Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 11:12 AM EST

PDB ID	:	1CAX
Title	:	DETERMINATION OF THREE CRYSTAL STRUCTURES OF CANAVALIN 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.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

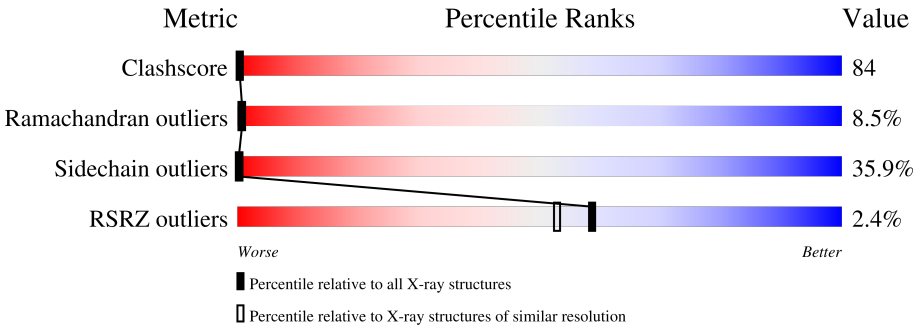
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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% 47% 30% 10%
1	C	181	2% 14% 43% 33% 10%
1	E	181	3% 19% 43% 29% 8%
2	B	184	2% 17% 41% 34% 8%
2	D	184	4% 17% 42% 32% 9%
2	F	184	3% 19% 39% 27% 15%

2 Entry composition (i)

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.

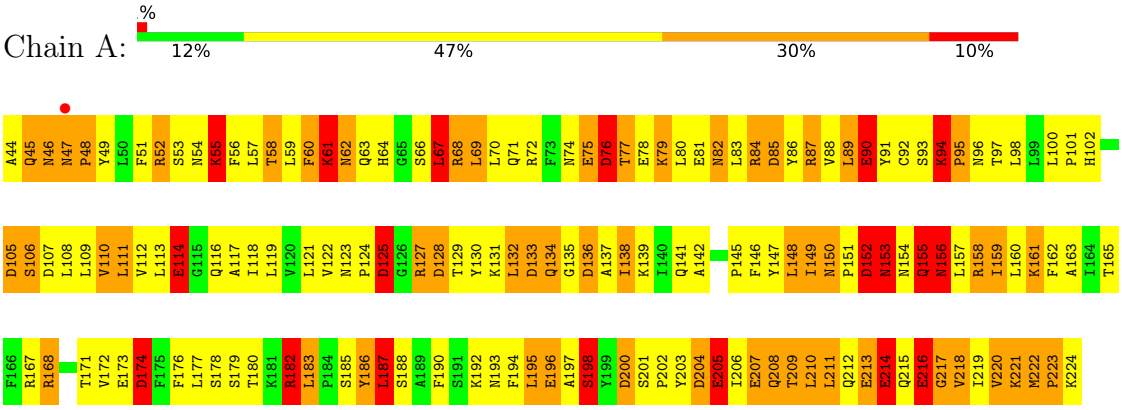
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1450	902	255	289	4			
2	D	184	Total	C	N	O	S	0	0	0
			1450	902	255	289	4			
2	F	184	Total	C	N	O	S	0	0	0
			1450	902	255	289	4			

3 Residue-property plots (i)

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.

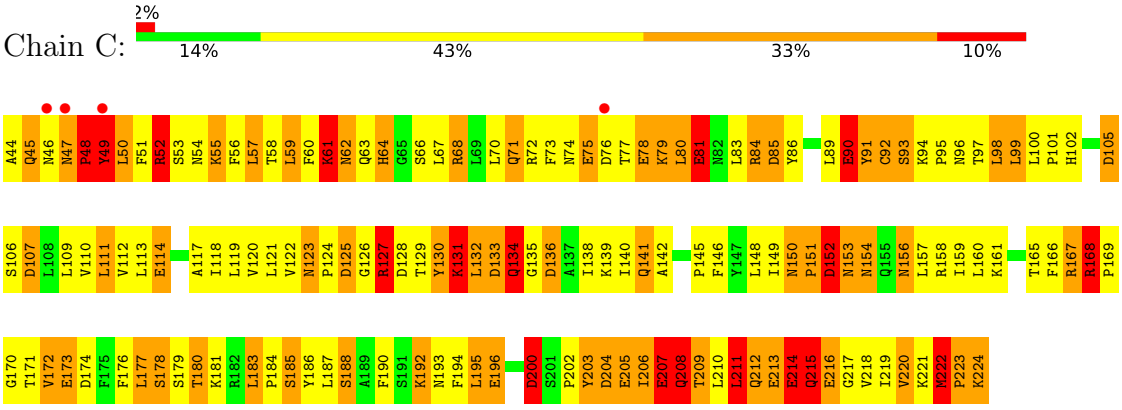
• Molecule 1: CANAVALIN

Chain A:



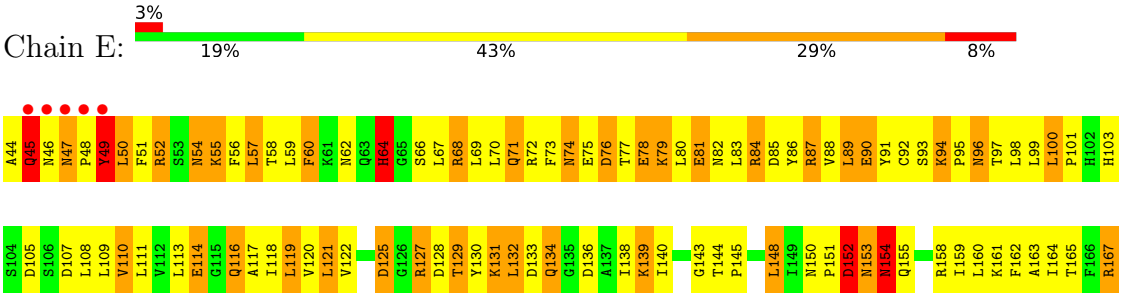
• Molecule 1: CANAVALIN

Chain C:



• Molecule 1: CANAVALIN

Chain E:

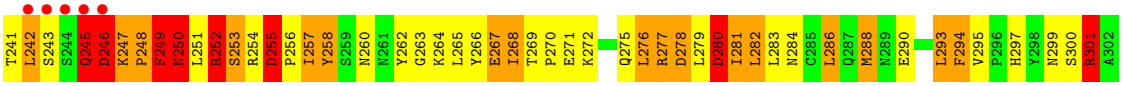


• Molecule 2: CANAVALIN

Chain B:

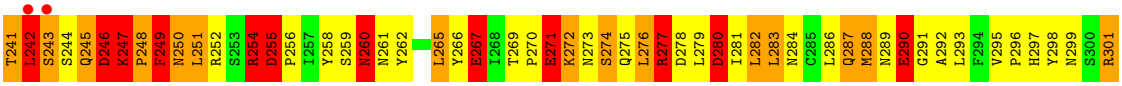
• Molecule 2: CANAVALIN

Chain D:



• Molecule 2: CANAVALIN

Chain F:



4 Data and refinement statistics (i)

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 32.31 – 2.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 66.0 (32.31-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.57Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.175 , (Not available) 0.186 , (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)	0.28 , 132.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.30	10/1511 (0.7%)	1.70	43/2046 (2.1%)
1	C	1.35	13/1511 (0.9%)	1.65	36/2046 (1.8%)
1	E	1.30	10/1511 (0.7%)	1.72	35/2046 (1.7%)
2	B	1.40	17/1472 (1.2%)	1.70	33/1992 (1.7%)
2	D	1.37	18/1472 (1.2%)	1.63	29/1992 (1.5%)
2	F	1.41	20/1472 (1.4%)	1.71	31/1992 (1.6%)
All	All	1.36	88/8949 (1.0%)	1.68	207/12114 (1.7%)

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 (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	GLU	CD-OE1	9.95	1.36	1.25
2	B	375	GLU	CD-OE2	9.47	1.36	1.25
2	F	321	GLU	CD-OE2	8.85	1.35	1.25
2	D	314	GLU	CD-OE2	8.54	1.35	1.25
1	E	90	GLU	CD-OE1	8.51	1.35	1.25
2	B	290	GLU	CD-OE1	8.40	1.34	1.25
1	C	90	GLU	CD-OE2	8.39	1.34	1.25
2	B	372	GLU	CD-OE1	8.20	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	GLU	CD-OE2	8.09	1.34	1.25
2	B	408	GLU	CD-OE1	8.09	1.34	1.25
1	A	90	GLU	CD-OE1	7.93	1.34	1.25
2	D	375	GLU	CD-OE1	7.92	1.34	1.25
1	C	173	GLU	CD-OE1	7.88	1.34	1.25
2	F	372	GLU	CD-OE1	7.87	1.34	1.25
1	E	205	GLU	CD-OE2	7.74	1.34	1.25
2	D	290	GLU	CD-OE2	7.64	1.34	1.25
2	F	415	GLU	CD-OE2	7.62	1.34	1.25
1	C	213	GLU	CD-OE2	7.57	1.33	1.25
1	A	213	GLU	CD-OE1	7.55	1.33	1.25
1	A	214	GLU	CD-OE2	7.50	1.33	1.25
2	F	329	GLU	CD-OE2	7.48	1.33	1.25
1	C	75	GLU	CD-OE2	7.47	1.33	1.25
2	D	271	GLU	CD-OE1	7.45	1.33	1.25
2	B	267	GLU	CD-OE2	7.38	1.33	1.25
1	C	196	GLU	CD-OE1	7.38	1.33	1.25
1	A	216	GLU	CD-OE2	7.30	1.33	1.25
2	F	375	GLU	CD-OE1	7.29	1.33	1.25
1	A	75	GLU	CD-OE1	7.29	1.33	1.25
2	F	267	GLU	CD-OE1	7.27	1.33	1.25
2	D	329	GLU	CD-OE1	7.22	1.33	1.25
1	E	207	GLU	CD-OE2	7.20	1.33	1.25
2	F	411	GLU	CD-OE2	7.09	1.33	1.25
2	D	411	GLU	CD-OE1	7.00	1.33	1.25
1	C	114	GLU	CD-OE2	6.96	1.33	1.25
1	E	216	GLU	CD-OE1	6.95	1.33	1.25
2	D	415	GLU	CD-OE1	6.93	1.33	1.25
2	D	267	GLU	CD-OE1	6.87	1.33	1.25
1	A	78	GLU	CD-OE1	6.85	1.33	1.25
1	E	52	ARG	NE-CZ	6.75	1.41	1.33
1	A	205	GLU	CD-OE1	6.71	1.33	1.25
2	D	404	GLU	CD-OE1	6.68	1.32	1.25
1	A	196	GLU	CD-OE1	6.67	1.32	1.25
2	B	329	GLU	CD-OE1	6.62	1.32	1.25
2	F	248	PRO	N-CA	-6.59	1.36	1.47
2	F	271	GLU	CD-OE1	6.57	1.32	1.25
2	F	342	GLU	CD-OE2	6.48	1.32	1.25
2	B	310	GLU	CD-OE1	6.46	1.32	1.25
1	E	81	GLU	CD-OE2	6.45	1.32	1.25
2	B	314	GLU	CD-OE2	6.45	1.32	1.25
2	F	407	GLU	CD-OE1	6.44	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	342	GLU	CD-OE2	6.37	1.32	1.25
2	B	411	GLU	CD-OE2	6.37	1.32	1.25
2	F	405	GLU	CD-OE2	6.29	1.32	1.25
1	C	205	GLU	CD-OE1	6.23	1.32	1.25
1	C	216	GLU	CD-OE2	6.20	1.32	1.25
2	D	316	GLU	CD-OE1	6.17	1.32	1.25
2	D	408	GLU	CD-OE2	6.17	1.32	1.25
2	F	290	GLU	CD-OE1	6.11	1.32	1.25
1	E	78	GLU	CD-OE1	6.10	1.32	1.25
2	D	310	GLU	CD-OE1	6.08	1.32	1.25
1	C	81	GLU	CD-OE1	6.03	1.32	1.25
1	C	214	GLU	CD-OE1	5.93	1.32	1.25
2	F	408	GLU	CD-OE2	5.90	1.32	1.25
1	A	114	GLU	CD-OE1	5.87	1.32	1.25
2	B	404	GLU	CD-OE1	5.82	1.32	1.25
2	F	384	GLU	CD-OE2	5.78	1.32	1.25
1	C	207	GLU	CD-OE1	5.73	1.31	1.25
2	D	384	GLU	CD-OE2	5.71	1.31	1.25
2	B	415	GLU	CD-OE1	5.69	1.31	1.25
2	B	407	GLU	CD-OE1	5.67	1.31	1.25
1	E	213	GLU	CD-OE2	5.67	1.31	1.25
2	B	342	GLU	CD-OE2	5.66	1.31	1.25
2	B	321	GLU	CD-OE1	5.59	1.31	1.25
2	B	271	GLU	CD-OE1	5.57	1.31	1.25
2	F	314	GLU	CD-OE2	5.56	1.31	1.25
1	A	81	GLU	CD-OE1	5.54	1.31	1.25
2	D	405	GLU	CD-OE2	5.52	1.31	1.25
2	D	372	GLU	CD-OE2	5.45	1.31	1.25
2	F	404	GLU	CD-OE1	5.41	1.31	1.25
2	D	407	GLU	CD-OE2	5.40	1.31	1.25
2	F	316	GLU	CD-OE1	5.38	1.31	1.25
2	F	254	ARG	CA-C	5.34	1.66	1.52
2	B	316	GLU	CD-OE2	5.26	1.31	1.25
2	F	243	SER	N-CA	-5.26	1.35	1.46
1	E	214	GLU	CD-OE2	5.23	1.31	1.25
2	D	321	GLU	CD-OE2	5.04	1.31	1.25
2	B	329	GLU	CB-CG	5.03	1.61	1.52
1	C	53	SER	CA-CB	5.01	1.60	1.52

All (207) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	222	MET	C-N-CD	-20.50	75.50	120.60
1	A	94	LYS	C-N-CD	-12.62	92.83	120.60
2	F	277	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	C	152	ASP	CB-CG-OD2	-9.96	109.33	118.30
2	F	249	PHE	N-CA-CB	9.91	128.44	110.60
1	A	136	ASP	CB-CG-OD1	-9.58	109.68	118.30
1	A	133	ASP	CB-CG-OD1	-9.12	110.09	118.30
2	F	278	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	E	223	PRO	CA-N-CD	-9.01	98.89	111.50
1	A	76	ASP	CB-CG-OD2	-8.96	110.24	118.30
2	B	361	ASP	CB-CG-OD1	-8.81	110.37	118.30
1	E	47	ASN	C-N-CD	-8.79	101.27	120.60
2	F	280	ASP	CB-CG-OD1	-8.66	110.50	118.30
1	A	213	GLU	N-CA-CB	8.45	125.80	110.60
1	C	204	ASP	CB-CG-OD2	8.41	125.87	118.30
1	E	174	ASP	CB-CG-OD2	-8.34	110.80	118.30
2	F	422	GLN	C-N-CD	-8.28	102.38	120.60
2	F	396	ASP	CB-CG-OD2	-8.13	110.98	118.30
2	B	245	GLN	N-CA-CB	-8.11	96.00	110.60
2	B	247	LYS	C-N-CD	-8.11	102.75	120.60
2	F	396	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	125	ASP	CB-CG-OD2	-8.00	111.11	118.30
1	C	49	TYR	CB-CG-CD1	7.96	125.77	121.00
2	B	246	ASP	CB-CG-OD2	-7.93	111.16	118.30
2	F	278	ASP	CB-CG-OD1	7.93	125.44	118.30
2	D	246	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	E	208	GLN	C-N-CA	7.87	141.38	121.70
1	E	168	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	C	85	ASP	CB-CG-OD1	7.73	125.26	118.30
2	D	301	ARG	NE-CZ-NH2	-7.71	116.44	120.30
2	D	280	ASP	N-CA-CB	7.52	124.13	110.60
2	F	361	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	E	72	ARG	NE-CZ-NH1	7.48	124.04	120.30
2	B	361	ASP	CB-CG-OD2	7.45	125.00	118.30
1	E	133	ASP	CB-CG-OD2	-7.39	111.64	118.30
2	B	280	ASP	CB-CG-OD1	-7.29	111.74	118.30
2	F	246	ASP	CB-CG-OD2	-7.24	111.79	118.30
2	F	277	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	C	204	ASP	CB-CG-OD1	-7.21	111.81	118.30
2	B	334	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	A	155	GLN	N-CA-CB	7.18	123.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	76	ASP	CB-CG-OD1	-7.15	111.87	118.30
1	A	128	ASP	CB-CG-OD1	-7.14	111.87	118.30
1	C	152	ASP	CB-CG-OD1	7.14	124.73	118.30
2	B	376	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	C	131	LYS	C-N-CA	-7.06	104.05	121.70
2	B	248	PRO	N-CA-C	-7.04	93.80	112.10
1	E	179	SER	N-CA-CB	7.03	121.05	110.50
2	D	246	ASP	N-CA-C	7.02	129.96	111.00
1	A	200	ASP	CB-CG-OD2	-7.02	111.98	118.30
2	F	390	ILE	C-N-CD	-7.01	105.17	120.60
1	C	127	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	105	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	E	125	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	125	ASP	CB-CG-OD1	6.92	124.53	118.30
2	D	334	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	D	252	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	F	344	ASP	CB-CG-OD1	6.87	124.48	118.30
1	E	105	ASP	CB-CG-OD2	6.85	124.46	118.30
1	A	200	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	128	ASP	CB-CG-OD1	-6.83	112.15	118.30
2	F	422	GLN	N-CA-CB	6.82	122.88	110.60
1	E	105	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	C	105	ASP	CB-CG-OD1	-6.75	112.23	118.30
1	A	174	ASP	CB-CG-OD2	-6.72	112.25	118.30
2	F	335	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	B	248	PRO	N-CA-CB	6.68	111.32	103.30
1	A	133	ASP	CB-CG-OD2	6.63	124.26	118.30
2	D	278	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	A	76	ASP	CB-CG-OD1	6.48	124.13	118.30
2	F	417	TYR	CB-CG-CD1	-6.47	117.12	121.00
2	B	245	GLN	CB-CA-C	-6.46	97.49	110.40
2	B	246	ASP	CB-CG-OD1	6.44	124.10	118.30
2	F	361	ASP	CB-CG-OD1	6.43	124.09	118.30
1	E	167	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	C	133	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	208	GLN	N-CA-CB	6.42	122.15	110.60
1	A	136	ASP	CB-CG-OD2	6.40	124.06	118.30
1	E	144	THR	C-N-CD	-6.37	106.58	120.60
2	F	420	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	116	GLN	CB-CA-C	6.32	123.04	110.40
1	C	85	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	C	136	ASP	CB-CG-OD2	-6.29	112.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	255	ASP	CB-CG-OD2	6.27	123.94	118.30
2	F	317	LEU	N-CA-CB	6.26	122.92	110.40
1	E	174	ASP	CB-CG-OD1	6.26	123.93	118.30
2	F	280	ASP	CB-CG-OD2	6.25	123.93	118.30
2	D	350	SER	N-CA-CB	6.23	119.84	110.50
2	D	393	GLN	N-CA-CB	6.21	121.78	110.60
1	E	212	GLN	C-N-CA	6.18	137.15	121.70
2	B	258	TYR	N-CA-CB	6.18	121.72	110.60
2	D	351	SER	N-CA-CB	6.18	119.77	110.50
1	C	52	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	B	361	ASP	N-CA-CB	6.15	121.68	110.60
1	C	48	PRO	C-N-CA	6.15	137.07	121.70
2	D	361	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	E	200	ASP	CB-CG-OD1	-6.14	112.78	118.30
1	E	209	THR	CA-CB-CG2	6.11	120.96	112.40
1	A	158	ARG	NE-CZ-NH2	-6.11	117.25	120.30
2	B	320	LEU	N-CA-C	-6.10	94.53	111.00
2	B	423	PRO	N-CA-CB	6.09	110.61	103.30
1	E	107	ASP	CB-CG-OD1	-6.09	112.82	118.30
2	F	344	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	107	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	E	133	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	151	PRO	C-N-CA	6.06	136.84	121.70
1	C	152	ASP	N-CA-C	6.00	127.20	111.00
2	B	405	GLU	N-CA-CB	-6.00	99.80	110.60
1	A	223	PRO	N-CA-C	-5.99	96.53	112.10
2	F	242	LEU	N-CA-CB	5.99	122.37	110.40
2	D	280	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	E	204	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	107	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	C	68	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	B	388	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	204	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	128	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	76	ASP	N-CA-CB	-5.93	99.93	110.60
1	A	158	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	F	420	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	200	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	E	52	ARG	CD-NE-CZ	5.89	131.85	123.60
1	A	152	ASP	CB-CG-OD1	-5.88	113.01	118.30
2	D	277	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	F	422	GLN	CB-CA-C	5.83	122.06	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	133	ASP	CB-CG-OD2	-5.82	113.06	118.30
2	B	361	ASP	CB-CA-C	5.82	122.04	110.40
1	C	204	ASP	CB-CA-C	5.82	122.04	110.40
1	A	211	LEU	CB-CA-C	5.79	121.19	110.20
1	E	152	ASP	CB-CG-OD1	5.76	123.48	118.30
2	D	280	ASP	CB-CA-C	5.75	121.91	110.40
2	F	242	LEU	CA-C-N	-5.75	104.54	117.20
1	E	200	ASP	CB-CG-OD2	5.75	123.47	118.30
2	B	301	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	209	THR	CA-CB-OG1	5.70	120.97	109.00
1	E	50	LEU	N-CA-CB	5.69	121.78	110.40
2	B	320	LEU	C-N-CA	-5.67	107.52	121.70
2	B	278	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	E	152	ASP	CB-CG-OD2	-5.66	113.20	118.30
2	B	277	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	D	396	ASP	CB-CG-OD2	5.61	123.35	118.30
1	E	68	ARG	NE-CZ-NH2	-5.59	117.51	120.30
2	B	246	ASP	N-CA-C	5.57	126.04	111.00
2	F	424	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	136	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	76	ASP	CB-CA-C	-5.55	99.30	110.40
1	E	52	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	D	255	ASP	CB-CG-OD1	5.51	123.26	118.30
2	D	420	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	E	50	LEU	N-CA-C	5.51	125.89	111.00
2	D	391	PRO	N-CA-CB	5.51	109.91	103.30
1	A	67	LEU	CB-CA-C	-5.50	99.75	110.20
2	D	282	LEU	N-CA-CB	5.49	121.39	110.40
2	F	255	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	153	ASN	N-CA-CB	5.49	120.48	110.60
2	B	244	SER	CB-CA-C	5.48	120.52	110.10
2	D	344	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	201	SER	C-N-CD	-5.48	108.54	120.60
1	C	105	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	198	SER	CB-CA-C	5.47	120.49	110.10
1	A	152	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	61	LYS	N-CA-CB	5.46	120.42	110.60
1	A	85	ASP	CB-CG-OD1	-5.45	113.39	118.30
2	B	416	SER	N-CA-C	5.45	125.71	111.00
1	E	203	TYR	CB-CA-C	5.44	121.28	110.40
2	D	321	GLU	N-CA-C	5.43	125.67	111.00
2	F	331	MET	N-CA-CB	5.42	120.35	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	416	SER	N-CA-C	5.41	125.60	111.00
2	D	344	ASP	CB-CG-OD1	5.39	123.15	118.30
2	D	341	SER	N-CA-CB	5.36	118.54	110.50
2	B	325	GLN	N-CA-CB	5.33	120.20	110.60
2	F	322	GLN	N-CA-C	5.33	125.39	111.00
1	C	68	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	131	LYS	O-C-N	-5.32	114.18	122.70
1	A	131	LYS	N-CA-CB	5.32	120.17	110.60
2	B	324	GLN	C-N-CA	5.31	134.97	121.70
1	E	76	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	55	LYS	N-CA-C	5.28	125.27	111.00
1	A	196	GLU	N-CA-CB	5.28	120.11	110.60
2	D	245	GLN	C-N-CA	5.27	134.88	121.70
1	C	125	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	127	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	D	280	ASP	CB-CG-OD1	5.23	123.00	118.30
1	C	174	ASP	CB-CG-OD1	5.22	123.00	118.30
2	D	249	PHE	N-CA-C	-5.21	96.93	111.00
1	A	63	GLN	N-CA-CB	5.18	119.93	110.60
1	A	223	PRO	CA-C-N	-5.18	105.80	117.20
1	C	222	MET	CA-CB-CG	-5.18	104.50	113.30
1	C	58	THR	N-CA-CB	5.17	120.12	110.30
2	F	254	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	105	ASP	N-CA-CB	-5.13	101.37	110.60
1	C	168	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	182	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	B	376	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	168	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	D	278	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	63	GLN	N-CA-CB	5.08	119.74	110.60
1	E	179	SER	CB-CA-C	5.07	119.73	110.10
1	C	180	THR	CA-CB-CG2	-5.06	105.31	112.40
2	F	331	MET	CB-CA-C	5.06	120.51	110.40
1	A	204	ASP	CB-CG-OD1	-5.04	113.77	118.30
2	B	335	ARG	N-CA-CB	5.04	119.66	110.60
2	B	344	ASP	CB-CG-OD2	5.03	122.83	118.30
2	B	245	GLN	N-CA-C	5.03	124.57	111.00
1	E	87	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	58	THR	N-CA-CB	5.02	119.84	110.30
2	D	396	ASP	CB-CG-OD1	-5.00	113.80	118.30

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
2	B	329	GLU	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1480	0	1473	280	0
1	C	1480	0	1473	286	0
1	E	1480	0	1473	277	0
2	B	1450	0	1425	275	1
2	D	1450	0	1425	286	0
2	F	1450	0	1425	294	1
All	All	8790	0	8694	1463	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 84.

All (1463) 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
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: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:A:88:VAL:C	1:A:89:LEU:HD23	1.89	0.93
2:B:389:GLN:C	1:E:127:ARG:HH21	1.72	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:D:267:GLU:C	2:D:268:ILE:HD13	1.95	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:A:47:ASN:CG	1:A:76:ASP:HB3	2.00	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
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:267:GLU:O	2:D:268:ILE:HD13	1.81	0.81
2:D:387:ILE:HA	2:D:390:ILE:HG13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:210:LEU:HD12	1:A:210:LEU:C	2.00	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
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
2:B:323:GLN:C	2:B:325:GLN:H	1.85	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:400:PRO:CG	1:E:212:GLN:HB2	2.12	0.80
1:C:212:GLN:HB2	2:F:400:PRO:HB3	1.64	0.80
2:F:306:LEU:HD13	2:F:364:MET:HE1	1.63	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:106:SER:C	1:C:142:ALA:HB2	2.03	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
1:E:213:GLU:O	1:E:213:GLU:HG2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:GLN:HG2	1:A:156:ASN:N	1.98	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
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
2:D:422:GLN:HG2	2:D:423:PRO:N	1.98	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:D:391:PRO:C	2:D:394:VAL:HG23	2.04	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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:70:LEU:HG	1:A:71:GLN:H	1.51	0.75
2:B:297:HIS:C	2:B:297:HIS:CD2	2.60	0.75
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: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:D:319:GLY:C	2:D:320:LEU:CD2	2.56	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
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:C:211:LEU:HD12	1:C:211:LEU:C	2.07	0.73
1:E:117:ALA:O	1:E:131:LYS:HA	1.89	0.73
1:C:47:ASN:C	1:C:49:TYR:H	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ALA:C	1:A:46:ASN:H	1.91	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
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: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
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
2:B:290:GLU:HB2	2:B:360:SER:C	2.10	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:D:319:GLY:C	2:D:320:LEU:HD22	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:69:LEU:HD12	1:A:69:LEU:C	2.09	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
2:F:282:LEU:C	2:F:282:LEU:HD23	2.11	0.70
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
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:331:MET:HE1	2:B:332:GLN:HE22	1.56	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
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
1:E:151:PRO:O	1:E:153:ASN:N	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:306:LEU:HD13	2:F:364:MET:HE2	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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:49:TYR:HE1	1:C:79:LYS:NZ	1.92	0.67
1:E:113:LEU:C	1:E:134:GLN:HE21	1.97	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
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:NZ	1:C:133:ASP:OD1	2.25	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
2:B:413:GLN:OE1	2:B:414:LYS:HG3	1.97	0.65
2:D:247:LYS:CG	2:D:248:PRO:N	2.59	0.65
2:B:251:LEU:HD22	2:B:273:ASN:HD21	1.60	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:C	1:A:217:GLY:H	2.00	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
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
2:B:328:LEU:C	2:B:330:SER:H	2.00	0.64
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:D:323:GLN:HG3	2:D:326:GLN:CD	2.17	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
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:F:310:GLU:HG3	2:F:310:GLU:O	1.95	0.64
2:F:422:GLN:CD	2:F:423:PRO:HD2	2.17	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
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
1:C:192:LYS:HZ3	1:C:192:LYS:HB2	1.63	0.64
1:E:180:THR:C	1:E:182:ARG:H	2.02	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:47:ASN:ND2	1:A:76:ASP:CG	2.52	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: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
2:F:422:GLN:HE21	2:F:422:GLN:C	2.01	0.63
1:A:49:TYR:HD2	2:B:336:TYR:HH	1.46	0.62
1:E:212:GLN:HG2	1:E:213:GLU:C	2.20	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
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
1:A:106:SER:C	1:A:142:ALA:HB2	2.20	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
2:F:306:LEU:HB3	2:F:364:MET:HE1	1.82	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
2:F:295:VAL:O	2:F:297:HIS:ND1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ASN:N	1:C:76:ASP:HB3	2.03	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: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
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:131:LYS:C	1:C:132:LEU:HD13	2.20	0.61
1:C:148:LEU:HD12	1:C:149:ILE:N	2.16	0.61
2:B:267:GLU:CD	2:B:376:ARG:HH22	2.04	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:316:GLU:CD	2:D:335:ARG:HD2	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
2:D:301:ARG:HG3	2:D:374:ASN:HB2	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: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
2:B:331:MET:HE1	2:B:332:GLN:NE2	2.17	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
2:D:319:GLY:C	2:D:320:LEU:HD23	2.20	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
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
1:A:210:LEU:C	1:A:210:LEU:CD1	2.70	0.59
2:B:328:LEU:CD2	1:E:182:ARG:HG3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLU:HB2	1:C:158:ARG:NH1	2.18	0.59
1:E:44:ALA:O	1:E:45:GLN:HB3	2.02	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
1:C:211:LEU:C	1:C:211:LEU:CD1	2.70	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
2:B:322:GLN:H	2:B:331:MET:HE1	1.67	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:114:GLU:CD	1:A:158:ARG:HD3	2.24	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
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: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
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
2:F:335:ARG:HG2	2:F:335:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:GLN:C	1:E:127:ARG:NH2	2.51	0.57
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:A:86:TYR:C	1:A:87:ARG:HG2	2.23	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: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
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:A:150:ASN:HD22	1:A:150:ASN:C	2.08	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
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:363:ASN:OD1	2:B:363:ASN:C	2.40	0.57
2:B:404:GLU:HG3	2:B:405:GLU:H	1.70	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
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
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
2:B:331:MET:CE	2:B:332:GLN:NE2	2.68	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:282:LEU:HD12	2:B:282:LEU:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:SER:OG	1:E:194:PHE:HB2	2.05	0.56
2:F:242:LEU:HD13	2:F:244:SER:C	2.26	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:D:260:ASN:CG	2:D:262:TYR:H	2.08	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
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
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
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:306:LEU:HD22	2:F:364:MET:HE2	1.87	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: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
2:D:408:GLU:C	2:D:410:LEU:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:54:ASN:C	1:A:55:LYS:HD2	2.27	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:B:328:LEU:O	2:B:329:GLU:CD	2.44	0.55
1:C:186:TYR:C	1:C:188:SER:H	2.10	0.55
2:F:325:GLN:HG3	2:F:331:MET:HB2	1.87	0.55
1:E:57:LEU:HB2	1:E:69:LEU:O	2.05	0.55
2:B:323:GLN:C	2:B:325:GLN:N	2.58	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
1:E:185:SER:O	1:E:187:LEU:N	2.40	0.55
2:F:322:GLN:H	2:F:331:MET:HE3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:247:LYS:CB	2:F:248:PRO:CD	2.85	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:322:GLN:N	2:B:331:MET:HE1	2.23	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
2:F:282:LEU:C	2:F:282:LEU:CD2	2.76	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
2:F:323:GLN:C	2:F:325:GLN:H	2.10	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:320:LEU:HA	2:D:331:MET:HE1	1.90	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
1:C:192:LYS:HB2	1:C:192:LYS:NZ	2.20	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
1:E:119:LEU:HD12	1:E:148:LEU:HD13	1.90	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:206:ILE:C	1:E:208:GLN:H	2.12	0.53
2:F:316:GLU:HG2	2:F:337:ALA:HB2	1.90	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:260:ASN:OD1	2:F:260:ASN:C	2.45	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:297:HIS:C	2:B:297:HIS:HD2	2.11	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
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:51:PHE:C	2:D:346:ILE:CD1	2.77	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
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:151:PRO:C	1:E:153:ASN:H	2.08	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
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
2:B:241:THR:O	2:B:241:THR:HG22	2.10	0.52
1:C:168:ARG:HH12	2:F:321:GLU:CB	2.19	0.52
2:D:386:VAL:C	2:D:388:ARG:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:408:GLU:C	2:D:410:LEU:N	2.63	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
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
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:B:331:MET:CE	2:B:332:GLN:HE22	2.23	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:132:LEU:CD1	2:D:250:ASN:ND2	2.73	0.52
1:C:139:LYS:HZ3	1:C:141:GLN:NE2	2.08	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:CE1	1:A:187:LEU:HD23	2.45	0.51
2:B:322:GLN:C	2:B:324:GLN:N	2.61	0.51
2:B:351:SER:HB3	1:E:103:HIS:CD2	2.45	0.51
2:B:366:GLY:C	2:B:367:ILE:HG13	2.31	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:96:ASN:C	1:C:222:MET:HB2	2.30	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
1:C:224:LYS:HD3	1:C:224:LYS:C	2.31	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
2:F:290:GLU:HB2	2:F:360:SER:C	2.31	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
1:A:67:LEU:C	1:A:68:ARG:HG3	2.30	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:H	2:B:322:GLN:HE21	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
2:F:315:VAL:O	2:F:337:ALA:HB1	2.10	0.51
2:F:325:GLN:OE1	2:F:331:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:220:VAL:CG1	1:A:221:LYS:N	2.74	0.51
2:B:347:VAL:O	2:B:349:PRO:HD2	2.11	0.51
1:A:59:LEU:O	1:A:60:PHE:HB2	2.11	0.50
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
2:F:247:LYS:N	2:F:247:LYS:CD	2.75	0.50
2:F:322:GLN:N	2:F:331:MET:HE3	2.26	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:B:424:ARG:HD3	1:E:196:GLU:CD	2.31	0.50
1:C:202:PRO:O	1:C:203:TYR:C	2.49	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:A:178:SER:OG	2:D:398:THR:O	2.25	0.50
1:C:213:GLU:HB3	1:C:215:GLN:OE1	2.11	0.50
2:D:246:ASP:CG	2:D:249:PHE:HD2	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:HIS:HD2	2:B:298:TYR:N	2.10	0.50
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:E:88:VAL:CG2	1:E:162:PHE:HD1	2.24	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:B:247:LYS:HA	2:B:247:LYS:HZ2	1.76	0.49
2:B:300:SER:C	2:B:301:ARG:HG3	2.31	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:D:413:GLN:CD	2:D:419:VAL:HG11	2.33	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:300:SER:OG	2:D:374:ASN:HA	2.13	0.48
2:D:383:LYS:CD	2:D:384:GLU:N	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:328:LEU:HD22	1:E:182:ARG:HD2	1.96	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:B:328:LEU:C	2:B:330:SER:N	2.67	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:288:MET:HE2	2:D:362:LEU:HD23	1.96	0.48
1:E:86:TYR:CE1	1:E:164:ILE:HG23	2.48	0.48
2:F:378:PHE:HB2	2:F:384:GLU:C	2.34	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:322:GLN:HE22	2:B:332:GLN:CD	2.17	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:82:ASN:C	1:E:84:ARG:H	2.17	0.48
1:E:220:VAL:HG13	1:E:221:LYS:C	2.34	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
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
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
2:F:386:VAL:C	2:F:388:ARG:H	2.17	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
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
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:222:MET:HB2	1:A:224:LYS:C	2.34	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
1:C:105:ASP:CB	2:F:351:SER:HB2	2.44	0.47
1:C:192:LYS:HZ2	2:F:424:ARG:NH2	2.13	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
2:B:328:LEU:CD2	1:E:182:ARG:CG	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:212:GLN:CD	1:C:213:GLU:H	2.18	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
2:F:325:GLN:CA	2:F:325:GLN:NE2	2.74	0.47
2:F:422:GLN:NE2	2:F:422:GLN:C	2.68	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:150:ASN:C	1:A:150:ASN:ND2	2.68	0.46
1:C:118:ILE:HA	1:C:130:TYR:O	2.15	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:F:242:LEU:HB3	2:F:244:SER:N	2.30	0.46
1:A:79:LYS:HD2	2:B:321:GLU:CD	2.37	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: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
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
2:D:386:VAL:C	2:D:388:ARG:N	2.69	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
2:B:368:GLY:O	2:B:371:ALA:HB2	2.16	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
2:F:413:GLN:OE1	2:F:413:GLN:CA	2.64	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
2:B:295:VAL:CG1	2:B:296:PRO:CD	2.91	0.45
2:B:312:ARG:HG2	2:B:313:ALA:N	2.32	0.45
2:B:381:GLY:O	2:B:385:ASN:ND2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:315:VAL:HG21	2:F:340:LEU:HD21	1.98	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
2:D:246:ASP:O	2:D:247:LYS:HB3	2.17	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:69:LEU:C	1:A:69:LEU:CD1	2.80	0.45
1:A:137:ALA:O	2:B:250:ASN:HB3	2.16	0.45
1:C:186:TYR:C	1:C:188:SER:N	2.69	0.45
1:E:100:LEU:HD12	1:E:218:VAL:HA	1.98	0.45
2:F:399:PHE:C	2:F:401:GLY:H	2.20	0.45
2:B:290:GLU:CB	2:B:360:SER:HA	2.47	0.45
2:B:295:VAL:CG1	2:B:296:PRO:N	2.80	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
2:D:334:ARG:HD2	2:D:335:ARG:O	2.17	0.45
2:B:288:MET:HE2	2:B:358:ALA:HB2	1.99	0.45
2:B:372:GLU:O	2:B:374:ASN:N	2.50	0.45
1:E:46:ASN:HD21	1:E:48:PRO:CG	2.29	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
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
2:D:242:LEU:HD23	2:D:245:GLN:HB3	1.98	0.44
2:D:413:GLN:C	2:D:415:GLU:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:LEU:HD21	2:B:283:LEU:HD12	1.99	0.44
1:C:149:ILE:CG2	1:C:150:ASN:N	2.79	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:C:106:SER:O	1:C:142:ALA:HB2	2.18	0.44
2:D:360:SER:O	2:D:361:ASP:C	2.56	0.44
1:E:46:ASN:HD21	1:E:48:PRO:HG3	1.82	0.44
2:B:335:ARG:HG2	2:B:336:TYR:N	2.32	0.44
2:B:404:GLU:HA	2:B:407:GLU:CB	2.44	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: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
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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:117:ALA:C	1:C:118:ILE:HD12	2.39	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:400:PRO:CG	1:E:212:GLN:N	2.79	0.43
1:E:187:LEU:HD23	1:E:187:LEU:HA	1.70	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
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
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
2:D:280:ASP:C	2:D:281:ILE:HG12	2.38	0.43
1:E:56:PHE:HB3	1:E:57:LEU:H	1.45	0.43
2:B:322:GLN:N	2:B:331:MET:CE	2.82	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:HG2	1:C:207:GLU:O	2.19	0.43
2:F:306:LEU:CD1	2:F:364:MET:HE1	2.41	0.43
2:F:335:ARG:CG	2:F:335:ARG:NH1	2.82	0.43
2:F:404:GLU:O	2:F:405:GLU:C	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:79:LYS:HD2	2:B:321:GLU:CG	2.48	0.43
1:A:96:ASN:C	1:A:97:THR:HG23	2.38	0.43
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: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
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
1:A:44:ALA:C	1:A:46:ASN:N	2.68	0.42
1:A:215:GLN:C	1:A:217:GLY:N	2.71	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
1:C:62:ASN:ND2	1:C:216:GLU:CD	2.72	0.42
2:F:254:ARG:HH11	2:F:254:ARG:CG	2.20	0.42
1:A:197:ALA:O	1:A:198:SER:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:324:GLN:CD	2:F:324:GLN:N	2.72	0.42
1:A:86:TYR:HB3	1:A:162:PHE:CE1	2.54	0.42
1:A:153:ASN:CG	1:A:154:ASN:H	2.16	0.42
1:C:60:PHE:CD1	2:F:328:LEU:HD11	2.54	0.42
2:D:286:LEU:CD1	2:D:288:MET:HE2	2.49	0.42
2:D:386:VAL:O	2:D:389:GLN:HG2	2.20	0.42
1:E:92:CYS:SG	1:E:93:SER:N	2.92	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
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
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
2:F:325:GLN:OE1	2:F:331:MET:CE	2.67	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: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
1:E:143:GLY:O	1:E:145:PRO:CD	2.66	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:325:GLN:C	2:D:330:SER:HB3	2.34	0.42
2:D:383:LYS:CB	2:D:416:SER:CB	2.97	0.42
1:E:153:ASN:C	1:E:155:GLN:H	2.22	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
2:D:242:LEU:CD2	2:D:245:GLN:CB	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:291:GLY:O	2:F:420:ASP:HA	2.19	0.42
1:A:151:PRO:O	1:A:152:ASP:C	2.58	0.42
1:C:138:ILE:HG13	1:C:139:LYS:N	2.35	0.42
1:C:148:LEU:HD12	1:C:148:LEU:C	2.40	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
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
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:60:PHE:CD1	1:A:60:PHE:C	2.93	0.41
1:A:124:PRO:CD	1:A:125:ASP:N	2.84	0.41
1:A:223:PRO:HG2	1:A:224:LYS:HG3	2.03	0.41
2:B:252:ARG:O	2:B:253:SER:OG	2.32	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: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: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:356:LEU:C	2:B:356:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:NZ	2:D:322:GLN:CD	2.74	0.41
2:D:295:VAL:CG1	2:D:380:ALA:HB3	2.36	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:107:ASP:N	1:C:142:ALA:HB2	2.35	0.41
1:C:220:VAL:HG11	2:F:397:LEU:HD22	2.03	0.41
2:D:306:LEU:HB2	2:D:346:ILE:CG2	2.51	0.41
1:A:186:TYR:C	1:A:188:SER:H	2.24	0.41
1:A:206:ILE:O	1:A:207:GLU:C	2.57	0.41
2:D:387:ILE:H	2:D:387:ILE:HG13	1.76	0.41
1:E:50:LEU:C	1:E:51:PHE:HD1	2.24	0.41
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
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:277:ARG:C	2:B:279:LEU:H	2.24	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: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: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:364:MET:HE3	2:F:364:MET:HB3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:387:ILE:C	2:B:390:ILE:HD12	2.42	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
2:F:329:GLU:O	2:F:330:SER:C	2.60	0.40
1:A:133:ASP:O	1:A:136:ASP:HB2	2.20	0.40
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:N	2:B:247:LYS:HD2	2.36	0.40
2:B:404:GLU:C	2:B:406:VAL:N	2.71	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
1:A:72:ARG:C	1:A:74:ASN:N	2.75	0.40
1:A:186:TYR:C	1:A:188:SER:N	2.74	0.40
1:C:54:ASN:HB2	2:D:344:ASP:OD2	2.21	0.40
1:C:213:GLU:C	1:C:215:GLN:N	2.75	0.40
2:D:387:ILE:C	2:D:390:ILE:HG13	2.42	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
2	B	182/184 (99%)	137 (75%)	31 (17%)	14 (8%)	1	1
2	D	182/184 (99%)	134 (74%)	32 (18%)	16 (9%)	1	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%)	1	1

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (i)

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%)	107 (64%)	60 (36%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	167/167 (100%)	113 (68%)	54 (32%)	0	0
1	E	167/167 (100%)	113 (68%)	54 (32%)	0	0
2	B	161/161 (100%)	106 (66%)	55 (34%)	0	0
2	D	161/161 (100%)	98 (61%)	63 (39%)	0	0
2	F	161/161 (100%)	94 (58%)	67 (42%)	0	0
All	All	984/984 (100%)	631 (64%)	353 (36%)	0	0

All (353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
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	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	92	CYS
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	125	ASP
1	A	127	ARG
1	A	128	ASP

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Mol	Chain	Res	Type
1	A	132	LEU
1	A	134	GLN
1	A	138	ILE
1	A	148	LEU
1	A	149	ILE
1	A	150	ASN
1	A	152	ASP
1	A	153	ASN
1	A	155	GLN
1	A	156	ASN
1	A	159	ILE
1	A	161	LYS
1	A	168	ARG
1	A	174	ASP
1	A	182	ARG
1	A	183	LEU
1	A	186	TYR
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	220	VAL
1	A	221	LYS
2	B	242	LEU
2	B	243	SER
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	258	TYR
2	B	259	SER
2	B	261	ASN

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Mol	Chain	Res	Type
2	B	265	LEU
2	B	272	LYS
2	B	275	GLN
2	B	278	ASP
2	B	279	LEU
2	B	281	ILE
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	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	350	SER
2	B	353	PRO
2	B	357	LYS
2	B	360	SER
2	B	364	MET
2	B	370	ASN
2	B	373	ASN
2	B	379	LEU
2	B	386	VAL
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

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Mol	Chain	Res	Type
2	B	424	ARG
1	C	49	TYR
1	C	52	ARG
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	90	GLU
1	C	91	TYR
1	C	92	CYS
1	C	93	SER
1	C	98	LEU
1	C	99	LEU
1	C	111	LEU
1	C	123	ASN
1	C	125	ASP
1	C	127	ARG
1	C	130	TYR
1	C	131	LYS
1	C	132	LEU
1	C	134	GLN
1	C	141	GLN
1	C	150	ASN
1	C	152	ASP
1	C	154	ASN
1	C	156	ASN
1	C	167	ARG
1	C	168	ARG
1	C	172	VAL
1	C	177	LEU
1	C	178	SER
1	C	181	LYS
1	C	183	LEU
1	C	185	SER

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Mol	Chain	Res	Type
1	C	188	SER
1	C	192	LYS
1	C	193	ASN
1	C	195	LEU
1	C	200	ASP
1	C	208	GLN
1	C	209	THR
1	C	211	LEU
1	C	212	GLN
1	C	215	GLN
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	246	ASP
2	D	249	PHE
2	D	250	ASN
2	D	251	LEU
2	D	252	ARG
2	D	253	SER
2	D	254	ARG
2	D	255	ASP
2	D	257	ILE
2	D	258	TYR
2	D	264	LYS
2	D	268	ILE
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
2	D	299	ASN
2	D	301	ARG
2	D	306	LEU

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Mol	Chain	Res	Type
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	365	VAL
2	D	370	ASN
2	D	374	ASN
2	D	376	ARG
2	D	377	ASN
2	D	379	LEU
2	D	383	LYS
2	D	386	VAL
2	D	387	ILE
2	D	388	ARG
2	D	389	GLN
2	D	390	ILE
2	D	393	GLN
2	D	394	VAL
2	D	395	SER
2	D	396	ASP
2	D	398	THR
2	D	413	GLN
2	D	414	LYS
2	D	415	GLU
2	D	417	TYR
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

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Mol	Chain	Res	Type
1	E	64	HIS
1	E	66	SER
1	E	71	GLN
1	E	74	ASN
1	E	79	LYS
1	E	84	ARG
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	127	ARG
1	E	129	THR
1	E	131	LYS
1	E	132	LEU
1	E	134	GLN
1	E	139	LYS
1	E	148	LEU
1	E	152	ASP
1	E	153	ASN
1	E	154	ASN
1	E	159	ILE
1	E	167	ARG
1	E	168	ARG
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	204	ASP
1	E	211	LEU
1	E	213	GLU
1	E	215	GLN
1	E	216	GLU

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Mol	Chain	Res	Type
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	251	LEU
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	274	SER
2	F	276	LEU
2	F	277	ARG
2	F	280	ASP
2	F	282	LEU
2	F	283	LEU
2	F	286	LEU
2	F	287	GLN
2	F	288	MET
2	F	289	ASN
2	F	290	GLU
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	334	ARG
2	F	335	ARG

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Mol	Chain	Res	Type
2	F	339	THR
2	F	340	LEU
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	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
2	F	397	LEU
2	F	404	GLU
2	F	407	GLU
2	F	408	GLU
2	F	413	GLN
2	F	422	GLN
2	F	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) 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

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Mol	Chain	Res	Type
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	96	ASN
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	370	ASN
2	D	377	ASN
2	D	382	HIS
1	E	45	GLN
1	E	71	GLN
1	E	116	GLN
1	E	134	GLN
1	E	208	GLN
1	E	212	GLN
2	F	245	GLN
2	F	289	ASN
2	F	309	ASN
2	F	323	GLN
2	F	324	GLN
2	F	326	GLN
2	F	377	ASN
2	F	422	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.91	1 (0%)	89	88	8, 20, 30, 41	0
1	C	181/181 (100%)	-0.72	4 (2%)	62	56	8, 20, 32, 39	0
1	E	181/181 (100%)	-0.70	5 (2%)	53	46	5, 18, 33, 42	0
2	B	184/184 (100%)	-0.69	4 (2%)	62	56	6, 17, 32, 40	0
2	D	184/184 (100%)	-0.79	7 (3%)	40	33	7, 20, 33, 41	0
2	F	184/184 (100%)	-0.77	5 (2%)	54	48	6, 20, 33, 42	0
All	All	1095/1095 (100%)	-0.76	26 (2%)	59	53	5, 19, 33, 42	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	48	PRO	5.3
1	C	47	ASN	4.1
2	B	243	SER	4.0
2	F	243	SER	3.8
2	D	243	SER	3.7
1	E	49	TYR	3.3
2	D	245	GLN	3.1
1	E	46	ASN	2.9
1	C	46	ASN	2.7
2	B	322	GLN	2.6
2	D	321	GLU	2.6
1	C	49	TYR	2.6
2	B	324	GLN	2.5
1	A	47	ASN	2.5
1	C	76	ASP	2.5
1	E	47	ASN	2.5
2	B	244	SER	2.4
2	F	326	GLN	2.4
2	F	323	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	325	GLN	2.3
2	D	322	GLN	2.3
1	E	45	GLN	2.2
2	D	242	LEU	2.2
2	F	242	LEU	2.2
2	D	244	SER	2.1
2	D	246	ASP	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 monosaccharides 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.