



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:58 PM UTC

PDB ID : 1CAX / pdb_00001cax
Title : DETERMINATION OF THREE CRYSTAL STRUCTURES OF
CANAVALLIN BY MOLECULAR REPLACEMENT
Authors : Ko, T-P.; Ng, J.D.; Day, J.; Greenwood, A.; McPherson, A.
Deposited on : 1993-06-10
Resolution : 2.60 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

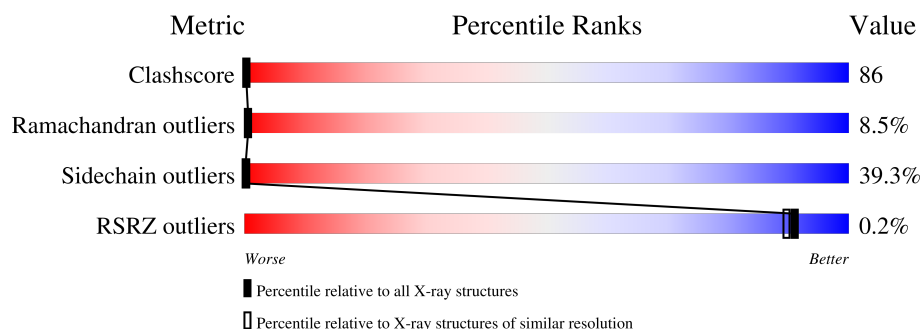
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	181	12% 36% 40% 13%
1	C	181	13% 39% 34% 14%
1	E	181	17% 36% 35% 12%
2	B	184	% 15% 41% 34% 10%
2	D	184	16% 39% 34% 11%
2	F	184	% 15% 38% 30% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8790 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 CANAVALIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1480	946	251	281	2			
1	C	181	Total	C	N	O	S	0	0	0
			1480	946	251	281	2			
1	E	181	Total	C	N	O	S	0	0	0
			1480	946	251	281	2			

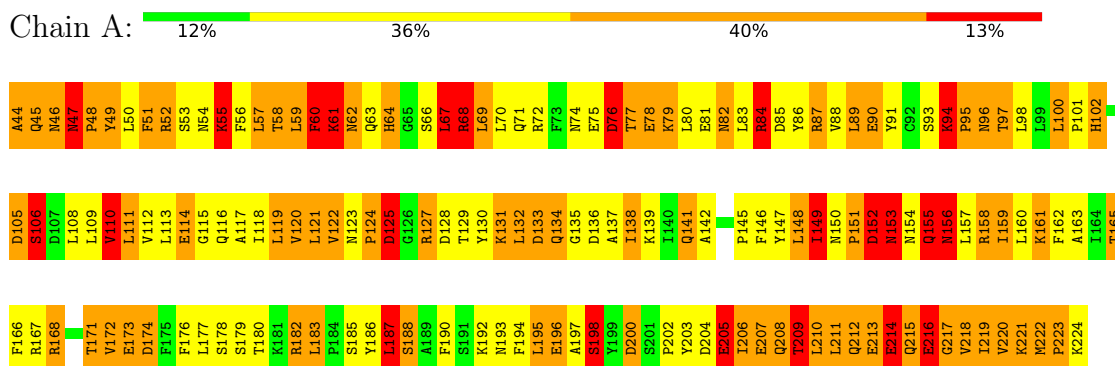
- Molecule 2 is a protein called CANAVALIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1450	902	255	289	4			
2	D	184	Total	C	N	O	S	0	0	0
			1450	902	255	289	4			
2	F	184	Total	C	N	O	S	0	0	0
			1450	902	255	289	4			

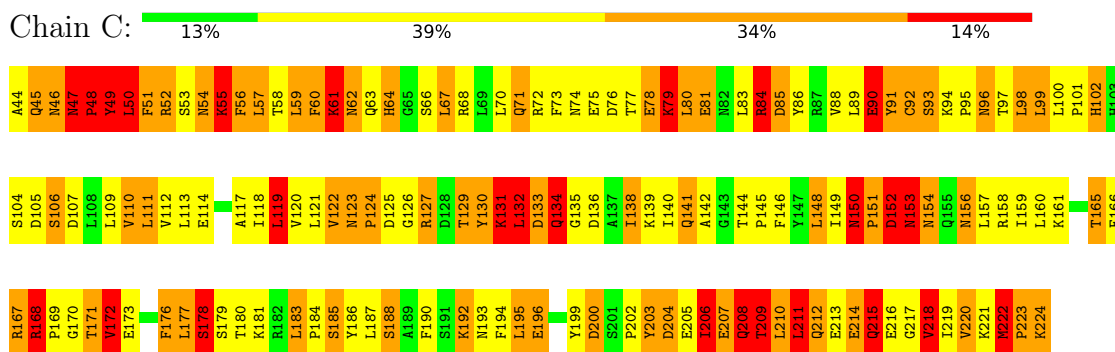
3 Residue-property plots

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.

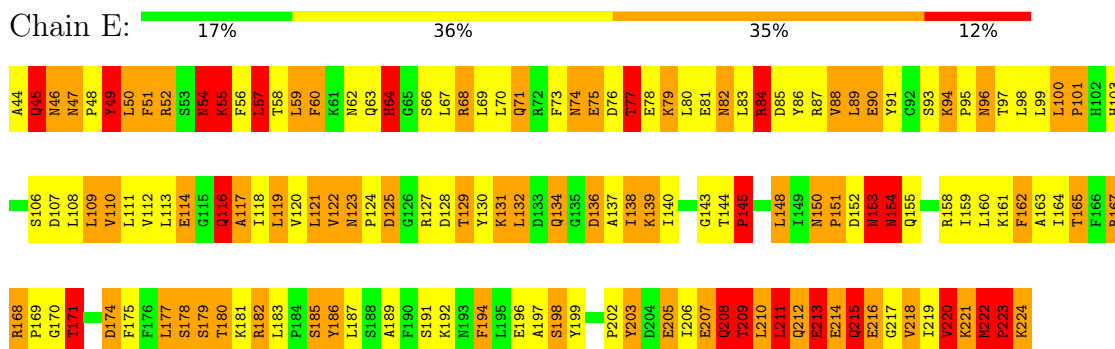
• Molecule 1: CANAVALIN



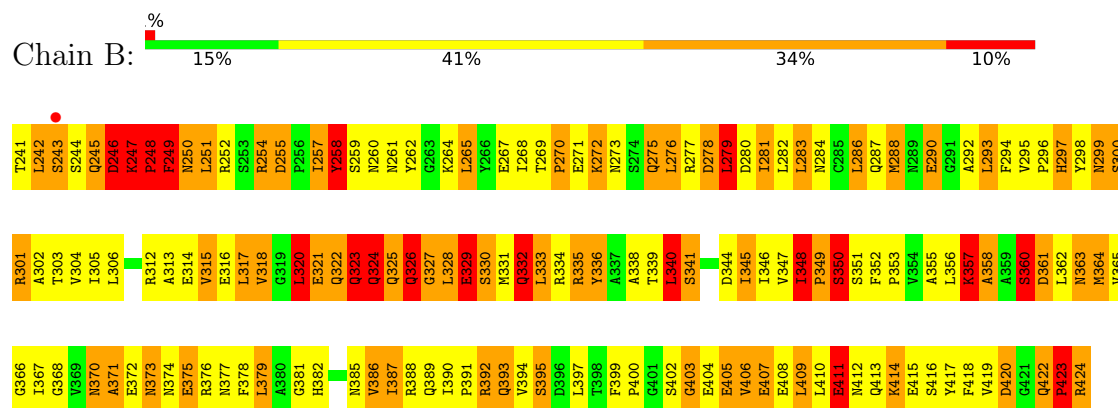
• Molecule 1: CANAVALIN



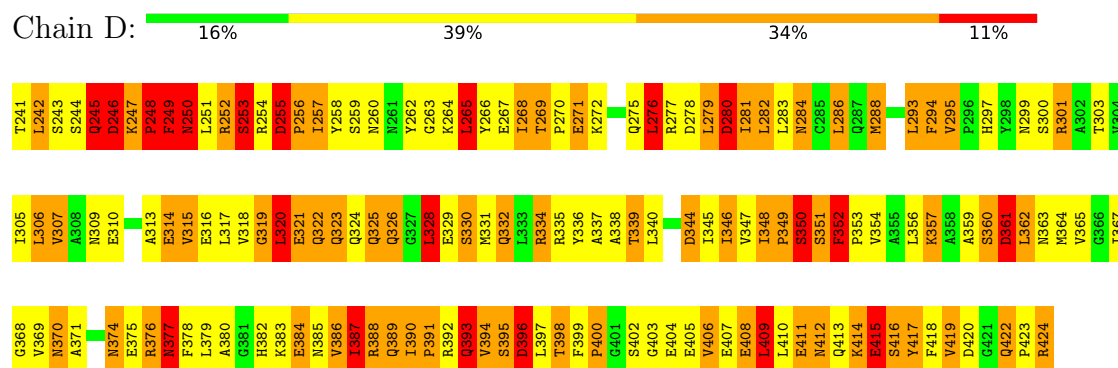
• Molecule 1: CANAVALIN



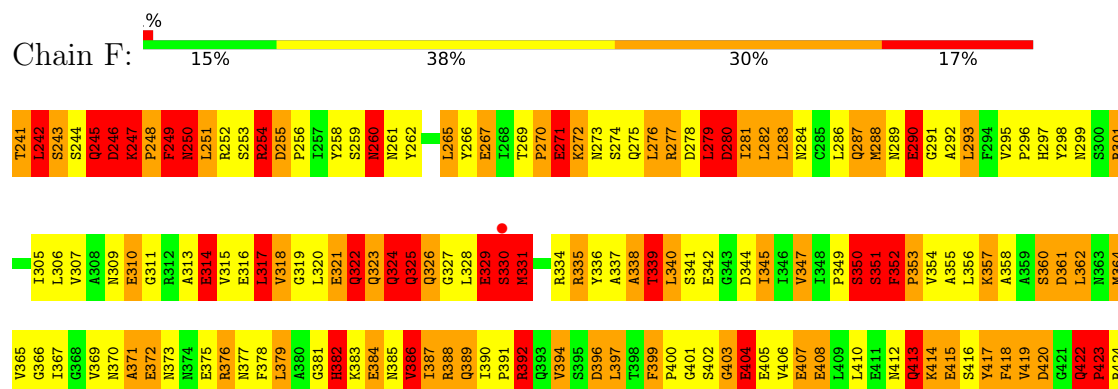
- Molecule 2: CANAVALIN



- Molecule 2: CANAVALIN



- Molecule 2: CANAVALIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	136.50Å 150.30Å 133.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 64.3 (8.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.57Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.175 , (Not available) 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 161.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8790	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.65	14/1511 (0.9%)	2.04	64/2046 (3.1%)
1	C	1.66	16/1511 (1.1%)	2.00	54/2046 (2.6%)
1	E	1.65	19/1511 (1.3%)	2.12	73/2046 (3.6%)
2	B	1.70	16/1472 (1.1%)	2.13	66/1992 (3.3%)
2	D	1.69	17/1472 (1.2%)	2.05	54/1992 (2.7%)
2	F	1.78	20/1472 (1.4%)	2.11	69/1992 (3.5%)
All	All	1.69	102/8949 (1.1%)	2.08	380/12114 (3.1%)

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	3	1
1	C	2	0
1	E	4	0
2	B	0	1
2	D	3	0
2	F	5	0
All	All	17	2

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	254	ARG	CA-C	10.50	1.66	1.52
2	F	248	PRO	N-CA	-9.17	1.36	1.47
2	F	367	ILE	C-N	-8.55	1.28	1.33
1	E	52	ARG	NE-CZ	7.97	1.41	1.33
1	E	75	GLU	N-CA	-7.78	1.38	1.46
2	F	321	GLU	CA-C	7.69	1.60	1.53
2	F	243	SER	N-CA	-7.69	1.35	1.46
2	F	417	TYR	CA-C	-7.21	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	353	PRO	N-CA	-7.14	1.40	1.46
2	D	318	VAL	CA-C	7.09	1.60	1.52
2	D	377	ASN	CA-C	-6.95	1.44	1.52
2	D	253	SER	CA-C	6.77	1.61	1.52
2	B	394	VAL	CA-CB	-6.73	1.46	1.54
2	B	329	GLU	CA-C	6.72	1.61	1.52
2	F	321	GLU	C-N	6.63	1.42	1.33
2	D	320	LEU	N-CA	6.57	1.54	1.46
2	F	420	ASP	N-CA	-6.51	1.38	1.46
2	D	344	ASP	CA-C	-6.48	1.44	1.52
2	F	314	GLU	CA-C	-6.35	1.45	1.52
1	C	210	LEU	N-CA	-6.29	1.38	1.46
2	B	329	GLU	CA-CB	6.26	1.64	1.53
1	C	210	LEU	CA-C	-6.23	1.44	1.52
2	D	322	GLN	N-CA	6.18	1.53	1.46
1	A	47	ASN	CA-C	6.07	1.59	1.52
1	E	107	ASP	CA-C	-6.01	1.45	1.52
1	C	151	PRO	N-CA	-6.00	1.39	1.47
1	C	52	ARG	N-CA	5.98	1.53	1.46
2	D	248	PRO	N-CA	-5.95	1.39	1.47
2	D	350	SER	CA-C	-5.95	1.44	1.52
1	A	198	SER	N-CA	-5.94	1.38	1.46
1	E	114	GLU	CD-OE1	5.92	1.36	1.25
1	E	137	ALA	CA-C	-5.90	1.45	1.52
1	E	167	ARG	CA-C	-5.90	1.45	1.52
1	C	150	ASN	C-N	-5.85	1.26	1.33
2	D	249	PHE	N-CA	-5.84	1.38	1.45
1	A	44	ALA	C-N	5.84	1.41	1.33
2	F	270	PRO	C-N	-5.84	1.25	1.33
2	F	325	GLN	CA-C	-5.83	1.45	1.52
2	B	371	ALA	C-N	-5.76	1.26	1.33
1	C	51	PHE	N-CA	-5.70	1.38	1.45
2	B	394	VAL	CA-C	-5.67	1.46	1.52
1	C	52	ARG	NE-CZ	5.66	1.39	1.33
2	B	375	GLU	CD-OE2	5.64	1.36	1.25
2	B	349	PRO	N-CA	-5.64	1.40	1.47
1	A	121	LEU	CA-C	-5.62	1.46	1.52
1	E	52	ARG	CD-NE	5.62	1.54	1.46
1	E	54	ASN	C-N	5.60	1.41	1.33
1	E	101	PRO	CA-C	-5.58	1.46	1.52
2	B	357	LYS	N-CA	5.57	1.52	1.46
2	D	319	GLY	C-N	5.55	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	295	VAL	N-CA	-5.52	1.41	1.47
1	A	158	ARG	CA-C	-5.52	1.46	1.52
1	E	82	ASN	CA-C	-5.49	1.45	1.52
2	B	293	LEU	CA-C	-5.49	1.46	1.53
1	E	138	ILE	CA-C	-5.49	1.47	1.52
1	C	54	ASN	N-CA	5.46	1.53	1.46
1	A	67	LEU	C-N	-5.44	1.25	1.33
2	B	286	LEU	CA-C	-5.43	1.46	1.52
2	F	243	SER	C-O	-5.42	1.17	1.24
1	C	104	SER	CA-C	-5.39	1.46	1.52
1	C	171	THR	N-CA	-5.37	1.39	1.46
1	C	144	THR	N-CA	5.35	1.52	1.46
1	A	214	GLU	N-CA	-5.34	1.40	1.46
2	D	265	LEU	CA-C	-5.34	1.46	1.52
1	A	173	GLU	CA-C	-5.33	1.46	1.52
1	E	169	PRO	N-CA	-5.29	1.41	1.47
2	B	280	ASP	CG-OD1	5.28	1.35	1.25
2	F	321	GLU	CD-OE2	5.28	1.35	1.25
1	C	55	LYS	CA-CB	-5.25	1.46	1.53
1	C	106	SER	CA-C	-5.23	1.46	1.52
1	C	172	VAL	CA-CB	-5.22	1.47	1.54
2	D	259	SER	C-N	5.22	1.38	1.33
2	B	360	SER	C-O	-5.21	1.18	1.23
2	D	252	ARG	NE-CZ	5.19	1.38	1.33
1	C	53	SER	CA-CB	5.19	1.60	1.52
2	D	244	SER	N-CA	-5.18	1.40	1.46
1	A	133	ASP	CA-C	-5.17	1.46	1.53
1	A	209	THR	CA-C	5.16	1.59	1.52
1	E	211	LEU	CA-CB	5.16	1.61	1.53
1	A	166	PHE	CA-C	5.16	1.57	1.52
1	A	67	LEU	CA-C	-5.12	1.46	1.52
1	E	171	THR	N-CA	-5.12	1.39	1.46
2	B	420	ASP	CG-OD1	5.12	1.35	1.25
2	D	314	GLU	CD-OE2	5.10	1.35	1.25
1	E	145	PRO	N-CA	-5.09	1.41	1.46
1	E	90	GLU	CD-OE1	5.08	1.35	1.25
2	F	245	GLN	CA-C	5.08	1.59	1.52
1	A	47	ASN	CA-CB	5.07	1.60	1.53
2	B	321	GLU	CA-C	-5.07	1.48	1.52
2	B	249	PHE	N-CA	-5.06	1.39	1.46
2	F	253	SER	C-N	5.06	1.40	1.33
1	E	107	ASP	CG-OD1	5.04	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	386	VAL	CA-C	5.03	1.59	1.52
2	F	251	LEU	CA-CB	5.03	1.61	1.53
2	F	375	GLU	C-N	-5.03	1.26	1.33
2	B	290	GLU	CD-OE1	5.02	1.34	1.25
1	C	90	GLU	CD-OE2	5.02	1.34	1.25
2	F	325	GLN	N-CA	-5.01	1.39	1.46
2	D	420	ASP	N-CA	-5.01	1.40	1.46
1	E	162	PHE	N-CA	5.01	1.53	1.46
1	A	68	ARG	CA-C	-5.00	1.46	1.52
1	E	109	LEU	CA-C	5.00	1.58	1.52

All (380) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	222	MET	CA-C-N	17.22	141.37	119.84
1	E	222	MET	C-N-CA	17.22	141.37	119.84
1	C	131	LYS	CA-C-N	-12.19	104.05	122.09
1	C	131	LYS	C-N-CA	-12.19	104.05	122.09
1	E	222	MET	C-N-CD	-12.07	75.50	125.00
1	A	206	ILE	N-CA-C	-11.82	99.31	110.42
2	F	322	GLN	N-CA-C	11.68	125.39	110.33
1	E	222	MET	O-C-N	11.22	130.22	121.47
1	A	223	PRO	N-CA-C	-10.72	96.53	114.75
2	F	249	PHE	N-CA-CB	10.70	128.44	111.43
1	A	55	LYS	N-CA-C	10.47	125.27	108.41
1	E	208	GLN	CA-C-N	10.39	141.38	121.54
1	E	208	GLN	C-N-CA	10.39	141.38	121.54
1	C	199	TYR	N-CA-C	10.37	122.58	111.28
2	B	320	LEU	CA-C-N	-10.03	107.52	122.56
2	B	320	LEU	C-N-CA	-10.03	107.52	122.56
1	E	212	GLN	CA-C-N	9.92	137.15	122.87
1	E	212	GLN	C-N-CA	9.92	137.15	122.87
2	B	246	ASP	N-CA-C	9.84	126.04	108.24
2	B	416	SER	N-CA-C	9.64	125.71	111.34
2	F	392	ARG	N-CA-C	9.62	122.96	111.33
2	B	320	LEU	N-CA-C	-9.58	94.53	109.76
1	A	84	ARG	N-CA-C	9.54	122.88	111.33
1	C	79	LYS	N-CA-C	9.51	121.65	111.28
2	F	278	ASP	CA-CB-CG	9.51	122.11	112.60
1	E	50	LEU	N-CA-C	9.48	125.89	109.96
2	D	321	GLU	N-CA-C	9.44	125.67	111.04
2	D	416	SER	N-CA-C	9.42	125.60	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	223	PRO	CA-N-CD	-9.36	98.89	112.00
2	B	248	PRO	N-CA-C	-9.07	93.80	112.47
1	C	55	LYS	N-CA-C	9.05	122.98	108.41
1	E	84	ARG	N-CA-C	9.02	122.09	111.71
2	D	246	ASP	N-CA-C	9.00	129.96	110.80
1	A	155	GLN	N-CA-CB	8.91	123.52	110.06
2	B	321	GLU	N-CA-C	8.89	124.31	112.13
2	B	362	LEU	N-CA-C	8.86	123.34	108.90
2	F	249	PHE	CA-CB-CG	8.85	122.65	113.80
1	A	213	GLU	N-CA-CB	8.67	125.80	110.80
2	B	245	GLN	N-CA-CB	-8.57	96.00	110.65
1	C	85	ASP	CA-CB-CG	8.51	121.11	112.60
2	B	324	GLN	CA-C-N	8.40	134.97	122.87
2	B	324	GLN	C-N-CA	8.40	134.97	122.87
2	F	250	ASN	CA-CB-CG	-8.40	104.20	112.60
1	A	64	HIS	CA-CB-CG	-8.35	105.45	113.80
2	F	243	SER	N-CA-C	-8.33	102.90	113.23
2	F	422	GLN	CB-CA-C	8.21	122.06	109.50
1	C	48	PRO	CA-C-N	8.13	137.07	121.54
1	C	48	PRO	C-N-CA	8.13	137.07	121.54
2	B	245	GLN	N-CA-C	8.12	124.57	113.21
1	C	58	THR	N-CA-C	8.04	123.05	108.17
1	E	46	ASN	N-CA-C	8.03	121.59	107.61
2	F	365	VAL	CA-C-N	-8.04	116.64	122.18
2	F	365	VAL	C-N-CA	-8.04	116.64	122.18
2	B	279	LEU	N-CA-C	-8.02	104.38	114.56
1	C	151	PRO	CA-C-N	8.01	136.84	121.54
1	C	151	PRO	C-N-CA	8.01	136.84	121.54
2	D	249	PHE	N-CA-C	-7.99	96.93	109.72
2	B	247	LYS	CA-C-N	7.97	129.81	119.84
2	B	247	LYS	C-N-CA	7.97	129.81	119.84
2	D	320	LEU	CA-C-N	7.91	132.75	120.89
2	D	320	LEU	C-N-CA	7.91	132.75	120.89
2	B	304	VAL	N-CA-C	7.89	119.27	107.51
1	A	94	LYS	C-N-CD	-7.84	92.83	125.00
1	A	97	THR	N-CA-C	7.83	120.97	109.07
2	F	422	GLN	N-CA-CB	7.74	122.88	109.57
2	D	315	VAL	N-CA-C	7.71	118.91	108.11
1	E	116	GLN	CA-C-N	-7.71	109.84	122.11
1	E	116	GLN	C-N-CA	-7.71	109.84	122.11
2	F	317	LEU	N-CA-CB	7.71	122.92	110.51
1	C	152	ASP	N-CA-C	7.70	127.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	248	PRO	N-CA-CB	7.69	111.32	103.25
1	C	208	GLN	N-CA-CB	7.66	122.15	110.28
2	D	279	LEU	N-CA-C	-7.63	104.10	113.41
2	D	391	PRO	N-CA-C	7.62	123.15	111.34
2	F	362	LEU	N-CA-C	7.61	121.95	109.24
1	C	47	ASN	CA-C-N	7.59	129.33	119.84
1	C	47	ASN	C-N-CA	7.59	129.33	119.84
1	E	209	THR	CA-CB-OG1	7.58	120.97	109.60
2	F	317	LEU	N-CA-C	-7.57	98.74	110.17
2	D	412	ASN	N-CA-C	7.48	122.07	112.34
2	D	295	VAL	CB-CA-C	7.47	118.20	110.88
1	C	178	SER	N-CA-C	7.41	122.41	109.96
2	D	393	GLN	N-CA-CB	7.35	121.78	110.46
1	C	56	PHE	CA-CB-CG	7.33	121.13	113.80
2	F	338	ALA	N-CA-C	7.33	117.68	108.45
2	F	278	ASP	CA-C-N	7.32	133.13	120.68
2	F	278	ASP	C-N-CA	7.32	133.13	120.68
2	D	322	GLN	N-CA-C	7.29	121.35	109.76
1	E	179	SER	N-CA-CB	7.28	121.05	110.06
2	D	280	ASP	N-CA-CB	7.28	124.13	111.40
1	C	60	PHE	CA-CB-CG	7.19	120.99	113.80
1	E	50	LEU	N-CA-CB	7.13	121.78	110.23
1	E	220	VAL	N-CA-CB	-7.12	103.42	112.60
2	B	340	LEU	N-CA-CB	7.10	120.39	110.17
1	A	196	GLU	N-CA-C	7.08	119.66	111.02
1	A	94	LYS	CA-C-N	7.05	128.66	119.84
1	A	94	LYS	C-N-CA	7.05	128.66	119.84
1	E	199	TYR	N-CA-C	7.05	118.61	111.07
1	E	211	LEU	N-CA-C	7.04	121.31	109.76
2	F	242	LEU	N-CA-CB	7.03	122.37	110.49
2	B	423	PRO	N-CA-CB	7.01	110.61	103.25
2	B	415	GLU	N-CA-C	6.99	120.69	109.86
2	D	245	GLN	CA-C-N	6.98	134.88	121.54
2	D	245	GLN	C-N-CA	6.98	134.88	121.54
1	C	78	GLU	CA-C-N	6.98	129.63	120.28
1	C	78	GLU	C-N-CA	6.98	129.63	120.28
2	F	319	GLY	CA-C-N	6.95	131.07	121.33
2	F	319	GLY	C-N-CA	6.95	131.07	121.33
2	B	407	GLU	CA-C-N	6.94	130.44	120.79
2	B	407	GLU	C-N-CA	6.94	130.44	120.79
2	D	391	PRO	N-CA-CB	6.93	109.91	103.39
1	E	170	GLY	N-CA-C	-6.92	105.77	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	350	SER	CA-C-N	-6.92	111.17	122.65
2	F	350	SER	C-N-CA	-6.92	111.17	122.65
2	F	321	GLU	N-CA-C	6.91	123.97	110.56
1	E	64	HIS	CA-CB-CG	6.90	120.70	113.80
2	B	382	HIS	CA-CB-CG	-6.87	106.93	113.80
2	B	244	SER	CB-CA-C	6.84	120.52	110.26
1	C	58	THR	N-CA-CB	6.80	120.12	110.46
1	A	211	LEU	CB-CA-C	6.79	121.19	110.19
1	C	131	LYS	O-C-N	-6.79	114.18	123.01
1	A	196	GLU	N-CA-CB	6.77	120.11	109.82
1	A	50	LEU	N-CA-C	6.76	120.84	109.76
2	B	258	TYR	N-CA-CB	6.72	121.72	110.77
1	A	51	PHE	N-CA-C	-6.71	105.07	112.72
2	F	351	SER	N-CA-C	6.69	120.43	112.93
2	B	330	SER	CA-C-N	6.69	132.43	123.00
2	B	330	SER	C-N-CA	6.69	132.43	123.00
2	D	351	SER	N-CA-CB	6.67	119.77	110.90
2	D	282	LEU	N-CA-CB	6.64	121.39	110.69
1	A	58	THR	N-CA-CB	6.63	119.84	109.83
2	B	345	ILE	N-CA-C	6.62	118.02	108.48
2	B	361	ASP	N-CA-CB	6.62	121.68	110.49
1	E	213	GLU	N-CA-C	-6.61	100.48	109.54
2	B	358	ALA	N-CA-C	6.59	119.59	107.73
1	A	215	GLN	N-CA-C	-6.58	103.72	111.03
2	D	399	PHE	N-CA-C	6.58	120.08	110.14
2	F	249	PHE	CA-C-N	-6.57	112.03	121.42
2	F	249	PHE	C-N-CA	-6.57	112.03	121.42
1	E	77	THR	N-CA-C	6.56	120.39	109.95
2	D	406	VAL	CB-CA-C	-6.49	103.58	111.88
1	A	153	ASN	CA-CB-CG	6.47	119.07	112.60
1	E	122	VAL	CB-CA-C	-6.46	102.67	111.33
1	E	51	PHE	CA-CB-CG	-6.41	107.39	113.80
2	D	244	SER	CA-C-N	6.38	130.47	120.89
2	D	244	SER	C-N-CA	6.38	130.47	120.89
2	B	361	ASP	CA-CB-CG	-6.38	106.22	112.60
1	E	117	ALA	N-CA-C	6.37	117.53	108.74
1	A	59	LEU	N-CA-C	-6.36	105.83	113.97
1	A	81	GLU	N-CA-C	6.35	119.88	111.75
2	F	318	VAL	CA-C-N	-6.34	113.91	122.03
2	F	318	VAL	C-N-CA	-6.34	113.91	122.03
1	E	212	GLN	CB-CA-C	-6.30	103.22	113.37
2	D	321	GLU	CA-C-N	6.30	130.51	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	321	GLU	C-N-CA	6.30	130.51	121.50
1	E	112	VAL	N-CA-C	6.27	117.12	108.84
1	A	76	ASP	N-CA-CB	-6.25	99.93	110.49
1	C	102	HIS	CA-CB-CG	-6.23	107.57	113.80
1	E	55	LYS	N-CA-C	6.21	118.90	108.02
1	E	212	GLN	O-C-N	6.21	129.68	122.84
1	A	58	THR	CB-CA-C	6.20	120.01	109.72
1	C	218	VAL	N-CA-C	6.19	122.39	113.16
2	F	418	PHE	CA-CB-CG	-6.19	107.61	113.80
2	F	415	GLU	N-CA-C	6.18	118.84	109.63
1	C	204	ASP	CB-CA-C	6.17	122.04	110.63
1	A	116	GLN	CB-CA-C	6.15	123.04	109.94
1	E	209	THR	CA-CB-CG2	6.15	120.96	110.50
1	E	151	PRO	N-CA-C	6.14	119.82	111.22
1	E	153	ASN	N-CA-C	6.14	119.54	109.72
2	F	322	GLN	N-CA-CB	6.13	118.62	110.29
2	F	325	GLN	N-CA-C	-6.12	97.76	110.80
1	A	115	GLY	N-CA-C	6.12	119.53	110.60
2	B	332	GLN	CB-CG-CD	6.11	122.99	112.60
1	E	124	PRO	N-CA-CB	6.11	109.15	103.41
1	A	124	PRO	CB-CA-C	-6.09	102.29	110.88
1	C	165	THR	N-CA-C	6.09	120.19	109.96
1	A	131	LYS	N-CA-CB	6.07	120.17	110.16
1	E	68	ARG	N-CA-C	6.05	118.76	108.90
1	E	179	SER	CB-CA-C	6.04	119.73	109.53
1	A	100	LEU	CA-C-N	6.02	126.37	119.93
1	A	100	LEU	C-N-CA	6.02	126.37	119.93
1	A	200	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	47	ASN	CA-CB-CG	6.00	118.60	112.60
1	C	67	LEU	CB-CA-C	5.99	118.61	110.94
1	E	124	PRO	N-CA-C	-5.99	106.67	114.03
2	D	319	GLY	CA-C-N	5.98	132.96	121.54
2	D	319	GLY	C-N-CA	5.98	132.96	121.54
2	D	350	SER	CA-C-N	-5.97	112.87	122.24
2	D	350	SER	C-N-CA	-5.97	112.87	122.24
1	E	151	PRO	CA-C-N	5.96	132.92	121.54
1	E	151	PRO	C-N-CA	5.96	132.92	121.54
2	B	270	PRO	CA-C-N	5.96	130.13	120.60
2	B	270	PRO	C-N-CA	5.96	130.13	120.60
2	B	411	GLU	N-CA-CB	5.93	119.17	110.57
1	C	51	PHE	N-CA-C	-5.93	106.02	113.72
1	E	211	LEU	CB-CA-C	5.93	119.44	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	SER	CA-C-N	-5.92	112.37	122.56
2	B	350	SER	C-N-CA	-5.92	112.37	122.56
1	A	153	ASN	N-CA-CB	5.91	120.48	110.49
2	F	352	PHE	CA-C-N	-5.90	114.48	120.85
2	F	352	PHE	C-N-CA	-5.90	114.48	120.85
1	A	155	GLN	N-CA-C	5.88	119.50	110.20
2	D	284	ASN	N-CA-C	5.88	118.23	108.99
2	F	392	ARG	N-CA-CB	5.88	118.87	110.06
1	E	136	ASP	CA-CB-CG	-5.88	106.72	112.60
2	B	245	GLN	CB-CA-C	-5.87	97.49	110.99
1	E	178	SER	N-CA-C	5.87	119.17	110.48
2	B	329	GLU	CA-C-N	5.85	130.78	121.18
2	B	329	GLU	C-N-CA	5.85	130.78	121.18
2	B	361	ASP	CB-CA-C	5.84	122.04	110.42
2	D	256	PRO	CB-CA-C	-5.83	101.94	111.56
2	F	331	MET	N-CA-CB	5.83	120.35	110.49
1	C	153	ASN	N-CA-C	5.83	123.21	110.80
1	C	132	LEU	N-CA-CB	5.82	119.66	110.23
2	F	375	GLU	CA-C-N	-5.80	114.83	123.00
2	F	375	GLU	C-N-CA	-5.80	114.83	123.00
1	A	120	VAL	N-CA-CB	5.79	117.94	110.99
1	E	47	ASN	C-N-CD	-5.79	101.27	125.00
1	A	96	ASN	CA-C-O	-5.78	114.82	122.44
1	E	169	PRO	N-CA-C	5.77	119.56	110.50
2	B	405	GLU	N-CA-CB	-5.76	99.80	110.18
1	A	119	LEU	CA-C-N	-5.75	115.68	122.93
1	A	119	LEU	C-N-CA	-5.75	115.68	122.93
1	C	63	GLN	N-CA-CB	5.75	119.74	110.42
2	B	323	GLN	O-C-N	5.74	129.79	122.33
2	F	382	HIS	CA-C-N	5.73	129.94	120.94
2	F	382	HIS	C-N-CA	5.73	129.94	120.94
2	D	400	PRO	N-CA-C	-5.72	102.21	111.14
1	E	153	ASN	CA-C-N	5.72	132.46	121.54
1	E	153	ASN	C-N-CA	5.72	132.46	121.54
2	F	339	THR	CA-C-N	-5.70	114.15	122.65
2	F	339	THR	C-N-CA	-5.70	114.15	122.65
1	A	49	TYR	CA-C-N	-5.69	114.17	122.65
1	A	49	TYR	C-N-CA	-5.69	114.17	122.65
1	A	84	ARG	N-CA-CB	5.68	118.58	110.06
1	A	57	LEU	CA-C-N	-5.68	112.65	120.71
1	A	57	LEU	C-N-CA	-5.68	112.65	120.71
2	D	348	ILE	CA-C-N	5.67	125.60	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	348	ILE	C-N-CA	5.67	125.60	119.76
1	A	149	ILE	CB-CA-C	-5.66	103.46	111.21
2	D	276	LEU	CA-C-N	5.64	128.63	120.79
2	D	276	LEU	C-N-CA	5.64	128.63	120.79
2	F	311	GLY	N-CA-C	5.64	118.11	111.63
1	A	102	HIS	CA-CB-CG	-5.63	108.17	113.80
2	B	363	ASN	CA-CB-CG	-5.63	106.97	112.60
1	A	188	SER	CA-C-N	-5.63	110.68	121.94
1	A	188	SER	C-N-CA	-5.63	110.68	121.94
2	B	325	GLN	N-CA-C	-5.61	101.85	109.54
1	C	208	GLN	N-CA-C	5.61	118.33	111.82
1	C	54	ASN	N-CA-C	5.61	120.12	113.28
2	F	279	LEU	N-CA-C	5.60	119.28	112.23
1	A	76	ASP	CB-CA-C	-5.59	99.30	110.42
1	A	63	GLN	N-CA-CB	5.59	119.93	110.49
1	A	223	PRO	CA-C-O	5.58	126.60	118.78
1	C	209	THR	CA-C-O	5.58	127.93	121.34
2	D	352	PHE	CA-C-N	5.57	125.33	119.76
2	D	352	PHE	C-N-CA	5.57	125.33	119.76
1	C	122	VAL	N-CA-C	5.57	116.75	108.23
2	B	363	ASN	N-CA-CB	5.56	119.49	110.77
1	E	205	GLU	CA-C-N	5.55	127.55	120.56
1	E	205	GLU	C-N-CA	5.55	127.55	120.56
2	F	314	GLU	N-CA-C	-5.54	100.26	109.46
1	C	96	ASN	N-CA-C	5.54	118.98	111.17
2	D	350	SER	N-CA-CB	5.53	119.84	110.49
1	E	57	LEU	CB-CA-C	-5.52	102.18	110.24
2	F	314	GLU	CA-C-O	-5.52	114.30	120.54
2	F	422	GLN	C-N-CD	-5.52	102.38	125.00
2	F	423	PRO	N-CA-CB	5.51	109.04	103.25
2	F	376	ARG	CB-CA-C	5.51	119.30	110.16
1	A	60	PHE	CA-CB-CG	-5.50	108.30	113.80
1	C	124	PRO	N-CA-C	5.50	121.08	113.98
2	B	247	LYS	O-C-N	5.49	127.63	121.32
2	D	408	GLU	CB-CA-C	5.49	118.62	109.56
1	E	220	VAL	CB-CA-C	-5.49	103.67	111.19
1	C	171	THR	CB-CA-C	5.48	118.45	109.90
2	F	280	ASP	CA-CB-CG	-5.47	107.13	112.60
1	E	203	TYR	CB-CA-C	5.46	121.28	110.42
1	C	46	ASN	N-CA-C	5.45	118.65	107.37
2	B	247	LYS	C-N-CD	-5.43	102.75	125.00
1	C	151	PRO	O-C-N	5.43	129.48	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	PHE	N-CA-C	5.43	119.08	109.96
1	E	123	ASN	CA-C-N	-5.42	114.23	119.87
1	E	123	ASN	C-N-CA	-5.42	114.23	119.87
2	B	254	ARG	N-CA-C	5.42	118.57	107.69
1	E	59	LEU	N-CA-C	-5.41	106.81	113.41
2	F	324	GLN	N-CA-C	-5.41	104.14	111.55
1	C	50	LEU	N-CA-C	5.40	122.31	110.80
1	A	105	ASP	N-CA-CB	-5.39	101.37	110.49
2	F	242	LEU	N-CA-C	5.39	122.28	110.80
1	E	205	GLU	N-CA-C	-5.37	105.08	111.69
2	F	373	ASN	CA-CB-CG	-5.36	107.24	112.60
1	C	84	ARG	N-CA-C	5.36	118.29	111.69
2	B	318	VAL	N-CA-C	5.36	116.30	108.53
1	C	119	LEU	CA-C-N	-5.35	115.25	122.91
1	C	119	LEU	C-N-CA	-5.35	115.25	122.91
2	B	335	ARG	N-CA-CB	5.35	119.66	110.68
1	E	169	PRO	CB-CA-C	5.35	117.39	111.56
1	E	208	GLN	O-C-N	5.33	129.22	122.28
2	F	271	GLU	N-CA-C	-5.33	106.28	112.89
1	A	151	PRO	N-CA-CB	5.33	108.30	103.34
1	C	171	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	198	SER	CB-CA-C	5.33	120.49	110.63
2	D	415	GLU	N-CA-C	5.33	117.28	109.24
1	E	52	ARG	CD-NE-CZ	5.32	131.85	124.40
1	C	134	GLN	N-CA-CB	5.31	119.47	110.49
2	D	284	ASN	CA-CB-CG	5.31	117.91	112.60
2	D	349	PRO	N-CA-CB	5.31	108.03	103.31
2	B	260	ASN	CA-CB-CG	5.29	117.89	112.60
1	C	196	GLU	N-CA-C	-5.29	104.41	111.24
2	B	357	LYS	CA-C-N	-5.28	115.09	123.12
2	B	357	LYS	C-N-CA	-5.28	115.09	123.12
1	E	68	ARG	CA-C-N	5.28	130.52	122.65
1	E	68	ARG	C-N-CA	5.28	130.52	122.65
2	F	253	SER	CA-C-N	5.28	131.63	121.54
2	F	253	SER	C-N-CA	5.28	131.63	121.54
1	E	150	ASN	CA-C-N	5.28	125.28	120.21
1	E	150	ASN	C-N-CA	5.28	125.28	120.21
2	D	250	ASN	N-CA-C	5.26	122.01	110.80
2	F	251	LEU	N-CA-CB	5.26	118.83	110.57
2	F	371	ALA	CA-C-N	-5.26	113.58	120.95
2	F	371	ALA	C-N-CA	-5.26	113.58	120.95
2	D	361	ASP	CA-CB-CG	-5.25	107.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	254	ARG	N-CA-C	5.24	121.95	110.80
2	F	399	PHE	CA-CB-CG	-5.23	108.57	113.80
2	D	280	ASP	CB-CA-C	5.22	121.91	112.30
1	E	77	THR	N-CA-CB	-5.22	102.50	110.85
2	B	332	GLN	CB-CA-C	-5.22	101.19	109.80
1	E	209	THR	N-CA-C	-5.22	99.69	110.80
2	F	404	GLU	N-CA-CB	5.21	118.02	110.26
1	A	61	LYS	N-CA-CB	5.21	120.42	111.00
1	C	134	GLN	N-CA-C	5.20	121.88	110.80
1	E	106	SER	N-CA-C	5.20	117.31	109.41
2	B	260	ASN	N-CA-C	-5.20	101.37	108.38
2	D	391	PRO	CB-CA-C	5.19	117.81	111.12
1	E	203	TYR	N-CA-CB	5.18	119.25	110.49
2	F	361	ASP	N-CA-C	-5.18	102.19	109.96
1	A	78	GLU	N-CA-C	-5.17	107.64	114.31
2	B	340	LEU	CB-CA-C	5.17	119.05	109.54
2	D	269	THR	CB-CA-C	-5.16	101.37	109.22
2	F	413	GLN	N-CA-C	5.16	117.11	108.23
1	A	212	GLN	CB-CA-C	-5.15	103.23	114.10
1	E	194	PHE	CA-CB-CG	5.15	118.95	113.80
2	F	242	LEU	CA-C-O	5.14	127.87	120.51
1	A	96	ASN	CB-CA-C	-5.14	103.27	112.27
1	C	200	ASP	CA-C-N	5.14	130.48	122.26
1	C	200	ASP	C-N-CA	5.14	130.48	122.26
2	D	249	PHE	CB-CA-C	5.14	119.45	109.33
1	A	212	GLN	N-CA-CB	-5.14	102.23	110.55
2	B	370	ASN	CA-C-N	5.14	127.88	120.38
2	B	370	ASN	C-N-CA	5.14	127.88	120.38
2	F	290	GLU	CB-CA-C	5.14	117.91	109.90
2	D	255	ASP	CA-C-N	5.13	126.25	119.84
2	D	255	ASP	C-N-CA	5.13	126.25	119.84
1	E	46	ASN	N-CA-CB	5.13	118.56	110.71
1	A	209	THR	CA-C-O	5.13	124.36	119.08
1	E	209	THR	N-CA-CB	5.12	119.14	110.49
1	C	167	ARG	N-CA-CB	5.12	119.14	110.49
2	F	416	SER	N-CA-C	5.12	121.70	110.80
2	D	326	GLN	N-CA-CB	5.12	118.97	110.63
2	B	348	ILE	CA-C-N	5.11	126.22	119.84
2	B	348	ILE	C-N-CA	5.11	126.22	119.84
1	C	133	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	47	ASN	N-CA-C	5.07	121.02	109.81
2	F	331	MET	CB-CA-C	5.07	120.51	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	351	SER	CB-CA-C	5.06	117.53	109.02
2	B	357	LYS	N-CA-C	5.06	118.06	109.76
1	A	110	VAL	N-CA-C	5.06	115.25	108.17
2	B	245	GLN	CA-C-N	-5.06	115.28	122.41
2	B	245	GLN	C-N-CA	-5.06	115.28	122.41
2	D	362	LEU	N-CA-C	5.05	117.97	110.14
1	A	223	PRO	CA-C-N	5.05	130.79	121.70
1	A	223	PRO	C-N-CA	5.05	130.79	121.70
2	B	329	GLU	CB-CG-CD	5.03	121.16	112.60
1	A	106	SER	N-CA-C	5.03	118.16	110.36
1	A	153	ASN	O-C-N	5.03	129.28	122.59
1	E	90	GLU	N-CA-CB	-5.03	102.36	110.81
1	E	181	LYS	N-CA-C	-5.02	107.43	113.21
2	F	329	GLU	N-CA-C	5.01	121.48	110.80
2	B	290	GLU	N-CA-CB	5.00	118.95	110.49
1	E	154	ASN	CA-CB-CG	-5.00	107.59	112.60

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	55	LYS	CA
1	A	155	GLN	CA
1	A	196	GLU	CA
1	C	58	THR	CA
1	C	208	GLN	CA
2	D	280	ASP	CA
2	D	393	GLN	CA
2	D	412	ASN	CA
1	E	50	LEU	CA
1	E	203	TYR	CA
1	E	209	THR	CB
1	E	211	LEU	CA
2	F	242	LEU	CA
2	F	322	GLN	CA
2	F	329	GLU	CA
2	F	392	ARG	CA
2	F	422	GLN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	SER	Mainchain

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Mol	Chain	Res	Type	Group
2	B	329	GLU	Sidechain

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	1480	0	1473	281	0
1	C	1480	0	1473	298	0
1	E	1480	0	1473	286	0
2	B	1450	0	1425	282	1
2	D	1450	0	1425	301	0
2	F	1450	0	1425	300	1
All	All	8790	0	8694	1509	1

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 86.

All (1509) 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)
2:D:402:SER:HB3	2:D:405:GLU:HB2	1.23	1.20
2:F:404:GLU:HA	2:F:407:GLU:HB2	1.23	1.20
1:E:222:MET:CG	1:E:223:PRO:HD3	1.71	1.19
1:A:168:ARG:HE	2:D:322:GLN:HA	1.08	1.18
1:E:222:MET:HG3	1:E:223:PRO:CD	1.75	1.14
1:E:168:ARG:HG3	1:E:168:ARG:HH11	1.14	1.12
1:A:210:LEU:HD12	1:A:211:LEU:N	1.63	1.11
2:D:340:LEU:HD13	2:D:344:ASP:HB2	1.28	1.11
1:C:48:PRO:HB2	1:C:50:LEU:HD23	1.28	1.10
1:E:77:THR:HG23	1:E:79:LYS:HG3	1.36	1.07
2:F:277:ARG:HG3	2:F:277:ARG:HH11	1.15	1.07
1:A:222:MET:HB3	1:A:223:PRO:HD2	1.31	1.07
2:B:295:VAL:HG13	2:B:296:PRO:HD2	1.34	1.07
2:D:383:LYS:HD2	2:D:384:GLU:H	1.13	1.06
1:C:47:ASN:H	1:C:76:ASP:HB3	1.20	1.05
2:F:245:GLN:HE21	2:F:249:PHE:HB3	1.14	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:PRO:HG3	1:E:212:GLN:HB2	1.39	1.04
1:A:111:LEU:HD12	1:A:160:LEU:HB3	1.36	1.04
1:C:57:LEU:HD11	2:F:326:GLN:HE21	1.21	1.03
2:D:320:LEU:HB2	2:D:331:MET:HG3	1.40	1.02
1:E:51:PHE:HE2	2:F:349:PRO:HG3	1.25	1.02
1:C:57:LEU:HD13	2:F:326:GLN:CB	1.89	1.02
1:A:155:GLN:HG2	1:A:156:ASN:H	1.23	1.02
2:D:323:GLN:HA	2:D:323:GLN:HE21	1.20	1.02
2:D:325:GLN:O	2:D:330:SER:HB3	1.58	1.02
2:D:314:GLU:HG3	2:D:359:ALA:HB2	1.41	1.01
1:C:55:LYS:HA	1:C:55:LYS:HE3	1.42	0.99
1:E:120:VAL:HG22	1:E:129:THR:HG22	1.43	0.99
2:D:307:VAL:HG22	2:D:345:ILE:HG12	1.41	0.98
1:C:72:ARG:HH22	2:F:323:GLN:HB3	1.28	0.98
1:C:52:ARG:HA	2:D:346:ILE:HD13	1.40	0.98
2:B:389:GLN:C	1:E:127:ARG:HH21	1.72	0.97
1:A:88:VAL:C	1:A:89:LEU:HD23	1.89	0.96
2:D:295:VAL:HG13	2:D:380:ALA:HB3	1.48	0.95
2:D:383:LYS:HD2	2:D:384:GLU:N	1.82	0.95
1:A:69:LEU:HD12	1:A:70:LEU:N	1.82	0.95
1:C:56:PHE:HE2	1:C:90:GLU:HB2	1.32	0.94
2:F:323:GLN:HE21	2:F:323:GLN:HA	1.30	0.94
2:B:249:PHE:HD1	2:B:249:PHE:H	1.10	0.94
2:D:320:LEU:N	2:D:320:LEU:HD23	1.81	0.93
1:C:57:LEU:HD13	2:F:326:GLN:HB3	1.48	0.92
2:F:306:LEU:HD13	2:F:364:MET:CE	1.99	0.92
2:B:329:GLU:HB3	1:E:182:ARG:HD2	1.50	0.92
2:D:267:GLU:C	2:D:268:ILE:HD13	1.95	0.92
2:B:328:LEU:H	2:B:331:MET:HB2	1.33	0.91
2:D:323:GLN:HG3	2:D:326:GLN:NE2	1.83	0.91
2:B:325:GLN:HB2	2:B:331:MET:SD	2.09	0.91
2:F:419:VAL:HG13	2:F:420:ASP:H	1.35	0.90
1:A:134:GLN:HE21	1:A:135:GLY:N	1.68	0.90
2:B:357:LYS:HB2	1:E:194:PHE:CE1	2.07	0.90
1:C:98:LEU:HD21	1:C:100:LEU:HD23	1.51	0.90
2:D:388:ARG:HH11	2:D:388:ARG:HB3	1.35	0.90
2:F:419:VAL:CG1	2:F:420:ASP:N	2.33	0.90
2:D:317:LEU:HD13	2:D:348:ILE:HD12	1.54	0.90
1:C:56:PHE:CE2	1:C:90:GLU:HB2	2.06	0.90
1:C:120:VAL:CG2	1:C:129:THR:HG23	2.02	0.89
2:B:320:LEU:HD22	1:E:175:PHE:CE2	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:TYR:CZ	1:C:207:GLU:HB2	2.07	0.89
2:F:262:TYR:HB2	2:F:418:PHE:HB3	1.54	0.89
1:C:98:LEU:HD23	1:C:220:VAL:HG11	1.54	0.89
1:E:182:ARG:HG2	1:E:182:ARG:HH11	1.38	0.89
1:C:183:LEU:HG	1:C:184:PRO:HD2	1.55	0.88
2:D:323:GLN:HA	2:D:323:GLN:NE2	1.84	0.88
1:A:112:VAL:CG1	1:A:134:GLN:HA	2.04	0.88
1:A:89:LEU:HD23	1:A:89:LEU:N	1.87	0.88
1:A:89:LEU:HB2	1:A:161:LYS:HB3	1.55	0.88
1:E:192:LYS:NZ	1:E:203:TYR:HB3	1.89	0.87
1:C:67:LEU:HD13	1:C:91:TYR:HB2	1.56	0.87
1:C:119:LEU:HD21	1:C:140:ILE:HD11	1.54	0.87
2:B:400:PRO:HG3	1:E:212:GLN:CB	2.05	0.87
1:A:47:ASN:CG	1:A:76:ASP:HB3	2.00	0.87
2:B:386:VAL:HG22	1:E:122:VAL:HG11	1.55	0.86
1:C:47:ASN:HB3	1:C:77:THR:HB	1.55	0.86
2:D:257:ILE:HD13	2:D:257:ILE:H	1.38	0.86
2:B:331:MET:HE3	2:B:332:GLN:NE2	1.89	0.86
1:A:111:LEU:CD1	1:A:160:LEU:HB3	2.04	0.86
2:F:254:ARG:HH11	2:F:254:ARG:HG2	1.41	0.86
1:A:210:LEU:HD12	1:A:210:LEU:C	2.00	0.85
2:F:306:LEU:HD13	2:F:364:MET:HE1	1.57	0.85
1:C:79:LYS:HG2	2:D:321:GLU:HB3	1.59	0.85
1:C:98:LEU:HB2	1:C:149:ILE:HG12	1.56	0.85
1:E:62:ASN:OD1	1:E:64:HIS:HB2	1.77	0.85
1:A:79:LYS:HE3	2:B:321:GLU:HG2	1.58	0.85
2:B:267:GLU:HG3	2:B:284:ASN:ND2	1.92	0.85
1:E:49:TYR:CD1	1:E:79:LYS:HE2	2.11	0.85
1:E:153:ASN:OD1	1:E:155:GLN:HB2	1.77	0.85
2:F:325:GLN:HA	2:F:330:SER:OG	1.76	0.85
2:B:316:GLU:HG3	1:E:194:PHE:CE2	2.11	0.85
2:B:386:VAL:HG22	1:E:122:VAL:CG1	2.07	0.85
1:C:48:PRO:HB2	1:C:50:LEU:CD2	2.05	0.85
1:C:57:LEU:HD13	2:F:326:GLN:CA	2.07	0.85
2:B:392:ARG:HH12	2:B:404:GLU:HA	1.40	0.85
1:E:120:VAL:HG22	1:E:129:THR:CG2	2.06	0.85
2:F:404:GLU:CA	2:F:407:GLU:HB2	2.04	0.85
1:A:177:LEU:HD21	2:D:387:ILE:HG12	1.56	0.85
1:C:203:TYR:CE2	1:C:207:GLU:HB2	2.12	0.85
1:E:212:GLN:CG	1:E:213:GLU:H	1.86	0.85
2:D:269:THR:HB	2:D:270:PRO:HD2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LEU:O	2:F:400:PRO:HG3	1.75	0.84
1:C:177:LEU:O	1:C:185:SER:HB2	1.77	0.84
2:B:363:ASN:OD1	2:B:364:MET:N	2.10	0.84
2:D:260:ASN:HD21	2:D:262:TYR:HB2	1.41	0.84
1:C:57:LEU:HD11	2:F:326:GLN:NE2	1.92	0.84
1:A:114:GLU:HB3	1:A:158:ARG:HB2	1.58	0.84
2:B:323:GLN:C	2:B:325:GLN:H	1.85	0.83
1:C:106:SER:C	1:C:142:ALA:HB2	2.03	0.83
1:E:192:LYS:HZ3	1:E:203:TYR:HD2	1.22	0.83
2:D:306:LEU:HB3	2:D:346:ILE:HG22	1.61	0.83
1:E:212:GLN:HG2	1:E:213:GLU:H	1.41	0.83
2:B:406:VAL:HG22	1:E:209:THR:HG23	1.61	0.83
1:E:95:PRO:HB3	1:E:153:ASN:O	1.78	0.83
2:F:379:LEU:HB3	2:F:387:ILE:HD11	1.59	0.83
2:D:293:LEU:HB2	2:D:357:LYS:HG3	1.60	0.82
2:F:404:GLU:HA	2:F:407:GLU:CB	2.08	0.82
1:A:113:LEU:HD11	1:A:160:LEU:HB2	1.62	0.82
2:D:242:LEU:HG	2:D:245:GLN:HB2	1.61	0.82
2:D:346:ILE:HD12	2:D:347:VAL:H	1.43	0.82
1:A:222:MET:HB3	1:A:223:PRO:CD	2.10	0.82
1:C:220:VAL:HG21	2:F:397:LEU:HD23	1.61	0.82
1:C:93:SER:O	1:C:156:ASN:HB3	1.79	0.82
1:E:56:PHE:CE2	1:E:70:LEU:HB2	2.15	0.82
1:C:212:GLN:HG3	1:C:214:GLU:H	1.44	0.81
2:D:314:GLU:HG2	2:D:339:THR:CG2	2.09	0.81
2:D:391:PRO:C	2:D:394:VAL:HG23	2.04	0.81
1:A:112:VAL:HG11	1:A:134:GLN:HA	1.58	0.81
2:B:257:ILE:HD13	2:B:267:GLU:HB2	1.61	0.81
2:D:387:ILE:HA	2:D:390:ILE:HG13	1.62	0.81
1:E:168:ARG:HG3	1:E:168:ARG:NH1	1.88	0.81
2:F:297:HIS:O	2:F:353:PRO:HA	1.79	0.81
2:B:249:PHE:N	2:B:249:PHE:CD1	2.48	0.81
1:C:207:GLU:HA	1:C:210:LEU:CD2	2.10	0.81
1:C:132:LEU:N	1:C:132:LEU:HD13	1.95	0.81
1:A:207:GLU:HG2	1:A:208:GLN:OE1	1.81	0.81
1:E:154:ASN:N	1:E:154:ASN:OD1	2.14	0.80
2:F:419:VAL:HG13	2:F:420:ASP:N	1.92	0.80
2:B:295:VAL:HG13	2:B:296:PRO:CD	2.10	0.80
1:E:67:LEU:CD1	1:E:91:TYR:HB2	2.11	0.80
2:D:402:SER:CB	2:D:405:GLU:HB2	2.08	0.80
1:E:113:LEU:O	1:E:134:GLN:NE2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:CD1	1:A:211:LEU:HB2	2.12	0.80
1:A:193:ASN:ND2	2:D:424:ARG:H	1.80	0.80
1:C:50:LEU:HD22	1:C:50:LEU:H	1.44	0.80
2:B:322:GLN:NE2	2:B:332:GLN:NE2	2.29	0.80
2:B:297:HIS:C	2:B:297:HIS:CD2	2.60	0.80
2:B:400:PRO:CG	1:E:212:GLN:HB2	2.12	0.80
1:C:211:LEU:HD12	1:C:211:LEU:C	2.07	0.80
1:C:212:GLN:HB2	2:F:400:PRO:HB3	1.64	0.80
2:D:247:LYS:O	2:D:249:PHE:N	2.15	0.79
2:F:315:VAL:HG12	2:F:316:GLU:H	1.47	0.79
2:D:320:LEU:N	2:D:320:LEU:CD2	2.45	0.79
1:C:52:ARG:CA	2:D:346:ILE:HD13	2.12	0.79
1:C:79:LYS:HG2	2:D:321:GLU:CB	2.12	0.79
2:D:293:LEU:HB2	2:D:357:LYS:CG	2.11	0.79
2:B:424:ARG:HD3	1:E:196:GLU:OE1	1.82	0.79
1:A:69:LEU:HD13	1:A:89:LEU:HD22	1.63	0.79
2:B:318:VAL:HG21	1:E:189:ALA:HB3	1.65	0.79
1:C:179:SER:HA	1:C:184:PRO:HA	1.64	0.79
2:F:266:TYR:O	2:F:284:ASN:HA	1.83	0.79
2:F:254:ARG:HG3	2:F:255:ASP:N	1.98	0.79
1:A:157:LEU:HD12	1:A:158:ARG:H	1.48	0.79
2:B:282:LEU:O	2:B:282:LEU:HD12	1.82	0.79
2:D:267:GLU:O	2:D:268:ILE:HD13	1.81	0.79
2:D:319:GLY:C	2:D:320:LEU:CD2	2.56	0.79
1:C:192:LYS:HZ3	1:C:192:LYS:HB2	1.49	0.78
1:E:213:GLU:O	1:E:213:GLU:HG2	1.84	0.78
1:C:47:ASN:C	1:C:49:TYR:H	1.89	0.78
1:C:81:GLU:O	1:C:84:ARG:HG2	1.82	0.78
2:F:293:LEU:HD12	2:F:357:LYS:HG3	1.65	0.78
2:F:378:PHE:O	2:F:385:ASN:HA	1.83	0.78
1:C:98:LEU:HD23	1:C:220:VAL:CG1	2.13	0.78
1:E:51:PHE:CE2	2:F:349:PRO:HG3	2.15	0.78
2:F:378:PHE:HD2	2:F:384:GLU:HB3	1.48	0.78
1:A:222:MET:HB2	1:A:224:LYS:O	1.84	0.78
1:A:56:PHE:CE1	1:A:70:LEU:HD13	2.19	0.78
2:D:388:ARG:HH11	2:D:388:ARG:CB	1.98	0.78
1:A:44:ALA:C	1:A:46:ASN:H	1.91	0.77
1:A:69:LEU:HD13	1:A:89:LEU:CD2	2.14	0.77
2:D:402:SER:OG	2:D:404:GLU:HG2	1.84	0.77
2:B:300:SER:OG	2:B:301:ARG:HG3	1.83	0.77
2:B:388:ARG:HG2	2:B:411:GLU:OE2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:THR:OG1	2:B:272:LYS:HD3	1.84	0.77
2:B:379:LEU:HD21	1:E:186:TYR:HE2	1.48	0.77
1:E:216:GLU:HG2	1:E:219:ILE:O	1.85	0.77
2:F:260:ASN:OD1	2:F:261:ASN:N	2.17	0.77
1:C:72:ARG:HH22	2:F:323:GLN:CB	1.98	0.77
2:B:276:LEU:HD11	2:B:283:LEU:HD11	1.65	0.77
2:B:320:LEU:HD13	2:B:320:LEU:N	2.00	0.77
2:B:322:GLN:N	2:B:331:MET:HE1	2.00	0.77
2:D:340:LEU:CD1	2:D:344:ASP:HB2	2.14	0.77
2:B:268:ILE:HG22	2:B:276:LEU:CD2	2.15	0.76
1:C:120:VAL:HG22	1:C:129:THR:HG23	1.67	0.76
1:E:89:LEU:HD12	1:E:161:LYS:O	1.83	0.76
1:C:47:ASN:OD1	1:C:50:LEU:HB2	1.85	0.76
1:E:100:LEU:HB3	1:E:101:PRO:HD2	1.66	0.76
2:F:250:ASN:OD1	2:F:250:ASN:N	2.16	0.76
2:B:290:GLU:HB2	2:B:360:SER:C	2.10	0.76
1:C:168:ARG:HH12	2:F:321:GLU:HB3	1.50	0.76
2:F:290:GLU:HB2	2:F:360:SER:HA	1.66	0.76
1:E:56:PHE:CD2	1:E:70:LEU:HB2	2.20	0.76
2:B:290:GLU:HB2	2:B:360:SER:CA	2.15	0.76
1:A:112:VAL:HG23	1:A:132:LEU:HD23	1.65	0.76
2:D:319:GLY:C	2:D:320:LEU:HD22	2.11	0.76
1:E:46:ASN:OD1	1:E:48:PRO:HD2	1.85	0.76
1:A:157:LEU:HD12	1:A:158:ARG:N	2.00	0.76
2:B:312:ARG:HD3	2:B:339:THR:CG2	2.16	0.76
1:A:112:VAL:CG2	1:A:132:LEU:HD23	2.16	0.76
2:B:346:ILE:HG23	2:B:348:ILE:HD11	1.65	0.76
1:A:69:LEU:HD12	1:A:69:LEU:C	2.09	0.75
2:D:314:GLU:HG2	2:D:339:THR:HG22	1.66	0.75
2:B:387:ILE:HA	2:B:390:ILE:CD1	2.17	0.75
1:E:83:LEU:HD11	2:F:347:VAL:HG11	1.67	0.75
1:A:123:ASN:HB3	1:A:124:PRO:CD	2.16	0.75
1:A:124:PRO:HG2	1:A:125:ASP:OD2	1.86	0.75
1:E:77:THR:HG23	1:E:79:LYS:H	1.50	0.75
1:C:118:ILE:HD11	1:C:151:PRO:HG3	1.66	0.75
1:E:114:GLU:HB2	1:E:158:ARG:HD3	1.66	0.75
2:D:388:ARG:HB3	2:D:388:ARG:NH1	2.00	0.75
1:A:212:GLN:HB3	2:D:400:PRO:HG3	1.66	0.75
2:D:320:LEU:HB3	2:D:332:GLN:O	1.85	0.75
2:F:322:GLN:H	2:F:331:MET:HE3	1.51	0.75
1:A:70:LEU:HG	1:A:71:GLN:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:LEU:HD23	1:E:163:ALA:HB2	1.69	0.75
2:B:389:GLN:O	1:E:127:ARG:NH2	2.19	0.75
2:D:293:LEU:HD23	2:D:293:LEU:O	1.87	0.75
2:F:282:LEU:C	2:F:282:LEU:HD23	2.11	0.75
2:B:325:GLN:HG3	2:B:332:GLN:HE21	1.52	0.74
2:D:383:LYS:HB3	2:D:416:SER:HB3	1.69	0.74
1:A:110:VAL:HG23	1:A:138:ILE:HG22	1.68	0.74
1:C:55:LYS:HA	1:C:55:LYS:CE	2.10	0.74
1:A:70:LEU:HG	1:A:71:GLN:N	2.02	0.74
2:B:404:GLU:HA	2:B:407:GLU:HB3	1.70	0.74
1:C:222:MET:SD	1:C:223:PRO:HD2	2.28	0.74
2:D:242:LEU:O	2:D:245:GLN:HB3	1.87	0.74
2:B:322:GLN:NE2	2:B:332:GLN:HE22	1.85	0.74
2:B:400:PRO:HG3	1:E:212:GLN:CA	2.18	0.74
1:A:108:LEU:HD22	1:A:161:LYS:CG	2.17	0.74
1:C:202:PRO:O	1:C:205:GLU:N	2.21	0.74
2:D:288:MET:HE2	2:D:362:LEU:HD23	1.68	0.74
1:E:74:ASN:O	1:E:74:ASN:ND2	2.20	0.74
2:F:422:GLN:NE2	2:F:423:PRO:HD2	2.03	0.74
1:A:91:TYR:HB3	1:A:159:ILE:HG22	1.70	0.73
1:A:122:VAL:HG12	2:D:386:VAL:HG22	1.69	0.73
1:E:98:LEU:H	1:E:220:VAL:HG12	1.52	0.73
1:A:57:LEU:HD12	1:A:69:LEU:O	1.89	0.73
1:A:58:THR:HG21	1:A:61:LYS:HE2	1.69	0.73
2:F:292:ALA:HA	2:F:419:VAL:O	1.88	0.73
2:F:388:ARG:HH11	2:F:388:ARG:HB3	1.52	0.73
1:A:47:ASN:ND2	1:A:76:ASP:OD2	2.22	0.73
1:A:179:SER:HB2	1:A:212:GLN:HG2	1.70	0.73
1:E:117:ALA:O	1:E:131:LYS:HA	1.89	0.73
2:D:422:GLN:HG2	2:D:423:PRO:N	1.98	0.73
1:E:220:VAL:HG13	1:E:221:LYS:N	2.03	0.73
1:A:168:ARG:NE	2:D:322:GLN:HA	1.94	0.73
2:D:404:GLU:HG3	2:D:405:GLU:N	2.02	0.73
1:C:148:LEU:HD21	1:C:159:ILE:HD12	1.69	0.73
1:E:51:PHE:HE2	2:F:349:PRO:CG	2.00	0.73
1:A:210:LEU:HD12	1:A:211:LEU:CA	2.19	0.73
2:B:413:GLN:OE1	2:B:414:LYS:HE2	1.89	0.73
1:E:62:ASN:HD21	1:E:219:ILE:HB	1.54	0.73
1:A:168:ARG:HE	2:D:322:GLN:CA	1.96	0.72
1:A:220:VAL:HG13	1:A:221:LYS:N	2.03	0.72
1:C:113:LEU:HD11	1:C:160:LEU:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:ASP:HA	2:D:249:PHE:HB3	1.71	0.72
2:F:277:ARG:HG3	2:F:277:ARG:NH1	1.90	0.72
1:C:120:VAL:HG23	1:C:129:THR:HG23	1.69	0.72
2:F:290:GLU:HB2	2:F:360:SER:CA	2.19	0.72
1:A:206:ILE:O	1:A:209:THR:N	2.20	0.72
2:B:400:PRO:HG3	1:E:212:GLN:N	2.05	0.72
1:E:192:LYS:O	1:E:196:GLU:HG3	1.89	0.72
2:F:325:GLN:CA	2:F:325:GLN:HE21	2.01	0.72
1:C:111:LEU:HD11	2:D:283:LEU:CD2	2.19	0.72
2:D:383:LYS:CD	2:D:384:GLU:H	1.96	0.72
2:F:280:ASP:O	2:F:281:ILE:HD12	1.89	0.72
2:F:288:MET:HE2	2:F:358:ALA:HB2	1.72	0.72
2:D:258:TYR:HD2	2:D:265:LEU:HB3	1.55	0.72
2:F:254:ARG:HG2	2:F:254:ARG:NH1	2.03	0.72
1:A:60:PHE:O	1:A:66:SER:HA	1.89	0.72
2:F:245:GLN:NE2	2:F:249:PHE:HB3	1.98	0.72
1:E:70:LEU:HD12	1:E:71:GLN:H	1.55	0.72
1:E:192:LYS:HZ3	1:E:203:TYR:HB3	1.55	0.72
1:A:155:GLN:HG2	1:A:156:ASN:N	1.98	0.72
2:B:306:LEU:O	2:B:345:ILE:HG23	1.90	0.72
2:B:378:PHE:CZ	2:B:417:TYR:HD2	2.07	0.72
2:D:242:LEU:O	2:D:242:LEU:HD23	1.89	0.72
1:E:182:ARG:HG2	1:E:182:ARG:NH1	2.00	0.72
1:E:113:LEU:C	1:E:134:GLN:HE21	1.97	0.71
2:F:323:GLN:HE21	2:F:323:GLN:CA	1.96	0.71
1:A:215:GLN:HG2	1:A:216:GLU:N	2.05	0.71
1:A:123:ASN:O	2:D:386:VAL:HG23	1.90	0.71
1:C:83:LEU:CD2	2:D:369:VAL:HG21	2.20	0.71
2:D:258:TYR:HD1	2:D:417:TYR:CE1	2.07	0.71
2:F:323:GLN:HA	2:F:323:GLN:NE2	2.04	0.71
2:B:247:LYS:HB3	2:B:248:PRO:HD2	1.72	0.71
1:E:77:THR:HG23	1:E:79:LYS:CG	2.17	0.71
2:B:318:VAL:CG2	1:E:189:ALA:HB3	2.20	0.71
1:C:214:GLU:O	1:C:217:GLY:N	2.23	0.71
1:E:64:HIS:NE2	1:E:221:LYS:HB2	2.05	0.71
2:F:290:GLU:HA	2:F:358:ALA:O	1.90	0.71
2:F:423:PRO:O	2:F:424:ARG:HB2	1.91	0.71
1:C:179:SER:OG	1:C:211:LEU:HA	1.90	0.71
2:F:325:GLN:O	2:F:326:GLN:HB2	1.89	0.71
1:A:168:ARG:HD3	2:D:321:GLU:O	1.90	0.70
2:D:245:GLN:HE21	2:D:246:ASP:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:ARG:HD3	1:E:189:ALA:O	1.91	0.70
1:C:122:VAL:O	1:C:145:PRO:HD2	1.91	0.70
2:B:247:LYS:HA	2:B:247:LYS:NZ	2.07	0.70
2:B:327:GLY:HA3	2:B:330:SER:HB2	1.73	0.70
1:E:130:TYR:HB3	2:F:241:THR:CG2	2.21	0.70
2:B:258:TYR:O	2:B:264:LYS:HA	1.90	0.70
1:E:48:PRO:O	1:E:49:TYR:HB2	1.91	0.70
1:A:215:GLN:C	1:A:217:GLY:H	2.00	0.70
2:B:257:ILE:CD1	2:B:267:GLU:HB2	2.20	0.70
1:C:131:LYS:HD2	1:C:131:LYS:O	1.92	0.70
2:D:315:VAL:O	2:D:337:ALA:HA	1.92	0.70
2:D:393:GLN:O	2:D:397:LEU:HD12	1.92	0.70
2:B:322:GLN:HE22	2:B:332:GLN:NE2	1.90	0.70
2:B:406:VAL:HG22	1:E:209:THR:CG2	2.22	0.70
2:D:313:ALA:HB3	2:D:340:LEU:HB2	1.73	0.70
1:E:131:LYS:H	2:F:241:THR:HG23	1.57	0.70
2:F:247:LYS:HB3	2:F:248:PRO:HD2	1.73	0.70
2:F:422:GLN:CD	2:F:423:PRO:HD2	2.17	0.70
1:A:111:LEU:HD11	1:A:160:LEU:HD23	1.73	0.69
1:A:139:LYS:HE3	1:A:141:GLN:HG3	1.73	0.69
1:A:185:SER:OG	1:A:187:LEU:HB2	1.91	0.69
1:A:108:LEU:HD22	1:A:161:LYS:HG2	1.72	0.69
2:D:347:VAL:O	2:D:349:PRO:HD3	1.92	0.69
2:B:331:MET:HE3	2:B:332:GLN:HE22	1.56	0.69
1:E:151:PRO:O	1:E:153:ASN:N	2.23	0.69
2:D:323:GLN:HG3	2:D:326:GLN:CD	2.17	0.69
1:A:117:ALA:HB2	1:A:157:LEU:HD22	1.74	0.69
1:A:179:SER:CB	1:A:211:LEU:HD12	2.21	0.69
2:B:328:LEU:C	2:B:330:SER:H	2.00	0.69
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.56	0.69
2:B:312:ARG:HD3	2:B:339:THR:HG22	1.74	0.69
2:B:322:GLN:O	2:B:325:GLN:HG2	1.93	0.69
2:D:247:LYS:HG3	2:D:248:PRO:N	2.08	0.69
2:D:377:ASN:N	2:D:377:ASN:HD22	1.91	0.69
2:F:295:VAL:HG22	2:F:417:TYR:O	1.93	0.69
1:A:196:GLU:OE2	1:A:203:TYR:HB2	1.91	0.69
1:E:48:PRO:HA	1:E:77:THR:OG1	1.93	0.69
1:A:60:PHE:CE1	1:A:62:ASN:HB3	2.28	0.68
1:C:94:LYS:HB3	1:C:95:PRO:HD2	1.75	0.68
1:A:215:GLN:HG2	1:A:216:GLU:H	1.58	0.68
2:B:348:ILE:HD12	2:B:348:ILE:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:ARG:HH12	2:B:404:GLU:CA	2.06	0.68
1:C:194:PHE:CZ	2:F:357:LYS:HB2	2.29	0.68
1:E:180:THR:C	1:E:182:ARG:H	2.02	0.68
1:E:207:GLU:HA	1:E:210:LEU:HB3	1.74	0.68
1:A:106:SER:HB3	1:A:165:THR:HA	1.76	0.68
2:D:248:PRO:HA	2:D:275:GLN:NE2	2.09	0.68
2:B:302:ALA:HB2	2:B:371:ALA:HA	1.75	0.68
1:C:212:GLN:HG3	1:C:214:GLU:N	2.08	0.68
2:D:260:ASN:OD1	2:D:263:GLY:N	2.26	0.68
1:A:47:ASN:ND2	1:A:76:ASP:CG	2.52	0.68
2:F:389:GLN:O	2:F:391:PRO:HD3	1.92	0.68
1:A:100:LEU:HB3	1:A:101:PRO:HD2	1.73	0.68
1:A:205:GLU:HA	1:A:208:GLN:CG	2.22	0.68
2:B:328:LEU:H	2:B:331:MET:CB	2.05	0.68
1:C:79:LYS:HE2	2:D:322:GLN:NE2	2.09	0.68
2:D:317:LEU:HD12	2:D:354:VAL:HB	1.74	0.68
2:D:391:PRO:O	2:D:394:VAL:HG23	1.93	0.68
1:E:132:LEU:CD2	2:F:250:ASN:HD22	2.06	0.68
1:E:136:ASP:OD1	2:F:252:ARG:HG3	1.94	0.68
1:A:47:ASN:ND2	1:A:76:ASP:HB3	2.09	0.68
1:C:57:LEU:HD13	2:F:326:GLN:HA	1.74	0.68
2:D:257:ILE:HG13	2:D:265:LEU:HD12	1.76	0.68
2:B:335:ARG:NH1	1:E:189:ALA:O	2.26	0.68
1:C:72:ARG:NH2	2:F:323:GLN:HB3	2.05	0.68
1:C:207:GLU:HA	1:C:210:LEU:HD23	1.76	0.68
2:D:286:LEU:O	2:D:363:ASN:HA	1.94	0.68
2:D:300:SER:HG	2:D:374:ASN:HA	1.58	0.68
1:E:96:ASN:HA	1:E:150:ASN:O	1.93	0.68
2:B:322:GLN:O	2:B:325:GLN:N	2.26	0.68
1:C:96:ASN:O	1:C:221:LYS:HG3	1.94	0.68
2:D:378:PHE:O	2:D:385:ASN:HA	1.94	0.68
1:E:153:ASN:HB2	1:E:154:ASN:OD1	1.94	0.67
2:F:422:GLN:HE21	2:F:422:GLN:C	2.01	0.67
1:A:114:GLU:OE1	1:A:158:ARG:NH1	2.27	0.67
2:D:391:PRO:CA	2:D:394:VAL:HG23	2.24	0.67
1:E:143:GLY:O	1:E:145:PRO:HD3	1.94	0.67
1:E:212:GLN:HE21	1:E:214:GLU:HB2	1.59	0.67
1:A:219:ILE:N	1:A:219:ILE:HD12	2.09	0.67
1:E:212:GLN:HG2	1:E:213:GLU:C	2.20	0.67
2:B:393:GLN:O	2:B:397:LEU:HG	1.95	0.67
1:A:176:PHE:CE2	1:A:218:VAL:HG13	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:HIS:HB2	1:C:97:THR:HG21	1.76	0.67
2:D:260:ASN:OD1	2:D:262:TYR:N	2.28	0.67
2:D:346:ILE:HD12	2:D:347:VAL:N	2.10	0.67
2:D:306:LEU:CB	2:D:346:ILE:HG22	2.24	0.67
1:A:106:SER:C	1:A:142:ALA:HB2	2.20	0.67
1:C:49:TYR:HE1	1:C:79:LYS:NZ	1.92	0.67
1:A:193:ASN:HD22	2:D:424:ARG:H	1.43	0.67
2:D:268:ILE:HD13	2:D:268:ILE:N	2.07	0.67
1:A:47:ASN:ND2	1:A:76:ASP:CB	2.58	0.66
1:A:45:GLN:O	1:A:76:ASP:HA	1.95	0.66
1:E:192:LYS:HZ2	1:E:203:TYR:HB3	1.59	0.66
2:B:313:ALA:O	2:B:340:LEU:N	2.28	0.66
2:B:389:GLN:HA	1:E:127:ARG:NH2	2.11	0.66
2:B:322:GLN:C	2:B:331:MET:HE1	2.21	0.66
1:C:149:ILE:HD13	1:C:222:MET:HE2	1.76	0.66
1:E:51:PHE:CZ	2:F:321:GLU:OE2	2.48	0.66
1:E:118:ILE:CD1	1:E:151:PRO:HG3	2.26	0.66
1:A:117:ALA:HB2	1:A:157:LEU:CD2	2.25	0.66
1:C:212:GLN:CG	1:C:214:GLU:H	2.06	0.66
2:F:247:LYS:H	2:F:247:LYS:HD2	1.61	0.66
2:B:328:LEU:HD21	1:E:182:ARG:HG3	1.78	0.66
2:F:273:ASN:HB3	2:F:276:LEU:HB2	1.77	0.66
1:C:131:LYS:C	1:C:132:LEU:HD13	2.20	0.66
1:C:131:LYS:NZ	1:C:133:ASP:OD1	2.25	0.66
2:B:267:GLU:CD	2:B:376:ARG:HH22	2.04	0.66
2:B:325:GLN:HB3	2:B:330:SER:O	1.96	0.66
1:C:89:LEU:HB2	1:C:161:LYS:HB2	1.78	0.66
1:C:211:LEU:O	1:C:211:LEU:HD12	1.95	0.66
1:C:187:LEU:HD11	2:F:387:ILE:CD1	2.26	0.65
2:D:242:LEU:HG	2:D:245:GLN:CB	2.26	0.65
2:B:360:SER:OG	2:B:361:ASP:N	2.28	0.65
2:D:386:VAL:O	2:D:388:ARG:N	2.29	0.65
1:E:119:LEU:HD12	1:E:148:LEU:CD1	2.25	0.65
1:E:151:PRO:O	1:E:153:ASN:ND2	2.28	0.65
1:A:210:LEU:C	1:A:210:LEU:CD1	2.70	0.65
2:B:413:GLN:OE1	2:B:414:LYS:HG3	1.97	0.65
2:B:251:LEU:HD22	2:B:273:ASN:HD21	1.60	0.65
2:D:316:GLU:CD	2:D:335:ARG:HD2	2.20	0.65
1:E:98:LEU:HB3	1:E:220:VAL:HG11	1.78	0.65
2:B:251:LEU:HD13	2:B:273:ASN:ND2	2.12	0.65
2:F:360:SER:OG	2:F:361:ASP:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:O	1:A:97:THR:HG23	1.97	0.65
1:A:102:HIS:ND1	1:A:102:HIS:N	2.45	0.65
1:A:127:ARG:NH1	2:D:389:GLN:HA	2.12	0.65
1:C:49:TYR:CE1	1:C:79:LYS:CE	2.80	0.65
1:E:130:TYR:HD1	2:F:241:THR:HG22	1.62	0.65
1:C:185:SER:O	1:C:188:SER:HB2	1.97	0.65
2:D:294:PHE:N	2:D:356:LEU:O	2.27	0.65
1:A:205:GLU:HA	1:A:208:GLN:HG3	1.77	0.65
2:D:245:GLN:NE2	2:D:246:ASP:H	1.93	0.65
2:D:247:LYS:CG	2:D:248:PRO:N	2.59	0.65
1:A:210:LEU:HD12	1:A:211:LEU:HB2	1.79	0.65
1:C:183:LEU:HG	1:C:184:PRO:CD	2.25	0.65
1:C:207:GLU:HA	1:C:210:LEU:HD22	1.78	0.65
2:F:242:LEU:HD13	2:F:244:SER:O	1.97	0.65
2:F:325:GLN:HA	2:F:325:GLN:HE21	1.60	0.65
1:C:50:LEU:HD22	1:C:50:LEU:N	2.11	0.64
1:C:102:HIS:HB3	1:C:176:PHE:CD1	2.33	0.64
2:B:341:SER:O	2:B:344:ASP:HB2	1.97	0.64
1:C:54:ASN:O	1:C:55:LYS:NZ	2.29	0.64
1:C:211:LEU:C	1:C:211:LEU:CD1	2.70	0.64
2:D:320:LEU:HB2	2:D:331:MET:CG	2.22	0.64
2:F:381:GLY:HA2	2:F:413:GLN:HG3	1.80	0.64
1:A:82:ASN:OD1	1:A:82:ASN:N	2.26	0.64
2:D:260:ASN:ND2	2:D:262:TYR:HB2	2.11	0.64
2:D:319:GLY:C	2:D:320:LEU:HD23	2.20	0.64
2:F:322:GLN:N	2:F:331:MET:HE3	2.10	0.64
1:C:97:THR:HA	1:C:221:LYS:HA	1.80	0.64
1:C:177:LEU:HB3	2:F:399:PHE:CZ	2.33	0.64
2:F:310:GLU:HG3	2:F:310:GLU:O	1.95	0.64
1:C:223:PRO:HG3	2:F:397:LEU:HD11	1.80	0.64
1:C:99:LEU:HD23	1:C:219:ILE:HG13	1.78	0.64
2:F:378:PHE:CD2	2:F:384:GLU:HB3	2.31	0.64
2:D:386:VAL:O	2:D:389:GLN:N	2.28	0.64
1:A:178:SER:OG	2:D:398:THR:HG22	1.98	0.64
2:F:269:THR:HB	2:F:270:PRO:HD2	1.80	0.64
1:A:105:ASP:O	1:A:142:ALA:HB1	1.98	0.63
2:D:377:ASN:N	2:D:377:ASN:ND2	2.45	0.63
1:A:212:GLN:HB3	2:D:400:PRO:CG	2.27	0.63
2:B:278:ASP:O	2:B:279:LEU:HD13	1.98	0.63
1:A:193:ASN:HD22	2:D:424:ARG:N	1.96	0.63
1:E:58:THR:HA	1:E:68:ARG:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:MET:HG3	1:E:223:PRO:HD3	0.80	0.63
2:F:245:GLN:HE21	2:F:249:PHE:CB	2.00	0.63
1:A:123:ASN:HB3	1:A:124:PRO:HD2	1.78	0.63
1:C:111:LEU:HD11	2:D:283:LEU:HD21	1.79	0.63
2:F:316:GLU:O	2:F:354:VAL:HG23	1.97	0.63
2:B:328:LEU:HA	2:B:331:MET:HB3	1.81	0.63
2:D:278:ASP:N	2:D:278:ASP:OD1	2.28	0.63
1:E:180:THR:OG1	1:E:183:LEU:O	2.09	0.63
1:A:114:GLU:CD	1:A:158:ARG:HD3	2.24	0.63
1:E:207:GLU:HA	1:E:210:LEU:CB	2.28	0.63
2:F:255:ASP:OD1	2:F:256:PRO:HD2	1.98	0.63
1:C:96:ASN:O	1:C:221:LYS:HE3	1.98	0.63
2:D:278:ASP:OD1	2:D:279:LEU:N	2.32	0.63
2:D:293:LEU:HA	2:D:356:LEU:O	1.99	0.63
1:E:91:TYR:CZ	1:E:93:SER:HB3	2.33	0.63
1:A:49:TYR:HD2	2:B:336:TYR:HH	1.46	0.62
2:F:265:LEU:HD11	2:F:284:ASN:HB2	1.81	0.62
1:A:54:ASN:O	1:A:55:LYS:NZ	2.26	0.62
2:F:314:GLU:HB2	2:F:357:LYS:HB3	1.81	0.62
2:F:419:VAL:HG12	2:F:420:ASP:N	2.12	0.62
1:C:72:ARG:NH1	2:F:324:GLN:HE22	1.98	0.62
1:E:67:LEU:HD13	1:E:91:TYR:HB2	1.81	0.62
1:A:86:TYR:C	1:A:87:ARG:HG2	2.23	0.62
2:B:328:LEU:CD2	1:E:182:ARG:HD2	2.30	0.62
2:B:335:ARG:HB2	1:E:189:ALA:HB1	1.80	0.62
2:D:408:GLU:O	2:D:410:LEU:N	2.32	0.62
2:F:306:LEU:HB3	2:F:364:MET:HE1	1.82	0.62
1:A:147:TYR:CZ	2:D:394:VAL:HG11	2.34	0.62
1:C:179:SER:CB	1:C:211:LEU:HA	2.29	0.62
1:E:55:LYS:NZ	1:E:55:LYS:HA	2.14	0.62
2:F:242:LEU:HB3	2:F:244:SER:H	1.64	0.62
1:A:52:ARG:HA	2:B:346:ILE:HD12	1.82	0.62
2:B:250:ASN:N	2:B:250:ASN:OD1	2.32	0.62
1:C:96:ASN:HD21	1:C:152:ASP:HA	1.64	0.62
1:C:220:VAL:HG21	2:F:397:LEU:CD2	2.30	0.62
1:E:151:PRO:C	1:E:153:ASN:H	2.08	0.62
2:F:306:LEU:HD13	2:F:364:MET:HE2	1.81	0.62
2:F:413:GLN:OE1	2:F:414:LYS:N	2.33	0.62
1:A:49:TYR:OH	2:B:322:GLN:NE2	2.33	0.62
1:A:54:ASN:O	1:A:55:LYS:HD2	1.99	0.62
1:E:79:LYS:O	1:E:80:LEU:HD23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:295:VAL:O	2:F:297:HIS:ND1	2.33	0.62
1:C:47:ASN:N	1:C:76:ASP:HB3	2.03	0.62
1:A:150:ASN:C	1:A:150:ASN:HD22	2.08	0.62
2:B:363:ASN:OD1	2:B:363:ASN:C	2.40	0.62
2:B:389:GLN:C	1:E:127:ARG:NH2	2.51	0.62
2:D:309:ASN:OD1	2:D:363:ASN:ND2	2.32	0.62
2:D:412:ASN:O	2:D:414:LYS:NZ	2.32	0.62
1:E:113:LEU:HA	1:E:134:GLN:NE2	2.15	0.62
2:F:246:ASP:CB	2:F:247:LYS:HE2	2.30	0.62
1:A:110:VAL:HG23	1:A:138:ILE:CG2	2.30	0.61
2:B:267:GLU:OE2	2:B:376:ARG:NH2	2.30	0.61
1:C:215:GLN:HG2	1:C:216:GLU:H	1.64	0.61
2:B:366:GLY:O	2:B:367:ILE:HG13	2.00	0.61
1:C:49:TYR:HE1	1:C:79:LYS:HZ2	1.48	0.61
1:E:113:LEU:CA	1:E:134:GLN:HE21	2.13	0.61
2:F:265:LEU:HD11	2:F:284:ASN:HD22	1.65	0.61
2:B:282:LEU:HD12	2:B:282:LEU:C	2.26	0.61
2:D:260:ASN:CG	2:D:262:TYR:H	2.08	0.61
2:D:307:VAL:HG22	2:D:345:ILE:CG1	2.23	0.61
1:E:113:LEU:HA	1:E:134:GLN:HE21	1.65	0.61
2:F:242:LEU:HD13	2:F:244:SER:C	2.26	0.61
1:A:162:PHE:HE2	2:B:281:ILE:HD11	1.65	0.61
1:E:109:LEU:HD22	2:F:281:ILE:HG21	1.83	0.61
1:A:196:GLU:OE2	2:D:424:ARG:HD3	2.01	0.61
1:C:73:PHE:HB3	1:C:80:LEU:CD1	2.30	0.61
1:C:83:LEU:HD21	2:D:369:VAL:HG21	1.82	0.61
1:C:148:LEU:HD12	1:C:149:ILE:N	2.16	0.61
1:C:157:LEU:HD12	1:C:158:ARG:N	2.16	0.61
2:D:245:GLN:CG	2:D:246:ASP:H	2.14	0.61
1:A:89:LEU:N	1:A:89:LEU:CD2	2.63	0.61
2:B:409:LEU:HA	2:B:412:ASN:ND2	2.16	0.61
1:C:167:ARG:HH22	1:C:168:ARG:HH11	1.49	0.61
2:F:258:TYR:CD1	2:F:417:TYR:CE2	2.88	0.61
1:A:176:PHE:CZ	1:A:218:VAL:HG13	2.36	0.60
2:D:245:GLN:HG2	2:D:246:ASP:N	2.15	0.60
2:F:301:ARG:HD3	2:F:372:GLU:O	2.00	0.60
2:D:307:VAL:CG2	2:D:345:ILE:HG12	2.24	0.60
2:D:387:ILE:HA	2:D:390:ILE:CG1	2.29	0.60
2:F:309:ASN:O	2:F:342:GLU:HG2	2.01	0.60
1:C:54:ASN:ND2	2:D:344:ASP:OD2	2.33	0.60
1:C:119:LEU:HD23	1:C:121:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:242:LEU:HD22	2:F:244:SER:N	2.16	0.60
1:A:102:HIS:HD2	1:A:174:ASP:OD1	1.84	0.60
1:A:216:GLU:O	1:A:220:VAL:HG23	2.02	0.60
2:B:281:ILE:HA	2:B:368:GLY:O	2.02	0.60
1:C:51:PHE:O	2:D:346:ILE:HD12	2.02	0.60
1:C:133:ASP:N	1:C:136:ASP:OD2	2.30	0.60
2:D:408:GLU:C	2:D:410:LEU:H	2.09	0.60
2:D:245:GLN:HG2	2:D:249:PHE:CD2	2.36	0.60
1:E:85:ASP:O	1:E:165:THR:HG23	2.02	0.60
2:B:333:LEU:CD1	1:E:186:TYR:HA	2.32	0.60
2:B:392:ARG:HG2	2:B:392:ARG:HH11	1.67	0.60
2:D:387:ILE:CA	2:D:390:ILE:HG13	2.32	0.60
2:B:314:GLU:HA	2:B:338:ALA:O	2.01	0.60
1:C:98:LEU:HD21	1:C:100:LEU:CD2	2.28	0.60
2:D:293:LEU:CB	2:D:357:LYS:HG3	2.31	0.60
2:D:334:ARG:HD3	2:D:335:ARG:N	2.17	0.60
1:E:108:LEU:CD2	1:E:163:ALA:HB2	2.31	0.60
2:F:242:LEU:HD22	2:F:244:SER:H	1.67	0.60
1:A:54:ASN:C	1:A:55:LYS:HD2	2.27	0.60
1:A:150:ASN:HD22	1:A:151:PRO:N	2.00	0.60
2:B:320:LEU:HD22	1:E:175:PHE:CD2	2.37	0.60
2:B:328:LEU:O	2:B:329:GLU:CD	2.44	0.60
2:B:351:SER:HB3	1:E:103:HIS:NE2	2.16	0.60
2:B:387:ILE:O	2:B:390:ILE:HD12	2.01	0.60
1:C:118:ILE:CD1	1:C:151:PRO:HG3	2.32	0.60
1:C:186:TYR:C	1:C:188:SER:H	2.10	0.60
2:D:301:ARG:HG3	2:D:374:ASN:HB2	1.84	0.60
2:D:320:LEU:HA	2:D:331:MET:HE2	1.84	0.60
1:C:49:TYR:CD1	1:C:79:LYS:HE3	2.37	0.59
2:F:265:LEU:CD1	2:F:284:ASN:HB2	2.32	0.59
1:A:168:ARG:NH1	1:A:168:ARG:HB3	2.17	0.59
1:A:192:LYS:O	1:A:196:GLU:HG3	2.03	0.59
2:B:323:GLN:C	2:B:325:GLN:N	2.58	0.59
2:F:242:LEU:CB	2:F:245:GLN:HG2	2.31	0.59
2:F:273:ASN:O	2:F:277:ARG:N	2.35	0.59
2:F:422:GLN:HB2	2:F:423:PRO:CD	2.31	0.59
1:C:73:PHE:HB3	1:C:80:LEU:HD13	1.84	0.59
1:C:110:VAL:HG13	1:C:111:LEU:N	2.17	0.59
1:C:110:VAL:O	1:C:111:LEU:HD12	2.02	0.59
1:E:49:TYR:HA	1:E:79:LYS:CD	2.32	0.59
2:F:326:GLN:O	2:F:328:LEU:N	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:GLU:HB2	2:B:360:SER:HA	1.82	0.59
2:B:320:LEU:N	2:B:320:LEU:CD1	2.65	0.59
2:B:323:GLN:O	2:B:326:GLN:N	2.35	0.59
1:C:126:GLY:HA2	2:F:389:GLN:OE1	2.02	0.59
2:D:408:GLU:O	2:D:411:GLU:N	2.27	0.59
2:F:242:LEU:HD22	2:F:244:SER:OG	2.01	0.59
2:B:328:LEU:CD2	1:E:182:ARG:HG3	2.32	0.59
1:C:114:GLU:HB2	1:C:158:ARG:NH1	2.18	0.59
1:E:130:TYR:CD1	2:F:241:THR:HG22	2.36	0.59
1:E:223:PRO:CG	1:E:224:LYS:H	2.14	0.59
2:F:246:ASP:HB2	2:F:247:LYS:HE2	1.85	0.59
2:B:300:SER:HB3	2:B:375:GLU:HG3	1.85	0.59
1:C:139:LYS:HZ3	1:C:141:GLN:NE2	2.00	0.59
2:D:245:GLN:HG2	2:D:246:ASP:H	1.68	0.59
1:E:108:LEU:HD23	1:E:163:ALA:CB	2.32	0.59
2:D:258:TYR:CE2	2:D:265:LEU:HD12	2.37	0.59
1:E:54:ASN:O	1:E:55:LYS:NZ	2.34	0.59
1:E:138:ILE:HG12	1:E:139:LYS:N	2.17	0.59
2:B:270:PRO:O	2:B:277:ARG:HB2	2.03	0.58
1:C:64:HIS:HD2	1:C:97:THR:HG22	1.68	0.58
1:C:209:THR:HG21	2:F:406:VAL:HG22	1.84	0.58
1:A:59:LEU:O	2:D:328:LEU:HB2	2.03	0.58
1:A:180:THR:HG22	1:A:214:GLU:HB3	1.85	0.58
1:C:153:ASN:OD1	1:C:154:ASN:N	2.36	0.58
1:A:60:PHE:HE1	1:A:62:ASN:HB3	1.69	0.58
1:A:203:TYR:O	1:A:207:GLU:HB3	2.02	0.58
1:C:130:TYR:HD1	2:D:242:LEU:HD11	1.68	0.58
2:B:357:LYS:HB2	1:E:194:PHE:CZ	2.38	0.58
2:B:387:ILE:HA	2:B:390:ILE:HD11	1.85	0.58
1:C:47:ASN:CB	1:C:77:THR:HB	2.29	0.58
1:E:44:ALA:O	1:E:45:GLN:HB3	2.02	0.58
2:F:325:GLN:NE2	2:F:330:SER:HB2	2.18	0.58
2:F:245:GLN:O	2:F:246:ASP:HB2	2.03	0.58
2:F:298:TYR:HE1	2:F:379:LEU:HD21	1.69	0.58
2:D:383:LYS:CB	2:D:416:SER:HB3	2.34	0.58
2:F:259:SER:O	2:F:260:ASN:HB3	2.03	0.58
2:F:282:LEU:C	2:F:282:LEU:CD2	2.76	0.58
2:F:299:ASN:O	2:F:350:SER:O	2.22	0.58
1:A:214:GLU:HG3	1:A:217:GLY:HA2	1.84	0.58
1:C:170:GLY:O	1:C:172:VAL:HG12	2.03	0.58
1:E:69:LEU:HD12	1:E:89:LEU:CD2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:402:SER:O	2:F:405:GLU:N	2.37	0.58
1:A:49:TYR:HD2	2:B:336:TYR:CE2	2.21	0.58
1:A:210:LEU:HD12	1:A:211:LEU:CB	2.33	0.58
2:D:257:ILE:HD13	2:D:257:ILE:N	2.14	0.58
1:E:192:LYS:HD3	1:E:196:GLU:OE2	2.04	0.58
1:E:206:ILE:C	1:E:208:GLN:H	2.12	0.58
2:F:260:ASN:OD1	2:F:260:ASN:C	2.45	0.58
2:F:335:ARG:HG2	2:F:335:ARG:HH11	1.68	0.58
1:C:98:LEU:CD2	1:C:100:LEU:HD23	2.31	0.57
1:C:152:ASP:OD1	1:C:153:ASN:N	2.37	0.57
1:E:209:THR:O	1:E:210:LEU:O	2.22	0.57
1:C:168:ARG:NH2	2:F:322:GLN:HB3	2.19	0.57
1:E:179:SER:O	1:E:214:GLU:HB3	2.04	0.57
1:A:149:ILE:HD13	1:A:149:ILE:N	2.18	0.57
1:C:51:PHE:C	2:D:346:ILE:CD1	2.77	0.57
1:E:153:ASN:H	1:E:153:ASN:HD22	1.51	0.57
1:A:101:PRO:HG2	2:D:398:THR:HG21	1.87	0.57
2:B:297:HIS:C	2:B:297:HIS:HD2	2.11	0.57
1:C:49:TYR:CE1	1:C:79:LYS:HE3	2.39	0.57
2:D:247:LYS:HG3	2:D:248:PRO:CD	2.35	0.57
1:E:214:GLU:OE1	1:E:215:GLN:HG3	2.05	0.57
2:F:315:VAL:CG2	2:F:340:LEU:HD22	2.33	0.57
2:F:388:ARG:HD2	2:F:410:LEU:HB3	1.85	0.57
1:A:44:ALA:O	1:A:46:ASN:N	2.21	0.57
2:B:267:GLU:HG3	2:B:284:ASN:HD21	1.69	0.57
2:B:327:GLY:O	2:B:328:LEU:O	2.22	0.57
2:D:407:GLU:O	2:D:411:GLU:OE1	2.23	0.57
1:A:62:ASN:ND2	1:A:216:GLU:HG3	2.20	0.57
1:C:148:LEU:CD2	1:C:159:ILE:HD12	2.35	0.57
2:D:281:ILE:HA	2:D:368:GLY:O	2.04	0.57
2:F:323:GLN:C	2:F:325:GLN:H	2.10	0.57
1:A:193:ASN:ND2	2:D:424:ARG:N	2.52	0.57
2:B:321:GLU:HB3	2:B:322:GLN:HE21	1.70	0.57
2:B:404:GLU:HG3	2:B:405:GLU:H	1.70	0.57
2:D:408:GLU:C	2:D:410:LEU:N	2.63	0.57
2:B:322:GLN:H	2:B:331:MET:HE1	1.69	0.57
1:C:59:LEU:HB2	1:C:67:LEU:O	2.04	0.57
2:B:387:ILE:HG22	2:B:410:LEU:HD11	1.86	0.57
2:D:386:VAL:C	2:D:388:ARG:H	2.11	0.57
1:E:116:GLN:HA	1:E:132:LEU:O	2.04	0.57
1:E:131:LYS:N	2:F:241:THR:HG23	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:MET:CB	1:A:223:PRO:HD2	2.20	0.56
2:B:320:LEU:CD2	1:E:175:PHE:CD2	2.88	0.56
1:C:209:THR:CG2	2:F:401:GLY:HA3	2.35	0.56
1:C:209:THR:HA	2:F:400:PRO:HG2	1.87	0.56
1:E:98:LEU:HB3	1:E:220:VAL:CG1	2.34	0.56
2:B:297:HIS:CD2	2:B:298:TYR:N	2.72	0.56
2:D:245:GLN:HE21	2:D:246:ASP:N	2.03	0.56
1:E:118:ILE:HD11	1:E:151:PRO:HG3	1.85	0.56
1:E:191:SER:OG	1:E:194:PHE:HB2	2.05	0.56
1:A:113:LEU:O	1:A:114:GLU:HB2	2.04	0.56
1:A:182:ARG:HG2	2:D:328:LEU:HD22	1.88	0.56
1:A:205:GLU:CA	1:A:208:GLN:HG2	2.36	0.56
2:B:357:LYS:HD3	2:B:358:ALA:H	1.70	0.56
2:B:357:LYS:HD3	2:B:358:ALA:N	2.21	0.56
2:D:246:ASP:OD1	2:D:247:LYS:N	2.27	0.56
1:E:49:TYR:HA	1:E:79:LYS:CE	2.35	0.56
1:E:130:TYR:HB3	2:F:241:THR:HG22	1.87	0.56
2:F:335:ARG:HH11	2:F:335:ARG:CG	2.16	0.56
2:B:320:LEU:CD1	2:B:333:LEU:HG	2.36	0.56
1:C:73:PHE:CZ	2:D:305:ILE:HD13	2.41	0.56
1:C:109:LEU:HD21	2:D:283:LEU:HD11	1.86	0.56
2:F:247:LYS:HD2	2:F:247:LYS:N	2.20	0.56
2:F:287:GLN:O	2:F:288:MET:HG3	2.05	0.56
1:C:224:LYS:HD3	1:C:224:LYS:C	2.31	0.56
2:D:246:ASP:OD1	2:D:249:PHE:HD2	1.88	0.56
1:A:122:VAL:HG12	2:D:386:VAL:CG2	2.36	0.56
1:A:179:SER:HB3	1:A:211:LEU:CD1	2.36	0.56
1:C:96:ASN:C	1:C:222:MET:HB2	2.30	0.56
2:D:257:ILE:H	2:D:257:ILE:CD1	2.03	0.56
2:D:269:THR:HB	2:D:270:PRO:CD	2.33	0.56
1:C:49:TYR:CE1	1:C:79:LYS:NZ	2.72	0.56
1:C:178:SER:O	1:C:180:THR:HG23	2.06	0.56
1:C:194:PHE:HZ	2:F:357:LYS:HB2	1.69	0.56
1:A:67:LEU:C	1:A:68:ARG:HG3	2.30	0.56
2:B:325:GLN:HG3	2:B:332:GLN:NE2	2.19	0.56
2:B:392:ARG:NH1	2:B:404:GLU:CA	2.69	0.56
1:C:57:LEU:CD1	2:F:326:GLN:HB3	2.28	0.56
1:C:96:ASN:ND2	1:C:152:ASP:HA	2.21	0.56
2:F:379:LEU:HB3	2:F:387:ILE:CD1	2.32	0.56
2:B:247:LYS:HB3	2:B:248:PRO:CD	2.36	0.56
2:B:322:GLN:C	2:B:324:GLN:N	2.61	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:ARG:HH11	2:B:392:ARG:CG	2.19	0.56
1:C:97:THR:HG22	1:C:220:VAL:O	2.06	0.56
2:F:254:ARG:HG3	2:F:255:ASP:H	1.69	0.56
2:B:276:LEU:HD11	2:B:283:LEU:CD1	2.34	0.55
1:C:112:VAL:HG21	1:C:132:LEU:HB2	1.86	0.55
1:C:139:LYS:NZ	1:C:141:GLN:NE2	2.54	0.55
1:C:167:ARG:HG2	2:F:350:SER:HB2	1.87	0.55
2:D:267:GLU:OE2	2:D:376:ARG:NH2	2.39	0.55
1:E:97:THR:HG22	1:E:220:VAL:O	2.06	0.55
2:B:329:GLU:HB3	1:E:182:ARG:CD	2.30	0.55
1:C:57:LEU:HD21	2:F:326:GLN:NE2	2.21	0.55
1:C:98:LEU:HG	1:C:99:LEU:N	2.20	0.55
1:C:119:LEU:HD12	1:C:148:LEU:HB2	1.89	0.55
2:D:297:HIS:HB3	2:D:378:PHE:CD1	2.41	0.55
1:E:114:GLU:CB	1:E:158:ARG:HD3	2.35	0.55
1:A:162:PHE:CE2	2:B:281:ILE:HD11	2.40	0.55
2:D:387:ILE:HA	2:D:390:ILE:CD1	2.37	0.55
2:D:395:SER:O	2:D:398:THR:N	2.40	0.55
1:E:49:TYR:HA	1:E:79:LYS:HD2	1.88	0.55
1:E:88:VAL:HG12	1:E:88:VAL:O	2.05	0.55
1:A:106:SER:O	1:A:142:ALA:HB2	2.07	0.55
1:A:151:PRO:O	1:A:152:ASP:O	2.23	0.55
2:B:258:TYR:CE2	2:B:265:LEU:HD23	2.41	0.55
2:B:366:GLY:C	2:B:367:ILE:HG13	2.31	0.55
1:C:157:LEU:HD12	1:C:158:ARG:H	1.70	0.55
2:D:258:TYR:HD2	2:D:265:LEU:CB	2.19	0.55
1:E:71:GLN:NE2	1:E:75:GLU:HB3	2.21	0.55
1:E:55:LYS:HA	1:E:55:LYS:HZ2	1.69	0.55
2:F:290:GLU:HB2	2:F:360:SER:C	2.31	0.55
1:A:110:VAL:O	1:A:137:ALA:HA	2.06	0.55
1:A:221:LYS:O	1:A:222:MET:O	2.25	0.55
2:F:325:GLN:HG3	2:F:331:MET:HB2	1.87	0.55
2:B:424:ARG:HD3	1:E:196:GLU:CD	2.31	0.55
1:C:202:PRO:O	1:C:203:TYR:C	2.49	0.55
1:E:57:LEU:HB2	1:E:69:LEU:O	2.05	0.55
2:D:246:ASP:CG	2:D:249:PHE:HD2	2.15	0.55
1:E:50:LEU:HD23	1:E:51:PHE:H	1.72	0.55
1:E:51:PHE:N	1:E:51:PHE:CD1	2.74	0.55
1:A:114:GLU:O	1:A:157:LEU:HD12	2.07	0.55
1:C:57:LEU:HD22	2:F:326:GLN:HB3	1.88	0.55
1:C:200:ASP:O	2:F:412:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:SER:O	1:E:187:LEU:N	2.40	0.55
1:A:49:TYR:HD2	2:B:336:TYR:OH	1.90	0.55
1:C:56:PHE:HB3	1:C:68:ARG:HB3	1.87	0.55
1:C:85:ASP:O	1:C:165:THR:OG1	2.24	0.55
1:C:168:ARG:NH2	2:F:322:GLN:CA	2.70	0.55
1:C:196:GLU:OE1	2:F:424:ARG:NH1	2.40	0.55
1:E:212:GLN:HG2	1:E:213:GLU:N	2.18	0.55
1:C:168:ARG:HH22	2:F:322:GLN:CA	2.20	0.54
2:F:247:LYS:CB	2:F:248:PRO:CD	2.85	0.54
2:F:306:LEU:HD22	2:F:364:MET:HE2	1.88	0.54
1:A:148:LEU:HD21	1:A:159:ILE:HD13	1.89	0.54
1:A:179:SER:HB3	1:A:211:LEU:HD12	1.89	0.54
1:A:205:GLU:N	1:A:208:GLN:HG2	2.23	0.54
1:C:49:TYR:CD1	1:C:79:LYS:HD3	2.42	0.54
2:F:382:HIS:HB2	2:F:415:GLU:O	2.07	0.54
1:A:80:LEU:O	1:A:83:LEU:HB2	2.07	0.54
2:B:300:SER:C	2:B:301:ARG:HG3	2.31	0.54
1:C:190:PHE:HB2	1:C:195:LEU:HD21	1.89	0.54
2:D:321:GLU:HG3	2:D:352:PHE:HZ	1.72	0.54
2:B:404:GLU:O	2:B:408:GLU:N	2.23	0.54
2:D:270:PRO:HG3	2:D:371:ALA:HB3	1.88	0.54
1:E:78:GLU:O	1:E:81:GLU:HG2	2.08	0.54
2:F:281:ILE:HD11	2:F:369:VAL:HG12	1.89	0.54
1:A:108:LEU:HD22	1:A:161:LYS:HG3	1.90	0.54
1:C:92:CYS:SG	1:C:93:SER:N	2.81	0.54
1:C:223:PRO:HG3	2:F:397:LEU:CD1	2.38	0.54
2:D:394:VAL:O	2:D:398:THR:OG1	2.25	0.54
2:F:262:TYR:CE2	2:F:420:ASP:HB2	2.42	0.54
1:E:158:ARG:HH12	2:F:309:ASN:HD21	1.54	0.54
2:B:357:LYS:HB2	1:E:194:PHE:HE1	1.71	0.54
1:C:178:SER:HB2	1:C:180:THR:CG2	2.38	0.54
2:D:389:GLN:O	2:D:391:PRO:HD3	2.07	0.54
1:A:79:LYS:CE	2:B:321:GLU:HG2	2.36	0.53
2:B:298:TYR:HB3	2:B:353:PRO:HA	1.90	0.53
2:D:413:GLN:OE1	2:D:415:GLU:N	2.40	0.53
1:E:212:GLN:HB3	1:E:214:GLU:N	2.24	0.53
2:B:292:ALA:O	2:B:358:ALA:N	2.34	0.53
2:B:386:VAL:HG22	1:E:122:VAL:HG12	1.86	0.53
2:D:257:ILE:HG12	2:D:265:LEU:O	2.07	0.53
2:D:413:GLN:CD	2:D:419:VAL:HG11	2.33	0.53
1:E:119:LEU:HD12	1:E:148:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:ARG:NH1	2:F:309:ASN:HD21	2.06	0.53
1:A:210:LEU:HD11	1:A:211:LEU:HB2	1.89	0.53
1:A:219:ILE:HD12	1:A:219:ILE:H	1.73	0.53
2:B:424:ARG:NH2	1:E:192:LYS:NZ	2.57	0.53
2:D:246:ASP:HA	2:D:249:PHE:CB	2.37	0.53
2:F:396:ASP:HB2	2:F:402:SER:HA	1.90	0.53
2:B:276:LEU:HG	2:B:281:ILE:O	2.07	0.53
1:C:136:ASP:OD1	2:D:252:ARG:HD3	2.08	0.53
1:E:119:LEU:HD12	1:E:148:LEU:HD11	1.89	0.53
1:C:94:LYS:HB3	1:C:95:PRO:CD	2.38	0.53
2:D:301:ARG:NH2	2:D:370:ASN:ND2	2.57	0.53
1:E:120:VAL:HA	1:E:128:ASP:O	2.09	0.53
2:F:316:GLU:HG2	2:F:337:ALA:HB2	1.90	0.53
2:F:386:VAL:C	2:F:388:ARG:H	2.17	0.53
2:B:247:LYS:HA	2:B:247:LYS:HZ2	1.72	0.53
1:C:131:LYS:O	1:C:131:LYS:CD	2.56	0.53
2:D:245:GLN:HG2	2:D:249:PHE:CG	2.43	0.53
1:E:132:LEU:CD2	2:F:250:ASN:ND2	2.71	0.53
2:F:388:ARG:HH11	2:F:388:ARG:CB	2.19	0.53
1:A:215:GLN:CG	1:A:216:GLU:H	2.22	0.53
2:B:325:GLN:O	2:B:327:GLY:N	2.39	0.53
1:E:192:LYS:HG3	1:E:203:TYR:CG	2.44	0.53
2:F:315:VAL:HG12	2:F:316:GLU:N	2.20	0.53
2:F:378:PHE:HB2	2:F:384:GLU:C	2.34	0.53
1:A:56:PHE:CE2	1:A:90:GLU:HB2	2.43	0.53
2:B:340:LEU:HD13	2:B:340:LEU:H	1.73	0.53
2:B:389:GLN:CA	1:E:127:ARG:NH2	2.71	0.53
1:C:213:GLU:O	1:C:215:GLN:N	2.42	0.53
2:D:257:ILE:HG13	2:D:265:LEU:CD1	2.38	0.53
2:D:297:HIS:O	2:D:353:PRO:HA	2.09	0.53
2:D:414:LYS:HZ2	2:D:414:LYS:N	2.05	0.53
2:B:322:GLN:HE22	2:B:332:GLN:CD	2.17	0.53
1:E:82:ASN:C	1:E:84:ARG:H	2.17	0.53
1:E:139:LYS:HD3	2:F:279:LEU:CD1	2.38	0.53
2:F:242:LEU:CB	2:F:244:SER:H	2.22	0.53
2:B:334:ARG:HD3	2:B:336:TYR:CE2	2.44	0.52
2:D:320:LEU:HA	2:D:331:MET:CE	2.39	0.52
1:E:220:VAL:HG13	1:E:221:LYS:C	2.34	0.52
2:B:299:ASN:HB3	2:B:374:ASN:OD1	2.09	0.52
2:B:399:PHE:HB3	1:E:209:THR:HA	1.91	0.52
1:E:81:GLU:O	1:E:84:ARG:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:LEU:HB3	1:E:101:PRO:CD	2.39	0.52
1:E:100:LEU:CB	1:E:101:PRO:HD2	2.39	0.52
1:A:222:MET:HB2	1:A:224:LYS:C	2.34	0.52
2:B:241:THR:O	2:B:241:THR:HG22	2.10	0.52
2:B:331:MET:CE	2:B:332:GLN:NE2	2.68	0.52
1:C:168:ARG:HH12	2:F:321:GLU:CB	2.19	0.52
1:E:109:LEU:HB3	1:E:162:PHE:HB3	1.91	0.52
1:A:52:ARG:NH1	1:A:54:ASN:OD1	2.43	0.52
1:A:172:VAL:CG2	1:A:173:GLU:N	2.73	0.52
1:C:122:VAL:HG12	2:F:386:VAL:HG22	1.90	0.52
1:E:119:LEU:HD11	1:E:140:ILE:HD11	1.90	0.52
2:F:422:GLN:HB2	2:F:423:PRO:HD3	1.91	0.52
2:F:422:GLN:O	2:F:423:PRO:O	2.28	0.52
2:B:424:ARG:NH2	1:E:192:LYS:HZ2	2.07	0.52
1:C:132:LEU:N	1:C:132:LEU:CD1	2.70	0.52
2:D:325:GLN:C	2:D:330:SER:HB3	2.34	0.52
1:E:212:GLN:NE2	1:E:214:GLU:HB2	2.22	0.52
2:F:269:THR:HB	2:F:270:PRO:CD	2.39	0.52
2:F:282:LEU:HB3	2:F:371:ALA:CB	2.40	0.52
2:F:422:GLN:NE2	2:F:422:GLN:C	2.68	0.52
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.23	0.52
1:E:118:ILE:HD12	1:E:151:PRO:HG3	1.91	0.52
1:E:196:GLU:HA	1:E:206:ILE:HD11	1.92	0.52
1:A:60:PHE:HD2	1:A:182:ARG:HE	1.58	0.52
2:D:387:ILE:HG22	2:D:387:ILE:O	2.09	0.52
1:A:101:PRO:HD2	2:D:398:THR:HG23	1.91	0.52
1:C:131:LYS:HZ2	1:C:133:ASP:CG	2.16	0.52
1:C:132:LEU:CD1	2:D:250:ASN:ND2	2.73	0.52
1:E:114:GLU:HB3	1:E:158:ARG:HG3	1.92	0.52
2:F:316:GLU:HG2	2:F:337:ALA:CB	2.40	0.52
1:C:49:TYR:CD2	2:D:336:TYR:OH	2.60	0.52
1:C:86:TYR:CE1	2:D:369:VAL:HG11	2.44	0.52
2:D:258:TYR:HD1	2:D:417:TYR:CZ	2.26	0.52
1:E:88:VAL:HG23	1:E:162:PHE:HD1	1.75	0.52
2:F:403:GLY:O	2:F:407:GLU:HB2	2.08	0.52
1:A:72:ARG:HH22	2:D:323:GLN:HB3	1.75	0.52
1:A:172:VAL:CG2	1:A:173:GLU:H	2.23	0.52
1:C:49:TYR:HE1	1:C:79:LYS:CE	2.21	0.52
1:E:158:ARG:HH12	2:F:309:ASN:ND2	2.08	0.52
1:A:72:ARG:NH1	2:D:323:GLN:O	2.30	0.51
1:A:127:ARG:HH12	2:D:389:GLN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:SER:O	2:B:245:GLN:NE2	2.43	0.51
2:B:290:GLU:N	2:B:361:ASP:OD1	2.43	0.51
1:C:47:ASN:ND2	1:C:50:LEU:O	2.42	0.51
1:C:105:ASP:N	1:C:105:ASP:OD1	2.43	0.51
1:C:212:GLN:CD	1:C:213:GLU:H	2.18	0.51
2:D:293:LEU:HB2	2:D:357:LYS:HA	1.91	0.51
1:E:51:PHE:N	1:E:51:PHE:HD1	2.08	0.51
1:E:134:GLN:O	2:F:252:ARG:HD3	2.10	0.51
1:A:182:ARG:HG2	2:D:328:LEU:CD2	2.40	0.51
1:A:186:TYR:CE1	1:A:187:LEU:HD23	2.45	0.51
2:B:351:SER:HB3	1:E:103:HIS:CD2	2.45	0.51
2:F:413:GLN:OE1	2:F:413:GLN:HA	2.10	0.51
1:A:122:VAL:O	1:A:145:PRO:HD2	2.10	0.51
2:B:321:GLU:HB3	2:B:322:GLN:NE2	2.25	0.51
2:B:328:LEU:N	2:B:331:MET:HB2	2.15	0.51
1:C:49:TYR:CD1	1:C:79:LYS:CD	2.93	0.51
1:C:168:ARG:HH22	2:F:322:GLN:N	2.07	0.51
1:C:212:GLN:CG	1:C:213:GLU:N	2.73	0.51
2:D:303:THR:O	2:D:368:GLY:HA2	2.10	0.51
2:D:323:GLN:HE21	2:D:323:GLN:CA	2.09	0.51
1:E:88:VAL:HG23	1:E:162:PHE:CD1	2.46	0.51
1:E:139:LYS:HD3	2:F:279:LEU:HD13	1.92	0.51
1:E:192:LYS:NZ	1:E:203:TYR:HD2	2.02	0.51
1:E:213:GLU:O	1:E:215:GLN:N	2.43	0.51
2:F:273:ASN:OD1	2:F:275:GLN:HB2	2.10	0.51
1:A:150:ASN:C	1:A:150:ASN:ND2	2.68	0.51
2:D:258:TYR:CD1	2:D:417:TYR:CE1	2.95	0.51
1:E:74:ASN:OD1	1:E:84:ARG:HB2	2.10	0.51
2:B:270:PRO:O	2:B:277:ARG:HD2	2.10	0.51
2:B:313:ALA:N	2:B:340:LEU:O	2.39	0.51
2:B:322:GLN:HE21	2:B:322:GLN:H	1.57	0.51
2:B:325:GLN:OE1	2:B:325:GLN:HA	2.10	0.51
1:C:44:ALA:O	1:C:45:GLN:HG3	2.11	0.51
2:F:306:LEU:HB3	2:F:364:MET:CE	2.40	0.51
1:A:111:LEU:HD11	1:A:160:LEU:CD2	2.39	0.51
1:A:127:ARG:CZ	2:D:389:GLN:HB3	2.41	0.51
2:F:262:TYR:HE2	2:F:420:ASP:HB2	1.75	0.51
1:A:134:GLN:NE2	1:A:135:GLY:N	2.49	0.51
2:B:317:LEU:HD23	2:B:318:VAL:N	2.25	0.51
1:C:112:VAL:HG21	1:C:132:LEU:CB	2.41	0.51
2:D:294:PHE:CD1	2:D:418:PHE:CE1	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:315:VAL:O	2:F:337:ALA:HB1	2.10	0.51
2:F:352:PHE:N	2:F:352:PHE:HD1	2.08	0.51
2:B:268:ILE:HG22	2:B:276:LEU:HD23	1.93	0.51
2:B:402:SER:O	2:B:404:GLU:N	2.44	0.51
1:C:121:LEU:HD11	1:C:140:ILE:HG12	1.93	0.51
1:E:117:ALA:N	1:E:132:LEU:O	2.44	0.51
1:E:121:LEU:HD13	1:E:121:LEU:N	2.25	0.51
1:E:138:ILE:CG1	1:E:139:LYS:N	2.74	0.51
2:B:413:GLN:OE1	2:B:414:LYS:N	2.44	0.51
1:E:67:LEU:HD12	1:E:90:GLU:O	2.11	0.51
1:A:94:LYS:HG2	1:A:95:PRO:HD3	1.93	0.51
2:B:347:VAL:O	2:B:349:PRO:HD2	2.11	0.51
1:C:186:TYR:C	1:C:188:SER:N	2.69	0.51
1:A:105:ASP:OD2	1:A:167:ARG:NH1	2.44	0.50
1:A:124:PRO:O	2:D:384:GLU:HA	2.11	0.50
1:C:132:LEU:HD11	2:D:250:ASN:ND2	2.26	0.50
2:F:422:GLN:CB	2:F:423:PRO:HD2	2.41	0.50
1:A:79:LYS:HD2	2:B:321:GLU:CD	2.37	0.50
2:F:247:LYS:N	2:F:247:LYS:CD	2.75	0.50
1:A:77:THR:HG21	1:A:80:LEU:CD1	2.41	0.50
1:A:147:TYR:CE2	2:D:394:VAL:HG11	2.47	0.50
2:D:245:GLN:CG	2:D:246:ASP:N	2.74	0.50
2:D:319:GLY:O	2:D:320:LEU:HD22	2.11	0.50
1:E:83:LEU:CD1	2:F:347:VAL:HG11	2.39	0.50
1:E:119:LEU:O	1:E:129:THR:HA	2.11	0.50
2:F:297:HIS:HB2	2:F:377:ASN:O	2.11	0.50
1:C:213:GLU:HB3	1:C:215:GLN:OE1	2.11	0.50
2:D:352:PHE:CD1	2:D:352:PHE:N	2.79	0.50
1:E:168:ARG:HB3	1:E:171:THR:HB	1.92	0.50
2:B:296:PRO:O	2:B:297:HIS:HB3	2.12	0.50
2:D:386:VAL:C	2:D:388:ARG:N	2.69	0.50
1:E:91:TYR:OH	1:E:93:SER:HB3	2.12	0.50
2:F:305:ILE:O	2:F:366:GLY:HA2	2.12	0.50
1:A:172:VAL:HG22	1:A:173:GLU:N	2.26	0.50
2:F:247:LYS:HB3	2:F:248:PRO:CD	2.42	0.50
2:F:420:ASP:OD1	2:F:422:GLN:N	2.45	0.50
1:C:84:ARG:HB2	1:C:84:ARG:CZ	2.41	0.50
2:D:247:LYS:HB2	2:D:248:PRO:HD2	1.94	0.50
1:E:206:ILE:O	1:E:208:GLN:N	2.45	0.50
1:A:72:ARG:NH2	1:A:171:THR:OG1	2.45	0.50
2:B:297:HIS:HD2	2:B:298:TYR:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:376:ARG:HG2	2:D:376:ARG:HH11	1.76	0.50
1:E:179:SER:CB	1:E:211:LEU:HB2	2.42	0.50
2:F:352:PHE:N	2:F:352:PHE:CD1	2.79	0.50
2:F:422:GLN:CB	2:F:423:PRO:CD	2.89	0.50
1:A:59:LEU:O	1:A:60:PHE:HB2	2.11	0.49
1:E:88:VAL:CG2	1:E:162:PHE:HD1	2.24	0.49
2:F:399:PHE:C	2:F:401:GLY:H	2.20	0.49
2:F:402:SER:O	2:F:404:GLU:N	2.45	0.49
2:B:248:PRO:CB	2:B:275:GLN:NE2	2.76	0.49
2:B:295:VAL:HG12	2:B:296:PRO:O	2.12	0.49
1:C:123:ASN:O	2:F:389:GLN:HG3	2.12	0.49
2:F:379:LEU:HA	2:F:385:ASN:OD1	2.12	0.49
1:A:51:PHE:HZ	2:B:321:GLU:OE2	1.96	0.49
1:A:176:PHE:CZ	1:A:218:VAL:CG1	2.95	0.49
1:A:179:SER:CB	1:A:211:LEU:CD1	2.90	0.49
2:B:322:GLN:NE2	2:B:322:GLN:H	2.11	0.49
2:B:268:ILE:HG22	2:B:276:LEU:HD22	1.93	0.49
1:C:95:PRO:O	1:C:221:LYS:NZ	2.41	0.49
2:D:248:PRO:HA	2:D:275:GLN:HE22	1.76	0.49
1:E:110:VAL:CG1	1:E:140:ILE:HG13	2.42	0.49
2:D:413:GLN:C	2:D:415:GLU:H	2.20	0.49
2:F:306:LEU:CD1	2:F:364:MET:HE1	2.36	0.49
2:B:331:MET:CE	2:B:332:GLN:HE22	2.23	0.49
2:D:396:ASP:OD2	2:D:403:GLY:N	2.46	0.49
1:E:69:LEU:HD12	1:E:89:LEU:HD23	1.93	0.49
1:E:130:TYR:CE1	2:F:242:LEU:HD12	2.48	0.49
2:F:317:LEU:HD13	2:F:336:TYR:HB2	1.95	0.49
2:D:383:LYS:HD2	2:D:384:GLU:HG3	1.95	0.49
1:E:177:LEU:O	1:E:185:SER:HB2	2.13	0.49
1:A:56:PHE:CD1	1:A:70:LEU:HD13	2.47	0.49
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.23	0.49
1:A:129:THR:HG22	1:A:130:TYR:N	2.27	0.49
1:E:60:PHE:CZ	1:E:67:LEU:HD23	2.48	0.49
2:F:296:PRO:HA	2:F:354:VAL:O	2.13	0.49
2:F:387:ILE:HA	2:F:390:ILE:HD12	1.94	0.49
1:C:130:TYR:HD1	2:D:242:LEU:CD1	2.26	0.49
2:F:242:LEU:HB2	2:F:245:GLN:HG2	1.94	0.49
2:F:325:GLN:NE2	2:F:330:SER:CB	2.76	0.49
2:B:269:THR:HB	2:B:270:PRO:HD2	1.95	0.48
2:B:363:ASN:OD1	2:B:364:MET:O	2.31	0.48
2:D:360:SER:O	2:D:361:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:383:LYS:CD	2:D:384:GLU:N	2.63	0.48
1:A:49:TYR:CD2	2:B:336:TYR:HE2	2.31	0.48
1:A:72:ARG:NH2	2:D:323:GLN:HB3	2.27	0.48
1:A:111:LEU:HB3	1:A:137:ALA:HB2	1.95	0.48
1:C:49:TYR:CD1	1:C:79:LYS:CE	2.96	0.48
2:D:280:ASP:C	2:D:281:ILE:HG12	2.38	0.48
1:E:192:LYS:HZ3	1:E:203:TYR:CB	2.25	0.48
2:F:315:VAL:HG21	2:F:340:LEU:CD2	2.43	0.48
2:F:420:ASP:OD1	2:F:422:GLN:HB3	2.13	0.48
1:A:100:LEU:HB3	1:A:101:PRO:CD	2.41	0.48
1:A:215:GLN:CG	1:A:216:GLU:N	2.76	0.48
1:E:109:LEU:HD21	2:F:283:LEU:HD21	1.94	0.48
2:F:328:LEU:HB3	2:F:329:GLU:OE2	2.14	0.48
1:A:93:SER:O	1:A:156:ASN:HB3	2.12	0.48
2:B:288:MET:HE2	2:B:358:ALA:HB2	1.95	0.48
2:B:328:LEU:HD22	1:E:182:ARG:HD2	1.96	0.48
1:C:117:ALA:C	1:C:118:ILE:HD12	2.39	0.48
2:D:242:LEU:CG	2:D:245:GLN:HB2	2.37	0.48
2:D:255:ASP:HA	2:D:256:PRO:HD3	1.63	0.48
2:D:404:GLU:CG	2:D:405:GLU:N	2.73	0.48
1:E:179:SER:HB2	1:E:211:LEU:HB2	1.95	0.48
2:F:265:LEU:HD12	2:F:266:TYR:N	2.28	0.48
2:F:394:VAL:O	2:F:397:LEU:N	2.38	0.48
1:A:86:TYR:HA	1:A:163:ALA:O	2.14	0.48
1:C:112:VAL:CG2	1:C:132:LEU:HB2	2.43	0.48
1:C:177:LEU:O	1:C:185:SER:CB	2.58	0.48
1:C:212:GLN:HG3	1:C:213:GLU:N	2.29	0.48
2:D:320:LEU:CB	2:D:331:MET:HE2	2.43	0.48
1:E:86:TYR:CE1	1:E:164:ILE:HG23	2.48	0.48
1:A:179:SER:O	1:A:180:THR:HG23	2.13	0.48
1:A:196:GLU:O	1:A:200:ASP:N	2.47	0.48
1:A:210:LEU:CD1	1:A:211:LEU:N	2.56	0.48
2:B:242:LEU:O	2:B:245:GLN:HB3	2.12	0.48
2:B:293:LEU:HD22	1:E:197:ALA:HB3	1.95	0.48
2:B:404:GLU:C	2:B:406:VAL:N	2.71	0.48
1:E:130:TYR:CB	2:F:241:THR:HG22	2.43	0.48
2:F:322:GLN:O	2:F:323:GLN:NE2	2.47	0.48
1:A:60:PHE:HA	1:A:182:ARG:HH21	1.79	0.48
1:A:69:LEU:C	1:A:69:LEU:CD1	2.80	0.48
2:B:297:HIS:HB2	2:B:377:ASN:O	2.14	0.48
2:B:389:GLN:CA	1:E:127:ARG:HH21	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:CD2	1:C:219:ILE:HG13	2.43	0.48
2:D:414:LYS:NZ	2:D:414:LYS:N	2.62	0.48
1:E:60:PHE:CZ	1:E:67:LEU:CD2	2.96	0.48
1:E:70:LEU:HD12	1:E:71:GLN:N	2.26	0.48
1:E:77:THR:CG2	1:E:79:LYS:HG3	2.25	0.48
2:F:404:GLU:O	2:F:405:GLU:C	2.57	0.48
1:C:83:LEU:HD21	2:D:369:VAL:CG2	2.43	0.48
1:C:156:ASN:OD1	1:C:156:ASN:N	2.46	0.48
2:D:300:SER:OG	2:D:374:ASN:HA	2.13	0.48
1:E:130:TYR:CE1	2:F:242:LEU:HB2	2.49	0.48
2:F:335:ARG:HG2	2:F:335:ARG:NH1	2.29	0.48
1:A:112:VAL:HG12	1:A:134:GLN:HB2	1.96	0.47
2:B:297:HIS:O	2:B:353:PRO:HA	2.14	0.47
2:D:258:TYR:CD2	2:D:265:LEU:HB3	2.42	0.47
2:F:282:LEU:HB3	2:F:371:ALA:HB1	1.96	0.47
1:A:96:ASN:C	1:A:97:THR:HG23	2.38	0.47
2:B:246:ASP:OD1	2:B:249:PHE:CZ	2.68	0.47
2:B:321:GLU:OE1	2:B:352:PHE:HE2	1.96	0.47
1:C:62:ASN:ND2	1:C:216:GLU:CD	2.72	0.47
1:A:111:LEU:CD2	2:B:283:LEU:HD22	2.44	0.47
2:D:260:ASN:HD21	2:D:418:PHE:HB2	1.80	0.47
1:E:94:LYS:HB3	1:E:95:PRO:HD2	1.96	0.47
2:F:388:ARG:HH11	2:F:388:ARG:CG	2.27	0.47
1:A:129:THR:CG2	1:A:130:TYR:N	2.76	0.47
1:C:100:LEU:HB3	1:C:101:PRO:HD2	1.96	0.47
2:B:296:PRO:HA	2:B:355:ALA:HB2	1.96	0.47
2:B:392:ARG:NH1	2:B:404:GLU:HA	2.20	0.47
1:C:179:SER:C	1:C:180:THR:CG2	2.87	0.47
2:B:318:VAL:HG22	1:E:189:ALA:CB	2.44	0.47
1:C:190:PHE:HB2	1:C:195:LEU:CD2	2.45	0.47
2:D:320:LEU:N	2:D:321:GLU:OE2	2.47	0.47
2:F:265:LEU:CD1	2:F:266:TYR:N	2.78	0.47
2:F:324:GLN:CD	2:F:324:GLN:N	2.72	0.47
1:A:49:TYR:CD2	2:B:336:TYR:CE2	3.03	0.47
1:A:182:ARG:CG	2:D:328:LEU:HD22	2.44	0.47
1:A:205:GLU:HA	1:A:208:GLN:HG2	1.92	0.47
1:A:215:GLN:C	1:A:217:GLY:N	2.71	0.47
2:B:361:ASP:N	2:B:361:ASP:OD1	2.45	0.47
1:C:57:LEU:CD1	2:F:326:GLN:HA	2.43	0.47
1:C:61:LYS:O	1:C:62:ASN:HB3	2.15	0.47
1:C:84:ARG:HH21	1:C:169:PRO:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ASP:CB	2:F:351:SER:HB2	2.44	0.47
2:D:258:TYR:CD1	2:D:417:TYR:CD1	3.03	0.47
2:D:293:LEU:HA	2:D:357:LYS:HA	1.96	0.47
2:F:381:GLY:HA2	2:F:413:GLN:CG	2.44	0.47
1:A:44:ALA:C	1:A:46:ASN:N	2.68	0.47
2:B:328:LEU:CD2	1:E:182:ARG:CG	2.93	0.47
2:D:337:ALA:O	2:D:338:ALA:HB2	2.15	0.47
1:E:202:PRO:HD2	1:E:205:GLU:OE1	2.15	0.47
2:F:325:GLN:HG3	2:F:331:MET:HG2	1.95	0.47
1:A:123:ASN:HB3	1:A:124:PRO:HD3	1.97	0.47
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.61	0.47
2:B:320:LEU:HD23	1:E:174:ASP:O	2.15	0.47
1:E:223:PRO:CG	1:E:224:LYS:N	2.78	0.47
1:A:214:GLU:HG3	1:A:217:GLY:CA	2.44	0.47
2:B:281:ILE:O	2:B:281:ILE:HG22	2.13	0.47
2:D:320:LEU:O	2:D:320:LEU:HG	2.15	0.47
1:E:153:ASN:C	1:E:155:GLN:H	2.22	0.47
2:B:321:GLU:HG3	2:B:322:GLN:HG3	1.98	0.46
2:D:306:LEU:CB	2:D:346:ILE:CG2	2.93	0.46
1:E:113:LEU:HD11	1:E:160:LEU:HB2	1.97	0.46
1:A:91:TYR:HB3	1:A:159:ILE:CG2	2.44	0.46
1:A:112:VAL:HG12	1:A:134:GLN:HA	1.95	0.46
1:A:151:PRO:O	1:A:152:ASP:C	2.58	0.46
1:C:118:ILE:HA	1:C:130:TYR:O	2.15	0.46
1:C:148:LEU:HD12	1:C:148:LEU:C	2.40	0.46
2:D:352:PHE:N	2:D:352:PHE:HD1	2.13	0.46
1:A:84:ARG:CG	1:A:84:ARG:NH1	2.76	0.46
1:A:153:ASN:CG	1:A:154:ASN:H	2.16	0.46
2:B:328:LEU:N	2:B:331:MET:CB	2.77	0.46
2:B:333:LEU:HD11	1:E:186:TYR:HA	1.98	0.46
2:B:392:ARG:NH1	2:B:404:GLU:HB3	2.30	0.46
2:B:404:GLU:O	2:B:407:GLU:N	2.48	0.46
1:C:142:ALA:HB3	1:C:166:PHE:CE2	2.51	0.46
1:E:130:TYR:CZ	2:F:242:LEU:HD12	2.50	0.46
1:A:152:ASP:O	1:A:153:ASN:CB	2.64	0.46
1:A:159:ILE:HG22	1:A:159:ILE:O	2.16	0.46
1:C:79:LYS:CE	2:D:322:GLN:NE2	2.76	0.46
1:C:118:ILE:CD1	1:C:151:PRO:CG	2.94	0.46
2:D:414:LYS:HA	2:D:414:LYS:HD3	1.67	0.46
1:A:56:PHE:HE2	1:A:90:GLU:HB2	1.80	0.46
1:A:60:PHE:CD1	1:A:60:PHE:C	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:TYR:HB3	2:F:241:THR:HG21	1.98	0.46
1:E:136:ASP:HA	2:F:251:LEU:O	2.15	0.46
1:A:70:LEU:CG	1:A:71:GLN:N	2.77	0.46
2:B:277:ARG:NH1	2:B:372:GLU:OE2	2.48	0.46
2:B:404:GLU:H	2:B:404:GLU:HG2	1.26	0.46
1:A:70:LEU:O	1:A:87:ARG:NH2	2.48	0.46
1:A:205:GLU:CA	1:A:208:GLN:CG	2.92	0.46
1:C:67:LEU:HD12	1:C:68:ARG:N	2.31	0.46
1:C:132:LEU:HB3	1:C:136:ASP:CB	2.45	0.46
1:C:142:ALA:HB3	1:C:166:PHE:CZ	2.49	0.46
2:D:258:TYR:HE2	2:D:265:LEU:HD12	1.79	0.46
2:F:282:LEU:HD23	2:F:282:LEU:O	2.16	0.46
2:B:356:LEU:C	2:B:356:LEU:HD23	2.41	0.46
1:E:180:THR:C	1:E:182:ARG:N	2.73	0.46
1:A:168:ARG:HB3	1:A:168:ARG:CZ	2.46	0.46
1:A:177:LEU:O	1:A:185:SER:HB2	2.15	0.46
1:A:206:ILE:O	1:A:207:GLU:C	2.57	0.46
1:C:73:PHE:O	1:C:80:LEU:HD11	2.16	0.46
2:D:408:GLU:HA	2:D:411:GLU:HG2	1.97	0.46
1:E:50:LEU:C	1:E:51:PHE:HD1	2.24	0.46
2:F:242:LEU:HB3	2:F:244:SER:N	2.30	0.46
1:A:186:TYR:C	1:A:188:SER:H	2.24	0.46
2:B:320:LEU:HD12	2:B:333:LEU:HG	1.97	0.46
1:C:47:ASN:H	1:C:76:ASP:CB	2.09	0.46
1:C:79:LYS:NZ	2:D:322:GLN:CD	2.74	0.46
1:C:168:ARG:NH2	2:F:322:GLN:CB	2.79	0.46
2:D:245:GLN:NE2	2:D:245:GLN:H	2.14	0.46
2:D:266:TYR:O	2:D:284:ASN:HB2	2.15	0.46
2:D:315:VAL:HB	2:D:356:LEU:CD2	2.46	0.46
2:F:325:GLN:OE1	2:F:331:MET:HG2	2.15	0.46
1:A:168:ARG:HH11	1:A:168:ARG:HG2	1.80	0.45
2:B:273:ASN:HB3	2:B:276:LEU:HB2	1.97	0.45
1:C:114:GLU:HB2	1:C:158:ARG:HH11	1.80	0.45
1:C:183:LEU:HA	1:C:184:PRO:HD3	1.84	0.45
1:E:206:ILE:C	1:E:208:GLN:N	2.74	0.45
2:B:300:SER:HB3	2:B:375:GLU:H	1.81	0.45
1:C:95:PRO:HA	1:C:150:ASN:ND2	2.32	0.45
1:C:209:THR:HG21	2:F:401:GLY:HA3	1.96	0.45
2:D:247:LYS:CB	2:D:248:PRO:HD2	2.46	0.45
1:A:68:ARG:NH1	1:A:90:GLU:OE1	2.49	0.45
1:A:86:TYR:O	1:A:87:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:GLY:O	2:B:371:ALA:HB2	2.16	0.45
1:C:192:LYS:HB2	1:C:192:LYS:NZ	2.20	0.45
2:D:316:GLU:HG2	2:D:337:ALA:HB2	1.97	0.45
1:A:127:ARG:NH1	2:D:389:GLN:CA	2.78	0.45
2:B:328:LEU:O	2:B:329:GLU:CB	2.62	0.45
1:C:64:HIS:CD2	1:C:97:THR:HG22	2.49	0.45
1:E:98:LEU:N	1:E:220:VAL:HG12	2.28	0.45
1:A:88:VAL:O	1:A:89:LEU:HD23	2.16	0.45
1:A:122:VAL:CG1	2:D:386:VAL:HG22	2.43	0.45
1:A:197:ALA:O	1:A:198:SER:C	2.56	0.45
2:B:295:VAL:CG1	2:B:296:PRO:CD	2.91	0.45
2:B:381:GLY:O	2:B:385:ASN:ND2	2.38	0.45
2:B:387:ILE:C	2:B:390:ILE:HD12	2.42	0.45
2:F:315:VAL:HG21	2:F:340:LEU:HD21	1.98	0.45
2:F:329:GLU:O	2:F:330:SER:C	2.60	0.45
2:F:402:SER:OG	2:F:405:GLU:HB2	2.17	0.45
1:A:134:GLN:O	1:A:134:GLN:HG3	2.15	0.45
2:B:325:GLN:CG	2:B:332:GLN:HE21	2.25	0.45
1:C:78:GLU:HB3	2:D:322:GLN:NE2	2.31	0.45
1:C:186:TYR:HE1	2:F:379:LEU:HD13	1.81	0.45
1:E:77:THR:HG23	1:E:79:LYS:N	2.24	0.45
1:E:196:GLU:HG2	1:E:203:TYR:HB2	1.99	0.45
1:A:137:ALA:O	2:B:250:ASN:HB3	2.16	0.45
1:E:100:LEU:HD12	1:E:218:VAL:HA	1.98	0.45
2:B:290:GLU:CB	2:B:360:SER:HA	2.47	0.45
2:B:422:GLN:O	2:B:423:PRO:O	2.34	0.45
1:C:46:ASN:HB3	1:C:76:ASP:O	2.17	0.45
1:C:52:ARG:N	2:D:346:ILE:CD1	2.80	0.45
1:C:109:LEU:CD2	2:D:283:LEU:HD11	2.47	0.45
1:C:122:VAL:HG13	2:F:389:GLN:HB3	1.99	0.45
1:C:168:ARG:HH21	2:F:322:GLN:HB3	1.82	0.45
1:C:194:PHE:CD2	2:F:316:GLU:OE2	2.70	0.45
1:C:213:GLU:C	1:C:215:GLN:N	2.75	0.45
2:D:334:ARG:HD2	2:D:335:ARG:O	2.17	0.45
2:D:387:ILE:C	2:D:390:ILE:HG13	2.42	0.45
2:B:372:GLU:O	2:B:374:ASN:N	2.50	0.45
1:C:96:ASN:C	1:C:222:MET:H	2.25	0.45
1:E:46:ASN:HD21	1:E:48:PRO:CG	2.29	0.45
2:B:328:LEU:C	2:B:330:SER:N	2.67	0.45
1:C:95:PRO:HA	1:C:150:ASN:HD21	1.81	0.45
2:D:245:GLN:NE2	2:D:246:ASP:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:O	1:A:49:TYR:HB2	2.16	0.44
2:B:328:LEU:HD21	1:E:182:ARG:CG	2.46	0.44
1:C:173:GLU:OE1	1:C:173:GLU:HA	2.17	0.44
1:C:202:PRO:O	1:C:204:ASP:N	2.50	0.44
1:C:212:GLN:CD	1:C:213:GLU:N	2.75	0.44
2:D:242:LEU:HD23	2:D:245:GLN:HB3	1.98	0.44
2:F:413:GLN:OE1	2:F:413:GLN:CA	2.64	0.44
1:A:77:THR:HG21	1:A:80:LEU:HD12	1.98	0.44
2:B:328:LEU:CD2	1:E:182:ARG:CD	2.95	0.44
1:C:47:ASN:HA	1:C:48:PRO:HD2	1.54	0.44
1:C:132:LEU:HB3	1:C:136:ASP:HB2	2.00	0.44
2:F:274:SER:O	2:F:277:ARG:HB3	2.17	0.44
2:F:293:LEU:CD1	2:F:357:LYS:HG3	2.42	0.44
2:B:276:LEU:HD21	2:B:283:LEU:HD12	1.99	0.44
2:B:282:LEU:C	2:B:282:LEU:CD1	2.90	0.44
1:C:149:ILE:CG2	1:C:150:ASN:N	2.79	0.44
1:C:212:GLN:CD	1:C:214:GLU:H	2.25	0.44
2:D:249:PHE:CD1	2:D:249:PHE:C	2.94	0.44
2:D:334:ARG:CD	2:D:334:ARG:C	2.90	0.44
1:E:69:LEU:CD1	1:E:89:LEU:CD2	2.95	0.44
1:E:69:LEU:CD2	1:E:87:ARG:NH2	2.81	0.44
2:F:379:LEU:HB3	2:F:387:ILE:CG1	2.48	0.44
1:A:69:LEU:HD13	1:A:89:LEU:HD21	1.96	0.44
1:A:186:TYR:C	1:A:188:SER:N	2.74	0.44
1:E:46:ASN:HD21	1:E:48:PRO:HG3	1.82	0.44
2:B:404:GLU:HA	2:B:407:GLU:CB	2.44	0.44
2:B:413:GLN:O	2:B:414:LYS:C	2.59	0.44
1:C:99:LEU:HD23	1:C:219:ILE:CG1	2.46	0.44
1:E:47:ASN:N	1:E:48:PRO:CD	2.80	0.44
1:A:49:TYR:HA	1:A:79:LYS:HE2	1.99	0.44
1:A:124:PRO:HB2	2:D:384:GLU:HB3	1.98	0.44
1:A:167:ARG:HG3	2:D:350:SER:OG	2.17	0.44
2:B:277:ARG:C	2:B:279:LEU:H	2.24	0.44
2:B:279:LEU:HD12	2:B:279:LEU:HA	1.68	0.44
1:C:57:LEU:CD1	2:F:326:GLN:CB	2.79	0.44
1:C:133:ASP:O	1:C:134:GLN:C	2.61	0.44
1:C:213:GLU:C	1:C:215:GLN:H	2.25	0.44
2:D:383:LYS:HD3	2:D:383:LYS:HA	1.79	0.44
2:F:245:GLN:O	2:F:246:ASP:CB	2.66	0.44
2:F:323:GLN:CA	2:F:323:GLN:NE2	2.71	0.44
2:F:404:GLU:O	2:F:408:GLU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLN:HE21	1:A:135:GLY:H	1.61	0.44
2:B:318:VAL:CG2	1:E:189:ALA:CB	2.92	0.44
2:B:357:LYS:CD	2:B:358:ALA:N	2.81	0.44
2:B:391:PRO:O	2:B:395:SER:HB3	2.17	0.44
2:D:246:ASP:O	2:D:247:LYS:HB3	2.17	0.44
2:D:257:ILE:CG1	2:D:265:LEU:HD12	2.45	0.44
1:E:80:LEU:HD23	1:E:80:LEU:HA	1.70	0.44
1:A:49:TYR:HD2	2:B:336:TYR:CZ	2.36	0.44
1:A:79:LYS:HD2	2:B:321:GLU:OE2	2.17	0.44
1:A:214:GLU:OE1	1:A:216:GLU:N	2.51	0.44
2:B:246:ASP:C	2:B:247:LYS:HD2	2.43	0.44
2:B:247:LYS:CB	2:B:248:PRO:CD	2.93	0.44
2:B:328:LEU:HD22	1:E:182:ARG:CD	2.48	0.44
2:B:334:ARG:CD	2:B:336:TYR:CE2	3.01	0.44
1:C:47:ASN:HB2	1:C:76:ASP:HB3	2.00	0.44
2:D:315:VAL:HB	2:D:356:LEU:HD21	1.99	0.44
2:D:352:PHE:HA	2:D:353:PRO:HD2	1.67	0.44
1:E:138:ILE:HG13	2:F:248:PRO:HB3	1.99	0.44
2:F:404:GLU:C	2:F:407:GLU:HB2	2.40	0.44
1:A:49:TYR:HA	1:A:79:LYS:NZ	2.33	0.44
1:A:105:ASP:OD1	1:A:167:ARG:NH1	2.51	0.44
2:B:406:VAL:O	2:B:410:LEU:HG	2.18	0.44
1:C:177:LEU:HB3	2:F:399:PHE:HZ	1.79	0.44
2:D:242:LEU:CD2	2:D:245:GLN:HB2	2.48	0.44
1:E:177:LEU:HD13	1:E:186:TYR:OH	2.17	0.44
2:F:246:ASP:N	2:F:247:LYS:HD2	2.33	0.44
1:A:46:ASN:HD22	1:A:46:ASN:HA	1.31	0.43
1:A:186:TYR:O	1:A:188:SER:N	2.51	0.43
2:B:397:LEU:HD12	1:E:98:LEU:CD2	2.48	0.43
2:D:257:ILE:CG1	2:D:265:LEU:CD1	2.96	0.43
1:E:60:PHE:CE2	1:E:67:LEU:CB	3.02	0.43
2:F:306:LEU:HD23	2:F:306:LEU:HA	1.58	0.43
2:F:329:GLU:O	2:F:331:MET:N	2.51	0.43
1:A:114:GLU:CB	1:A:158:ARG:HB2	2.40	0.43
2:B:295:VAL:CG1	2:B:296:PRO:N	2.80	0.43
2:B:400:PRO:CG	1:E:212:GLN:N	2.79	0.43
1:C:51:PHE:C	2:D:346:ILE:HD12	2.44	0.43
1:E:187:LEU:HD23	1:E:187:LEU:HA	1.70	0.43
2:F:383:LYS:C	2:F:385:ASN:H	2.25	0.43
1:A:194:PHE:O	1:A:198:SER:HB2	2.18	0.43
1:A:219:ILE:N	1:A:219:ILE:CD1	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:GLU:HA	2:B:339:THR:HA	2.00	0.43
1:C:179:SER:HB2	1:C:211:LEU:HA	1.99	0.43
1:E:120:VAL:HG13	1:E:129:THR:HG23	2.00	0.43
2:F:410:LEU:N	2:F:410:LEU:HD23	2.33	0.43
2:F:413:GLN:OE1	2:F:413:GLN:C	2.62	0.43
1:A:45:GLN:CG	1:A:75:GLU:HG2	2.49	0.43
1:A:192:LYS:HD2	2:D:424:ARG:HD3	1.99	0.43
2:B:348:ILE:HA	2:B:349:PRO:HD2	1.38	0.43
1:C:121:LEU:HD12	1:C:146:PHE:HB2	1.99	0.43
1:C:168:ARG:HB3	1:C:171:THR:HB	2.00	0.43
1:E:56:PHE:HB3	1:E:57:LEU:H	1.45	0.43
2:F:325:GLN:OE1	2:F:331:MET:CE	2.67	0.43
2:F:386:VAL:C	2:F:388:ARG:N	2.76	0.43
2:B:312:ARG:HG2	2:B:313:ALA:N	2.32	0.43
1:C:96:ASN:O	1:C:222:MET:N	2.49	0.43
1:C:110:VAL:O	1:C:110:VAL:HG12	2.12	0.43
1:C:176:PHE:CZ	1:C:218:VAL:HG11	2.53	0.43
1:C:207:GLU:O	1:C:207:GLU:HG2	2.19	0.43
2:D:364:MET:HB3	2:D:364:MET:HE2	1.82	0.43
2:F:335:ARG:CG	2:F:335:ARG:NH1	2.82	0.43
1:A:62:ASN:HD21	1:A:216:GLU:HG3	1.83	0.43
1:A:96:ASN:O	1:A:97:THR:CG2	2.64	0.43
1:A:168:ARG:HD3	2:D:321:GLU:C	2.43	0.43
2:B:262:TYR:CZ	2:B:420:ASP:HB2	2.53	0.43
1:C:102:HIS:HB3	1:C:176:PHE:CE1	2.53	0.43
1:C:117:ALA:O	1:C:118:ILE:HG13	2.19	0.43
1:C:206:ILE:O	1:C:208:GLN:N	2.52	0.43
2:D:258:TYR:CD1	2:D:417:TYR:CZ	3.06	0.43
1:E:49:TYR:CE1	2:F:336:TYR:OH	2.68	0.43
1:E:138:ILE:HD11	2:F:248:PRO:HB2	2.01	0.43
1:A:178:SER:OG	2:D:398:THR:O	2.25	0.43
2:B:328:LEU:O	2:B:329:GLU:OE1	2.36	0.43
2:D:325:GLN:OE1	2:D:331:MET:SD	2.77	0.43
1:E:77:THR:CG2	1:E:79:LYS:H	2.26	0.43
1:E:94:LYS:HB3	1:E:95:PRO:CD	2.49	0.43
1:E:103:HIS:CE1	1:E:175:PHE:HB2	2.54	0.43
2:F:242:LEU:HB3	2:F:245:GLN:HG2	2.00	0.43
2:F:292:ALA:CA	2:F:419:VAL:O	2.64	0.43
2:F:340:LEU:HD13	2:F:340:LEU:N	2.34	0.43
2:F:422:GLN:O	2:F:423:PRO:C	2.61	0.43
1:A:79:LYS:HD2	2:B:321:GLU:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD22	1:A:187:LEU:HA	1.80	0.43
2:B:290:GLU:HG3	2:B:360:SER:HA	2.00	0.43
1:C:74:ASN:OD1	1:C:74:ASN:N	2.45	0.43
2:D:247:LYS:C	2:D:249:PHE:N	2.76	0.43
2:D:402:SER:O	2:D:406:VAL:HG23	2.19	0.43
1:E:45:GLN:HB3	1:E:45:GLN:HE21	1.67	0.43
1:A:105:ASP:HB2	1:A:173:GLU:O	2.19	0.43
2:B:288:MET:CE	2:B:294:PHE:HB2	2.48	0.43
1:C:98:LEU:HD23	1:C:220:VAL:HG12	1.99	0.43
1:E:46:ASN:CG	1:E:48:PRO:HD2	2.43	0.43
2:F:313:ALA:O	2:F:339:THR:HA	2.19	0.43
1:A:56:PHE:CD1	1:A:70:LEU:CD1	3.01	0.42
1:A:114:GLU:OE1	1:A:158:ARG:HD3	2.19	0.42
2:B:333:LEU:HA	2:B:333:LEU:HD23	1.57	0.42
1:C:139:LYS:HB3	2:D:275:GLN:OE1	2.19	0.42
2:D:306:LEU:HA	2:D:306:LEU:HD12	1.44	0.42
2:F:422:GLN:HB2	2:F:423:PRO:HD2	2.00	0.42
2:B:258:TYR:HB2	2:B:418:PHE:CE2	2.54	0.42
2:B:320:LEU:HD11	2:B:333:LEU:HG	2.00	0.42
2:B:378:PHE:O	2:B:385:ASN:HA	2.19	0.42
2:F:254:ARG:HH11	2:F:254:ARG:CG	2.20	0.42
1:C:54:ASN:CG	2:D:344:ASP:OD2	2.62	0.42
1:C:119:LEU:CD2	1:C:121:LEU:HD13	2.47	0.42
1:C:127:ARG:HD2	2:F:391:PRO:HG3	2.01	0.42
1:C:187:LEU:HD11	2:F:387:ILE:HD11	1.99	0.42
1:C:222:MET:O	1:C:224:LYS:N	2.53	0.42
2:D:382:HIS:CD2	2:D:413:GLN:O	2.73	0.42
2:F:307:VAL:HG22	2:F:345:ILE:HD13	2.01	0.42
1:A:86:TYR:HB3	1:A:162:PHE:CE1	2.54	0.42
2:B:400:PRO:HG2	1:E:211:LEU:C	2.44	0.42
1:C:60:PHE:CD1	2:F:328:LEU:HD11	2.54	0.42
2:D:386:VAL:O	2:D:389:GLN:HG2	2.20	0.42
1:E:212:GLN:HB3	1:E:214:GLU:H	1.83	0.42
2:F:325:GLN:HE21	2:F:325:GLN:N	2.17	0.42
2:F:341:SER:O	2:F:344:ASP:HB2	2.19	0.42
1:C:119:LEU:CD2	1:C:121:LEU:CD1	2.97	0.42
1:C:123:ASN:HB2	1:C:124:PRO:HD2	2.02	0.42
1:C:133:ASP:H	1:C:136:ASP:CG	2.26	0.42
2:D:340:LEU:HD13	2:D:344:ASP:CB	2.21	0.42
1:E:86:TYR:HE1	1:E:164:ILE:HG23	1.83	0.42
1:E:121:LEU:N	1:E:128:ASP:O	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:HD13	1:E:186:TYR:CZ	2.55	0.42
2:F:314:GLU:HA	2:F:338:ALA:O	2.19	0.42
1:A:196:GLU:OE2	2:D:424:ARG:CD	2.67	0.42
2:B:267:GLU:CG	2:B:284:ASN:HD21	2.31	0.42
2:B:413:GLN:NE2	2:B:419:VAL:HG11	2.33	0.42
1:C:119:LEU:N	1:C:130:TYR:O	2.44	0.42
1:C:206:ILE:C	1:C:208:GLN:N	2.78	0.42
1:E:123:ASN:C	1:E:125:ASP:N	2.76	0.42
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.88	0.42
2:B:403:GLY:O	2:B:407:GLU:HB2	2.19	0.42
1:C:114:GLU:HB3	1:C:158:ARG:HB2	2.01	0.42
1:C:129:THR:O	2:D:242:LEU:HD12	2.20	0.42
2:D:408:GLU:O	2:D:409:LEU:C	2.63	0.42
1:E:143:GLY:O	1:E:145:PRO:CD	2.66	0.42
2:F:265:LEU:CD1	2:F:265:LEU:C	2.92	0.42
2:F:316:GLU:OE1	2:F:335:ARG:HD2	2.20	0.42
2:F:354:VAL:HG22	2:F:355:ALA:N	2.35	0.42
2:B:300:SER:CB	2:B:375:GLU:HG3	2.49	0.42
1:C:64:HIS:HD2	1:C:97:THR:CG2	2.33	0.42
2:D:242:LEU:HD23	2:D:245:GLN:CB	2.49	0.42
2:D:276:LEU:HD12	2:D:276:LEU:HA	1.86	0.42
2:D:383:LYS:CB	2:D:416:SER:CB	2.97	0.42
2:F:242:LEU:CD2	2:F:244:SER:H	2.31	0.42
1:A:49:TYR:HA	1:A:79:LYS:CE	2.50	0.42
1:A:105:ASP:CG	1:A:167:ARG:NH1	2.78	0.42
2:D:242:LEU:CD2	2:D:245:GLN:CB	2.98	0.42
1:E:120:VAL:C	1:E:121:LEU:HD13	2.45	0.42
1:E:207:GLU:C	1:E:208:GLN:HG3	2.44	0.42
2:F:291:GLY:O	2:F:420:ASP:HA	2.19	0.42
1:A:51:PHE:HZ	2:B:321:GLU:CD	2.28	0.42
1:C:138:ILE:HG13	1:C:139:LYS:N	2.35	0.42
1:C:150:ASN:HB2	1:C:157:LEU:HD22	2.02	0.42
1:E:116:GLN:HE21	1:E:116:GLN:HB2	1.54	0.42
1:E:136:ASP:OD1	2:F:252:ARG:CG	2.66	0.42
2:F:335:ARG:HH11	2:F:335:ARG:CB	2.33	0.42
2:B:405:GLU:O	2:B:408:GLU:HB3	2.20	0.41
2:D:413:GLN:C	2:D:415:GLU:N	2.76	0.41
1:E:194:PHE:O	1:E:198:SER:OG	2.36	0.41
2:F:325:GLN:HA	2:F:330:SER:HG	1.83	0.41
1:A:105:ASP:HA	2:D:351:SER:OG	2.19	0.41
2:B:306:LEU:HD23	2:B:306:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:GLU:OE1	2:B:352:PHE:CE2	2.72	0.41
1:C:79:LYS:NZ	2:D:322:GLN:NE2	2.67	0.41
1:C:111:LEU:HD11	2:D:283:LEU:HD23	2.01	0.41
1:C:215:GLN:CG	1:C:216:GLU:H	2.33	0.41
2:D:306:LEU:HD22	2:D:348:ILE:HG12	2.02	0.41
1:E:114:GLU:OE1	1:E:158:ARG:CD	2.69	0.41
2:F:325:GLN:HG3	2:F:331:MET:CB	2.50	0.41
1:A:186:TYR:CD1	1:A:187:LEU:N	2.89	0.41
2:B:424:ARG:NE	1:E:196:GLU:OE2	2.53	0.41
1:C:50:LEU:HA	1:C:50:LEU:HD13	1.64	0.41
1:C:185:SER:O	1:C:188:SER:CB	2.67	0.41
2:D:321:GLU:N	2:D:331:MET:SD	2.93	0.41
2:D:340:LEU:HD12	2:D:344:ASP:O	2.21	0.41
1:E:69:LEU:CD1	1:E:89:LEU:HD23	2.50	0.41
1:E:182:ARG:HD3	1:E:182:ARG:HA	1.79	0.41
2:F:340:LEU:N	2:F:340:LEU:CD1	2.83	0.41
1:A:72:ARG:C	1:A:74:ASN:N	2.75	0.41
1:A:223:PRO:HG2	1:A:224:LYS:HG3	2.03	0.41
2:B:315:VAL:N	2:B:338:ALA:O	2.49	0.41
2:B:346:ILE:HD12	2:B:346:ILE:HA	1.85	0.41
1:C:134:GLN:C	1:C:136:ASP:H	2.28	0.41
1:E:46:ASN:ND2	1:E:48:PRO:CD	2.84	0.41
2:F:293:LEU:N	2:F:419:VAL:O	2.51	0.41
2:F:325:GLN:OE1	2:F:331:MET:HE2	2.20	0.41
2:F:388:ARG:HG3	2:F:410:LEU:HB3	2.02	0.41
1:A:102:HIS:HB3	1:A:176:PHE:CD2	2.55	0.41
2:B:290:GLU:HA	2:B:358:ALA:O	2.20	0.41
2:B:328:LEU:C	2:B:328:LEU:HD23	2.46	0.41
2:D:295:VAL:CG1	2:D:380:ALA:HB3	2.36	0.41
2:D:330:SER:O	2:D:331:MET:C	2.61	0.41
1:E:48:PRO:HD3	1:E:76:ASP:HB3	2.03	0.41
2:F:392:ARG:H	2:F:392:ARG:HG3	1.79	0.41
1:A:121:LEU:CD2	1:A:146:PHE:HB3	2.51	0.41
1:C:47:ASN:O	1:C:49:TYR:N	2.53	0.41
1:C:70:LEU:HD12	1:C:71:GLN:H	1.85	0.41
1:C:220:VAL:HG11	2:F:397:LEU:HD22	2.03	0.41
2:D:270:PRO:O	2:D:271:GLU:C	2.62	0.41
2:D:306:LEU:HB2	2:D:346:ILE:CG2	2.51	0.41
2:F:402:SER:O	2:F:403:GLY:C	2.63	0.41
1:C:214:GLU:O	1:C:215:GLN:C	2.64	0.41
2:D:387:ILE:H	2:D:387:ILE:HG13	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:PHE:CD2	1:E:67:LEU:HB3	2.55	0.41
1:E:64:HIS:CE1	1:E:216:GLU:OE2	2.74	0.41
1:E:223:PRO:HG2	1:E:224:LYS:H	1.82	0.41
1:A:49:TYR:CD2	2:B:336:TYR:OH	2.67	0.41
1:A:222:MET:CB	1:A:223:PRO:CD	2.86	0.41
1:C:59:LEU:O	2:F:328:LEU:HD12	2.20	0.41
1:C:94:LYS:HA	1:C:156:ASN:HD22	1.86	0.41
2:D:396:ASP:CG	2:D:403:GLY:N	2.78	0.41
1:E:47:ASN:H	1:E:76:ASP:CG	2.28	0.41
1:A:79:LYS:H	1:A:79:LYS:HG2	1.41	0.41
2:B:269:THR:HB	2:B:271:GLU:OE1	2.21	0.41
2:B:346:ILE:CG2	2:B:348:ILE:HD11	2.43	0.41
1:C:57:LEU:H	1:C:57:LEU:HG	1.69	0.41
1:C:134:GLN:HE21	1:C:135:GLY:H	1.68	0.41
2:D:347:VAL:C	2:D:348:ILE:HD13	2.45	0.41
2:D:377:ASN:HD22	2:D:377:ASN:H	1.65	0.41
2:D:391:PRO:CA	2:D:394:VAL:CG2	2.95	0.41
1:E:49:TYR:CD1	2:F:336:TYR:OH	2.70	0.41
1:E:73:PHE:CD2	1:E:83:LEU:HB3	2.56	0.41
1:E:114:GLU:OE1	1:E:158:ARG:HD2	2.21	0.41
1:E:185:SER:C	1:E:187:LEU:N	2.79	0.41
1:E:192:LYS:HG3	1:E:203:TYR:CD2	2.56	0.41
2:F:271:GLU:H	2:F:271:GLU:HG2	1.27	0.41
2:F:313:ALA:O	2:F:340:LEU:N	2.48	0.41
2:F:399:PHE:C	2:F:401:GLY:N	2.79	0.41
2:B:242:LEU:HD23	2:B:242:LEU:N	2.36	0.41
2:D:279:LEU:HB3	2:D:281:ILE:HG13	2.03	0.41
2:F:267:GLU:HA	2:F:283:LEU:O	2.21	0.41
2:F:417:TYR:CD1	2:F:417:TYR:N	2.85	0.41
1:A:207:GLU:CG	1:A:208:GLN:N	2.84	0.40
1:A:207:GLU:HG3	1:A:208:GLN:N	2.31	0.40
1:C:96:ASN:O	1:C:221:LYS:CG	2.67	0.40
2:D:334:ARG:HD3	2:D:334:ARG:C	2.46	0.40
1:E:49:TYR:CA	1:E:79:LYS:HD2	2.51	0.40
1:A:64:HIS:O	1:A:93:SER:HA	2.22	0.40
1:A:171:THR:HA	2:D:323:GLN:HB2	2.03	0.40
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.86	0.40
1:C:133:ASP:O	1:C:136:ASP:HB2	2.21	0.40
1:C:180:THR:HB	1:C:217:GLY:HA2	2.02	0.40
2:F:325:GLN:HB2	2:F:326:GLN:H	1.68	0.40
1:A:133:ASP:O	1:A:136:ASP:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HA	1:A:148:LEU:HD12	1.82	0.40
2:B:243:SER:O	2:B:245:GLN:HB3	2.21	0.40
2:B:247:LYS:HD2	2:B:247:LYS:N	2.36	0.40
2:B:317:LEU:HD23	2:B:317:LEU:C	2.45	0.40
2:B:335:ARG:HG2	2:B:336:TYR:N	2.32	0.40
1:C:64:HIS:CD2	1:C:97:THR:CG2	3.04	0.40
1:C:132:LEU:HD12	2:D:250:ASN:ND2	2.36	0.40
2:D:294:PHE:CE1	2:D:418:PHE:CE1	3.10	0.40
1:E:103:HIS:CE1	1:E:175:PHE:CB	3.04	0.40
1:A:45:GLN:HG3	1:A:75:GLU:HG2	2.02	0.40
2:D:307:VAL:CG2	2:D:345:ILE:CD1	2.99	0.40
2:D:376:ARG:NH1	2:D:376:ARG:CG	2.83	0.40
2:F:272:LYS:NZ	2:F:272:LYS:HB3	2.35	0.40
2:B:325:GLN:C	2:B:327:GLY:N	2.79	0.40
1:C:54:ASN:HB2	2:D:344:ASP:OD2	2.21	0.40
1:C:107:ASP:N	1:C:142:ALA:HB2	2.35	0.40
1:E:46:ASN:CG	1:E:48:PRO:CD	2.95	0.40

All (1) 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)
2:B:273:ASN:OD1	2:F:243:SER:O[3_655]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	179/181 (99%)	134 (75%)	28 (16%)	17 (10%)	0 0
1	C	179/181 (99%)	134 (75%)	26 (14%)	19 (11%)	0 0
1	E	179/181 (99%)	139 (78%)	27 (15%)	13 (7%)	1 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	182/184 (99%)	137 (75%)	31 (17%)	14 (8%)	1	1
2	D	182/184 (99%)	134 (74%)	32 (18%)	16 (9%)	0	0
2	F	182/184 (99%)	140 (77%)	29 (16%)	13 (7%)	1	1
All	All	1083/1095 (99%)	818 (76%)	173 (16%)	92 (8%)	0	0

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	152	ASP
1	A	153	ASN
1	A	217	GLY
1	A	222	MET
2	B	247	LYS
2	B	326	GLN
2	B	373	ASN
2	B	403	GLY
2	B	423	PRO
1	C	45	GLN
1	C	49	TYR
1	C	50	LEU
1	C	61	LYS
1	C	152	ASP
1	C	153	ASN
1	C	211	LEU
1	C	214	GLU
1	C	215	GLN
1	C	222	MET
2	D	246	ASP
2	D	247	LYS
2	D	250	ASN
2	D	253	SER
2	D	320	LEU
2	D	330	SER
2	D	387	ILE
1	E	45	GLN
1	E	152	ASP
1	E	186	TYR
1	E	210	LEU
1	E	215	GLN
1	E	223	PRO

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Mol	Chain	Res	Type
2	F	242	LEU
2	F	246	ASP
2	F	247	LYS
2	F	254	ARG
2	F	329	GLU
2	F	330	SER
2	F	331	MET
2	F	423	PRO
1	A	95	PRO
1	A	114	GLU
1	A	156	ASN
1	A	205	GLU
2	B	243	SER
2	B	297	HIS
2	B	324	GLN
2	B	328	LEU
2	B	350	SER
1	C	48	PRO
1	C	134	GLN
1	C	207	GLU
2	D	361	ASP
2	D	396	ASP
1	E	49	TYR
1	E	64	HIS
1	E	154	ASN
1	E	207	GLU
1	E	209	THR
1	E	217	GLY
2	F	326	GLN
2	F	327	GLY
2	F	403	GLY
1	A	125	ASP
1	A	187	LEU
1	A	190	PHE
2	B	248	PRO
2	B	252	ARG
1	C	223	PRO
2	D	248	PRO
2	D	409	LEU
1	E	214	GLU
2	F	350	SER
1	A	60	PHE

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Mol	Chain	Res	Type
1	A	202	PRO
1	A	216	GLU
2	B	255	ASP
1	C	47	ASN
2	D	255	ASP
2	D	328	LEU
2	D	350	SER
2	D	360	SER
2	F	260	ASN
1	A	218	VAL
1	C	62	ASN
1	C	203	TYR
2	B	327	GLY
1	C	206	ILE
1	A	48	PRO
1	C	168	ARG
2	D	419	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/167 (100%)	101 (60%)	66 (40%)	0	0
1	C	167/167 (100%)	108 (65%)	59 (35%)	0	0
1	E	167/167 (100%)	107 (64%)	60 (36%)	0	0
2	B	161/161 (100%)	100 (62%)	61 (38%)	0	0
2	D	161/161 (100%)	92 (57%)	69 (43%)	0	0
2	F	161/161 (100%)	89 (55%)	72 (45%)	0	0
All	All	984/984 (100%)	597 (61%)	387 (39%)	0	0

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN

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Mol	Chain	Res	Type
1	A	47	ASN
1	A	52	ARG
1	A	53	SER
1	A	55	LYS
1	A	61	LYS
1	A	62	ASN
1	A	67	LEU
1	A	68	ARG
1	A	69	LEU
1	A	76	ASP
1	A	77	THR
1	A	78	GLU
1	A	79	LYS
1	A	82	ASN
1	A	84	ARG
1	A	85	ASP
1	A	87	ARG
1	A	89	LEU
1	A	90	GLU
1	A	94	LYS
1	A	98	LEU
1	A	106	SER
1	A	110	VAL
1	A	111	LEU
1	A	118	ILE
1	A	119	LEU
1	A	120	VAL
1	A	122	VAL
1	A	125	ASP
1	A	127	ARG
1	A	128	ASP
1	A	131	LYS
1	A	132	LEU
1	A	134	GLN
1	A	138	ILE
1	A	141	GLN
1	A	148	LEU
1	A	149	ILE
1	A	152	ASP
1	A	153	ASN
1	A	155	GLN
1	A	156	ASN

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Mol	Chain	Res	Type
1	A	159	ILE
1	A	161	LYS
1	A	165	THR
1	A	168	ARG
1	A	171	THR
1	A	172	VAL
1	A	174	ASP
1	A	182	ARG
1	A	183	LEU
1	A	187	LEU
1	A	195	LEU
1	A	204	ASP
1	A	205	GLU
1	A	207	GLU
1	A	208	GLN
1	A	209	THR
1	A	210	LEU
1	A	213	GLU
1	A	214	GLU
1	A	216	GLU
1	A	219	ILE
1	A	220	VAL
1	A	221	LYS
2	B	242	LEU
2	B	246	ASP
2	B	247	LYS
2	B	249	PHE
2	B	250	ASN
2	B	251	LEU
2	B	254	ARG
2	B	255	ASP
2	B	257	ILE
2	B	258	TYR
2	B	259	SER
2	B	261	ASN
2	B	265	LEU
2	B	272	LYS
2	B	275	GLN
2	B	276	LEU
2	B	278	ASP
2	B	279	LEU
2	B	281	ILE

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Mol	Chain	Res	Type
2	B	283	LEU
2	B	286	LEU
2	B	287	GLN
2	B	288	MET
2	B	299	ASN
2	B	300	SER
2	B	301	ARG
2	B	303	THR
2	B	305	ILE
2	B	315	VAL
2	B	317	LEU
2	B	320	LEU
2	B	322	GLN
2	B	323	GLN
2	B	324	GLN
2	B	326	GLN
2	B	329	GLU
2	B	332	GLN
2	B	333	LEU
2	B	336	TYR
2	B	340	LEU
2	B	341	SER
2	B	348	ILE
2	B	350	SER
2	B	357	LYS
2	B	360	SER
2	B	364	MET
2	B	365	VAL
2	B	370	ASN
2	B	373	ASN
2	B	379	LEU
2	B	386	VAL
2	B	387	ILE
2	B	392	ARG
2	B	393	GLN
2	B	395	SER
2	B	406	VAL
2	B	409	LEU
2	B	411	GLU
2	B	414	LYS
2	B	422	GLN
2	B	424	ARG

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Mol	Chain	Res	Type
1	C	49	TYR
1	C	55	LYS
1	C	57	LEU
1	C	59	LEU
1	C	61	LYS
1	C	64	HIS
1	C	66	SER
1	C	71	GLN
1	C	75	GLU
1	C	79	LYS
1	C	80	LEU
1	C	81	GLU
1	C	84	ARG
1	C	88	VAL
1	C	90	GLU
1	C	91	TYR
1	C	92	CYS
1	C	93	SER
1	C	98	LEU
1	C	99	LEU
1	C	110	VAL
1	C	111	LEU
1	C	119	LEU
1	C	123	ASN
1	C	125	ASP
1	C	127	ARG
1	C	129	THR
1	C	130	TYR
1	C	131	LYS
1	C	132	LEU
1	C	134	GLN
1	C	138	ILE
1	C	141	GLN
1	C	148	LEU
1	C	150	ASN
1	C	152	ASP
1	C	154	ASN
1	C	156	ASN
1	C	168	ARG
1	C	172	VAL
1	C	177	LEU
1	C	178	SER

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Mol	Chain	Res	Type
1	C	181	LYS
1	C	183	LEU
1	C	185	SER
1	C	188	SER
1	C	192	LYS
1	C	193	ASN
1	C	195	LEU
1	C	206	ILE
1	C	208	GLN
1	C	209	THR
1	C	211	LEU
1	C	212	GLN
1	C	215	GLN
1	C	218	VAL
1	C	220	VAL
1	C	222	MET
1	C	224	LYS
2	D	241	THR
2	D	242	LEU
2	D	243	SER
2	D	245	GLN
2	D	249	PHE
2	D	250	ASN
2	D	251	LEU
2	D	253	SER
2	D	254	ARG
2	D	255	ASP
2	D	257	ILE
2	D	264	LYS
2	D	265	LEU
2	D	268	ILE
2	D	271	GLU
2	D	272	LYS
2	D	276	LEU
2	D	277	ARG
2	D	280	ASP
2	D	281	ILE
2	D	282	LEU
2	D	286	LEU
2	D	288	MET
2	D	293	LEU
2	D	294	PHE

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Mol	Chain	Res	Type
2	D	299	ASN
2	D	301	ARG
2	D	306	LEU
2	D	307	VAL
2	D	310	GLU
2	D	320	LEU
2	D	323	GLN
2	D	324	GLN
2	D	325	GLN
2	D	328	LEU
2	D	329	GLU
2	D	332	GLN
2	D	334	ARG
2	D	339	THR
2	D	346	ILE
2	D	352	PHE
2	D	357	LYS
2	D	365	VAL
2	D	367	ILE
2	D	370	ASN
2	D	374	ASN
2	D	375	GLU
2	D	376	ARG
2	D	377	ASN
2	D	379	LEU
2	D	384	GLU
2	D	386	VAL
2	D	387	ILE
2	D	388	ARG
2	D	389	GLN
2	D	390	ILE
2	D	392	ARG
2	D	393	GLN
2	D	394	VAL
2	D	395	SER
2	D	396	ASP
2	D	398	THR
2	D	409	LEU
2	D	411	GLU
2	D	414	LYS
2	D	415	GLU
2	D	417	TYR

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Mol	Chain	Res	Type
2	D	422	GLN
2	D	424	ARG
1	E	45	GLN
1	E	49	TYR
1	E	52	ARG
1	E	54	ASN
1	E	55	LYS
1	E	57	LEU
1	E	59	LEU
1	E	60	PHE
1	E	63	GLN
1	E	64	HIS
1	E	66	SER
1	E	71	GLN
1	E	74	ASN
1	E	77	THR
1	E	79	LYS
1	E	84	ARG
1	E	88	VAL
1	E	89	LEU
1	E	94	LYS
1	E	96	ASN
1	E	99	LEU
1	E	100	LEU
1	E	110	VAL
1	E	111	LEU
1	E	116	GLN
1	E	119	LEU
1	E	121	LEU
1	E	125	ASP
1	E	129	THR
1	E	131	LYS
1	E	132	LEU
1	E	134	GLN
1	E	139	LYS
1	E	144	THR
1	E	145	PRO
1	E	148	LEU
1	E	153	ASN
1	E	154	ASN
1	E	159	ILE
1	E	165	THR

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Mol	Chain	Res	Type
1	E	167	ARG
1	E	168	ARG
1	E	171	THR
1	E	174	ASP
1	E	177	LEU
1	E	178	SER
1	E	180	THR
1	E	182	ARG
1	E	185	SER
1	E	198	SER
1	E	208	GLN
1	E	211	LEU
1	E	213	GLU
1	E	215	GLN
1	E	216	GLU
1	E	218	VAL
1	E	220	VAL
1	E	221	LYS
1	E	222	MET
1	E	224	LYS
2	F	241	THR
2	F	245	GLN
2	F	246	ASP
2	F	247	LYS
2	F	249	PHE
2	F	250	ASN
2	F	254	ARG
2	F	255	ASP
2	F	260	ASN
2	F	265	LEU
2	F	267	GLU
2	F	271	GLU
2	F	272	LYS
2	F	276	LEU
2	F	277	ARG
2	F	279	LEU
2	F	280	ASP
2	F	281	ILE
2	F	282	LEU
2	F	283	LEU
2	F	286	LEU
2	F	287	GLN

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Mol	Chain	Res	Type
2	F	288	MET
2	F	289	ASN
2	F	290	GLU
2	F	293	LEU
2	F	301	ARG
2	F	310	GLU
2	F	314	GLU
2	F	317	LEU
2	F	318	VAL
2	F	320	LEU
2	F	322	GLN
2	F	323	GLN
2	F	324	GLN
2	F	325	GLN
2	F	330	SER
2	F	331	MET
2	F	334	ARG
2	F	335	ARG
2	F	339	THR
2	F	340	LEU
2	F	345	ILE
2	F	347	VAL
2	F	351	SER
2	F	352	PHE
2	F	356	LEU
2	F	357	LYS
2	F	360	SER
2	F	362	LEU
2	F	364	MET
2	F	370	ASN
2	F	372	GLU
2	F	376	ARG
2	F	379	LEU
2	F	382	HIS
2	F	384	GLU
2	F	386	VAL
2	F	387	ILE
2	F	388	ARG
2	F	389	GLN
2	F	392	ARG
2	F	394	VAL
2	F	396	ASP

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Mol	Chain	Res	Type
2	F	397	LEU
2	F	404	GLU
2	F	407	GLU
2	F	408	GLU
2	F	413	GLN
2	F	414	LYS
2	F	419	VAL
2	F	422	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	134	GLN
1	A	141	GLN
1	A	150	ASN
1	A	153	ASN
1	A	155	GLN
1	A	156	ASN
1	A	193	ASN
2	B	245	GLN
2	B	273	ASN
2	B	275	GLN
2	B	284	ASN
2	B	297	HIS
2	B	322	GLN
2	B	325	GLN
2	B	332	GLN
2	B	393	GLN
1	C	71	GLN
1	C	102	HIS
1	C	134	GLN
1	C	141	GLN
1	C	150	ASN
1	C	208	GLN
2	D	245	GLN
2	D	261	ASN
2	D	322	GLN
2	D	323	GLN
2	D	332	GLN
2	D	370	ASN
2	D	377	ASN

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Mol	Chain	Res	Type
2	D	382	HIS
2	D	393	GLN
1	E	45	GLN
1	E	46	ASN
1	E	71	GLN
1	E	116	GLN
1	E	123	ASN
1	E	134	GLN
1	E	208	GLN
1	E	212	GLN
2	F	245	GLN
2	F	250	ASN
2	F	289	ASN
2	F	309	ASN
2	F	323	GLN
2	F	324	GLN
2	F	325	GLN
2	F	326	GLN
2	F	332	GLN
2	F	363	ASN
2	F	422	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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	181/181 (100%)	-0.95	0 100 100	8, 20, 30, 41	0
1	C	181/181 (100%)	-0.85	0 100 100	8, 20, 32, 39	0
1	E	181/181 (100%)	-0.94	0 100 100	5, 18, 33, 42	0
2	B	184/184 (100%)	-0.89	1 (0%) 87 85	6, 17, 32, 40	0
2	D	184/184 (100%)	-0.88	0 100 100	7, 20, 33, 41	0
2	F	184/184 (100%)	-0.84	1 (0%) 87 85	6, 20, 33, 42	0
All	All	1095/1095 (100%)	-0.89	2 (0%) 91 90	5, 19, 33, 42	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	330	SER	2.4
2	B	243	SER	2.1

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.