



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:51 AM UTC

PDB ID : 5XDA / pdb_00005xda
Title : Structural basis for Ufm1 recognition by UfSP
Authors : Kim, K.H.; Ha, B.H.; Kim, E.E.
Deposited on : 2017-03-28
Resolution : 3.29 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

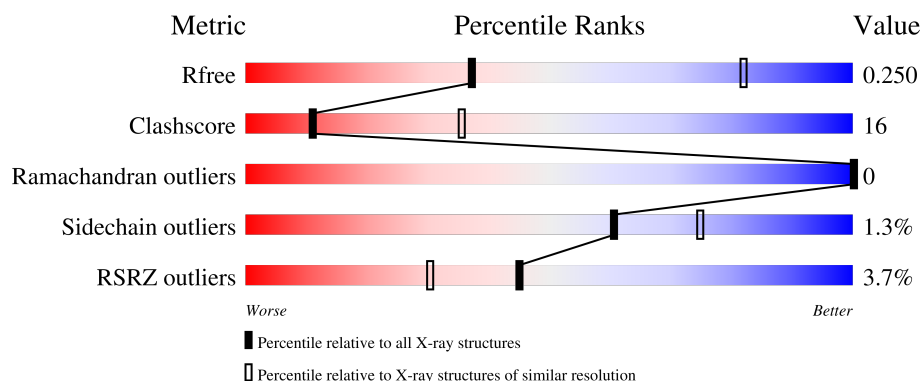
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	565	
1	B	565	
1	C	565	
1	D	565	
1	E	565	

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Mol	Chain	Length	Quality of chain
1	F	565	7% 68% 24% 5%
2	G	84	% 79% 21%
2	H	84	2% 88% 12%
2	I	84	4% 81% 14% 5%
2	J	84	2% 71% 23% 6%
2	K	84	2% 95% 5%
2	L	84	% 85% 13% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29730 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 Ufm1-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4306	2733	755	802	16			
1	B	542	Total	C	N	O	S	0	0	0
			4342	2754	762	810	16			
1	C	541	Total	C	N	O	S	0	0	0
			4332	2748	759	809	16			
1	D	538	Total	C	N	O	S	0	0	0
			4312	2736	756	804	16			
1	E	535	Total	C	N	O	S	0	0	0
			4289	2723	751	799	16			
1	F	535	Total	C	N	O	S	0	0	0
			4289	2723	752	798	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	SER	CYS	engineered mutation	UNP Q94218
B	407	SER	CYS	engineered mutation	UNP Q94218
C	407	SER	CYS	engineered mutation	UNP Q94218
D	407	SER	CYS	engineered mutation	UNP Q94218
E	407	SER	CYS	engineered mutation	UNP Q94218
F	407	SER	CYS	engineered mutation	UNP Q94218

- Molecule 2 is a protein called Ubiquitin-fold modifier 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	84	Total	C	N	O	0	0	0
			627	405	106	116			
2	H	84	Total	C	N	O	0	0	0
			627	405	106	116			
2	I	84	Total	C	N	O	0	0	0
			627	405	106	116			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	84	Total	C	N	O	0	0	0
			627	405	106	116			
2	K	84	Total	C	N	O	0	0	0
			627	405	106	116			
2	L	84	Total	C	N	O	0	0	0
			627	405	106	116			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	94	GLY	HIS	engineered mutation	UNP P34661
H	94	GLY	HIS	engineered mutation	UNP P34661
I	94	GLY	HIS	engineered mutation	UNP P34661
J	94	GLY	HIS	engineered mutation	UNP P34661
K	94	GLY	HIS	engineered mutation	UNP P34661
L	94	GLY	HIS	engineered mutation	UNP P34661

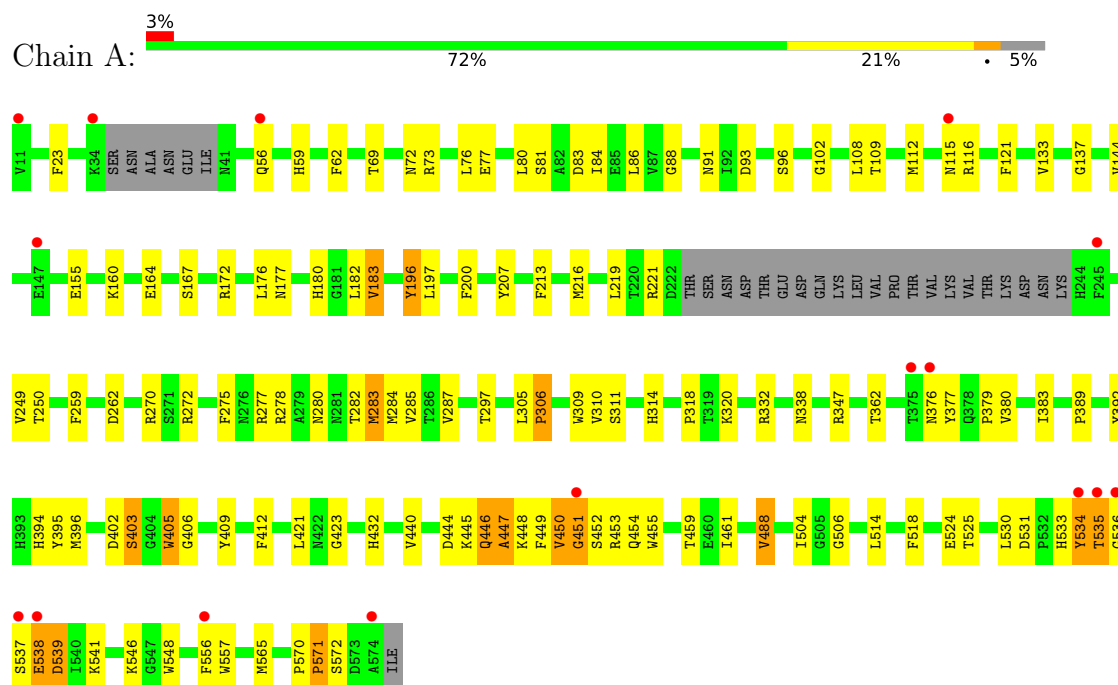
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	19	Total	O	0	0
			19	19		
3	C	27	Total	O	0	0
			27	27		
3	D	6	Total	O	0	0
			6	6		
3	E	11	Total	O	0	0
			11	11		
3	F	5	Total	O	0	0
			5	5		
3	G	4	Total	O	0	0
			4	4		
3	H	2	Total	O	0	0
			2	2		
3	I	4	Total	O	0	0
			4	4		
3	L	2	Total	O	0	0
			2	2		

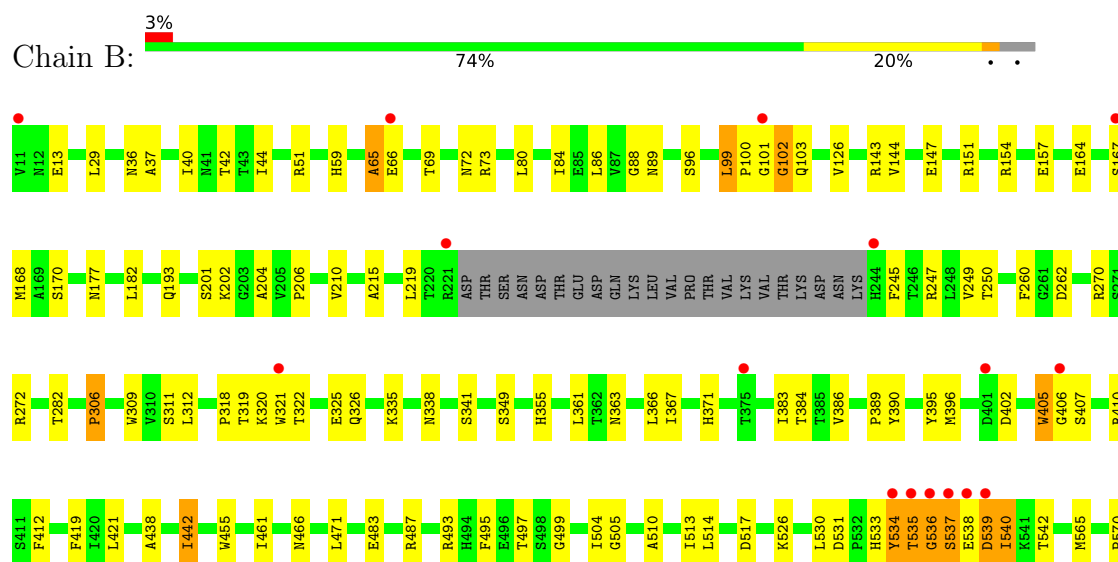
3 Residue-property plots [i](#)

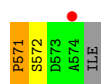
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ufm1-specific protease

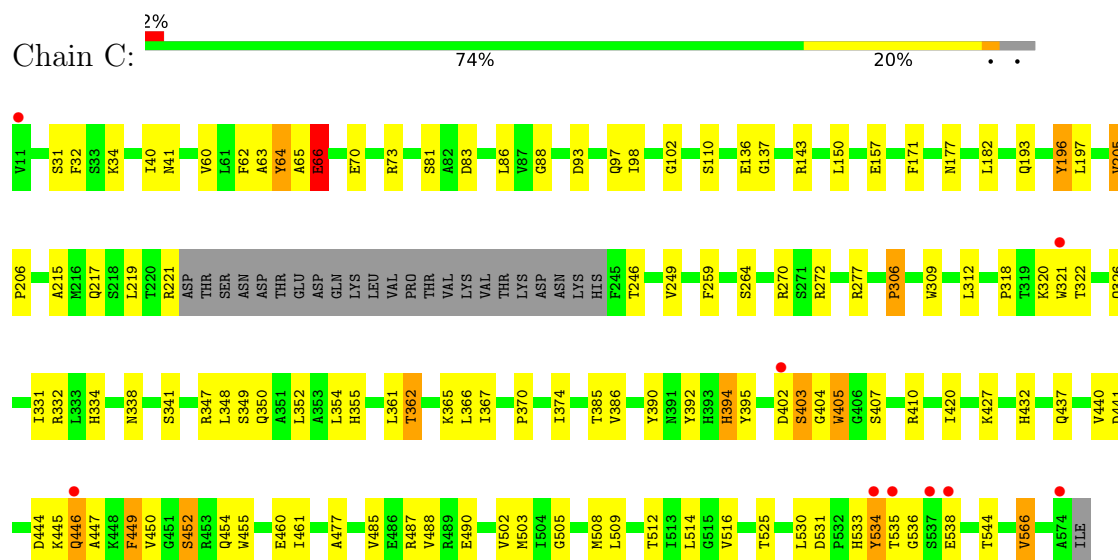


• Molecule 1: Ufm1-specific protease

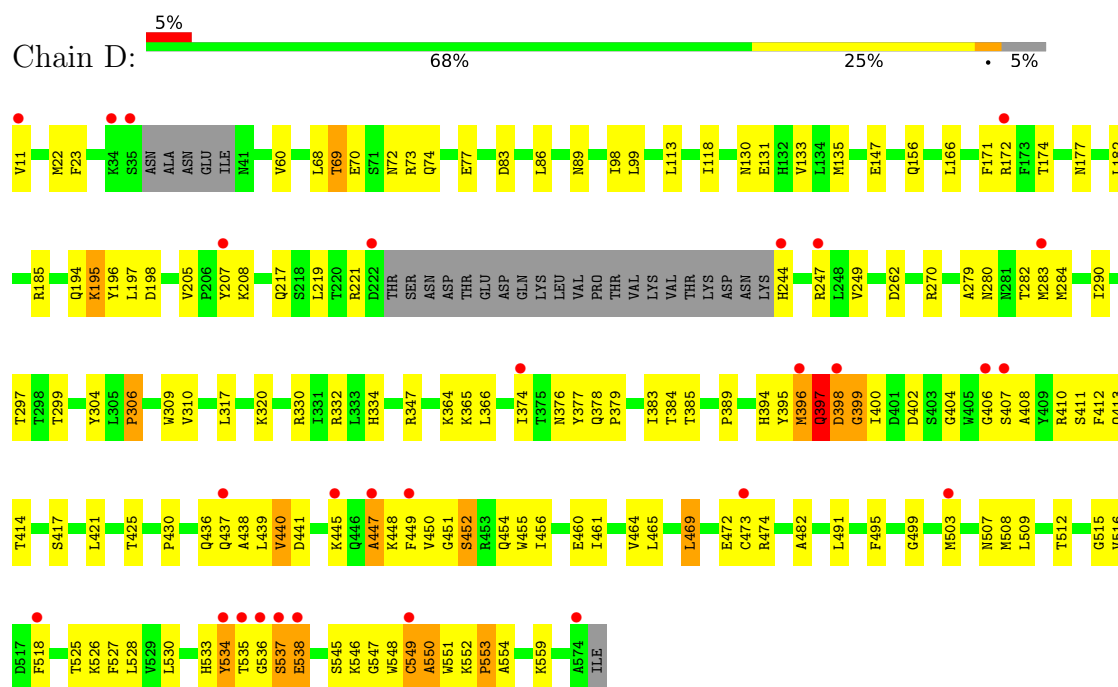




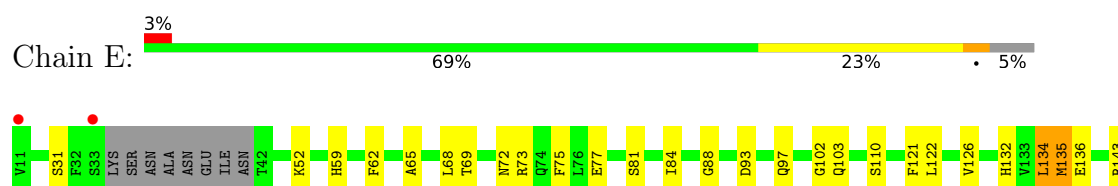
• Molecule 1: Ufm1-specific protease

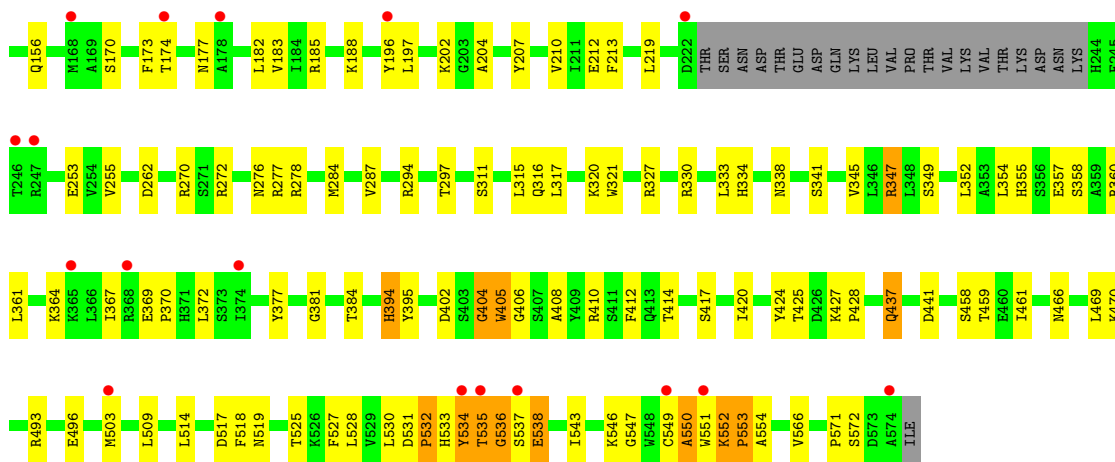


• Molecule 1: Ufm1-specific protease

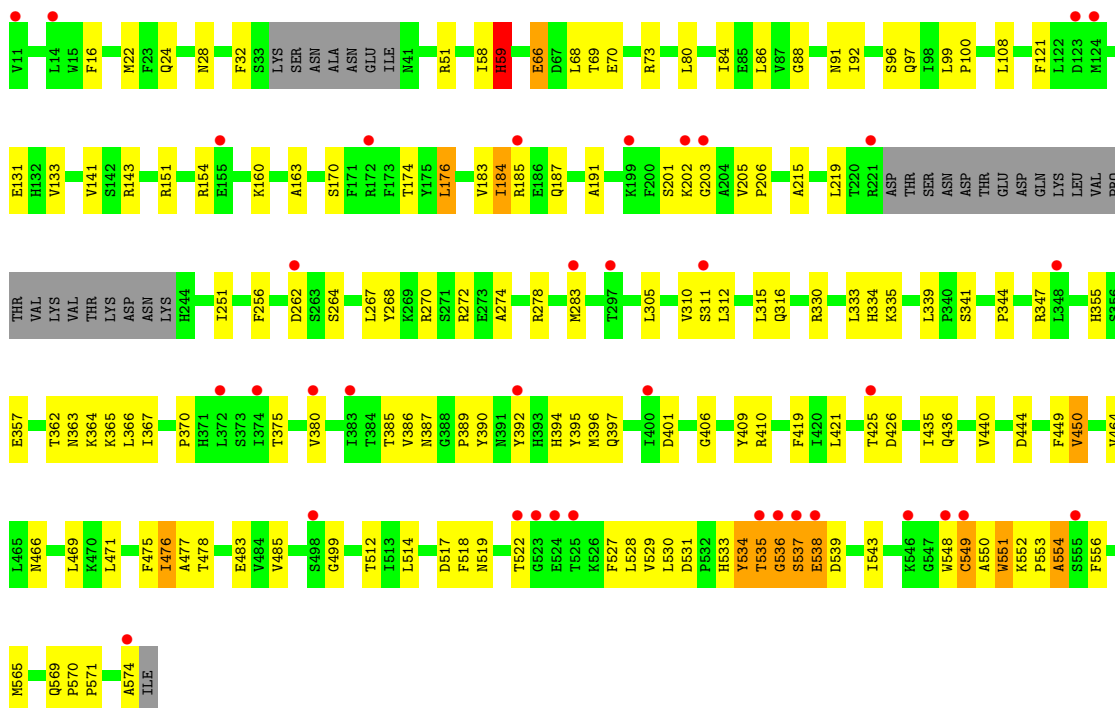


• Molecule 1: Ufm1-specific protease

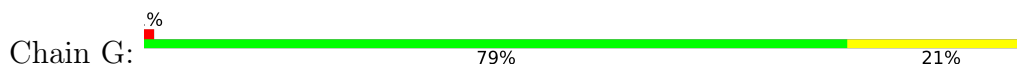




• Molecule 1: Ufm1-specific protease



• Molecule 2: Ubiquitin-fold modifier 1

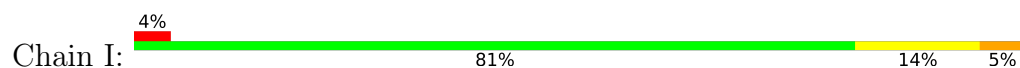


• Molecule 2: Ubiquitin-fold modifier 1





- Molecule 2: Ubiquitin-fold modifier 1



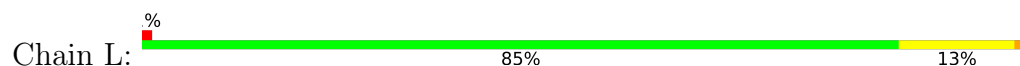
- Molecule 2: Ubiquitin-fold modifier 1



- Molecule 2: Ubiquitin-fold modifier 1



- Molecule 2: Ubiquitin-fold modifier 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	267.45Å 455.33Å 195.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 3.29 46.16 – 3.29	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.16-3.29) 95.9 (46.16-3.29)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.207 , 0.243 0.218 , 0.250	Depositor DCC
R_{free} test set	2018 reflections (1.12%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.045 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29730	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/4407	0.93	20/5968 (0.3%)
1	B	0.42	1/4444 (0.0%)	1.15	27/6020 (0.4%)
1	C	0.55	8/4433 (0.2%)	0.94	19/6005 (0.3%)
1	D	0.48	6/4413 (0.1%)	1.02	32/5976 (0.5%)
1	E	0.46	4/4390 (0.1%)	1.05	37/5946 (0.6%)
1	F	0.39	3/4390 (0.1%)	1.08	23/5946 (0.4%)
2	G	0.65	0/641	0.77	0/870
2	H	0.30	0/641	0.80	1/870 (0.1%)
2	I	0.52	1/641 (0.2%)	1.16	6/870 (0.7%)
2	J	0.32	0/641	0.94	6/870 (0.7%)
2	K	0.31	0/641	0.77	0/870
2	L	0.30	0/641	0.86	2/870 (0.2%)
All	All	0.45	23/30323 (0.1%)	1.01	173/41081 (0.4%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	566	VAL	C-O	12.39	1.38	1.24
1	D	69	THR	CA-C	8.91	1.64	1.52
1	C	331	ILE	CB-CG1	8.53	1.70	1.53
2	I	88	PRO	N-CD	-8.37	1.36	1.47
1	C	331	ILE	CA-CB	-8.27	1.44	1.54
1	C	64	TYR	CA-C	-8.20	1.42	1.53
1	D	69	THR	N-CA	8.19	1.56	1.46
1	E	405	TRP	C-N	-7.36	1.22	1.33
1	D	447	ALA	C-O	6.96	1.32	1.24
1	D	447	ALA	CA-C	6.85	1.62	1.52
1	C	64	TYR	C-O	-6.65	1.15	1.23
1	B	29	LEU	CA-CB	-6.58	1.42	1.53
1	D	399	GLY	C-N	-6.39	1.25	1.33
1	F	534	TYR	N-CA	5.87	1.52	1.45
1	D	447	ALA	N-CA	5.85	1.53	1.46
1	C	60	VAL	CB-CG1	5.67	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	537	SER	C-N	-5.55	1.22	1.34
1	F	59	HIS	CA-C	-5.41	1.45	1.52
1	E	553	PRO	CA-C	-5.23	1.46	1.52
1	F	59	HIS	CG-ND1	-5.21	1.32	1.38
1	E	394	HIS	CG-ND1	-5.14	1.32	1.38
1	C	66	GLU	C-O	-5.13	1.17	1.24
1	C	65	ALA	C-O	-5.01	1.18	1.24

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	SER	N-CA-C	29.82	147.41	111.33
1	B	536	GLY	N-CA-C	-22.50	83.12	112.14
1	F	535	THR	N-CA-C	-22.31	74.84	109.65
1	C	403	SER	N-CA-C	21.20	133.75	111.07
1	E	404	GLY	N-CA-C	-20.52	79.58	111.18
1	B	538	GLU	N-CA-CB	-20.50	80.25	110.80
1	B	36	ASN	CB-CA-C	-20.47	77.49	111.68
1	F	550	ALA	N-CA-CB	-19.93	76.81	110.49
1	F	202	LYS	CB-CA-C	-19.89	77.66	110.29
1	F	537	SER	N-CA-C	-19.24	76.75	107.73
1	B	571	PRO	CB-CA-C	-17.56	82.34	110.25
1	B	101	GLY	N-CA-C	17.27	154.10	113.18
1	F	537	SER	CB-CA-C	17.26	143.01	110.56
1	C	446	GLN	N-CA-C	17.00	132.26	110.33
1	E	550	ALA	N-CA-CB	-16.44	82.97	111.08
1	F	536	GLY	N-CA-C	15.56	150.06	113.18
1	F	534	TYR	N-CA-C	-15.43	85.33	110.17
1	D	69	THR	N-CA-C	15.37	131.26	110.35
1	E	553	PRO	CB-CA-C	-15.37	91.29	111.12
1	B	99	LEU	CB-CA-C	15.12	131.92	109.09
1	E	534	TYR	N-CA-C	15.11	132.48	109.96
2	I	93	GLY	CA-C-N	-14.86	94.95	121.70
2	I	93	GLY	C-N-CA	-14.86	94.95	121.70
1	B	534	TYR	N-CA-C	14.69	130.31	109.15
1	F	550	ALA	CB-CA-C	-14.54	81.49	110.42
1	B	99	LEU	N-CA-C	-14.54	91.36	110.40
1	B	572	SER	N-CA-C	14.31	134.63	108.58
1	E	537	SER	N-CA-C	-14.28	86.43	108.14
1	D	194	GLN	N-CA-C	14.17	126.72	111.28
1	C	452	SER	N-CA-C	14.11	127.69	110.19
1	F	476	ILE	N-CA-C	-13.97	89.91	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	438	ALA	N-CA-C	-13.84	96.45	114.31
1	D	553	PRO	CB-CA-C	-13.62	90.59	110.75
1	A	376	ASN	N-CA-C	13.32	129.48	113.23
1	D	538	GLU	N-CA-C	13.30	130.14	111.52
1	D	397	GLN	CB-CA-C	-13.26	87.93	109.80
1	A	405	TRP	N-CA-C	12.93	128.53	113.02
1	E	572	SER	N-CA-C	12.61	126.79	111.40
1	F	538	GLU	N-CA-CB	-12.45	90.21	109.88
1	F	554	ALA	N-CA-C	-12.23	98.39	113.18
1	C	362	THR	CB-CA-C	-11.71	91.70	111.26
1	B	537	SER	N-CA-CB	-11.68	92.54	110.06
1	B	540	ILE	N-CA-C	-11.57	97.21	113.07
1	B	572	SER	N-CA-CB	-11.46	91.39	110.42
1	C	64	TYR	N-CA-C	-11.30	94.76	110.35
1	B	37	ALA	N-CA-C	10.95	128.78	113.56
1	A	571	PRO	CB-CA-C	-10.87	96.72	110.95
1	D	447	ALA	N-CA-C	10.81	124.15	111.71
1	E	538	GLU	N-CA-CB	-10.80	95.11	111.64
1	A	448	LYS	N-CA-C	-10.76	100.29	113.41
1	D	549	CYS	N-CA-C	-10.72	97.62	111.02
1	E	554	ALA	N-CA-C	10.52	125.63	113.01
1	A	572	SER	N-CA-C	10.40	123.75	110.65
1	C	403	SER	CB-CA-C	-10.06	95.08	110.88
1	A	377	TYR	N-CA-C	9.73	124.45	109.96
1	D	399	GLY	N-CA-C	-9.70	90.20	113.18
1	D	440	VAL	N-CA-C	-9.66	104.08	111.90
1	E	126	VAL	N-CA-C	9.62	119.65	110.42
1	A	405	TRP	N-CA-CB	-9.51	96.67	110.47
1	E	571	PRO	CB-CA-C	-9.39	96.85	110.75
1	D	397	GLN	N-CA-C	-9.31	95.99	110.42
1	E	204	ALA	N-CA-C	9.30	124.29	110.52
1	A	572	SER	N-CA-CB	-9.23	99.74	110.35
1	B	539	ASP	N-CA-C	-9.21	95.88	109.15
1	A	539	ASP	N-CA-CB	9.09	125.84	110.49
1	A	447	ALA	CB-CA-C	-9.03	92.45	110.42
1	A	534	TYR	N-CA-C	8.92	129.79	110.80
1	A	196	TYR	N-CA-C	8.84	121.00	111.36
2	J	65	VAL	N-CA-CB	8.79	123.76	112.34
1	E	537	SER	O-C-N	-8.78	114.51	123.29
1	D	398	ASP	N-CA-C	8.63	123.30	111.90
1	C	365	LYS	N-CA-C	-8.58	100.34	113.89
1	F	201	SER	N-CA-C	8.48	125.08	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	532	PRO	CB-CA-C	-8.41	98.34	111.04
1	E	405	TRP	N-CA-C	8.31	129.91	113.29
1	D	537	SER	N-CA-C	-8.24	91.59	107.57
1	D	306	PRO	CB-CA-C	8.22	120.95	110.92
1	F	476	ILE	CB-CA-C	8.21	126.48	111.30
1	A	538	GLU	N-CA-C	-8.14	93.46	110.80
1	B	535	THR	CA-C-N	-8.04	112.71	120.34
1	B	535	THR	C-N-CA	-8.04	112.71	120.34
2	J	93	GLY	N-CA-C	-7.96	97.19	110.80
1	E	135	MET	N-CA-C	7.88	120.87	111.02
1	C	405	TRP	N-CA-C	-7.86	104.57	114.56
1	B	338	ASN	OD1-CG-ND2	7.83	130.43	122.60
1	A	535	THR	N-CA-CB	-7.82	98.58	110.07
1	E	405	TRP	O-C-N	-7.81	113.53	121.88
1	D	554	ALA	N-CA-C	7.71	120.58	111.71
1	A	446	GLN	N-CA-C	7.59	121.99	111.74
2	J	65	VAL	N-CA-C	-7.45	94.29	107.18
1	C	534	TYR	N-CA-C	7.41	120.59	109.25
1	F	549	CYS	N-CA-C	7.41	122.77	113.43
1	E	204	ALA	N-CA-CB	-7.39	98.63	110.46
2	I	88	PRO	CB-CA-C	7.33	120.90	110.20
1	E	536	GLY	N-CA-C	7.31	130.50	113.18
1	E	136	GLU	N-CA-C	7.29	121.83	113.15
1	D	69	THR	CB-CA-C	-7.22	96.69	109.62
1	E	572	SER	N-CA-CB	-7.10	99.63	110.13
1	C	65	ALA	N-CA-C	6.99	118.98	111.36
1	D	194	GLN	CB-CA-C	-6.92	99.31	110.79
1	C	362	THR	N-CA-C	6.88	121.63	113.23
1	D	306	PRO	CA-C-N	6.84	128.38	119.84
1	D	306	PRO	C-N-CA	6.84	128.38	119.84
1	E	554	ALA	N-CA-CB	-6.81	98.47	110.39
1	C	196	TYR	N-CA-C	6.78	118.36	110.97
1	D	534	TYR	N-CA-C	6.69	119.33	108.63
1	E	534	TYR	N-CA-CB	-6.61	99.07	109.51
1	F	549	CYS	CB-CA-C	6.59	120.73	109.65
1	D	538	GLU	N-CA-CB	-6.58	101.92	111.91
1	D	550	ALA	N-CA-C	-6.56	99.44	109.41
1	F	477	ALA	N-CA-CB	6.54	121.80	110.81
1	B	99	LEU	CA-C-N	6.52	127.69	120.45
1	B	99	LEU	C-N-CA	6.52	127.69	120.45
2	H	56	THR	N-CA-C	-6.47	105.12	114.12
1	C	452	SER	N-CA-CB	-6.41	101.54	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	93	GLY	N-CA-C	-6.35	101.10	110.87
1	A	451	GLY	N-CA-C	-6.34	98.15	113.18
1	A	450	VAL	CB-CA-C	-6.19	104.05	111.97
1	F	380	VAL	N-CA-C	-6.17	106.72	112.83
1	E	535	THR	N-CA-C	-6.14	95.53	107.62
1	E	405	TRP	CB-CA-C	-6.07	98.76	110.35
1	E	553	PRO	N-CA-C	-6.06	101.95	111.34
1	E	202	LYS	CB-CA-C	-6.05	99.64	110.70
1	E	550	ALA	CB-CA-C	6.04	121.24	109.33
2	J	64	GLY	N-CA-C	-6.01	98.92	113.18
2	L	90	ASP	N-CA-C	5.97	119.48	107.41
1	F	554	ALA	N-CA-CB	5.97	120.44	110.41
1	F	538	GLU	N-CA-C	-5.92	99.15	108.63
1	D	447	ALA	CA-C-O	5.92	126.79	120.10
1	C	64	TYR	CA-C-O	-5.90	115.21	121.88
1	E	188	LYS	CA-C-N	5.90	127.22	119.84
1	E	188	LYS	C-N-CA	5.90	127.22	119.84
1	E	134	LEU	N-CA-C	5.76	118.25	110.88
1	B	65	ALA	N-CA-C	5.75	119.77	112.87
1	E	550	ALA	N-CA-C	-5.72	100.57	109.72
1	F	551	TRP	N-CA-CB	-5.69	100.87	110.49
1	B	102	GLY	N-CA-C	-5.64	102.72	111.12
1	D	399	GLY	O-C-N	-5.62	115.39	122.70
1	E	552	LYS	N-CA-C	5.62	118.81	110.32
1	D	398	ASP	CA-C-N	5.62	132.43	121.41
1	D	398	ASP	C-N-CA	5.62	132.43	121.41
1	B	405	TRP	CB-CA-C	-5.61	99.26	110.42
1	C	331	ILE	CB-CA-C	-5.57	104.62	112.14
1	B	13	GLU	N-CA-C	-5.52	99.80	108.63
1	C	449	PHE	N-CA-CB	5.51	118.22	110.12
2	L	89	ARG	CB-CA-C	-5.51	99.89	109.64
1	F	203	GLY	N-CA-C	-5.49	106.44	114.90
1	D	396	MET	N-CA-C	5.45	122.00	113.72
1	D	452	SER	N-CA-C	-5.44	101.41	110.17
2	J	23	ASP	CA-C-N	5.42	125.24	119.28
2	J	23	ASP	C-N-CA	5.42	125.24	119.28
1	D	398	ASP	N-CA-CB	5.40	120.24	112.08
1	E	394	HIS	N-CA-C	5.40	115.16	108.19
1	D	469	LEU	CB-CA-C	5.36	119.03	109.38
1	D	195	LYS	N-CA-CB	5.36	119.55	110.49
1	E	408	ALA	N-CA-C	-5.36	105.88	112.90
1	B	535	THR	O-C-N	-5.30	116.26	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	87	ILE	CB-CA-C	-5.28	101.76	111.36
1	B	570	PRO	CB-CA-C	-5.25	104.51	110.92
1	E	552	LYS	CA-C-N	5.25	125.53	119.92
1	E	552	LYS	C-N-CA	5.25	125.53	119.92
1	D	450	VAL	CB-CA-C	-5.23	103.31	111.26
1	E	202	LYS	N-CA-C	5.22	118.11	111.69
2	I	88	PRO	N-CA-CB	-5.20	96.68	102.72
1	A	403	SER	CB-CA-C	5.16	118.98	110.88
1	F	569	GLN	CA-C-N	5.14	123.36	119.66
1	F	569	GLN	C-N-CA	5.14	123.36	119.66
1	A	306	PRO	O-C-N	5.14	123.67	121.31
1	C	306	PRO	O-C-N	5.12	123.66	121.31
1	C	205	VAL	CA-C-N	5.05	125.33	119.47
1	C	205	VAL	C-N-CA	5.05	125.33	119.47
1	B	306	PRO	O-C-N	5.02	123.62	121.31
1	A	447	ALA	N-CA-C	5.01	121.48	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4306	0	4218	153	0
1	B	4342	0	4254	122	0
1	C	4332	0	4247	156	0
1	D	4312	0	4223	211	0
1	E	4289	0	4199	132	0
1	F	4289	0	4201	152	0
2	G	627	0	652	15	0
2	H	627	0	652	7	0
2	I	627	0	652	41	0
2	J	627	0	652	31	0
2	K	627	0	652	3	0
2	L	627	0	652	8	0
3	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	0	0	0
3	C	27	0	0	1	0
3	D	6	0	0	1	0
3	E	11	0	0	1	0
3	F	5	0	0	0	0
3	G	4	0	0	0	0
3	H	2	0	0	0	0
3	I	4	0	0	0	0
3	L	2	0	0	0	0
All	All	29730	0	29254	968	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (968) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:SER:HB3	1:D:503:MET:CE	1.32	1.59
1:D:411:SER:CB	1:D:503:MET:HE1	1.32	1.57
1:C:321:TRP:HE1	1:C:326:GLN:CB	1.15	1.52
1:A:394:HIS:CE1	1:A:535:THR:HB	1.45	1.50
1:C:321:TRP:NE1	1:C:326:GLN:HB2	1.21	1.44
1:B:321:TRP:NE1	1:B:326:GLN:HB2	1.42	1.35
1:F:367:ILE:HD11	1:F:538:GLU:CG	1.53	1.35
1:C:392:TYR:HE2	1:C:394:HIS:ND1	1.25	1.32
1:D:535:THR:OG1	1:D:548:TRP:CE3	1.72	1.32
1:D:398:ASP:O	1:D:400:ILE:HG13	1.17	1.30
1:B:319:THR:N	1:B:321:TRP:HZ3	1.31	1.29
1:F:58:ILE:HG22	1:F:59:HIS:CE1	1.69	1.27
1:C:392:TYR:CE2	1:C:394:HIS:ND1	2.00	1.27
1:D:172:ARG:HD2	1:D:221:ARG:NE	1.46	1.27
2:I:87:ILE:CG2	2:I:88:PRO:HD2	1.62	1.26
1:B:321:TRP:HE1	1:B:326:GLN:CB	1.50	1.24
1:A:176:LEU:HD12	1:A:182:LEU:O	1.20	1.24
1:D:411:SER:CB	1:D:503:MET:CE	2.01	1.23
1:F:392:TYR:CE2	1:F:394:HIS:ND1	2.09	1.21
1:F:367:ILE:CG1	1:F:538:GLU:HG3	1.71	1.19
1:D:535:THR:OG1	1:D:548:TRP:CZ3	1.94	1.19
1:D:547:GLY:C	1:D:550:ALA:HB2	1.68	1.19
1:C:477:ALA:CB	2:I:87:ILE:HD13	1.72	1.18
1:A:394:HIS:CE1	1:A:535:THR:CB	2.27	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ILE:CD1	1:F:538:GLU:CG	2.22	1.17
1:B:319:THR:CA	1:B:321:TRP:HZ3	1.57	1.16
1:B:405:TRP:O	1:B:405:TRP:CE3	1.99	1.16
1:C:318:PRO:O	1:C:321:TRP:CZ3	1.99	1.16
1:A:405:TRP:CE2	1:A:453:ARG:HG3	1.79	1.15
1:D:207:TYR:CE1	1:D:208:LYS:HE2	1.80	1.14
1:C:318:PRO:O	1:C:321:TRP:HZ3	1.29	1.13
1:C:460:GLU:HG3	2:I:89:ARG:NH1	1.63	1.13
1:A:396:MET:SD	1:A:534:TYR:CE1	2.41	1.12
1:B:395:TYR:CB	1:B:534:TYR:HB2	1.79	1.11
1:A:172:ARG:HH22	1:A:221:ARG:NH2	1.48	1.11
1:D:449:PHE:HE1	1:D:454:GLN:HB3	1.10	1.11
1:D:550:ALA:HB3	1:D:552:LYS:HE2	1.30	1.11
1:B:318:PRO:C	1:B:321:TRP:CZ3	2.29	1.10
1:E:532:PRO:HD2	1:E:533:HIS:H	1.07	1.10
1:E:547:GLY:HA2	1:E:550:ALA:HB2	1.26	1.10
1:A:172:ARG:NH2	1:A:221:ARG:HH21	1.48	1.10
1:C:440:VAL:HG21	1:C:450:VAL:HG23	1.25	1.09
1:C:321:TRP:HE1	1:C:326:GLN:CA	1.65	1.09
1:A:379:PRO:HB3	1:A:383:ILE:HD11	1.26	1.09
1:A:556:PHE:HE2	1:A:557:TRP:CZ3	1.71	1.09
1:B:395:TYR:HB2	1:B:534:TYR:HB2	1.12	1.09
1:C:395:TYR:CB	1:C:534:TYR:HB2	1.81	1.08
1:A:449:PHE:CE1	1:A:454:GLN:HB3	1.88	1.08
1:B:319:THR:CA	1:B:321:TRP:CZ3	2.36	1.08
1:F:367:ILE:HG12	1:F:538:GLU:HG3	1.24	1.08
1:C:66:GLU:N	1:C:66:GLU:OE1	1.87	1.07
1:B:319:THR:N	1:B:321:TRP:CZ3	2.21	1.07
1:F:66:GLU:OE1	1:F:66:GLU:N	1.87	1.05
2:I:87:ILE:HG23	2:I:88:PRO:HD2	1.12	1.05
1:E:547:GLY:HA2	1:E:550:ALA:CB	1.85	1.05
1:F:58:ILE:C	1:F:59:HIS:ND1	2.15	1.05
1:C:395:TYR:HB2	1:C:534:TYR:CB	1.85	1.05
1:A:394:HIS:ND1	1:A:535:THR:HB	1.71	1.04
1:A:283:MET:HE3	1:A:284:MET:HG2	1.40	1.04
1:B:367:ILE:HD11	1:B:537:SER:O	1.56	1.04
1:D:196:TYR:CD2	1:D:197:LEU:HD13	1.92	1.04
2:G:53:PRO:HG2	2:G:56:THR:OG1	1.59	1.03
1:C:460:GLU:CD	2:I:89:ARG:HH11	1.67	1.03
1:D:195:LYS:HG2	1:D:198:ASP:OD2	1.58	1.03
1:F:367:ILE:CD1	1:F:538:GLU:HG2	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:HB3	1:A:116:ARG:HD3	1.39	1.02
1:D:172:ARG:HD2	1:D:221:ARG:HE	0.87	1.02
1:D:411:SER:OG	1:D:503:MET:HE2	1.59	1.02
1:A:176:LEU:HD13	1:A:183:VAL:HB	1.40	1.02
1:B:405:TRP:O	1:B:405:TRP:CD2	2.12	1.02
1:D:449:PHE:CE1	1:D:454:GLN:HB3	1.95	1.02
1:C:420:ILE:HD11	1:C:427:LYS:O	1.60	1.01
1:F:174:THR:HG22	1:F:185:ARG:HB2	1.42	1.01
2:I:87:ILE:CG2	2:I:88:PRO:CD	2.37	1.01
1:D:196:TYR:CD2	1:D:197:LEU:CD1	2.44	1.01
1:C:477:ALA:HB2	2:I:87:ILE:HD13	1.39	1.01
1:B:504:ILE:HG12	1:B:565:MET:HG2	1.43	1.00
1:C:485:VAL:O	1:C:488:VAL:HG23	1.60	1.00
1:D:474:ARG:HG2	2:J:64:GLY:O	1.62	1.00
1:D:135:MET:HE1	1:D:207:TYR:CE2	1.97	0.99
1:E:196:TYR:CD2	1:E:197:LEU:HD12	1.97	0.99
1:F:174:THR:HG22	1:F:185:ARG:CB	1.91	0.99
1:C:460:GLU:CG	2:I:89:ARG:NH1	2.26	0.99
1:C:477:ALA:HB2	2:I:87:ILE:CD1	1.92	0.99
1:C:460:GLU:CG	2:I:89:ARG:HH11	1.75	0.98
1:A:172:ARG:NH1	1:A:221:ARG:HD3	1.77	0.98
1:F:160:LYS:HG3	1:F:283:MET:HE1	1.43	0.98
1:A:405:TRP:CG	1:A:453:ARG:HG2	1.98	0.98
1:A:396:MET:SD	1:A:534:TYR:HE1	1.80	0.97
1:D:195:LYS:CG	1:D:198:ASP:OD2	2.13	0.97
1:E:404:GLY:O	1:E:405:TRP:CD1	2.18	0.97
1:E:528:LEU:HD13	1:E:551:TRP:NE1	1.79	0.97
1:A:556:PHE:CE2	1:A:557:TRP:CZ3	2.51	0.97
1:D:398:ASP:O	1:D:400:ILE:CG1	2.11	0.97
1:D:395:TYR:HB2	1:D:534:TYR:HB2	1.47	0.96
1:E:532:PRO:CD	1:E:533:HIS:H	1.77	0.96
1:F:552:LYS:HB3	1:F:553:PRO:CD	1.95	0.96
1:B:504:ILE:HD11	1:B:513:ILE:HD12	1.47	0.96
1:F:32:PHE:CD2	1:F:341:SER:HB3	1.99	0.96
1:A:444:ASP:O	1:A:445:LYS:HG2	1.66	0.96
1:D:205:VAL:HB	1:D:207:TYR:CE2	2.00	0.96
1:E:196:TYR:CD2	1:E:197:LEU:CD1	2.49	0.95
1:F:392:TYR:CE2	1:F:394:HIS:CE1	2.53	0.95
1:B:395:TYR:HB2	1:B:534:TYR:CB	1.95	0.95
2:J:20:LEU:CD1	2:J:23:ASP:H	1.79	0.95
1:F:552:LYS:HB3	1:F:553:PRO:HD2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:LYS:HB3	1:E:553:PRO:HD2	1.46	0.95
1:C:477:ALA:CB	2:I:87:ILE:CD1	2.44	0.95
1:D:425:THR:HG21	1:D:469:LEU:CD2	1.96	0.94
1:A:176:LEU:CD1	1:A:182:LEU:O	2.14	0.94
1:B:318:PRO:C	1:B:321:TRP:HZ3	1.71	0.94
1:F:367:ILE:HD11	1:F:538:GLU:HG2	0.95	0.94
1:A:280:ASN:O	1:A:283:MET:HG3	1.67	0.93
1:D:172:ARG:CD	1:D:221:ARG:NE	2.31	0.93
1:D:528:LEU:HB2	1:D:551:TRP:CZ3	2.04	0.92
1:F:365:LYS:O	1:F:538:GLU:CD	2.11	0.92
1:F:174:THR:HG21	1:F:185:ARG:HE	1.33	0.92
1:E:534:TYR:CZ	1:E:536:GLY:HA3	2.04	0.92
1:C:508:MET:C	2:I:92:VAL:HB	1.95	0.92
1:D:551:TRP:C	1:D:552:LYS:HD3	1.93	0.92
1:D:550:ALA:HB3	1:D:552:LYS:CE	2.00	0.91
1:C:460:GLU:OE2	2:I:89:ARG:NH1	2.04	0.91
1:D:172:ARG:CD	1:D:221:ARG:HE	1.82	0.91
1:B:349:SER:OG	1:B:361:LEU:HD23	1.71	0.91
1:F:58:ILE:HG22	1:F:59:HIS:HE1	1.15	0.90
1:F:367:ILE:HD13	1:F:538:GLU:OE2	1.69	0.90
1:D:247:ARG:NH1	1:D:249:VAL:CG2	2.35	0.90
1:F:58:ILE:CG2	1:F:59:HIS:CE1	2.55	0.90
1:F:392:TYR:CD2	1:F:394:HIS:ND1	2.40	0.90
1:C:321:TRP:NE1	1:C:326:GLN:CB	1.98	0.89
1:E:534:TYR:CE1	1:E:536:GLY:HA2	2.06	0.89
1:B:319:THR:HA	1:B:321:TRP:CZ3	2.07	0.89
1:F:553:PRO:HD2	1:F:556:PHE:HB2	1.54	0.89
1:D:547:GLY:CA	1:D:550:ALA:HB2	2.02	0.89
1:D:196:TYR:HD2	1:D:197:LEU:HD13	1.37	0.89
2:I:87:ILE:HG22	2:I:88:PRO:CD	2.00	0.89
1:D:280:ASN:O	1:D:283:MET:HG3	1.71	0.89
1:B:321:TRP:HE1	1:B:326:GLN:HB2	0.73	0.89
1:D:196:TYR:CE2	1:D:197:LEU:CD1	2.56	0.89
1:C:460:GLU:CD	2:I:89:ARG:NH1	2.29	0.89
1:C:440:VAL:HG21	1:C:450:VAL:CG2	2.02	0.89
1:A:405:TRP:CE2	1:A:453:ARG:CG	2.56	0.88
1:C:392:TYR:HD1	1:C:530:LEU:HD11	1.35	0.88
1:F:536:GLY:O	1:F:537:SER:OG	1.91	0.88
1:D:247:ARG:NH1	1:D:249:VAL:HG23	1.88	0.88
1:D:551:TRP:O	1:D:552:LYS:HD3	1.73	0.88
1:C:477:ALA:HB1	2:I:87:ILE:HD13	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:395:TYR:HB2	1:F:534:TYR:HB3	1.56	0.87
1:D:411:SER:OG	1:D:503:MET:CE	2.17	0.87
2:I:87:ILE:HG22	2:I:88:PRO:N	1.87	0.87
1:F:392:TYR:CD2	1:F:394:HIS:CE1	2.63	0.86
1:A:449:PHE:HE1	1:A:454:GLN:HB3	1.34	0.86
1:A:394:HIS:CE1	1:A:535:THR:CG2	2.57	0.86
1:E:420:ILE:HG22	1:E:425:THR:O	1.75	0.86
1:D:448:LYS:O	1:D:452:SER:OG	1.94	0.85
1:E:458:SER:HA	1:E:503:MET:HE3	1.57	0.85
1:D:195:LYS:CB	1:D:198:ASP:OD2	2.25	0.85
1:D:411:SER:CB	1:D:503:MET:HE2	2.01	0.85
1:C:534:TYR:O	1:C:534:TYR:CD1	2.30	0.85
1:D:508:MET:O	2:J:93:GLY:O	1.95	0.85
1:A:531:ASP:OD1	1:A:533:HIS:HB2	1.75	0.85
1:B:504:ILE:HD11	1:B:513:ILE:CD1	2.06	0.84
1:C:321:TRP:CE2	1:C:326:GLN:HB2	2.11	0.84
1:E:532:PRO:HD2	1:E:533:HIS:N	1.89	0.84
1:D:445:LYS:NZ	1:D:449:PHE:CE2	2.45	0.84
1:A:23:PHE:CB	1:A:116:ARG:HD3	2.06	0.84
1:C:534:TYR:CZ	1:C:535:THR:O	2.30	0.84
2:I:87:ILE:HG22	2:I:88:PRO:HD2	1.57	0.84
1:D:538:GLU:O	1:D:538:GLU:HG2	1.75	0.84
1:A:405:TRP:CD2	1:A:453:ARG:HG3	2.12	0.84
1:A:449:PHE:O	1:A:452:SER:OG	1.95	0.84
1:D:425:THR:HG21	1:D:469:LEU:HD22	1.60	0.83
1:D:547:GLY:C	1:D:550:ALA:CB	2.51	0.83
2:J:20:LEU:HD12	2:J:23:ASP:H	1.39	0.83
1:C:321:TRP:NE1	1:C:326:GLN:CA	2.33	0.83
1:D:207:TYR:HE1	1:D:208:LYS:HE2	1.37	0.83
1:A:444:ASP:C	1:A:445:LYS:HG2	2.02	0.82
1:F:392:TYR:CD1	1:F:530:LEU:HD11	2.15	0.82
1:C:318:PRO:C	1:C:321:TRP:HZ3	1.88	0.82
1:E:535:THR:HG21	1:E:543:ILE:HG22	1.60	0.82
1:A:23:PHE:HB3	1:A:116:ARG:CD	2.09	0.82
1:A:405:TRP:CD2	1:A:453:ARG:CG	2.61	0.81
2:J:20:LEU:HD13	2:J:20:LEU:C	2.06	0.81
1:C:534:TYR:CE2	1:C:535:THR:O	2.33	0.81
1:E:553:PRO:O	1:E:553:PRO:HG2	1.80	0.81
1:A:379:PRO:HB3	1:A:383:ILE:CD1	2.10	0.81
1:B:571:PRO:O	1:B:571:PRO:HG2	1.81	0.81
1:C:392:TYR:CD2	1:C:394:HIS:ND1	2.48	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:531:ASP:OD1	1:E:532:PRO:HD2	1.81	0.81
1:F:365:LYS:O	1:F:538:GLU:OE2	1.98	0.81
1:B:318:PRO:O	1:B:321:TRP:CH2	2.33	0.80
1:C:395:TYR:HB2	1:C:534:TYR:HB2	0.91	0.80
1:D:547:GLY:HA2	1:D:550:ALA:CB	2.10	0.80
1:A:449:PHE:HE1	1:A:454:GLN:CB	1.95	0.80
1:C:404:GLY:O	2:I:94:GLY:N	2.15	0.80
1:E:532:PRO:CD	1:E:533:HIS:N	2.39	0.80
1:A:389:PRO:HG2	1:A:421:LEU:HB3	1.65	0.79
1:F:367:ILE:CD1	1:F:538:GLU:HG3	2.00	0.78
1:A:556:PHE:CE2	1:A:557:TRP:CE3	2.70	0.78
1:D:207:TYR:CE1	1:D:208:LYS:CE	2.64	0.78
1:F:58:ILE:CG2	1:F:59:HIS:HE1	1.91	0.78
1:C:488:VAL:HG13	1:C:516:VAL:HG21	1.66	0.78
1:A:283:MET:HE3	1:A:284:MET:CG	2.13	0.78
1:F:58:ILE:O	1:F:59:HIS:ND1	2.16	0.78
1:E:458:SER:HA	1:E:503:MET:CE	2.13	0.77
1:D:205:VAL:HG21	1:D:207:TYR:CZ	2.20	0.77
1:F:392:TYR:HE2	1:F:394:HIS:CE1	2.02	0.77
1:D:547:GLY:O	1:D:550:ALA:CB	2.31	0.77
1:A:396:MET:SD	1:A:534:TYR:CD1	2.77	0.77
1:D:547:GLY:HA2	1:D:550:ALA:HB2	1.65	0.77
1:C:392:TYR:CD1	1:C:530:LEU:HD11	2.20	0.76
1:E:528:LEU:HD13	1:E:551:TRP:CD1	2.20	0.76
1:E:530:LEU:CD1	1:E:549:CYS:SG	2.74	0.76
2:J:20:LEU:CD1	2:J:23:ASP:N	2.47	0.76
1:B:321:TRP:CD1	1:B:326:GLN:HB2	2.19	0.76
1:D:425:THR:HG21	1:D:469:LEU:HD21	1.64	0.76
1:E:196:TYR:HD2	1:E:197:LEU:CD1	1.99	0.76
1:A:394:HIS:NE2	1:A:535:THR:HG21	2.01	0.76
1:A:394:HIS:NE2	1:A:535:THR:CG2	2.49	0.76
1:A:394:HIS:NE2	1:A:535:THR:HB	1.98	0.76
1:E:534:TYR:CZ	1:E:536:GLY:CA	2.68	0.76
1:D:402:ASP:HB3	1:D:406:GLY:HA3	1.65	0.76
1:B:535:THR:HG22	1:B:536:GLY:O	1.84	0.76
2:I:61:THR:HG23	2:I:63:ASP:H	1.50	0.76
1:D:509:LEU:HD23	2:J:94:GLY:HA2	1.66	0.75
1:D:395:TYR:CB	1:D:534:TYR:HB2	2.16	0.75
1:D:247:ARG:HH12	1:D:249:VAL:HG21	1.51	0.75
1:E:404:GLY:O	1:E:405:TRP:HD1	1.69	0.75
1:E:534:TYR:CE1	1:E:536:GLY:CA	2.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:THR:HG22	1:F:185:ARG:HB3	1.69	0.75
1:D:247:ARG:HH12	1:D:249:VAL:CG2	2.00	0.75
1:F:367:ILE:CD1	1:F:538:GLU:OE2	2.35	0.75
1:C:420:ILE:CD1	1:C:427:LYS:O	2.35	0.74
1:C:460:GLU:HG3	2:I:89:ARG:HH12	1.50	0.74
1:D:207:TYR:CZ	1:D:208:LYS:HE2	2.21	0.74
1:E:182:LEU:HA	1:E:196:TYR:OH	1.87	0.74
1:D:508:MET:O	2:J:92:VAL:HG13	1.87	0.74
1:D:530:LEU:HD13	1:D:549:CYS:SG	2.28	0.74
1:F:436:GLN:NE2	1:F:449:PHE:O	2.20	0.74
1:D:445:LYS:NZ	1:D:449:PHE:HE2	1.83	0.74
1:B:99:LEU:HD12	1:B:100:PRO:HD2	1.70	0.73
1:D:445:LYS:HD3	1:D:449:PHE:CD2	2.23	0.73
1:A:405:TRP:CD1	1:A:453:ARG:CG	2.70	0.73
1:E:553:PRO:O	1:E:553:PRO:CG	2.34	0.73
1:C:318:PRO:C	1:C:321:TRP:CZ3	2.65	0.73
1:C:404:GLY:O	2:I:93:GLY:C	2.32	0.73
1:B:66:GLU:HG3	1:C:332:ARG:HG3	1.70	0.73
1:B:99:LEU:HD12	1:B:100:PRO:CD	2.19	0.73
1:B:319:THR:C	1:B:321:TRP:CZ3	2.67	0.73
1:B:405:TRP:O	1:B:405:TRP:CG	2.37	0.72
1:D:283:MET:SD	1:D:284:MET:HG3	2.28	0.72
1:A:405:TRP:CG	1:A:453:ARG:CG	2.72	0.72
1:D:73:ARG:NH2	1:D:77:GLU:OE2	2.23	0.72
1:A:556:PHE:HE2	1:A:557:TRP:CE3	2.08	0.72
1:B:318:PRO:O	1:B:321:TRP:CZ3	2.43	0.72
1:A:405:TRP:CD2	1:A:453:ARG:HG2	2.24	0.72
1:D:449:PHE:HA	1:D:452:SER:OG	1.90	0.72
1:F:367:ILE:CG1	1:F:538:GLU:CG	2.50	0.71
1:F:389:PRO:HB2	1:F:421:LEU:HD23	1.71	0.71
1:D:280:ASN:HA	1:D:283:MET:CG	2.20	0.71
1:A:405:TRP:CD1	1:A:453:ARG:HG2	2.25	0.71
1:D:69:THR:OG1	1:D:72:ASN:ND2	2.20	0.71
1:A:537:SER:O	1:A:538:GLU:C	2.33	0.71
1:D:280:ASN:C	1:D:283:MET:HG3	2.16	0.71
1:D:535:THR:OG1	1:D:548:TRP:CD2	2.33	0.71
1:F:187:GLN:NE2	1:F:191:ALA:O	2.23	0.71
1:F:389:PRO:HG2	1:F:421:LEU:HB3	1.73	0.71
1:B:99:LEU:CG	1:B:100:PRO:HD2	2.20	0.71
1:C:534:TYR:CD1	1:C:534:TYR:C	2.68	0.71
1:F:517:ASP:HB2	1:F:551:TRP:CH2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:LYS:HZ3	1:D:449:PHE:HE2	1.33	0.71
1:D:508:MET:C	2:J:92:VAL:HG13	2.14	0.71
1:F:425:THR:HG21	1:F:469:LEU:CD2	2.21	0.71
1:D:436:GLN:OE1	1:D:451:GLY:N	2.24	0.70
1:D:530:LEU:CD1	1:D:549:CYS:SG	2.79	0.70
1:A:172:ARG:HH22	1:A:221:ARG:HH21	0.79	0.70
1:C:361:LEU:O	1:C:362:THR:OG1	2.08	0.70
1:D:528:LEU:HB2	1:D:551:TRP:CH2	2.26	0.70
1:D:135:MET:CE	1:D:207:TYR:CE2	2.74	0.70
1:C:392:TYR:HE2	1:C:394:HIS:CG	2.06	0.70
1:D:207:TYR:HE1	1:D:208:LYS:CE	2.03	0.70
1:E:327:ARG:HG3	1:E:347:ARG:HH22	1.55	0.70
1:A:144:VAL:HG11	1:A:275:PHE:HE1	1.54	0.69
1:A:219:LEU:HD13	1:B:144:VAL:HG13	1.74	0.69
1:F:392:TYR:HE2	1:F:394:HIS:ND1	1.87	0.69
1:D:135:MET:CE	1:D:207:TYR:HE2	2.05	0.69
1:A:405:TRP:NE1	1:A:453:ARG:HD3	2.06	0.69
1:A:449:PHE:HE1	1:A:454:GLN:CG	2.04	0.69
1:D:547:GLY:CA	1:D:550:ALA:CB	2.69	0.69
1:D:547:GLY:O	1:D:550:ALA:HB2	1.88	0.69
1:B:99:LEU:CD1	1:B:100:PRO:HD2	2.21	0.69
1:D:461:ILE:HD12	1:D:503:MET:HG2	1.74	0.69
1:F:58:ILE:HG22	1:F:59:HIS:ND1	2.06	0.69
1:D:280:ASN:O	1:D:283:MET:CG	2.41	0.69
1:F:367:ILE:CD1	1:F:538:GLU:CD	2.66	0.69
1:F:552:LYS:CB	1:F:553:PRO:CD	2.68	0.69
1:D:135:MET:HE1	1:D:207:TYR:HE2	1.52	0.69
1:C:196:TYR:HD2	1:C:197:LEU:HG	1.57	0.68
1:A:73:ARG:NH1	1:A:77:GLU:OE2	2.27	0.68
1:D:474:ARG:CG	2:J:64:GLY:O	2.40	0.68
2:J:20:LEU:HD13	2:J:22:SER:N	2.09	0.68
1:C:392:TYR:CE2	1:C:394:HIS:CG	2.81	0.68
1:F:392:TYR:HD1	1:F:530:LEU:HD11	1.59	0.68
1:F:531:ASP:OD1	1:F:533:HIS:ND1	2.26	0.67
1:A:556:PHE:CD2	1:A:557:TRP:CE3	2.83	0.67
1:D:89:ASN:ND2	1:D:98:ILE:HG23	2.09	0.67
1:D:195:LYS:HB3	1:D:198:ASP:OD2	1.92	0.67
1:E:395:TYR:HB2	1:E:534:TYR:HB2	1.77	0.67
1:F:32:PHE:HD2	1:F:341:SER:HB3	1.57	0.67
1:A:394:HIS:NE2	1:A:535:THR:CB	2.56	0.67
1:C:509:LEU:C	2:I:92:VAL:HG21	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:THR:HG1	1:D:72:ASN:HD22	1.43	0.67
1:E:173:PHE:HE1	1:F:219:LEU:HD21	1.60	0.66
1:A:172:ARG:CZ	1:A:221:ARG:HD3	2.26	0.66
1:C:446:GLN:O	1:C:449:PHE:N	2.28	0.66
1:F:163:ALA:CB	1:F:283:MET:SD	2.83	0.66
1:B:396:MET:HB2	1:B:534:TYR:CE1	2.29	0.66
1:A:449:PHE:CE1	1:A:454:GLN:CB	2.69	0.66
1:B:535:THR:O	1:B:536:GLY:C	2.35	0.66
1:B:99:LEU:HG	1:B:100:PRO:HD2	1.78	0.66
1:B:262:ASP:OD2	1:B:270:ARG:NH2	2.29	0.66
1:C:196:TYR:CE2	1:C:197:LEU:HD21	2.31	0.66
1:F:160:LYS:CG	1:F:283:MET:HE1	2.23	0.66
1:D:205:VAL:CB	1:D:207:TYR:CE2	2.76	0.66
1:D:205:VAL:HG21	1:D:207:TYR:OH	1.96	0.65
1:F:425:THR:HG21	1:F:469:LEU:HD22	1.78	0.65
1:A:389:PRO:HB2	1:A:421:LEU:HD23	1.78	0.65
1:F:160:LYS:HG3	1:F:283:MET:CE	2.21	0.65
1:D:547:GLY:O	1:D:550:ALA:HB3	1.97	0.65
1:E:538:GLU:CG	1:E:538:GLU:O	2.44	0.65
1:E:528:LEU:HD13	1:E:551:TRP:CE2	2.32	0.65
1:A:506:GLY:H	2:G:92:VAL:HG11	1.62	0.65
1:D:412:PHE:HD1	1:D:461:ILE:HG23	1.62	0.65
1:E:534:TYR:OH	1:E:536:GLY:HA3	1.96	0.65
2:J:20:LEU:HD12	2:J:23:ASP:N	2.10	0.65
1:A:394:HIS:CE1	1:A:536:GLY:H	2.14	0.65
1:B:395:TYR:HB3	1:B:534:TYR:HB2	1.77	0.65
1:E:547:GLY:CA	1:E:550:ALA:CB	2.70	0.65
1:A:537:SER:O	1:A:539:ASP:N	2.30	0.65
1:B:177:ASN:HB3	1:B:182:LEU:HB2	1.77	0.65
1:F:367:ILE:HD11	1:F:538:GLU:CD	2.20	0.65
1:F:551:TRP:H	1:F:551:TRP:CD1	2.14	0.65
1:A:405:TRP:NE1	1:A:453:ARG:CG	2.60	0.64
1:B:89:ASN:ND2	1:B:99:LEU:O	2.30	0.64
1:C:535:THR:HG22	1:C:536:GLY:N	2.11	0.64
1:C:460:GLU:HG3	2:I:89:ARG:HH11	1.33	0.64
1:D:395:TYR:OH	1:D:407:SER:OG	2.14	0.64
1:F:160:LYS:HA	1:F:283:MET:CE	2.27	0.64
1:F:59:HIS:ND1	1:F:59:HIS:N	2.43	0.64
1:A:556:PHE:HD2	1:A:557:TRP:CD2	2.15	0.64
1:B:371:HIS:HD1	1:B:390:TYR:HH	1.36	0.64
1:E:272:ARG:O	1:E:276:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:VAL:CG1	1:C:516:VAL:HG21	2.27	0.63
1:D:482:ALA:HB2	1:D:559:LYS:HD2	1.80	0.63
1:E:278:ARG:NH1	1:E:316:GLN:OE1	2.31	0.63
1:A:182:LEU:HA	1:A:196:TYR:OH	1.97	0.63
1:E:424:TYR:O	1:E:425:THR:CG2	2.46	0.63
1:F:528:LEU:HD23	1:F:551:TRP:CD1	2.33	0.63
1:A:69:THR:OG1	1:A:72:ASN:HB2	1.99	0.63
1:C:440:VAL:CG2	1:C:450:VAL:HG23	2.16	0.63
1:C:509:LEU:O	2:I:92:VAL:HG21	1.99	0.63
1:F:552:LYS:CB	1:F:553:PRO:HD2	2.25	0.63
1:A:395:TYR:CE2	1:A:403:SER:O	2.51	0.63
1:D:205:VAL:HB	1:D:207:TYR:HE2	1.58	0.63
1:F:440:VAL:HG21	1:F:450:VAL:HG12	1.80	0.63
1:A:394:HIS:HE1	1:A:536:GLY:H	1.47	0.62
1:C:503:MET:HG3	1:C:566:VAL:HG12	1.81	0.62
1:D:526:LYS:HB2	1:D:552:LYS:O	1.99	0.62
1:E:183:VAL:N	1:E:196:TYR:OH	2.32	0.62
1:A:59:HIS:HE1	1:A:311:SER:HB3	1.65	0.62
1:E:297:THR:HB	1:E:320:LYS:HB2	1.81	0.62
1:B:320:LYS:N	1:B:321:TRP:CE3	2.67	0.62
1:C:460:GLU:OE2	2:I:89:ARG:CZ	2.47	0.62
1:D:395:TYR:HB2	1:D:534:TYR:CB	2.24	0.62
1:D:396:MET:HG3	1:D:396:MET:O	1.99	0.62
1:F:527:PHE:O	1:F:551:TRP:HA	2.00	0.62
1:D:395:TYR:HH	1:D:407:SER:HG	1.45	0.62
1:F:24:GLN:O	1:F:28:ASN:ND2	2.27	0.62
1:C:531:ASP:OD1	1:C:533:HIS:ND1	2.29	0.62
1:D:280:ASN:HA	1:D:283:MET:HG2	1.80	0.62
1:D:527:PHE:N	1:D:552:LYS:O	2.32	0.62
1:B:321:TRP:NE1	1:B:326:GLN:CB	2.30	0.62
1:B:504:ILE:CD1	1:B:513:ILE:CD1	2.78	0.62
1:A:394:HIS:CG	1:A:535:THR:HB	2.34	0.61
1:E:156:GLN:HG3	1:E:287:VAL:HG13	1.81	0.61
1:B:335:LYS:NZ	1:C:41:ASN:OD1	2.34	0.61
1:C:206:PRO:HB3	1:C:312:LEU:HD11	1.82	0.61
1:E:424:TYR:C	1:E:425:THR:HG23	2.25	0.61
2:J:20:LEU:CD1	2:J:20:LEU:C	2.73	0.61
1:B:147:GLU:OE1	1:B:247:ARG:NH1	2.29	0.61
1:F:392:TYR:CE2	1:F:394:HIS:CG	2.88	0.61
1:E:81:SER:O	1:E:277:ARG:NH1	2.34	0.61
1:A:280:ASN:HA	1:A:283:MET:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:LYS:HD3	1:D:449:PHE:CE2	2.35	0.61
1:E:530:LEU:HD12	1:E:549:CYS:SG	2.39	0.61
1:D:68:LEU:O	1:D:99:LEU:HD22	2.00	0.61
1:F:476:ILE:HG23	1:F:565:MET:HB2	1.82	0.61
1:C:321:TRP:CD1	1:C:326:GLN:N	2.69	0.61
1:F:278:ARG:NH1	1:F:316:GLN:OE1	2.33	0.61
1:C:171:PHE:HB3	1:C:272:ARG:HE	1.65	0.61
1:E:73:ARG:NH1	1:E:77:GLU:OE2	2.30	0.61
1:D:172:ARG:HD2	1:D:221:ARG:CZ	2.26	0.61
1:D:196:TYR:CE2	1:D:197:LEU:HD11	2.35	0.60
1:A:262:ASP:OD2	1:A:270:ARG:NH2	2.34	0.60
1:D:332:ARG:NH1	3:D:601:HOH:O	2.34	0.60
1:E:367:ILE:HG21	1:E:370:PRO:HB3	1.83	0.60
1:E:381:GLY:HA3	1:E:519:ASN:HB2	1.84	0.60
1:E:88:GLY:HA2	1:E:102:GLY:HA3	1.83	0.60
1:D:280:ASN:O	1:D:283:MET:SD	2.60	0.60
1:F:552:LYS:HB3	1:F:553:PRO:HD3	1.81	0.60
1:A:405:TRP:CD1	1:A:453:ARG:CD	2.85	0.60
1:B:466:ASN:HA	1:B:471:LEU:H	1.67	0.60
1:E:412:PHE:HD1	1:E:461:ILE:HG23	1.67	0.60
1:D:394:HIS:NE2	1:D:536:GLY:O	2.33	0.60
1:E:527:PHE:N	1:E:552:LYS:O	2.28	0.60
2:G:67:VAL:HG13	2:G:76:ILE:HD11	1.83	0.60
1:E:182:LEU:CA	1:E:196:TYR:OH	2.48	0.60
1:A:306:PRO:HG2	1:A:309:TRP:CD2	2.36	0.60
2:J:20:LEU:HD13	2:J:21:THR:N	2.17	0.60
1:E:547:GLY:CA	1:E:550:ALA:HB2	2.18	0.59
1:A:196:TYR:HD2	1:A:197:LEU:HG	1.67	0.59
1:D:205:VAL:CG2	1:D:207:TYR:CZ	2.86	0.59
2:L:57:SER:HB3	2:L:86:LEU:HD11	1.84	0.59
1:C:73:ARG:HD2	1:C:86:LEU:HG	1.83	0.59
1:D:377:TYR:CG	1:D:551:TRP:CD1	2.91	0.59
1:A:23:PHE:HB3	1:A:116:ARG:HG2	1.84	0.59
1:D:196:TYR:CD2	1:D:197:LEU:HD12	2.32	0.59
1:F:365:LYS:O	1:F:538:GLU:OE1	2.19	0.59
1:D:425:THR:CG2	1:D:469:LEU:HD22	2.31	0.59
1:D:538:GLU:O	1:D:538:GLU:CG	2.46	0.59
1:E:528:LEU:HD22	1:E:551:TRP:CZ2	2.37	0.59
1:D:247:ARG:NH1	1:D:249:VAL:HG21	2.12	0.59
1:D:247:ARG:HH11	1:D:249:VAL:CG2	2.16	0.59
1:D:247:ARG:HH11	1:D:249:VAL:HG23	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:PHE:HD1	1:D:525:THR:HG22	1.68	0.59
1:D:550:ALA:HB3	1:D:552:LYS:NZ	2.17	0.59
1:F:32:PHE:CE1	1:F:335:LYS:HG2	2.37	0.59
1:F:529:VAL:O	1:F:549:CYS:HB2	2.02	0.59
1:F:70:GLU:OE1	1:F:73:ARG:NH1	2.35	0.58
1:F:160:LYS:HA	1:F:283:MET:HE3	1.85	0.58
1:F:32:PHE:CD2	1:F:341:SER:CB	2.82	0.58
1:A:412:PHE:HD2	1:A:461:ILE:HG23	1.67	0.58
1:D:553:PRO:O	1:D:553:PRO:HG2	2.01	0.58
1:E:425:THR:HG21	1:E:469:LEU:HD22	1.85	0.58
1:B:405:TRP:O	1:B:405:TRP:HE3	1.79	0.58
1:C:404:GLY:HA3	2:I:94:GLY:O	2.04	0.58
1:E:31:SER:OG	1:E:341:SER:OG	2.21	0.58
1:C:402:ASP:OD2	1:C:432:HIS:NE2	2.37	0.58
1:A:176:LEU:HD12	1:A:182:LEU:C	2.18	0.58
1:B:170:SER:OG	1:B:272:ARG:NH1	2.37	0.58
1:A:176:LEU:CD1	1:A:183:VAL:HB	2.24	0.58
1:C:196:TYR:CD2	1:C:197:LEU:CD2	2.87	0.58
1:A:405:TRP:NE1	1:A:453:ARG:CD	2.67	0.57
1:D:262:ASP:OD2	1:D:270:ARG:NH2	2.36	0.57
1:D:550:ALA:CB	1:D:552:LYS:HE2	2.21	0.57
2:G:43:LEU:HD23	2:G:59:ILE:HG12	1.84	0.57
1:C:392:TYR:HD1	1:C:530:LEU:CD1	2.13	0.57
1:D:547:GLY:HA2	1:D:550:ALA:HB1	1.84	0.57
2:L:90:ASP:OD1	2:L:90:ASP:N	2.36	0.57
1:C:534:TYR:OH	1:C:536:GLY:HA2	2.05	0.57
1:B:395:TYR:O	1:B:534:TYR:HD1	1.88	0.57
1:C:321:TRP:NE1	1:C:326:GLN:HA	2.20	0.57
1:E:196:TYR:CD2	1:E:197:LEU:HD11	2.36	0.57
1:A:23:PHE:HB3	1:A:116:ARG:CG	2.34	0.57
1:A:440:VAL:HG22	1:A:447:ALA:H	1.69	0.57
1:A:450:VAL:HG23	1:A:451:GLY:N	2.19	0.57
1:D:166:LEU:HD23	1:D:279:ALA:HB1	1.85	0.56
1:F:370:PRO:HG3	1:F:392:TYR:HB2	1.88	0.56
1:C:349:SER:CB	1:C:361:LEU:HD23	2.35	0.56
1:C:306:PRO:HG2	1:C:309:TRP:CD2	2.41	0.56
1:C:349:SER:HB3	1:C:361:LEU:HD23	1.87	0.56
1:D:83:ASP:HB3	1:D:270:ARG:HD3	1.86	0.56
1:E:535:THR:HG21	1:E:543:ILE:CG2	2.33	0.56
1:F:347:ARG:NH1	1:F:426:ASP:OD2	2.38	0.56
1:F:362:THR:HG21	1:F:421:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:HG21	1:A:282:THR:HG21	1.86	0.56
1:A:440:VAL:HG21	1:A:450:VAL:HG13	1.88	0.56
1:B:363:ASN:HB3	1:B:366:LEU:HG	1.87	0.56
1:D:472:GLU:O	1:D:473:CYS:SG	2.63	0.56
2:G:21:THR:HG21	2:G:85:ARG:HE	1.69	0.56
1:A:405:TRP:CZ2	1:A:453:ARG:HG3	2.40	0.56
1:C:488:VAL:HG21	1:C:525:THR:HG21	1.87	0.56
1:D:455:TRP:HZ3	1:D:508:MET:HG2	1.71	0.56
1:E:531:ASP:OD1	1:E:533:HIS:ND1	2.37	0.56
1:C:437:GLN:NE2	1:C:441:ASP:OD1	2.34	0.56
1:D:207:TYR:CD1	1:D:208:LYS:HG2	2.40	0.56
1:C:321:TRP:HD1	1:C:322:THR:O	1.89	0.56
1:E:461:ILE:HB	1:E:503:MET:HE1	1.85	0.56
1:B:40:ILE:HD12	1:C:341:SER:HB2	1.88	0.55
1:B:51:ARG:HG3	1:B:84:ILE:HG22	1.87	0.55
2:J:20:LEU:HD11	2:J:23:ASP:N	2.19	0.55
2:J:63:ASP:O	2:J:65:VAL:N	2.39	0.55
1:D:398:ASP:O	1:D:399:GLY:C	2.48	0.55
1:E:461:ILE:CB	1:E:503:MET:HE1	2.13	0.55
1:B:389:PRO:HG2	1:B:421:LEU:HB3	1.89	0.55
1:D:445:LYS:CD	1:D:449:PHE:CD2	2.90	0.55
1:C:34:LYS:NZ	3:C:605:HOH:O	2.39	0.55
1:C:485:VAL:O	1:C:488:VAL:CG2	2.46	0.55
1:D:439:LEU:HD13	1:D:445:LYS:HZ2	1.71	0.55
1:E:552:LYS:CB	1:E:553:PRO:HD2	2.15	0.55
2:J:61:THR:OG1	2:J:63:ASP:O	2.24	0.55
1:C:404:GLY:CA	2:I:94:GLY:O	2.55	0.55
1:D:147:GLU:OE2	1:D:247:ARG:HD2	2.07	0.55
1:B:151:ARG:HH21	1:B:154:ARG:HD3	1.71	0.55
1:C:217:GLN:HB2	1:D:219:LEU:HD21	1.88	0.55
1:F:91:ASN:OD1	1:F:96:SER:OG	2.22	0.55
1:C:455:TRP:HB2	2:I:91:ARG:HD2	1.89	0.55
1:E:424:TYR:O	1:E:425:THR:HG23	2.07	0.55
1:B:80:LEU:HB3	1:B:84:ILE:HD11	1.88	0.54
1:E:395:TYR:HD2	1:E:534:TYR:HB2	1.73	0.54
1:F:396:MET:HG3	1:F:401:ASP:HA	1.88	0.54
1:F:406:GLY:HA2	1:F:409:TYR:HD2	1.73	0.54
2:J:20:LEU:CD1	2:J:22:SER:N	2.70	0.54
1:D:445:LYS:CD	1:D:449:PHE:CE2	2.89	0.54
1:E:170:SER:HA	1:E:173:PHE:HE2	1.71	0.54
1:C:63:ALA:C	1:C:64:TYR:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:TRP:CD1	1:C:322:THR:O	2.61	0.54
1:C:395:TYR:CG	1:C:534:TYR:HB2	2.42	0.54
1:A:539:ASP:OD1	1:A:541:LYS:HG3	2.07	0.54
1:B:88:GLY:HA2	1:B:102:GLY:HA3	1.88	0.54
1:D:408:ALA:HB1	1:D:456:ILE:HG12	1.89	0.54
1:E:62:PHE:N	1:E:338:ASN:OD1	2.40	0.54
1:F:394:HIS:O	1:F:397:GLN:HG2	2.07	0.54
1:E:395:TYR:CB	1:E:534:TYR:HB2	2.38	0.54
1:B:341:SER:HB2	1:C:40:ILE:HD12	1.90	0.54
1:C:509:LEU:N	2:I:92:VAL:HB	2.22	0.54
1:C:534:TYR:O	1:C:534:TYR:HD1	1.87	0.54
1:D:205:VAL:CG2	1:D:207:TYR:CE2	2.91	0.53
1:E:121:PHE:HD2	1:E:122:LEU:HD12	1.73	0.53
1:F:364:LYS:HD2	1:F:364:LYS:H	1.73	0.53
1:F:536:GLY:C	1:F:537:SER:HG	1.96	0.53
1:A:402:ASP:HA	1:A:405:TRP:NE1	2.24	0.53
1:E:294:ARG:HD2	1:E:321:TRP:CD1	2.43	0.53
1:C:137:GLY:HA3	1:C:259:PHE:HD1	1.74	0.53
1:D:70:GLU:HA	1:D:73:ARG:HG2	1.91	0.53
1:E:59:HIS:NE2	1:E:311:SER:HB3	2.23	0.53
1:B:99:LEU:HD12	1:B:100:PRO:HD3	1.88	0.53
1:B:193:GLN:OE1	1:B:193:GLN:N	2.40	0.53
1:C:349:SER:HB3	1:C:361:LEU:CD2	2.39	0.53
1:A:59:HIS:CE1	1:A:311:SER:HB3	2.44	0.53
1:E:532:PRO:CG	1:E:533:HIS:N	2.71	0.53
1:E:532:PRO:HD2	1:E:533:HIS:HD1	1.74	0.53
1:A:88:GLY:HA2	1:A:102:GLY:HA3	1.90	0.53
1:A:133:VAL:HG12	1:A:310:VAL:HG21	1.91	0.52
1:F:16:PHE:HD2	1:F:131:GLU:HB2	1.73	0.52
1:F:514:LEU:HD11	1:F:530:LEU:HD22	1.90	0.52
1:A:449:PHE:HE1	1:A:454:GLN:HG2	1.73	0.52
1:C:177:ASN:HB3	1:C:182:LEU:HB2	1.91	0.52
1:C:449:PHE:CE1	1:C:454:GLN:HB2	2.44	0.52
1:D:374:ILE:HD11	1:D:549:CYS:O	2.09	0.52
1:D:553:PRO:O	1:D:553:PRO:CG	2.57	0.52
1:E:531:ASP:OD1	1:E:532:PRO:CD	2.56	0.52
1:E:369:GLU:HB3	1:E:372:LEU:HD13	1.91	0.52
1:E:384:THR:HG21	1:E:496:GLU:HG3	1.91	0.52
1:F:392:TYR:HD2	1:F:394:HIS:CE1	2.22	0.52
1:B:306:PRO:HG2	1:B:309:TRP:CD2	2.44	0.52
1:D:22:MET:HG3	1:D:60:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ARG:HG3	1:F:84:ILE:HG22	1.91	0.52
1:B:407:SER:HB3	1:B:510:ALA:HB3	1.92	0.52
1:A:518:PHE:HD1	1:A:525:THR:HG22	1.75	0.52
1:D:550:ALA:CB	1:D:552:LYS:NZ	2.73	0.52
1:F:99:LEU:HD22	1:F:100:PRO:HD2	1.91	0.52
2:I:87:ILE:HG23	2:I:88:PRO:CD	2.06	0.52
1:A:394:HIS:CE1	1:A:535:THR:HG22	2.44	0.52
1:B:319:THR:HA	1:B:321:TRP:CH2	2.44	0.52
1:C:514:LEU:HD11	1:C:530:LEU:HB2	1.92	0.52
1:F:553:PRO:CD	1:F:556:PHE:HB2	2.34	0.52
1:B:483:GLU:HG2	1:B:487:ARG:HD3	1.92	0.52
1:D:548:TRP:O	1:D:549:CYS:C	2.47	0.52
1:B:164:GLU:O	1:B:167:SER:OG	2.22	0.51
1:B:395:TYR:HB2	1:B:534:TYR:CA	2.40	0.51
1:D:437:GLN:O	1:D:441:ASP:OD2	2.29	0.51
1:E:395:TYR:CD2	1:E:534:TYR:HB2	2.44	0.51
1:F:444:ASP:OD1	2:L:89:ARG:NH2	2.37	0.51
1:A:556:PHE:CD2	1:A:557:TRP:CD2	2.98	0.51
1:E:182:LEU:HA	1:E:196:TYR:HH	1.75	0.51
2:G:53:PRO:HG2	2:G:56:THR:HG1	1.74	0.51
1:D:385:THR:HG22	1:D:515:GLY:HA3	1.92	0.51
1:F:174:THR:CG2	1:F:185:ARG:HE	2.14	0.51
1:F:176:LEU:HD13	1:F:183:VAL:HG22	1.92	0.51
1:F:344:PRO:HG3	1:F:574:ALA:HA	1.92	0.51
1:B:571:PRO:O	1:B:571:PRO:CG	2.36	0.51
1:C:62:PHE:N	1:C:338:ASN:OD1	2.41	0.51
1:C:321:TRP:HZ2	1:C:326:GLN:HG3	1.76	0.51
1:C:385:THR:OG1	1:C:386:VAL:N	2.43	0.51
1:A:91:ASN:OD1	1:A:96:SER:OG	2.23	0.51
1:A:93:ASP:N	1:A:108:LEU:O	2.44	0.51
1:D:533:HIS:O	1:D:548:TRP:HZ3	1.93	0.51
1:F:133:VAL:HG12	1:F:310:VAL:HG11	1.91	0.51
1:C:193:GLN:H	1:C:264:SER:HB3	1.76	0.51
1:F:529:VAL:O	1:F:549:CYS:O	2.28	0.51
2:J:29:LYS:HG3	2:J:49:GLU:HG2	1.92	0.51
1:A:402:ASP:OD2	1:A:432:HIS:NE2	2.42	0.51
1:F:163:ALA:HB3	1:F:283:MET:SD	2.49	0.50
1:D:410:ARG:NH1	1:D:413:GLN:OE1	2.40	0.50
1:D:461:ILE:CD1	1:D:503:MET:HE3	2.41	0.50
1:E:360:ARG:HD2	1:E:364:LYS:HG2	1.93	0.50
2:H:34:PRO:HB2	2:H:37:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD12	1:B:215:ALA:HB1	1.93	0.50
1:B:250:THR:HG21	1:B:282:THR:HG21	1.94	0.50
1:A:394:HIS:CD2	1:A:535:THR:HB	2.46	0.50
1:C:93:ASP:OD2	1:C:110:SER:OG	2.21	0.50
1:D:166:LEU:HD23	1:D:279:ALA:CB	2.41	0.50
1:E:317:LEU:HD13	1:E:330:ARG:HH12	1.77	0.50
1:F:262:ASP:OD2	1:F:270:ARG:NH2	2.42	0.50
1:C:367:ILE:HD11	1:C:538:GLU:HA	1.93	0.50
1:C:402:ASP:OD2	1:C:410:ARG:NE	2.45	0.50
1:E:405:TRP:O	1:E:405:TRP:CE3	2.65	0.50
1:E:553:PRO:O	1:E:553:PRO:CD	2.55	0.50
1:A:56:GLN:OE1	1:A:133:VAL:HG22	2.11	0.50
1:C:402:ASP:OD1	1:C:402:ASP:O	2.30	0.50
1:D:512:THR:HB	1:D:530:LEU:HB3	1.94	0.50
1:F:363:ASN:HB3	1:F:366:LEU:HD23	1.94	0.50
1:A:392:TYR:OH	1:A:531:ASP:O	2.16	0.50
1:C:535:THR:CG2	1:C:536:GLY:N	2.74	0.50
1:B:318:PRO:O	1:B:321:TRP:HH2	1.92	0.49
1:B:535:THR:CG2	1:B:536:GLY:O	2.57	0.49
1:C:449:PHE:CE1	1:C:454:GLN:CB	2.95	0.49
1:B:73:ARG:HD3	1:B:86:LEU:HD22	1.95	0.49
1:E:81:SER:HB2	1:E:84:ILE:HD13	1.94	0.49
1:E:424:TYR:C	1:E:425:THR:CG2	2.85	0.49
1:A:144:VAL:HG11	1:A:275:PHE:CE1	2.42	0.49
1:A:196:TYR:CD2	1:A:197:LEU:HG	2.47	0.49
1:D:507:ASN:O	1:D:508:MET:HB2	2.12	0.49
1:A:167:SER:O	1:A:272:ARG:NH2	2.45	0.49
1:A:455:TRP:HB2	2:G:91:ARG:HG2	1.95	0.49
1:A:406:GLY:HA2	1:A:409:TYR:HD2	1.78	0.49
1:C:392:TYR:CE2	1:C:394:HIS:HB3	2.47	0.49
1:D:73:ARG:HE	1:D:86:LEU:HD22	1.78	0.49
1:D:280:ASN:CA	1:D:283:MET:HG3	2.43	0.49
1:E:132:HIS:O	1:E:134:LEU:HG	2.12	0.49
2:J:12:SER:OG	2:J:13:LYS:N	2.46	0.49
1:A:172:ARG:CZ	1:A:221:ARG:HH21	2.22	0.49
1:D:330:ARG:O	1:D:334:HIS:ND1	2.31	0.49
1:A:80:LEU:HB3	1:A:84:ILE:HD11	1.95	0.49
1:B:504:ILE:CD1	1:B:513:ILE:HD12	2.31	0.49
1:C:321:TRP:HZ2	1:C:326:GLN:CG	2.26	0.49
1:B:154:ARG:HH21	1:B:157:GLU:HG3	1.78	0.49
1:C:404:GLY:O	2:I:94:GLY:CA	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:MET:HG2	1:D:310:VAL:HA	1.95	0.49
1:D:207:TYR:CE1	1:D:208:LYS:HG2	2.47	0.49
1:E:349:SER:HB3	1:E:361:LEU:HD22	1.95	0.49
1:F:174:THR:CG2	1:F:185:ARG:HB2	2.30	0.49
1:B:402:ASP:HB2	1:B:406:GLY:HA3	1.94	0.48
1:F:151:ARG:HH21	1:F:154:ARG:HH11	1.61	0.48
1:A:394:HIS:HE1	1:A:536:GLY:N	2.09	0.48
1:D:280:ASN:HA	1:D:283:MET:HG3	1.93	0.48
1:A:73:ARG:HD2	1:A:86:LEU:HD13	1.94	0.48
1:D:365:LYS:O	1:D:538:GLU:OE1	2.32	0.48
1:F:475:PHE:N	2:L:64:GLY:O	2.43	0.48
1:F:92:ILE:HG22	1:F:108:LEU:HB2	1.94	0.48
1:F:370:PRO:HD2	1:F:390:TYR:CE2	2.47	0.48
2:I:43:LEU:HD13	2:I:59:ILE:HG13	1.96	0.48
1:A:446:GLN:O	1:A:447:ALA:HB3	2.13	0.48
1:E:174:THR:HG23	1:E:185:ARG:HB3	1.94	0.48
2:J:90:ASP:N	2:J:90:ASP:OD1	2.47	0.48
1:B:514:LEU:HD11	1:B:530:LEU:HB2	1.96	0.48
1:D:171:PHE:CE1	1:D:172:ARG:CG	2.96	0.48
1:D:526:LYS:CB	1:D:552:LYS:O	2.61	0.48
2:I:61:THR:HG22	2:I:65:VAL:H	1.78	0.48
1:B:322:THR:HG23	1:B:325:GLU:H	1.79	0.48
1:C:321:TRP:NE1	1:C:326:GLN:N	2.62	0.48
1:D:171:PHE:CD1	1:D:172:ARG:HG2	2.49	0.48
1:D:495:PHE:HA	1:D:499:GLY:HA2	1.96	0.48
1:D:408:ALA:HB2	2:J:92:VAL:O	2.14	0.48
1:E:402:ASP:HB2	1:E:406:GLY:HA3	1.95	0.48
1:A:347:ARG:HD2	1:A:423:GLY:O	2.14	0.48
1:A:533:HIS:O	1:A:548:TRP:CZ3	2.67	0.48
1:B:396:MET:HB2	1:B:534:TYR:CD1	2.49	0.48
1:A:455:TRP:HB2	2:G:91:ARG:CG	2.44	0.47
1:B:321:TRP:HE1	1:B:326:GLN:CG	2.21	0.47
1:F:143:ARG:NH1	1:F:357:GLU:OE1	2.47	0.47
1:F:174:THR:HG21	1:F:185:ARG:NE	2.16	0.47
1:A:172:ARG:CZ	1:A:221:ARG:CD	2.92	0.47
1:F:184:ILE:HD11	1:F:268:TYR:HA	1.96	0.47
1:D:196:TYR:CE2	1:D:197:LEU:HD12	2.48	0.47
1:F:206:PRO:HB3	1:F:312:LEU:HD11	1.95	0.47
1:F:466:ASN:HA	1:F:471:LEU:H	1.79	0.47
1:A:533:HIS:NE2	2:G:94:GLY:OXT	2.47	0.47
1:D:130:ASN:OD1	1:D:131:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:THR:CG2	1:F:185:ARG:HB3	2.42	0.47
1:C:318:PRO:O	1:C:321:TRP:CH2	2.60	0.47
1:C:461:ILE:HD12	1:C:503:MET:HG2	1.96	0.47
2:L:27:PRO:HB2	2:L:50:PHE:HE1	1.79	0.47
1:C:487:ARG:NE	1:C:490:GLU:OE2	2.39	0.47
1:D:548:TRP:O	1:D:549:CYS:HB2	2.14	0.47
1:E:459:THR:HG21	2:K:89:ARG:HG2	1.96	0.47
1:B:412:PHE:HD2	1:B:461:ILE:HG23	1.80	0.47
1:A:280:ASN:O	1:A:284:MET:HG3	2.14	0.47
1:D:182:LEU:HA	1:D:196:TYR:OH	2.15	0.47
1:D:528:LEU:CB	1:D:551:TRP:CZ3	2.91	0.47
1:F:394:HIS:CD2	1:F:534:TYR:HA	2.50	0.47
1:D:389:PRO:HG2	1:D:421:LEU:HB3	1.97	0.47
1:E:177:ASN:HB2	1:E:213:PHE:CE1	2.50	0.47
1:F:32:PHE:CE2	1:F:341:SER:HB3	2.48	0.47
2:I:31:LEU:HD22	2:I:42:VAL:HG13	1.97	0.47
1:A:506:GLY:N	2:G:92:VAL:HG11	2.29	0.46
1:E:69:THR:OG1	1:E:72:ASN:OD1	2.32	0.46
1:F:32:PHE:CZ	1:F:335:LYS:HG2	2.51	0.46
1:F:385:THR:OG1	1:F:386:VAL:N	2.46	0.46
1:A:297:THR:HB	1:A:320:LYS:HB2	1.95	0.46
1:A:362:THR:HG21	1:A:421:LEU:HD11	1.97	0.46
1:B:455:TRP:HB2	2:H:91:ARG:HG2	1.96	0.46
1:B:539:ASP:HB3	1:B:542:THR:HG23	1.96	0.46
1:D:135:MET:HE1	1:D:207:TYR:CD2	2.48	0.46
1:E:514:LEU:HD11	1:E:530:LEU:HD22	1.96	0.46
1:B:371:HIS:ND1	1:B:390:TYR:OH	2.29	0.46
1:E:207:TYR:HB2	1:E:352:LEU:HD21	1.97	0.46
1:E:458:SER:CA	1:E:503:MET:HE3	2.39	0.46
1:F:143:ARG:HB2	1:F:355:HIS:NE2	2.30	0.46
1:D:461:ILE:O	1:D:465:LEU:HD12	2.16	0.46
1:E:68:LEU:HD23	1:E:68:LEU:HA	1.77	0.46
1:F:527:PHE:O	1:F:552:LYS:N	2.44	0.46
1:D:533:HIS:C	1:D:548:TRP:HZ3	2.23	0.46
1:A:115:ASN:O	1:A:116:ARG:HB2	2.15	0.46
1:A:459:THR:OG1	2:G:89:ARG:HG2	2.15	0.46
1:D:508:MET:HB2	1:D:508:MET:HE3	1.82	0.46
1:B:405:TRP:H	2:H:94:GLY:H	1.62	0.46
1:D:552:LYS:HB3	1:D:553:PRO:HD2	1.97	0.46
1:E:52:LYS:HD3	1:E:103:GLN:HE22	1.81	0.46
1:F:535:THR:HG22	1:F:548:TRP:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:OG1	1:A:72:ASN:CB	2.64	0.46
1:D:396:MET:O	1:D:396:MET:CG	2.63	0.46
2:J:20:LEU:HD13	2:J:22:SER:H	1.80	0.46
1:A:450:VAL:CG2	1:A:451:GLY:N	2.79	0.46
1:B:154:ARG:HE	1:B:157:GLU:HG3	1.80	0.46
1:C:321:TRP:CZ2	1:C:326:GLN:CG	2.99	0.46
1:E:427:LYS:HA	1:E:428:PRO:HD3	1.77	0.46
1:F:187:GLN:NE2	1:F:264:SER:OG	2.37	0.46
1:A:83:ASP:HB3	1:A:270:ARG:HD3	1.98	0.45
1:B:69:THR:HG23	1:B:72:ASN:H	1.81	0.45
1:B:504:ILE:HG12	1:B:565:MET:CG	2.30	0.45
1:C:440:VAL:CG2	1:C:450:VAL:CG2	2.86	0.45
1:C:505:GLY:HA3	2:I:90:ASP:OD2	2.17	0.45
1:E:196:TYR:CE2	1:E:197:LEU:HD11	2.51	0.45
1:A:81:SER:O	1:A:277:ARG:NH1	2.49	0.45
1:C:157:GLU:OE1	1:C:157:GLU:N	2.49	0.45
1:D:207:TYR:CE1	1:D:208:LYS:CD	3.00	0.45
1:D:282:THR:HG23	1:D:299:THR:HG21	1.99	0.45
1:E:330:ARG:HE	1:E:347:ARG:HH21	1.64	0.45
1:C:81:SER:O	1:C:277:ARG:NH1	2.49	0.45
1:C:150:LEU:HB2	1:C:246:THR:HG23	1.97	0.45
1:E:530:LEU:HD13	1:E:549:CYS:SG	2.56	0.45
1:F:32:PHE:HD2	1:F:341:SER:CB	2.26	0.45
2:G:79:LYS:HE3	2:G:79:LYS:HB2	1.85	0.45
1:B:517:ASP:HB3	1:B:526:LYS:HB2	1.97	0.45
1:C:88:GLY:HA2	1:C:102:GLY:HA3	1.99	0.45
1:C:444:ASP:OD2	1:C:445:LYS:HG3	2.17	0.45
1:A:23:PHE:CB	1:A:116:ARG:CD	2.81	0.45
1:B:505:GLY:HA3	2:H:90:ASP:OD2	2.17	0.45
1:B:535:THR:HG22	1:B:536:GLY:N	2.32	0.45
1:B:103:GLN:H	1:B:103:GLN:HG2	1.64	0.45
1:B:206:PRO:HB3	1:B:312:LEU:HD21	1.99	0.45
1:C:352:LEU:HD23	1:C:354:LEU:HD21	1.98	0.45
1:C:395:TYR:OH	1:C:407:SER:HB3	2.17	0.45
1:D:383:ILE:O	1:D:384:THR:HG23	2.17	0.45
1:F:478:THR:HB	1:F:483:GLU:HB3	1.99	0.45
1:F:485:VAL:HG11	1:F:554:ALA:HB1	1.99	0.45
1:B:386:VAL:HG12	1:B:514:LEU:O	2.17	0.45
1:B:386:VAL:HG23	1:B:499:GLY:O	2.17	0.45
1:D:171:PHE:CE1	1:D:172:ARG:HG2	2.52	0.45
1:D:545:SER:HB2	1:D:546:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:ASP:OD2	1:E:410:ARG:NH2	2.50	0.45
1:A:570:PRO:HA	1:A:571:PRO:HD3	1.84	0.45
1:D:177:ASN:HB3	1:D:182:LEU:HB2	1.99	0.45
1:E:253:GLU:OE2	1:E:358:SER:OG	2.21	0.45
1:E:394:HIS:NE2	1:E:535:THR:O	2.50	0.45
1:F:22:MET:HE1	1:F:121:PHE:CE1	2.52	0.45
1:E:493:ARG:NH1	3:E:601:HOH:O	2.51	0.44
1:C:392:TYR:CD2	1:C:394:HIS:CE1	3.03	0.44
1:D:306:PRO:HG2	1:D:309:TRP:CD2	2.52	0.44
1:B:320:LYS:N	1:B:321:TRP:HE3	2.15	0.44
1:B:384:THR:HG22	1:B:495:PHE:HB2	1.99	0.44
1:E:424:TYR:O	1:E:425:THR:HG22	2.16	0.44
1:F:184:ILE:HD12	1:F:267:LEU:HB3	1.99	0.44
1:A:488:VAL:HG11	1:A:518:PHE:HB2	1.99	0.44
1:D:366:LEU:HD21	1:D:397:GLN:NE2	2.33	0.44
1:E:414:THR:O	1:E:417:SER:OG	2.32	0.44
1:F:570:PRO:HA	1:F:571:PRO:HD3	1.86	0.44
1:B:349:SER:OG	1:B:361:LEU:CD2	2.55	0.44
1:B:493:ARG:O	1:B:497:THR:HG22	2.17	0.44
1:B:504:ILE:HD11	1:B:513:ILE:HD11	1.93	0.44
1:C:485:VAL:C	1:C:488:VAL:HG23	2.36	0.44
1:D:397:GLN:O	1:D:410:ARG:NH2	2.51	0.44
1:E:518:PHE:HB2	1:E:525:THR:HG22	1.99	0.44
1:F:425:THR:CG2	1:F:469:LEU:HD22	2.45	0.44
1:B:531:ASP:OD1	1:B:533:HIS:ND1	2.45	0.44
1:B:535:THR:C	1:B:536:GLY:O	2.41	0.44
1:E:262:ASP:OD2	1:E:270:ARG:NH2	2.51	0.44
2:H:59:ILE:HD11	2:H:84:LEU:HB3	1.98	0.44
1:B:202:LYS:HA	1:B:260:PHE:HD2	1.82	0.44
1:C:32:PHE:HZ	1:C:334:HIS:HB3	1.82	0.44
1:C:477:ALA:CB	2:I:87:ILE:HD11	2.43	0.44
1:E:538:GLU:O	1:E:538:GLU:HG3	2.15	0.44
1:F:170:SER:OG	1:F:272:ARG:NH1	2.51	0.44
1:F:311:SER:OG	1:F:312:LEU:N	2.49	0.44
1:C:320:LYS:O	1:C:321:TRP:HB3	2.18	0.44
1:D:156:GLN:HB2	1:D:290:ILE:HG21	2.00	0.44
1:F:80:LEU:HB3	1:F:84:ILE:HD11	1.99	0.44
1:F:256:PHE:HB3	1:F:274:ALA:HB2	2.00	0.44
1:F:330:ARG:O	1:F:334:HIS:HD2	2.00	0.44
2:J:57:SER:HB3	2:J:86:LEU:HD11	1.99	0.44
1:A:182:LEU:CA	1:A:196:TYR:OH	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:TYR:O	1:A:534:TYR:CD2	2.71	0.43
1:B:325:GLU:HA	1:C:97:GLN:HE21	1.83	0.43
1:B:389:PRO:HB2	1:B:421:LEU:HD23	1.99	0.43
1:C:196:TYR:CD2	1:C:197:LEU:HG	2.46	0.43
1:D:474:ARG:CB	2:J:64:GLY:O	2.66	0.43
1:E:93:ASP:OD2	1:E:110:SER:OG	2.26	0.43
1:F:69:THR:OG1	1:F:70:GLU:N	2.49	0.43
1:F:425:THR:HG21	1:F:469:LEU:HD21	1.99	0.43
2:J:37:THR:O	2:J:73:ALA:N	2.42	0.43
1:B:219:LEU:HD23	1:B:219:LEU:HA	1.87	0.43
1:C:196:TYR:CE2	1:C:197:LEU:CD2	3.01	0.43
1:D:436:GLN:O	1:D:440:VAL:HG23	2.18	0.43
1:E:121:PHE:CD2	1:E:122:LEU:HD12	2.52	0.43
1:E:509:LEU:HD22	1:E:533:HIS:CE1	2.53	0.43
1:F:517:ASP:HB2	1:F:551:TRP:CZ3	2.53	0.43
1:C:347:ARG:HB2	1:C:350:GLN:HG3	2.00	0.43
1:D:465:LEU:O	1:D:469:LEU:O	2.36	0.43
1:D:491:LEU:HD23	1:D:516:VAL:HG11	2.01	0.43
1:E:135:MET:HE1	1:E:207:TYR:HE2	1.82	0.43
1:E:461:ILE:CB	1:E:503:MET:CE	2.92	0.43
1:E:503:MET:HE2	1:E:566:VAL:HG11	1.98	0.43
1:F:151:ARG:NH2	1:F:154:ARG:HH11	2.17	0.43
1:F:519:ASN:HB3	1:F:522:THR:HG23	2.00	0.43
1:A:280:ASN:O	1:A:283:MET:CG	2.52	0.43
1:C:374:ILE:HG12	1:C:544:THR:HG23	1.98	0.43
1:E:404:GLY:O	1:E:405:TRP:CG	2.69	0.43
1:F:315:LEU:HD13	1:F:333:LEU:HD13	2.00	0.43
1:C:508:MET:CA	2:I:92:VAL:HB	2.48	0.43
1:D:413:GLN:NE2	1:D:430:PRO:O	2.43	0.43
1:D:550:ALA:CB	1:D:552:LYS:CE	2.85	0.43
1:F:86:LEU:HD23	1:F:88:GLY:H	1.84	0.43
2:G:13:LYS:HB3	2:G:34:PRO:HA	1.99	0.43
1:A:112:MET:HE1	1:A:121:PHE:HB2	2.01	0.43
1:B:164:GLU:O	1:B:168:MET:HG2	2.19	0.43
1:C:348:LEU:HD23	1:C:348:LEU:HA	1.85	0.43
1:E:219:LEU:HD12	1:F:215:ALA:HB1	2.01	0.43
1:F:387:ASN:HB3	1:F:499:GLY:HA3	1.99	0.43
1:A:283:MET:HG3	1:A:284:MET:N	2.33	0.43
1:C:143:ARG:HB2	1:C:355:HIS:CE1	2.54	0.43
1:F:514:LEU:HB2	1:F:528:LEU:HD12	2.00	0.43
1:A:172:ARG:NH1	1:A:221:ARG:CD	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:THR:HB	1:B:65:ALA:HB3	2.00	0.43
1:C:349:SER:HB2	1:C:361:LEU:HD23	2.00	0.43
1:C:512:THR:HB	1:C:530:LEU:HB3	2.01	0.43
1:E:75:PHE:HA	1:E:284:MET:HE1	2.01	0.43
1:E:143:ARG:NH2	1:E:357:GLU:OE1	2.38	0.43
1:E:437:GLN:NE2	1:E:441:ASP:OD2	2.52	0.43
2:J:23:ASP:HA	2:J:24:PRO:HD3	1.81	0.43
1:B:419:PHE:CZ	1:B:471:LEU:HD21	2.54	0.43
1:B:495:PHE:CZ	1:B:513:ILE:HG22	2.54	0.43
1:D:280:ASN:CA	1:D:283:MET:CG	2.96	0.43
1:D:537:SER:O	1:D:538:GLU:HB3	2.19	0.43
1:F:32:PHE:HE1	1:F:335:LYS:HG2	1.81	0.43
1:B:495:PHE:HZ	1:B:513:ILE:HG22	1.84	0.42
2:L:34:PRO:HG2	2:L:37:THR:OG1	2.19	0.42
1:A:207:TYR:HB3	1:A:305:LEU:HD12	2.00	0.42
1:A:546:LYS:HB2	1:A:548:TRP:CD1	2.54	0.42
1:D:174:THR:HG23	1:D:185:ARG:HB3	2.01	0.42
1:F:396:MET:H	1:F:410:ARG:HH21	1.67	0.42
1:F:419:PHE:CZ	1:F:471:LEU:HD21	2.53	0.42
1:F:435:ILE:HG23	1:F:464:VAL:HG21	2.01	0.42
2:L:33:VAL:HG11	2:L:42:VAL:HG22	2.01	0.42
1:B:59:HIS:CE1	1:B:311:SER:HB3	2.54	0.42
1:C:395:TYR:CE2	1:C:403:SER:O	2.71	0.42
1:D:304:TYR:OH	1:D:317:LEU:HD11	2.19	0.42
2:G:90:ASP:OD1	2:G:90:ASP:N	2.38	0.42
1:D:74:GLN:HB3	1:D:284:MET:HE1	2.01	0.42
1:E:315:LEU:HD13	1:E:333:LEU:HD13	2.00	0.42
2:I:61:THR:HG22	2:I:65:VAL:N	2.34	0.42
1:A:405:TRP:CD1	1:A:405:TRP:H	2.37	0.42
1:C:31:SER:OG	1:C:341:SER:OG	2.27	0.42
1:E:255:VAL:HG11	1:E:354:LEU:HD13	2.02	0.42
1:F:539:ASP:O	1:F:543:ILE:HG13	2.19	0.42
1:A:109:THR:OG1	1:A:112:MET:HG2	2.20	0.42
1:A:160:LYS:O	1:A:164:GLU:HG3	2.19	0.42
1:A:514:LEU:HD11	1:A:530:LEU:HB2	2.01	0.42
1:C:509:LEU:C	2:I:92:VAL:CG2	2.91	0.42
1:C:535:THR:HG22	1:C:536:GLY:H	1.82	0.42
1:E:65:ALA:HB1	1:E:97:GLN:HG3	2.01	0.42
1:A:177:ASN:HB2	1:A:213:PHE:CE1	2.55	0.42
1:B:99:LEU:HD12	1:B:99:LEU:HA	1.72	0.42
1:E:395:TYR:CD2	1:E:534:TYR:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:60:ILE:HD13	2:J:87:ILE:HD13	2.02	0.42
2:G:39:PHE:CD1	2:G:76:ILE:HG21	2.55	0.42
2:H:28:PHE:HA	2:H:50:PHE:HZ	1.85	0.42
1:A:62:PHE:N	1:A:338:ASN:OD1	2.38	0.41
1:A:285:VAL:HG21	1:A:318:PRO:HD3	2.02	0.41
1:C:370:PRO:HD2	1:C:390:TYR:CE2	2.55	0.41
1:C:534:TYR:CE1	1:C:535:THR:O	2.72	0.41
1:D:404:GLY:HA2	2:J:94:GLY:OXT	2.20	0.41
1:F:32:PHE:O	1:F:32:PHE:CD1	2.73	0.41
2:J:20:LEU:HD12	2:J:23:ASP:CB	2.50	0.41
1:A:76:LEU:O	1:A:80:LEU:HG	2.20	0.41
1:B:44:ILE:O	1:B:96:SER:OG	2.26	0.41
1:B:201:SER:HA	1:B:204:ALA:HB2	2.02	0.41
1:B:320:LYS:N	1:B:321:TRP:CZ3	2.87	0.41
1:C:405:TRP:CD1	1:C:405:TRP:N	2.88	0.41
1:A:504:ILE:HB	1:A:565:MET:HG2	2.02	0.41
1:A:394:HIS:CE1	1:A:536:GLY:N	2.84	0.41
1:C:215:ALA:HB1	1:D:219:LEU:HD12	2.02	0.41
1:C:321:TRP:HZ2	1:C:326:GLN:CD	2.29	0.41
1:C:321:TRP:CZ2	1:C:326:GLN:CD	2.98	0.41
1:E:294:ARG:NH1	1:E:294:ARG:HG3	2.35	0.41
1:E:334:HIS:HE1	1:E:345:VAL:HB	1.84	0.41
1:F:512:THR:HB	1:F:530:LEU:HB3	2.02	0.41
1:A:160:LYS:HB2	1:A:160:LYS:HE3	1.87	0.41
1:A:180:HIS:CD2	1:A:200:PHE:HZ	2.38	0.41
1:A:380:VAL:HG21	1:A:524:GLU:CD	2.45	0.41
1:B:438:ALA:O	1:B:442:ILE:HG12	2.21	0.41
1:C:205:VAL:HA	1:C:206:PRO:HD3	1.91	0.41
1:C:447:ALA:O	1:C:450:VAL:HB	2.21	0.41
1:F:174:THR:CG2	1:F:185:ARG:CB	2.81	0.41
1:A:278:ARG:CZ	1:A:314:HIS:HB3	2.51	0.41
1:B:402:ASP:OD2	1:B:410:ARG:NE	2.54	0.41
1:C:219:LEU:HD13	1:D:217:GLN:HB2	2.02	0.41
1:D:447:ALA:C	1:D:449:PHE:N	2.78	0.41
1:E:170:SER:HA	1:E:173:PHE:CE2	2.54	0.41
1:E:377:TYR:OH	1:E:517:ASP:OD2	2.37	0.41
1:E:404:GLY:HA2	2:K:94:GLY:C	2.46	0.41
1:E:546:LYS:HA	1:E:546:LYS:HD3	1.91	0.41
1:F:205:VAL:HA	1:F:206:PRO:HD3	1.84	0.41
1:F:436:GLN:O	1:F:440:VAL:HG23	2.20	0.41
1:D:133:VAL:HG13	1:D:310:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ARG:HD3	1:D:347:ARG:HA	1.96	0.41
1:C:502:VAL:HG13	1:C:566:VAL:O	2.21	0.41
1:D:171:PHE:CE1	1:D:172:ARG:HG3	2.55	0.41
1:E:395:TYR:HB2	1:E:534:TYR:CB	2.46	0.41
1:F:68:LEU:HD13	1:F:97:GLN:O	2.21	0.41
1:A:137:GLY:HA3	1:A:259:PHE:HD1	1.86	0.41
1:B:245:PHE:CD1	1:B:245:PHE:C	2.99	0.41
1:C:83:ASP:HB3	1:C:270:ARG:HD3	2.03	0.41
1:C:362:THR:O	1:C:366:LEU:HD12	2.20	0.41
1:D:297:THR:OG1	1:D:320:LYS:HB2	2.21	0.41
1:D:378:GLN:HA	1:D:379:PRO:HD3	1.89	0.41
1:D:445:LYS:CE	1:D:449:PHE:CE2	3.04	0.41
1:E:394:HIS:O	1:E:410:ARG:NE	2.54	0.41
1:E:466:ASN:O	1:E:470:LYS:HD3	2.21	0.41
2:I:78:LEU:HB2	2:K:33:VAL:HG12	2.03	0.41
2:J:20:LEU:HD12	2:J:23:ASP:HB3	2.03	0.41
1:A:216:MET:HE3	1:A:216:MET:HB2	1.92	0.41
1:F:392:TYR:CE1	1:F:530:LEU:HD11	2.55	0.41
1:B:306:PRO:HG2	1:B:309:TRP:CG	2.55	0.40
1:B:318:PRO:HB2	1:B:321:TRP:CE3	2.56	0.40
1:C:70:GLU:OE1	1:C:73:ARG:NH2	2.54	0.40
1:C:321:TRP:CZ2	1:C:326:GLN:HG3	2.55	0.40
1:F:485:VAL:HG12	1:F:527:PHE:HE1	1.85	0.40
1:B:419:PHE:CE1	1:B:471:LEU:HD21	2.56	0.40
1:D:364:LYS:H	1:D:364:LYS:HG2	1.70	0.40
1:D:377:TYR:CD2	1:D:551:TRP:NE1	2.89	0.40
1:D:551:TRP:C	1:D:552:LYS:CD	2.81	0.40
2:L:14:VAL:HG22	2:L:33:VAL:O	2.22	0.40
1:A:283:MET:O	1:A:287:VAL:HG23	2.21	0.40
1:B:143:ARG:HB2	1:B:355:HIS:CE1	2.57	0.40
1:D:23:PHE:HE2	1:D:118:ILE:HG12	1.87	0.40
1:D:414:THR:O	1:D:417:SER:OG	2.35	0.40
1:D:534:TYR:O	1:D:534:TYR:CD2	2.74	0.40
1:E:212:GLU:OE1	1:E:355:HIS:ND1	2.54	0.40
2:H:90:ASP:OD1	2:H:90:ASP:N	2.49	0.40
1:E:531:ASP:OD1	1:E:533:HIS:HB2	2.21	0.40
1:C:446:GLN:O	1:C:449:PHE:CB	2.69	0.40
1:C:449:PHE:O	1:C:452:SER:OG	2.29	0.40
1:D:460:GLU:O	1:D:464:VAL:HG23	2.22	0.40
1:D:533:HIS:HB2	1:D:548:TRP:CZ3	2.56	0.40
1:D:551:TRP:O	1:D:552:LYS:CD	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:HIS:HA	1:F:339:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

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	531/565 (94%)	490 (92%)	41 (8%)	0	100	100
1	B	538/565 (95%)	509 (95%)	29 (5%)	0	100	100
1	C	537/565 (95%)	508 (95%)	29 (5%)	0	100	100
1	D	532/565 (94%)	495 (93%)	37 (7%)	0	100	100
1	E	529/565 (94%)	497 (94%)	32 (6%)	0	100	100
1	F	529/565 (94%)	471 (89%)	58 (11%)	0	100	100
2	G	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
2	H	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
2	I	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
2	J	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	K	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	L	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
All	All	3688/3894 (95%)	3442 (93%)	246 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	468/495 (94%)	462 (99%)	6 (1%)	61	75
1	B	472/495 (95%)	466 (99%)	6 (1%)	61	75
1	C	471/495 (95%)	465 (99%)	6 (1%)	61	75
1	D	469/495 (95%)	464 (99%)	5 (1%)	65	76
1	E	466/495 (94%)	463 (99%)	3 (1%)	78	82
1	F	466/495 (94%)	456 (98%)	10 (2%)	47	67
2	G	69/69 (100%)	68 (99%)	1 (1%)	59	74
2	H	69/69 (100%)	69 (100%)	0	100	100
2	I	69/69 (100%)	68 (99%)	1 (1%)	59	74
2	J	69/69 (100%)	67 (97%)	2 (3%)	37	62
2	K	69/69 (100%)	68 (99%)	1 (1%)	59	74
2	L	69/69 (100%)	68 (99%)	1 (1%)	59	74
All	All	3226/3384 (95%)	3184 (99%)	42 (1%)	61	75

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	GLU
1	A	183	VAL
1	A	249	VAL
1	A	283	MET
1	A	332	ARG
1	A	488	VAL
1	B	126	VAL
1	B	210	VAL
1	B	249	VAL
1	B	383	ILE
1	B	442	ILE
1	B	540	ILE
1	C	66	GLU
1	C	98	ILE
1	C	136	GLU
1	C	221	ARG
1	C	249	VAL
1	C	394	HIS

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Mol	Chain	Res	Type
1	D	11	VAL
1	D	113	LEU
1	D	244	HIS
1	D	376	ASN
1	D	397	GLN
1	E	210	VAL
1	E	347	ARG
1	E	437	GLN
1	F	59	HIS
1	F	66	GLU
1	F	141	VAL
1	F	176	LEU
1	F	184	ILE
1	F	251	ILE
1	F	305	LEU
1	F	375	THR
1	F	450	VAL
1	F	518	PHE
2	G	49	GLU
2	I	91	ARG
2	J	20	LEU
2	J	76	ILE
2	K	29	LYS
2	L	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	394	HIS
1	A	446	GLN
1	B	280	ASN
1	B	437	GLN
1	C	20	GLN
1	C	130	ASN
1	C	180	HIS
1	C	324	ASN
1	C	363	ASN
1	D	59	HIS
1	D	72	ASN
1	D	454	GLN
1	E	20	GLN

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Mol	Chain	Res	Type
1	E	324	ASN
1	E	350	GLN
1	F	432	HIS
1	F	437	GLN
1	F	466	ASN
1	F	561	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	537/565 (95%)	-0.11	16 (2%)	52	35	6, 35, 74, 110	0
1	B	542/565 (95%)	-0.25	17 (3%)	51	34	7, 27, 76, 117	0
1	C	541/565 (95%)	-0.26	9 (1%)	69	50	6, 31, 77, 120	0
1	D	538/565 (95%)	0.21	28 (5%)	33	22	19, 58, 105, 131	0
1	E	535/565 (94%)	0.14	19 (3%)	46	31	16, 53, 94, 128	0
1	F	535/565 (94%)	0.52	37 (6%)	23	16	31, 72, 111, 134	0
2	G	84/84 (100%)	-0.52	1 (1%)	76	58	10, 23, 50, 87	0
2	H	84/84 (100%)	-0.45	2 (2%)	59	40	15, 28, 49, 83	0
2	I	84/84 (100%)	-0.28	3 (3%)	46	31	5, 24, 48, 84	0
2	J	84/84 (100%)	0.04	2 (2%)	59	40	33, 62, 88, 131	0
2	K	84/84 (100%)	-0.56	2 (2%)	59	40	9, 27, 53, 91	0
2	L	84/84 (100%)	0.26	1 (1%)	76	58	24, 70, 90, 100	0
All	All	3732/3894 (95%)	0.00	137 (3%)	45	30	5, 45, 95, 134	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	574	ALA	7.3
2	I	94	GLY	7.3
1	A	538	GLU	7.1
1	A	536	GLY	7.0
1	D	549	CYS	5.8
1	B	537	SER	5.8
1	F	536	GLY	5.5
1	F	574	ALA	5.3
1	E	503	MET	5.2
1	D	537	SER	5.2
1	D	11	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	549	CYS	5.0
1	D	536	GLY	4.6
1	D	574	ALA	4.5
1	D	374	ILE	4.5
1	A	574	ALA	4.4
1	A	115	ASN	4.2
1	B	101	GLY	4.2
1	F	523	GLY	4.2
1	A	535	THR	4.1
1	E	222	ASP	4.0
1	D	534	TYR	4.0
1	F	380	VAL	4.0
1	B	401	ASP	3.9
1	F	538	GLU	3.9
1	D	396	MET	3.9
1	D	503	MET	3.9
1	E	168	MET	3.8
1	A	534	TYR	3.8
1	B	321	TRP	3.7
1	A	556	PHE	3.7
1	D	407	SER	3.6
1	C	574	ALA	3.6
1	D	535	THR	3.6
1	B	375	THR	3.6
1	A	451	GLY	3.5
1	D	445	LYS	3.5
1	E	11	VAL	3.4
1	D	283	MET	3.4
1	D	398	ASP	3.3
1	B	534	TYR	3.3
1	B	535	THR	3.2
1	D	35	SER	3.2
1	F	549	CYS	3.2
1	F	11	VAL	3.2
2	J	64	GLY	3.1
2	K	93	GLY	3.1
1	B	538	GLU	3.1
1	F	525	THR	3.1
1	C	538	GLU	3.1
1	F	546	LYS	3.0
1	E	537	SER	3.0
1	F	348	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	33	SER	3.0
1	A	34	LYS	2.9
1	B	167	SER	2.9
1	D	34	LYS	2.9
1	D	207	TYR	2.9
1	E	196	TYR	2.9
1	D	406	GLY	2.9
1	F	522	THR	2.8
1	E	374	ILE	2.8
1	E	247	ARG	2.8
1	F	537	SER	2.8
1	D	244	HIS	2.7
1	F	555	SER	2.7
2	H	11	GLY	2.7
1	F	535	THR	2.7
1	D	437	GLN	2.7
1	E	246	THR	2.6
1	A	11	VAL	2.6
1	C	11	VAL	2.6
1	C	534	TYR	2.6
1	F	185	ARG	2.6
1	B	11	VAL	2.6
1	B	574	ALA	2.6
1	A	376	ASN	2.5
1	B	539	ASP	2.5
1	F	524	GLU	2.5
1	D	447	ALA	2.5
1	B	244	HIS	2.5
2	G	93	GLY	2.5
2	I	92	VAL	2.5
1	F	400	ILE	2.4
1	F	124	MET	2.4
1	D	449	PHE	2.4
1	F	392	TYR	2.4
1	E	178	ALA	2.4
1	E	365	LYS	2.4
1	F	548	TRP	2.4
1	F	383	ILE	2.4
1	A	147	GLU	2.4
1	F	221	ARG	2.3
1	A	537	SER	2.3
1	D	247	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	203	GLY	2.3
1	F	262	ASP	2.3
1	F	372	LEU	2.3
1	B	221	ARG	2.3
2	K	11	GLY	2.3
1	C	535	THR	2.3
1	F	297	THR	2.3
1	C	446	GLN	2.3
1	F	172	ARG	2.3
1	F	425	THR	2.3
1	A	245	PHE	2.3
1	F	498	SER	2.3
1	A	56	GLN	2.3
1	F	14	LEU	2.2
1	C	537	SER	2.2
1	D	473	CYS	2.2
1	D	538	GLU	2.2
1	D	172	ARG	2.2
2	I	11	GLY	2.2
1	F	123	ASP	2.2
1	F	311	SER	2.2
1	B	406	GLY	2.2
1	A	375	THR	2.1
1	B	66	GLU	2.1
1	D	518	PHE	2.1
1	D	222	ASP	2.1
1	F	155	GLU	2.1
1	E	534	TYR	2.1
2	H	94	GLY	2.1
1	F	199	LYS	2.1
1	E	174	THR	2.1
1	E	368	ARG	2.1
1	E	535	THR	2.1
1	F	283	MET	2.1
1	E	551	TRP	2.0
1	C	402	ASP	2.0
1	B	536	GLY	2.0
2	J	94	GLY	2.0
2	L	11	GLY	2.0
1	F	202	LYS	2.0
1	F	374	ILE	2.0
1	C	321	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.