



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:42 AM UTC

PDB ID : 1W91 / pdb_00001w91
Title : crystal structure of 1,4-BETA-D-XYLAN XYLOHYDROLASE solve using anomalous signal from Seleniomethionine
Authors : Jakoncic, J.; Shoham, G.; Stojanoff, V.
Deposited on : 2004-10-05
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

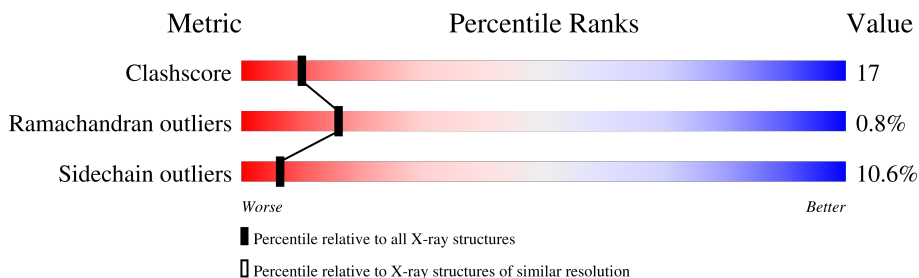
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	503	64% 28% 6% ..
1	B	503	69% 24% 5% ..
1	C	503	66% 27% 5% ..
1	D	503	68% 23% 7% ..
1	E	503	69% 25% . ..
1	F	503	70% 23% . ..
1	G	503	68% 24% 6% ..
1	H	503	72% 22% . ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35545 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 BETA-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	B	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	C	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	D	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	E	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	F	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	G	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			
1	H	499	Total	C	N	O	S	0	0	0
			4082	2640	691	740	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	ARG	PRO	conflict	UNP Q9ZFM2
A	446	GLN	SER	conflict	UNP Q9ZFM2
B	445	ARG	PRO	conflict	UNP Q9ZFM2
B	446	GLN	SER	conflict	UNP Q9ZFM2
C	445	ARG	PRO	conflict	UNP Q9ZFM2
C	446	GLN	SER	conflict	UNP Q9ZFM2
D	445	ARG	PRO	conflict	UNP Q9ZFM2
D	446	GLN	SER	conflict	UNP Q9ZFM2
E	445	ARG	PRO	conflict	UNP Q9ZFM2
E	446	GLN	SER	conflict	UNP Q9ZFM2
F	445	ARG	PRO	conflict	UNP Q9ZFM2
F	446	GLN	SER	conflict	UNP Q9ZFM2
G	445	ARG	PRO	conflict	UNP Q9ZFM2

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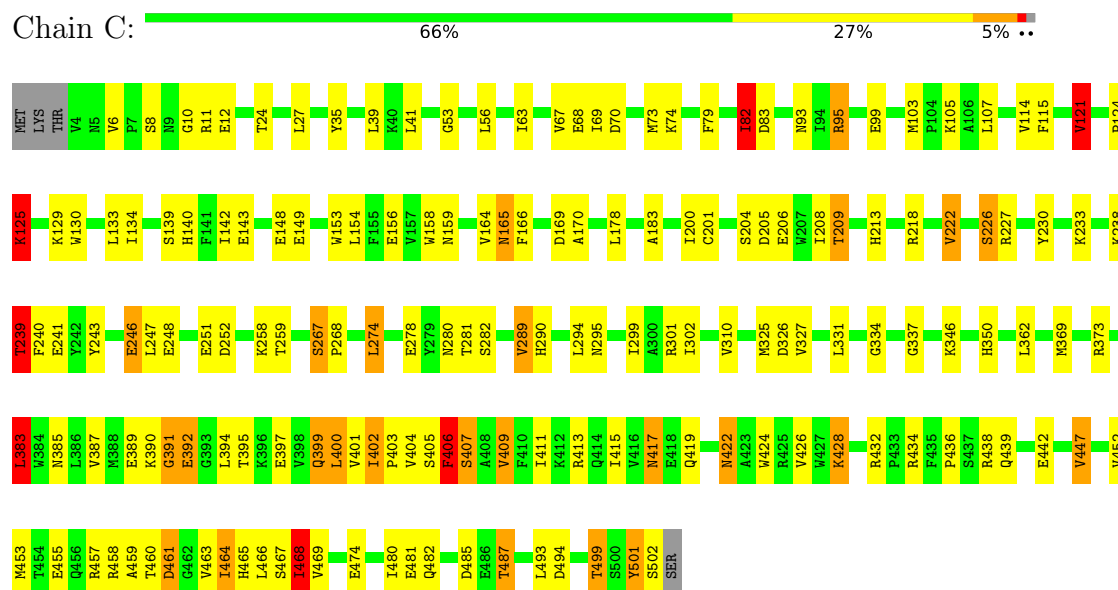
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Chain	Residue	Modelled	Actual	Comment	Reference
G	446	GLN	SER	conflict	UNP Q9ZFM2
H	445	ARG	PRO	conflict	UNP Q9ZFM2
H	446	GLN	SER	conflict	UNP Q9ZFM2

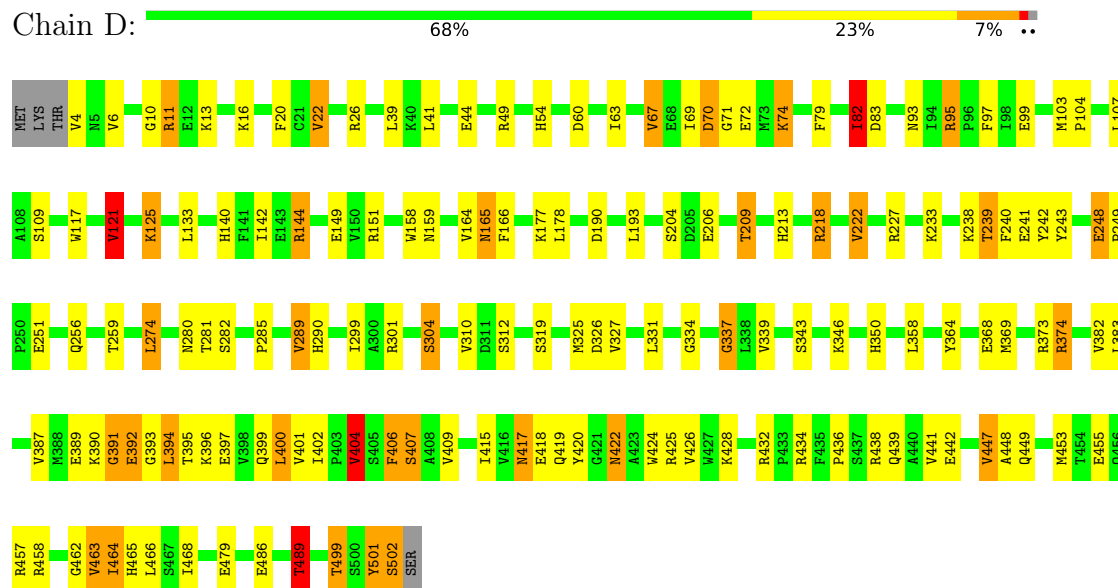
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	363	Total	O	0	0
			363	363		
2	B	317	Total	O	0	0
			317	317		
2	C	371	Total	O	0	0
			371	371		
2	D	340	Total	O	0	0
			340	340		
2	E	347	Total	O	0	0
			347	347		
2	F	414	Total	O	0	0
			414	414		
2	G	340	Total	O	0	0
			340	340		
2	H	397	Total	O	0	0
			397	397		

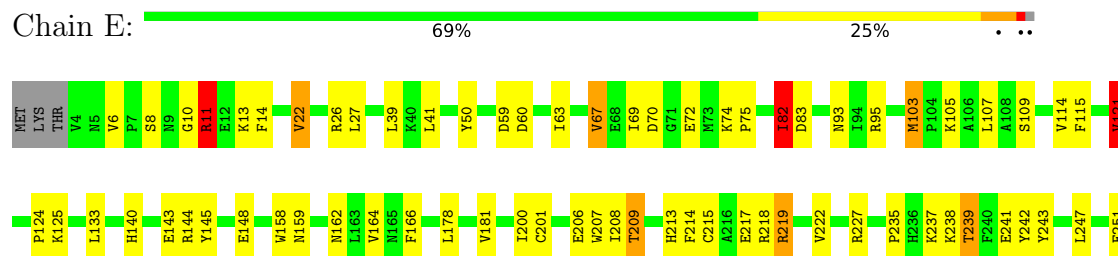
• Molecule 1: BETA-XYLOSIDASE

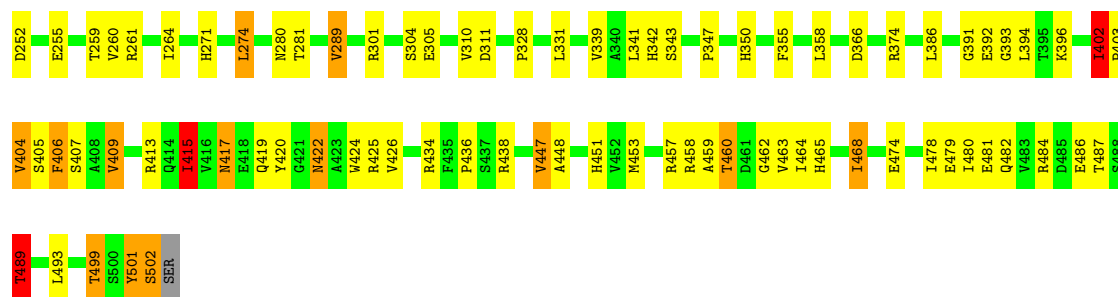


• Molecule 1: BETA-XYLOSIDASE



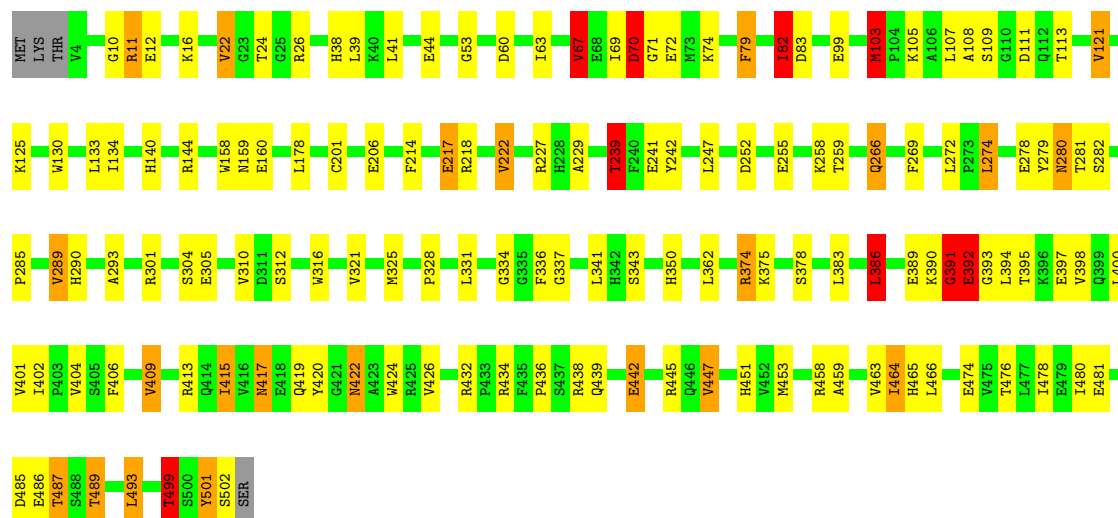
• Molecule 1: BETA-XYLOSIDASE





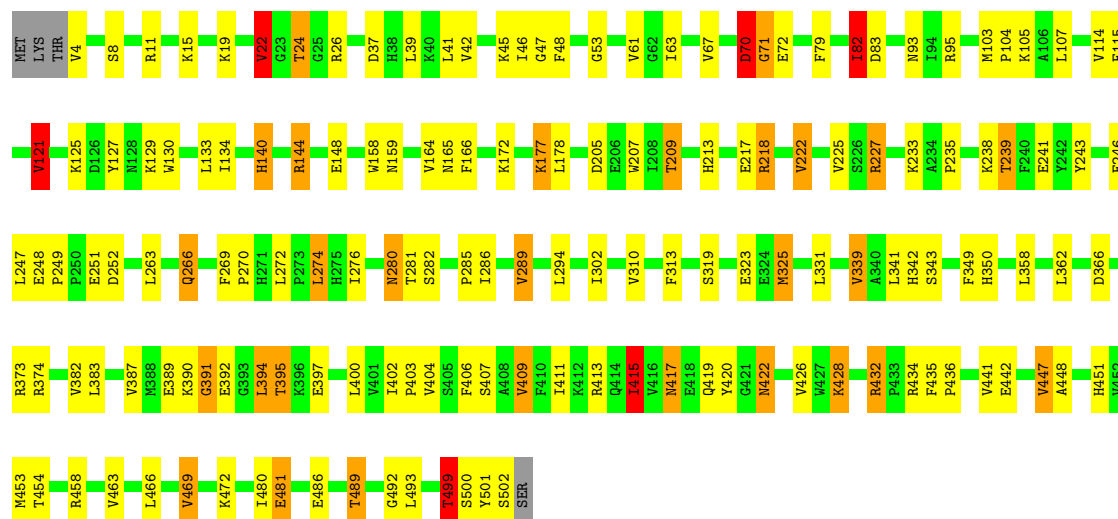
• Molecule 1: BETA-XYLOSIDASE

Chain F: 70% 23%



• Molecule 1: BETA-XYLOSIDASE

Chain G: 68% 24% 6%

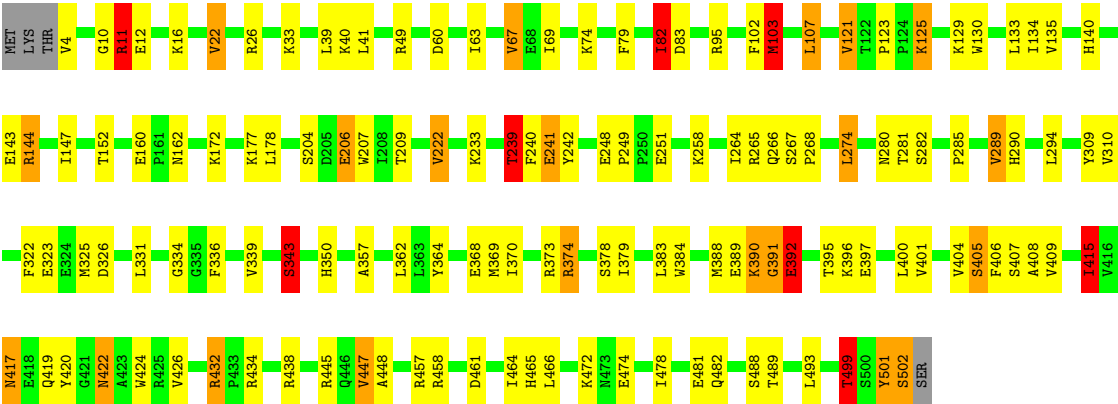


• Molecule 1: BETA-XYLOSIDASE

Chain H:

72%

22%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.70Å 166.02Å 313.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	100.0 (8.00-2.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	35545	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.25	8/4198 (0.2%)	1.22	25/5699 (0.4%)
1	B	1.24	5/4198 (0.1%)	1.26	11/5699 (0.2%)
1	C	1.31	7/4198 (0.2%)	1.24	19/5699 (0.3%)
1	D	1.25	6/4197 (0.1%)	1.21	22/5696 (0.4%)
1	E	1.31	5/4198 (0.1%)	1.25	20/5699 (0.4%)
1	F	1.32	11/4198 (0.3%)	1.27	23/5699 (0.4%)
1	G	1.20	10/4198 (0.2%)	1.30	24/5699 (0.4%)
1	H	1.32	13/4198 (0.3%)	1.31	24/5699 (0.4%)
All	All	1.27	65/33583 (0.2%)	1.26	168/45589 (0.4%)

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	B	0	1
1	F	0	3
1	H	0	2
All	All	0	6

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	TYR	C-N	25.81	1.69	1.33
1	E	501	TYR	C-N	25.40	1.69	1.33
1	F	501	TYR	C-N	19.53	1.60	1.33
1	A	501	TYR	C-N	16.28	1.56	1.33
1	B	501	TYR	C-N	13.27	1.51	1.33
1	H	501	TYR	C-N	10.13	1.47	1.33
1	D	432	ARG	C-O	9.25	1.28	1.23
1	C	432	ARG	C-O	8.65	1.28	1.23
1	E	235	PRO	C-O	8.22	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	103	MET	CB-CG	8.10	1.76	1.52
1	F	103	MET	CB-CG	7.87	1.76	1.52
1	E	415	ILE	CA-CB	7.42	1.65	1.54
1	D	432	ARG	N-CA	7.21	1.51	1.46
1	A	339	VAL	CA-CB	7.15	1.62	1.54
1	H	432	ARG	C-O	6.90	1.27	1.23
1	B	432	ARG	N-CA	6.86	1.51	1.46
1	F	160	GLU	C-O	-6.68	1.20	1.23
1	C	302	ILE	CA-CB	6.65	1.62	1.54
1	C	183	ALA	CA-CB	6.58	1.63	1.53
1	H	391	GLY	CA-C	-6.38	1.46	1.52
1	H	322	PHE	N-CA	6.24	1.53	1.46
1	G	61	VAL	CA-CB	6.21	1.63	1.54
1	F	321	VAL	CA-CB	6.08	1.62	1.54
1	G	501	TYR	C-N	6.01	1.41	1.33
1	G	499	THR	CA-CB	5.99	1.62	1.53
1	F	442	GLU	CG-CD	5.96	1.67	1.52
1	F	476	THR	N-CA	-5.93	1.38	1.46
1	G	209	THR	CA-CB	5.77	1.62	1.53
1	A	344	ILE	CA-CB	5.71	1.59	1.53
1	H	147	ILE	CA-CB	5.70	1.62	1.54
1	F	38	HIS	C-O	-5.69	1.17	1.24
1	B	20	PHE	C-O	-5.67	1.17	1.24
1	E	181	VAL	CA-CB	5.62	1.60	1.54
1	F	478	ILE	CA-CB	5.60	1.61	1.54
1	A	348	THR	N-CA	5.60	1.53	1.46
1	G	442	GLU	CG-CD	5.51	1.65	1.52
1	E	75	PRO	C-O	-5.48	1.17	1.23
1	C	82	ILE	CA-CB	5.45	1.62	1.54
1	H	160	GLU	N-CA	5.43	1.50	1.46
1	C	82	ILE	CB-CG2	5.40	1.70	1.52
1	H	123	PRO	CA-C	5.31	1.57	1.52
1	D	289	VAL	CA-CB	5.30	1.62	1.54
1	H	152	THR	CA-CB	5.30	1.62	1.53
1	B	321	VAL	C-O	5.25	1.30	1.24
1	D	142	ILE	CA-CB	5.24	1.60	1.54
1	A	442	GLU	CG-CD	5.23	1.65	1.52
1	G	339	VAL	CA-CB	5.22	1.60	1.54
1	C	142	ILE	CA-CB	5.16	1.60	1.54
1	A	147	ILE	CA-CB	5.16	1.60	1.54
1	H	370	ILE	CA-CB	5.14	1.61	1.54
1	F	432	ARG	CZ-NH1	5.13	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	432	ARG	CZ-NH1	5.12	1.40	1.32
1	F	499	THR	CA-CB	5.12	1.61	1.53
1	G	37	ASP	CA-C	5.12	1.59	1.52
1	G	249	PRO	CA-C	5.12	1.56	1.52
1	D	442	GLU	CG-CD	5.11	1.64	1.52
1	H	488	SER	N-CA	5.11	1.52	1.46
1	A	181	VAL	CA-CB	5.08	1.60	1.54
1	H	135	VAL	CA-C	5.08	1.59	1.52
1	D	463	VAL	CA-CB	5.07	1.61	1.54
1	A	348	THR	CA-CB	5.06	1.61	1.53
1	G	140	HIS	C-O	-5.05	1.18	1.24
1	B	249	PRO	CA-C	5.04	1.56	1.52
1	F	293	ALA	CA-C	5.02	1.59	1.52
1	H	357	ALA	CA-C	5.00	1.59	1.52

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	501	TYR	O-C-N	-27.96	90.40	122.84
1	C	501	TYR	O-C-N	-25.34	93.45	122.84
1	B	501	TYR	CA-C-N	24.46	165.72	121.70
1	B	501	TYR	C-N-CA	24.46	165.72	121.70
1	H	501	TYR	CA-C-N	23.86	164.65	121.70
1	H	501	TYR	C-N-CA	23.86	164.65	121.70
1	F	501	TYR	O-C-N	-23.65	92.63	122.43
1	G	501	TYR	CA-C-N	23.07	163.22	121.70
1	G	501	TYR	C-N-CA	23.07	163.22	121.70
1	G	501	TYR	O-C-N	-12.66	108.76	122.94
1	C	501	TYR	CA-C-N	11.79	142.92	121.70
1	C	501	TYR	C-N-CA	11.79	142.92	121.70
1	B	501	TYR	O-C-N	-11.63	109.89	123.03
1	H	289	VAL	CB-CA-C	-10.72	96.39	112.05
1	D	289	VAL	CB-CA-C	-10.16	96.41	112.16
1	A	222	VAL	CB-CA-C	-10.03	94.43	110.28
1	G	289	VAL	CB-CA-C	-9.93	96.77	112.16
1	F	289	VAL	CB-CA-C	-9.87	97.64	112.05
1	C	289	VAL	CB-CA-C	-9.68	97.15	112.16
1	A	289	VAL	CB-CA-C	-9.55	98.11	112.05
1	E	289	VAL	CB-CA-C	-9.54	98.11	112.05
1	H	222	VAL	CB-CA-C	-9.37	95.92	111.29
1	H	22	VAL	CB-CA-C	-9.13	96.68	110.55
1	F	222	VAL	CB-CA-C	-9.09	94.65	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	22	VAL	CB-CA-C	-8.93	96.41	110.69
1	G	222	VAL	CB-CA-C	-8.91	96.21	110.28
1	G	22	VAL	CB-CA-C	-8.76	96.68	110.69
1	F	337	GLY	N-CA-C	8.54	121.35	111.36
1	F	121	VAL	N-CA-CB	-7.85	101.74	111.94
1	H	103	MET	CB-CG-SD	-7.76	89.41	112.70
1	D	121	VAL	N-CA-CB	-7.75	101.86	111.94
1	C	121	VAL	N-CA-CB	-7.70	101.93	111.94
1	F	239	THR	N-CA-C	-7.68	97.51	108.96
1	D	22	VAL	CB-CA-C	-7.63	98.95	110.55
1	F	103	MET	CG-SD-CE	-7.63	84.11	100.90
1	B	222	VAL	CB-CA-C	-7.49	98.44	110.28
1	F	103	MET	CB-CG-SD	-7.40	90.50	112.70
1	A	501	TYR	CA-C-N	7.39	135.00	121.70
1	A	501	TYR	C-N-CA	7.39	135.00	121.70
1	F	22	VAL	CB-CA-C	-7.33	97.92	110.30
1	A	26	ARG	NE-CZ-NH1	-7.22	114.28	121.50
1	E	402	ILE	CA-C-N	7.19	127.16	119.76
1	E	402	ILE	C-N-CA	7.19	127.16	119.76
1	C	267	SER	CA-C-N	7.18	126.88	119.56
1	C	267	SER	C-N-CA	7.18	126.88	119.56
1	E	121	VAL	N-CA-CB	-6.95	102.91	111.94
1	H	82	ILE	CB-CA-C	-6.93	101.03	112.26
1	F	386	LEU	CA-CB-CG	6.86	140.30	116.30
1	G	415	ILE	CG1-CB-CG2	-6.75	90.46	110.70
1	A	460	THR	N-CA-C	6.69	119.43	109.59
1	D	222	VAL	CB-CA-C	-6.69	99.71	110.28
1	B	121	VAL	N-CA-CB	-6.67	103.27	111.94
1	E	144	ARG	NE-CZ-NH2	-6.67	113.19	119.20
1	B	82	ILE	CB-CA-C	-6.62	101.53	112.26
1	D	327	VAL	CA-C-N	6.62	127.01	119.93
1	D	327	VAL	C-N-CA	6.62	127.01	119.93
1	C	222	VAL	CB-CA-C	-6.60	99.85	110.28
1	G	121	VAL	N-CA-CB	-6.57	103.61	112.22
1	G	82	ILE	CB-CA-C	-6.56	101.99	112.16
1	H	415	ILE	CG1-CB-CG2	-6.53	91.11	110.70
1	D	432	ARG	CA-C-N	-6.52	113.04	119.76
1	D	432	ARG	C-N-CA	-6.52	113.04	119.76
1	H	343	SER	CA-C-N	6.51	127.28	122.59
1	H	343	SER	C-N-CA	6.51	127.28	122.59
1	E	489	THR	N-CA-CB	-6.48	99.64	110.39
1	A	121	VAL	N-CA-CB	-6.47	103.53	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	PRO	CA-C-N	-6.47	113.63	120.03
1	A	123	PRO	C-N-CA	-6.47	113.63	120.03
1	E	105	LYS	N-CA-C	6.46	118.86	111.11
1	H	67	VAL	CB-CA-C	6.44	119.74	110.33
1	H	390	LYS	CA-C-N	-6.43	116.41	121.82
1	H	390	LYS	C-N-CA	-6.43	116.41	121.82
1	F	217	GLU	N-CA-C	6.41	118.27	111.28
1	H	103	MET	CG-SD-CE	-6.28	87.08	100.90
1	H	239	THR	N-CA-C	-6.28	99.87	109.41
1	G	144	ARG	NE-CZ-NH2	-6.25	113.57	119.20
1	C	468	ILE	CB-CA-C	6.25	119.11	110.99
1	D	337	GLY	N-CA-C	6.17	119.94	111.54
1	A	26	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	B	82	ILE	CG1-CB-CG2	6.11	129.04	110.70
1	E	67	VAL	CB-CA-C	6.06	119.83	110.50
1	E	103	MET	CA-C-N	-6.06	113.52	119.76
1	E	103	MET	C-N-CA	-6.06	113.52	119.76
1	H	289	VAL	N-CA-CB	6.03	120.01	110.54
1	A	435	PHE	CA-C-N	6.01	125.97	119.78
1	A	435	PHE	C-N-CA	6.01	125.97	119.78
1	D	501	TYR	CA-C-O	-5.99	114.09	121.88
1	E	289	VAL	N-CA-CB	5.99	119.94	110.54
1	A	499	THR	CB-CA-C	5.98	118.38	110.06
1	D	82	ILE	CB-CA-C	-5.91	102.69	112.26
1	B	26	ARG	NE-CZ-NH1	-5.90	115.60	121.50
1	A	82	ILE	CB-CG1-CD1	-5.90	101.42	113.80
1	G	37	ASP	CB-CA-C	-5.89	101.64	110.88
1	F	22	VAL	CG1-CB-CG2	5.88	123.73	110.80
1	F	67	VAL	CB-CA-C	5.87	119.54	110.50
1	D	449	GLN	CA-C-N	-5.87	113.74	119.78
1	D	449	GLN	C-N-CA	-5.87	113.74	119.78
1	C	289	VAL	CG1-CB-CG2	5.86	123.69	110.80
1	G	144	ARG	CG-CD-NE	-5.86	99.12	112.00
1	D	22	VAL	CG1-CB-CG2	5.85	123.67	110.80
1	D	289	VAL	N-CA-CB	5.82	120.61	110.65
1	C	239	THR	N-CA-C	-5.79	100.61	109.41
1	G	177	LYS	N-CA-C	5.78	117.26	111.07
1	C	327	VAL	CA-C-N	5.77	125.79	119.90
1	C	327	VAL	C-N-CA	5.77	125.79	119.90
1	A	144	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	A	289	VAL	CG1-CB-CG2	5.72	123.39	110.80
1	E	289	VAL	CG1-CB-CG2	5.72	123.39	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	241	GLU	CB-CA-C	-5.70	99.50	109.07
1	F	82	ILE	CB-CA-C	-5.66	103.10	112.26
1	G	415	ILE	N-CA-C	5.65	116.88	108.46
1	A	131	ARG	CG-CD-NE	-5.65	99.57	112.00
1	C	82	ILE	N-CA-CB	5.65	120.99	110.77
1	H	144	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	C	299	ILE	N-CA-C	5.63	116.36	110.62
1	H	22	VAL	CG1-CB-CG2	5.62	123.17	110.80
1	G	432	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	F	289	VAL	N-CA-CB	5.59	119.31	110.54
1	H	239	THR	N-CA-CB	-5.57	102.58	111.43
1	A	280	ASN	N-CA-C	-5.57	100.03	107.88
1	F	82	ILE	CG1-CB-CG2	5.51	127.24	110.70
1	D	97	PHE	CA-C-N	5.47	128.75	120.77
1	D	97	PHE	C-N-CA	5.47	128.75	120.77
1	G	289	VAL	CG1-CB-CG2	5.43	122.75	110.80
1	H	49	ARG	N-CA-C	5.43	118.37	111.69
1	F	121	VAL	CG1-CB-CG2	5.43	122.74	110.80
1	A	121	VAL	CB-CA-C	5.42	119.78	112.36
1	D	304	SER	N-CA-C	5.40	117.59	111.11
1	F	280	ASN	N-CA-C	-5.37	100.30	107.88
1	A	205	ASP	N-CA-C	5.36	119.44	113.01
1	B	174	GLU	N-CA-C	-5.35	105.53	111.36
1	E	82	ILE	CG1-CB-CG2	5.34	126.72	110.70
1	C	383	LEU	CA-CB-CG	5.33	134.95	116.30
1	C	432	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	B	280	ASN	N-CA-C	-5.30	100.40	107.88
1	D	489	THR	N-CA-CB	-5.29	101.61	110.39
1	G	302	ILE	N-CA-C	5.29	115.50	110.53
1	D	441	VAL	N-CA-C	5.28	115.49	110.42
1	A	449	GLN	N-CA-C	5.27	117.56	110.29
1	E	289	VAL	CA-CB-CG2	5.27	119.35	110.40
1	G	82	ILE	N-CA-CB	5.25	119.63	110.65
1	F	501	TYR	CA-C-N	5.24	131.13	121.70
1	F	501	TYR	C-N-CA	5.24	131.13	121.70
1	F	289	VAL	CG1-CB-CG2	5.22	122.28	110.80
1	H	67	VAL	N-CA-CB	-5.19	103.94	111.52
1	G	22	VAL	CG1-CB-CG2	5.18	122.20	110.80
1	G	435	PHE	CA-C-N	5.17	125.07	119.85
1	G	435	PHE	C-N-CA	5.17	125.07	119.85
1	A	125	LYS	N-CA-C	-5.16	106.49	112.89
1	G	395	THR	N-CA-C	5.13	117.11	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	LYS	N-CA-C	-5.13	105.87	111.82
1	A	239	THR	N-CA-C	-5.12	101.97	109.81
1	A	62	GLY	N-CA-C	5.10	122.94	115.08
1	B	319	SER	N-CA-C	5.10	116.82	108.76
1	E	501	TYR	CA-C-O	-5.10	115.42	121.89
1	H	499	THR	CB-CA-C	5.09	117.48	109.84
1	H	82	ILE	N-CA-CB	5.09	119.98	110.77
1	E	59	ASP	N-CA-C	5.09	118.75	112.54
1	G	209	THR	CB-CA-C	5.08	119.49	110.85
1	G	441	VAL	N-CA-C	5.08	115.30	110.42
1	E	460	THR	N-CA-C	5.08	117.02	109.25
1	F	79	PHE	N-CA-C	5.07	119.10	113.02
1	E	502	SER	CA-C-O	-5.07	112.19	120.80
1	D	289	VAL	CG1-CB-CG2	5.04	121.90	110.80
1	C	82	ILE	CB-CA-C	-5.03	104.12	112.26
1	D	144	ARG	NE-CZ-NH2	-5.03	114.68	119.20
1	A	489	THR	N-CA-CB	-5.01	102.50	110.22
1	F	442	GLU	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	69	ILE	Peptide
1	F	391	GLY	Peptide
1	F	501	TYR	Mainchain
1	F	71	GLY	Peptide
1	H	390	LYS	Peptide
1	H	501	TYR	Peptide

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	4082	0	3992	161	0
1	B	4082	0	3992	134	0
1	C	4082	0	3992	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4082	0	3991	157	0
1	E	4082	0	3992	144	0
1	F	4082	0	3992	143	0
1	G	4082	0	3992	119	0
1	H	4082	0	3992	142	0
2	A	363	0	0	43	1
2	B	317	0	0	26	0
2	C	371	0	0	37	0
2	D	340	0	0	38	1
2	E	347	0	0	41	0
2	F	414	0	0	48	1
2	G	340	0	0	25	1
2	H	397	0	0	42	0
All	All	35545	0	31935	1125	2

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 17.

All (1125) 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:F:103:MET:HE3	1:F:103:MET:CB	1.19	1.62
1:F:103:MET:CB	1:F:103:MET:CG	1.76	1.60
1:H:103:MET:CG	1:H:103:MET:CB	1.76	1.54
1:H:103:MET:CB	1:H:103:MET:HE3	1.27	1.54
1:E:501:TYR:C	1:E:502:SER:N	1.68	1.51
1:H:103:MET:HB3	1:H:103:MET:CE	1.02	1.47
1:A:103:MET:CE	1:A:104:PRO:HD2	1.45	1.46
1:C:501:TYR:C	1:C:502:SER:N	1.69	1.45
1:F:103:MET:HB3	1:F:103:MET:CE	0.95	1.42
1:H:103:MET:CB	1:H:103:MET:CE	1.83	1.28
1:A:103:MET:HE3	1:A:104:PRO:CD	1.65	1.26
1:F:386:LEU:HB2	2:F:2385:HOH:O	1.32	1.26
1:E:201:CYS:HB2	2:E:2185:HOH:O	1.39	1.19
1:E:358:LEU:HD12	2:E:2259:HOH:O	1.43	1.18
1:F:103:MET:CB	1:F:103:MET:CE	1.74	1.15
1:A:272:LEU:HB3	2:A:2226:HOH:O	1.44	1.14
1:C:205:ASP:OD1	1:C:227:ARG:NH1	1.82	1.13
1:D:103:MET:HE2	1:D:107:LEU:HB3	1.23	1.12
1:A:26:ARG:NH1	1:A:60:ASP:OD2	1.82	1.12
1:C:439:GLN:HG3	2:C:2331:HOH:O	1.47	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ILE:HD11	1:E:420:TYR:HD1	1.14	1.11
1:F:415:ILE:CD1	1:F:451:HIS:HB3	1.79	1.11
1:B:392:GLU:HG2	1:B:393:GLY:H	1.06	1.09
1:F:252:ASP:HB3	2:F:2254:HOH:O	1.50	1.08
1:B:103:MET:HE3	1:B:104:PRO:HD2	1.12	1.08
1:H:405:SER:HA	2:H:2313:HOH:O	1.55	1.07
1:G:252:ASP:HB3	2:G:2206:HOH:O	1.53	1.07
1:G:103:MET:CE	1:G:107:LEU:HB3	1.85	1.06
1:G:274:LEU:HD13	1:G:310:VAL:HG12	1.33	1.06
1:H:392:GLU:HA	2:H:2305:HOH:O	1.55	1.05
1:B:274:LEU:HD13	1:B:310:VAL:HG12	1.32	1.05
1:E:219:ARG:HG2	1:E:219:ARG:HH11	1.13	1.04
1:H:103:MET:CB	1:H:103:MET:SD	2.45	1.04
1:A:103:MET:HE3	1:A:104:PRO:HD2	1.08	1.04
1:H:10:GLY:O	1:H:11:ARG:HB3	1.52	1.04
1:A:413:ARG:HD3	1:A:453:MET:HE2	1.40	1.03
1:D:238:LYS:HE2	1:D:243:TYR:CZ	1.94	1.03
1:C:148:GLU:HB2	2:C:2162:HOH:O	1.57	1.02
1:H:364:TYR:CE2	1:H:369:MET:HE2	1.94	1.02
1:F:103:MET:CB	1:F:103:MET:SD	2.48	1.02
1:A:10:GLY:O	1:A:11:ARG:HB3	1.57	1.02
1:A:103:MET:HE2	1:A:104:PRO:HD2	1.37	1.02
1:H:4:VAL:HG11	1:H:369:MET:HE1	1.33	1.02
1:D:274:LEU:HD13	1:D:310:VAL:HG12	1.41	1.02
1:F:26:ARG:NH1	1:F:60:ASP:OD2	1.93	1.01
1:D:103:MET:CE	1:D:104:PRO:HD2	1.91	1.01
1:B:26:ARG:NH1	1:B:60:ASP:OD2	1.94	1.01
1:H:4:VAL:HG11	1:H:369:MET:CE	1.91	1.01
1:D:238:LYS:HE2	1:D:243:TYR:CE1	1.96	1.01
1:H:103:MET:HB3	1:H:103:MET:HE2	1.40	1.01
1:H:83:ASP:OD1	1:H:140:HIS:HE1	1.44	1.00
1:B:252:ASP:HB3	2:B:2192:HOH:O	1.58	1.00
1:D:69:ILE:HD12	1:D:69:ILE:O	1.61	1.00
1:D:103:MET:HE3	1:D:104:PRO:CD	1.90	1.00
1:F:201:CYS:HB3	2:F:2180:HOH:O	1.58	1.00
1:F:350:HIS:HD2	2:F:2315:HOH:O	1.45	0.99
1:A:15:LYS:HD2	2:A:2240:HOH:O	1.60	0.99
1:E:103:MET:CE	1:E:107:LEU:HB3	1.92	0.99
1:B:103:MET:CE	1:B:104:PRO:HD2	1.92	0.99
1:B:392:GLU:HG2	1:B:393:GLY:N	1.67	0.99
1:C:205:ASP:CG	1:C:227:ARG:HH12	1.68	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:MET:SD	2:A:2121:HOH:O	2.20	0.99
1:F:415:ILE:HD13	1:F:451:HIS:HB3	1.40	0.98
1:D:280:ASN:HD22	1:D:281:THR:H	1.05	0.98
1:F:103:MET:HB3	1:F:103:MET:HE2	1.43	0.98
1:E:259:THR:HG22	2:E:2187:HOH:O	1.62	0.97
1:A:103:MET:CE	1:A:104:PRO:CD	2.33	0.97
1:E:103:MET:HE3	1:E:107:LEU:CB	1.94	0.97
1:G:266:GLN:HG3	2:G:2213:HOH:O	1.65	0.97
1:D:103:MET:HE2	1:D:107:LEU:CB	1.93	0.97
1:B:103:MET:HE3	1:B:104:PRO:CD	1.95	0.97
1:G:239:THR:HG22	1:G:241:GLU:H	1.24	0.96
1:B:364:TYR:CE2	1:B:369:MET:HE2	2.01	0.96
1:E:103:MET:HE3	1:E:107:LEU:HB2	1.45	0.96
1:E:274:LEU:HD13	1:E:310:VAL:HG12	1.47	0.96
1:F:12:GLU:HG2	2:F:2015:HOH:O	1.66	0.96
1:D:501:TYR:C	1:D:502:SER:N	2.24	0.96
1:F:406:PHE:HE2	1:F:409:VAL:HG23	1.31	0.95
1:C:274:LEU:HD13	1:C:310:VAL:HG12	1.47	0.95
1:D:364:TYR:CE2	1:D:369:MET:HE2	2.02	0.95
1:C:103:MET:CE	1:C:107:LEU:HB3	1.96	0.95
1:A:239:THR:HG22	1:A:241:GLU:H	1.30	0.94
1:E:426:VAL:HG21	1:E:447:VAL:HG11	1.49	0.94
1:B:350:HIS:HD2	2:B:2233:HOH:O	1.50	0.94
1:E:415:ILE:HD11	1:E:420:TYR:CD1	2.02	0.93
1:H:206:GLU:HB2	2:H:2196:HOH:O	1.67	0.93
1:H:395:THR:HG22	2:H:2309:HOH:O	1.67	0.93
1:F:274:LEU:HD13	1:F:310:VAL:HG12	1.49	0.93
1:D:239:THR:HG22	1:D:242:TYR:H	1.33	0.93
1:E:239:THR:HG22	1:E:242:TYR:H	1.30	0.93
1:B:239:THR:HG22	1:B:242:TYR:H	1.34	0.93
1:F:103:MET:CB	1:F:103:MET:HE2	1.94	0.93
1:B:280:ASN:HD22	1:B:281:THR:H	1.14	0.93
1:D:103:MET:HE3	1:D:104:PRO:HD2	0.96	0.92
1:F:69:ILE:HD12	1:F:69:ILE:O	1.70	0.91
1:G:390:LYS:O	1:G:391:GLY:O	1.84	0.91
1:H:274:LEU:HD13	1:H:310:VAL:HG12	1.50	0.91
1:D:26:ARG:NH1	1:D:60:ASP:OD2	2.04	0.91
1:C:390:LYS:O	1:C:391:GLY:O	1.87	0.91
1:D:301:ARG:HB2	2:D:2230:HOH:O	1.70	0.91
1:G:4:VAL:N	2:G:2001:HOH:O	2.05	0.90
1:C:239:THR:HG22	1:C:241:GLU:H	1.33	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:LEU:HD23	2:H:2136:HOH:O	1.71	0.90
1:F:481:GLU:HG3	2:F:2388:HOH:O	1.72	0.90
1:G:26:ARG:NH2	1:G:323:GLU:OE1	2.05	0.90
1:A:280:ASN:HD22	1:A:281:THR:H	1.19	0.89
1:C:485:ASP:OD1	1:C:487:THR:HG23	1.73	0.89
1:E:280:ASN:HD22	1:E:281:THR:H	1.21	0.88
1:C:280:ASN:HD22	1:C:281:THR:H	1.21	0.88
1:F:415:ILE:HD11	1:F:451:HIS:HB3	1.55	0.88
1:H:389:GLU:HG2	2:H:2299:HOH:O	1.73	0.88
1:A:413:ARG:HD3	1:A:453:MET:CE	2.02	0.88
1:D:439:GLN:HG3	2:D:2296:HOH:O	1.74	0.88
1:F:390:LYS:O	1:F:391:GLY:O	1.92	0.87
1:F:445:ARG:NH1	2:F:2368:HOH:O	2.07	0.87
1:H:368:GLU:OE2	1:H:396:LYS:NZ	2.08	0.87
1:C:69:ILE:HB	1:C:74:LYS:HD2	1.55	0.86
1:F:280:ASN:HD22	1:F:281:THR:H	1.20	0.86
1:E:218:ARG:HG2	2:E:2191:HOH:O	1.76	0.86
1:A:12:GLU:HG2	2:A:2008:HOH:O	1.74	0.86
1:B:489:THR:CG2	1:D:434:ARG:HE	1.86	0.86
1:E:255:GLU:HG2	2:E:2214:HOH:O	1.73	0.86
1:B:249:PRO:HA	1:B:388:MET:HE1	1.58	0.86
1:H:350:HIS:HD2	2:H:2282:HOH:O	1.58	0.85
1:E:93:ASN:HB3	2:E:2092:HOH:O	1.75	0.85
1:F:485:ASP:OD1	1:F:487:THR:HG23	1.75	0.85
1:B:392:GLU:CG	1:B:393:GLY:H	1.90	0.85
1:E:103:MET:CE	1:E:107:LEU:CB	2.53	0.85
1:E:301:ARG:HB2	2:E:2229:HOH:O	1.74	0.85
1:C:274:LEU:CD1	1:C:310:VAL:HG12	2.06	0.85
1:F:10:GLY:O	1:F:11:ARG:HB3	1.76	0.85
1:E:350:HIS:HD2	2:E:2257:HOH:O	1.60	0.84
1:F:105:LYS:HE2	2:F:2078:HOH:O	1.74	0.84
1:E:501:TYR:O	1:E:502:SER:N	2.10	0.84
1:F:439:GLN:HG3	2:F:2364:HOH:O	1.77	0.84
1:F:489:THR:CG2	1:H:434:ARG:HE	1.91	0.84
1:E:26:ARG:NH1	1:E:60:ASP:OD2	2.10	0.84
1:E:434:ARG:HE	1:G:489:THR:CG2	1.89	0.84
1:A:4:VAL:N	2:A:2001:HOH:O	2.09	0.84
1:E:481:GLU:HG3	2:E:2328:HOH:O	1.76	0.84
1:A:489:THR:CG2	1:C:434:ARG:HE	1.90	0.84
1:F:390:LYS:O	1:F:391:GLY:C	2.18	0.84
1:F:438:ARG:CD	2:F:2363:HOH:O	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:MET:HE2	1:B:107:LEU:HB3	1.60	0.84
1:B:364:TYR:CD2	1:B:369:MET:HE2	2.13	0.83
1:H:408:ALA:HB1	2:H:2356:HOH:O	1.79	0.83
1:E:219:ARG:HH11	1:E:219:ARG:CG	1.91	0.83
1:H:103:MET:HE3	1:H:103:MET:CA	2.08	0.82
1:A:69:ILE:O	1:A:69:ILE:HG13	1.79	0.82
1:H:280:ASN:HD22	1:H:281:THR:H	1.26	0.82
1:B:489:THR:HG21	1:D:434:ARG:HE	1.43	0.82
1:D:213:HIS:HD2	2:D:2191:HOH:O	1.61	0.82
1:E:403:PRO:HA	1:E:462:GLY:O	1.80	0.81
1:C:238:LYS:HD3	1:C:243:TYR:CE1	2.14	0.81
1:F:406:PHE:CE2	1:F:409:VAL:HG23	2.15	0.81
1:D:364:TYR:CD2	1:D:369:MET:HE2	2.15	0.81
1:C:399:GLN:HE21	1:C:467:SER:HB3	1.43	0.81
1:E:239:THR:HG22	1:E:242:TYR:N	1.95	0.81
1:A:350:HIS:HD2	2:A:2271:HOH:O	1.62	0.81
1:A:274:LEU:HD13	1:A:310:VAL:HG12	1.63	0.80
1:A:270:PRO:HG2	2:A:2224:HOH:O	1.82	0.80
1:G:280:ASN:HD22	1:G:281:THR:H	1.28	0.80
1:C:205:ASP:CG	1:C:227:ARG:NH1	2.34	0.80
1:C:415:ILE:CD1	1:C:453:MET:HE2	2.12	0.80
1:F:386:LEU:HD13	2:F:2331:HOH:O	1.81	0.80
1:A:209:THR:HG21	2:A:2178:HOH:O	1.81	0.80
1:A:426:VAL:HG21	1:A:447:VAL:HG11	1.62	0.80
1:F:259:THR:HG22	2:F:2220:HOH:O	1.83	0.80
1:C:201:CYS:HB2	2:C:2206:HOH:O	1.81	0.79
1:H:239:THR:HG22	1:H:241:GLU:H	1.47	0.79
1:D:69:ILE:HD11	1:D:74:LYS:NZ	1.97	0.79
1:C:103:MET:HE2	1:C:107:LEU:HB3	1.65	0.79
1:C:501:TYR:O	1:C:502:SER:N	2.16	0.79
1:F:79:PHE:HD2	1:F:82:ILE:HD11	1.47	0.79
1:D:93:ASN:HB3	2:D:2105:HOH:O	1.82	0.78
1:H:438:ARG:NE	2:H:2330:HOH:O	2.06	0.78
1:A:369:MET:HE3	1:A:371:VAL:CG2	2.12	0.78
1:B:125:LYS:HD2	2:B:2111:HOH:O	1.82	0.78
1:F:103:MET:HE3	1:F:103:MET:CA	2.10	0.78
1:A:468:ILE:HD13	1:A:478:ILE:HD13	1.65	0.78
1:D:69:ILE:CD1	1:D:74:LYS:HZ3	1.97	0.78
1:H:374:ARG:HD3	1:H:378:SER:OG	1.84	0.77
1:F:130:TRP:NE1	1:F:134:ILE:HD11	1.99	0.77
1:F:391:GLY:HA3	1:F:394:LEU:HD11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:HA	2:A:2226:HOH:O	1.83	0.77
1:H:265:ARG:HD2	2:H:2236:HOH:O	1.85	0.77
1:E:404:VAL:O	1:E:462:GLY:HA2	1.84	0.77
1:D:280:ASN:HD22	1:D:281:THR:N	1.83	0.76
1:F:83:ASP:OD1	1:F:140:HIS:HE1	1.66	0.76
1:D:390:LYS:O	1:D:391:GLY:O	2.03	0.76
1:E:271:HIS:HB2	2:E:2220:HOH:O	1.83	0.76
1:E:493:LEU:HD22	2:G:2284:HOH:O	1.84	0.76
1:H:407:SER:O	1:H:458:ARG:HG3	1.85	0.76
1:F:239:THR:HG22	1:F:241:GLU:H	1.48	0.76
1:F:434:ARG:HH21	1:H:489:THR:HG22	1.50	0.76
1:D:239:THR:HG22	1:D:241:GLU:H	1.51	0.76
1:G:238:LYS:HD3	1:G:243:TYR:CE1	2.19	0.76
1:A:239:THR:CG2	1:A:241:GLU:H	1.99	0.75
1:C:148:GLU:CB	2:C:2162:HOH:O	2.24	0.75
1:C:103:MET:HE3	1:C:107:LEU:HB3	1.67	0.75
1:F:438:ARG:HD2	2:F:2363:HOH:O	1.87	0.75
1:A:399:GLN:HG3	1:A:467:SER:HB3	1.68	0.74
1:B:486:GLU:O	1:B:489:THR:HB	1.86	0.74
1:F:397:GLU:HB3	2:F:2380:HOH:O	1.87	0.74
1:G:285:PRO:HG2	1:G:325:MET:HG3	1.70	0.74
1:G:103:MET:HE3	1:G:107:LEU:HB3	1.68	0.74
1:B:130:TRP:CE2	1:B:134:ILE:HD11	2.22	0.74
1:D:69:ILE:O	1:D:69:ILE:CD1	2.35	0.73
1:A:103:MET:HE3	1:A:104:PRO:HD3	1.68	0.73
1:C:233:LYS:HD2	1:C:246:GLU:HG2	1.70	0.73
1:B:4:VAL:HG11	1:B:369:MET:HE1	1.69	0.73
1:E:239:THR:CG2	1:E:241:GLU:H	2.01	0.73
1:F:144:ARG:NH2	1:G:436:PRO:O	2.22	0.73
1:H:266:GLN:HB2	2:H:2234:HOH:O	1.88	0.73
1:D:415:ILE:HD11	1:D:453:MET:HE1	1.70	0.73
1:B:438:ARG:CZ	2:B:2264:HOH:O	2.36	0.73
1:D:69:ILE:HG12	1:D:74:LYS:HG3	1.70	0.73
1:D:280:ASN:ND2	1:D:281:THR:H	1.85	0.73
1:C:83:ASP:OD1	1:C:140:HIS:HE1	1.72	0.73
1:G:103:MET:HE2	1:G:107:LEU:HB3	1.68	0.73
1:E:219:ARG:HG2	1:E:219:ARG:NH1	1.89	0.72
1:F:206:GLU:HB2	2:F:2221:HOH:O	1.89	0.72
1:A:489:THR:HG21	1:C:434:ARG:HE	1.52	0.72
1:B:434:ARG:HE	1:D:489:THR:CG2	2.02	0.72
1:C:99:GLU:OE1	2:C:2121:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:LYS:O	1:D:391:GLY:C	2.33	0.72
1:D:404:VAL:O	1:D:462:GLY:HA2	1.88	0.72
1:E:10:GLY:O	1:E:11:ARG:HB2	1.88	0.72
1:D:69:ILE:CG1	1:D:74:LYS:HG3	2.19	0.72
1:A:364:TYR:CD2	1:A:369:MET:HE2	2.25	0.72
1:G:426:VAL:HG21	1:G:447:VAL:HG11	1.70	0.72
1:A:83:ASP:OD1	1:A:140:HIS:HE1	1.73	0.71
2:A:2205:HOH:O	1:C:499:THR:CG2	2.37	0.71
2:F:2252:HOH:O	1:H:499:THR:HB	1.89	0.71
1:G:350:HIS:HD2	2:G:2255:HOH:O	1.71	0.71
1:B:239:THR:HG22	1:B:242:TYR:N	2.05	0.71
1:E:215:CYS:SG	1:E:222:VAL:CG2	2.78	0.71
1:E:434:ARG:HE	1:G:489:THR:HG21	1.55	0.71
1:H:103:MET:CB	1:H:103:MET:HE2	2.07	0.71
1:F:63:ILE:HD11	1:F:82:ILE:HG12	1.71	0.71
1:A:99:GLU:OE1	2:A:2104:HOH:O	2.09	0.71
2:A:2207:HOH:O	1:C:499:THR:HB	1.89	0.71
1:C:200:ILE:HD11	1:C:208:ILE:CD1	2.20	0.71
1:C:415:ILE:HD12	1:C:453:MET:HE2	1.73	0.71
1:H:438:ARG:NH2	2:H:2330:HOH:O	2.24	0.71
1:B:103:MET:HE2	1:B:107:LEU:CB	2.20	0.71
1:D:240:PHE:CE2	1:D:241:GLU:HG3	2.27	0.70
1:G:125:LYS:O	1:G:125:LYS:HG3	1.91	0.70
1:A:148:GLU:HG3	2:A:2146:HOH:O	1.90	0.70
1:D:501:TYR:O	1:D:502:SER:N	2.24	0.70
1:F:391:GLY:HA3	1:F:394:LEU:CD1	2.21	0.70
1:F:350:HIS:CD2	2:F:2315:HOH:O	2.31	0.70
1:D:400:LEU:HD23	1:D:468:ILE:HD12	1.74	0.69
1:H:16:LYS:HD2	2:H:2286:HOH:O	1.92	0.69
1:D:426:VAL:HG21	1:D:447:VAL:HG11	1.74	0.69
1:D:49:ARG:HD2	2:D:2056:HOH:O	1.91	0.69
1:E:415:ILE:CD1	1:E:420:TYR:CD1	2.75	0.69
1:F:474:GLU:OE1	2:F:2386:HOH:O	2.09	0.69
1:E:215:CYS:SG	1:E:222:VAL:HG21	2.33	0.69
2:F:2248:HOH:O	1:H:499:THR:HG22	1.92	0.69
1:G:107:LEU:HD22	2:G:2112:HOH:O	1.91	0.69
1:D:350:HIS:HD2	2:D:2261:HOH:O	1.74	0.69
1:B:130:TRP:NE1	1:B:134:ILE:HD11	2.07	0.69
1:C:426:VAL:HG21	1:C:447:VAL:HG11	1.75	0.69
1:D:227:ARG:NH2	1:D:256:GLN:HE21	1.91	0.69
1:H:69:ILE:HD11	1:H:74:LYS:HE2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:GLU:OE1	2:C:2358:HOH:O	2.09	0.69
1:D:213:HIS:CD2	2:D:2191:HOH:O	2.39	0.69
1:A:486:GLU:O	1:A:489:THR:HB	1.91	0.69
1:B:201:CYS:HB2	2:B:2162:HOH:O	1.93	0.69
1:H:177:LYS:HE3	2:H:2180:HOH:O	1.93	0.69
1:D:400:LEU:HD23	1:D:468:ILE:CD1	2.23	0.68
1:D:44:GLU:HG3	2:D:2050:HOH:O	1.91	0.68
1:E:438:ARG:HD3	2:E:2304:HOH:O	1.92	0.68
1:F:125:LYS:HD2	2:F:2150:HOH:O	1.94	0.68
1:A:388:MET:HE2	2:A:2134:HOH:O	1.92	0.68
2:A:2205:HOH:O	1:C:499:THR:HG23	1.92	0.68
1:B:285:PRO:HG2	1:B:325:MET:HG3	1.74	0.68
1:D:121:VAL:HG22	1:D:166:PHE:O	1.93	0.68
1:E:489:THR:CG2	1:G:434:ARG:HE	2.06	0.68
1:A:417:ASN:ND2	1:A:420:TYR:H	1.92	0.68
1:C:259:THR:HG22	2:C:2210:HOH:O	1.94	0.68
1:H:121:VAL:O	1:H:121:VAL:CG1	2.40	0.68
1:A:282:SER:HB3	1:A:290:HIS:CE1	2.28	0.68
1:B:145:TYR:HE2	1:C:438:ARG:HH22	1.40	0.68
1:G:103:MET:HE3	1:G:107:LEU:CB	2.24	0.68
1:B:239:THR:HG22	1:B:241:GLU:H	1.57	0.67
1:D:103:MET:CE	1:D:107:LEU:HB3	2.13	0.67
1:H:83:ASP:OD1	1:H:140:HIS:CE1	2.36	0.67
1:A:449:GLN:HG3	2:A:2324:HOH:O	1.93	0.67
1:E:206:GLU:HB2	2:E:2188:HOH:O	1.93	0.67
1:B:4:VAL:HG11	1:B:369:MET:CE	2.24	0.67
1:B:227:ARG:CD	1:B:260:VAL:HG21	2.24	0.67
1:E:486:GLU:O	1:E:489:THR:HB	1.95	0.67
1:F:406:PHE:HE2	1:F:409:VAL:CG2	2.05	0.67
1:H:143:GLU:HG3	2:H:2145:HOH:O	1.95	0.67
1:C:239:THR:HG21	2:C:2236:HOH:O	1.95	0.67
1:C:125:LYS:HD2	2:C:2138:HOH:O	1.95	0.67
1:C:373:ARG:HD2	2:C:2005:HOH:O	1.94	0.67
1:E:63:ILE:HD11	1:E:82:ILE:HG12	1.76	0.67
1:G:130:TRP:NE1	1:G:134:ILE:HD11	2.10	0.66
1:B:400:LEU:HB3	1:B:402:ILE:HD11	1.77	0.66
1:H:69:ILE:HG12	1:H:74:LYS:HG2	1.78	0.66
1:C:280:ASN:HD22	1:C:281:THR:N	1.94	0.66
1:F:11:ARG:HG2	2:F:2013:HOH:O	1.96	0.66
1:D:71:GLY:N	2:D:2086:HOH:O	2.19	0.66
1:E:274:LEU:CD1	1:E:310:VAL:HG12	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:MET:HE1	1:A:130:TRP:CE3	2.30	0.66
1:F:386:LEU:CD1	2:F:2331:HOH:O	2.39	0.66
1:C:415:ILE:HD11	1:C:453:MET:HE2	1.76	0.66
1:F:417:ASN:ND2	1:F:419:GLN:H	1.94	0.66
1:B:239:THR:CG2	1:B:241:GLU:H	2.09	0.66
1:C:301:ARG:HB2	2:C:2264:HOH:O	1.95	0.66
1:D:239:THR:CG2	1:D:241:GLU:H	2.08	0.65
1:G:413:ARG:HD3	1:G:453:MET:CE	2.25	0.65
1:C:10:GLY:O	1:C:11:ARG:HB3	1.95	0.65
1:F:436:PRO:O	1:G:144:ARG:NH2	2.27	0.65
1:D:501:TYR:C	1:D:502:SER:CA	2.69	0.65
1:E:355:PHE:HD2	2:E:2259:HOH:O	1.79	0.65
1:F:239:THR:HG22	1:F:242:TYR:H	1.59	0.65
1:A:369:MET:HE3	1:A:371:VAL:HG23	1.77	0.65
1:C:417:ASN:HD22	1:C:419:GLN:H	1.44	0.65
1:G:24:THR:HG23	1:G:53:GLY:HA3	1.79	0.65
1:D:70:ASP:O	2:D:2084:HOH:O	2.14	0.65
1:E:103:MET:HE2	1:E:107:LEU:HB3	1.79	0.65
1:F:99:GLU:OE1	2:F:2123:HOH:O	2.15	0.65
1:A:209:THR:CG2	2:A:2178:HOH:O	2.41	0.65
1:E:355:PHE:CD2	2:E:2259:HOH:O	2.49	0.65
1:A:239:THR:HG22	1:A:241:GLU:N	2.07	0.65
1:E:402:ILE:HD12	1:E:480:ILE:HD13	1.79	0.65
1:C:259:THR:CG2	2:C:2210:HOH:O	2.45	0.64
1:D:79:PHE:HD2	1:D:82:ILE:HD11	1.62	0.64
1:H:26:ARG:NH2	1:H:323:GLU:OE1	2.31	0.64
1:F:301:ARG:HB2	2:F:2283:HOH:O	1.97	0.64
1:G:8:SER:O	1:G:373:ARG:NH2	2.29	0.64
1:G:8:SER:HB3	1:G:403:PRO:CB	2.27	0.64
1:A:209:THR:HB	2:A:2216:HOH:O	1.96	0.64
1:C:455:GLU:OE2	1:C:457:ARG:NH2	2.28	0.64
1:C:417:ASN:ND2	1:C:419:GLN:H	1.94	0.64
1:D:93:ASN:CB	2:D:2105:HOH:O	2.40	0.64
1:A:392:GLU:O	1:A:392:GLU:HG2	1.98	0.64
1:D:406:PHE:O	1:D:407:SER:CB	2.45	0.64
1:C:206:GLU:HB2	2:C:2213:HOH:O	1.97	0.64
1:E:145:TYR:HE2	1:H:438:ARG:HH21	1.46	0.64
1:F:392:GLU:H	1:F:394:LEU:HD12	1.63	0.64
1:B:168:LYS:HE3	2:B:2139:HOH:O	1.98	0.63
1:H:474:GLU:OE1	2:H:2370:HOH:O	2.15	0.63
1:E:413:ARG:HD3	1:E:453:MET:CE	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:HD22	1:A:281:THR:N	1.95	0.63
1:F:341:LEU:CD1	2:F:2179:HOH:O	2.47	0.63
1:G:103:MET:CE	1:G:107:LEU:CB	2.70	0.63
1:G:481:GLU:HG2	2:G:2315:HOH:O	1.97	0.63
1:H:69:ILE:HD11	1:H:74:LYS:CE	2.28	0.63
1:D:204:SER:CB	2:D:2184:HOH:O	2.46	0.63
1:A:63:ILE:HD11	1:A:82:ILE:HG12	1.80	0.63
1:A:404:VAL:HG11	1:A:459:ALA:CB	2.29	0.63
1:G:339:VAL:CG1	1:G:343:SER:HA	2.29	0.63
1:G:407:SER:O	1:G:458:ARG:HG3	1.99	0.63
1:C:205:ASP:OD2	1:C:227:ARG:NH1	2.27	0.63
1:E:109:SER:HA	1:E:125:LYS:HG3	1.81	0.63
1:B:99:GLU:OE1	2:B:2087:HOH:O	2.16	0.62
1:A:408:ALA:HB2	1:A:458:ARG:HE	1.64	0.62
1:F:301:ARG:CB	2:F:2283:HOH:O	2.46	0.62
1:C:93:ASN:HB3	2:C:2114:HOH:O	1.98	0.62
1:D:165:ASN:H	1:D:165:ASN:ND2	1.96	0.62
1:E:13:LYS:HE3	2:E:2003:HOH:O	1.97	0.62
1:G:82:ILE:HD12	1:G:83:ASP:N	2.14	0.62
1:G:83:ASP:OD1	1:G:140:HIS:HE1	1.82	0.62
1:G:274:LEU:HD13	1:G:310:VAL:CG1	2.21	0.62
1:H:4:VAL:CG1	1:H:369:MET:HE1	2.20	0.62
1:D:417:ASN:ND2	1:D:419:GLN:H	1.98	0.62
1:F:422:ASN:C	1:F:422:ASN:HD22	2.06	0.62
1:H:406:PHE:CD1	1:H:482:GLN:NE2	2.68	0.62
1:F:103:MET:CG	1:F:103:MET:CA	2.71	0.62
1:F:417:ASN:HD22	1:F:417:ASN:C	2.07	0.62
1:E:70:ASP:HB3	2:E:2073:HOH:O	2.00	0.62
1:A:79:PHE:HD2	1:A:82:ILE:HD11	1.65	0.62
1:B:426:VAL:HG21	1:B:447:VAL:HG11	1.81	0.62
1:F:415:ILE:HD11	1:F:420:TYR:CD1	2.35	0.62
1:C:415:ILE:HD11	1:C:453:MET:CE	2.30	0.61
1:F:499:THR:HG22	2:H:2223:HOH:O	2.00	0.61
1:G:286:ILE:HG12	1:G:325:MET:HE3	1.82	0.61
1:F:130:TRP:CE2	1:F:134:ILE:HD11	2.35	0.61
1:F:393:GLY:C	1:F:394:LEU:HG	2.25	0.61
1:F:247:LEU:HG	1:H:499:THR:HG21	1.80	0.61
1:H:364:TYR:CD2	1:H:369:MET:HE2	2.35	0.61
1:H:482:GLN:CD	2:H:2377:HOH:O	2.44	0.61
1:A:205:ASP:HB3	1:A:263:LEU:HD11	1.82	0.61
1:B:280:ASN:HD22	1:B:281:THR:N	1.92	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:LEU:HD13	2:G:2284:HOH:O	1.99	0.61
1:H:445:ARG:NH1	2:H:2338:HOH:O	2.11	0.61
1:A:144:ARG:NH2	1:D:436:PRO:O	2.33	0.61
1:A:213:HIS:ND1	2:A:2182:HOH:O	2.31	0.61
1:B:227:ARG:NE	1:B:260:VAL:HG21	2.15	0.61
1:F:417:ASN:ND2	1:F:420:TYR:H	1.98	0.61
1:H:404:VAL:CG2	1:H:406:PHE:CE2	2.83	0.61
1:A:6:VAL:HG21	1:A:402:ILE:HD13	1.82	0.61
1:C:411:ILE:HD13	1:C:466:LEU:HD21	1.83	0.61
1:C:103:MET:HE1	1:C:107:LEU:HD13	1.82	0.61
1:D:239:THR:HG22	1:D:242:TYR:N	2.11	0.61
1:E:438:ARG:CD	2:E:2304:HOH:O	2.46	0.61
1:F:489:THR:HG21	1:H:434:ARG:HE	1.66	0.61
1:G:417:ASN:ND2	1:G:420:TYR:H	1.98	0.61
1:H:290:HIS:HD2	1:H:334:GLY:O	1.84	0.61
1:D:457:ARG:HD2	1:D:464:ILE:HD11	1.82	0.60
1:E:213:HIS:NE2	1:E:217:GLU:OE2	2.33	0.60
1:H:417:ASN:ND2	1:H:419:GLN:H	1.98	0.60
1:G:8:SER:HB3	1:G:403:PRO:HB2	1.82	0.60
1:A:95:ARG:NH1	2:A:2103:HOH:O	2.35	0.60
1:C:238:LYS:HD3	1:C:243:TYR:HE1	1.61	0.60
1:E:280:ASN:HD22	1:E:281:THR:N	1.97	0.60
1:F:398:VAL:HG12	1:F:400:LEU:HD13	1.83	0.60
1:G:213:HIS:HE1	2:G:2175:HOH:O	1.83	0.60
1:A:251:GLU:HG2	1:A:301:ARG:HH12	1.67	0.60
1:D:501:TYR:C	1:D:502:SER:HA	2.27	0.60
1:C:406:PHE:O	1:C:407:SER:HB3	2.00	0.60
1:D:165:ASN:H	1:D:165:ASN:HD22	1.50	0.60
1:D:248:GLU:HG3	1:D:249:PRO:HD2	1.83	0.60
1:F:325:MET:HE2	2:F:2277:HOH:O	2.01	0.60
1:H:392:GLU:HG3	2:H:2304:HOH:O	2.01	0.60
1:D:4:VAL:HG11	1:D:369:MET:HE1	1.83	0.60
1:E:239:THR:HG22	1:E:241:GLU:H	1.66	0.60
1:E:417:ASN:ND2	1:E:419:GLN:H	2.00	0.60
1:F:255:GLU:HG2	2:F:2258:HOH:O	2.01	0.60
1:E:239:THR:HG23	1:E:241:GLU:H	1.65	0.60
1:B:103:MET:HE1	1:B:130:TRP:CE3	2.37	0.59
1:C:130:TRP:CE2	1:C:134:ILE:HD11	2.36	0.59
1:F:280:ASN:HD22	1:F:281:THR:N	1.97	0.59
1:G:130:TRP:CE2	1:G:134:ILE:HD11	2.37	0.59
1:B:439:GLN:NE2	2:B:2265:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:LEU:HD12	2:F:2179:HOH:O	2.03	0.59
1:A:391:GLY:HA3	1:A:394:LEU:HD11	1.83	0.59
1:D:63:ILE:HD11	1:D:82:ILE:HG12	1.83	0.59
1:E:145:TYR:HE2	1:H:438:ARG:NH2	2.00	0.59
1:D:6:VAL:HG21	1:D:402:ILE:HD13	1.84	0.59
1:E:436:PRO:O	1:H:144:ARG:NH2	2.35	0.59
1:H:438:ARG:CZ	2:H:2330:HOH:O	2.43	0.59
1:A:399:GLN:NE2	2:A:2289:HOH:O	2.36	0.59
1:F:426:VAL:HG21	1:F:447:VAL:HG11	1.84	0.59
1:C:464:ILE:CD1	1:C:466:LEU:HG	2.33	0.59
1:A:426:VAL:CG2	1:A:447:VAL:HG11	2.33	0.59
1:B:438:ARG:NH2	2:B:2263:HOH:O	2.36	0.59
1:D:391:GLY:O	1:D:392:GLU:HB2	2.02	0.59
1:F:402:ILE:HB	1:F:464:ILE:CD1	2.32	0.59
1:F:486:GLU:O	1:F:489:THR:HB	2.02	0.59
1:C:350:HIS:ND1	2:C:2292:HOH:O	2.32	0.58
1:D:10:GLY:O	1:D:11:ARG:HB3	2.02	0.58
1:E:499:THR:CG2	2:G:2199:HOH:O	2.50	0.58
1:A:10:GLY:O	1:A:11:ARG:CB	2.40	0.58
1:C:502:SER:HA	2:C:2371:HOH:O	2.03	0.58
1:G:274:LEU:CD1	1:G:310:VAL:HG12	2.22	0.58
1:A:417:ASN:ND2	1:A:419:GLN:H	2.01	0.58
1:D:238:LYS:CE	1:D:243:TYR:CE1	2.80	0.58
1:C:301:ARG:CB	2:C:2264:HOH:O	2.50	0.58
1:D:4:VAL:HG11	1:D:369:MET:CE	2.33	0.58
1:D:103:MET:CE	1:D:107:LEU:CB	2.78	0.58
1:A:404:VAL:N	1:A:462:GLY:O	2.36	0.58
1:C:240:PHE:CE2	1:C:241:GLU:HG3	2.38	0.58
1:C:165:ASN:ND2	1:C:165:ASN:H	2.01	0.58
1:E:214:PHE:CE1	1:E:218:ARG:HD3	2.39	0.58
1:E:499:THR:HG21	1:G:247:LEU:HG	1.86	0.58
1:A:449:GLN:CD	2:A:2324:HOH:O	2.47	0.57
1:F:109:SER:HA	1:F:125:LYS:HG2	1.84	0.57
1:D:69:ILE:HD11	1:D:74:LYS:HZ2	1.69	0.57
1:E:417:ASN:ND2	1:E:420:TYR:H	2.02	0.57
1:G:107:LEU:CD2	2:G:2112:HOH:O	2.51	0.57
1:A:489:THR:CG2	1:C:434:ARG:HH21	2.17	0.57
1:B:103:MET:HE1	1:B:130:TRP:HE3	1.70	0.57
1:H:69:ILE:CD1	1:H:74:LYS:HG3	2.34	0.57
1:H:63:ILE:HD11	1:H:82:ILE:HG12	1.85	0.57
1:B:286:ILE:HG12	1:B:325:MET:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2341:HOH:O	1:G:239:THR:HG21	2.03	0.57
1:D:274:LEU:CD1	1:D:310:VAL:HG12	2.26	0.57
1:C:121:VAL:HG22	1:C:166:PHE:O	2.05	0.57
1:G:481:GLU:CG	2:G:2315:HOH:O	2.50	0.57
1:B:107:LEU:HD21	1:B:129:LYS:HB3	1.86	0.57
1:E:474:GLU:OE1	2:E:2325:HOH:O	2.17	0.57
1:E:487:THR:HG23	2:G:2284:HOH:O	2.03	0.57
1:C:70:ASP:CG	1:C:70:ASP:O	2.48	0.57
1:E:426:VAL:HG21	1:E:447:VAL:CG1	2.30	0.57
1:F:398:VAL:CG1	1:F:400:LEU:CD1	2.83	0.57
1:C:267:SER:HB2	1:C:268:PRO:HD2	1.85	0.56
1:D:16:LYS:HE3	2:D:2023:HOH:O	2.05	0.56
1:A:368:GLU:OE1	1:A:396:LYS:HE2	2.05	0.56
1:A:411:ILE:HD11	1:A:464:ILE:HD11	1.88	0.56
1:E:301:ARG:HH21	1:E:305:GLU:CD	2.13	0.56
1:F:398:VAL:HG12	1:F:400:LEU:CD1	2.35	0.56
1:H:432:ARG:NE	2:H:2324:HOH:O	2.03	0.56
1:C:83:ASP:OD1	1:C:140:HIS:CE1	2.57	0.56
1:D:103:MET:HE1	1:D:107:LEU:CD1	2.36	0.56
1:D:392:GLU:CD	1:D:393:GLY:H	2.13	0.56
1:E:409:VAL:HG11	1:E:464:ILE:HD13	1.87	0.56
1:A:239:THR:HG22	1:A:242:TYR:H	1.68	0.56
1:B:434:ARG:HE	1:D:489:THR:HG23	1.70	0.56
1:D:158:TRP:CD1	1:D:159:ASN:H	2.23	0.56
1:F:386:LEU:CD2	2:F:2385:HOH:O	2.54	0.56
1:H:364:TYR:HE2	1:H:369:MET:HE2	1.61	0.56
1:B:144:ARG:HB2	2:B:2123:HOH:O	2.04	0.56
1:C:401:VAL:HG22	1:C:465:HIS:CD2	2.40	0.56
1:E:227:ARG:HD2	1:E:260:VAL:HG21	1.88	0.56
1:F:493:LEU:C	1:F:493:LEU:HD23	2.31	0.56
1:H:129:LYS:NZ	2:H:2139:HOH:O	2.39	0.56
1:H:404:VAL:HG22	1:H:406:PHE:CE2	2.41	0.56
1:H:422:ASN:HD21	1:H:424:TRP:HB3	1.70	0.56
1:A:200:ILE:HD11	1:A:208:ILE:HG13	1.88	0.56
1:C:103:MET:HE3	1:C:107:LEU:CB	2.35	0.56
1:C:252:ASP:HB3	2:C:2243:HOH:O	2.04	0.56
1:D:69:ILE:CD1	1:D:74:LYS:NZ	2.62	0.56
1:E:10:GLY:O	1:E:11:ARG:CB	2.54	0.56
1:H:130:TRP:NE1	1:H:134:ILE:HD11	2.21	0.56
1:H:417:ASN:ND2	1:H:420:TYR:H	2.03	0.56
1:A:285:PRO:HG2	1:A:325:MET:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ASP:OD1	1:B:227:ARG:NH1	2.39	0.56
1:H:481:GLU:HG2	2:H:2374:HOH:O	2.05	0.56
1:A:103:MET:HE1	1:A:130:TRP:HE3	1.69	0.56
1:D:415:ILE:HD11	1:D:453:MET:CE	2.36	0.56
1:G:422:ASN:HD22	1:G:422:ASN:C	2.13	0.56
1:A:227:ARG:NH2	1:A:256:GLN:OE1	2.37	0.55
1:E:350:HIS:CD2	2:E:2257:HOH:O	2.45	0.55
1:F:79:PHE:CD2	1:F:82:ILE:HD11	2.35	0.55
1:B:249:PRO:CA	1:B:388:MET:HE1	2.32	0.55
1:C:82:ILE:HD12	1:C:83:ASP:N	2.22	0.55
1:C:103:MET:HE1	1:C:124:PRO:HB3	1.89	0.55
1:E:407:SER:O	1:E:458:ARG:HD3	2.06	0.55
1:F:438:ARG:O	1:F:442:GLU:HG3	2.06	0.55
1:H:266:GLN:CB	2:H:2234:HOH:O	2.51	0.55
1:E:350:HIS:HE1	1:E:448:ALA:O	1.89	0.55
1:A:290:HIS:HD2	1:A:334:GLY:O	1.89	0.55
1:B:105:LYS:HG3	2:B:2053:HOH:O	2.06	0.55
1:C:413:ARG:NH2	1:C:468:ILE:HD12	2.21	0.55
1:E:501:TYR:C	1:E:502:SER:CA	2.74	0.55
1:H:426:VAL:HG21	1:H:447:VAL:HG11	1.89	0.55
1:C:206:GLU:HG3	2:C:2212:HOH:O	2.05	0.55
1:F:105:LYS:HG3	2:F:2079:HOH:O	2.07	0.55
1:G:387:VAL:HG11	1:G:394:LEU:HD13	1.89	0.55
1:B:392:GLU:CG	1:B:393:GLY:N	2.52	0.55
1:C:413:ARG:CZ	1:C:468:ILE:HD12	2.36	0.55
1:E:252:ASP:CG	2:E:2210:HOH:O	2.49	0.55
1:G:63:ILE:HD11	1:G:82:ILE:HG12	1.89	0.55
1:G:103:MET:HE3	1:G:104:PRO:HD2	1.89	0.55
1:H:233:LYS:HE3	1:H:248:GLU:OE2	2.07	0.55
1:A:493:LEU:C	1:A:493:LEU:HD23	2.33	0.54
1:B:499:THR:HG23	2:D:2209:HOH:O	2.06	0.54
1:G:19:LYS:HE3	1:G:46:ILE:O	2.07	0.54
1:H:264:ILE:CD1	1:H:274:LEU:HG	2.38	0.54
1:D:364:TYR:CD2	1:D:369:MET:CE	2.87	0.54
1:E:404:VAL:H	1:E:462:GLY:C	2.15	0.54
1:C:466:LEU:HD11	1:C:480:ILE:HD11	1.89	0.54
1:D:374:ARG:NH2	1:D:479:GLU:OE1	2.36	0.54
1:F:266:GLN:HG3	2:F:2265:HOH:O	2.07	0.54
1:H:422:ASN:C	1:H:422:ASN:HD22	2.15	0.54
1:B:417:ASN:ND2	1:B:419:GLN:H	2.05	0.54
1:B:418:GLU:O	1:B:425:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:LYS:HD3	1:E:243:TYR:CE1	2.43	0.54
1:F:269:PHE:HB3	1:F:272:LEU:HG	1.90	0.54
1:H:391:GLY:HA3	1:H:472:LYS:NZ	2.22	0.54
1:C:399:GLN:NE2	1:C:467:SER:HB3	2.19	0.54
1:D:417:ASN:HD22	1:D:419:GLN:H	1.56	0.54
1:G:15:LYS:HD2	2:G:2223:HOH:O	2.08	0.54
1:A:103:MET:HE2	1:A:107:LEU:HB3	1.89	0.54
1:A:409:VAL:HG11	1:A:464:ILE:HD12	1.90	0.54
1:B:130:TRP:NE1	1:B:134:ILE:CD1	2.71	0.54
1:A:489:THR:CG2	1:C:434:ARG:NE	2.67	0.54
1:F:312:SER:OG	2:F:2292:HOH:O	2.18	0.54
1:F:214:PHE:CE1	1:F:218:ARG:HD3	2.43	0.54
1:A:24:THR:HG23	1:A:53:GLY:HA3	1.90	0.53
1:E:366:ASP:OD1	1:E:366:ASP:C	2.50	0.53
1:A:103:MET:HE3	1:A:103:MET:HA	1.90	0.53
1:D:213:HIS:HB3	2:D:2192:HOH:O	2.07	0.53
1:G:397:GLU:HG3	1:G:469:VAL:HG13	1.90	0.53
1:H:69:ILE:HG12	1:H:74:LYS:CG	2.38	0.53
1:A:389:GLU:CD	1:A:389:GLU:H	2.15	0.53
1:B:387:VAL:HG11	1:B:394:LEU:HD13	1.90	0.53
1:E:350:HIS:CE1	1:E:448:ALA:O	2.61	0.53
1:G:406:PHE:HE2	1:G:409:VAL:HG22	1.74	0.53
1:A:489:THR:HG23	1:C:434:ARG:HH21	1.73	0.53
1:B:79:PHE:HD2	1:B:82:ILE:HD11	1.72	0.53
1:G:93:ASN:HB3	2:G:2089:HOH:O	2.07	0.53
1:A:272:LEU:HD13	2:A:2226:HOH:O	2.06	0.53
1:C:68:GLU:HG3	1:C:73:MET:SD	2.48	0.53
1:E:209:THR:HB	2:E:2218:HOH:O	2.09	0.53
1:F:70:ASP:HB2	2:F:2097:HOH:O	2.09	0.53
1:B:489:THR:CG2	1:D:434:ARG:HH21	2.22	0.53
1:E:417:ASN:C	1:E:417:ASN:HD22	2.16	0.53
1:H:249:PRO:HB3	1:H:388:MET:HE1	1.90	0.53
1:D:95:ARG:CZ	2:D:2108:HOH:O	2.57	0.53
1:E:83:ASP:OD1	1:E:140:HIS:HE1	1.92	0.53
1:E:252:ASP:HB3	2:E:2210:HOH:O	2.08	0.53
1:A:26:ARG:NH1	1:A:60:ASP:CG	2.65	0.53
1:D:70:ASP:HA	2:D:2084:HOH:O	2.07	0.53
1:B:481:GLU:HG3	2:B:2286:HOH:O	2.09	0.53
1:E:391:GLY:CA	2:E:2279:HOH:O	2.57	0.53
1:A:481:GLU:HG3	2:A:2292:HOH:O	2.09	0.53
1:A:499:THR:CG2	2:C:2240:HOH:O	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:VAL:HG11	1:D:394:LEU:HD13	1.90	0.53
1:G:417:ASN:HD22	1:G:420:TYR:H	1.56	0.53
1:H:11:ARG:HG2	1:H:12:GLU:N	2.23	0.53
1:B:72:GLU:OE1	1:G:270:PRO:HG3	2.09	0.52
1:E:391:GLY:C	2:E:2279:HOH:O	2.51	0.52
1:G:172:LYS:HA	1:G:207:TRP:CH2	2.43	0.52
1:H:121:VAL:O	1:H:121:VAL:HG13	2.09	0.52
1:G:125:LYS:HE2	2:G:2097:HOH:O	2.10	0.52
1:H:285:PRO:HG2	1:H:325:MET:HG3	1.90	0.52
1:B:144:ARG:NH2	1:C:436:PRO:O	2.41	0.52
1:B:202:GLY:HA2	1:B:227:ARG:HH12	1.74	0.52
1:B:481:GLU:CG	2:B:2286:HOH:O	2.57	0.52
1:A:426:VAL:HG21	1:A:447:VAL:CG1	2.37	0.52
1:B:40:LYS:HE3	2:B:2037:HOH:O	2.09	0.52
1:G:158:TRP:CD1	1:G:159:ASN:H	2.28	0.52
1:C:8:SER:OG	1:C:403:PRO:HB2	2.10	0.52
2:E:2208:HOH:O	1:G:499:THR:HB	2.07	0.52
1:F:11:ARG:CG	2:F:2013:HOH:O	2.55	0.52
1:G:269:PHE:HB3	1:G:272:LEU:HG	1.90	0.52
1:H:239:THR:HG21	2:H:2217:HOH:O	2.08	0.52
1:B:10:GLY:O	1:B:11:ARG:HB2	2.09	0.52
1:C:233:LYS:CD	1:C:246:GLU:HG2	2.38	0.52
1:E:264:ILE:CD1	1:E:274:LEU:HG	2.39	0.52
2:E:2206:HOH:O	1:G:499:THR:CG2	2.57	0.52
1:D:70:ASP:HB2	2:D:2085:HOH:O	2.10	0.52
1:H:432:ARG:NH2	2:H:2324:HOH:O	2.38	0.52
1:A:390:LYS:HD3	1:C:501:TYR:O	2.10	0.52
1:C:465:HIS:HB3	2:C:2311:HOH:O	2.09	0.52
1:F:103:MET:HE1	1:F:108:ALA:HA	1.90	0.52
1:H:121:VAL:O	1:H:121:VAL:HG12	2.09	0.52
1:A:239:THR:HG21	2:A:2201:HOH:O	2.09	0.52
1:E:415:ILE:HD13	1:E:451:HIS:HB3	1.91	0.52
1:C:56:LEU:CD1	1:C:82:ILE:HG21	2.39	0.51
1:E:339:VAL:CG1	1:E:343:SER:HA	2.40	0.51
1:F:325:MET:CE	2:F:2277:HOH:O	2.56	0.51
1:A:127:TYR:CE1	1:A:177:LYS:HE3	2.44	0.51
1:D:72:GLU:HG2	1:D:74:LYS:HG2	1.92	0.51
1:D:422:ASN:ND2	2:D:2282:HOH:O	2.43	0.51
1:D:486:GLU:O	1:D:489:THR:HB	2.10	0.51
1:B:489:THR:CG2	1:D:434:ARG:NE	2.66	0.51
1:C:290:HIS:HD2	1:C:334:GLY:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:LEU:CD2	1:D:468:ILE:HD12	2.39	0.51
1:A:214:PHE:CE1	1:A:218:ARG:HD3	2.45	0.51
1:B:331:LEU:HD13	1:B:332:PHE:CE1	2.45	0.51
2:F:2248:HOH:O	1:H:499:THR:CG2	2.52	0.51
1:B:350:HIS:CD2	2:B:2233:HOH:O	2.39	0.51
1:B:451:HIS:HD2	2:D:2157:HOH:O	1.94	0.51
1:F:290:HIS:HD2	1:F:334:GLY:O	1.93	0.51
1:F:415:ILE:CD1	1:F:451:HIS:CB	2.72	0.51
1:H:350:HIS:CD2	2:H:2282:HOH:O	2.45	0.51
1:A:499:THR:HG21	1:C:247:LEU:HG	1.91	0.51
1:C:251:GLU:HB2	2:C:2242:HOH:O	2.09	0.51
1:A:240:PHE:CD2	1:D:67:VAL:HG11	2.46	0.51
1:D:71:GLY:CA	2:D:2086:HOH:O	2.56	0.51
1:E:69:ILE:HG12	1:E:74:LYS:HG3	1.92	0.51
1:E:457:ARG:NH1	1:E:465:HIS:O	2.42	0.51
1:G:8:SER:HB3	1:G:403:PRO:CG	2.41	0.51
1:G:82:ILE:HD12	1:G:83:ASP:H	1.73	0.51
1:E:280:ASN:ND2	1:E:281:THR:H	2.01	0.51
1:F:44:GLU:HG3	2:F:2052:HOH:O	2.10	0.51
1:G:247:LEU:HD21	2:G:2198:HOH:O	2.11	0.51
1:H:481:GLU:CG	2:H:2374:HOH:O	2.59	0.51
1:A:265:ARG:HD2	2:A:2217:HOH:O	2.12	0.51
1:E:374:ARG:NH2	1:E:479:GLU:OE1	2.36	0.51
1:H:69:ILE:HD11	1:H:74:LYS:HG3	1.93	0.50
1:B:240:PHE:CD1	1:C:69:ILE:HD11	2.46	0.50
2:B:2187:HOH:O	1:D:499:THR:HG23	2.10	0.50
1:C:424:TRP:CH2	1:C:428:LYS:HE2	2.46	0.50
1:D:70:ASP:N	2:D:2085:HOH:O	2.43	0.50
1:F:16:LYS:HE2	2:F:2318:HOH:O	2.11	0.50
1:G:426:VAL:HG21	1:G:447:VAL:CG1	2.41	0.50
1:A:173:GLN:HG2	2:A:2168:HOH:O	2.11	0.50
1:A:350:HIS:HE1	1:A:448:ALA:O	1.94	0.50
1:A:404:VAL:CG1	1:A:459:ALA:HB1	2.42	0.50
1:C:200:ILE:HD11	1:C:208:ILE:HD12	1.93	0.50
1:D:82:ILE:HD12	1:D:83:ASP:N	2.26	0.50
1:A:14:PHE:HE2	2:A:2020:HOH:O	1.94	0.50
1:A:266:GLN:NE2	2:A:2218:HOH:O	2.43	0.50
1:A:499:THR:HG22	2:C:2240:HOH:O	2.10	0.50
1:B:278:GLU:HG2	1:B:316:TRP:CE3	2.46	0.50
1:C:103:MET:CE	1:C:107:LEU:HD13	2.41	0.50
1:E:413:ARG:HD3	1:E:453:MET:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:ASP:O	1:G:71:GLY:O	2.29	0.50
1:C:369:MET:HE3	1:C:383:LEU:HD13	1.93	0.50
1:E:14:PHE:HE2	2:E:2259:HOH:O	1.94	0.50
1:E:404:VAL:N	1:E:462:GLY:O	2.43	0.50
1:F:158:TRP:CD1	1:F:159:ASN:H	2.30	0.50
1:H:103:MET:CG	1:H:103:MET:CA	2.80	0.50
1:C:63:ILE:HD11	1:C:82:ILE:HG12	1.94	0.50
1:C:417:ASN:HD22	1:C:417:ASN:C	2.20	0.50
1:D:373:ARG:HG2	2:D:2264:HOH:O	2.12	0.50
1:H:26:ARG:NH1	2:H:2034:HOH:O	2.37	0.50
1:A:69:ILE:HD11	1:A:74:LYS:HZ3	1.77	0.50
2:B:2187:HOH:O	1:D:499:THR:CG2	2.59	0.50
1:C:218:ARG:HD2	2:C:2217:HOH:O	2.11	0.50
1:C:413:ARG:CZ	1:C:468:ILE:CD1	2.89	0.50
1:E:145:TYR:CE2	1:H:438:ARG:NH2	2.79	0.50
1:F:499:THR:HB	2:H:2228:HOH:O	2.11	0.50
1:H:239:THR:CG2	2:H:2217:HOH:O	2.59	0.50
1:A:305:GLU:HB3	2:A:2238:HOH:O	2.11	0.50
1:F:393:GLY:O	1:F:394:LEU:HG	2.12	0.50
1:H:103:MET:HE3	1:H:103:MET:C	2.35	0.50
1:E:402:ILE:HD12	1:E:480:ILE:CD1	2.40	0.50
1:G:205:ASP:HB3	1:G:263:LEU:HD11	1.94	0.50
1:H:364:TYR:CD2	1:H:369:MET:CE	2.95	0.50
1:E:499:THR:HG23	2:G:2199:HOH:O	2.12	0.49
1:A:436:PRO:O	1:D:144:ARG:NH2	2.45	0.49
1:A:499:THR:HB	2:C:2241:HOH:O	2.13	0.49
1:E:392:GLU:HG2	1:E:393:GLY:H	1.76	0.49
1:E:422:ASN:ND2	1:E:425:ARG:H	2.11	0.49
1:E:426:VAL:CG2	1:E:447:VAL:HG11	2.31	0.49
1:G:404:VAL:HG12	1:G:406:PHE:H	1.77	0.49
1:B:417:ASN:ND2	1:B:420:TYR:H	2.10	0.49
1:D:209:THR:CG2	2:D:2185:HOH:O	2.60	0.49
1:F:374:ARG:HD3	1:F:378:SER:OG	2.12	0.49
1:G:239:THR:HG22	1:G:241:GLU:N	2.09	0.49
1:C:82:ILE:HD12	1:C:83:ASP:H	1.77	0.49
1:C:93:ASN:CB	2:C:2114:HOH:O	2.57	0.49
1:E:200:ILE:HD11	1:E:208:ILE:HG13	1.95	0.49
1:E:341:LEU:O	1:E:342:HIS:HB2	2.13	0.49
1:G:130:TRP:O	1:G:134:ILE:HD12	2.12	0.49
1:A:402:ILE:HB	1:A:464:ILE:CG2	2.43	0.49
1:B:158:TRP:CD1	1:B:159:ASN:H	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ARG:NH1	1:B:465:HIS:O	2.43	0.49
1:A:269:PHE:HB3	1:A:272:LEU:HG	1.95	0.49
1:H:79:PHE:HD2	1:H:82:ILE:HD11	1.78	0.49
1:A:158:TRP:CD1	1:A:159:ASN:H	2.31	0.49
1:C:246:GLU:HG3	1:C:247:LEU:N	2.28	0.49
1:B:83:ASP:OD1	1:B:140:HIS:HE1	1.95	0.49
1:C:442:GLU:HG2	2:C:2336:HOH:O	2.11	0.49
1:F:489:THR:HG22	1:H:434:ARG:HE	1.71	0.49
1:G:114:VAL:O	1:G:115:PHE:HB2	2.13	0.49
1:A:364:TYR:HD2	1:A:369:MET:HE2	1.77	0.49
1:C:485:ASP:OD1	1:C:487:THR:CG2	2.55	0.49
1:E:114:VAL:O	1:E:115:PHE:HB2	2.12	0.49
1:E:264:ILE:HD11	1:E:274:LEU:HG	1.95	0.49
1:C:24:THR:HG23	1:C:53:GLY:HA3	1.94	0.49
1:D:103:MET:HE1	1:D:107:LEU:HD13	1.94	0.49
1:D:125:LYS:HD3	2:D:2129:HOH:O	2.12	0.49
1:F:434:ARG:HE	1:H:489:THR:HG21	1.77	0.49
1:A:401:VAL:HG22	1:A:465:HIS:HD2	1.78	0.48
1:A:411:ILE:HD13	1:A:466:LEU:HD21	1.94	0.48
1:B:417:ASN:HD22	1:B:419:GLN:H	1.61	0.48
1:C:213:HIS:HB3	2:C:2216:HOH:O	2.13	0.48
1:C:413:ARG:NH2	1:C:474:GLU:OE2	2.47	0.48
1:A:126:ASP:N	2:A:2122:HOH:O	2.45	0.48
1:G:22:VAL:HG13	1:G:48:PHE:CZ	2.49	0.48
1:A:83:ASP:OD1	1:A:140:HIS:CE1	2.60	0.48
1:C:391:GLY:HA3	1:C:394:LEU:HD11	1.94	0.48
1:C:413:ARG:NH2	1:C:468:ILE:CD1	2.76	0.48
1:E:402:ILE:CD1	1:E:480:ILE:HD13	2.44	0.48
1:D:422:ASN:C	1:D:422:ASN:HD22	2.21	0.48
1:C:406:PHE:HB3	1:C:482:GLN:HG3	1.95	0.48
1:D:438:ARG:NE	2:D:2295:HOH:O	2.43	0.48
1:C:422:ASN:C	1:C:422:ASN:HD22	2.22	0.48
1:D:109:SER:HA	1:D:125:LYS:HG2	1.95	0.48
1:D:239:THR:HG22	1:D:241:GLU:N	2.26	0.48
1:E:422:ASN:HD22	1:E:422:ASN:C	2.22	0.48
1:F:422:ASN:HD21	1:F:424:TRP:HB3	1.77	0.48
1:A:397:GLU:HG2	2:A:2289:HOH:O	2.14	0.48
1:C:130:TRP:NE1	1:C:134:ILE:HD11	2.29	0.48
1:D:20:PHE:HB3	1:D:312:SER:HB2	1.96	0.48
1:H:415:ILE:HG21	1:H:415:ILE:HD12	1.39	0.48
1:A:69:ILE:HD11	1:A:74:LYS:NZ	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:VAL:HG22	1:A:465:HIS:CD2	2.48	0.48
1:E:489:THR:HG21	1:G:434:ARG:HE	1.78	0.48
1:F:402:ILE:HB	1:F:464:ILE:HD11	1.95	0.48
1:F:415:ILE:HD13	1:F:451:HIS:CB	2.28	0.48
1:H:391:GLY:HA3	1:H:472:LYS:HZ2	1.79	0.48
1:H:417:ASN:HD22	1:H:419:GLN:H	1.62	0.48
1:B:406:PHE:HD2	1:B:409:VAL:CG2	2.26	0.47
1:E:140:HIS:HD2	2:E:2135:HOH:O	1.96	0.47
1:E:143:GLU:HG3	2:E:2133:HOH:O	2.14	0.47
1:F:130:TRP:NE1	1:F:134:ILE:CD1	2.74	0.47
1:G:451:HIS:HD2	2:G:2136:HOH:O	1.97	0.47
1:H:373:ARG:NH1	1:H:379:ILE:HD11	2.29	0.47
1:E:422:ASN:HD21	1:E:424:TRP:HB3	1.79	0.47
1:H:458:ARG:HG2	2:H:2361:HOH:O	2.13	0.47
1:B:301:ARG:CB	2:B:2209:HOH:O	2.61	0.47
1:C:238:LYS:CD	1:C:243:TYR:CE1	2.94	0.47
1:C:405:SER:O	1:C:406:PHE:O	2.32	0.47
1:F:402:ILE:HB	1:F:464:ILE:HD13	1.95	0.47
1:G:341:LEU:O	1:G:342:HIS:HB2	2.14	0.47
1:G:387:VAL:HB	1:G:472:LYS:HG3	1.95	0.47
1:G:79:PHE:HD2	1:G:82:ILE:HD11	1.78	0.47
1:B:63:ILE:HD11	1:B:82:ILE:HG12	1.96	0.47
1:B:460:THR:O	1:B:461:ASP:C	2.57	0.47
1:A:489:THR:HG23	1:C:434:ARG:HE	1.74	0.47
1:B:82:ILE:HD12	1:B:83:ASP:N	2.28	0.47
1:B:233:LYS:HD3	1:B:246:GLU:HG2	1.97	0.47
1:C:233:LYS:CE	1:C:246:GLU:HG2	2.44	0.47
1:C:274:LEU:HD13	1:C:310:VAL:CG1	2.31	0.47
1:F:239:THR:CG2	2:F:2244:HOH:O	2.62	0.47
1:H:239:THR:CG2	1:H:241:GLU:H	2.22	0.47
1:H:373:ARG:CZ	1:H:379:ILE:HD11	2.44	0.47
1:A:201:CYS:HB2	2:A:2176:HOH:O	2.13	0.47
1:A:404:VAL:CG1	1:A:459:ALA:CB	2.92	0.47
1:A:446:GLN:HG2	1:C:452:VAL:HG21	1.96	0.47
1:B:103:MET:HE1	1:B:107:LEU:HD13	1.97	0.47
1:G:24:THR:HG23	1:G:53:GLY:CA	2.45	0.47
1:C:129:LYS:HE3	2:C:2078:HOH:O	2.15	0.47
1:D:394:LEU:HD12	2:D:2276:HOH:O	2.14	0.47
1:G:233:LYS:HD3	1:G:246:GLU:OE1	2.14	0.47
1:G:415:ILE:HG23	1:G:415:ILE:HD13	1.29	0.47
1:H:69:ILE:O	1:H:69:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:VAL:HG21	1:C:402:ILE:HD13	1.97	0.47
1:G:486:GLU:O	1:G:489:THR:HB	2.15	0.47
1:C:6:VAL:O	1:C:403:PRO:HD3	2.15	0.47
1:H:384:TRP:HA	1:H:474:GLU:O	2.14	0.47
1:A:404:VAL:HG11	1:A:459:ALA:HB1	1.96	0.46
1:C:415:ILE:CD1	1:C:453:MET:CE	2.88	0.46
1:D:140:HIS:HD2	2:D:2144:HOH:O	1.98	0.46
1:D:406:PHE:O	1:D:407:SER:HB3	2.14	0.46
1:E:164:VAL:HG13	2:E:2107:HOH:O	2.15	0.46
1:E:261:ARG:NH2	1:E:311:ASP:OD2	2.44	0.46
1:G:428:LYS:HD3	1:G:432:ARG:NH1	2.31	0.46
1:E:158:TRP:CD1	1:E:159:ASN:H	2.33	0.46
1:B:406:PHE:HB3	1:B:482:GLN:HG3	1.97	0.46
2:B:2305:HOH:O	1:D:239:THR:HG21	2.15	0.46
1:G:45:LYS:HD3	2:G:2041:HOH:O	2.14	0.46
1:A:457:ARG:HH11	1:A:466:LEU:HD23	1.81	0.46
1:B:493:LEU:HD23	1:B:493:LEU:C	2.40	0.46
1:F:434:ARG:HE	1:H:489:THR:CG2	2.29	0.46
1:A:364:TYR:CE2	1:A:369:MET:HE2	2.51	0.46
1:E:438:ARG:NE	2:E:2302:HOH:O	2.48	0.46
1:G:107:LEU:HD21	1:G:129:LYS:HB3	1.97	0.46
1:G:426:VAL:CG2	1:G:447:VAL:HG11	2.43	0.46
1:C:24:THR:OG1	1:C:35:TYR:OH	2.29	0.46
1:D:339:VAL:CG1	1:D:343:SER:HA	2.45	0.46
1:F:398:VAL:CG1	1:F:400:LEU:HD13	2.42	0.46
1:B:402:ILE:HA	1:B:403:PRO:HD2	1.80	0.46
1:B:325:MET:HE2	2:B:2203:HOH:O	2.16	0.46
1:C:103:MET:HE2	1:C:124:PRO:HA	1.97	0.46
1:D:337:GLY:O	1:D:346:LYS:HD2	2.15	0.46
1:D:417:ASN:HD22	1:D:417:ASN:C	2.24	0.46
1:D:426:VAL:HG21	1:D:447:VAL:CG1	2.44	0.46
1:E:69:ILE:CG1	1:E:74:LYS:HG3	2.46	0.46
1:E:342:HIS:HD2	2:E:2007:HOH:O	1.98	0.46
1:H:339:VAL:CG1	1:H:343:SER:HA	2.46	0.46
1:H:389:GLU:OE2	2:H:2301:HOH:O	2.20	0.46
1:A:238:LYS:HD3	1:A:243:TYR:CE1	2.51	0.46
1:D:394:LEU:HD23	2:D:2277:HOH:O	2.16	0.46
1:G:93:ASN:CB	2:G:2089:HOH:O	2.63	0.46
1:G:417:ASN:ND2	1:G:419:GLN:H	2.14	0.46
1:H:162:ASN:ND2	1:H:204:SER:OG	2.45	0.46
1:A:12:GLU:CG	2:A:2008:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:THR:HB	1:B:51:ILE:HD11	1.98	0.46
1:C:95:ARG:HD3	1:C:149:GLU:OE2	2.16	0.46
1:C:325:MET:O	1:C:326:ASP:CB	2.63	0.46
1:C:406:PHE:HD2	1:C:409:VAL:HG23	1.81	0.46
1:C:460:THR:O	1:C:461:ASP:HB2	2.16	0.46
1:G:493:LEU:HD23	1:G:493:LEU:C	2.41	0.46
1:H:239:THR:HG22	1:H:241:GLU:N	2.23	0.46
1:B:87:ASP:OD1	1:C:438:ARG:NH2	2.49	0.45
1:B:459:ALA:HA	1:B:464:ILE:HG22	1.98	0.45
1:C:143:GLU:HG3	2:C:2151:HOH:O	2.16	0.45
1:B:261:ARG:O	1:B:265:ARG:HG3	2.16	0.45
1:B:445:ARG:NH1	2:B:2269:HOH:O	2.03	0.45
1:D:227:ARG:NH2	1:D:256:GLN:NE2	2.62	0.45
1:D:350:HIS:HE1	1:D:448:ALA:O	2.00	0.45
1:D:404:VAL:O	1:D:462:GLY:CA	2.61	0.45
1:E:252:ASP:CB	2:E:2210:HOH:O	2.64	0.45
1:F:413:ARG:NH2	1:F:474:GLU:OE2	2.46	0.45
1:A:383:LEU:HD23	1:A:383:LEU:N	2.31	0.45
1:A:397:GLU:HB3	2:A:2289:HOH:O	2.16	0.45
1:D:325:MET:O	1:D:326:ASP:CB	2.64	0.45
1:G:83:ASP:OD1	1:G:140:HIS:CE1	2.68	0.45
1:A:417:ASN:HD22	1:A:417:ASN:C	2.24	0.45
1:B:406:PHE:CE1	1:B:482:GLN:HB2	2.52	0.45
1:C:369:MET:HE3	1:C:383:LEU:CD1	2.47	0.45
1:C:406:PHE:HB2	1:C:407:SER:H	1.51	0.45
1:F:481:GLU:CD	2:F:2390:HOH:O	2.60	0.45
1:A:148:GLU:CG	2:A:2146:HOH:O	2.57	0.45
1:D:151:ARG:HD2	2:D:2153:HOH:O	2.15	0.45
1:H:438:ARG:HD2	2:H:2331:HOH:O	2.16	0.45
1:A:114:VAL:O	1:A:115:PHE:HB2	2.17	0.45
1:B:350:HIS:CE1	1:B:448:ALA:O	2.69	0.45
1:C:407:SER:HA	1:C:459:ALA:HB3	1.99	0.45
1:C:426:VAL:HG21	1:C:447:VAL:CG1	2.43	0.45
1:D:350:HIS:CE1	1:D:448:ALA:O	2.69	0.45
1:D:406:PHE:O	1:D:407:SER:OG	2.34	0.45
1:F:10:GLY:O	1:F:11:ARG:CB	2.50	0.45
1:A:406:PHE:CG	1:A:482:GLN:HG3	2.52	0.45
1:A:417:ASN:HD22	1:A:420:TYR:H	1.61	0.45
1:B:95:ARG:HD3	1:B:149:GLU:OE2	2.17	0.45
1:E:103:MET:HE1	1:E:124:PRO:HB3	1.99	0.45
1:E:121:VAL:HG22	1:E:166:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:THR:CG2	1:F:241:GLU:H	2.24	0.45
1:H:26:ARG:NH1	1:H:60:ASP:OD2	2.48	0.45
1:H:280:ASN:HD22	1:H:281:THR:N	2.04	0.45
1:B:69:ILE:HG13	1:B:74:LYS:HG3	1.99	0.45
1:C:280:ASN:ND2	1:C:281:THR:H	2.02	0.45
1:E:69:ILE:HD11	1:E:74:LYS:NZ	2.32	0.45
1:H:240:PHE:CE2	1:H:241:GLU:HG3	2.52	0.45
1:A:121:VAL:HG22	1:A:166:PHE:O	2.17	0.45
1:B:206:GLU:HB2	2:B:2165:HOH:O	2.16	0.45
1:G:350:HIS:CE1	1:G:448:ALA:O	2.70	0.45
1:H:493:LEU:C	1:H:493:LEU:HD23	2.41	0.45
1:D:417:ASN:ND2	1:D:420:TYR:H	2.15	0.45
1:A:103:MET:HE2	1:A:107:LEU:CB	2.46	0.44
1:A:408:ALA:HB2	1:A:458:ARG:NE	2.30	0.44
1:B:417:ASN:HD22	1:B:420:TYR:H	1.64	0.44
1:B:438:ARG:NH2	2:B:2264:HOH:O	2.47	0.44
1:D:285:PRO:HG2	1:D:325:MET:HG3	2.00	0.44
1:E:239:THR:HG22	1:E:241:GLU:N	2.30	0.44
1:G:502:SER:HB2	2:G:2339:HOH:O	2.16	0.44
1:A:369:MET:CE	1:A:371:VAL:CG2	2.91	0.44
1:D:455:GLU:CD	1:D:457:ARG:HH21	2.25	0.44
1:E:162:ASN:HA	1:E:207:TRP:CZ2	2.52	0.44
1:E:438:ARG:NH1	2:E:2304:HOH:O	2.50	0.44
1:F:415:ILE:HD11	1:F:451:HIS:CB	2.37	0.44
1:G:225:VAL:HG23	1:G:272:LEU:HD13	1.99	0.44
1:H:369:MET:HE1	1:H:400:LEU:CD1	2.47	0.44
1:C:79:PHE:HD2	1:C:82:ILE:HD11	1.82	0.44
1:C:426:VAL:CG2	1:C:447:VAL:HG11	2.46	0.44
1:D:99:GLU:OE1	2:D:2111:HOH:O	2.21	0.44
1:D:368:GLU:OE2	1:D:396:LYS:HE3	2.17	0.44
1:E:14:PHE:CE2	2:E:2259:HOH:O	2.57	0.44
1:F:285:PRO:HB3	1:F:336:PHE:CE1	2.52	0.44
1:A:102:PHE:HB3	1:A:120:ASN:O	2.18	0.44
1:D:177:LYS:HE3	2:D:2172:HOH:O	2.16	0.44
1:G:148:GLU:HB3	2:G:2126:HOH:O	2.16	0.44
1:G:411:ILE:O	1:G:454:THR:HA	2.17	0.44
1:A:247:LEU:HG	1:C:499:THR:HG21	2.00	0.44
1:A:382:VAL:C	1:A:383:LEU:HD23	2.42	0.44
1:B:285:PRO:CG	1:B:325:MET:HG3	2.45	0.44
1:C:406:PHE:O	1:C:407:SER:CB	2.66	0.44
1:D:95:ARG:NH2	2:D:2108:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ARG:O	1:D:304:SER:HB3	2.17	0.44
1:E:468:ILE:HD12	1:E:478:ILE:HD13	2.00	0.44
1:F:258:LYS:HE2	2:F:2258:HOH:O	2.17	0.44
1:H:417:ASN:HD22	1:H:420:TYR:H	1.66	0.44
1:H:457:ARG:NH1	1:H:465:HIS:O	2.47	0.44
1:B:499:THR:CG2	2:D:2209:HOH:O	2.64	0.44
1:C:464:ILE:HD13	1:C:466:LEU:HG	2.00	0.44
1:G:235:PRO:HG2	1:G:238:LYS:HE2	1.99	0.44
1:B:205:ASP:HB3	1:B:263:LEU:HD11	1.99	0.44
1:B:374:ARG:HD3	1:B:378:SER:OG	2.17	0.44
1:B:426:VAL:CG2	1:B:447:VAL:HG11	2.46	0.44
1:C:438:ARG:HD3	2:C:2327:HOH:O	2.17	0.44
1:B:400:LEU:HB3	1:B:402:ILE:CD1	2.46	0.44
1:C:385:ASN:ND2	1:C:394:LEU:O	2.49	0.44
1:C:406:PHE:CD1	1:C:406:PHE:N	2.85	0.44
1:D:209:THR:HB	2:D:2218:HOH:O	2.17	0.44
1:E:392:GLU:HG2	1:E:393:GLY:N	2.32	0.44
1:F:466:LEU:HD11	1:F:480:ILE:HD11	1.99	0.44
1:F:485:ASP:OD1	1:F:487:THR:CG2	2.55	0.44
1:H:392:GLU:CA	2:H:2305:HOH:O	2.36	0.44
1:B:350:HIS:HE1	1:B:448:ALA:O	2.01	0.44
1:C:204:SER:CB	2:C:2207:HOH:O	2.66	0.44
1:E:208:ILE:HD13	1:E:260:VAL:HG13	1.99	0.44
1:G:121:VAL:HG22	1:G:166:PHE:O	2.17	0.44
1:G:406:PHE:CE2	1:G:409:VAL:CG2	3.01	0.44
1:A:26:ARG:HD3	1:A:117:TRP:CE2	2.53	0.43
1:C:369:MET:HE1	1:C:400:LEU:HD21	2.00	0.43
1:D:103:MET:HE2	1:D:107:LEU:HB2	1.93	0.43
1:F:459:ALA:HA	1:F:464:ILE:HG22	2.00	0.43
1:G:213:HIS:NE2	1:G:217:GLU:OE2	2.51	0.43
1:A:24:THR:CG2	1:A:53:GLY:HA3	2.47	0.43
1:D:424:TRP:O	1:D:428:LYS:HG3	2.19	0.43
1:D:426:VAL:CG2	1:D:447:VAL:HG11	2.47	0.43
1:E:237:LYS:NZ	1:G:492:GLY:O	2.44	0.43
1:E:247:LEU:HG	1:G:499:THR:HG21	2.00	0.43
1:G:406:PHE:HE2	1:G:409:VAL:CG2	2.31	0.43
1:A:239:THR:HG22	1:A:242:TYR:N	2.33	0.43
1:A:350:HIS:CE1	1:A:448:ALA:O	2.71	0.43
1:B:290:HIS:HD2	1:B:334:GLY:O	2.00	0.43
1:B:391:GLY:HA3	1:B:394:LEU:HD11	2.00	0.43
1:C:397:GLU:HG2	1:C:469:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:HIS:HD2	1:D:334:GLY:O	2.01	0.43
1:B:26:ARG:HD3	1:B:117:TRP:CE2	2.54	0.43
1:D:26:ARG:HD3	1:D:117:TRP:CE2	2.53	0.43
1:D:218:ARG:HE	1:D:218:ARG:HB3	1.46	0.43
1:E:13:LYS:CE	2:E:2003:HOH:O	2.62	0.43
1:E:404:VAL:HG11	1:E:459:ALA:CB	2.48	0.43
1:H:79:PHE:HA	1:H:82:ILE:HD11	2.00	0.43
1:A:493:LEU:HD23	1:A:494:ASP:N	2.33	0.43
1:B:20:PHE:HB3	1:B:312:SER:HB2	1.99	0.43
1:B:489:THR:HG22	1:D:434:ARG:HH21	1.82	0.43
1:D:227:ARG:HH21	1:D:256:GLN:HE21	1.65	0.43
1:F:285:PRO:HG2	1:F:325:MET:HG3	2.00	0.43
1:H:125:LYS:HA	1:H:125:LYS:HD3	1.71	0.43
1:H:239:THR:HG22	1:H:242:TYR:H	1.84	0.43
1:B:417:ASN:HB3	1:B:474:GLU:HG3	2.01	0.43
1:C:209:THR:HB	2:C:2252:HOH:O	2.19	0.43
1:F:266:GLN:NE2	2:F:2265:HOH:O	2.51	0.43
1:F:389:GLU:HG3	2:F:2334:HOH:O	2.17	0.43
1:F:392:GLU:N	1:F:394:LEU:HD12	2.32	0.43
1:B:93:ASN:HB3	2:B:2085:HOH:O	2.17	0.43
1:D:457:ARG:NH1	1:D:466:LEU:HD23	2.34	0.43
1:E:69:ILE:HG13	1:E:69:ILE:O	2.19	0.43
1:G:218:ARG:HE	1:G:218:ARG:HB3	1.34	0.43
1:H:172:LYS:HA	1:H:207:TRP:CH2	2.54	0.43
1:D:82:ILE:HD12	1:D:83:ASP:H	1.83	0.43
1:D:165:ASN:ND2	1:D:165:ASN:N	2.66	0.43
1:E:493:LEU:C	1:E:493:LEU:HD23	2.43	0.43
1:E:499:THR:HG22	2:G:2199:HOH:O	2.17	0.43
1:F:125:LYS:CD	2:F:2150:HOH:O	2.59	0.43
1:B:258:LYS:HD3	1:B:309:TYR:CE2	2.53	0.43
1:B:445:ARG:HH11	1:B:445:ARG:HD2	1.58	0.43
1:D:16:LYS:HD2	2:D:2263:HOH:O	2.19	0.43
1:F:502:SER:HA	2:H:2158:HOH:O	2.18	0.43
1:B:434:ARG:HE	1:D:489:THR:HG21	1.82	0.43
1:C:125:LYS:HD3	1:C:125:LYS:HA	1.88	0.43
1:B:458:ARG:HD3	1:B:458:ARG:HA	1.62	0.42
1:F:239:THR:HG23	2:F:2244:HOH:O	2.19	0.42
1:F:301:ARG:HH21	1:F:305:GLU:CD	2.27	0.42
1:H:502:SER:HA	2:H:2397:HOH:O	2.19	0.42
1:A:26:ARG:HH11	1:A:26:ARG:HD2	1.53	0.42
1:A:162:ASN:ND2	1:A:204:SER:OG	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:HB2	2:B:2209:HOH:O	2.19	0.42
1:B:404:VAL:HG13	1:B:406:PHE:HB2	2.01	0.42
1:C:130:TRP:NE1	1:C:134:ILE:CD1	2.82	0.42
1:C:230:TYR:OH	1:C:278:GLU:OE1	2.20	0.42
1:G:415:ILE:HG21	1:G:415:ILE:HD12	1.43	0.42
1:H:103:MET:HE3	1:H:103:MET:HB3	0.43	0.42
1:H:285:PRO:HB3	1:H:336:PHE:CE1	2.54	0.42
1:A:287:ASN:CG	1:A:289:VAL:HG22	2.45	0.42
1:B:107:LEU:HD21	1:B:129:LYS:CB	2.48	0.42
1:E:50:TYR:HA	1:E:95:ARG:O	2.18	0.42
1:F:103:MET:HE3	1:F:103:MET:C	2.43	0.42
1:A:301:ARG:CB	2:A:2235:HOH:O	2.67	0.42
1:B:308:ASP:OD2	1:B:365:ARG:NH2	2.53	0.42
1:B:364:TYR:HE2	1:B:369:MET:HE2	1.72	0.42
1:D:418:GLU:O	1:D:425:ARG:HD3	2.18	0.42
1:H:82:ILE:HD12	1:H:83:ASP:N	2.34	0.42
1:A:79:PHE:CD2	1:A:82:ILE:HD11	2.51	0.42
1:A:103:MET:HE1	1:A:130:TRP:CZ3	2.54	0.42
1:A:415:ILE:HG23	1:A:415:ILE:HD13	1.73	0.42
1:B:227:ARG:O	1:B:276:ILE:HA	2.19	0.42
1:C:281:THR:OG1	1:C:295:ASN:ND2	2.47	0.42
1:E:392:GLU:CG	1:E:393:GLY:H	2.31	0.42
2:E:2341:HOH:O	1:G:239:THR:CG2	2.66	0.42
1:F:438:ARG:HD3	2:F:2361:HOH:O	2.18	0.42
1:H:325:MET:O	1:H:326:ASP:CB	2.67	0.42
1:A:374:ARG:NH2	1:A:479:GLU:OE1	2.33	0.42
1:C:156:GLU:OE1	1:C:226:SER:OG	2.29	0.42
1:F:438:ARG:HD3	2:F:2363:HOH:O	2.09	0.42
1:B:227:ARG:HD3	1:B:260:VAL:HG21	2.01	0.42
1:C:158:TRP:CD1	1:C:159:ASN:H	2.37	0.42
1:C:493:LEU:HD23	1:C:494:ASP:N	2.35	0.42
1:D:358:LEU:HD21	1:D:382:VAL:HG23	2.01	0.42
1:F:278:GLU:HG2	1:F:316:TRP:CE3	2.54	0.42
1:G:366:ASP:OD1	1:G:366:ASP:C	2.63	0.42
1:B:123:PRO:CD	1:B:168:LYS:HE2	2.50	0.42
1:E:13:LYS:NZ	2:E:2003:HOH:O	2.50	0.42
1:H:267:SER:HB2	1:H:268:PRO:HD2	2.02	0.42
1:H:415:ILE:HG23	1:H:415:ILE:HD13	1.24	0.42
1:B:123:PRO:HD2	1:B:168:LYS:HE2	2.01	0.42
1:D:392:GLU:O	1:D:394:LEU:N	2.49	0.42
2:E:2206:HOH:O	1:G:499:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:VAL:HG22	1:F:465:HIS:CD2	2.55	0.42
1:G:466:LEU:HD11	1:G:480:ILE:HD11	2.01	0.42
1:C:125:LYS:CG	2:C:2123:HOH:O	2.67	0.41
1:C:438:ARG:CD	2:C:2327:HOH:O	2.68	0.41
1:F:282:SER:HB3	1:F:290:HIS:CE1	2.55	0.41
1:H:4:VAL:HG11	1:H:369:MET:HE2	1.92	0.41
1:H:33:LYS:HD2	2:H:2048:HOH:O	2.19	0.41
1:H:417:ASN:HD22	1:H:417:ASN:C	2.28	0.41
1:B:274:LEU:CD1	1:B:310:VAL:HG12	2.24	0.41
1:B:417:ASN:HD22	1:B:417:ASN:C	2.27	0.41
1:C:8:SER:OG	1:C:403:PRO:CB	2.68	0.41
1:F:451:HIS:HD2	2:H:2165:HOH:O	2.03	0.41
1:A:449:GLN:NE2	2:A:2324:HOH:O	2.53	0.41
1:E:251:GLU:HG2	1:E:301:ARG:NH1	2.36	0.41
1:H:251:GLU:HB2	2:H:2229:HOH:O	2.20	0.41
1:A:287:ASN:OD1	1:A:289:VAL:HG22	2.21	0.41
1:B:374:ARG:NH2	1:B:479:GLU:OE1	2.44	0.41
1:C:82:ILE:HD12	1:C:82:ILE:C	2.45	0.41
1:C:107:LEU:HD21	1:C:129:LYS:HB3	2.03	0.41
1:C:169:ASP:O	1:C:170:ALA:C	2.64	0.41
1:C:413:ARG:HD3	1:C:453:MET:HE3	2.01	0.41
1:G:19:LYS:HE2	1:G:47:GLY:O	2.20	0.41
1:G:121:VAL:HG13	1:G:121:VAL:O	2.20	0.41
1:G:164:VAL:HG12	2:G:2103:HOH:O	2.20	0.41
1:A:325:MET:O	1:A:326:ASP:CB	2.69	0.41
1:B:205:ASP:HB3	1:B:263:LEU:CD1	2.50	0.41
1:C:457:ARG:NH1	1:C:465:HIS:O	2.54	0.41
1:F:422:ASN:C	1:F:422:ASN:ND2	2.78	0.41
1:H:401:VAL:HG22	1:H:465:HIS:CD2	2.56	0.41
1:A:445:ARG:HD2	2:A:2316:HOH:O	2.20	0.41
1:B:358:LEU:HD21	1:B:382:VAL:HG23	2.03	0.41
1:C:153:TRP:O	1:C:154:LEU:HD23	2.20	0.41
1:C:337:GLY:O	1:C:346:LYS:HD2	2.20	0.41
1:D:190:ASP:HB3	1:D:193:LEU:HG	2.03	0.41
1:G:103:MET:HE3	1:G:107:LEU:HB2	2.01	0.41
1:H:264:ILE:HD11	1:H:274:LEU:HG	2.03	0.41
1:C:267:SER:HB2	1:C:268:PRO:CD	2.49	0.41
1:C:424:TRP:CZ2	1:C:428:LYS:HE2	2.55	0.41
1:D:93:ASN:CG	2:D:2105:HOH:O	2.62	0.41
1:D:206:GLU:HG3	2:D:2187:HOH:O	2.20	0.41
1:D:401:VAL:HG22	1:D:465:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:ARG:HG3	2:E:2293:HOH:O	2.19	0.41
1:G:79:PHE:CD2	1:G:82:ILE:HD11	2.55	0.41
1:F:111:ASP:O	1:F:113:THR:HG23	2.19	0.41
1:G:227:ARG:O	1:G:276:ILE:HA	2.20	0.41
1:A:143:GLU:OE1	2:A:2137:HOH:O	2.22	0.41
1:D:227:ARG:HH21	1:D:256:GLN:NE2	2.19	0.41
1:F:67:VAL:HG13	1:F:69:ILE:HG23	2.03	0.41
1:G:127:TYR:CE1	1:G:177:LYS:HE3	2.56	0.41
1:G:165:ASN:H	1:G:165:ASN:ND2	2.19	0.41
1:G:417:ASN:HD22	1:G:417:ASN:C	2.29	0.41
1:H:40:LYS:HE3	2:H:2047:HOH:O	2.20	0.41
1:H:258:LYS:HG3	1:H:309:TYR:CD2	2.55	0.41
1:C:395:THR:HG23	2:C:2309:HOH:O	2.20	0.41
1:F:229:ALA:O	1:F:279:TYR:HA	2.21	0.41
1:G:45:LYS:HD2	1:G:349:PHE:CZ	2.55	0.41
1:A:65:ARG:HG2	2:A:2071:HOH:O	2.19	0.40
1:A:423:ALA:HB2	1:A:448:ALA:HB2	2.03	0.40
1:B:239:THR:HG21	2:B:2183:HOH:O	2.22	0.40
1:C:399:GLN:HE21	1:C:467:SER:CB	2.25	0.40
1:D:95:ARG:HD3	1:D:149:GLU:OE2	2.21	0.40
1:G:358:LEU:HD21	1:G:382:VAL:HG23	2.01	0.40
1:A:389:GLU:CD	1:A:389:GLU:N	2.79	0.40
1:A:481:GLU:CG	2:A:2292:HOH:O	2.68	0.40
1:B:69:ILE:CG1	1:B:74:LYS:HG3	2.50	0.40
1:C:387:VAL:HG11	1:C:394:LEU:HD13	2.03	0.40
1:H:350:HIS:CE1	1:H:448:ALA:O	2.74	0.40
1:C:114:VAL:O	1:C:115:PHE:HB2	2.22	0.40
1:C:387:VAL:HG13	1:C:394:LEU:HD22	2.04	0.40
1:D:54:HIS:HE1	1:D:159:ASN:OD1	2.04	0.40
1:A:126:ASP:C	1:A:126:ASP:OD1	2.64	0.40
1:E:6:VAL:HB	1:E:402:ILE:HG22	2.03	0.40
1:F:24:THR:HG23	1:F:53:GLY:HA3	2.04	0.40
1:H:464:ILE:HD12	1:H:466:LEU:HD21	2.04	0.40
1:A:65:ARG:CG	2:A:2071:HOH:O	2.69	0.40
1:A:278:GLU:HG2	1:A:316:TRP:CE3	2.57	0.40
1:C:239:THR:CG2	2:C:2236:HOH:O	2.60	0.40
1:E:406:PHE:CD1	1:E:406:PHE:N	2.89	0.40
1:F:280:ASN:ND2	1:F:281:THR:H	2.01	0.40
1:H:69:ILE:CG1	1:H:74:LYS:HG2	2.47	0.40

All (2) 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:D:2193:HOH:O	2:G:2069:HOH:O[3_645]	1.99	0.21
2:A:2007:HOH:O	2:F:2015:HOH:O[4_556]	2.18	0.02

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	497/503 (99%)	467 (94%)	27 (5%)	3 (1%)	21	23
1	B	497/503 (99%)	473 (95%)	18 (4%)	6 (1%)	10	8
1	C	497/503 (99%)	469 (94%)	24 (5%)	4 (1%)	16	16
1	D	496/503 (99%)	468 (94%)	22 (4%)	6 (1%)	10	8
1	E	497/503 (99%)	475 (96%)	21 (4%)	1 (0%)	43	51
1	F	497/503 (99%)	468 (94%)	25 (5%)	4 (1%)	16	16
1	G	497/503 (99%)	474 (95%)	20 (4%)	3 (1%)	21	23
1	H	497/503 (99%)	476 (96%)	18 (4%)	3 (1%)	21	23
All	All	3975/4024 (99%)	3770 (95%)	175 (4%)	30 (1%)	16	16

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	GLY
1	B	406	PHE
1	B	461	ASP
1	C	391	GLY
1	C	406	PHE
1	C	407	SER
1	D	70	ASP
1	D	392	GLU
1	D	407	SER
1	F	392	GLU
1	G	391	GLY

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Mol	Chain	Res	Type
1	H	392	GLU
1	A	11	ARG
1	B	391	GLY
1	C	392	GLU
1	D	391	GLY
1	E	11	ARG
1	F	11	ARG
1	F	391	GLY
1	G	70	ASP
1	G	71	GLY
1	H	11	ARG
1	B	70	ASP
1	B	392	GLU
1	B	407	SER
1	D	406	PHE
1	F	70	ASP
1	A	70	ASP
1	H	102	PHE
1	D	404	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	439/443 (99%)	385 (88%)	54 (12%)	4	4
1	B	439/443 (99%)	394 (90%)	45 (10%)	7	7
1	C	439/443 (99%)	390 (89%)	49 (11%)	6	5
1	D	439/443 (99%)	391 (89%)	48 (11%)	6	6
1	E	439/443 (99%)	398 (91%)	41 (9%)	8	9
1	F	439/443 (99%)	394 (90%)	45 (10%)	7	7
1	G	439/443 (99%)	386 (88%)	53 (12%)	5	4
1	H	439/443 (99%)	401 (91%)	38 (9%)	9	10
All	All	3512/3544 (99%)	3139 (89%)	373 (11%)	6	6

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	39	LEU
1	A	41	LEU
1	A	67	VAL
1	A	68	GLU
1	A	69	ILE
1	A	82	ILE
1	A	95	ARG
1	A	107	LEU
1	A	121	VAL
1	A	131	ARG
1	A	133	LEU
1	A	139	SER
1	A	147	ILE
1	A	164	VAL
1	A	178	LEU
1	A	206	GLU
1	A	209	THR
1	A	217	GLU
1	A	222	VAL
1	A	227	ARG
1	A	239	THR
1	A	265	ARG
1	A	274	LEU
1	A	280	ASN
1	A	289	VAL
1	A	294	LEU
1	A	299	ILE
1	A	313	PHE
1	A	319	SER
1	A	325	MET
1	A	331	LEU
1	A	362	LEU
1	A	368	GLU
1	A	383	LEU
1	A	386	LEU
1	A	389	GLU
1	A	392	GLU
1	A	395	THR
1	A	397	GLU
1	A	402	ILE
1	A	404	VAL

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Mol	Chain	Res	Type
1	A	409	VAL
1	A	415	ILE
1	A	417	ASN
1	A	422	ASN
1	A	447	VAL
1	A	463	VAL
1	A	464	ILE
1	A	481	GLU
1	A	484	ARG
1	A	489	THR
1	A	499	THR
1	A	502	SER
1	B	13	LYS
1	B	15	LYS
1	B	27	LEU
1	B	39	LEU
1	B	41	LEU
1	B	67	VAL
1	B	68	GLU
1	B	69	ILE
1	B	70	ASP
1	B	74	LYS
1	B	82	ILE
1	B	121	VAL
1	B	125	LYS
1	B	133	LEU
1	B	164	VAL
1	B	165	ASN
1	B	178	LEU
1	B	222	VAL
1	B	226	SER
1	B	239	THR
1	B	251	GLU
1	B	255	GLU
1	B	259	THR
1	B	265	ARG
1	B	274	LEU
1	B	280	ASN
1	B	319	SER
1	B	325	MET
1	B	331	LEU
1	B	374	ARG

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Mol	Chain	Res	Type
1	B	383	LEU
1	B	389	GLU
1	B	392	GLU
1	B	395	THR
1	B	396	LYS
1	B	399	GLN
1	B	404	VAL
1	B	409	VAL
1	B	417	ASN
1	B	422	ASN
1	B	447	VAL
1	B	463	VAL
1	B	481	GLU
1	B	489	THR
1	B	499	THR
1	C	12	GLU
1	C	27	LEU
1	C	39	LEU
1	C	41	LEU
1	C	67	VAL
1	C	82	ILE
1	C	95	ARG
1	C	105	LYS
1	C	121	VAL
1	C	125	LYS
1	C	133	LEU
1	C	139	SER
1	C	164	VAL
1	C	165	ASN
1	C	178	LEU
1	C	209	THR
1	C	222	VAL
1	C	226	SER
1	C	239	THR
1	C	246	GLU
1	C	248	GLU
1	C	258	LYS
1	C	274	LEU
1	C	282	SER
1	C	289	VAL
1	C	294	LEU
1	C	331	LEU

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Mol	Chain	Res	Type
1	C	362	LEU
1	C	383	LEU
1	C	389	GLU
1	C	392	GLU
1	C	399	GLN
1	C	400	LEU
1	C	402	ILE
1	C	404	VAL
1	C	406	PHE
1	C	409	VAL
1	C	417	ASN
1	C	422	ASN
1	C	428	LYS
1	C	447	VAL
1	C	458	ARG
1	C	461	ASP
1	C	463	VAL
1	C	464	ILE
1	C	468	ILE
1	C	481	GLU
1	C	487	THR
1	C	499	THR
1	D	11	ARG
1	D	13	LYS
1	D	22	VAL
1	D	39	LEU
1	D	41	LEU
1	D	67	VAL
1	D	74	LYS
1	D	82	ILE
1	D	95	ARG
1	D	121	VAL
1	D	125	LYS
1	D	133	LEU
1	D	164	VAL
1	D	165	ASN
1	D	178	LEU
1	D	209	THR
1	D	218	ARG
1	D	222	VAL
1	D	233	LYS
1	D	239	THR

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Mol	Chain	Res	Type
1	D	248	GLU
1	D	251	GLU
1	D	259	THR
1	D	274	LEU
1	D	282	SER
1	D	289	VAL
1	D	299	ILE
1	D	319	SER
1	D	331	LEU
1	D	374	ARG
1	D	383	LEU
1	D	389	GLU
1	D	394	LEU
1	D	395	THR
1	D	397	GLU
1	D	399	GLN
1	D	400	LEU
1	D	404	VAL
1	D	409	VAL
1	D	417	ASN
1	D	422	ASN
1	D	447	VAL
1	D	458	ARG
1	D	463	VAL
1	D	464	ILE
1	D	489	THR
1	D	499	THR
1	D	502	SER
1	E	8	SER
1	E	11	ARG
1	E	22	VAL
1	E	27	LEU
1	E	39	LEU
1	E	41	LEU
1	E	67	VAL
1	E	72	GLU
1	E	82	ILE
1	E	121	VAL
1	E	133	LEU
1	E	148	GLU
1	E	178	LEU
1	E	209	THR

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Mol	Chain	Res	Type
1	E	219	ARG
1	E	239	THR
1	E	274	LEU
1	E	289	VAL
1	E	304	SER
1	E	328	PRO
1	E	331	LEU
1	E	347	PRO
1	E	386	LEU
1	E	394	LEU
1	E	396	LYS
1	E	402	ILE
1	E	404	VAL
1	E	405	SER
1	E	406	PHE
1	E	409	VAL
1	E	415	ILE
1	E	417	ASN
1	E	422	ASN
1	E	447	VAL
1	E	460	THR
1	E	463	VAL
1	E	468	ILE
1	E	482	GLN
1	E	484	ARG
1	E	489	THR
1	E	499	THR
1	F	22	VAL
1	F	39	LEU
1	F	41	LEU
1	F	67	VAL
1	F	70	ASP
1	F	72	GLU
1	F	74	LYS
1	F	82	ILE
1	F	103	MET
1	F	107	LEU
1	F	121	VAL
1	F	133	LEU
1	F	178	LEU
1	F	217	GLU
1	F	222	VAL

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Mol	Chain	Res	Type
1	F	227	ARG
1	F	239	THR
1	F	266	GLN
1	F	274	LEU
1	F	289	VAL
1	F	304	SER
1	F	328	PRO
1	F	331	LEU
1	F	343	SER
1	F	362	LEU
1	F	374	ARG
1	F	375	LYS
1	F	383	LEU
1	F	386	LEU
1	F	392	GLU
1	F	395	THR
1	F	404	VAL
1	F	409	VAL
1	F	415	ILE
1	F	417	ASN
1	F	422	ASN
1	F	447	VAL
1	F	453	MET
1	F	458	ARG
1	F	463	VAL
1	F	464	ILE
1	F	487	THR
1	F	489	THR
1	F	493	LEU
1	F	499	THR
1	G	11	ARG
1	G	22	VAL
1	G	24	THR
1	G	39	LEU
1	G	41	LEU
1	G	42	VAL
1	G	67	VAL
1	G	70	ASP
1	G	72	GLU
1	G	82	ILE
1	G	95	ARG
1	G	105	LYS

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Mol	Chain	Res	Type
1	G	121	VAL
1	G	133	LEU
1	G	178	LEU
1	G	209	THR
1	G	218	ARG
1	G	222	VAL
1	G	227	ARG
1	G	239	THR
1	G	248	GLU
1	G	251	GLU
1	G	266	GLN
1	G	274	LEU
1	G	280	ASN
1	G	282	SER
1	G	289	VAL
1	G	294	LEU
1	G	313	PHE
1	G	319	SER
1	G	325	MET
1	G	331	LEU
1	G	362	LEU
1	G	374	ARG
1	G	383	LEU
1	G	389	GLU
1	G	392	GLU
1	G	394	LEU
1	G	395	THR
1	G	400	LEU
1	G	402	ILE
1	G	409	VAL
1	G	415	ILE
1	G	417	ASN
1	G	422	ASN
1	G	428	LYS
1	G	447	VAL
1	G	463	VAL
1	G	469	VAL
1	G	481	GLU
1	G	489	THR
1	G	499	THR
1	G	500	SER
1	H	11	ARG

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Mol	Chain	Res	Type
1	H	22	VAL
1	H	39	LEU
1	H	41	LEU
1	H	67	VAL
1	H	82	ILE
1	H	95	ARG
1	H	103	MET
1	H	107	LEU
1	H	121	VAL
1	H	125	LYS
1	H	133	LEU
1	H	178	LEU
1	H	206	GLU
1	H	209	THR
1	H	222	VAL
1	H	239	THR
1	H	274	LEU
1	H	282	SER
1	H	289	VAL
1	H	294	LEU
1	H	331	LEU
1	H	343	SER
1	H	362	LEU
1	H	374	ARG
1	H	383	LEU
1	H	392	GLU
1	H	397	GLU
1	H	405	SER
1	H	409	VAL
1	H	415	ILE
1	H	417	ASN
1	H	422	ASN
1	H	447	VAL
1	H	461	ASP
1	H	478	ILE
1	H	499	THR
1	H	502	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

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Mol	Chain	Res	Type
1	A	93	ASN
1	A	112	GLN
1	A	128	ASN
1	A	140	HIS
1	A	165	ASN
1	A	194	GLN
1	A	280	ASN
1	A	290	HIS
1	A	295	ASN
1	A	342	HIS
1	A	350	HIS
1	A	385	ASN
1	A	414	GLN
1	A	417	ASN
1	A	422	ASN
1	A	465	HIS
1	B	140	HIS
1	B	165	ASN
1	B	280	ASN
1	B	290	HIS
1	B	295	ASN
1	B	350	HIS
1	B	385	ASN
1	B	414	GLN
1	B	417	ASN
1	B	422	ASN
1	B	451	HIS
1	C	140	HIS
1	C	165	ASN
1	C	194	GLN
1	C	280	ASN
1	C	290	HIS
1	C	295	ASN
1	C	342	HIS
1	C	399	GLN
1	C	417	ASN
1	C	422	ASN
1	C	451	HIS
1	C	465	HIS
1	D	54	HIS
1	D	165	ASN
1	D	256	GLN

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Mol	Chain	Res	Type
1	D	280	ASN
1	D	290	HIS
1	D	295	ASN
1	D	350	HIS
1	D	385	ASN
1	D	417	ASN
1	D	422	ASN
1	D	451	HIS
1	D	465	HIS
1	D	482	GLN
1	E	5	ASN
1	E	165	ASN
1	E	173	GLN
1	E	194	GLN
1	E	280	ASN
1	E	290	HIS
1	E	350	HIS
1	E	385	ASN
1	E	417	ASN
1	E	422	ASN
1	F	140	HIS
1	F	165	ASN
1	F	213	HIS
1	F	280	ASN
1	F	290	HIS
1	F	295	ASN
1	F	342	HIS
1	F	350	HIS
1	F	385	ASN
1	F	417	ASN
1	F	422	ASN
1	F	465	HIS
1	F	482	GLN
1	G	112	GLN
1	G	140	HIS
1	G	165	ASN
1	G	266	GLN
1	G	280	ASN
1	G	290	HIS
1	G	295	ASN
1	G	350	HIS
1	G	385	ASN

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Mol	Chain	Res	Type
1	G	417	ASN
1	G	422	ASN
1	G	451	HIS
1	G	482	GLN
1	H	5	ASN
1	H	9	ASN
1	H	140	HIS
1	H	194	GLN
1	H	280	ASN
1	H	290	HIS
1	H	295	ASN
1	H	350	HIS
1	H	385	ASN
1	H	417	ASN
1	H	422	ASN
1	H	429	GLN
1	H	451	HIS
1	H	456	GLN
1	H	465	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	C	1
1	E	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	501:TYR	C	502:SER	N	2.24
1	C	501:TYR	C	502:SER	N	1.69
1	E	501:TYR	C	502:SER	N	1.68
1	F	501:TYR	C	502:SER	N	1.60

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.