3	1.62	0.64
2:D:880:ARG:CZ	2:D:1471:LEU:HG	2.27	0.64
3:E:107:ALA:C	3:E:130:ARG:NH1	2.55	0.64
1:A:197:GLU:OE1	1:A:198:LEU:HD12	1.98	0.64
2:B:962:ILE:HG13	2:B:1330:PHE:O	1.97	0.64
2:B:1356:LEU:HD13	2:B:1357:THR:H	1.61	0.64
1:C:508:ARG:HH12	1:C:512:GLN:C	2.06	0.64
1:A:239:THR:OG1	1:A:252:GLU:HG2	1.98	0.64
1:A:274:GLY:HA3	1:A:325:TYR:CZ	2.32	0.64
2:D:766:GLU:CB	2:D:796:LYS:HZ1	2.08	0.64
2:D:905:THR:HA	2:D:931:VAL:HG23	1.79	0.64
3:E:223:ILE:O	3:E:223:ILE:HG13	1.98	0.64
1:C:625:ILE:HD12	1:C:643:GLY:HA3	1.80	0.64
2:B:1392:TYR:CD1	2:B:1398:ALA:HB2	2.32	0.64
2:D:1249:VAL:HG22	2:D:1250:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLN:HE21	1:A:218:PHE:HE1	1.46	0.64
1:A:466:ARG:HG3	1:A:556:LYS:CD	2.16	0.64
2:B:940:LYS:HD3	2:B:940:LYS:N	2.13	0.64
2:B:991:THR:HG22	2:B:1282:TYR:CE2	2.34	0.64
1:C:302:LEU:HD21	1:C:307:LEU:HB2	1.79	0.64
2:D:971:VAL:HG12	2:D:1349:HIS:HB2	1.80	0.64
2:D:1423:ASN:O	2:D:1423:ASN:ND2	2.26	0.64
1:A:404:ASP:OD1	1:A:406:VAL:HG12	1.97	0.63
2:B:761:ILE:HD12	2:B:761:ILE:O	1.97	0.63
2:D:1291:GLU:OE2	2:D:1337:LYS:HB3	1.99	0.63
2:D:1368:LYS:HB2	2:D:1385:ILE:HD11	1.80	0.63
2:D:1506:CYS:HG	2:D:1511:CYS:HB2	1.58	0.63
2:B:1411:PHE:CZ	2:B:1465:GLN:HB3	2.33	0.63
2:B:1516:GLU:OE1	2:B:1624:LYS:HG2	1.98	0.63
2:D:1552:VAL:HG12	2:D:1561:TYR:HD1	1.63	0.63
2:B:1405:ILE:HG12	2:B:1477:VAL:HG22	1.80	0.63
3:E:146:LEU:CD1	3:E:150:LYS:HB2	2.29	0.63
3:E:195:LYS:HE3	3:E:197:PHE:CE1	2.34	0.63
1:A:456:LEU:HB2	1:A:535:TYR:HE2	1.63	0.63
2:B:1188:THR:HA	2:B:1191:ILE:HD11	1.80	0.63
2:D:1292:LEU:HB2	2:D:1313:TRP:HB2	1.79	0.63
1:C:148:ARG:HG3	2:D:773:TRP:CZ2	2.33	0.63
1:C:205:LYS:CE	1:C:219:SER:HB3	2.28	0.63
2:D:1604:MET:HA	2:D:1627:TRP:O	1.99	0.63
1:A:83:MET:CE	1:A:505:ARG:HH11	2.11	0.63
2:D:853:ASN:HD22	2:D:888:ILE:HG23	1.62	0.63
2:D:1066:PHE:CB	2:D:1078:LEU:HD11	2.29	0.63
2:D:1533:LEU:HD23	2:D:1656:MET:HE2	1.81	0.63
2:B:1503:ASN:ND2	2:B:1589:LYS:HE3	2.14	0.63
2:D:1148:LEU:O	2:D:1152:GLN:HG2	1.99	0.63
3:F:121:VAL:HA	3:F:145:CYS:SG	2.39	0.63
3:F:222:GLU:OE2	3:F:224:TYR:OH	2.13	0.63
3:F:199:SER:OG	3:F:201:SER:O	2.15	0.63
1:C:69:LEU:HD21	1:C:91:PRO:CD	2.28	0.62
2:D:763:SER:HB3	2:D:926:ARG:HB2	1.80	0.62
1:A:45:GLU:OE2	1:A:491:THR:HG21	1.98	0.62
1:A:181:SER:CB	3:E:246:ARG:NH2	2.63	0.62
2:B:761:ILE:HG21	2:B:913:LYS:HE3	1.81	0.62
2:B:1174:ASP:OD1	2:B:1175:PHE:CD2	2.53	0.62
2:B:1187:TYR:HD1	2:B:1232:ALA:HB2	1.65	0.62
2:D:1310:ARG:HD2	2:D:1312:HIS:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:259:MET:SD	3:F:281:PRO:HB2	2.39	0.62
2:B:871:ALA:O	2:B:903:LEU:N	2.28	0.62
1:C:566:LYS:HB2	1:C:584:LYS:HE2	1.81	0.62
2:D:996:ASP:OD1	2:D:1036:LYS:HE2	1.98	0.62
2:D:1108:ILE:HD11	2:D:1151:LEU:HD21	1.81	0.62
2:B:1136:ASN:HA	2:B:1139:LYS:NZ	2.14	0.62
2:D:1089:ALA:HA	2:D:1092:LEU:HD13	1.79	0.62
2:D:1313:TRP:CZ3	2:D:1318:LEU:HD11	2.34	0.62
2:D:1420:GLN:O	2:D:1423:ASN:ND2	2.31	0.62
2:D:756:ILE:HD11	2:D:760:ASN:OD1	2.00	0.62
2:D:1492:PHE:HE2	2:D:1500:GLY:O	1.82	0.62
2:D:1496:GLU:O	2:D:1498:GLU:N	2.32	0.62
2:B:1436:LYS:O	2:B:1441:ARG:NH2	2.33	0.62
2:B:1532:ARG:NH2	2:B:1629:GLU:OE2	2.31	0.62
2:D:957:VAL:HG21	2:D:1335:GLU:HA	1.82	0.62
2:B:1082:VAL:O	2:B:1086:PHE:HD1	1.82	0.62
1:C:120:VAL:O	1:C:656:GLN:NE2	2.30	0.62
2:D:1291:GLU:OE2	2:D:1338:GLY:N	2.33	0.62
2:D:1659:PHE:HE2	2:D:1662:PRO:HD3	1.63	0.62
3:E:163:CYS:HB2	3:E:180:ILE:O	2.00	0.62
3:F:232:ASP:O	3:F:233:ASN:OD1	2.18	0.62
2:B:1144:THR:O	2:B:1148:LEU:HB2	1.98	0.62
2:B:1189:VAL:HG11	2:B:1213:THR:HG21	1.82	0.62
2:D:886:VAL:HG21	2:D:894:LEU:CD2	2.29	0.62
2:D:987:VAL:HG22	2:D:988:ALA:N	2.15	0.62
2:D:1210:PHE:CE1	2:D:1220:TRP:HH2	2.18	0.62
3:E:141:PRO:HA	3:E:157:PHE:HD2	1.63	0.62
3:E:145:CYS:HB2	3:E:151:TRP:CZ3	2.35	0.62
1:A:502:LYS:NZ	1:A:503:ALA:O	2.30	0.62
1:C:146:LEU:HD13	2:D:773:TRP:CD2	2.34	0.62
2:D:800:THR:HG22	2:D:801:THR:H	1.64	0.62
1:A:376:VAL:CG1	1:A:401:THR:HG21	2.30	0.61
2:B:1303:ARG:NH1	2:B:1306:LYS:HA	2.13	0.61
2:B:1538:GLU:O	2:B:1541:VAL:HG12	2.00	0.61
3:E:130:ARG:NH1	3:E:130:ARG:HG3	2.15	0.61
2:B:939:ASN:C	2:B:940:LYS:HD3	2.25	0.61
2:B:945:ARG:HD2	2:B:960:GLU:OE1	1.99	0.61
1:C:496:ASN:C	1:C:498:GLY:H	2.08	0.61
2:D:985:THR:HG22	2:D:987:VAL:HG12	1.82	0.61
1:A:155:LYS:HG2	1:A:499:ARG:HE	1.64	0.61
1:A:364:PHE:CE2	1:A:366:PRO:HA	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:GLN:HG2	2:B:1341:THR:HB	1.81	0.61
2:D:1214:ALA:HB2	2:D:1220:TRP:HE1	1.65	0.61
2:D:1643:GLN:HG3	2:D:1644:LYS:HD2	1.82	0.61
1:A:148:ARG:CZ	1:A:594:VAL:HB	2.30	0.61
2:D:1060:ARG:HG3	2:D:1060:ARG:HH11	1.65	0.61
1:A:167:ILE:HG12	1:A:176:LYS:HB3	1.83	0.61
1:A:181:SER:HB3	3:E:246:ARG:NH2	2.14	0.61
2:B:1469:VAL:HG13	2:B:1472:ILE:HG22	1.81	0.61
2:D:937:ARG:HH21	2:D:1349:HIS:CE1	2.17	0.61
2:D:1202:LEU:CD1	2:D:1243:LEU:HD21	2.27	0.61
2:B:1554:LEU:CD1	2:B:1591:ARG:HH12	2.11	0.61
1:C:449:VAL:HG21	1:C:545:GLU:HG3	1.83	0.61
1:C:646:PHE:H	1:C:654:THR:HG21	1.65	0.61
2:D:756:ILE:HD12	3:F:134:ARG:HH22	1.65	0.61
2:D:1301:PRO:HD2	2:D:1328:GLU:OE2	2.01	0.61
1:A:76:LEU:HG	1:A:82:HIS:HA	1.83	0.61
1:A:647:THR:HG22	1:A:653:GLN:HE22	1.64	0.61
2:B:1548:ARG:HD2	2:B:1566:GLU:OE2	2.01	0.61
2:D:1528:THR:OG1	2:D:1529:LEU:N	2.32	0.61
2:B:780:GLU:OE2	2:B:789:LYS:HD3	2.00	0.61
2:B:1643:GLN:HG3	2:B:1644:LYS:N	2.16	0.61
1:C:487:ILE:H	1:C:487:ILE:HD12	1.65	0.61
2:D:997:ALA:H	2:D:1036:LYS:HE2	1.66	0.61
1:A:125:LEU:CD1	1:A:125:LEU:H	2.12	0.61
1:A:622:LYS:HD2	1:A:622:LYS:O	2.01	0.61
2:B:1496:GLU:HG2	2:B:1497:LYS:H	1.65	0.61
2:D:1433:GLU:CD	2:D:1445:ILE:H	2.08	0.61
1:C:135:ASP:HB3	1:C:146:LEU:HD11	1.82	0.61
2:D:1033:GLN:HB3	2:D:1036:LYS:HZ2	1.64	0.61
2:D:1507:ARG:O	2:D:1508:ASP:OD1	2.18	0.61
1:A:42:MET:HB3	1:A:86:VAL:HG23	1.83	0.60
2:B:1138:GLU:HG3	2:B:1188:THR:HG21	1.83	0.60
1:C:479:MET:HG3	1:C:480:ASP:OD1	2.01	0.60
1:A:591:ALA:HB2	2:B:810:SER:HB2	1.82	0.60
2:B:1576:VAL:CA	2:B:1580:GLN:HE22	2.15	0.60
2:D:1131:GLY:O	2:D:1228:TYR:HE1	1.84	0.60
1:C:67:LEU:CD2	1:C:67:LEU:CD1	2.71	0.60
3:E:146:LEU:CG	3:E:150:LYS:HB2	2.30	0.60
2:B:800:THR:OG1	2:B:801:THR:N	2.25	0.60
1:C:599:ASP:OD1	2:D:800:THR:HG21	2.01	0.60
2:D:759:GLU:HG2	2:D:760:ASN:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1061:GLN:HG3	2:D:1062:PRO:HD2	1.83	0.60
2:D:1397:ASP:CB	2:D:1450:LYS:HE2	2.32	0.60
3:F:109:LEU:HB2	3:F:114:ILE:HG12	1.81	0.60
2:B:904:LYS:HG3	2:B:908:GLN:OE1	2.00	0.60
2:B:1202:LEU:HD12	2:B:1202:LEU:O	2.01	0.60
1:C:365:LYS:NZ	1:C:457:HIS:HA	2.16	0.60
2:D:778:LEU:HG	2:D:787:SER:HB3	1.82	0.60
1:A:364:PHE:CE1	1:A:420:LEU:HG	2.36	0.60
2:D:1148:LEU:HD11	2:D:1195:ALA:HB1	1.83	0.60
2:D:1187:TYR:HD1	2:D:1232:ALA:HB2	1.67	0.60
2:D:1487:GLU:N	2:D:1487:GLU:OE1	2.35	0.60
3:E:226:PRO:O	3:E:276:TRP:CZ2	2.54	0.60
1:A:83:MET:HG3	1:A:505:ARG:HD2	1.81	0.60
2:B:1136:ASN:O	2:B:1185:ARG:NH1	2.35	0.60
2:B:1497:LYS:HZ1	2:B:1501:LYS:C	2.09	0.60
2:D:1013:GLU:O	2:D:1016:ILE:HG22	2.01	0.60
1:A:36:LEU:CD2	1:A:125:LEU:HA	2.31	0.60
1:A:133:GLN:HG3	1:A:133:GLN:O	2.02	0.60
2:B:872:PHE:CD1	2:B:902:PRO:HA	2.37	0.60
2:B:1382:ASN:OD1	2:B:1383:THR:N	2.34	0.60
2:B:1521:GLN:H	2:B:1521:GLN:CD	2.08	0.60
2:B:1543:TYR:HB2	2:B:1545:TYR:CZ	2.36	0.60
2:D:947:LEU:N	2:D:947:LEU:HD12	2.17	0.60
2:D:990:MET:N	2:D:991:THR:HA	2.17	0.60
2:B:1274:MET:SD	2:B:1277:GLN:NE2	2.75	0.60
2:B:1303:ARG:HH12	2:B:1307:ILE:N	1.99	0.60
2:B:1317:SER:OG	2:B:1320:ARG:NH2	2.35	0.60
2:D:1217:LYS:HG3	2:D:1248:PHE:CE2	2.37	0.60
2:D:1241:LEU:HD21	2:D:1285:ASP:HB2	1.83	0.60
2:D:1610:ASP:HA	2:D:1621:ILE:HD11	1.83	0.60
3:E:106:SER:O	3:E:130:ARG:N	2.30	0.60
3:F:233:ASN:ND2	3:F:257:PHE:CD2	2.69	0.60
2:B:1429:ILE:HD11	2:B:1433:GLU:HG3	1.83	0.60
2:D:899:VAL:HG23	2:D:1473:GLN:HE21	1.67	0.60
2:D:987:VAL:CG2	2:D:988:ALA:H	2.13	0.60
2:D:1130:ILE:HD12	2:D:1133:LEU:HB2	1.84	0.60
2:D:1233:THR:HG22	2:D:1256:LEU:HD11	1.84	0.60
3:F:186:ILE:HD13	3:F:213:TRP:CH2	2.35	0.60
1:A:62:PHE:CE2	2:B:1039:LEU:HD11	2.36	0.59
1:C:465:LEU:CD1	1:C:555:VAL:HG22	2.32	0.59
1:C:558:SER:O	1:C:617:TRP:NE1	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1104:VAL:O	2:D:1108:ILE:HG12	2.02	0.59
2:D:1128:GLU:OE2	2:D:1267:GLY:HA3	2.01	0.59
2:D:1600:LYS:HD2	2:D:1633:GLU:OE2	2.02	0.59
1:A:105:PHE:HE2	1:A:122:LEU:HG	1.67	0.59
2:B:872:PHE:HD1	2:B:902:PRO:HA	1.66	0.59
2:B:1078:LEU:HD21	2:B:1124:VAL:HG21	1.84	0.59
2:B:1171:LYS:O	2:B:1174:ASP:OD1	2.20	0.59
2:B:1197:ALA:HA	2:B:1202:LEU:HG	1.83	0.59
2:B:1636:GLU:OE2	2:B:1642:ASN:ND2	2.35	0.59
1:C:157:LEU:HD11	2:D:811:ASP:C	2.27	0.59
1:C:207:ARG:NH1	1:C:219:SER:HG	1.95	0.59
1:C:484:GLU:OE1	1:C:484:GLU:N	2.32	0.59
2:D:756:ILE:CG1	3:F:134:ARG:HH22	2.15	0.59
2:B:1240:LEU:HA	2:B:1243:LEU:HB2	1.85	0.59
1:C:196:PRO:HD2	1:C:199:VAL:HG21	1.83	0.59
1:C:455:TYR:HB2	1:C:478:ARG:HB3	1.84	0.59
3:F:180:ILE:HD11	3:F:213:TRP:CH2	2.36	0.59
2:D:1185:ARG:O	2:D:1189:VAL:HG22	2.02	0.59
2:D:1240:LEU:HD23	2:D:1249:VAL:HG12	1.83	0.59
2:D:1392:TYR:CD1	2:D:1398:ALA:HB2	2.37	0.59
1:A:227:TYR:OH	2:B:769:GLU:OE1	2.18	0.59
1:A:611:LEU:HG	2:B:817:VAL:HG21	1.83	0.59
2:B:1117:VAL:HG22	2:B:1144:THR:HG21	1.83	0.59
2:B:1214:ALA:HB2	2:B:1220:TRP:CE2	2.38	0.59
2:B:1607:LEU:CD2	2:B:1608:SER:H	2.15	0.59
1:C:100:LYS:HD3	2:D:1313:TRP:CZ2	2.37	0.59
2:D:1128:GLU:OE1	2:D:1267:GLY:HA3	2.03	0.59
2:D:1149:ILE:CD1	2:D:1194:TYR:HE2	2.12	0.59
2:B:982:LEU:HD21	2:B:1296:VAL:HG21	1.82	0.59
2:B:1007:PRO:HB2	2:B:1055:GLN:NE2	2.18	0.59
2:B:1075:SER:HB3	2:B:1078:LEU:HD12	1.84	0.59
2:D:761:ILE:HG22	2:D:762:VAL:N	2.18	0.59
2:D:877:THR:HG23	2:D:879:LYS:H	1.68	0.59
2:D:1506:CYS:HB3	2:D:1511:CYS:HB2	1.82	0.59
1:A:471:LEU:HD13	1:A:473:VAL:HG23	1.85	0.59
2:D:877:THR:OG1	2:D:878:THR:N	2.34	0.59
2:B:1303:ARG:HH12	2:B:1306:LYS:C	2.11	0.59
2:D:755:ILE:CG2	2:D:756:ILE:H	2.15	0.59
2:D:1515:GLU:HA	2:D:1589:LYS:NZ	2.18	0.59
2:B:1582:ARG:HD2	2:B:1620:TYR:HE1	1.68	0.59
2:D:1397:ASP:OD1	2:D:1453:HIS:ND1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:113:TYR:CD1	3:E:125:VAL:HG12	2.38	0.59
3:E:171:ASN:ND2	3:E:194:TYR:CZ	2.69	0.59
1:A:81:ASN:O	1:A:82:HIS:CG	2.56	0.58
2:D:1562:ILE:HG13	2:D:1562:ILE:O	2.02	0.58
2:D:1148:LEU:HD11	2:D:1195:ALA:CB	2.32	0.58
2:D:1253:VAL:HA	2:D:1256:LEU:HD22	1.85	0.58
1:A:140:THR:O	1:A:195:ILE:HD11	2.03	0.58
1:A:389:VAL:HG12	1:A:426:THR:HG22	1.85	0.58
2:B:1015:MET:HG2	2:B:1056:GLN:HE22	1.69	0.58
1:C:28:ILE:HD12	1:C:29:ILE:H	1.68	0.58
1:C:449:VAL:O	1:C:452:SER:OG	2.22	0.58
2:D:1311:ILE:HD11	2:D:1318:LEU:HA	1.85	0.58
1:A:628:THR:CG2	1:A:641:ASP:HB3	2.33	0.58
2:B:1130:ILE:HG13	2:B:1133:LEU:HB2	1.84	0.58
1:A:340:GLN:OE1	1:A:340:GLN:HA	2.04	0.58
2:B:971:VAL:HB	2:B:1349:HIS:NE2	2.18	0.58
2:B:1587:PRO:HG2	2:B:1590:CYS:SG	2.44	0.58
2:B:1639:ASP:HB3	2:B:1641:GLU:OE1	2.04	0.58
1:C:28:ILE:HD12	1:C:29:ILE:N	2.18	0.58
2:D:756:ILE:CD1	3:F:134:ARG:HH12	2.16	0.58
2:D:937:ARG:NH2	2:D:1349:HIS:HE1	2.00	0.58
2:B:1112:GLN:HA	2:B:1112:GLN:OE1	2.03	0.58
2:B:1631:TRP:CD1	2:B:1649:LEU:HD13	2.38	0.58
1:C:30:THR:HG23	1:C:645:THR:OG1	2.03	0.58
1:C:135:ASP:OD1	1:C:139:TYR:OH	2.17	0.58
1:C:337:ASP:OD2	2:D:834:ARG:NE	2.37	0.58
2:D:757:ALA:O	2:D:761:ILE:HD13	2.03	0.58
2:D:780:GLU:OE1	2:D:780:GLU:N	2.36	0.58
1:A:169:ASN:HB2	1:A:170:PRO:HD2	1.86	0.58
1:A:252:GLU:OE1	1:A:252:GLU:N	2.25	0.58
1:A:496:ASN:C	1:A:498:GLY:H	2.12	0.58
2:B:1152:GLN:NE2	2:B:1198:GLN:HE22	2.02	0.58
2:B:1202:LEU:CA	2:B:1206:LEU:HD11	2.33	0.58
2:B:1357:THR:HA	2:B:1358:CYS:C	2.29	0.58
1:C:47:HIS:ND1	1:C:489:TYR:OH	2.34	0.58
1:C:72:GLU:HB2	1:C:86:VAL:HG21	1.85	0.58
2:D:1600:LYS:HE3	2:D:1630:HIS:NE2	2.19	0.58
2:D:1631:TRP:CD1	2:D:1649:LEU:CD2	2.86	0.58
3:F:187:SER:C	3:F:188:PHE:HD1	2.11	0.58
1:A:45:GLU:OE1	1:A:534:TYR:OH	2.22	0.58
1:A:122:LEU:HD21	1:A:657:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD12	1:A:337:ASP:HB2	1.84	0.58
1:A:359:LYS:HD2	1:A:552:TRP:CZ3	2.38	0.58
2:B:1049:ILE:HG22	2:B:1093:ILE:HD13	1.84	0.58
2:B:1592:GLU:O	2:B:1595:LYS:NZ	2.28	0.58
1:C:39:GLU:OE1	1:C:39:GLU:N	2.24	0.58
1:C:324:LEU:HB2	1:C:346:ILE:CG1	2.34	0.58
3:F:186:ILE:HD11	3:F:202:SER:HB2	1.84	0.58
2:B:958:GLN:N	2:B:958:GLN:OE1	2.37	0.58
2:D:1067:ALA:HA	2:D:1078:LEU:HD21	1.86	0.58
2:D:1096:ASP:OD2	2:D:1098:GLN:NE2	2.37	0.58
2:D:1255:TRP:HE3	2:D:1256:LEU:HD12	1.67	0.58
2:D:1550:VAL:CG2	2:D:1581:GLN:NE2	2.67	0.58
3:E:197:PHE:HE2	3:E:221:ARG:HD2	1.67	0.58
1:A:104:LYS:CG	1:A:105:PHE:N	2.66	0.58
1:A:563:LEU:HD22	2:B:808:SER:HB3	1.85	0.58
1:C:552:TRP:CH2	1:C:554:ASP:HB2	2.38	0.58
2:D:841:ARG:HH12	2:D:903:LEU:C	2.12	0.58
2:D:1105:LYS:CE	2:D:1106:TRP:HE1	2.12	0.58
2:D:1416:ASP:OD1	2:D:1417:ASP:N	2.37	0.58
1:C:119:LYS:NZ	1:C:654:THR:O	2.36	0.57
2:D:1494:HIS:CD2	2:D:1497:LYS:HD2	2.39	0.57
3:E:224:TYR:HD2	3:E:242:HIS:HB3	1.67	0.57
3:F:135:ARG:HE	3:F:141:PRO:HB3	1.68	0.57
2:B:1554:LEU:HD12	2:B:1555:SER:H	1.69	0.57
1:C:125:LEU:HB2	1:C:215:GLN:NE2	2.19	0.57
2:D:1240:LEU:HD11	2:D:1248:PHE:HB3	1.85	0.57
2:D:1475:GLY:HA3	2:D:1493:TYR:CZ	2.39	0.57
1:A:650:SER:HG	1:A:652:GLN:HE22	1.48	0.57
2:D:794:PHE:CE2	3:F:176:VAL:HB	2.39	0.57
2:D:1035:GLU:HA	2:D:1039:LEU:HD11	1.86	0.57
1:A:57:VAL:HG21	1:A:86:VAL:HG21	1.86	0.57
1:A:135:ASP:OD1	1:A:139:TYR:OH	2.22	0.57
2:B:1043:GLN:O	2:B:1046:LEU:HG	2.04	0.57
2:B:1496:GLU:HG2	2:B:1497:LYS:N	2.20	0.57
2:D:835:LEU:HD23	2:D:929:LEU:HB3	1.86	0.57
1:A:272:ILE:HG22	1:A:327:SER:HB3	1.87	0.57
2:B:1084:LYS:HE2	2:B:1273:PHE:CE2	2.40	0.57
2:B:1549:LEU:HD13	2:B:1563:MET:CE	2.33	0.57
3:F:233:ASN:HD21	3:F:283:CYS:C	2.08	0.57
2:B:846:GLU:OE2	2:B:897:PRO:HB3	2.05	0.57
1:C:560:VAL:CG2	2:D:813:LYS:HZ1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:763:SER:OG	2:D:911:GLU:OE2	2.14	0.57
2:D:1597:GLU:HG3	2:D:1600:LYS:CG	2.34	0.57
1:C:560:VAL:HG13	2:D:813:LYS:HE3	1.85	0.57
2:D:951:ARG:O	2:D:952:LEU:HG	2.05	0.57
2:D:975:GLU:OE1	2:D:975:GLU:N	2.26	0.57
2:D:1027:TYR:CZ	2:D:1031:THR:HG21	2.40	0.57
2:D:1190:ALA:HB2	2:D:1220:TRP:HE3	1.70	0.57
2:D:1217:LYS:HG2	2:D:1217:LYS:O	2.05	0.57
2:D:1382:ASN:OD1	2:D:1383:THR:N	2.38	0.57
2:D:1644:LYS:HA	2:D:1647:GLN:OE1	2.04	0.57
2:B:1112:GLN:NE2	2:B:1116:GLY:C	2.63	0.57
1:C:66:LYS:HE3	3:E:147:GLN:N	2.20	0.57
1:C:508:ARG:HH22	1:C:512:GLN:N	2.03	0.57
2:D:1547:THR:HB	2:D:1563:MET:HG3	1.87	0.57
2:D:1577:GLN:N	2:D:1580:GLN:HE21	1.86	0.57
2:B:801:THR:OG1	2:B:824:THR:HG22	2.05	0.57
2:B:1015:MET:CG	2:B:1056:GLN:HE22	2.18	0.57
1:C:146:LEU:HD13	2:D:773:TRP:CE3	2.39	0.57
2:D:1149:ILE:HD11	2:D:1153:GLU:OE2	2.04	0.57
1:A:209:TYR:CD2	1:A:214:PRO:HA	2.39	0.57
2:B:1292:LEU:O	2:B:1313:TRP:CE3	2.57	0.57
1:C:600:LYS:NZ	2:D:822:GLU:OE2	2.23	0.57
3:E:224:TYR:CE2	3:E:242:HIS:HB3	2.40	0.57
2:B:878:THR:HG21	2:B:1624:LYS:HZ1	1.70	0.56
2:D:962:ILE:HD11	2:D:1330:PHE:CD2	2.40	0.56
3:E:282:GLU:OE2	3:E:284:ARG:HG2	2.04	0.56
3:F:188:PHE:CD2	3:F:218:PRO:HD2	2.39	0.56
1:A:125:LEU:H	1:A:125:LEU:HD12	1.69	0.56
2:B:865:GLU:CD	2:B:883:GLN:HE21	2.13	0.56
2:B:938:MET:HA	2:B:938:MET:HE2	1.86	0.56
1:C:26:TYR:O	1:C:649:SER:N	2.38	0.56
2:D:1065:ALA:HB3	2:D:1074:PRO:HB3	1.87	0.56
1:A:28:ILE:HD12	1:A:43:VAL:O	2.05	0.56
1:A:30:THR:HG22	1:A:645:THR:OG1	2.06	0.56
1:A:372:LEU:HD11	1:A:422:ILE:HG12	1.87	0.56
2:B:879:LYS:NZ	2:B:1521:GLN:HE22	2.03	0.56
2:B:904:LYS:HE3	2:B:908:GLN:HE22	1.69	0.56
2:B:949:PRO:HG3	2:B:958:GLN:HE22	1.70	0.56
2:B:1237:LEU:O	2:B:1241:LEU:HG	2.05	0.56
2:B:1240:LEU:C	2:B:1240:LEU:HD12	2.30	0.56
2:B:1516:GLU:CD	2:B:1624:LYS:HG2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:LYS:HD2	2:D:854:TYR:CE1	2.40	0.56
1:C:365:LYS:HZ1	1:C:549:ASP:CG	2.13	0.56
1:C:599:ASP:HB2	2:D:802:TRP:CZ3	2.40	0.56
2:D:756:ILE:HB	3:F:134:ARG:NH2	2.19	0.56
2:D:1117:VAL:HA	2:D:1144:THR:HG21	1.86	0.56
2:D:1148:LEU:HD21	2:D:1195:ALA:HB1	1.85	0.56
2:D:1216:ASP:OD2	2:D:1219:ARG:NH1	2.38	0.56
2:D:1217:LYS:HG3	2:D:1248:PHE:CZ	2.39	0.56
2:D:1298:LEU:CD1	2:D:1307:ILE:HB	2.35	0.56
2:D:1551:LYS:HE3	2:D:1562:ILE:HD13	1.86	0.56
3:F:239:GLU:OE1	3:F:240:ARG:O	2.23	0.56
1:A:366:PRO:HD2	1:A:455:TYR:CE1	2.41	0.56
1:A:390:ALA:HB3	1:A:427:LYS:HE3	1.86	0.56
1:C:196:PRO:HD2	1:C:199:VAL:CG2	2.36	0.56
2:D:1654:GLU:O	2:D:1658:VAL:HG13	2.05	0.56
3:E:203:PHE:HB3	3:E:214:SER:HB3	1.87	0.56
3:E:248:SER:OG	3:E:266:TYR:HB3	2.05	0.56
3:F:186:ILE:HG13	3:F:188:PHE:CE1	2.41	0.56
2:D:826:MET:HG2	2:D:827:GLN:N	2.19	0.56
2:D:912:VAL:HG13	2:D:925:VAL:HG23	1.87	0.56
1:A:178:ASP:OD2	3:E:247:GLN:NE2	2.39	0.56
2:B:1209:LYS:O	2:B:1213:THR:OG1	2.18	0.56
1:C:477:LEU:HD11	1:C:479:MET:HE2	1.88	0.56
2:D:904:LYS:HG3	2:D:908:GLN:NE2	2.21	0.56
2:D:1241:LEU:HD11	2:D:1285:ASP:HB3	1.85	0.56
3:F:186:ILE:HD13	3:F:213:TRP:CZ3	2.41	0.56
1:A:25:MET:HE2	1:A:47:HIS:HD2	1.70	0.56
1:A:235:ILE:HD11	1:A:256:THR:HB	1.88	0.56
2:B:1367:ILE:HD11	2:B:1384:MET:HB2	1.88	0.56
1:C:523:THR:CB	1:C:560:VAL:HG23	2.31	0.56
2:D:856:GLN:OE1	2:D:856:GLN:N	2.35	0.56
2:D:945:ARG:HB2	2:D:1342:LEU:HD23	1.88	0.56
3:F:124:VAL:HA	3:F:143:LEU:O	2.05	0.56
2:B:1086:PHE:O	2:B:1095:ILE:HD12	2.06	0.56
2:D:1004:ILE:O	2:D:1004:ILE:HG13	2.05	0.56
2:D:1210:PHE:CD1	2:D:1220:TRP:HH2	2.23	0.56
2:D:1255:TRP:HA	2:D:1258:GLU:CD	2.30	0.56
3:F:190:CYS:SG	3:F:196:LEU:HD12	2.45	0.56
2:B:1303:ARG:NH1	2:B:1306:LYS:CA	2.69	0.56
2:D:1255:TRP:CE3	2:D:1256:LEU:HD12	2.40	0.56
3:E:116:GLN:HG2	3:E:119:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1607:LEU:HD22	2:B:1609:SER:H	1.71	0.56
1:C:182:SER:O	1:C:185:GLN:HB2	2.06	0.56
1:C:397:VAL:HG13	1:C:409:LEU:HD22	1.87	0.56
1:C:650:SER:OG	1:C:652:GLN:OE1	2.10	0.56
1:A:140:THR:HG23	1:A:227:TYR:CZ	2.40	0.55
1:A:496:ASN:O	1:A:498:GLY:N	2.39	0.55
2:B:1549:LEU:HD13	2:B:1563:MET:HE2	1.88	0.55
1:C:365:LYS:NZ	1:C:456:LEU:O	2.36	0.55
2:D:802:TRP:HB2	2:D:823:VAL:HG23	1.86	0.55
2:D:937:ARG:NH2	2:D:1349:HIS:CE1	2.73	0.55
2:D:945:ARG:HB2	2:D:1342:LEU:CD2	2.36	0.55
3:F:157:PHE:HD1	3:F:157:PHE:H	1.53	0.55
2:B:1507:ARG:NH1	2:B:1508:ASP:OD1	2.39	0.55
1:C:35:ARG:NH2	1:C:498:GLY:O	2.38	0.55
1:C:201:MET:HE1	1:C:226:GLU:H	1.71	0.55
1:A:37:GLU:CD	1:A:161:ARG:NH1	2.63	0.55
1:A:166:ASN:OD1	1:A:167:ILE:N	2.40	0.55
1:A:332:LEU:CD1	1:A:337:ASP:HB2	2.36	0.55
1:C:57:VAL:O	1:C:71:SER:HA	2.06	0.55
1:C:397:VAL:HG12	1:C:409:LEU:HD22	1.88	0.55
2:D:1218:ASN:HB2	2:D:1251:PRO:O	2.07	0.55
1:A:31:PRO:HA	1:A:644:LEU:HD23	1.89	0.55
1:A:462:ARG:HH21	1:A:463:THR:C	2.13	0.55
2:B:757:ALA:N	2:B:760:ASN:HD21	2.03	0.55
2:D:1016:ILE:O	2:D:1016:ILE:HD12	2.07	0.55
3:E:233:ASN:HB2	3:E:283:CYS:SG	2.46	0.55
3:F:180:ILE:C	3:F:180:ILE:HD12	2.28	0.55
2:B:761:ILE:HG21	2:B:913:LYS:CE	2.37	0.55
2:B:1014:ASN:HD22	2:B:1055:GLN:HG3	1.72	0.55
2:B:1052:GLY:O	2:B:1056:GLN:HG2	2.07	0.55
1:C:190:PRO:HD2	3:F:246:ARG:NH2	2.22	0.55
2:D:1636:GLU:OE1	2:D:1636:GLU:N	2.39	0.55
3:E:273:GLU:CG	3:E:275:GLU:OE2	2.54	0.55
1:A:263:LYS:HG3	2:B:854:TYR:CE1	2.42	0.55
1:A:595:LEU:HD11	2:B:791:MET:HE1	1.88	0.55
2:B:1203:LYS:O	2:B:1206:LEU:HG	2.07	0.55
2:B:1507:ARG:HD2	2:B:1508:ASP:OD1	2.06	0.55
2:B:1544:VAL:HG13	2:B:1570:LYS:CB	2.37	0.55
2:B:1608:SER:O	2:B:1611:PHE:HD2	1.89	0.55
1:C:394:GLU:HB3	1:C:397:VAL:HG23	1.87	0.55
1:C:488:ARG:NH2	1:C:509:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1118:PHE:N	2:D:1144:THR:HG23	2.21	0.55
2:D:1564:ALA:HB2	2:D:1581:GLN:HE22	1.71	0.55
3:E:107:ALA:C	3:E:130:ARG:HH12	2.15	0.55
3:E:197:PHE:CE2	3:E:221:ARG:HD2	2.41	0.55
3:E:245:TYR:CD1	3:E:245:TYR:C	2.84	0.55
2:B:1012:GLU:OE2	2:B:1068:ALA:HB2	2.06	0.55
2:B:1085:VAL:HG12	2:B:1086:PHE:CD1	2.41	0.55
2:D:768:PRO:HD3	2:D:796:LYS:NZ	2.21	0.55
2:D:1233:THR:CG2	2:D:1256:LEU:HD11	2.36	0.55
1:A:196:PRO:HD2	1:A:199:VAL:CG2	2.35	0.55
2:B:1263:GLY:CA	2:B:1272:THR:HG22	2.36	0.55
1:C:95:GLU:O	1:C:97:LYS:N	2.40	0.55
2:D:846:GLU:OE2	2:D:897:PRO:HB3	2.07	0.55
2:B:1300:LEU:CD1	2:B:1303:ARG:HE	2.20	0.55
1:A:628:THR:HG21	1:A:641:ASP:HB3	1.88	0.55
2:B:962:ILE:HG12	2:B:1330:PHE:CE1	2.42	0.55
2:B:967:LEU:CD1	2:B:1327:ASN:HD22	2.19	0.55
2:D:1132:GLY:HA2	2:D:1228:TYR:CE1	2.42	0.55
2:D:1597:GLU:OE2	2:D:1600:LYS:HE2	2.07	0.55
2:B:1497:LYS:NZ	2:B:1501:LYS:O	2.35	0.54
1:C:540:ALA:HB3	1:C:543:GLN:HG2	1.89	0.54
2:D:761:ILE:CG2	2:D:762:VAL:N	2.70	0.54
2:D:1355:GLN:HA	2:D:1357:THR:HG23	1.89	0.54
3:E:276:TRP:H	3:E:276:TRP:HE3	1.54	0.54
3:F:106:SER:HA	3:F:133:TYR:CD2	2.42	0.54
1:A:566:LYS:HE3	1:A:584:LYS:CD	2.37	0.54
2:B:1136:ASN:HD22	2:B:1139:LYS:HZ3	1.55	0.54
2:B:1558:PHE:CD1	2:B:1587:PRO:HA	2.41	0.54
1:C:54:PRO:HG2	1:C:113:GLY:HA2	1.89	0.54
2:D:766:GLU:CB	2:D:796:LYS:NZ	2.66	0.54
2:D:905:THR:HA	2:D:931:VAL:CG2	2.36	0.54
2:D:1492:PHE:HE2	2:D:1500:GLY:C	2.16	0.54
3:E:109:LEU:O	3:E:114:ILE:HD11	2.08	0.54
3:E:130:ARG:HG3	3:E:130:ARG:HH11	1.72	0.54
1:A:471:LEU:HD21	1:A:519:LEU:HD23	1.89	0.54
2:D:1135:ASN:O	2:D:1136:ASN:HB2	2.07	0.54
2:D:1517:ASN:ND2	2:D:1521:GLN:HB2	2.20	0.54
1:A:60:HIS:ND1	1:A:67:LEU:O	2.34	0.54
2:D:1194:TYR:OH	2:D:1198:GLN:NE2	2.40	0.54
1:A:462:ARG:NH2	1:A:463:THR:O	2.30	0.54
2:B:830:PHE:CE1	2:B:852:TYR:HD2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1475:GLY:HA3	2:B:1493:TYR:CZ	2.43	0.54
2:B:1521:GLN:OE1	2:B:1521:GLN:N	2.25	0.54
1:C:50:GLN:NE2	1:C:51:GLY:H	1.98	0.54
3:E:175:ASP:HB3	3:E:187:SER:OG	2.07	0.54
2:B:980:ILE:HG22	2:B:1344:VAL:HG22	1.89	0.54
2:B:1152:GLN:HE21	2:B:1198:GLN:HE22	1.54	0.54
1:C:368:MET:O	1:C:413:THR:HG22	2.07	0.54
2:D:1015:MET:HE2	2:D:1015:MET:HA	1.88	0.54
2:D:1061:GLN:C	2:D:1063:SER:N	2.61	0.54
2:B:897:PRO:O	2:B:1473:GLN:NE2	2.41	0.54
1:C:36:LEU:HD11	1:C:91:PRO:C	2.33	0.54
2:D:1436:LYS:O	2:D:1441:ARG:NH2	2.36	0.54
3:E:143:LEU:HD11	3:E:151:TRP:CE3	2.43	0.54
1:A:221:GLU:HB2	1:A:609:ASN:ND2	2.23	0.54
2:B:1202:LEU:HD11	2:B:1243:LEU:CD2	2.30	0.54
1:C:32:ASN:HD22	1:C:33:ILE:HG12	1.73	0.54
3:E:156:GLU:OE2	3:E:158:CYS:O	2.26	0.54
3:F:113:TYR:HA	3:F:116:GLN:CG	2.37	0.54
2:B:1082:VAL:HG13	2:B:1086:PHE:CE1	2.43	0.54
2:B:1238:LEU:CD1	2:B:1277:GLN:HE21	2.17	0.54
2:B:1259:GLN:C	2:B:1260:ARG:HG3	2.33	0.54
2:B:1429:ILE:HD11	2:B:1433:GLU:HB2	1.89	0.54
1:C:66:LYS:NZ	1:C:66:LYS:O	2.34	0.54
1:C:95:GLU:C	1:C:97:LYS:H	2.16	0.54
2:D:1417:ASP:OD1	2:D:1418:LEU:N	2.41	0.54
3:E:170:ARG:HG3	3:E:170:ARG:NH1	2.16	0.54
1:A:28:ILE:HD11	1:A:42:MET:CG	2.38	0.54
1:A:44:LEU:HD12	1:A:44:LEU:N	2.23	0.54
1:A:412:ASN:ND2	3:F:101:PRO:O	2.40	0.54
2:D:1562:ILE:HG13	2:D:1581:GLN:HE21	1.71	0.54
2:B:974:THR:HG21	2:B:1349:HIS:CD2	2.43	0.53
2:B:1012:GLU:CD	2:B:1124:VAL:HG22	2.33	0.53
2:B:1358:CYS:HB3	2:B:1361:PHE:O	2.07	0.53
1:C:657:ARG:NE	1:C:659:GLU:O	2.38	0.53
1:A:26:TYR:HD2	1:A:112:PHE:CD2	2.26	0.53
1:A:412:ASN:OD1	3:F:103:ARG:HB2	2.09	0.53
1:C:169:ASN:HB2	1:C:170:PRO:HD2	1.90	0.53
1:C:273:PHE:CE2	1:C:326:VAL:HG22	2.43	0.53
2:D:1106:TRP:CD1	2:D:1106:TRP:H	2.24	0.53
2:D:1192:ALA:HA	2:D:1195:ALA:HB3	1.89	0.53
3:F:282:GLU:OE2	3:F:284:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLN:H	1:C:183:GLN:CD	2.14	0.53
2:D:758:GLU:HG2	2:D:867:LEU:HG	1.90	0.53
2:D:810:SER:CB	2:D:813:LYS:HB3	2.30	0.53
2:D:1180:TYR:CD2	2:D:1206:LEU:HG	2.43	0.53
2:D:1352:ALA:HB3	2:D:1353:LYS:HA	1.90	0.53
1:C:132:ILE:HD13	1:C:206:ILE:HG22	1.91	0.53
2:B:929:LEU:HD12	2:B:930:LYS:N	2.23	0.53
2:B:977:GLU:OE2	2:B:979:ARG:NE	2.42	0.53
2:B:1554:LEU:CD1	2:B:1591:ARG:HH22	2.21	0.53
1:C:37:GLU:OE2	1:C:212:ASN:ND2	2.41	0.53
2:D:1280:ALA:O	2:D:1283:GLN:NE2	2.41	0.53
3:F:126:GLU:HG3	3:F:142:LYS:HG2	1.90	0.53
3:F:233:ASN:HD21	3:F:283:CYS:HB3	1.71	0.53
1:A:647:THR:CB	1:A:653:GLN:HE22	2.21	0.53
2:B:764:ARG:N	2:B:924:GLY:O	2.31	0.53
2:D:1407:MET:HE2	2:D:1493:TYR:OH	2.08	0.53
2:D:1417:ASP:OD2	2:D:1461:PHE:HB2	2.08	0.53
2:D:1517:ASN:ND2	2:D:1519:PHE:O	2.42	0.53
3:E:104:LEU:O	3:E:130:ARG:CZ	2.56	0.53
1:A:61:ASP:OD1	1:A:65:LYS:N	2.42	0.53
2:B:1411:PHE:C	2:B:1466:TYR:HE1	2.17	0.53
2:B:1496:GLU:O	2:B:1497:LYS:C	2.52	0.53
2:B:1561:TYR:HB3	2:B:1563:MET:HE3	1.91	0.53
2:B:1576:VAL:HA	2:B:1580:GLN:HE22	1.74	0.53
2:B:1634:GLU:C	2:B:1634:GLU:CD	2.77	0.53
2:D:841:ARG:HH22	2:D:903:LEU:HA	1.73	0.53
2:D:1089:ALA:HA	2:D:1092:LEU:CD1	2.38	0.53
2:D:1554:LEU:HD11	2:D:1591:ARG:CZ	2.39	0.53
1:A:126:GLN:HE21	1:A:154:HIS:CD2	2.26	0.53
1:A:181:SER:CB	3:E:246:ARG:HE	2.15	0.53
2:B:874:SER:HB3	2:B:900:ILE:HG22	1.89	0.53
2:B:1105:LYS:HG2	2:B:1162:VAL:CG2	2.37	0.53
1:C:565:VAL:HG13	2:D:821:PHE:HB2	1.90	0.53
2:D:1252:VAL:O	2:D:1256:LEU:HD13	2.09	0.53
1:A:125:LEU:CD2	1:A:215:GLN:HE22	2.22	0.53
1:A:235:ILE:CD1	1:A:256:THR:HB	2.38	0.53
1:A:242:PHE:CD2	1:A:379:PRO:HG2	2.44	0.53
2:B:1255:TRP:O	2:B:1259:GLN:HG2	2.09	0.53
2:D:1047:GLU:HG3	2:D:1051:LYS:NZ	2.23	0.53
2:D:1298:LEU:HD12	2:D:1307:ILE:HB	1.90	0.53
2:D:1414:ASP:O	2:D:1417:ASP:OD1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1533:LEU:HA	2:D:1652:PHE:HE1	1.73	0.53
1:C:373:MET:HE3	1:C:462:ARG:NH1	2.24	0.53
1:C:567:SER:O	1:C:584:LYS:NZ	2.38	0.53
2:D:1001:LYS:O	2:D:1004:ILE:HG12	2.09	0.53
3:F:133:TYR:O	3:F:134:ARG:HD2	2.09	0.53
1:A:130:LEU:HD21	1:A:163:VAL:CG1	2.38	0.52
2:B:886:VAL:HG11	2:B:894:LEU:HD22	1.90	0.52
2:B:957:VAL:HG21	2:B:1335:GLU:HG3	1.91	0.52
2:B:1045:ALA:O	2:B:1049:ILE:HD12	2.09	0.52
1:C:573:ARG:HE	1:C:579:GLN:HE21	1.58	0.52
2:D:831:ILE:HG13	2:D:923:ASP:OD2	2.09	0.52
2:D:1172:ALA:O	2:D:1176:LEU:HD13	2.08	0.52
3:F:187:SER:C	3:F:188:PHE:CD1	2.87	0.52
1:A:35:ARG:HG2	1:A:124:SER:HB3	1.91	0.52
2:B:907:LEU:HD12	2:B:907:LEU:O	2.09	0.52
2:B:1112:GLN:HE22	2:B:1117:VAL:N	2.08	0.52
1:C:43:VAL:HG11	1:C:493:LEU:HD21	1.91	0.52
2:D:1313:TRP:HA	2:D:1313:TRP:CE3	2.44	0.52
2:D:1494:HIS:CE1	2:D:1496:GLU:OE1	2.62	0.52
3:F:246:ARG:HH11	3:F:246:ARG:HB3	1.74	0.52
2:B:978:THR:OG1	2:B:1346:THR:HG22	2.10	0.52
2:D:1077:TRP:CD2	2:D:1130:ILE:HG22	2.44	0.52
2:D:1215:LYS:HD2	2:D:1215:LYS:C	2.34	0.52
1:A:261:TYR:CD2	2:B:826:MET:SD	3.03	0.52
1:A:326:VAL:CG2	1:A:343:ARG:HB3	2.39	0.52
1:A:481:ARG:HA	1:A:484:GLU:CD	2.34	0.52
2:B:1174:ASP:HA	2:B:1201:ARG:NH2	2.21	0.52
2:B:1291:GLU:OE1	2:B:1291:GLU:N	2.43	0.52
1:C:230:PRO:HB2	1:C:339:VAL:CG2	2.40	0.52
2:D:872:PHE:CD1	2:D:902:PRO:HA	2.44	0.52
2:D:1423:ASN:HD22	2:D:1423:ASN:C	2.18	0.52
2:D:1495:PRO:HG2	2:D:1496:GLU:OE1	2.10	0.52
3:E:116:GLN:O	3:E:117:ASN:ND2	2.42	0.52
3:E:156:GLU:OE2	3:E:158:CYS:N	2.43	0.52
2:B:1576:VAL:CG1	2:B:1582:ARG:HE	2.22	0.52
2:D:764:ARG:HB3	2:D:767:PHE:CZ	2.44	0.52
2:D:957:VAL:CG2	2:D:1335:GLU:HA	2.39	0.52
2:D:980:ILE:HD11	2:D:1322:GLU:HB2	1.90	0.52
2:D:1132:GLY:HA2	2:D:1228:TYR:CD1	2.45	0.52
2:B:761:ILE:CG2	2:B:913:LYS:HE3	2.39	0.52
1:C:183:GLN:HG3	3:F:266:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ASN:O	1:C:498:GLY:N	2.42	0.52
2:D:1310:ARG:NH2	3:F:235:ILE:HG12	2.24	0.52
3:F:188:PHE:CD1	3:F:188:PHE:N	2.78	0.52
1:A:376:VAL:HG11	1:A:401:THR:HG21	1.90	0.52
2:B:1149:ILE:CA	2:B:1152:GLN:HE22	2.23	0.52
1:C:36:LEU:HD12	1:C:90:ILE:O	2.10	0.52
2:D:758:GLU:CA	2:D:913:LYS:HZ3	2.08	0.52
2:D:1190:ALA:HB2	2:D:1220:TRP:CE3	2.45	0.52
2:B:1577:GLN:N	2:B:1580:GLN:HE22	2.08	0.52
1:C:96:PHE:HD1	1:C:104:LYS:HG2	1.74	0.52
1:C:148:ARG:NH2	2:D:773:TRP:CZ3	2.78	0.52
1:C:175:VAL:HB	2:D:979:ARG:CZ	2.40	0.52
1:C:479:MET:HE1	1:C:487:ILE:CD1	2.40	0.52
2:D:1102:GLY:HA2	2:D:1105:LYS:HE2	1.92	0.52
2:D:1197:ALA:HB2	2:D:1202:LEU:CD2	2.38	0.52
3:E:194:TYR:CD1	3:E:222:GLU:HA	2.45	0.52
1:A:129:TYR:HA	1:A:218:PHE:CE2	2.44	0.52
1:A:181:SER:HB3	3:E:246:ARG:CZ	2.40	0.52
1:A:431:LEU:C	1:A:431:LEU:HD12	2.35	0.52
2:B:1202:LEU:HB2	2:B:1206:LEU:HD11	1.91	0.52
1:C:596:VAL:O	2:D:804:ILE:HA	2.10	0.52
2:D:1174:ASP:HA	2:D:1177:GLU:HG2	1.90	0.52
2:D:1254:ARG:O	2:D:1258:GLU:OE1	2.27	0.52
1:A:496:ASN:C	1:A:496:ASN:OD1	2.52	0.52
2:B:760:ASN:OD1	2:B:761:ILE:HG23	2.10	0.52
2:B:811:ASP:OD1	2:B:811:ASP:N	2.42	0.52
2:B:1549:LEU:HD12	2:B:1550:VAL:N	2.25	0.52
1:C:491:THR:HG22	1:C:505:ARG:NE	2.25	0.52
2:D:979:ARG:HG3	2:D:1323:GLU:HG3	1.91	0.52
2:D:1544:VAL:HG23	2:D:1570:LYS:HG2	1.91	0.52
3:F:139:LEU:HD11	3:F:155:VAL:HG21	1.92	0.52
1:A:474:ASN:OD1	1:A:516:VAL:HG12	2.10	0.51
1:A:610:LYS:O	1:A:615:LYS:NZ	2.43	0.51
2:B:935:GLY:HA3	2:B:1349:HIS:CE1	2.45	0.51
2:B:1312:HIS:HA	2:B:1313:TRP:CE3	2.46	0.51
2:B:1577:GLN:N	2:B:1580:GLN:NE2	2.59	0.51
3:F:116:GLN:HG3	3:F:119:PHE:CE1	2.45	0.51
3:F:135:ARG:HH12	3:F:137:PRO:HA	1.75	0.51
1:A:103:ASN:N	1:A:103:ASN:OD1	2.40	0.51
1:A:448:THR:HG23	1:A:451:ASN:HA	1.92	0.51
2:B:938:MET:C	2:B:940:LYS:HZ3	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:VAL:CG2	1:C:394:GLU:HB2	2.40	0.51
2:D:1063:SER:O	2:D:1065:ALA:N	2.43	0.51
2:D:1145:ALA:O	2:D:1149:ILE:HG22	2.10	0.51
3:E:235:ILE:HG22	3:E:236:ILE:H	1.74	0.51
2:B:764:ARG:HD2	2:B:797:ASP:O	2.09	0.51
2:B:1084:LYS:HE3	2:B:1149:ILE:HD13	1.91	0.51
2:B:1248:PHE:O	2:B:1251:PRO:HD2	2.10	0.51
2:B:1317:SER:O	2:B:1319:LEU:HG	2.10	0.51
2:D:756:ILE:CD1	3:F:134:ARG:HH22	2.23	0.51
2:D:1149:ILE:HA	2:D:1152:GLN:HE21	1.75	0.51
2:D:1159:GLU:OE2	2:D:1165:LEU:HD23	2.11	0.51
3:E:107:ALA:N	3:E:130:ARG:NH1	2.58	0.51
3:E:235:ILE:HG22	3:E:236:ILE:N	2.26	0.51
1:A:540:ALA:HB3	1:A:543:GLN:HG2	1.91	0.51
2:B:1226:GLN:O	2:B:1230:VAL:HG23	2.11	0.51
2:D:1065:ALA:CB	2:D:1074:PRO:HB3	2.41	0.51
2:D:1313:TRP:HZ3	2:D:1318:LEU:HD11	1.73	0.51
2:D:1423:ASN:O	2:D:1425:VAL:HG12	2.10	0.51
2:D:1547:THR:HG22	2:D:1565:ILE:HD13	1.93	0.51
1:A:28:ILE:CG1	1:A:42:MET:HE3	2.39	0.51
2:B:1192:ALA:O	2:B:1196:LEU:HG	2.10	0.51
2:B:1261:TYR:OH	2:B:1268:SER:HB2	2.11	0.51
1:C:148:ARG:CZ	1:C:594:VAL:CG2	2.88	0.51
1:C:489:TYR:CD2	1:C:505:ARG:HD2	2.46	0.51
2:D:756:ILE:CB	3:F:134:ARG:HH22	2.24	0.51
3:E:232:ASP:O	3:E:283:CYS:SG	2.69	0.51
3:F:203:PHE:O	3:F:214:SER:N	2.36	0.51
1:C:508:ARG:HH12	1:C:512:GLN:HB2	1.76	0.51
2:D:841:ARG:HH12	2:D:903:LEU:CA	2.23	0.51
2:D:1216:ASP:OD1	2:D:1218:ASN:OD1	2.29	0.51
2:D:1639:ASP:OD2	2:D:1642:ASN:HB2	2.11	0.51
3:E:107:ALA:HB1	3:E:127:TYR:HB3	1.91	0.51
1:A:368:MET:O	1:A:413:THR:HG22	2.09	0.51
2:B:1313:TRP:O	2:B:1314:GLU:HB2	2.11	0.51
2:B:1541:VAL:HG13	2:B:1570:LYS:HZ1	1.76	0.51
2:B:1634:GLU:OE2	2:B:1638:GLN:NE2	2.44	0.51
1:A:646:PHE:H	1:A:654:THR:HG21	1.76	0.51
2:B:1149:ILE:HA	2:B:1152:GLN:NE2	2.24	0.51
1:C:41:THR:HG22	1:C:500:LEU:HB2	1.92	0.51
1:C:42:MET:HB3	1:C:86:VAL:HG12	1.91	0.51
1:C:466:ARG:H	1:C:469:GLU:CD	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HG22	1:A:255:ILE:HD13	1.93	0.51
2:B:1118:PHE:HZ	2:B:1151:LEU:HD11	1.76	0.51
2:B:1435:ASP:OD1	2:B:1435:ASP:N	2.43	0.51
1:C:355:ILE:HG12	1:C:376:VAL:HG22	1.91	0.51
2:D:1588:ILE:HG22	2:D:1591:ARG:HH21	1.75	0.51
3:E:276:TRP:N	3:E:276:TRP:CD2	2.77	0.51
3:F:107:ALA:HB1	3:F:127:TYR:HB3	1.93	0.51
3:F:258:THR:O	3:F:283:CYS:HA	2.11	0.51
1:A:462:ARG:NH2	1:A:463:THR:C	2.69	0.51
2:B:967:LEU:HD22	2:B:1348:TYR:HD2	1.71	0.51
2:B:1060:ARG:NH2	2:B:1099:VAL:HA	2.26	0.51
2:B:1407:MET:SD	2:B:1413:PRO:HD3	2.51	0.51
2:B:1508:ASP:OD1	2:B:1508:ASP:N	2.40	0.51
2:B:1559:ASP:OD1	2:B:1586:SER:O	2.29	0.51
1:C:201:MET:HE1	1:C:225:LYS:CA	2.34	0.51
2:D:764:ARG:HH12	2:D:923:ASP:CG	2.12	0.51
2:D:996:ASP:O	2:D:999:ARG:HB2	2.11	0.51
2:D:1505:LEU:CD1	2:D:1585:ILE:HD11	2.39	0.51
2:D:1547:THR:HB	2:D:1563:MET:CG	2.41	0.51
2:D:1631:TRP:HZ3	2:D:1633:GLU:HA	1.75	0.51
3:F:195:LYS:HD2	3:F:196:LEU:N	2.24	0.51
1:C:429:GLN:C	1:C:431:LEU:H	2.20	0.50
2:D:1156:ASP:OD1	2:D:1157:ILE:HG13	2.11	0.50
3:F:129:CYS:HB3	3:F:133:TYR:HB2	1.91	0.50
1:A:39:GLU:HG3	1:A:87:THR:HG22	1.93	0.50
1:A:376:VAL:HG12	1:A:401:THR:HG21	1.93	0.50
2:B:1191:ILE:HG22	2:B:1235:TYR:CD1	2.47	0.50
1:C:465:LEU:HD11	1:C:555:VAL:HG22	1.93	0.50
2:D:1252:VAL:O	2:D:1255:TRP:HB3	2.11	0.50
2:D:1533:LEU:HD21	2:D:1655:SER:OG	2.11	0.50
1:A:362:LYS:NZ	1:A:442:GLN:O	2.30	0.50
1:A:397:VAL:HG12	1:A:409:LEU:HD23	1.93	0.50
2:B:841:ARG:NH2	2:B:903:LEU:HA	2.26	0.50
2:B:1116:GLY:HA2	2:B:1171:LYS:HG2	1.94	0.50
1:C:104:LYS:O	1:C:122:LEU:HD12	2.10	0.50
1:C:167:ILE:O	1:C:175:VAL:HG22	2.11	0.50
1:C:198:LEU:HD11	2:D:1349:HIS:NE2	2.27	0.50
1:C:460:VAL:HG13	1:C:462:ARG:HD3	1.92	0.50
2:D:798:SER:HB2	2:D:802:TRP:CZ2	2.47	0.50
2:D:979:ARG:HG3	2:D:1323:GLU:CG	2.42	0.50
2:D:1392:TYR:CE1	2:D:1398:ALA:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:THR:CG2	1:A:653:GLN:HE22	2.24	0.50
2:B:870:PRO:O	2:B:903:LEU:HD12	2.12	0.50
2:D:1128:GLU:OE1	2:D:1267:GLY:CA	2.59	0.50
2:D:1133:LEU:O	2:D:1139:LYS:HE3	2.11	0.50
2:D:1210:PHE:O	2:D:1213:THR:HG22	2.11	0.50
3:E:156:GLU:OE2	3:E:156:GLU:C	2.55	0.50
3:F:113:TYR:HA	3:F:116:GLN:CD	2.36	0.50
3:F:241:ASP:N	3:F:241:ASP:OD1	2.43	0.50
1:A:36:LEU:O	1:A:37:GLU:HG2	2.12	0.50
1:A:39:GLU:OE1	1:A:89:THR:HG23	2.12	0.50
2:B:831:ILE:HD12	2:B:925:VAL:HG23	1.92	0.50
2:B:1281:GLN:OE1	2:B:1284:LYS:HE2	2.11	0.50
1:C:456:LEU:HB2	1:C:535:TYR:HE2	1.77	0.50
3:F:157:PHE:C	3:F:159:LYS:HZ1	2.11	0.50
1:A:59:VAL:HG13	1:A:106:VAL:HG21	1.94	0.50
1:A:83:MET:HE3	1:A:505:ARG:CD	2.40	0.50
2:B:967:LEU:HD22	2:B:1348:TYR:CE2	2.47	0.50
2:B:1141:MET:HE2	2:B:1141:MET:HA	1.93	0.50
2:B:1206:LEU:HD12	2:B:1206:LEU:C	2.36	0.50
2:B:1608:SER:HA	2:B:1611:PHE:CE2	2.46	0.50
1:C:508:ARG:NH1	1:C:508:ARG:CG	2.68	0.50
2:D:1060:ARG:NH2	2:D:1099:VAL:HA	2.27	0.50
3:F:204:CYS:SG	3:F:211:VAL:HG21	2.51	0.50
1:A:166:ASN:HD21	1:A:174:PRO:CG	2.25	0.50
1:A:232:PHE:HE2	1:A:330:VAL:CG2	2.25	0.50
2:B:826:MET:HG3	2:B:827:GLN:H	1.77	0.50
2:B:1076:THR:OG1	2:B:1120:GLU:OE1	2.27	0.50
2:B:1643:GLN:HG3	2:B:1644:LYS:H	1.75	0.50
1:C:338:MET:HE1	2:D:1480:TYR:OH	2.11	0.50
2:D:757:ALA:O	2:D:761:ILE:CD1	2.59	0.50
1:C:97:LYS:CG	2:D:1314:GLU:HB3	2.42	0.50
1:C:313:ASN:ND2	1:C:318:ASP:HB2	2.27	0.50
1:C:365:LYS:HZ3	1:C:457:HIS:HA	1.75	0.50
1:C:460:VAL:CG2	1:C:471:LEU:HD21	2.41	0.50
2:D:761:ILE:HD13	2:D:913:LYS:NZ	2.27	0.50
2:D:1348:TYR:HE1	2:D:1350:ALA:HB2	1.76	0.50
3:E:171:ASN:ND2	3:E:194:TYR:CE1	2.80	0.50
3:F:116:GLN:HG3	3:F:119:PHE:CZ	2.46	0.50
1:A:35:ARG:HH22	1:A:498:GLY:HA3	1.76	0.50
1:A:63:PRO:HD3	2:B:1034:TRP:CZ3	2.46	0.50
1:A:380:ASP:OD1	1:A:381:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:752:ASP:HB3	2:B:753:GLU:OE1	2.12	0.50
2:B:1497:LYS:NZ	2:B:1502:LEU:HA	2.26	0.50
2:B:1551:LYS:HD2	2:B:1552:VAL:H	1.76	0.50
1:C:475:PHE:HB2	1:C:515:VAL:HG13	1.94	0.50
1:C:496:ASN:C	1:C:498:GLY:N	2.70	0.50
2:D:811:ASP:N	2:D:811:ASP:OD1	2.44	0.50
2:D:1210:PHE:CE1	2:D:1220:TRP:CH2	3.00	0.50
2:D:1313:TRP:CE3	2:D:1318:LEU:HD21	2.47	0.50
3:E:101:PRO:HB3	3:E:143:LEU:HD21	1.94	0.50
1:A:329:THR:HA	1:A:340:GLN:OE1	2.12	0.49
2:B:1032:GLU:HA	2:B:1034:TRP:CE3	2.47	0.49
2:D:1472:ILE:HD11	2:D:1494:HIS:NE2	2.27	0.49
3:E:133:TYR:O	3:E:161:LYS:HE3	2.12	0.49
3:F:246:ARG:CB	3:F:246:ARG:NH1	2.74	0.49
1:A:37:GLU:CD	1:A:161:ARG:HH12	2.20	0.49
1:A:484:GLU:O	1:A:487:ILE:HG22	2.12	0.49
1:A:489:TYR:CD2	1:A:505:ARG:NH2	2.80	0.49
2:B:755:ILE:HD12	2:B:756:ILE:O	2.12	0.49
2:B:1300:LEU:HD11	2:B:1303:ARG:CG	2.23	0.49
2:D:1037:PHE:O	2:D:1041:LYS:HD2	2.13	0.49
3:E:222:GLU:HG2	3:E:224:TYR:CE1	2.47	0.49
1:A:122:LEU:H	1:A:122:LEU:HD12	1.77	0.49
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.95	0.49
2:B:795:LEU:HD11	2:B:825:VAL:HB	1.93	0.49
1:C:72:GLU:HB2	1:C:86:VAL:CG2	2.42	0.49
2:D:763:SER:CB	2:D:926:ARG:HB2	2.43	0.49
2:D:841:ARG:NH1	2:D:903:LEU:C	2.70	0.49
2:D:971:VAL:HA	2:D:1351:LYS:HE3	1.94	0.49
2:D:972:PRO:HD3	2:D:1351:LYS:HE3	1.93	0.49
2:D:996:ASP:OD1	2:D:1036:LYS:CE	2.60	0.49
2:D:1294:LEU:HB3	2:D:1311:ILE:CG2	2.41	0.49
3:E:132:GLY:HA2	3:E:161:LYS:NZ	2.27	0.49
2:B:1299:GLN:HA	2:B:1303:ARG:HH21	1.76	0.49
1:C:453:ASN:OD1	1:C:455:TYR:HE2	1.95	0.49
2:D:898:TYR:HA	2:D:1473:GLN:HE22	1.78	0.49
2:D:1029:ASP:OD1	2:D:1034:TRP:NE1	2.32	0.49
2:D:1060:ARG:HD2	2:D:1064:SER:HA	1.94	0.49
3:F:157:PHE:CD1	3:F:157:PHE:N	2.81	0.49
3:F:224:TYR:CD1	3:F:242:HIS:HB3	2.47	0.49
1:A:326:VAL:O	1:A:342:GLU:HA	2.12	0.49
2:B:1159:GLU:OE2	2:B:1166:PRO:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1249:VAL:HB	2:B:1250:PRO:CD	2.42	0.49
2:B:1512:ARG:NH1	2:B:1621:ILE:HD11	2.28	0.49
1:C:355:ILE:HG23	1:C:374:VAL:HG13	1.94	0.49
1:C:625:ILE:CD1	1:C:643:GLY:HA3	2.42	0.49
2:D:1047:GLU:O	2:D:1050:LYS:HG2	2.12	0.49
2:D:1249:VAL:HG23	2:D:1250:PRO:HD3	1.92	0.49
2:D:1249:VAL:O	2:D:1252:VAL:HG12	2.13	0.49
2:D:1295:ASP:HB2	2:D:1335:GLU:HB3	1.94	0.49
2:D:1601:HIS:HB2	2:D:1631:TRP:HB3	1.94	0.49
2:B:1027:TYR:CZ	2:B:1031:THR:HG21	2.46	0.49
2:B:1082:VAL:O	2:B:1086:PHE:CD1	2.65	0.49
2:B:1420:GLN:O	2:B:1423:ASN:OD1	2.31	0.49
1:C:59:VAL:CG1	1:C:70:SER:H	2.25	0.49
1:C:67:LEU:CD2	1:C:67:LEU:CB	2.82	0.49
2:D:1063:SER:HA	2:D:1106:TRP:HZ3	1.78	0.49
1:A:105:PHE:CE2	1:A:122:LEU:HG	2.46	0.49
2:B:1022:VAL:HG22	2:B:1049:ILE:HG12	1.94	0.49
2:B:1532:ARG:HH21	2:B:1629:GLU:CD	2.20	0.49
2:B:1601:HIS:HB2	2:B:1631:TRP:HB3	1.95	0.49
2:B:1607:LEU:C	2:B:1610:ASP:OD1	2.56	0.49
1:C:367:GLY:H	1:C:413:THR:HG23	1.77	0.49
2:D:1303:ARG:NH2	3:F:241:ASP:HA	2.27	0.49
1:A:586:GLU:HG2	2:B:788:THR:HG23	1.95	0.49
2:B:1018:MET:HE3	2:B:1085:VAL:HG11	1.94	0.49
2:B:1554:LEU:HD13	2:B:1591:ARG:HH22	1.78	0.49
2:B:1638:GLN:OE1	2:B:1638:GLN:N	2.38	0.49
2:D:778:LEU:CG	2:D:787:SER:HB3	2.42	0.49
2:D:802:TRP:HB2	2:D:823:VAL:CG2	2.43	0.49
3:E:156:GLU:C	3:E:156:GLU:CD	2.81	0.49
3:F:180:ILE:HD12	3:F:180:ILE:O	2.13	0.49
1:A:126:GLN:HG2	1:A:154:HIS:NE2	2.27	0.49
1:A:130:LEU:HD13	1:A:210:TYR:CZ	2.48	0.49
1:A:431:LEU:HD11	1:A:436:GLN:NE2	2.27	0.49
2:B:753:GLU:O	2:B:754:ASP:OD1	2.30	0.49
2:B:846:GLU:OE1	2:B:1476:ALA:HB3	2.13	0.49
2:B:1053:TYR:HD2	2:B:1086:PHE:CE2	2.30	0.49
2:B:1130:ILE:HG23	2:B:1133:LEU:HB2	1.95	0.49
1:C:236:VAL:HG22	1:C:255:ILE:HD13	1.93	0.49
2:D:936:ILE:HG13	2:D:937:ARG:N	2.27	0.49
2:D:1063:SER:O	2:D:1063:SER:OG	2.18	0.49
3:E:105:ASN:OD1	3:E:105:ASN:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:N	3:E:246:ARG:CZ	2.75	0.49
2:B:1238:LEU:HD21	2:B:1278:ALA:HA	1.94	0.49
1:C:45:GLU:OE1	1:C:534:TYR:OH	2.27	0.49
1:C:78:PRO:HA	1:C:82:HIS:CE1	2.48	0.49
1:C:230:PRO:HB2	1:C:339:VAL:HG22	1.95	0.49
1:C:272:ILE:HG22	1:C:327:SER:HB3	1.94	0.49
1:C:385:TYR:CD1	1:C:386:ARG:HG3	2.47	0.49
1:C:398:GLN:CD	1:C:427:LYS:HE2	2.38	0.49
1:A:37:GLU:OE1	1:A:161:ARG:NH1	2.45	0.48
1:A:59:VAL:HG13	1:A:106:VAL:CG2	2.42	0.48
2:B:800:THR:H	2:B:825:VAL:HG13	1.77	0.48
1:C:489:TYR:HD2	1:C:505:ARG:HD2	1.78	0.48
2:D:758:GLU:H	2:D:881:ARG:HH12	1.61	0.48
2:D:1158:CYS:HA	2:D:1161:GLN:HE22	1.75	0.48
3:E:170:ARG:C	3:E:171:ASN:OD1	2.56	0.48
1:A:119:LYS:HB2	1:A:647:THR:HG21	1.95	0.48
1:A:130:LEU:HD21	1:A:163:VAL:HG12	1.94	0.48
1:A:335:GLY:HA3	2:B:1404:ASP:OD2	2.14	0.48
2:B:877:THR:HG23	2:B:879:LYS:N	2.28	0.48
2:B:1084:LYS:HE2	2:B:1273:PHE:HE2	1.77	0.48
2:B:1115:ASP:O	2:B:1175:PHE:CD2	2.66	0.48
2:B:1136:ASN:HD22	2:B:1139:LYS:HZ1	1.57	0.48
2:B:1149:ILE:O	2:B:1152:GLN:NE2	2.46	0.48
1:C:355:ILE:HD11	1:C:426:THR:HG23	1.95	0.48
2:D:1078:LEU:C	2:D:1078:LEU:HD12	2.38	0.48
3:F:194:TYR:CE1	3:F:222:GLU:HB3	2.48	0.48
1:A:365:LYS:HD3	1:A:365:LYS:N	2.28	0.48
1:A:484:GLU:OE1	1:A:484:GLU:N	2.41	0.48
2:B:937:ARG:NH1	2:B:1347:MET:HE1	2.28	0.48
2:B:1554:LEU:HD12	2:B:1555:SER:O	2.13	0.48
2:B:1607:LEU:HD13	2:B:1609:SER:OG	2.14	0.48
1:C:29:ILE:HB	1:C:43:VAL:HG13	1.94	0.48
1:C:50:GLN:HE21	1:C:51:GLY:N	1.95	0.48
1:C:183:GLN:O	1:C:185:GLN:HG2	2.13	0.48
1:C:634:ASP:O	1:C:638:VAL:HG23	2.13	0.48
2:D:1061:GLN:O	2:D:1062:PRO:C	2.55	0.48
2:D:1157:ILE:O	2:D:1161:GLN:NE2	2.35	0.48
2:D:1512:ARG:NH1	2:D:1621:ILE:HD13	2.29	0.48
2:D:1543:TYR:HB2	2:D:1545:TYR:CZ	2.48	0.48
3:E:170:ARG:CG	3:E:170:ARG:NH1	2.71	0.48
1:A:85:ASN:N	1:A:85:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:826:MET:CG	2:B:827:GLN:H	2.27	0.48
2:B:868:HIS:CD2	2:B:877:THR:HA	2.48	0.48
2:B:913:LYS:HD2	2:B:914:ALA:H	1.79	0.48
1:C:175:VAL:HB	2:D:979:ARG:NH1	2.27	0.48
1:C:385:TYR:HD2	1:C:403:GLY:HA2	1.77	0.48
2:B:1061:GLN:OE1	2:B:1074:PRO:HG3	2.13	0.48
2:B:1436:LYS:HB3	2:B:1441:ARG:HE	1.79	0.48
2:B:1505:LEU:HG	2:B:1612:TRP:CH2	2.49	0.48
2:B:1557:ASP:O	2:B:1588:ILE:HG23	2.12	0.48
1:C:77:THR:O	1:C:80:THR:HG22	2.14	0.48
2:D:756:ILE:CD1	2:D:761:ILE:HG13	2.39	0.48
2:D:1246:PHE:CE1	2:D:1286:ALA:HB3	2.48	0.48
3:E:146:LEU:N	3:E:150:LYS:O	2.41	0.48
1:A:487:ILE:CD1	1:A:535:TYR:HB2	2.42	0.48
2:B:996:ASP:OD1	2:B:999:ARG:HB2	2.13	0.48
1:C:209:TYR:CD2	1:C:214:PRO:HA	2.48	0.48
1:C:479:MET:HG3	1:C:480:ASP:N	2.29	0.48
2:D:1643:GLN:HE21	2:D:1644:LYS:NZ	2.12	0.48
1:A:471:LEU:HD12	1:A:471:LEU:O	2.14	0.48
1:A:628:THR:HG23	1:A:630:GLY:H	1.79	0.48
2:B:1507:ARG:CZ	2:B:1508:ASP:OD1	2.62	0.48
2:B:1544:VAL:CG1	2:B:1570:LYS:HB3	2.42	0.48
2:B:1574:ASP:O	2:B:1576:VAL:HG22	2.14	0.48
1:C:140:THR:O	1:C:143:SER:OG	2.26	0.48
1:C:332:LEU:C	1:C:334:SER:H	2.21	0.48
2:D:796:LYS:HG3	2:D:797:ASP:H	1.78	0.48
2:D:1202:LEU:O	2:D:1207:LEU:HB2	2.14	0.48
2:D:1508:ASP:CG	2:D:1509:GLU:N	2.70	0.48
2:B:971:VAL:HG21	2:B:1349:HIS:CE1	2.48	0.48
2:B:1032:GLU:HA	2:B:1034:TRP:CZ3	2.49	0.48
2:B:1576:VAL:HG11	2:B:1582:ARG:HE	1.78	0.48
1:C:115:GLN:HG2	1:C:649:SER:HB2	1.94	0.48
1:C:189:LEU:CD1	3:F:246:ARG:HH12	2.26	0.48
1:C:527:PRO:O	1:C:555:VAL:N	2.34	0.48
2:D:796:LYS:HA	2:D:796:LYS:HD2	1.57	0.48
2:D:888:ILE:HD12	2:D:889:PRO:HD2	1.96	0.48
2:D:1470:GLU:HG3	2:D:1471:LEU:HD22	1.94	0.48
3:E:222:GLU:HB3	3:E:224:TYR:HE1	1.78	0.48
1:A:119:LYS:CB	1:A:647:THR:HG21	2.43	0.48
1:A:130:LEU:CB	1:A:218:PHE:HD2	2.26	0.48
2:B:965:ALA:H	2:B:1327:ASN:HD21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1348:TYR:HD1	2:B:1349:HIS:C	2.22	0.48
1:C:28:ILE:HD13	1:C:44:LEU:HD23	1.94	0.48
1:C:508:ARG:NH1	1:C:512:GLN:HB2	2.28	0.48
1:C:532:VAL:HG11	1:C:644:LEU:HD12	1.96	0.48
1:C:561:GLY:HA3	2:D:813:LYS:CE	2.42	0.48
1:C:617:TRP:HA	1:C:617:TRP:CE3	2.49	0.48
2:D:856:GLN:HG2	2:D:857:ASN:N	2.28	0.48
2:D:1250:PRO:O	2:D:1254:ARG:HG2	2.14	0.48
2:D:1508:ASP:OD1	2:D:1509:GLU:N	2.40	0.48
3:E:203:PHE:O	3:E:214:SER:N	2.40	0.48
1:A:144:THR:HG23	1:A:194:ASP:OD1	2.13	0.48
1:A:476:LEU:HD13	1:A:514:LEU:CD1	2.44	0.48
1:A:487:ILE:HD11	1:A:535:TYR:HB2	1.95	0.48
1:A:502:LYS:HD2	1:A:503:ALA:N	2.29	0.48
2:B:1136:ASN:HA	2:B:1139:LYS:CE	2.43	0.48
2:B:1635:ASP:CA	2:B:1638:GLN:HE22	2.16	0.48
1:C:275:ILE:HG13	1:C:282:ILE:HB	1.95	0.48
1:C:488:ARG:HH12	1:C:507:VAL:CG1	2.27	0.48
2:D:1060:ARG:HG3	2:D:1060:ARG:NH1	2.28	0.48
3:F:222:GLU:OE2	3:F:224:TYR:CZ	2.67	0.48
1:A:132:ILE:HD13	1:A:206:ILE:HG22	1.95	0.47
1:A:166:ASN:HD21	1:A:174:PRO:HB3	1.79	0.47
2:B:974:THR:HG21	2:B:1349:HIS:HD2	1.79	0.47
2:B:980:ILE:HG13	2:B:1322:GLU:O	2.14	0.47
2:B:1152:GLN:HE21	2:B:1153:GLU:HG2	1.79	0.47
2:B:1166:PRO:O	2:B:1170:THR:OG1	2.30	0.47
2:B:1191:ILE:HG22	2:B:1235:TYR:CE1	2.48	0.47
1:C:588:ASP:O	2:D:778:LEU:HD23	2.14	0.47
1:C:599:ASP:C	1:C:601:GLY:N	2.70	0.47
3:E:222:GLU:HB3	3:E:224:TYR:CE1	2.49	0.47
3:F:188:PHE:CE2	3:F:218:PRO:HD2	2.48	0.47
1:A:191:LEU:HD12	1:A:192:SER:H	1.79	0.47
2:B:1031:THR:HB	2:B:1033:GLN:HE21	1.79	0.47
2:B:1044:GLY:O	2:B:1048:LEU:HD13	2.14	0.47
1:C:23:SER:O	1:C:544:ARG:NH2	2.42	0.47
1:C:36:LEU:HD21	1:C:92:ALA:HA	1.97	0.47
1:C:346:ILE:HG13	1:C:346:ILE:O	2.14	0.47
2:D:911:GLU:HB2	2:D:926:ARG:HG3	1.96	0.47
3:E:124:VAL:HA	3:E:143:LEU:O	2.14	0.47
3:E:260:ILE:CD1	3:E:284:ARG:HD3	2.35	0.47
3:F:231:ILE:HD11	3:F:234:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:O	1:A:37:GLU:CG	2.62	0.47
1:A:496:ASN:ND2	1:A:501:LEU:HD22	2.22	0.47
2:B:1152:GLN:NE2	2:B:1153:GLU:HG2	2.28	0.47
2:B:1233:THR:CG2	2:B:1256:LEU:HD11	2.38	0.47
2:B:1494:HIS:CD2	2:B:1495:PRO:HD2	2.39	0.47
1:C:312:GLN:H	1:C:312:GLN:CD	2.16	0.47
2:D:794:PHE:CZ	3:F:176:VAL:HB	2.49	0.47
2:D:1538:GLU:HB3	2:D:1539:PRO:HD2	1.96	0.47
3:F:255:LYS:HB2	3:F:255:LYS:HE2	1.58	0.47
2:B:1051:LYS:O	2:B:1055:GLN:HG2	2.15	0.47
2:B:1130:ILE:HA	2:B:1130:ILE:HD12	1.54	0.47
2:B:1431:LYS:O	2:B:1434:LEU:HB2	2.13	0.47
1:C:275:ILE:HG22	1:C:324:LEU:CD2	2.44	0.47
2:D:1002:HIS:NE2	2:D:1262:TYR:O	2.40	0.47
2:D:1056:GLN:HE22	2:D:1082:VAL:HG22	1.79	0.47
2:D:1186:SER:HA	2:D:1189:VAL:CG2	2.43	0.47
2:D:1328:GLU:OE1	2:D:1330:PHE:HB3	2.14	0.47
2:D:1485:LEU:HD12	2:D:1486:GLU:N	2.27	0.47
2:D:1636:GLU:O	2:D:1639:ASP:HB3	2.14	0.47
1:A:29:ILE:HG12	1:A:646:PHE:HD2	1.79	0.47
1:A:652:GLN:H	1:A:652:GLN:CD	2.19	0.47
2:B:949:PRO:O	2:B:950:GLU:HG2	2.15	0.47
2:B:1077:TRP:CD1	2:B:1130:ILE:HD11	2.50	0.47
2:D:753:GLU:O	2:D:753:GLU:HG2	2.13	0.47
2:D:755:ILE:CG2	2:D:756:ILE:N	2.77	0.47
2:D:764:ARG:HB3	2:D:767:PHE:HZ	1.79	0.47
2:D:975:GLU:H	2:D:975:GLU:CD	2.20	0.47
2:D:1018:MET:HE1	2:D:1086:PHE:CE1	2.50	0.47
3:F:245:TYR:O	3:F:245:TYR:CG	2.68	0.47
2:B:833:LEU:HG	2:B:835:LEU:HD13	1.97	0.47
2:B:1157:ILE:HD12	2:B:1158:CYS:SG	2.53	0.47
2:B:1237:LEU:HD23	2:B:1278:ALA:HB1	1.96	0.47
2:B:1312:HIS:HE1	3:E:237:GLN:HE22	1.62	0.47
2:B:1356:LEU:HD13	2:B:1357:THR:N	2.27	0.47
2:D:759:GLU:O	2:D:760:ASN:CG	2.57	0.47
2:D:1056:GLN:NE2	2:D:1082:VAL:HG22	2.29	0.47
2:D:1186:SER:O	2:D:1189:VAL:HG23	2.13	0.47
2:D:1193:GLY:O	2:D:1202:LEU:HD23	2.14	0.47
3:E:182:PHE:CE1	3:E:206:ILE:HG22	2.50	0.47
2:B:949:PRO:HG3	2:B:958:GLN:OE1	2.15	0.47
2:B:960:GLU:HB3	2:B:1332:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:PHE:CZ	1:C:658:ALA:HA	2.50	0.47
1:C:203:GLN:NE2	1:C:223:GLU:OE1	2.47	0.47
1:C:386:ARG:HG2	1:C:400:LEU:HD21	1.96	0.47
1:C:465:LEU:HD12	1:C:555:VAL:HG22	1.96	0.47
1:C:508:ARG:HH12	1:C:512:GLN:CB	2.27	0.47
2:D:752:ASP:CG	2:D:753:GLU:H	2.23	0.47
2:D:831:ILE:N	2:D:923:ASP:OD2	2.47	0.47
2:D:1310:ARG:HH21	3:F:235:ILE:HG12	1.80	0.47
2:D:1536:ALA:HB3	2:D:1656:MET:HE3	1.95	0.47
3:F:136:GLU:HB2	3:F:159:LYS:HZ1	1.80	0.47
1:A:169:ASN:HD21	1:A:173:ILE:HB	1.79	0.47
1:A:385:TYR:C	1:A:386:ARG:HG2	2.40	0.47
1:A:491:THR:O	1:A:533:ALA:HA	2.14	0.47
2:B:1434:LEU:HD23	2:B:1434:LEU:HA	1.81	0.47
1:C:135:ASP:HB3	1:C:146:LEU:CD1	2.42	0.47
1:C:229:LEU:CD2	1:C:601:GLY:HA3	2.45	0.47
2:D:932:VAL:HG13	2:D:933:PRO:HD2	1.96	0.47
2:D:934:GLU:HG2	2:D:1352:ALA:O	2.14	0.47
2:D:995:VAL:HG13	2:D:1027:TYR:CE2	2.50	0.47
2:D:1261:TYR:OH	2:D:1268:SER:HB3	2.14	0.47
3:E:107:ALA:N	3:E:130:ARG:HH12	2.13	0.47
3:F:105:ASN:OD1	3:F:106:SER:N	2.48	0.47
1:A:151:THR:HG21	1:A:182:SER:HB3	1.95	0.47
1:C:463:THR:O	1:C:465:LEU:N	2.48	0.47
2:D:985:THR:HA	2:D:986:PRO:HD3	1.83	0.47
2:D:1061:GLN:CG	2:D:1062:PRO:HD2	2.45	0.47
2:D:1102:GLY:HA2	2:D:1105:LYS:CE	2.45	0.47
2:D:1470:GLU:C	2:D:1471:LEU:HD22	2.40	0.47
1:A:35:ARG:HD3	1:A:154:HIS:CD2	2.49	0.47
1:A:458:LEU:HD11	1:A:533:ALA:HB3	1.97	0.47
1:A:492:TYR:HB2	1:A:531:LEU:HD11	1.96	0.47
2:D:772:LEU:O	2:D:774:ASN:N	2.47	0.47
2:D:1136:ASN:CA	2:D:1139:LYS:HE2	2.45	0.47
2:D:1160:GLU:OE2	3:E:117:ASN:HB2	2.15	0.47
3:E:104:LEU:O	3:E:130:ARG:NH2	2.48	0.47
2:B:913:LYS:HG3	2:B:914:ALA:N	2.30	0.46
2:B:970:GLN:NE2	2:B:974:THR:O	2.48	0.46
2:B:980:ILE:HG22	2:B:1344:VAL:HG13	1.97	0.46
2:B:1039:LEU:HA	2:B:1039:LEU:HD12	1.57	0.46
1:C:32:ASN:HD21	1:C:657:ARG:CD	2.01	0.46
1:C:150:PHE:CZ	2:D:807:VAL:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:PRO:HG2	2:D:824:THR:O	2.16	0.46
1:C:636:ALA:HB1	1:C:654:THR:HA	1.96	0.46
1:C:647:THR:HG23	1:C:653:GLN:HB3	1.97	0.46
2:D:904:LYS:HG3	2:D:908:GLN:HE22	1.79	0.46
2:D:1366:THR:OG1	2:D:1387:GLU:HB3	2.15	0.46
1:A:130:LEU:HB2	1:A:218:PHE:HD2	1.80	0.46
1:A:299:GLU:OE1	1:A:299:GLU:N	2.48	0.46
2:B:833:LEU:HD21	2:B:910:VAL:HG12	1.96	0.46
2:B:861:LYS:HD3	2:B:887:THR:HG23	1.96	0.46
2:B:1084:LYS:HZ3	2:B:1274:MET:HE1	1.81	0.46
2:B:1533:LEU:HD23	2:B:1656:MET:HE2	1.97	0.46
1:C:157:LEU:HD21	2:D:811:ASP:O	2.15	0.46
1:C:463:THR:O	1:C:465:LEU:HD23	2.15	0.46
1:C:659:GLU:N	1:C:659:GLU:CD	2.72	0.46
2:D:877:THR:HG23	2:D:879:LYS:N	2.30	0.46
2:D:894:LEU:HD12	2:D:894:LEU:HA	1.72	0.46
2:D:1217:LYS:NZ	2:D:1251:PRO:HG2	2.30	0.46
2:D:1450:LYS:HG3	2:D:1451:VAL:N	2.25	0.46
3:F:226:PRO:O	3:F:276:TRP:NE1	2.44	0.46
1:A:104:LYS:HG2	1:A:105:PHE:N	2.30	0.46
1:A:215:GLN:HG2	1:A:216:GLN:H	1.79	0.46
1:A:471:LEU:HD12	1:A:471:LEU:C	2.41	0.46
1:A:612:THR:HG23	1:A:615:LYS:HZ3	1.79	0.46
2:B:1191:ILE:H	2:B:1191:ILE:HG13	1.43	0.46
2:B:1413:PRO:HD2	2:B:1441:ARG:HD2	1.96	0.46
1:C:36:LEU:HD11	1:C:92:ALA:N	2.30	0.46
1:A:195:ILE:HG13	1:A:195:ILE:O	2.15	0.46
1:A:456:LEU:HB2	1:A:535:TYR:CE2	2.47	0.46
2:B:1060:ARG:CZ	2:B:1099:VAL:HG13	2.45	0.46
1:C:201:MET:HE3	1:C:201:MET:HB3	1.43	0.46
1:C:353:TYR:CE1	1:C:387:VAL:HG21	2.49	0.46
1:C:569:GLN:HB2	1:C:570:SER:H	1.49	0.46
2:D:1131:GLY:C	2:D:1228:TYR:HE1	2.22	0.46
2:D:1294:LEU:HB3	2:D:1311:ILE:HG23	1.97	0.46
2:D:1554:LEU:HD12	2:D:1555:SER:N	2.30	0.46
2:D:1640:GLU:O	2:D:1643:GLN:HG2	2.15	0.46
2:B:1174:ASP:OD1	2:B:1175:PHE:HD2	1.98	0.46
2:B:1265:GLY:N	2:B:1268:SER:OG	2.48	0.46
2:B:1512:ARG:HH12	2:B:1610:ASP:HA	1.80	0.46
2:D:974:THR:HB	2:D:1349:HIS:HD2	1.80	0.46
2:D:1066:PHE:CE1	2:D:1082:VAL:HG11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1152:GLN:O	2:D:1155:LYS:HB2	2.16	0.46
2:D:1216:ASP:OD1	2:D:1216:ASP:C	2.57	0.46
2:D:1275:VAL:HG13	2:D:1276:PHE:CD1	2.51	0.46
2:D:1492:PHE:N	2:D:1492:PHE:CD1	2.63	0.46
3:E:107:ALA:O	3:E:130:ARG:NH1	2.49	0.46
2:B:878:THR:HG21	2:B:1624:LYS:NZ	2.30	0.46
2:B:1541:VAL:HG13	2:B:1570:LYS:NZ	2.30	0.46
1:C:457:HIS:C	1:C:457:HIS:ND1	2.73	0.46
1:C:484:GLU:HA	1:C:487:ILE:CD1	2.46	0.46
3:F:136:GLU:CB	3:F:159:LYS:HE2	2.39	0.46
1:A:303:SER:OG	1:A:306:VAL:HG12	2.16	0.46
1:A:332:LEU:C	1:A:334:SER:H	2.24	0.46
2:B:1243:LEU:HA	2:B:1243:LEU:HD23	1.50	0.46
2:B:1311:ILE:HD11	2:B:1320:ARG:HD2	1.98	0.46
1:C:599:ASP:O	1:C:601:GLY:N	2.48	0.46
2:D:1015:MET:CE	2:D:1018:MET:HE2	2.45	0.46
2:D:1207:LEU:HD12	2:D:1207:LEU:HA	1.52	0.46
2:D:1469:VAL:HG13	2:D:1472:ILE:HG22	1.97	0.46
1:A:167:ILE:HD12	1:A:193:TRP:CE2	2.51	0.46
1:A:273:PHE:CE1	1:A:326:VAL:HG12	2.51	0.46
2:B:1136:ASN:CA	2:B:1139:LYS:HZ1	2.20	0.46
2:B:1189:VAL:CG1	2:B:1213:THR:HG21	2.43	0.46
2:B:1268:SER:O	2:B:1272:THR:HG23	2.16	0.46
1:C:175:VAL:O	2:D:979:ARG:NH1	2.48	0.46
1:C:631:SER:O	1:C:641:ASP:OD2	2.33	0.46
2:D:841:ARG:NH1	2:D:902:PRO:O	2.49	0.46
2:D:978:THR:HG1	2:D:1324:THR:HG23	1.78	0.46
2:D:1413:PRO:HD2	2:D:1441:ARG:HD2	1.97	0.46
3:F:175:ASP:HB3	3:F:187:SER:OG	2.16	0.46
1:A:104:LYS:HG3	1:A:105:PHE:H	1.81	0.46
1:A:492:TYR:CZ	1:A:504:GLY:HA3	2.51	0.46
2:B:999:ARG:NH1	2:B:1262:TYR:CZ	2.84	0.46
2:D:1025:VAL:HG23	2:D:1026:HIS:N	2.30	0.46
2:D:1472:ILE:HD11	2:D:1494:HIS:CD2	2.51	0.46
3:F:245:TYR:N	3:F:245:TYR:CD1	2.84	0.46
1:A:260:LEU:O	2:B:801:THR:OG1	2.33	0.46
2:B:977:GLU:HG2	2:B:1347:MET:HG2	1.98	0.46
2:B:1312:HIS:CE1	3:E:237:GLN:HE22	2.34	0.46
2:D:979:ARG:NH1	2:D:979:ARG:HG3	2.31	0.46
2:D:1492:PHE:CE2	2:D:1500:GLY:HA3	2.51	0.46
3:E:131:PRO:HA	3:E:132:GLY:HA2	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:149:LEU:HD12	3:F:149:LEU:HA	1.48	0.46
1:A:67:LEU:CD2	1:A:68:VAL:H	2.29	0.45
1:A:467:PRO:HA	1:A:521:ILE:HG22	1.97	0.45
1:A:478:ARG:NH1	1:A:479:MET:O	2.49	0.45
2:B:949:PRO:HG3	2:B:958:GLN:NE2	2.30	0.45
2:B:1264:GLY:H	2:B:1272:THR:HG21	1.81	0.45
2:B:1478:LYS:HA	2:B:1489:CYS:O	2.16	0.45
2:B:1594:LEU:HB3	2:B:1596:LEU:HG	1.98	0.45
2:D:1190:ALA:HA	2:D:1220:TRP:CZ3	2.34	0.45
2:B:1453:HIS:C	2:B:1453:HIS:ND1	2.74	0.45
2:B:1524:ASP:HA	2:B:1527:VAL:CG2	2.46	0.45
1:C:135:ASP:OD1	1:C:135:ASP:N	2.47	0.45
2:D:1215:LYS:HD2	2:D:1216:ASP:N	2.31	0.45
2:D:1494:HIS:CE1	2:D:1496:GLU:CD	2.94	0.45
3:F:188:PHE:HD1	3:F:188:PHE:N	2.11	0.45
1:C:148:ARG:NH2	2:D:773:TRP:CE3	2.84	0.45
3:F:163:CYS:HB2	3:F:180:ILE:O	2.16	0.45
2:B:982:LEU:HG	2:B:1311:ILE:HD13	1.98	0.45
2:B:1014:ASN:ND2	2:B:1055:GLN:HG3	2.31	0.45
2:B:1326:GLU:OE1	2:B:1326:GLU:N	2.49	0.45
2:D:1317:SER:OG	2:D:1320:ARG:NH2	2.50	0.45
2:D:1397:ASP:OD1	2:D:1453:HIS:N	2.49	0.45
3:E:245:TYR:CD1	3:E:246:ARG:HB2	2.51	0.45
3:F:197:PHE:CB	3:F:221:ARG:NH1	2.79	0.45
1:A:35:ARG:NH2	1:A:498:GLY:HA3	2.32	0.45
1:A:169:ASN:HB2	1:A:170:PRO:CD	2.46	0.45
1:A:240:GLU:HB3	1:A:242:PHE:CE1	2.52	0.45
1:A:575:PRO:HA	1:A:579:GLN:OE1	2.17	0.45
2:B:772:LEU:O	2:B:774:ASN:N	2.49	0.45
2:B:1084:LYS:NZ	2:B:1274:MET:HE1	2.32	0.45
2:B:1367:ILE:HD12	2:B:1385:ILE:O	2.17	0.45
2:B:1429:ILE:HD13	2:B:1445:ILE:O	2.17	0.45
1:C:351:SER:C	1:C:353:TYR:H	2.23	0.45
1:C:427:LYS:HE3	1:C:427:LYS:HB3	1.74	0.45
1:C:573:ARG:NE	1:C:579:GLN:HE21	2.15	0.45
2:D:1554:LEU:CD1	2:D:1591:ARG:CZ	2.95	0.45
1:A:143:SER:H	1:A:195:ILE:HD11	1.81	0.45
2:B:1308:THR:O	3:E:238:GLY:HA2	2.17	0.45
2:B:1384:MET:HE1	2:B:1495:PRO:HG3	1.98	0.45
2:D:1105:LYS:HB2	2:D:1162:VAL:HG21	1.97	0.45
2:D:1108:ILE:HD12	2:D:1168:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:203:PHE:CD2	3:E:205:LEU:HB3	2.52	0.45
3:F:198:GLY:HA3	3:F:218:PRO:HB3	1.99	0.45
1:A:93:ASN:ND2	1:A:95:GLU:HG2	2.31	0.45
2:B:1534:ASP:OD1	2:B:1535:LYS:N	2.50	0.45
2:D:1484:ASN:HB3	2:D:1487:GLU:CD	2.42	0.45
2:D:1554:LEU:HD12	2:D:1555:SER:H	1.81	0.45
2:D:1577:GLN:OE1	2:D:1577:GLN:N	2.49	0.45
3:E:132:GLY:O	3:E:161:LYS:HB2	2.16	0.45
1:A:76:LEU:HG	1:A:82:HIS:CA	2.46	0.45
2:B:949:PRO:HD3	2:B:958:GLN:HE22	1.81	0.45
2:B:1300:LEU:HD23	2:B:1324:THR:CG2	2.39	0.45
2:B:1544:VAL:HB	2:B:1605:TRP:HB3	1.97	0.45
2:D:781:PRO:HA	2:D:782:PRO:HD3	1.78	0.45
2:D:1542:ASP:O	2:D:1570:LYS:HE2	2.17	0.45
2:D:1544:VAL:HG22	2:D:1605:TRP:CB	2.46	0.45
1:A:293:ILE:HG13	1:A:293:ILE:O	2.17	0.45
2:B:913:LYS:HZ2	2:B:913:LYS:HG2	1.34	0.45
2:B:1117:VAL:CA	2:B:1144:THR:HG21	2.45	0.45
2:B:1180:TYR:CZ	2:B:1189:VAL:HG22	2.52	0.45
2:B:1245:ASP:O	2:B:1249:VAL:HG23	2.17	0.45
2:B:1403:LEU:HB2	2:B:1446:ILE:O	2.17	0.45
2:B:1489:CYS:SG	2:B:1491:ARG:NH1	2.90	0.45
1:C:225:LYS:HG2	1:C:226:GLU:N	2.31	0.45
1:C:569:GLN:N	1:C:582:THR:OG1	2.50	0.45
1:C:579:GLN:H	2:D:795:LEU:HD11	1.82	0.45
2:D:983:GLN:HB3	2:D:1341:THR:HG1	1.81	0.45
2:D:1138:GLU:OE2	2:D:1185:ARG:HD2	2.17	0.45
3:E:226:PRO:CD	3:E:276:TRP:HH2	2.29	0.45
1:A:70:SER:OG	1:A:88:PHE:HB2	2.17	0.45
1:A:496:ASN:C	1:A:498:GLY:N	2.74	0.45
1:A:569:GLN:N	1:A:582:THR:OG1	2.49	0.45
2:B:1053:TYR:CD2	2:B:1086:PHE:HE2	2.35	0.45
2:B:1202:LEU:CB	2:B:1206:LEU:HD11	2.46	0.45
2:B:1207:LEU:HA	2:B:1207:LEU:HD12	1.42	0.45
2:B:1415:THR:HG23	2:B:1416:ASP:N	2.32	0.45
2:B:1549:LEU:O	2:B:1599:LYS:N	2.37	0.45
2:D:810:SER:O	2:D:814:GLY:N	2.46	0.45
2:D:1497:LYS:O	2:D:1500:GLY:N	2.50	0.45
2:D:1550:VAL:CG2	2:D:1581:GLN:HE22	2.29	0.45
2:D:1558:PHE:N	2:D:1558:PHE:CD1	2.85	0.45
2:D:1564:ALA:HB2	2:D:1581:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:195:LYS:CE	3:E:197:PHE:HE1	2.27	0.45
3:F:156:GLU:OE2	3:F:158:CYS:O	2.35	0.45
1:A:93:ASN:CG	1:A:95:GLU:HG2	2.43	0.44
1:A:125:LEU:HD12	1:A:125:LEU:N	2.31	0.44
2:B:945:ARG:HD2	2:B:960:GLU:OE2	2.16	0.44
2:B:1577:GLN:O	2:B:1580:GLN:NE2	2.50	0.44
2:B:1662:PRO:O	2:B:1663:ASN:HB2	2.16	0.44
1:C:76:LEU:HD13	1:C:82:HIS:O	2.17	0.44
1:C:479:MET:HE1	1:C:487:ILE:HD11	1.99	0.44
2:D:1536:ALA:HB2	2:D:1605:TRP:CZ3	2.52	0.44
3:E:226:PRO:N	3:E:276:TRP:CH2	2.78	0.44
3:F:246:ARG:HG2	3:F:246:ARG:NH1	2.29	0.44
1:A:167:ILE:CG1	1:A:176:LYS:HB3	2.47	0.44
1:A:185:GLN:NE2	3:E:245:TYR:CE1	2.86	0.44
2:B:1418:LEU:HA	2:B:1421:LEU:HD22	2.00	0.44
2:B:1494:HIS:ND1	2:B:1497:LYS:CB	2.79	0.44
1:C:106:VAL:HG12	1:C:123:VAL:HG23	1.99	0.44
2:D:999:ARG:HG3	2:D:999:ARG:NH1	2.31	0.44
1:A:137:THR:OG1	1:A:606:ASN:O	2.32	0.44
1:A:646:PHE:H	1:A:654:THR:CG2	2.30	0.44
2:B:1060:ARG:HG3	2:B:1060:ARG:NH1	2.30	0.44
2:B:1086:PHE:O	2:B:1090:VAL:HG13	2.16	0.44
2:B:1561:TYR:HB3	2:B:1563:MET:CE	2.47	0.44
2:B:1576:VAL:HB	2:B:1580:GLN:NE2	2.33	0.44
1:C:324:LEU:HB2	1:C:346:ILE:HG13	1.99	0.44
1:C:389:VAL:HG12	1:C:426:THR:HG22	1.98	0.44
2:D:812:LYS:HD2	2:D:812:LYS:HA	1.69	0.44
2:D:1328:GLU:OE1	2:D:1330:PHE:HD2	1.99	0.44
2:D:1365:VAL:HG13	2:D:1386:LEU:HD11	1.99	0.44
3:E:231:ILE:HD11	3:E:234:GLY:HA3	1.98	0.44
3:E:236:ILE:HB	3:E:239:GLU:HG2	1.99	0.44
3:F:136:GLU:CB	3:F:159:LYS:HZ1	2.30	0.44
3:F:233:ASN:CG	3:F:283:CYS:HB3	2.41	0.44
1:A:386:ARG:HH11	1:A:386:ARG:HG3	1.82	0.44
2:B:1076:THR:H	2:B:1076:THR:HG23	1.39	0.44
1:C:32:ASN:ND2	1:C:32:ASN:C	2.75	0.44
1:C:186:LEU:HD13	1:C:186:LEU:HA	1.69	0.44
2:D:911:GLU:HA	2:D:925:VAL:O	2.17	0.44
2:D:994:ALA:HB1	2:D:1027:TYR:OH	2.18	0.44
2:D:1492:PHE:CZ	2:D:1499:ASP:O	2.71	0.44
2:B:948:ASP:OD2	2:B:951:ARG:NE	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1015:MET:CG	2:B:1056:GLN:NE2	2.80	0.44
2:D:1153:GLU:N	2:D:1153:GLU:OE1	2.50	0.44
2:D:1651:ALA:O	2:D:1655:SER:HB3	2.18	0.44
1:A:268:THR:HB	2:B:1447:TYR:OH	2.18	0.44
2:B:951:ARG:HH21	2:B:1339:GLN:CG	2.17	0.44
2:B:1312:HIS:CA	2:B:1313:TRP:CE3	3.00	0.44
2:B:1407:MET:CE	2:B:1463:VAL:HB	2.48	0.44
1:C:561:GLY:N	2:D:813:LYS:CE	2.80	0.44
2:D:1067:ALA:CA	2:D:1078:LEU:HD21	2.47	0.44
2:D:1190:ALA:CA	2:D:1220:TRP:HZ3	2.22	0.44
1:A:169:ASN:ND2	1:A:173:ILE:HB	2.33	0.44
2:B:879:LYS:HZ3	2:B:1521:GLN:HE22	1.64	0.44
2:B:992:GLU:OE1	2:B:992:GLU:HA	2.18	0.44
2:B:1266:TYR:CD1	2:B:1266:TYR:C	2.96	0.44
2:D:833:LEU:HG	2:D:835:LEU:HD13	1.98	0.44
2:D:929:LEU:C	2:D:929:LEU:HD12	2.43	0.44
2:D:997:ALA:O	2:D:1037:PHE:HE2	2.00	0.44
3:E:165:ASN:OD1	3:E:166:PRO:HD2	2.18	0.44
1:A:161:ARG:HH22	1:A:212:ASN:ND2	2.16	0.44
1:A:465:LEU:HD11	1:A:521:ILE:HD13	1.99	0.44
1:A:479:MET:CG	1:A:484:GLU:HG3	2.48	0.44
2:B:1136:ASN:HA	2:B:1139:LYS:HE3	1.99	0.44
2:B:1230:VAL:HG12	2:B:1275:VAL:CG2	2.47	0.44
2:B:1312:HIS:HA	2:B:1313:TRP:HE3	1.81	0.44
2:B:1363:LEU:HD21	2:B:1477:VAL:HG12	1.98	0.44
1:C:55:VAL:HA	1:C:111:THR:O	2.18	0.44
1:C:67:LEU:HD12	1:C:68:VAL:N	2.27	0.44
1:C:291:ILE:HA	1:C:292:PRO:HD3	1.70	0.44
1:C:385:TYR:CD2	1:C:403:GLY:HA2	2.52	0.44
1:C:496:ASN:CB	1:C:501:LEU:HG	2.34	0.44
2:D:793:ILE:HD12	2:D:794:PHE:H	1.83	0.44
2:D:795:LEU:CD1	2:D:795:LEU:C	2.91	0.44
2:D:947:LEU:HD12	2:D:947:LEU:H	1.80	0.44
3:E:146:LEU:HD12	3:E:150:LYS:H	1.83	0.44
3:E:282:GLU:OE2	3:E:284:ARG:CG	2.66	0.44
1:A:242:PHE:HD2	1:A:379:PRO:HG2	1.81	0.44
1:A:351:SER:OG	1:A:353:TYR:O	2.36	0.44
2:B:1077:TRP:CE2	2:B:1130:ILE:CD1	3.00	0.44
2:B:1444:LEU:HG	2:B:1445:ILE:N	2.32	0.44
2:B:1554:LEU:HD13	2:B:1591:ARG:CZ	2.48	0.44
1:C:26:TYR:HB2	1:C:649:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASN:CG	1:C:94:ARG:N	2.75	0.44
1:C:106:VAL:HG12	1:C:123:VAL:CG2	2.48	0.44
1:C:181:SER:HG	1:C:183:GLN:CD	2.11	0.44
1:C:198:LEU:HD13	2:D:975:GLU:OE2	2.18	0.44
2:D:771:TRP:CE3	2:D:772:LEU:HB2	2.53	0.44
2:D:1300:LEU:HD12	2:D:1300:LEU:O	2.18	0.44
3:F:110:LYS:O	3:F:114:ILE:HG13	2.18	0.44
2:B:838:SER:HB2	2:B:932:VAL:CG2	2.47	0.43
2:B:1479:VAL:HG12	2:B:1480:TYR:N	2.33	0.43
1:C:169:ASN:HB2	1:C:170:PRO:CD	2.48	0.43
1:C:420:LEU:HD11	1:C:422:ILE:HD11	2.00	0.43
1:C:480:ASP:OD1	1:C:480:ASP:N	2.50	0.43
2:D:761:ILE:HD13	2:D:913:LYS:HZ2	1.83	0.43
2:D:1047:GLU:HG3	2:D:1051:LYS:HZ2	1.83	0.43
2:D:1063:SER:HA	2:D:1106:TRP:CZ3	2.53	0.43
2:D:1641:GLU:OE1	2:D:1641:GLU:N	2.50	0.43
3:E:212:GLN:HG3	3:E:213:TRP:N	2.33	0.43
1:A:270:PHE:CE1	1:A:290:ARG:HD3	2.53	0.43
2:B:943:ALA:O	2:B:1343:SER:HA	2.19	0.43
2:B:1264:GLY:H	2:B:1272:THR:CG2	2.31	0.43
1:C:563:LEU:HB3	2:D:818:ALA:HB2	1.98	0.43
2:D:813:LYS:HA	2:D:813:LYS:HD2	1.80	0.43
2:D:1554:LEU:HD12	2:D:1554:LEU:HA	1.48	0.43
1:A:77:THR:OG1	1:A:80:THR:HG23	2.17	0.43
2:B:1077:TRP:NE1	2:B:1146:PHE:CZ	2.86	0.43
2:B:1358:CYS:CB	2:B:1361:PHE:O	2.66	0.43
2:B:1368:LYS:O	2:B:1385:ILE:HG22	2.18	0.43
2:B:1429:ILE:HD11	2:B:1433:GLU:CB	2.48	0.43
2:B:1558:PHE:HD1	2:B:1587:PRO:HA	1.81	0.43
1:C:60:HIS:NE2	1:C:109:GLN:HB2	2.33	0.43
1:C:77:THR:H	1:C:80:THR:HG22	1.83	0.43
1:C:135:ASP:CG	1:C:136:LYS:H	2.26	0.43
1:C:270:PHE:HE1	2:D:1400:MET:HE2	1.84	0.43
1:C:357:PHE:CE1	1:C:441:MET:HE1	2.54	0.43
2:D:942:VAL:HG21	2:D:1346:THR:HG23	2.00	0.43
2:D:997:ALA:H	2:D:1036:LYS:CE	2.30	0.43
2:D:1492:PHE:CE2	2:D:1500:GLY:C	2.96	0.43
1:A:552:TRP:CH2	1:A:554:ASP:HB2	2.54	0.43
2:B:1238:LEU:HD11	2:B:1277:GLN:NE2	2.25	0.43
2:B:1465:GLN:HG2	2:B:1465:GLN:O	2.18	0.43
2:B:1503:ASN:OD1	2:B:1515:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1506:CYS:HA	2:B:1511:CYS:HA	2.00	0.43
2:D:1303:ARG:NH1	3:F:241:ASP:OD1	2.52	0.43
1:A:130:LEU:HD13	1:A:210:TYR:OH	2.18	0.43
2:B:792:ASN:O	2:B:792:ASN:ND2	2.26	0.43
2:B:884:GLN:HG3	2:B:885:THR:N	2.33	0.43
2:B:1300:LEU:HD12	2:B:1300:LEU:C	2.42	0.43
2:B:1549:LEU:HD13	2:B:1563:MET:HE1	2.00	0.43
1:C:263:LYS:HB2	1:C:263:LYS:HE3	1.63	0.43
2:D:979:ARG:NH1	2:D:1323:GLU:CD	2.77	0.43
2:D:1317:SER:OG	2:D:1318:LEU:N	2.51	0.43
3:F:106:SER:HB3	3:F:158:CYS:HB2	1.99	0.43
1:A:227:TYR:CD1	1:A:227:TYR:C	2.96	0.43
1:A:648:SER:OG	1:A:652:GLN:CD	2.62	0.43
2:B:932:VAL:HG12	2:B:933:PRO:HD2	2.00	0.43
2:B:1300:LEU:CD1	2:B:1300:LEU:O	2.63	0.43
2:B:1312:HIS:C	2:B:1313:TRP:HE3	2.21	0.43
2:B:1360:LYS:HG3	2:B:1487:GLU:HB3	2.01	0.43
2:B:1502:LEU:HA	2:B:1502:LEU:HD12	1.79	0.43
2:B:1559:ASP:OD1	2:B:1586:SER:N	2.51	0.43
1:C:599:ASP:C	1:C:601:GLY:H	2.25	0.43
2:D:756:ILE:HG12	2:D:761:ILE:HD11	2.00	0.43
2:D:856:GLN:HG2	2:D:857:ASN:H	1.83	0.43
2:D:899:VAL:HG23	2:D:1473:GLN:NE2	2.32	0.43
2:D:971:VAL:HG12	2:D:1349:HIS:CB	2.48	0.43
2:D:1214:ALA:HB2	2:D:1220:TRP:NE1	2.31	0.43
2:D:1397:ASP:CG	2:D:1453:HIS:ND1	2.77	0.43
3:E:223:ILE:HD11	3:E:269:VAL:CG2	2.42	0.43
3:E:226:PRO:O	3:E:276:TRP:CH2	2.71	0.43
3:F:116:GLN:NE2	3:F:119:PHE:HE1	2.15	0.43
2:B:831:ILE:CD1	2:B:925:VAL:HG23	2.48	0.43
2:B:1083:VAL:HG13	2:B:1100:LEU:HD11	2.00	0.43
2:B:1214:ALA:HB2	2:B:1220:TRP:CD2	2.54	0.43
2:B:1360:LYS:HA	2:B:1360:LYS:HE2	2.01	0.43
1:C:58:THR:OG1	1:C:60:HIS:HE1	2.02	0.43
1:C:508:ARG:HH22	1:C:512:GLN:C	2.27	0.43
2:D:1015:MET:HA	2:D:1015:MET:CE	2.49	0.43
2:D:1348:TYR:CD1	2:D:1348:TYR:C	2.97	0.43
2:D:1536:ALA:HB3	2:D:1652:PHE:HZ	1.83	0.43
2:D:1542:ASP:C	2:D:1570:LYS:HE2	2.43	0.43
3:E:197:PHE:HB2	3:E:219:GLU:HG2	2.01	0.43
1:A:27:SER:OG	1:A:45:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:HA	1:A:100:LYS:HA	1.72	0.43
1:A:166:ASN:HD21	1:A:174:PRO:CB	2.31	0.43
1:A:181:SER:H	3:E:246:ARG:NE	2.17	0.43
1:A:471:LEU:CB	1:A:521:ILE:HD11	2.43	0.43
1:A:634:ASP:OD1	1:A:637:GLY:N	2.51	0.43
2:B:753:GLU:O	2:B:755:ILE:HG23	2.18	0.43
1:C:120:VAL:HB	1:C:656:GLN:NE2	2.34	0.43
1:C:120:VAL:C	1:C:656:GLN:HE22	2.23	0.43
2:D:1207:LEU:O	2:D:1210:PHE:HB3	2.18	0.43
2:D:1464:HIS:HB2	2:D:1466:TYR:CZ	2.53	0.43
3:E:146:LEU:HG	3:E:150:LYS:CB	2.40	0.43
3:E:193:GLY:O	3:E:223:ILE:HG23	2.19	0.43
3:E:236:ILE:CG2	3:E:239:GLU:HG2	2.49	0.43
2:B:807:VAL:HG22	2:B:817:VAL:HG22	2.01	0.43
2:B:949:PRO:CG	2:B:958:GLN:HE22	2.31	0.43
2:B:1060:ARG:NH1	2:B:1099:VAL:HG13	2.34	0.43
2:B:1154:ALA:O	2:B:1157:ILE:HG13	2.19	0.43
2:B:1206:LEU:HD12	2:B:1207:LEU:N	2.34	0.43
2:B:1425:VAL:O	2:B:1426:ASP:HB2	2.18	0.43
1:C:90:ILE:O	1:C:90:ILE:HG13	2.19	0.43
1:C:175:VAL:HB	2:D:979:ARG:NH2	2.34	0.43
1:C:205:LYS:HD2	1:C:221:GLU:HG2	2.01	0.43
2:D:759:GLU:O	2:D:760:ASN:ND2	2.52	0.43
2:D:813:LYS:O	2:D:813:LYS:HG3	2.18	0.43
2:D:1136:ASN:C	2:D:1139:LYS:HE2	2.44	0.43
2:D:1507:ARG:O	2:D:1507:ARG:HG3	2.19	0.43
2:D:1574:ASP:CG	2:D:1582:ARG:NH1	2.67	0.43
3:E:224:TYR:CD1	3:E:224:TYR:N	2.87	0.43
3:F:245:TYR:HD1	3:F:245:TYR:H	1.65	0.43
1:A:26:TYR:N	1:A:26:TYR:CD1	2.87	0.43
1:A:550:SER:OG	1:A:631:SER:N	2.52	0.43
2:B:1576:VAL:HG12	2:B:1582:ARG:HH21	1.82	0.43
2:D:872:PHE:HE1	2:D:902:PRO:HB3	1.84	0.43
2:D:962:ILE:HG12	2:D:1330:PHE:CE1	2.53	0.43
2:D:1237:LEU:HD22	2:D:1256:LEU:CD2	2.48	0.43
2:D:1268:SER:O	2:D:1272:THR:OG1	2.36	0.43
2:D:1496:GLU:HG2	2:D:1497:LYS:N	2.34	0.43
3:E:120:PRO:HG2	3:E:123:THR:CG2	2.49	0.43
1:A:161:ARG:O	1:A:181:SER:HA	2.19	0.42
1:A:490:TYR:OH	1:A:508:ARG:HD2	2.19	0.42
2:B:781:PRO:HA	2:B:782:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LYS:HD3	3:E:147:GLN:HG2	2.00	0.42
1:C:70:SER:OG	1:C:88:PHE:HB2	2.19	0.42
1:C:388:PRO:HG2	1:C:427:LYS:C	2.44	0.42
2:D:851:LEU:HD23	2:D:862:VAL:HG21	2.01	0.42
2:D:1023:ILE:HD12	2:D:1023:ILE:HA	1.91	0.42
2:D:1310:ARG:CD	2:D:1312:HIS:NE2	2.82	0.42
3:E:125:VAL:HG23	3:E:143:LEU:HG	2.01	0.42
3:E:132:GLY:HA2	3:E:161:LYS:HZ3	1.84	0.42
3:F:232:ASP:C	3:F:233:ASN:OD1	2.62	0.42
1:A:111:THR:CG2	1:A:116:VAL:HG23	2.42	0.42
1:A:277:ASP:O	1:A:280:GLN:HG2	2.18	0.42
1:A:420:LEU:O	1:A:443:ALA:N	2.48	0.42
1:A:637:GLY:O	1:A:641:ASP:HB2	2.19	0.42
2:B:783:LYS:HE3	3:F:197:PHE:CD1	2.55	0.42
2:B:1115:ASP:O	2:B:1175:PHE:CG	2.71	0.42
2:B:1118:PHE:N	2:B:1144:THR:CG2	2.79	0.42
2:B:1429:ILE:HD11	2:B:1433:GLU:CG	2.48	0.42
2:B:1559:ASP:OD2	2:B:1561:TYR:CZ	2.71	0.42
1:C:66:LYS:HE3	3:E:146:LEU:C	2.43	0.42
1:C:449:VAL:O	1:C:449:VAL:HG23	2.19	0.42
2:D:874:SER:HB3	2:D:900:ILE:HG22	2.01	0.42
2:D:916:VAL:HG22	2:D:921:ILE:O	2.19	0.42
2:D:1208:ASN:O	2:D:1211:LEU:HG	2.18	0.42
2:D:1225:LYS:HE3	2:D:1227:LEU:CD1	2.48	0.42
2:D:1328:GLU:CD	2:D:1330:PHE:HB3	2.44	0.42
2:D:1351:LYS:HA	2:D:1352:ALA:C	2.44	0.42
2:D:1400:MET:CE	2:D:1447:TYR:HB3	2.40	0.42
2:D:1659:PHE:CE2	2:D:1662:PRO:HD3	2.49	0.42
3:F:97:SER:OG	3:F:98:CYS:O	2.36	0.42
1:A:46:ALA:HB3	1:A:76:LEU:HD11	2.01	0.42
1:A:366:PRO:HD2	1:A:455:TYR:CZ	2.54	0.42
1:A:532:VAL:HG11	1:A:644:LEU:HD12	2.01	0.42
2:B:982:LEU:HD22	2:B:1296:VAL:HG11	2.00	0.42
2:B:1128:GLU:HG3	2:B:1267:GLY:HA2	2.00	0.42
2:B:1303:ARG:CZ	2:B:1307:ILE:HG12	2.49	0.42
2:B:1652:PHE:CE1	2:B:1656:MET:HE3	2.54	0.42
1:C:230:PRO:O	1:C:231:SER:OG	2.33	0.42
1:C:373:MET:HE1	1:C:408:LYS:HD2	2.01	0.42
1:C:641:ASP:OD1	1:C:642:ALA:N	2.53	0.42
2:D:756:ILE:HD11	3:F:134:ARG:HH12	1.82	0.42
2:D:839:VAL:HG22	2:D:929:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1061:GLN:OE1	2:D:1061:GLN:HA	2.20	0.42
2:D:1494:HIS:ND1	2:D:1496:GLU:OE1	2.52	0.42
2:D:1507:ARG:NH1	2:D:1613:GLY:HA2	2.34	0.42
3:F:222:GLU:CD	3:F:224:TYR:CZ	2.98	0.42
1:A:444:LEU:HG	1:A:445:PRO:HD2	2.00	0.42
1:A:568:GLY:C	3:F:271:ASN:HD21	2.14	0.42
2:B:896:VAL:HA	2:B:897:PRO:HD3	1.76	0.42
2:B:1010:CYS:O	2:B:1012:GLU:N	2.53	0.42
2:B:1408:MET:HG3	2:B:1411:PHE:HB2	2.01	0.42
1:C:488:ARG:O	1:C:508:ARG:N	2.48	0.42
2:D:1258:GLU:OE1	2:D:1258:GLU:N	2.49	0.42
3:F:131:PRO:HA	3:F:132:GLY:HA2	1.35	0.42
1:A:120:VAL:HG11	2:B:1039:LEU:HD23	2.01	0.42
1:A:147:TYR:CZ	1:A:191:LEU:HG	2.54	0.42
2:B:1117:VAL:HA	2:B:1144:THR:CG2	2.47	0.42
2:D:948:ASP:OD2	2:D:951:ARG:CZ	2.67	0.42
2:D:959:LYS:HE3	2:D:961:ASP:OD1	2.20	0.42
2:D:1033:GLN:HB3	2:D:1036:LYS:HZ3	1.80	0.42
2:D:1368:LYS:O	2:D:1385:ILE:HG13	2.19	0.42
2:D:1501:LYS:HD2	2:D:1557:ASP:OD2	2.19	0.42
2:D:1603:LEU:HD22	2:D:1649:LEU:CD1	2.49	0.42
3:E:157:PHE:CD1	3:E:157:PHE:N	2.84	0.42
3:E:258:THR:O	3:E:283:CYS:HA	2.19	0.42
1:A:354:GLN:O	1:A:376:VAL:HA	2.18	0.42
1:A:428:LYS:O	1:A:431:LEU:HG	2.20	0.42
1:A:534:TYR:CD1	1:A:534:TYR:C	2.98	0.42
1:C:65:LYS:HE3	1:C:65:LYS:HB3	1.48	0.42
1:C:182:SER:C	1:C:185:GLN:HB2	2.45	0.42
2:D:985:THR:HB	2:D:1339:GLN:O	2.19	0.42
2:D:1118:PHE:HD2	2:D:1144:THR:CG2	2.32	0.42
2:D:1544:VAL:CG2	2:D:1570:LYS:HD3	2.46	0.42
3:E:143:LEU:CD1	3:E:151:TRP:CE3	3.03	0.42
1:A:43:VAL:HG21	1:A:493:LEU:HD23	2.00	0.42
2:B:1167:GLY:O	2:B:1171:LYS:HB2	2.20	0.42
1:C:422:ILE:HG23	1:C:422:ILE:HD12	1.67	0.42
1:C:529:PHE:CZ	1:C:553:VAL:HG11	2.55	0.42
2:D:1237:LEU:HD22	2:D:1256:LEU:HD21	2.02	0.42
2:D:1562:ILE:O	2:D:1562:ILE:CG1	2.67	0.42
2:D:1640:GLU:O	2:D:1641:GLU:C	2.61	0.42
1:A:28:ILE:HD12	1:A:28:ILE:HA	1.75	0.42
1:A:46:ALA:O	1:A:82:HIS:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:CE1	1:A:339:VAL:HG23	2.55	0.42
1:A:253:VAL:CG1	1:A:300:VAL:HG13	2.50	0.42
1:A:429:GLN:C	1:A:431:LEU:H	2.28	0.42
2:B:996:ASP:OD1	2:B:996:ASP:C	2.63	0.42
2:B:1084:LYS:HE3	2:B:1149:ILE:CD1	2.49	0.42
2:B:1141:MET:HG3	2:B:1183:LEU:HD11	2.02	0.42
1:C:35:ARG:NH1	1:C:40:GLU:OE2	2.37	0.42
1:C:391:VAL:HG13	1:C:397:VAL:HG11	2.02	0.42
1:C:569:GLN:CD	1:C:581:MET:SD	3.03	0.42
2:D:841:ARG:HH22	2:D:903:LEU:C	2.27	0.42
2:D:1300:LEU:HD11	2:D:1303:ARG:HB2	2.00	0.42
2:D:1403:LEU:HB2	2:D:1446:ILE:O	2.19	0.42
3:E:157:PHE:H	3:E:157:PHE:HD1	1.65	0.42
3:F:136:GLU:O	3:F:137:PRO:C	2.62	0.42
3:F:245:TYR:O	3:F:246:ARG:HB2	2.19	0.42
1:A:37:GLU:OE2	1:A:127:SER:HB3	2.19	0.42
1:A:88:PHE:HE2	1:A:90:ILE:HD11	1.85	0.42
2:B:1144:THR:HB	2:B:1176:LEU:HD11	2.02	0.42
2:B:1149:ILE:HA	2:B:1152:GLN:OE1	2.19	0.42
2:B:1554:LEU:HD13	2:B:1591:ARG:NH2	2.34	0.42
1:C:102:ARG:NH2	2:D:1035:GLU:HB3	2.35	0.42
1:C:473:VAL:HG11	1:C:517:LEU:HD23	2.01	0.42
2:D:877:THR:HG23	2:D:880:ARG:H	1.85	0.42
2:D:1225:LYS:HE2	2:D:1228:TYR:CZ	2.55	0.42
3:E:135:ARG:CZ	3:E:137:PRO:HA	2.49	0.42
3:E:237:GLN:HB3	3:E:250:THR:CG2	2.42	0.42
3:F:156:GLU:O	3:F:159:LYS:HE3	2.19	0.42
1:A:28:ILE:HD11	1:A:42:MET:HG3	2.01	0.42
1:A:449:VAL:HG23	1:A:449:VAL:O	2.20	0.42
2:B:960:GLU:O	2:B:960:GLU:HG3	2.20	0.42
2:B:981:LEU:HD11	2:B:1343:SER:OG	2.19	0.42
2:B:1502:LEU:HD11	2:B:1515:GLU:HG3	2.02	0.42
1:C:324:LEU:HB2	1:C:346:ILE:HD11	2.02	0.42
2:D:962:ILE:HD11	2:D:1330:PHE:CE2	2.54	0.42
2:D:1313:TRP:HE3	2:D:1318:LEU:HD21	1.83	0.42
2:D:1408:MET:HB2	2:D:1411:PHE:CD1	2.55	0.42
2:D:1537:CYS:SG	2:D:1656:MET:HE1	2.60	0.42
2:D:1544:VAL:HG23	2:D:1570:LYS:CD	2.45	0.42
3:E:246:ARG:CZ	3:E:266:TYR:HB2	2.50	0.42
3:F:109:LEU:HD22	3:F:125:VAL:CG1	2.50	0.42
3:F:113:TYR:CA	3:F:116:GLN:HG2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:MET:HE3	1:A:495:MET:HB3	1.95	0.41
2:B:911:GLU:HA	2:B:925:VAL:O	2.19	0.41
1:C:55:VAL:HG23	1:C:74:THR:HG22	2.02	0.41
1:C:293:ILE:O	1:C:293:ILE:HG13	2.20	0.41
2:D:948:ASP:OD2	2:D:951:ARG:NH2	2.53	0.41
2:D:1027:TYR:CE2	2:D:1031:THR:HG21	2.54	0.41
2:D:1310:ARG:HH21	3:F:235:ILE:CG1	2.33	0.41
2:D:1471:LEU:HA	2:D:1471:LEU:HD13	1.58	0.41
2:D:1479:VAL:O	2:D:1480:TYR:HB3	2.19	0.41
3:E:243:TYR:CZ	3:E:249:VAL:HG12	2.55	0.41
2:B:752:ASP:HB3	2:B:753:GLU:H	1.54	0.41
2:B:1111:LYS:HA	2:B:1111:LYS:HD2	1.64	0.41
2:B:1549:LEU:HD11	2:B:1551:LYS:O	2.20	0.41
1:C:244:TYR:CE2	1:C:246:TYR:HB2	2.56	0.41
2:D:951:ARG:HH22	2:D:1339:GLN:HB3	1.84	0.41
2:D:1077:TRP:CE2	2:D:1130:ILE:HG22	2.55	0.41
2:D:1220:TRP:CE3	2:D:1236:ALA:HB2	2.56	0.41
2:D:1496:GLU:O	2:D:1497:LYS:C	2.63	0.41
3:F:103:ARG:O	3:F:104:LEU:HD23	2.20	0.41
3:F:206:ILE:O	3:F:206:ILE:HG13	2.20	0.41
3:F:207:SER:OG	3:F:208:GLY:N	2.51	0.41
1:A:65:LYS:HB2	1:A:65:LYS:HE3	1.69	0.41
1:A:67:LEU:HD23	1:A:68:VAL:H	1.85	0.41
1:A:185:GLN:NE2	3:E:245:TYR:HE1	2.18	0.41
1:A:332:LEU:C	1:A:334:SER:N	2.79	0.41
2:B:1023:ILE:HG13	2:B:1276:PHE:HB2	2.03	0.41
2:B:1348:TYR:HE1	2:B:1350:ALA:HB2	1.85	0.41
2:B:1505:LEU:HD23	2:B:1621:ILE:HG21	2.03	0.41
2:B:1592:GLU:O	2:B:1595:LYS:HD2	2.20	0.41
3:E:224:TYR:CD2	3:E:242:HIS:CD2	3.08	0.41
1:A:36:LEU:C	1:A:37:GLU:HG2	2.45	0.41
1:A:475:PHE:HB2	1:A:515:VAL:HG23	2.02	0.41
1:A:535:TYR:CZ	1:A:547:VAL:HB	2.56	0.41
2:B:875:LEU:HA	2:B:875:LEU:HD23	1.74	0.41
2:B:1512:ARG:HH12	2:B:1609:SER:C	2.24	0.41
1:C:230:PRO:CB	1:C:339:VAL:HG22	2.50	0.41
2:D:798:SER:HB2	2:D:802:TRP:HZ2	1.85	0.41
2:D:841:ARG:HH12	2:D:902:PRO:C	2.29	0.41
2:D:1136:ASN:O	2:D:1137:ASN:HB2	2.20	0.41
3:F:194:TYR:HE1	3:F:222:GLU:HB3	1.85	0.41
1:A:414:HIS:HA	1:A:415:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ILE:HA	1:A:487:ILE:HD12	1.83	0.41
1:A:608:LYS:HE2	1:A:608:LYS:HB3	1.84	0.41
2:B:783:LYS:NZ	3:F:197:PHE:HD1	2.18	0.41
2:B:1187:TYR:CD1	2:B:1232:ALA:HB2	2.50	0.41
2:B:1403:LEU:HD12	2:B:1448:LEU:HD11	2.02	0.41
1:C:181:SER:C	1:C:183:GLN:OE1	2.64	0.41
1:C:332:LEU:C	1:C:334:SER:N	2.78	0.41
1:C:599:ASP:HB2	2:D:802:TRP:HZ3	1.83	0.41
2:D:983:GLN:OE1	2:D:1319:LEU:HD21	2.20	0.41
2:D:1117:VAL:HG12	2:D:1175:PHE:CD2	2.55	0.41
3:E:139:LEU:HD12	3:E:139:LEU:HA	1.81	0.41
3:E:206:ILE:O	3:E:206:ILE:HG13	2.16	0.41
3:F:98:CYS:HA	3:F:149:LEU:HD11	2.02	0.41
3:F:268:THR:HG22	3:F:275:GLU:O	2.20	0.41
1:A:125:LEU:HD12	1:A:126:GLN:H	1.86	0.41
1:A:159:VAL:O	1:A:182:SER:OG	2.38	0.41
1:A:273:PHE:CD1	1:A:326:VAL:HG12	2.55	0.41
2:B:938:MET:CB	2:B:940:LYS:HZ2	2.34	0.41
2:B:1128:GLU:HA	2:B:1134:ARG:CZ	2.50	0.41
1:C:100:LYS:HD3	2:D:1313:TRP:CH2	2.55	0.41
1:C:144:THR:HG22	1:C:194:ASP:OD1	2.20	0.41
1:C:368:MET:O	1:C:413:THR:CG2	2.68	0.41
2:D:833:LEU:HD13	2:D:912:VAL:HG11	2.03	0.41
2:D:863:ARG:HG2	2:D:915:ALA:O	2.21	0.41
2:D:888:ILE:HA	2:D:889:PRO:HD3	1.89	0.41
2:D:897:PRO:C	2:D:1473:GLN:HE22	2.28	0.41
2:D:909:GLU:OE2	2:D:926:ARG:HD2	2.20	0.41
2:D:1425:VAL:O	2:D:1426:ASP:HB2	2.20	0.41
2:D:1545:TYR:CG	2:D:1565:ILE:HD12	2.55	0.41
2:B:841:ARG:O	2:B:842:ASN:OD1	2.39	0.41
2:B:981:LEU:O	2:B:1342:LEU:HD12	2.20	0.41
1:C:275:ILE:CG1	1:C:282:ILE:HB	2.51	0.41
2:D:860:LEU:O	2:D:888:ILE:HG22	2.20	0.41
2:D:880:ARG:HH11	2:D:880:ARG:HD3	1.72	0.41
2:D:913:LYS:HB2	2:D:913:LYS:HE3	1.60	0.41
3:E:120:PRO:HD2	3:E:123:THR:HG21	2.03	0.41
3:E:250:THR:HA	3:E:264:SER:HB2	2.01	0.41
1:A:161:ARG:NH2	1:A:212:ASN:ND2	2.69	0.41
1:A:178:ASP:OD1	1:A:179:SER:N	2.53	0.41
1:A:232:PHE:CZ	1:A:339:VAL:HG23	2.55	0.41
1:A:273:PHE:CG	1:A:302:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1436:LYS:HE3	2:B:1440:ASP:C	2.46	0.41
1:C:134:THR:HG22	1:C:147:TYR:HB3	2.02	0.41
1:C:156:LEU:HA	1:C:156:LEU:HD23	1.77	0.41
1:C:479:MET:CE	1:C:487:ILE:HD11	2.50	0.41
1:C:491:THR:HG22	1:C:505:ARG:CD	2.50	0.41
2:D:958:GLN:O	2:D:1333:THR:OG1	2.33	0.41
2:D:1107:LEU:HD23	2:D:1107:LEU:C	2.45	0.41
2:D:1476:ALA:HA	2:D:1492:PHE:HA	2.02	0.41
3:E:109:LEU:CB	3:E:114:ILE:HG12	2.43	0.41
3:F:110:LYS:HG3	3:F:126:GLU:O	2.20	0.41
3:F:120:PRO:HG2	3:F:123:THR:OG1	2.21	0.41
1:A:59:VAL:HG12	1:A:69:LEU:HB2	2.03	0.41
1:A:104:LYS:CG	1:A:105:PHE:H	2.33	0.41
1:A:104:LYS:HB2	1:A:104:LYS:HE3	1.70	0.41
1:A:252:GLU:H	1:A:252:GLU:CD	2.23	0.41
1:A:253:VAL:HG12	1:A:300:VAL:HG13	2.03	0.41
1:A:338:MET:CE	2:B:1485:LEU:HB2	2.34	0.41
1:A:473:VAL:HG21	1:A:531:LEU:CD2	2.51	0.41
1:A:617:TRP:CE3	1:A:617:TRP:HA	2.56	0.41
2:B:1256:LEU:HD13	2:B:1256:LEU:N	2.36	0.41
2:B:1559:ASP:OD2	2:B:1561:TYR:CE2	2.74	0.41
1:C:25:MET:HE2	1:C:47:HIS:CD2	2.50	0.41
1:C:170:PRO:HD3	1:C:204:TRP:CE2	2.55	0.41
2:D:1062:PRO:O	2:D:1106:TRP:CZ3	2.74	0.41
2:D:1197:ALA:HA	2:D:1202:LEU:HG	2.02	0.41
2:D:1311:ILE:CD1	2:D:1318:LEU:HA	2.50	0.41
2:D:1313:TRP:CG	2:D:1314:GLU:N	2.88	0.41
2:D:1550:VAL:HG23	2:D:1562:ILE:HG13	2.02	0.41
2:D:1631:TRP:CZ3	2:D:1633:GLU:HA	2.54	0.41
3:E:146:LEU:HD12	3:E:150:LYS:N	2.35	0.41
3:E:156:GLU:CD	3:E:158:CYS:O	2.64	0.41
3:F:181:LEU:HA	3:F:181:LEU:HD23	1.60	0.41
1:A:291:ILE:HA	1:A:292:PRO:HD3	1.71	0.41
1:A:360:THR:HG21	1:A:372:LEU:HD23	2.02	0.41
2:B:1325:LYS:HB3	2:B:1325:LYS:HE2	1.81	0.41
2:B:1417:ASP:O	2:B:1421:LEU:HD22	2.21	0.41
2:B:1418:LEU:HA	2:B:1418:LEU:HD23	2.00	0.41
2:B:1471:LEU:HD13	2:B:1471:LEU:HA	1.95	0.41
2:B:1636:GLU:O	2:B:1639:ASP:HB2	2.21	0.41
1:C:569:GLN:OE1	1:C:581:MET:SD	2.79	0.41
1:C:592:ARG:HB2	2:D:777:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1124:VAL:O	2:D:1127:GLN:HG2	2.21	0.41
2:D:1291:GLU:O	2:D:1292:LEU:C	2.64	0.41
2:D:1505:LEU:HD23	2:D:1505:LEU:HA	1.67	0.41
3:E:249:VAL:CG2	3:E:265:ILE:HG22	2.50	0.41
3:F:116:GLN:NE2	3:F:119:PHE:CE1	2.89	0.41
3:F:143:LEU:HA	3:F:143:LEU:HD23	1.76	0.41
1:A:139:TYR:C	1:A:227:TYR:HE2	2.28	0.40
1:A:261:TYR:HD2	2:B:826:MET:SD	2.45	0.40
1:A:449:VAL:HG21	1:A:545:GLU:CG	2.45	0.40
1:A:576:VAL:HG13	1:A:577:PRO:HD2	2.03	0.40
2:B:753:GLU:OE1	2:B:753:GLU:N	2.45	0.40
2:B:996:ASP:OD1	2:B:999:ARG:N	2.54	0.40
2:B:1403:LEU:HD23	2:B:1479:VAL:HG22	2.03	0.40
2:B:1420:GLN:O	2:B:1420:GLN:CD	2.64	0.40
2:B:1576:VAL:C	2:B:1580:GLN:HE22	2.29	0.40
1:C:55:VAL:CG2	1:C:74:THR:HG22	2.50	0.40
1:C:646:PHE:H	1:C:654:THR:HG23	1.80	0.40
2:D:762:VAL:O	2:D:924:GLY:HA3	2.21	0.40
2:D:934:GLU:HB2	2:D:1354:ASP:O	2.22	0.40
2:D:967:LEU:HD22	2:D:1348:TYR:CD2	2.56	0.40
2:D:1171:LYS:O	2:D:1174:ASP:HB2	2.21	0.40
2:D:1240:LEU:CD1	2:D:1248:PHE:HB3	2.51	0.40
2:D:1496:GLU:HG2	2:D:1497:LYS:H	1.86	0.40
3:E:229:PRO:HG2	3:E:280:PRO:CG	2.46	0.40
3:F:193:GLY:C	3:F:223:ILE:HD12	2.46	0.40
1:A:240:GLU:C	1:A:242:PHE:H	2.28	0.40
2:B:1382:ASN:OD1	2:B:1383:THR:HG22	2.21	0.40
1:C:180:LEU:HD22	1:C:191:LEU:HD11	2.04	0.40
1:C:449:VAL:HG21	1:C:545:GLU:CG	2.50	0.40
1:C:607:LYS:O	1:C:607:LYS:HG3	2.21	0.40
2:D:796:LYS:HE2	3:F:168:GLU:OE2	2.21	0.40
2:D:1149:ILE:CD1	2:D:1153:GLU:OE2	2.69	0.40
2:D:1494:HIS:CE1	2:D:1497:LYS:HG3	2.56	0.40
2:B:945:ARG:NH1	2:B:962:ILE:HG22	2.37	0.40
1:C:98:SER:C	1:C:100:LYS:HA	2.45	0.40
1:C:135:ASP:OD2	1:C:136:LYS:HG3	2.21	0.40
1:C:229:LEU:HD21	1:C:601:GLY:HA3	2.04	0.40
1:C:274:GLY:HA3	1:C:325:TYR:CZ	2.56	0.40
1:C:579:GLN:HE21	1:C:581:MET:HE1	1.87	0.40
2:D:756:ILE:HD12	3:F:134:ARG:NH2	2.34	0.40
2:D:935:GLY:CA	2:D:1353:LYS:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1018:MET:HE1	2:D:1086:PHE:HE1	1.85	0.40
2:D:1066:PHE:HB2	2:D:1078:LEU:CD1	2.47	0.40
2:D:1175:PHE:CE1	2:D:1179:ASN:ND2	2.90	0.40
2:D:1227:LEU:C	2:D:1227:LEU:HD12	2.47	0.40
2:D:1258:GLU:HA	2:D:1260:ARG:HH11	1.76	0.40
2:D:1310:ARG:HD2	2:D:1312:HIS:CD2	2.56	0.40
2:D:1367:ILE:HD12	2:D:1367:ILE:HG23	1.83	0.40
3:F:127:TYR:HE2	3:F:143:LEU:HD12	1.87	0.40
1:A:183:GLN:O	1:A:184:ASN:OD1	2.40	0.40
1:A:477:LEU:HD11	1:A:487:ILE:HG21	2.04	0.40
2:B:962:ILE:HD12	2:B:962:ILE:C	2.46	0.40
2:B:990:MET:HE2	2:B:1283:GLN:OE1	2.20	0.40
2:B:1130:ILE:CG2	2:B:1134:ARG:H	2.35	0.40
2:B:1135:ASN:HB2	2:B:1185:ARG:NH2	2.37	0.40
2:B:1253:VAL:H	2:B:1253:VAL:HG23	1.57	0.40
2:B:1411:PHE:C	2:B:1466:TYR:CE1	2.98	0.40
2:B:1521:GLN:CD	2:B:1521:GLN:N	2.76	0.40
1:C:104:LYS:HA	1:C:104:LYS:HD2	1.81	0.40
1:C:229:LEU:HD22	1:C:231:SER:H	1.86	0.40
1:C:269:ALA:HB2	1:C:330:VAL:HG22	2.03	0.40
1:C:456:LEU:HB2	1:C:535:TYR:CE2	2.57	0.40
1:C:589:HIS:HB2	2:D:782:PRO:HB3	2.02	0.40
2:D:778:LEU:HD12	2:D:778:LEU:HA	1.83	0.40
2:D:898:TYR:CA	2:D:1473:GLN:HE22	2.34	0.40
2:D:1132:GLY:HA3	2:D:1187:TYR:CZ	2.57	0.40
2:D:1352:ALA:N	2:D:1353:LYS:HA	2.36	0.40
2:D:1544:VAL:HG22	2:D:1605:TRP:HB2	2.04	0.40
3:E:133:TYR:CB	3:E:158:CYS:HB3	2.47	0.40
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.88	0.40
1:A:464:GLU:CB	1:A:556:LYS:HE3	2.49	0.40
1:A:480:ASP:O	1:A:484:GLU:OE1	2.38	0.40
1:A:615:LYS:HE2	1:A:615:LYS:HB2	1.69	0.40
2:B:792:ASN:HD22	2:B:792:ASN:C	2.13	0.40
2:B:1249:VAL:O	2:B:1253:VAL:HG23	2.21	0.40
2:B:1422:ALA:CB	2:B:1429:ILE:HG22	2.52	0.40
2:B:1653:THR:HG23	2:B:1654:GLU:HG2	2.03	0.40
1:C:27:SER:OG	1:C:45:GLU:HB2	2.21	0.40
1:C:67:LEU:HD21	1:C:69:LEU:HD12	2.03	0.40
2:D:1066:PHE:HB3	2:D:1078:LEU:HD11	2.02	0.40
2:D:1137:ASN:HB2	2:D:1185:ARG:HE	1.86	0.40
2:D:1217:LYS:O	2:D:1251:PRO:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1241:LEU:HD12	2:D:1241:LEU:HA	1.64	0.40
3:F:106:SER:CB	3:F:158:CYS:HB2	2.52	0.40
3:F:143:LEU:HD22	3:F:152:SER:O	2.22	0.40

All (4) 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:A:77:THR:OG1	2:B:954:ARG:NH2[3_455]	2.06	0.14
2:B:1577:GLN:NE2	3:E:133:TYR:OH[3_565]	2.15	0.05
1:C:413:THR:O	1:C:512:GLN:NE2[2_755]	2.15	0.05
1:A:435:GLU:OE2	2:D:1431:LYS:NZ[2_755]	2.19	0.01

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	640/645 (99%)	598 (93%)	37 (6%)	5 (1%)	16	52
1	C	640/645 (99%)	599 (94%)	34 (5%)	7 (1%)	11	45
2	B	898/915 (98%)	822 (92%)	58 (6%)	18 (2%)	6	32
2	D	898/915 (98%)	818 (91%)	57 (6%)	23 (3%)	4	26
3	E	187/194 (96%)	165 (88%)	17 (9%)	5 (3%)	4	26
3	F	187/194 (96%)	165 (88%)	17 (9%)	5 (3%)	4	26
All	All	3450/3508 (98%)	3167 (92%)	220 (6%)	63 (2%)	6	34

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	950	GLU
2	B	1137	ASN

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Mol	Chain	Res	Type
2	B	1286	ALA
2	B	1287	PRO
2	B	1573	SER
1	C	397	VAL
1	C	497	LYS
2	D	950	GLU
2	D	988	ALA
2	D	1497	LYS
3	E	239	GLU
3	F	239	GLU
1	A	397	VAL
1	A	497	LYS
1	A	540	ALA
2	B	957	VAL
2	B	992	GLU
2	B	1011	GLY
2	B	1264	GLY
2	B	1301	PRO
1	C	96	PHE
1	C	540	ALA
2	D	757	ALA
2	D	957	VAL
2	D	989	GLN
2	D	1011	GLY
2	D	1264	GLY
2	D	1289	HIS
2	D	1301	PRO
2	D	1358	CYS
1	A	600	LYS
2	B	1135	ASN
1	C	333	HIS
2	D	1498	GLU
2	D	1633	GLU
3	E	131	PRO
3	F	131	PRO
2	B	1317	SER
2	B	1354	ASP
2	B	1480	TYR
1	C	569	GLN
1	C	600	LYS
2	D	760	ASN
2	D	1064	SER

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Mol	Chain	Res	Type
2	D	1480	TYR
2	D	1499	ASP
3	E	156	GLU
3	E	237	GLN
3	F	237	GLN
2	B	796	LYS
2	B	935	GLY
2	B	1508	ASP
2	D	1136	ASN
2	D	1286	ALA
2	D	1287	PRO
2	D	1317	SER
2	D	1508	ASP
1	A	333	HIS
2	D	1399	THR
3	F	137	PRO
3	F	155	VAL
3	E	137	PRO
2	B	1520	ILE

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	564/567 (100%)	514 (91%)	50 (9%)	9	29
1	C	564/567 (100%)	518 (92%)	46 (8%)	10	32
2	B	791/810 (98%)	706 (89%)	85 (11%)	6	23
2	D	787/810 (97%)	702 (89%)	85 (11%)	6	22
3	E	166/167 (99%)	131 (79%)	35 (21%)	1	7
3	F	166/167 (99%)	132 (80%)	34 (20%)	1	8
All	All	3038/3088 (98%)	2703 (89%)	335 (11%)	6	22

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	TYR
1	A	30	THR
1	A	59	VAL
1	A	67	LEU
1	A	68	VAL
1	A	71	SER
1	A	76	LEU
1	A	83	MET
1	A	85	ASN
1	A	87	THR
1	A	89	THR
1	A	116	VAL
1	A	117	VAL
1	A	122	LEU
1	A	125	LEU
1	A	130	LEU
1	A	133	GLN
1	A	134	THR
1	A	136	LYS
1	A	163	VAL
1	A	177	GLN
1	A	186	LEU
1	A	213	SER
1	A	217	VAL
1	A	228	VAL
1	A	234	VAL
1	A	235	ILE
1	A	239	THR
1	A	252	GLU
1	A	293	ILE
1	A	306	VAL
1	A	330	VAL
1	A	413	THR
1	A	421	SER
1	A	423	THR
1	A	448	THR
1	A	462	ARG
1	A	463	THR
1	A	465	LEU
1	A	471	LEU
1	A	491	THR
1	A	496	ASN
1	A	556	LYS

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Mol	Chain	Res	Type
1	A	583	LEU
1	A	604	VAL
1	A	605	LEU
1	A	621	GLU
1	A	622	LYS
1	A	650	SER
1	A	656	GLN
2	B	755	ILE
2	B	759	GLU
2	B	761	ILE
2	B	763	SER
2	B	774	ASN
2	B	792	ASN
2	B	795	LEU
2	B	831	ILE
2	B	841	ARG
2	B	850	VAL
2	B	899	VAL
2	B	901	VAL
2	B	929	LEU
2	B	932	VAL
2	B	939	ASN
2	B	941	THR
2	B	946	THR
2	B	952	LEU
2	B	957	VAL
2	B	962	ILE
2	B	980	ILE
2	B	981	LEU
2	B	982	LEU
2	B	983	GLN
2	B	991	THR
2	B	995	VAL
2	B	996	ASP
2	B	1016	ILE
2	B	1046	LEU
2	B	1048	LEU
2	B	1049	ILE
2	B	1051	LYS
2	B	1070	VAL
2	B	1085	VAL
2	B	1095	ILE

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Mol	Chain	Res	Type
2	B	1117	VAL
2	B	1130	ILE
2	B	1157	ILE
2	B	1170	THR
2	B	1189	VAL
2	B	1191	ILE
2	B	1206	LEU
2	B	1207	LEU
2	B	1250	PRO
2	B	1253	VAL
2	B	1256	LEU
2	B	1260	ARG
2	B	1269	THR
2	B	1274	MET
2	B	1291	GLU
2	B	1292	LEU
2	B	1298	LEU
2	B	1300	LEU
2	B	1311	ILE
2	B	1319	LEU
2	B	1320	ARG
2	B	1349	HIS
2	B	1356	LEU
2	B	1357	THR
2	B	1366	THR
2	B	1384	MET
2	B	1407	MET
2	B	1414	ASP
2	B	1421	LEU
2	B	1451	VAL
2	B	1453	HIS
2	B	1462	LYS
2	B	1499	ASP
2	B	1503	ASN
2	B	1504	LYS
2	B	1507	ARG
2	B	1508	ASP
2	B	1511	CYS
2	B	1521	GLN
2	B	1522	LYS
2	B	1525	ASP
2	B	1544	VAL

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Mol	Chain	Res	Type
2	B	1550	VAL
2	B	1610	ASP
2	B	1622	ILE
2	B	1624	LYS
2	B	1628	VAL
2	B	1633	GLU
2	B	1634	GLU
2	B	1637	CYS
1	C	30	THR
1	C	35	ARG
1	C	41	THR
1	C	60	HIS
1	C	67	LEU
1	C	71	SER
1	C	77	THR
1	C	86	VAL
1	C	90	ILE
1	C	94	ARG
1	C	95	GLU
1	C	97	LYS
1	C	106	VAL
1	C	127	SER
1	C	136	LYS
1	C	138	ILE
1	C	146	LEU
1	C	191	LEU
1	C	226	GLU
1	C	229	LEU
1	C	293	ILE
1	C	301	VAL
1	C	302	LEU
1	C	338	MET
1	C	343	ARG
1	C	346	ILE
1	C	365	LYS
1	C	398	GLN
1	C	413	THR
1	C	431	LEU
1	C	441	MET
1	C	457	HIS
1	C	465	LEU
1	C	470	THR

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Mol	Chain	Res	Type
1	C	473	VAL
1	C	501	LEU
1	C	508	ARG
1	C	546	VAL
1	C	547	VAL
1	C	560	VAL
1	C	563	LEU
1	C	581	MET
1	C	594	VAL
1	C	605	LEU
1	C	625	ILE
1	C	659	GLU
2	D	753	GLU
2	D	756	ILE
2	D	762	VAL
2	D	793	ILE
2	D	795	LEU
2	D	796	LYS
2	D	800	THR
2	D	807	VAL
2	D	824	THR
2	D	831	ILE
2	D	862	VAL
2	D	883	GLN
2	D	885	THR
2	D	886	VAL
2	D	904	LYS
2	D	907	LEU
2	D	912	VAL
2	D	936	ILE
2	D	937	ARG
2	D	939	ASN
2	D	946	THR
2	D	995	VAL
2	D	1016	ILE
2	D	1021	THR
2	D	1039	LEU
2	D	1050	LYS
2	D	1078	LEU
2	D	1105	LYS
2	D	1107	LEU
2	D	1109	LEU

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Mol	Chain	Res	Type
2	D	1117	VAL
2	D	1125	ILE
2	D	1144	THR
2	D	1148	LEU
2	D	1149	ILE
2	D	1151	LEU
2	D	1152	GLN
2	D	1153	GLU
2	D	1159	GLU
2	D	1161	GLN
2	D	1189	VAL
2	D	1191	ILE
2	D	1215	LYS
2	D	1244	LYS
2	D	1256	LEU
2	D	1297	SER
2	D	1298	LEU
2	D	1302	SER
2	D	1311	ILE
2	D	1315	SER
2	D	1320	ARG
2	D	1324	THR
2	D	1331	THR
2	D	1341	THR
2	D	1342	LEU
2	D	1356	LEU
2	D	1366	THR
2	D	1395	ASP
2	D	1423	ASN
2	D	1435	ASP
2	D	1440	ASP
2	D	1450	LYS
2	D	1462	LYS
2	D	1472	ILE
2	D	1477	VAL
2	D	1485	LEU
2	D	1487	GLU
2	D	1491	ARG
2	D	1492	PHE
2	D	1506	CYS
2	D	1511	CYS
2	D	1516	GLU

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Mol	Chain	Res	Type
2	D	1528	THR
2	D	1529	LEU
2	D	1548	ARG
2	D	1550	VAL
2	D	1551	LYS
2	D	1552	VAL
2	D	1558	PHE
2	D	1563	MET
2	D	1585	ILE
2	D	1621	ILE
2	D	1624	LYS
2	D	1628	VAL
2	D	1658	VAL
3	E	100	VAL
3	E	102	THR
3	E	104	LEU
3	E	105	ASN
3	E	129	CYS
3	E	143	LEU
3	E	144	THR
3	E	146	LEU
3	E	150	LYS
3	E	156	GLU
3	E	159	LYS
3	E	160	LYS
3	E	163	CYS
3	E	170	ARG
3	E	171	ASN
3	E	174	ILE
3	E	180	ILE
3	E	181	LEU
3	E	185	THR
3	E	186	ILE
3	E	192	THR
3	E	196	LEU
3	E	199	SER
3	E	205	LEU
3	E	206	ILE
3	E	223	ILE
3	E	225	CYS
3	E	231	ILE
3	E	241	ASP

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Mol	Chain	Res	Type
3	E	245	TYR
3	E	246	ARG
3	E	248	SER
3	E	253	CYS
3	E	265	ILE
3	E	283	CYS
3	F	100	VAL
3	F	102	THR
3	F	104	LEU
3	F	106	SER
3	F	113	TYR
3	F	135	ARG
3	F	144	THR
3	F	145	CYS
3	F	146	LEU
3	F	155	VAL
3	F	156	GLU
3	F	157	PHE
3	F	159	LYS
3	F	160	LYS
3	F	163	CYS
3	F	174	ILE
3	F	180	ILE
3	F	185	THR
3	F	188	PHE
3	F	195	LYS
3	F	196	LEU
3	F	206	ILE
3	F	217	LEU
3	F	222	GLU
3	F	225	CYS
3	F	231	ILE
3	F	235	ILE
3	F	246	ARG
3	F	253	CYS
3	F	255	LYS
3	F	265	ILE
3	F	269	VAL
3	F	272	ASP
3	F	283	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	126	GLN
1	A	184	ASN
1	A	200	ASN
1	A	212	ASN
1	A	216	GLN
1	A	354	GLN
1	A	356	HIS
1	A	453	ASN
1	A	580	GLN
1	A	609	ASN
2	B	774	ASN
2	B	842	ASN
2	B	1055	GLN
2	B	1056	GLN
2	B	1136	ASN
2	B	1152	GLN
2	B	1277	GLN
2	B	1339	GLN
2	B	1349	HIS
2	B	1420	GLN
2	B	1453	HIS
2	B	1473	GLN
2	B	1580	GLN
2	B	1642	ASN
1	C	32	ASN
1	C	50	GLN
1	C	60	HIS
1	C	82	HIS
1	C	126	GLN
1	C	185	GLN
1	C	203	GLN
1	C	215	GLN
1	C	354	GLN
1	C	356	HIS
1	C	580	GLN
1	C	589	HIS
1	C	656	GLN
2	D	842	ASN
2	D	908	GLN
2	D	1014	ASN
2	D	1043	GLN
2	D	1152	GLN

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Mol	Chain	Res	Type
2	D	1198	GLN
2	D	1208	ASN
2	D	1259	GLN
2	D	1277	GLN
2	D	1349	HIS
2	D	1464	HIS
2	D	1473	GLN
2	D	1503	ASN
2	D	1517	ASN
2	D	1580	GLN
2	D	1581	GLN
2	D	1643	GLN
3	E	116	GLN
3	E	117	ASN
3	E	237	GLN
3	E	242	HIS
3	E	254	ASN
3	F	173	GLN
3	F	230	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	642/645 (99%)	0.17	11 (1%) 69 54	19, 107, 194, 287	0
1	C	642/645 (99%)	0.25	20 (3%) 51 39	16, 91, 178, 269	0
2	B	902/915 (98%)	0.28	16 (1%) 67 53	21, 143, 235, 308	0
2	D	902/915 (98%)	0.36	43 (4%) 35 31	16, 124, 224, 358	0
3	E	189/194 (97%)	0.30	6 (3%) 50 39	45, 129, 218, 254	0
3	F	189/194 (97%)	0.37	5 (2%) 57 44	38, 139, 231, 279	0
All	All	3466/3508 (98%)	0.28	101 (2%) 53 41	16, 118, 221, 358	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1569	ILE	5.6
1	A	96	PHE	5.0
1	C	460	VAL	4.6
2	D	1477	VAL	4.5
1	C	319	LEU	4.2
2	D	947	LEU	4.1
1	C	255	ILE	4.0
2	D	1309	HIS	3.9
3	E	131	PRO	3.9
2	D	1546	LYS	3.8
3	E	132	GLY	3.8
2	D	982	LEU	3.8
3	F	154	ALA	3.6
1	A	299	GLU	3.6
3	F	157	PHE	3.5
2	B	910	VAL	3.3
1	C	646	PHE	3.3
2	D	1141	MET	3.2
2	D	1346	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	519	LEU	3.0
2	D	1142	ALA	2.9
3	E	101	PRO	2.9
2	D	1365	VAL	2.8
1	C	471	LEU	2.8
2	D	1594	LEU	2.8
2	D	1176	LEU	2.8
1	A	460	VAL	2.8
2	D	1288	ASP	2.7
1	C	531	LEU	2.7
2	B	772	LEU	2.7
3	E	155	VAL	2.6
2	D	1363	LEU	2.5
2	D	1479	VAL	2.5
1	C	557	ASP	2.5
1	C	65	LYS	2.5
2	D	760	ASN	2.5
1	C	514	LEU	2.5
2	B	1418	LEU	2.5
2	D	835	LEU	2.5
2	D	1164	SER	2.5
2	D	1342	LEU	2.5
1	C	54	PRO	2.5
2	D	1354	ASP	2.4
2	D	1620	TYR	2.4
1	A	71	SER	2.4
2	D	1527	VAL	2.4
1	A	396	THR	2.4
2	B	1271	ALA	2.4
2	D	1290	GLN	2.3
3	E	102	THR	2.3
2	D	752	ASP	2.3
3	F	125	VAL	2.3
3	F	138	SER	2.3
3	F	206	ILE	2.3
2	D	1133	LEU	2.3
1	C	96	PHE	2.3
1	A	85	ASN	2.3
1	C	353	TYR	2.3
2	D	1347	MET	2.3
3	E	182	PHE	2.2
2	B	959	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	623	ALA	2.2
2	D	1296	VAL	2.2
1	A	275	ILE	2.2
2	B	804	ILE	2.2
2	B	1298	LEU	2.2
2	D	1596	LEU	2.2
2	D	847	ILE	2.2
2	D	1126	HIS	2.2
2	D	1439	SER	2.2
2	B	1596	LEU	2.2
2	D	989	GLN	2.2
2	B	785	GLY	2.2
2	D	1008	SER	2.2
1	A	501	LEU	2.2
1	C	411	ILE	2.2
1	C	67	LEU	2.1
2	D	839	VAL	2.1
1	C	229	LEU	2.1
2	D	1094	ALA	2.1
2	B	1388	ILE	2.1
2	D	967	LEU	2.1
2	B	1230	VAL	2.1
2	B	1441	ARG	2.1
2	D	1437	ALA	2.1
1	A	273	PHE	2.1
2	B	1505	LEU	2.1
1	C	53	VAL	2.1
1	A	660	LEU	2.1
1	C	513	ASP	2.1
2	D	1316	ALA	2.1
2	D	1438	PHE	2.1
1	C	326	VAL	2.1
2	D	1156	ASP	2.0
2	B	1069	PHE	2.0
2	D	1492	PHE	2.0
1	A	358	THR	2.0
2	B	1395	ASP	2.0
2	D	1101	CYS	2.0
2	D	1545	TYR	2.0
2	B	1008	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.