



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:15 PM UTC

PDB ID : 3K4A / pdb_00003k4a
Title : Crystal structure of selenomethionine substituted E. coli beta-glucuronidase
Authors : Wallace, B.D.; Orans, J.; Redinbo, M.R.
Deposited on : 2009-10-05
Resolution : 2.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

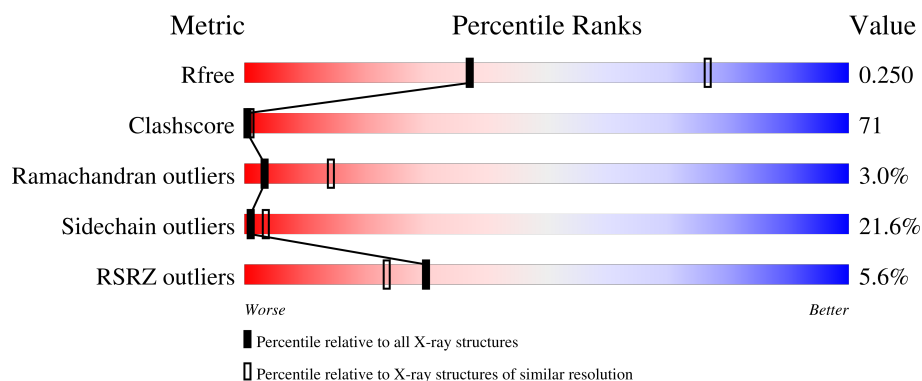
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	605	4% 30% 47% 19% ..
1	B	605	6% 22% 52% 20% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9761 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-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	Se	0	0	0
			4779	3034	827	896	9	13			
1	B	597	Total	C	N	O	S	Se	0	0	0
			4768	3026	826	894	9	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P05804
A	0	HIS	-	expression tag	UNP P05804
B	-1	SER	-	expression tag	UNP P05804
B	0	HIS	-	expression tag	UNP P05804

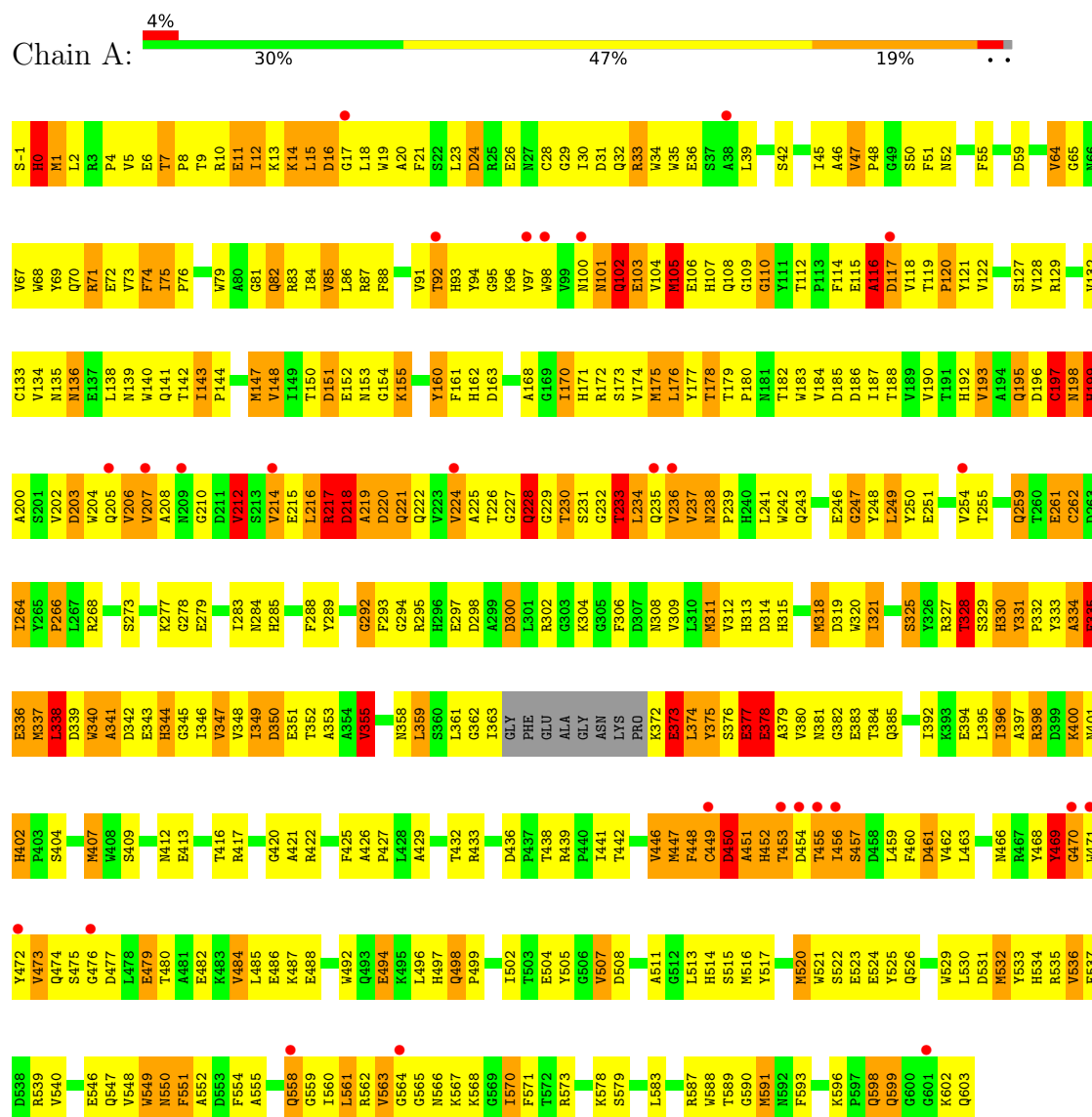
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	123	Total	O	0	0
			123	123		
2	B	91	Total	O	0	0
			91	91		

3 Residue-property plots

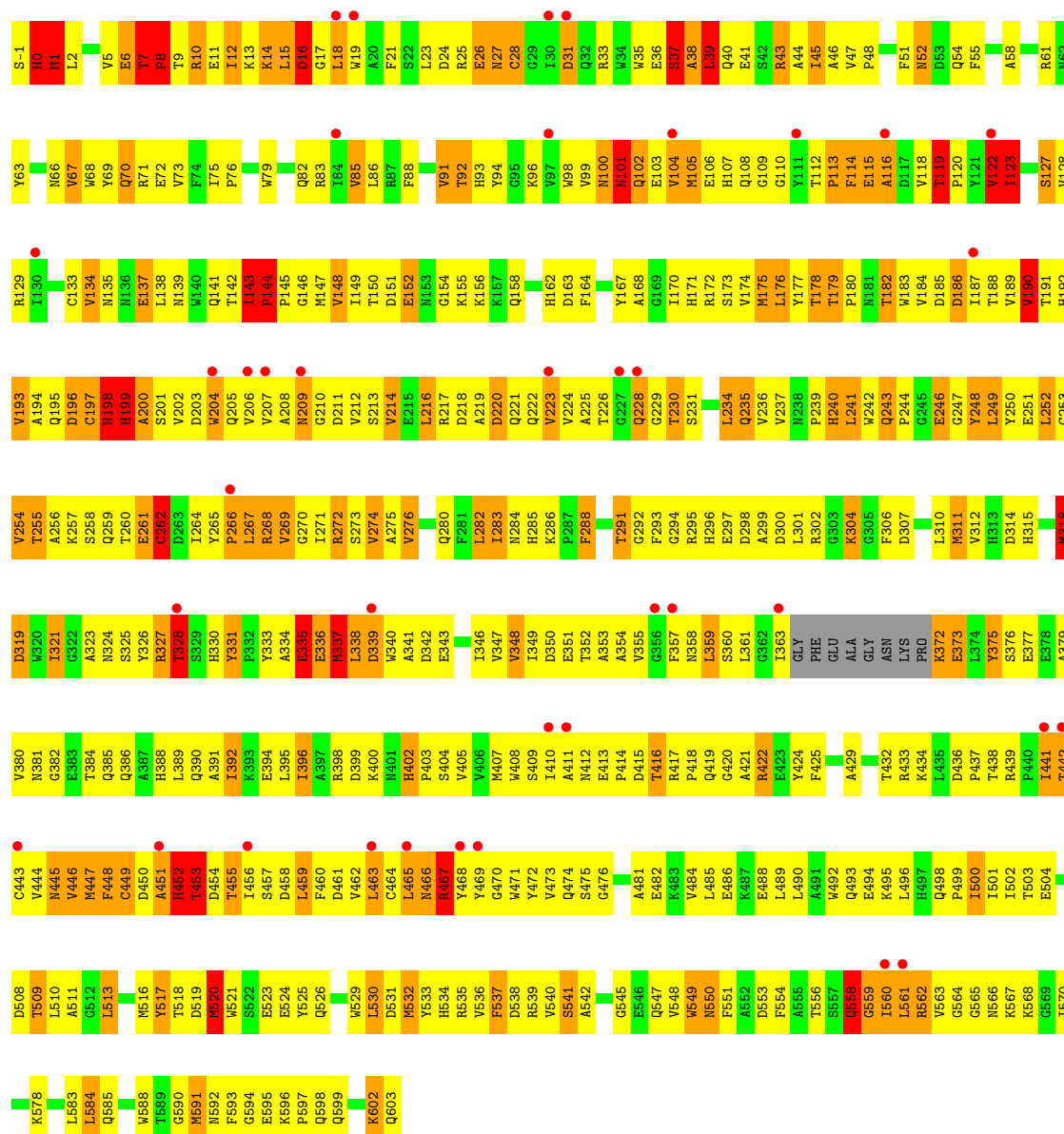
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.00Å 77.26Å 126.58Å 90.00° 125.02° 90.00°	Depositor
Resolution (Å)	32.11 – 2.90 32.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.11-2.90) 98.8 (32.11-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.242 , 0.282 0.251 , 0.250	Depositor DCC
R_{free} test set	1495 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9761	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.24	33/4893 (0.7%)	1.48	80/6636 (1.2%)
1	B	1.05	19/4882 (0.4%)	1.35	69/6623 (1.0%)
All	All	1.15	52/9775 (0.5%)	1.42	149/13259 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
All	All	0	11

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	GLU	N-CA	7.76	1.54	1.45
1	A	105	MSE	SE-CE	-7.04	1.74	1.95
1	A	1	MSE	CG-SE	-7.00	1.74	1.95
1	A	212	VAL	CA-CB	6.87	1.62	1.53
1	B	311	MSE	SE-CE	-6.86	1.74	1.95
1	B	1	MSE	CG-SE	-6.67	1.75	1.95
1	A	532	MSE	CG-SE	-6.65	1.75	1.95
1	A	175	MSE	SE-CE	-6.57	1.75	1.95
1	A	311	MSE	CG-SE	-6.48	1.76	1.95
1	A	147	MSE	SE-CE	-6.40	1.76	1.95
1	B	105	MSE	SE-CE	-6.34	1.76	1.95
1	B	91	VAL	CA-CB	-6.34	1.46	1.54
1	A	520	MSE	SE-CE	-6.19	1.76	1.95
1	A	377	GLU	CA-C	6.17	1.60	1.52
1	A	516	MSE	CG-SE	-6.12	1.77	1.95
1	A	318	MSE	SE-CE	-6.04	1.77	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MSE	SE-CE	-6.02	1.77	1.95
1	B	0	HIS	CA-C	-5.97	1.45	1.52
1	B	175	MSE	CG-SE	-5.92	1.77	1.95
1	A	407	MSE	SE-CE	-5.88	1.77	1.95
1	A	337	MSE	CG-SE	-5.87	1.77	1.95
1	A	148	VAL	CA-CB	5.85	1.61	1.54
1	A	334	ALA	CA-C	-5.83	1.45	1.52
1	A	516	MSE	SE-CE	-5.81	1.78	1.95
1	A	335	GLU	N-CA	5.78	1.55	1.46
1	B	532	MSE	SE-CE	-5.76	1.78	1.95
1	A	447	MSE	SE-CE	-5.73	1.78	1.95
1	A	340	TRP	N-CA	-5.72	1.39	1.46
1	A	520	MSE	CG-SE	-5.69	1.78	1.95
1	B	1	MSE	SE-CE	-5.64	1.78	1.95
1	A	591	MSE	SE-CE	-5.62	1.78	1.95
1	B	311	MSE	CG-SE	-5.57	1.78	1.95
1	B	237	VAL	CA-CB	5.54	1.61	1.54
1	A	318	MSE	CG-SE	-5.44	1.79	1.95
1	B	318	MSE	SE-CE	-5.41	1.79	1.95
1	B	122	VAL	CA-C	5.40	1.59	1.52
1	A	532	MSE	SE-CE	-5.39	1.79	1.95
1	A	175	MSE	CG-SE	-5.38	1.79	1.95
1	B	447	MSE	SE-CE	-5.31	1.79	1.95
1	A	340	TRP	CB-CG	-5.30	1.33	1.50
1	B	337	MSE	CG-SE	-5.29	1.79	1.95
1	A	105	MSE	CG-SE	-5.25	1.79	1.95
1	B	591	MSE	SE-CE	-5.24	1.79	1.95
1	A	407	MSE	CG-SE	-5.23	1.79	1.95
1	A	374	LEU	N-CA	5.18	1.52	1.46
1	B	122	VAL	CA-CB	5.14	1.63	1.54
1	A	147	MSE	CG-SE	-5.12	1.80	1.95
1	B	520	MSE	SE-CE	-5.12	1.80	1.95
1	A	337	MSE	SE-CE	-5.11	1.80	1.95
1	B	337	MSE	SE-CE	-5.06	1.80	1.95
1	B	516	MSE	CG-SE	-5.01	1.80	1.95
1	A	238	ASN	CA-C	5.01	1.59	1.52

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	LEU	N-CA-C	18.37	133.55	111.33
1	A	198	ASN	N-CA-C	13.36	131.25	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	CYS	N-CA-C	12.06	128.98	112.93
1	A	64	VAL	N-CA-C	11.14	124.44	113.53
1	B	336	GLU	N-CA-C	-10.93	100.06	113.50
1	A	92	THR	N-CA-C	10.60	122.91	111.36
1	A	199	HIS	N-CA-C	10.21	132.56	110.80
1	B	199	HIS	N-CA-C	9.95	125.25	111.92
1	A	218	ASP	N-CA-C	9.35	123.70	108.55
1	B	101	ASN	N-CA-C	9.30	124.22	111.39
1	B	452	HIS	N-CA-C	9.13	123.29	108.41
1	A	336	GLU	N-CA-C	-9.10	101.73	112.92
1	A	341	ALA	N-CA-C	-8.97	102.47	113.50
1	A	448	PHE	CB-CA-C	-8.88	98.45	110.79
1	A	382	GLY	N-CA-C	-8.84	104.59	114.40
1	B	453	THR	N-CA-C	-8.83	91.98	110.80
1	A	338	LEU	N-CA-C	-8.68	99.54	112.04
1	B	331	TYR	CA-C-N	8.67	128.43	119.76
1	B	331	TYR	C-N-CA	8.67	128.43	119.76
1	A	217	ARG	N-CA-C	8.44	124.27	113.88
1	A	335	GLU	N-CA-C	8.36	122.84	112.47
1	A	294	GLY	N-CA-C	-8.35	95.18	112.04
1	A	452	HIS	N-CA-C	-8.25	99.13	110.35
1	A	450	ASP	N-CA-C	-8.25	102.09	112.90
1	A	117	ASP	N-CA-C	8.20	122.83	109.72
1	B	26	GLU	N-CA-C	-8.13	102.94	112.86
1	B	119	THR	CA-C-N	-8.12	109.69	119.84
1	B	119	THR	C-N-CA	-8.12	109.69	119.84
1	A	448	PHE	CA-C-N	-8.02	109.15	122.79
1	A	448	PHE	C-N-CA	-8.02	109.15	122.79
1	B	38	ALA	N-CA-C	7.99	121.51	110.24
1	A	377	GLU	N-CA-C	7.96	122.48	110.14
1	B	402	HIS	CA-C-N	7.87	127.54	119.82
1	B	402	HIS	C-N-CA	7.87	127.54	119.82
1	B	7	THR	CA-C-N	-7.80	110.09	119.84
1	B	7	THR	C-N-CA	-7.80	110.09	119.84
1	B	91	VAL	N-CA-C	-7.68	97.42	108.48
1	A	110	GLY	N-CA-C	7.62	123.05	114.67
1	A	0	HIS	N-CA-C	7.61	127.02	110.80
1	B	52	ASN	N-CA-C	7.53	119.39	111.03
1	A	196	ASP	N-CA-C	7.50	125.06	113.28
1	A	558	GLN	N-CA-C	7.50	121.07	110.50
1	B	204	TRP	N-CA-C	7.47	119.93	108.42
1	A	292	GLY	N-CA-C	7.47	120.67	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	GLN	CA-C-N	-7.44	112.34	119.85
1	A	498	GLN	C-N-CA	-7.44	112.34	119.85
1	A	457	SER	N-CA-C	-7.41	102.90	112.23
1	B	177	TYR	N-CA-C	7.40	120.17	109.14
1	A	1	MSE	N-CA-C	7.35	121.33	110.46
1	A	300	ASP	N-CA-C	7.31	120.68	111.69
1	B	122	VAL	CB-CA-C	7.28	121.62	110.55
1	A	469	TYR	CB-CA-C	-7.21	99.92	111.39
1	B	261	GLU	N-CA-C	7.04	120.78	111.28
1	A	328	THR	N-CA-C	-6.97	99.11	109.15
1	A	373	GLU	CA-C-N	6.91	129.84	120.38
1	A	373	GLU	C-N-CA	6.91	129.84	120.38
1	A	470	GLY	N-CA-C	-6.86	104.00	112.77
1	A	220	ASP	N-CA-C	-6.85	99.14	110.17
1	B	85	VAL	N-CA-C	6.79	117.81	108.84
1	B	328	THR	N-CA-C	-6.79	99.84	109.96
1	A	551	PHE	N-CA-C	-6.69	103.68	110.97
1	A	219	ALA	N-CA-C	-6.68	105.13	113.55
1	B	6	GLU	N-CA-C	6.62	118.58	109.18
1	B	549	TRP	CA-C-N	-6.53	113.46	122.93
1	B	549	TRP	C-N-CA	-6.53	113.46	122.93
1	A	453	THR	CB-CA-C	6.50	123.36	110.42
1	A	446	VAL	CB-CA-C	-6.47	100.68	111.29
1	B	116	ALA	N-CA-C	6.47	124.58	110.80
1	B	39	LEU	N-CA-C	6.42	124.47	110.80
1	B	197	CYS	CA-C-N	6.37	133.17	121.70
1	B	197	CYS	C-N-CA	6.37	133.17	121.70
1	A	331	TYR	N-CA-C	-6.35	102.42	108.07
1	A	334	ALA	CA-C-O	-6.32	113.49	120.38
1	B	186	ASP	N-CA-C	6.30	119.87	111.30
1	A	451	ALA	N-CA-C	-6.26	105.61	113.18
1	A	599	GLN	N-CA-C	-6.25	97.50	110.80
1	B	335	GLU	N-CA-C	6.24	124.09	110.80
1	A	461	ASP	N-CA-C	6.19	120.96	113.41
1	B	563	VAL	N-CA-C	6.17	116.75	107.80
1	A	373	GLU	N-CA-C	6.16	123.93	110.80
1	A	589	THR	N-CA-C	-6.15	105.94	113.50
1	B	442	THR	N-CA-C	6.11	117.47	108.86
1	B	15	LEU	N-CA-C	-6.08	97.52	108.58
1	A	116	ALA	N-CA-C	6.08	121.21	113.55
1	B	112	THR	CA-C-N	6.06	126.25	120.31
1	B	112	THR	C-N-CA	6.06	126.25	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLN	N-CA-C	-6.05	99.33	109.07
1	B	274	VAL	N-CA-C	6.03	116.29	107.37
1	B	559	GLY	N-CA-C	6.02	122.42	112.30
1	B	113	PRO	N-CA-C	5.99	120.67	111.57
1	A	590	GLY	N-CA-C	-5.97	106.94	114.16
1	B	201	SER	N-CA-C	5.94	118.64	109.07
1	A	197	CYS	CA-C-N	-5.81	114.58	121.90
1	A	197	CYS	C-N-CA	-5.81	114.58	121.90
1	A	402	HIS	CA-C-N	-5.81	113.69	119.56
1	A	402	HIS	C-N-CA	-5.81	113.69	119.56
1	B	154	GLY	N-CA-C	5.81	124.02	115.08
1	B	312	VAL	O-C-N	5.80	127.50	121.87
1	A	91	VAL	N-CA-C	-5.79	99.71	108.17
1	A	350	ASP	N-CA-C	5.78	118.66	109.24
1	A	425	PHE	N-CA-C	5.78	119.51	112.23
1	B	16	ASP	N-CA-C	-5.70	101.52	110.36
1	A	75	ILE	N-CA-C	5.70	114.53	108.95
1	A	449	CYS	CA-CB-SG	-5.66	101.39	114.40
1	B	294	GLY	N-CA-C	-5.61	103.91	111.54
1	B	558	GLN	N-CA-C	5.60	122.72	110.80
1	B	291	THR	CB-CA-C	-5.57	102.00	111.02
1	B	421	ALA	N-CA-C	5.56	117.20	111.03
1	A	325	SER	N-CA-C	5.54	117.61	109.24
1	A	198	ASN	CA-C-N	-5.51	111.01	121.54
1	A	198	ASN	C-N-CA	-5.51	111.01	121.54
1	B	467	ARG	N-CA-C	5.49	116.61	108.86
1	A	355	VAL	CB-CA-C	-5.49	104.24	111.70
1	A	24	ASP	N-CA-C	-5.48	101.40	109.62
1	B	7	THR	CB-CA-C	5.48	120.96	110.17
1	B	144	PRO	CB-CA-C	5.47	117.59	110.92
1	B	602	LYS	N-CA-C	5.43	117.95	110.35
1	B	549	TRP	N-CA-CB	5.37	119.57	110.49
1	A	349	ILE	CA-C-N	-5.36	115.33	122.72
1	A	349	ILE	C-N-CA	-5.36	115.33	122.72
1	B	262	CYS	N-CA-C	5.36	117.79	110.24
1	A	452	HIS	N-CA-CB	5.33	117.88	110.04
1	B	338	LEU	N-CA-C	-5.30	105.19	110.97
1	A	238	ASN	N-CA-C	5.30	121.52	109.81
1	A	593	PHE	N-CA-C	5.30	118.16	110.42
1	A	340	TRP	N-CA-CB	-5.29	108.14	114.17
1	B	200	ALA	N-CA-C	5.28	117.14	110.33
1	B	549	TRP	CA-CB-CG	-5.27	103.59	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	HIS	N-CA-C	5.24	121.99	114.39
1	A	1	MSE	N-CA-CB	-5.16	102.46	110.46
1	B	304	LYS	CB-CA-C	-5.15	103.58	111.66
1	B	58	ALA	N-CA-C	5.13	116.68	111.14
1	B	359	LEU	N-CA-C	-5.12	106.72	113.17
1	A	573	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	B	70	GLN	N-CA-C	5.11	116.74	108.26
1	A	233	THR	N-CA-C	5.10	116.17	108.07
1	A	16	ASP	N-CA-C	-5.09	106.90	113.01
1	A	355	VAL	N-CA-C	-5.09	102.06	109.29
1	A	247	GLY	N-CA-C	-5.09	101.13	113.18
1	B	550	ASN	N-CA-C	5.08	117.76	109.59
1	B	228	GLN	N-CA-C	5.07	117.35	107.71
1	B	144	PRO	CA-N-CD	-5.06	104.92	112.00
1	A	559	GLY	N-CA-C	5.05	116.97	110.96
1	A	602	LYS	N-CA-C	-5.02	100.42	108.55
1	B	312	VAL	CA-C-N	5.01	127.44	120.63
1	B	312	VAL	C-N-CA	5.01	127.44	120.63
1	B	300	ASP	CA-C-N	-5.01	112.22	122.58
1	B	300	ASP	C-N-CA	-5.01	112.22	122.58
1	B	220	ASP	N-CA-C	5.00	118.68	112.58

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ALA	Peptide
1	A	197	CYS	Peptide
1	A	373	GLU	Peptide
1	A	378	GLU	Peptide
1	A	455	THR	Peptide
1	A	549	TRP	Peptide
1	B	143	ILE	Peptide
1	B	17	GLY	Peptide
1	B	37	SER	Peptide
1	B	451	ALA	Peptide
1	B	8	PRO	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	4779	0	4554	619	1
1	B	4768	0	4532	710	4
2	A	123	0	0	74	3
2	B	91	0	0	59	0
All	All	9761	0	9086	1318	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

All (1318) 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:B:502:ILE:HD12	1:B:537:PHE:CE2	1.49	1.48
1:A:455:THR:CG2	1:A:456:ILE:HG22	1.50	1.41
1:B:198:ASN:CB	1:B:236:VAL:HG22	1.59	1.32
1:B:444:VAL:CG1	1:B:466:ASN:HD21	1.47	1.26
1:A:456:ILE:CG1	1:A:459:LEU:HB2	1.64	1.26
1:A:238:ASN:CG	1:A:239:PRO:HD3	1.63	1.23
1:B:449:CYS:SG	1:B:488:GLU:OE1	1.97	1.21
1:B:444:VAL:HG13	1:B:466:ASN:ND2	1.55	1.21
1:A:92:THR:HG21	1:A:171:HIS:ND1	1.56	1.20
1:B:452:HIS:O	1:B:453:THR:HG23	1.44	1.16
1:B:253:CYS:SG	1:B:264:ILE:HG22	1.85	1.15
1:A:502:ILE:HD13	1:A:537:PHE:CE2	1.80	1.15
1:A:448:PHE:HB3	1:A:452:HIS:HA	1.15	1.15
1:A:402:HIS:CD2	2:A:673:HOH:O	1.94	1.14
1:A:139:ASN:O	1:A:142:THR:HG22	1.46	1.14
1:B:92:THR:HG22	2:B:680:HOH:O	1.45	1.14
1:A:448:PHE:O	1:A:452:HIS:HB2	1.48	1.13
1:B:416:THR:HG21	1:B:453:THR:HA	1.28	1.13
1:A:237:VAL:CG1	1:A:238:ASN:H	1.61	1.12
1:B:273:SER:HB3	1:B:284:ASN:H	1.09	1.11
1:B:335:GLU:HA	2:B:662:HOH:O	0.94	1.10
1:A:456:ILE:HG13	1:A:459:LEU:HB2	1.27	1.10
1:B:213:SER:HB3	1:B:255:THR:HB	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:HB2	1:A:155:LYS:HB3	1.23	1.10
1:A:402:HIS:HD2	2:A:673:HOH:O	1.31	1.10
1:B:36:GLU:HG3	1:B:129:ARG:HH22	1.16	1.09
1:A:92:THR:HG21	1:A:171:HIS:CE1	1.88	1.09
1:A:455:THR:CG2	1:A:456:ILE:CG2	2.31	1.09
1:A:328:THR:C	2:A:711:HOH:O	1.92	1.09
1:B:198:ASN:HB2	1:B:236:VAL:HG22	1.17	1.09
1:B:466:ASN:HB2	1:B:504:GLU:HB2	1.30	1.09
1:A:151:ASP:CB	1:A:155:LYS:HB3	1.83	1.08
1:A:92:THR:O	1:A:110:GLY:CA	2.01	1.08
1:A:183:TRP:HB3	2:A:715:HOH:O	1.52	1.07
1:B:444:VAL:HG13	1:B:466:ASN:HD21	0.92	1.07
1:B:36:GLU:HG3	1:B:129:ARG:NH2	1.68	1.07
1:B:69:TYR:CD1	1:B:170:ILE:HD12	1.88	1.07
1:A:361:LEU:HA	2:A:717:HOH:O	1.52	1.06
1:A:448:PHE:HB3	1:A:452:HIS:CA	1.85	1.06
1:B:502:ILE:CD1	1:B:537:PHE:HE2	1.68	1.06
1:B:566:ASN:HB3	1:B:568:LYS:HD2	1.36	1.05
1:A:455:THR:HG22	1:A:456:ILE:HG22	1.09	1.05
1:A:455:THR:HG23	1:A:456:ILE:CG2	1.87	1.05
1:B:447:MSE:HE3	1:B:467:ARG:HB3	1.34	1.05
1:B:144:PRO:HD2	1:B:353:ALA:O	1.55	1.04
1:B:502:ILE:CD1	1:B:537:PHE:CE2	2.41	1.04
1:B:69:TYR:CE1	1:B:170:ILE:HD12	1.91	1.04
1:A:17:GLY:HA2	1:A:47:VAL:HG13	1.04	1.03
1:A:455:THR:HG23	1:A:456:ILE:HG22	1.38	1.03
1:A:494:GLU:HG2	2:A:713:HOH:O	1.57	1.03
1:B:273:SER:O	1:B:283:ILE:HA	1.55	1.03
1:A:14:LYS:NZ	1:A:14:LYS:HB3	1.70	1.02
1:B:416:THR:CG2	1:B:453:THR:HA	1.88	1.02
1:A:338:LEU:HG	1:A:339:ASP:N	1.74	1.02
1:A:237:VAL:HG12	1:A:238:ASN:N	1.63	1.02
1:A:335:GLU:HA	2:A:614:HOH:O	0.84	1.01
1:B:92:THR:O	1:B:110:GLY:HA3	1.60	1.01
1:A:83:ARG:HB3	1:A:179:THR:O	1.57	1.00
1:A:92:THR:O	1:A:110:GLY:HA3	1.61	1.00
1:A:343:GLU:OE1	2:A:615:HOH:O	1.77	1.00
1:B:549:TRP:HZ3	1:B:568:LYS:NZ	1.58	1.00
1:B:337:MSE:HE1	1:B:348:VAL:HG21	1.41	0.99
1:A:179:THR:HB	2:A:715:HOH:O	1.61	0.99
1:A:10:ARG:HD2	1:A:79:TRP:HE1	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:HH11	1:B:334:ALA:HB2	1.25	0.99
1:B:143:ILE:HG23	1:B:353:ALA:O	1.62	0.98
1:B:14:LYS:HD3	1:B:174:VAL:O	1.62	0.98
1:B:282:LEU:HD23	1:B:285:HIS:HA	1.43	0.98
1:B:198:ASN:HB3	1:B:236:VAL:HG22	1.43	0.97
1:B:273:SER:HB3	1:B:284:ASN:N	1.79	0.97
1:A:14:LYS:HD2	1:A:176:LEU:HB2	1.45	0.97
1:A:92:THR:HG22	2:A:666:HOH:O	1.62	0.97
1:B:15:LEU:CD2	1:B:173:SER:HB3	1.94	0.97
1:B:559:GLY:H	1:B:562:ARG:HH22	1.05	0.97
1:A:142:THR:HG23	1:A:144:PRO:O	1.65	0.97
1:A:456:ILE:HG12	1:A:459:LEU:HB2	1.42	0.97
1:A:233:THR:O	1:A:234:LEU:HD23	1.64	0.96
1:A:315:HIS:HD1	1:A:340:TRP:CD1	1.83	0.96
1:B:172:ARG:NH1	1:B:334:ALA:HB2	1.81	0.96
1:A:5:VAL:HG11	1:A:266:PRO:HD2	1.46	0.96
1:A:92:THR:CG2	1:A:171:HIS:ND1	2.28	0.96
1:A:39:LEU:HD22	1:A:70:GLN:HB2	1.45	0.96
1:A:92:THR:O	1:A:110:GLY:HA2	1.66	0.96
1:A:17:GLY:CA	1:A:47:VAL:HG13	1.95	0.95
1:B:36:GLU:HB2	1:B:101:ASN:HD21	1.28	0.95
1:B:96:LYS:HE2	1:B:103:GLU:OE2	1.66	0.95
1:B:15:LEU:HD22	1:B:173:SER:HA	1.48	0.95
1:B:118:VAL:C	1:B:120:PRO:HD3	1.92	0.95
1:B:92:THR:O	1:B:110:GLY:CA	2.15	0.95
1:B:299:ALA:HB2	1:B:310:LEU:HD11	1.47	0.94
1:B:502:ILE:HD12	1:B:537:PHE:CZ	2.01	0.94
1:A:237:VAL:HG12	1:A:238:ASN:H	0.78	0.94
1:A:502:ILE:CD1	1:A:537:PHE:CE2	2.49	0.94
1:B:15:LEU:HD22	1:B:173:SER:CB	1.98	0.94
1:B:325:SER:N	2:B:691:HOH:O	2.01	0.94
1:B:272:ARG:HG3	1:B:274:VAL:HG23	1.51	0.93
1:A:199:HIS:CE1	1:A:236:VAL:CG2	2.52	0.93
1:B:197:CYS:HB3	1:B:198:ASN:CG	1.93	0.93
1:A:8:PRO:HB2	2:A:610:HOH:O	1.68	0.93
1:B:197:CYS:HB3	1:B:198:ASN:CB	1.99	0.93
1:A:118:VAL:HG23	1:A:120:PRO:HD2	1.50	0.92
1:B:10:ARG:H	1:B:178:THR:HG22	1.34	0.92
1:A:101:ASN:OD1	1:A:129:ARG:NH2	2.01	0.92
1:B:15:LEU:HD22	1:B:173:SER:CA	1.99	0.92
1:B:462:VAL:HG22	1:B:499:PRO:HG2	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HG	1:A:339:ASP:H	1.35	0.92
1:B:144:PRO:CD	1:B:353:ALA:O	2.19	0.91
1:B:108:GLN:HG3	2:B:617:HOH:O	1.69	0.91
1:A:449:CYS:O	1:A:449:CYS:SG	2.30	0.90
1:A:378:GLU:O	1:A:378:GLU:HG3	1.71	0.90
1:B:417:ARG:HG2	1:B:418:PRO:HD3	1.53	0.90
1:B:465:LEU:H	1:B:465:LEU:HD12	1.37	0.90
1:A:328:THR:HG22	1:A:333:TYR:CG	2.07	0.90
1:B:198:ASN:CB	1:B:236:VAL:CG2	2.48	0.90
1:B:449:CYS:CB	1:B:488:GLU:OE1	2.20	0.90
1:A:455:THR:HG22	1:A:456:ILE:CG2	1.96	0.89
1:A:548:VAL:HG11	1:A:570:ILE:HD11	1.53	0.89
1:B:96:LYS:NZ	2:B:648:HOH:O	1.98	0.89
1:A:342:ASP:OD2	2:A:673:HOH:O	1.89	0.89
1:B:197:CYS:HB3	1:B:198:ASN:ND2	1.87	0.89
1:A:102:GLN:OE1	1:A:102:GLN:HA	1.74	0.88
1:A:110:GLY:O	2:A:666:HOH:O	1.89	0.88
1:A:14:LYS:HB3	1:A:14:LYS:HZ3	1.37	0.88
1:A:327:ARG:HH21	1:A:412:ASN:HD21	1.15	0.88
1:A:456:ILE:HG13	1:A:459:LEU:CB	2.04	0.88
1:B:429:ALA:O	1:B:433:ARG:HG2	1.74	0.88
1:A:327:ARG:HH21	1:A:412:ASN:ND2	1.70	0.88
1:B:191:THR:HG22	1:B:200:ALA:HB2	1.56	0.88
1:B:197:CYS:HB3	1:B:198:ASN:HB3	1.56	0.87
1:B:10:ARG:HB2	1:B:10:ARG:HH11	1.34	0.87
1:B:382:GLY:O	1:B:386:GLN:HG2	1.74	0.87
1:B:253:CYS:SG	1:B:264:ILE:CG2	2.62	0.86
1:B:101:ASN:N	1:B:101:ASN:HD22	1.73	0.86
1:B:10:ARG:HH11	1:B:10:ARG:CB	1.87	0.86
1:B:311:MSE:HE2	1:B:336:GLU:HG2	1.56	0.86
1:B:470:GLY:H	1:B:529:TRP:HH2	1.23	0.86
1:A:548:VAL:HG11	1:A:570:ILE:CD1	2.06	0.86
1:B:105:MSE:SE	1:B:114:PHE:HB3	2.26	0.85
1:A:95:GLY:HA2	1:A:133:CYS:O	1.76	0.85
1:B:447:MSE:HE3	1:B:467:ARG:CB	2.05	0.85
1:A:15:LEU:HD23	1:A:173:SER:OG	1.77	0.85
1:B:86:LEU:O	1:B:105:MSE:HE1	1.77	0.85
1:B:101:ASN:HD22	1:B:101:ASN:H	1.25	0.85
1:B:302:ARG:HD3	2:B:645:HOH:O	1.77	0.84
1:A:74:PHE:CZ	1:B:7:THR:HA	2.11	0.84
1:A:84:ILE:HG22	1:A:176:LEU:HD11	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:CYS:HB2	1:A:198:ASN:OD1	1.75	0.84
1:B:451:ALA:HB2	2:B:677:HOH:O	1.76	0.84
1:B:10:ARG:HH12	1:B:79:TRP:HE1	1.26	0.84
1:B:15:LEU:CD2	1:B:173:SER:CB	2.54	0.84
1:A:17:GLY:HA3	1:A:47:VAL:H	1.41	0.84
1:B:36:GLU:HB2	1:B:101:ASN:ND2	1.92	0.84
1:B:471:TRP:HZ3	1:B:520:MSE:HG2	1.42	0.84
1:B:184:VAL:HG21	1:B:254:VAL:HG12	1.60	0.84
1:A:33:ARG:HB3	1:A:36:GLU:OE2	1.78	0.84
1:B:172:ARG:HH11	1:B:334:ALA:CB	1.89	0.84
1:B:198:ASN:HB3	1:B:236:VAL:CG2	2.06	0.83
1:B:328:THR:HA	1:B:333:TYR:CZ	2.13	0.83
1:B:45:ILE:HG13	1:B:55:PHE:HZ	1.43	0.83
1:A:186:ASP:HB3	1:A:206:VAL:CG1	2.08	0.83
1:B:10:ARG:NH1	1:B:79:TRP:HE1	1.75	0.83
1:B:172:ARG:NH1	1:B:334:ALA:CB	2.42	0.83
1:B:453:THR:HG21	1:B:456:ILE:HB	1.60	0.83
1:A:0:HIS:NE2	1:A:186:ASP:OD2	2.11	0.82
1:B:5:VAL:HG12	1:B:6:GLU:N	1.93	0.82
1:A:199:HIS:CE1	1:A:236:VAL:HG21	2.15	0.82
1:B:143:ILE:HG23	1:B:144:PRO:HD2	1.58	0.82
1:B:376:SER:HB2	2:B:643:HOH:O	1.78	0.82
1:B:327:ARG:NH1	1:B:503:THR:HB	1.93	0.82
1:A:45:ILE:HD12	1:A:55:PHE:CZ	2.15	0.82
1:B:241:LEU:H	1:B:241:LEU:HD23	1.45	0.82
1:B:400:LYS:HA	1:B:439:ARG:HH12	1.43	0.82
1:A:243:GLN:O	1:A:246:GLU:O	1.98	0.82
1:B:511:ALA:O	1:B:523:GLU:OE1	1.97	0.82
1:A:217:ARG:O	1:A:222:GLN:O	1.97	0.82
1:B:502:ILE:HD12	1:B:537:PHE:HE2	0.90	0.82
1:A:228:GLN:HA	1:A:228:GLN:NE2	1.95	0.81
1:B:83:ARG:HA	1:B:119:THR:OG1	1.78	0.81
1:B:143:ILE:HD11	1:B:388:HIS:HA	1.59	0.81
1:A:14:LYS:NZ	1:A:14:LYS:CB	2.42	0.81
1:A:218:ASP:HB2	1:A:221:GLN:HA	1.62	0.81
1:A:339:ASP:CB	2:A:722:HOH:O	2.28	0.81
1:A:297:GLU:O	1:A:304:LYS:HD3	1.81	0.81
1:A:361:LEU:HD23	2:A:717:HOH:O	1.80	0.81
1:B:15:LEU:HB3	1:B:174:VAL:H	1.46	0.81
1:A:332:PRO:HG3	1:A:395:LEU:HD12	1.61	0.81
1:A:566:ASN:HB3	2:A:635:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:THR:H	1:A:448:PHE:HE2	1.28	0.81
1:A:448:PHE:CB	1:A:452:HIS:HA	2.05	0.81
1:A:502:ILE:HD13	1:A:537:PHE:HE2	1.46	0.81
1:B:202:VAL:HG23	1:B:234:LEU:CD2	2.11	0.81
1:A:329:SER:O	1:A:330:HIS:ND1	2.13	0.80
1:B:392:ILE:O	1:B:396:ILE:HG13	1.81	0.80
1:B:272:ARG:HH21	1:B:439:ARG:HH21	1.28	0.80
1:B:21:PHE:CD2	1:B:45:ILE:HD12	2.16	0.80
1:B:465:LEU:HD12	1:B:465:LEU:N	1.97	0.80
1:B:36:GLU:HG2	1:B:37:SER:H	1.47	0.80
1:B:328:THR:HA	1:B:333:TYR:CE2	2.17	0.80
1:B:549:TRP:CZ3	1:B:568:LYS:NZ	2.42	0.79
1:B:341:ALA:HB1	1:B:404:SER:HB3	1.62	0.79
1:B:36:GLU:HG2	1:B:37:SER:N	1.97	0.79
1:B:327:ARG:HH12	1:B:504:GLU:HG3	1.46	0.79
1:B:466:ASN:HB3	1:B:504:GLU:H	1.47	0.79
1:B:375:TYR:CE1	1:B:379:ALA:HB2	2.18	0.79
1:B:470:GLY:N	1:B:529:TRP:HH2	1.80	0.79
1:A:105:MSE:HE1	1:A:115:GLU:HA	1.62	0.79
1:A:64:VAL:O	1:A:136:ASN:ND2	2.16	0.79
1:A:513:LEU:HD23	1:A:521:TRP:O	1.82	0.79
1:B:225:ALA:HB1	1:B:235:GLN:HG3	1.65	0.79
1:A:202:VAL:HG22	1:A:234:LEU:CD2	2.13	0.79
1:A:340:TRP:C	2:A:695:HOH:O	2.24	0.79
1:B:444:VAL:CG1	1:B:466:ASN:ND2	2.28	0.79
1:A:199:HIS:ND1	1:A:236:VAL:HB	1.98	0.79
1:B:202:VAL:HG23	1:B:234:LEU:HD21	1.64	0.79
1:B:466:ASN:HB3	1:B:504:GLU:N	1.98	0.78
1:A:172:ARG:NE	1:A:334:ALA:HB2	1.98	0.78
1:B:92:THR:CG2	1:B:93:HIS:N	2.47	0.78
1:A:17:GLY:HA2	1:A:47:VAL:CG1	2.01	0.78
1:A:45:ILE:HD12	1:A:55:PHE:HZ	1.46	0.78
1:A:71:ARG:HG2	1:A:71:ARG:HH11	1.49	0.78
1:B:92:THR:HA	2:B:657:HOH:O	1.82	0.78
1:B:466:ASN:HB2	1:B:504:GLU:CB	2.14	0.78
1:B:449:CYS:HB2	1:B:488:GLU:OE1	1.83	0.78
1:B:549:TRP:CD1	1:B:549:TRP:O	2.36	0.78
1:B:92:THR:HG23	1:B:93:HIS:N	1.97	0.78
1:B:590:GLY:O	2:B:641:HOH:O	2.00	0.78
1:A:199:HIS:HE1	1:A:236:VAL:HG21	1.49	0.77
1:A:340:TRP:O	1:A:346:ILE:HD12	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ILE:HG21	1:A:432:THR:HG22	1.66	0.77
1:B:315:HIS:HE1	1:B:336:GLU:OE1	1.67	0.77
1:B:52:ASN:HD21	1:B:168:ALA:H	1.30	0.77
1:A:238:ASN:CB	1:A:239:PRO:HD3	2.13	0.77
1:A:327:ARG:NH2	1:A:412:ASN:HD21	1.83	0.77
1:B:99:VAL:HG12	1:B:100:ASN:N	1.99	0.77
1:B:452:HIS:O	1:B:453:THR:CG2	2.32	0.77
1:B:508:ASP:OD2	1:B:568:LYS:HG2	1.84	0.77
1:A:15:LEU:HD22	1:A:48:PRO:HD3	1.67	0.76
1:B:122:VAL:CG2	1:B:123:ILE:HD12	2.16	0.76
1:A:392:ILE:HD13	1:A:432:THR:CG2	2.16	0.76
1:B:167:TYR:HB2	1:B:304:LYS:HG3	1.67	0.76
1:B:500:ILE:N	2:B:665:HOH:O	2.10	0.76
1:A:218:ASP:HB2	1:A:220:ASP:O	1.83	0.76
1:A:100:ASN:HA	1:A:129:ARG:HH21	1.51	0.75
1:B:139:ASN:O	1:B:142:THR:HG22	1.85	0.75
1:A:216:LEU:HD21	1:A:250:TYR:HB3	1.68	0.75
1:B:105:MSE:HE2	1:B:116:ALA:HB3	1.67	0.75
1:B:498:GLN:HB2	1:B:499:PRO:HD2	1.66	0.75
1:B:436:ASP:OD2	1:B:438:THR:N	2.19	0.75
1:A:17:GLY:O	1:A:46:ALA:HA	1.87	0.75
1:A:15:LEU:CD2	1:A:173:SER:OG	2.34	0.75
1:B:5:VAL:HG12	1:B:6:GLU:H	1.49	0.75
1:A:373:GLU:OE1	1:A:374:LEU:HD23	1.87	0.75
1:B:202:VAL:CG2	1:B:234:LEU:HD21	2.16	0.75
1:A:203:ASP:OD1	1:A:233:THR:OG1	2.04	0.75
1:A:416:THR:HB	1:A:455:THR:HB	1.69	0.75
1:B:379:ALA:HA	1:B:381:ASN:HD22	1.51	0.74
1:A:433:ARG:NH1	1:A:461:ASP:OD1	2.21	0.74
1:A:242:TRP:CZ2	1:A:345:GLY:HA2	2.23	0.74
1:B:359:LEU:CD1	1:B:372:LYS:HZ3	1.99	0.74
1:A:328:THR:HG22	1:A:333:TYR:CD2	2.21	0.74
1:A:36:GLU:C	1:A:129:ARG:HH12	1.95	0.74
1:B:311:MSE:CE	1:B:336:GLU:HG2	2.18	0.74
1:B:562:ARG:HH11	1:B:562:ARG:CG	2.01	0.74
1:A:198:ASN:O	1:A:237:VAL:O	2.06	0.73
1:B:400:LYS:O	1:B:439:ARG:NH2	2.16	0.73
1:B:559:GLY:H	1:B:562:ARG:NH2	1.83	0.73
1:A:105:MSE:HB3	1:A:116:ALA:HB2	1.70	0.73
1:A:453:THR:CA	2:A:707:HOH:O	2.35	0.73
1:B:272:ARG:HH21	1:B:439:ARG:NH2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LYS:C	1:B:439:ARG:HH22	1.95	0.73
1:A:328:THR:O	2:A:711:HOH:O	1.94	0.73
1:A:452:HIS:ND1	1:A:453:THR:N	2.37	0.73
1:A:598:GLN:O	1:A:599:GLN:HG2	1.88	0.73
1:B:449:CYS:SG	1:B:488:GLU:CD	2.71	0.73
1:B:463:LEU:HD21	1:B:492:TRP:CZ3	2.23	0.73
1:B:562:ARG:HA	1:B:566:ASN:CG	2.14	0.73
1:A:311:MSE:SE	2:A:722:HOH:O	2.55	0.73
1:A:378:GLU:O	1:A:378:GLU:CG	2.36	0.73
1:B:292:GLY:O	1:B:547:GLN:HA	1.88	0.72
1:A:470:GLY:HA3	1:A:529:TRP:CH2	2.23	0.72
1:B:417:ARG:NH2	2:B:632:HOH:O	2.22	0.72
1:B:99:VAL:O	1:B:100:ASN:C	2.30	0.72
1:B:325:SER:OG	2:B:691:HOH:O	2.05	0.72
1:B:465:LEU:O	1:B:502:ILE:HG23	1.89	0.72
1:B:462:VAL:HG13	1:B:499:PRO:O	1.88	0.72
1:B:451:ALA:HA	1:B:495:LYS:HD2	1.69	0.72
1:A:84:ILE:CG2	1:A:176:LEU:HD11	2.19	0.72
1:B:195:GLN:CD	1:B:195:GLN:H	1.98	0.72
1:B:566:ASN:HB3	1:B:568:LYS:CD	2.18	0.72
1:B:547:GLN:CB	2:B:666:HOH:O	2.38	0.72
1:B:466:ASN:OD1	2:B:678:HOH:O	2.08	0.72
1:B:413:GLU:HG2	2:B:678:HOH:O	1.91	0.71
1:A:14:LYS:CB	1:A:14:LYS:HZ2	2.03	0.71
1:B:475:SER:HB2	1:B:520:MSE:HE1	1.73	0.71
1:A:207:VAL:CG1	1:A:210:GLY:H	2.04	0.71
1:A:228:GLN:HA	1:A:228:GLN:HE21	1.53	0.71
1:A:469:TYR:HE2	1:A:485:LEU:HD13	1.56	0.71
1:B:8:PRO:O	2:B:634:HOH:O	2.07	0.71
1:A:328:THR:OG1	1:A:350:ASP:HA	1.90	0.71
1:A:335:GLU:O	1:A:339:ASP:CB	2.39	0.71
1:B:449:CYS:SG	1:B:450:ASP:N	2.64	0.71
1:B:550:ASN:ND2	1:B:554:PHE:CE2	2.58	0.71
1:A:9:THR:HG23	1:A:178:THR:O	1.91	0.71
1:B:103:GLU:HB2	2:B:647:HOH:O	1.90	0.70
1:B:10:ARG:HH12	1:B:79:TRP:NE1	1.88	0.70
1:B:38:ALA:HB1	1:B:70:GLN:OE1	1.91	0.70
1:B:338:LEU:HB2	2:B:653:HOH:O	1.91	0.70
1:A:172:ARG:CD	1:A:334:ALA:HB2	2.21	0.70
1:A:363:ILE:O	1:A:561:LEU:HG	1.91	0.70
1:B:455:THR:O	1:B:459:LEU:HD12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:THR:HG22	1:A:395:LEU:HD13	1.72	0.70
1:B:447:MSE:HA	1:B:467:ARG:HD3	1.73	0.70
1:B:172:ARG:HD3	1:B:334:ALA:HB2	1.72	0.70
1:A:30:ILE:HA	1:A:35:TRP:HZ3	1.57	0.70
1:A:450:ASP:OD1	2:A:671:HOH:O	2.08	0.69
1:A:10:ARG:HB3	1:A:10:ARG:CZ	2.23	0.69
1:B:548:VAL:HG21	1:B:584:LEU:HD21	1.74	0.69
1:A:12:ILE:HG22	1:A:79:TRP:HH2	1.57	0.69
1:B:105:MSE:SE	1:B:114:PHE:CB	2.90	0.69
1:A:10:ARG:HD2	1:A:79:TRP:NE1	2.04	0.69
1:B:43:ARG:HD3	1:B:55:PHE:CE1	2.27	0.69
1:A:151:ASP:OD1	1:A:155:LYS:NZ	2.15	0.69
1:A:144:PRO:HG3	1:A:353:ALA:O	1.91	0.69
1:A:381:ASN:CB	1:A:383:GLU:HB2	2.21	0.69
1:B:15:LEU:HD13	1:B:48:PRO:HD3	1.73	0.69
1:B:197:CYS:CB	1:B:198:ASN:HB3	2.23	0.69
1:B:359:LEU:CD1	1:B:372:LYS:NZ	2.56	0.69
1:B:584:LEU:O	1:B:588:TRP:HB2	1.93	0.69
1:A:336:GLU:HA	2:A:722:HOH:O	1.91	0.69
1:A:232:GLY:O	1:A:233:THR:OG1	2.09	0.69
1:B:15:LEU:O	1:B:15:LEU:HD12	1.92	0.69
1:B:272:ARG:NH2	1:B:439:ARG:HH21	1.91	0.68
1:B:372:LYS:NZ	1:B:372:LYS:HB2	2.07	0.68
1:A:470:GLY:O	1:A:471:TRP:C	2.36	0.68
1:A:502:ILE:HD13	1:A:537:PHE:CZ	2.28	0.68
1:A:455:THR:C	1:A:456:ILE:HG22	2.19	0.68
1:B:45:ILE:HG13	1:B:55:PHE:CZ	2.27	0.68
1:B:413:GLU:CG	2:B:678:HOH:O	2.41	0.68
1:A:330:HIS:N	2:A:711:HOH:O	2.26	0.68
1:A:376:SER:O	1:A:380:VAL:HG23	1.93	0.68
1:A:198:ASN:HB3	1:A:199:HIS:HD2	1.58	0.68
1:A:199:HIS:CE1	1:A:236:VAL:HG23	2.28	0.68
1:A:207:VAL:HG11	1:A:210:GLY:H	1.58	0.68
1:B:5:VAL:CG1	1:B:6:GLU:H	2.06	0.68
1:B:33:ARG:NH1	1:B:36:GLU:HB3	2.09	0.68
1:B:358:ASN:HB3	1:B:360:SER:H	1.59	0.68
1:B:474:GLN:N	2:B:670:HOH:O	2.27	0.68
1:A:17:GLY:O	1:A:45:ILE:O	2.12	0.68
1:A:381:ASN:CB	1:A:383:GLU:H	2.05	0.68
1:B:216:LEU:H	1:B:226:THR:HG22	1.59	0.68
1:A:295:ARG:O	1:A:329:SER:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:CE2	1:A:97:VAL:HG21	2.29	0.68
1:B:92:THR:O	1:B:110:GLY:HA2	1.94	0.68
1:B:202:VAL:CG1	1:B:204:TRP:HZ3	2.07	0.68
1:B:273:SER:CB	1:B:284:ASN:H	1.97	0.68
1:B:562:ARG:HH11	1:B:562:ARG:CB	2.05	0.68
1:A:247:GLY:C	2:A:693:HOH:O	2.37	0.67
1:B:212:VAL:HG11	1:B:230:THR:N	2.09	0.67
1:B:549:TRP:CD1	1:B:549:TRP:C	2.66	0.67
1:A:456:ILE:HB	1:A:459:LEU:HD12	1.76	0.67
1:B:91:VAL:CG1	1:B:134:VAL:CG1	2.72	0.67
1:B:341:ALA:HA	1:B:346:ILE:HB	1.75	0.67
1:B:338:LEU:HD12	1:B:339:ASP:N	2.09	0.67
1:A:238:ASN:CG	1:A:239:PRO:CD	2.57	0.67
1:B:462:VAL:HG22	1:B:499:PRO:CG	2.24	0.67
1:A:93:HIS:N	2:A:704:HOH:O	2.20	0.67
1:B:5:VAL:CG1	1:B:6:GLU:N	2.58	0.67
1:B:197:CYS:CB	1:B:198:ASN:ND2	2.57	0.67
1:A:83:ARG:HD3	1:A:179:THR:OG1	1.93	0.66
1:A:497:HIS:HD2	2:A:687:HOH:O	1.77	0.66
1:A:315:HIS:O	1:A:319:ASP:HB2	1.95	0.66
1:B:493:GLN:HG3	2:B:644:HOH:O	1.96	0.66
1:A:94:TYR:HB3	1:A:135:ASN:HB3	1.76	0.66
1:A:118:VAL:HG23	1:A:120:PRO:CD	2.22	0.66
1:A:457:SER:HB2	1:A:496:LEU:HD11	1.76	0.66
1:B:202:VAL:HG12	1:B:230:THR:O	1.95	0.66
1:B:52:ASN:ND2	1:B:168:ALA:H	1.94	0.66
1:B:296:HIS:HD2	1:B:550:ASN:HD21	1.43	0.66
1:B:302:ARG:CG	1:B:302:ARG:O	2.43	0.66
1:B:337:MSE:CE	1:B:348:VAL:HG21	2.21	0.66
1:B:190:VAL:HG21	1:B:438:THR:HG21	1.76	0.66
1:A:190:VAL:HG13	1:A:438:THR:HG21	1.76	0.66
1:B:184:VAL:HG12	1:B:185:ASP:N	2.11	0.66
1:B:288:PHE:HZ	1:B:347:VAL:HG21	1.61	0.66
1:B:355:VAL:HA	2:B:683:HOH:O	1.96	0.66
1:B:455:THR:O	1:B:459:LEU:CD1	2.43	0.66
1:A:93:HIS:C	2:A:705:HOH:O	2.39	0.65
1:B:333:TYR:O	1:B:398:ARG:NH2	2.29	0.65
1:A:187:ILE:HG22	1:A:188:THR:N	2.11	0.65
1:A:456:ILE:HG23	1:A:456:ILE:O	1.95	0.65
1:B:432:THR:OG1	1:B:441:ILE:HD13	1.96	0.65
1:A:187:ILE:HG22	1:A:188:THR:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:HH11	1:B:503:THR:HB	1.60	0.65
1:A:278:GLY:O	1:A:279:GLU:HB3	1.96	0.65
1:B:122:VAL:HG23	1:B:123:ILE:HD12	1.79	0.65
1:B:12:ILE:HG23	1:B:12:ILE:O	1.95	0.65
1:B:449:CYS:C	1:B:452:HIS:HB2	2.21	0.65
1:A:20:ALA:HB3	1:A:70:GLN:HB3	1.79	0.65
1:A:136:ASN:C	1:A:136:ASN:HD22	2.05	0.65
1:A:381:ASN:HB2	1:A:383:GLU:HB2	1.77	0.65
1:A:17:GLY:HA3	1:A:47:VAL:O	1.96	0.65
1:B:115:GLU:OE1	1:B:115:GLU:HA	1.96	0.65
1:B:448:PHE:HD1	1:B:448:PHE:O	1.79	0.65
1:B:547:GLN:HB3	2:B:666:HOH:O	1.97	0.65
1:B:559:GLY:N	1:B:562:ARG:HH22	1.87	0.65
1:B:191:THR:HG22	1:B:200:ALA:CB	2.27	0.65
1:A:195:GLN:O	1:A:195:GLN:HG3	1.97	0.64
1:A:107:HIS:HE1	1:A:394:GLU:OE1	1.81	0.64
1:B:442:THR:OG1	1:B:443:CYS:N	2.26	0.64
1:A:436:ASP:OD1	1:A:439:ARG:NH1	2.30	0.64
1:A:546:GLU:OE2	1:A:587:ARG:NH1	2.30	0.64
1:A:33:ARG:HB3	1:A:36:GLU:CD	2.22	0.64
1:B:150:THR:O	2:B:642:HOH:O	2.14	0.64
1:B:414:PRO:HA	2:B:679:HOH:O	1.97	0.64
1:A:5:VAL:HG11	1:A:266:PRO:CD	2.26	0.64
1:B:241:LEU:H	1:B:241:LEU:CD2	2.11	0.64
1:B:542:ALA:O	2:B:665:HOH:O	2.15	0.64
1:B:14:LYS:CD	1:B:174:VAL:O	2.42	0.64
1:B:351:GLU:HG2	1:B:409:SER:HB3	1.80	0.64
1:A:238:ASN:CB	1:A:239:PRO:CD	2.76	0.64
1:A:497:HIS:CD2	2:A:687:HOH:O	2.50	0.64
1:B:292:GLY:HA2	1:B:323:ALA:HB1	1.80	0.64
1:B:560:ILE:O	1:B:562:ARG:N	2.31	0.64
1:B:466:ASN:CB	1:B:504:GLU:H	2.11	0.63
1:A:82:GLN:HA	1:A:82:GLN:NE2	2.11	0.63
1:A:14:LYS:HE2	1:A:73:VAL:HG21	1.80	0.63
1:A:172:ARG:HD3	1:A:334:ALA:HB2	1.81	0.63
1:B:33:ARG:HA	1:B:35:TRP:CZ3	2.34	0.63
1:B:359:LEU:HD12	1:B:372:LYS:NZ	2.13	0.63
1:A:340:TRP:O	1:A:340:TRP:HD1	1.82	0.63
1:B:482:GLU:HG3	1:B:536:VAL:HG21	1.80	0.63
1:B:517:TYR:O	1:B:519:ASP:N	2.32	0.63
1:B:526:GLN:O	1:B:530:LEU:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ARG:O	1:B:539:ARG:HB2	1.99	0.63
1:A:102:GLN:HG3	1:A:121:TYR:CD1	2.34	0.63
1:B:355:VAL:HG23	1:B:412:ASN:HD22	1.63	0.63
1:B:562:ARG:HH11	1:B:562:ARG:HG3	1.62	0.63
1:A:30:ILE:HB	2:A:694:HOH:O	1.98	0.63
1:A:186:ASP:HB3	1:A:206:VAL:HG11	1.80	0.63
1:A:455:THR:O	1:A:456:ILE:HG22	1.98	0.63
1:A:455:THR:HG23	1:A:456:ILE:HG21	1.80	0.63
1:B:468:TYR:N	1:B:468:TYR:CD2	2.67	0.63
1:B:501:ILE:HG12	1:B:545:GLY:HA3	1.81	0.63
1:A:9:THR:CG2	1:A:178:THR:O	2.47	0.63
1:A:485:LEU:HD23	1:A:536:VAL:HG11	1.80	0.63
1:B:69:TYR:CD1	1:B:170:ILE:CD1	2.75	0.63
1:A:329:SER:N	2:A:711:HOH:O	2.19	0.62
1:A:186:ASP:HB3	1:A:206:VAL:HG13	1.81	0.62
1:B:61:ARG:NH1	2:B:624:HOH:O	2.32	0.62
1:B:359:LEU:HD11	1:B:372:LYS:HZ3	1.62	0.62
1:B:392:ILE:HD13	1:B:410:ILE:HG23	1.80	0.62
1:A:279:GLU:O	1:A:279:GLU:HG2	1.99	0.62
1:B:31:ASP:HB2	2:B:675:HOH:O	1.99	0.62
1:B:402:HIS:CE1	2:B:638:HOH:O	2.52	0.62
1:A:476:GLY:N	1:A:520:MSE:HE2	2.14	0.62
1:B:465:LEU:HD11	1:B:500:ILE:HG12	1.81	0.62
1:A:7:THR:O	1:A:9:THR:O	2.17	0.62
1:A:73:VAL:HG22	1:A:74:PHE:H	1.64	0.62
1:A:136:ASN:ND2	1:A:136:ASN:C	2.57	0.62
1:A:447:MSE:O	1:A:448:PHE:HD1	1.82	0.62
1:B:99:VAL:CG1	1:B:100:ASN:N	2.62	0.62
1:B:591:MSE:HE2	1:B:597:PRO:HD3	1.81	0.62
1:A:351:GLU:HG2	1:A:409:SER:OG	2.00	0.62
1:A:455:THR:HG22	1:A:455:THR:O	1.98	0.62
1:B:151:ASP:OD1	1:B:152:GLU:N	2.31	0.62
1:B:241:LEU:O	1:B:243:GLN:HG3	1.99	0.62
1:A:217:ARG:HG3	1:A:218:ASP:HB3	1.80	0.62
2:A:662:HOH:O	1:B:12:ILE:HD11	1.99	0.62
1:B:-1:SER:C	1:B:0:HIS:ND1	2.57	0.62
1:B:36:GLU:CG	1:B:37:SER:H	2.13	0.62
1:B:36:GLU:HA	1:B:129:ARG:NH1	2.15	0.62
1:A:520:MSE:O	1:A:521:TRP:HB2	1.99	0.62
1:B:119:THR:N	1:B:120:PRO:HD3	2.15	0.62
1:A:14:LYS:HB3	1:A:14:LYS:HZ2	1.56	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:THR:C	2:A:707:HOH:O	2.42	0.61
1:B:119:THR:HG21	2:B:693:HOH:O	2.00	0.61
1:B:182:THR:HG21	1:B:258:SER:HB2	1.81	0.61
1:B:372:LYS:N	1:B:373:GLU:HA	2.15	0.61
1:B:570:ILE:HD13	1:B:584:LEU:HD22	1.81	0.61
1:A:207:VAL:HG11	1:A:210:GLY:O	2.00	0.61
1:A:340:TRP:CD1	1:A:340:TRP:O	2.53	0.61
1:A:372:LYS:HB2	1:A:373:GLU:OE2	2.00	0.61
1:A:525:TYR:O	1:A:526:GLN:C	2.40	0.61
1:A:51:PHE:C	1:A:51:PHE:CD1	2.78	0.61
1:A:452:HIS:CD2	1:A:492:TRP:HH2	2.18	0.61
1:A:525:TYR:HB3	2:A:708:HOH:O	1.98	0.61
1:B:94:TYR:HB2	1:B:108:GLN:OE1	2.00	0.61
1:B:321:ILE:HG12	1:B:321:ILE:O	1.99	0.61
1:A:218:ASP:CB	1:A:221:GLN:HA	2.29	0.61
1:B:21:PHE:CE2	1:B:45:ILE:HD12	2.35	0.61
1:B:139:ASN:HA	1:B:146:GLY:O	2.00	0.61
1:B:172:ARG:NH1	1:B:334:ALA:N	2.48	0.61
1:B:212:VAL:HG22	1:B:230:THR:HG22	1.83	0.61
1:B:375:TYR:CD1	1:B:379:ALA:HB2	2.35	0.61
1:B:509:THR:HG21	1:B:526:GLN:HB2	1.83	0.61
1:A:228:GLN:NE2	1:A:228:GLN:CA	2.63	0.61
1:A:452:HIS:CE1	1:A:453:THR:O	2.54	0.61
1:B:212:VAL:CG2	1:B:230:THR:HG22	2.31	0.61
1:A:214:VAL:HG12	1:A:227:GLY:HA3	1.83	0.61
1:B:388:HIS:HD2	1:B:392:ILE:HD11	1.65	0.61
1:B:519:ASP:O	1:B:525:TYR:HB2	2.01	0.61
1:B:386:GLN:O	1:B:389:LEU:HB3	2.01	0.60
1:A:304:LYS:NZ	2:A:656:HOH:O	2.34	0.60
1:A:562:ARG:NH1	1:A:566:ASN:HD22	1.99	0.60
1:B:92:THR:CG2	1:B:93:HIS:H	2.14	0.60
1:B:187:ILE:HA	1:B:204:TRP:HB2	1.83	0.60
1:B:195:GLN:CD	1:B:195:GLN:N	2.58	0.60
1:B:293:PHE:HZ	1:B:321:ILE:HD13	1.66	0.60
1:A:422:ARG:HB2	1:A:454:ASP:HB2	1.83	0.60
1:A:468:TYR:OH	1:A:568:LYS:HD3	2.02	0.60
1:A:476:GLY:N	1:A:520:MSE:CE	2.64	0.60
1:A:550:ASN:ND2	1:A:554:PHE:CE2	2.70	0.60
1:B:357:PHE:C	1:B:358:ASN:OD1	2.44	0.60
1:B:402:HIS:CG	2:B:654:HOH:O	2.54	0.60
1:B:445:ASN:C	1:B:445:ASN:OD1	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HD12	2:A:698:HOH:O	2.01	0.60
1:B:105:MSE:HE2	1:B:116:ALA:CB	2.31	0.60
1:A:10:ARG:CD	1:A:79:TRP:HE1	2.08	0.60
1:A:376:SER:O	1:A:380:VAL:CG2	2.49	0.60
1:B:467:ARG:HB2	1:B:469:TYR:CZ	2.37	0.60
1:A:-1:SER:O	1:A:0:HIS:CB	2.48	0.60
1:A:450:ASP:O	1:A:452:HIS:O	2.19	0.60
1:B:143:ILE:CG2	1:B:144:PRO:HD2	2.30	0.59
1:B:379:ALA:HA	1:B:381:ASN:ND2	2.17	0.59
1:B:33:ARG:HA	1:B:35:TRP:CH2	2.37	0.59
1:B:184:VAL:HG12	1:B:185:ASP:H	1.67	0.59
1:B:341:ALA:HB1	1:B:404:SER:CB	2.30	0.59
1:B:444:VAL:HA	1:B:464:CYS:O	2.02	0.59
1:A:172:ARG:HD3	1:A:334:ALA:CB	2.32	0.59
1:A:238:ASN:OD1	1:A:239:PRO:HD3	1.98	0.59
1:A:469:TYR:CE2	1:A:485:LEU:HD13	2.35	0.59
1:B:143:ILE:HD13	1:B:391:ALA:HB2	1.85	0.59
1:B:417:ARG:CG	1:B:418:PRO:HD3	2.30	0.59
1:B:547:GLN:HB2	2:B:666:HOH:O	1.99	0.59
1:B:562:ARG:HG2	1:B:566:ASN:ND2	2.16	0.59
1:A:105:MSE:CE	1:A:114:PHE:O	2.50	0.59
1:B:184:VAL:HG21	1:B:254:VAL:CG1	2.29	0.59
1:B:99:VAL:HG23	1:B:104:VAL:HG21	1.84	0.59
1:B:455:THR:CG2	1:B:456:ILE:HG13	2.33	0.59
1:A:202:VAL:HG22	1:A:234:LEU:HD22	1.85	0.59
1:A:202:VAL:HG22	1:A:234:LEU:HD21	1.81	0.59
1:B:91:VAL:HG22	1:B:170:ILE:HG12	1.84	0.59
1:B:562:ARG:HH11	1:B:562:ARG:HB2	1.67	0.59
1:A:321:ILE:O	1:A:321:ILE:HG23	2.02	0.59
1:B:470:GLY:N	1:B:529:TRP:CH2	2.66	0.59
1:B:68:TRP:CZ3	1:B:133:CYS:HB2	2.37	0.59
1:B:359:LEU:HD11	1:B:372:LYS:NZ	2.17	0.59
1:B:494:GLU:O	1:B:495:LYS:C	2.45	0.59
1:A:216:LEU:HD21	1:A:250:TYR:CB	2.33	0.59
1:B:520:MSE:HB3	1:B:521:TRP:HD1	1.66	0.59
1:B:99:VAL:HG12	1:B:100:ASN:H	1.67	0.58
1:A:456:ILE:O	1:A:460:PHE:HD2	1.86	0.58
1:B:211:ASP:O	1:B:256:ALA:HA	2.04	0.58
1:B:273:SER:HB3	1:B:284:ASN:CA	2.33	0.58
1:B:295:ARG:HH12	1:B:314:ASP:HB3	1.69	0.58
1:B:299:ALA:CB	1:B:310:LEU:HD11	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:TRP:CE3	1:B:184:VAL:O	2.56	0.58
1:B:184:VAL:CG1	1:B:185:ASP:H	2.15	0.58
1:B:416:THR:HG23	1:B:453:THR:HA	1.83	0.58
1:A:36:GLU:HB2	2:A:714:HOH:O	2.04	0.58
1:B:102:GLN:HB2	2:B:668:HOH:O	2.02	0.58
1:A:36:GLU:C	1:A:129:ARG:NH1	2.62	0.58
1:A:249:LEU:HG	2:A:693:HOH:O	2.01	0.58
1:B:0:HIS:ND1	1:B:0:HIS:N	2.52	0.58
1:B:510:LEU:HD23	1:B:513:LEU:HD12	1.85	0.58
1:B:465:LEU:O	1:B:502:ILE:HA	2.03	0.58
1:A:143:ILE:HG22	1:A:353:ALA:HB3	1.84	0.58
1:B:206:VAL:HG13	1:B:206:VAL:O	2.03	0.58
1:A:0:HIS:CD2	1:A:186:ASP:CG	2.82	0.58
1:A:338:LEU:O	1:A:342:ASP:HB2	2.04	0.58
1:A:486:GLU:OE2	1:A:539:ARG:HD2	2.04	0.58
1:B:91:VAL:O	1:B:110:GLY:HA2	2.03	0.58
1:B:453:THR:CG2	1:B:456:ILE:HB	2.30	0.58
1:A:104:VAL:O	2:A:655:HOH:O	2.16	0.57
1:B:298:ASP:OD2	1:B:554:PHE:HA	2.03	0.57
1:A:278:GLY:HA2	2:A:709:HOH:O	2.04	0.57
1:A:441:ILE:HD12	1:A:460:PHE:CE1	2.38	0.57
1:B:43:ARG:HD3	1:B:55:PHE:CD1	2.40	0.57
1:B:302:ARG:CD	2:B:645:HOH:O	2.44	0.57
1:B:412:ASN:O	2:B:683:HOH:O	2.17	0.57
1:A:315:HIS:HD1	1:A:340:TRP:CG	2.22	0.57
1:B:36:GLU:CG	1:B:37:SER:N	2.66	0.57
1:A:195:GLN:O	1:A:195:GLN:CG	2.52	0.57
1:A:469:TYR:CD2	1:A:533:TYR:OH	2.57	0.57
1:B:466:ASN:CB	1:B:504:GLU:N	2.67	0.57
1:A:219:ALA:N	2:A:686:HOH:O	2.30	0.57
1:A:279:GLU:O	1:A:279:GLU:CG	2.52	0.57
1:B:292:GLY:HA3	1:B:325:SER:O	2.04	0.57
1:B:328:THR:OG1	1:B:331:TYR:O	2.20	0.57
1:A:94:TYR:O	1:A:134:VAL:HA	2.05	0.57
1:A:205:GLN:HB2	1:A:231:SER:H	1.69	0.57
1:A:343:GLU:N	2:A:695:HOH:O	2.36	0.57
1:A:187:ILE:HG12	1:A:205:GLN:NE2	2.19	0.57
1:A:468:TYR:CE2	1:A:549:TRP:HD1	2.23	0.57
1:B:83:ARG:NE	1:B:179:THR:HG23	2.20	0.57
1:B:208:ALA:O	1:B:210:GLY:N	2.35	0.57
1:B:216:LEU:HA	1:B:252:LEU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ARG:HE	1:B:439:ARG:HE	1.52	0.57
1:A:138:LEU:HD22	1:A:144:PRO:O	2.05	0.57
1:A:470:GLY:CA	1:A:529:TRP:CH2	2.88	0.57
1:B:82:GLN:CD	1:B:82:GLN:N	2.63	0.57
1:B:288:PHE:C	1:B:288:PHE:CD2	2.82	0.57
1:B:388:HIS:CD2	1:B:392:ILE:HD11	2.40	0.57
1:A:563:VAL:HG23	1:A:566:ASN:OD1	2.04	0.57
2:A:608:HOH:O	1:B:340:TRP:HH2	1.88	0.57
1:B:243:GLN:OE1	1:B:246:GLU:HB2	2.04	0.57
1:A:313:HIS:CD2	1:B:301:LEU:HD22	2.40	0.56
1:A:11:GLU:O	1:A:11:GLU:HG2	2.01	0.56
1:A:328:THR:HG22	1:A:333:TYR:CD1	2.39	0.56
1:B:217:ARG:HD3	1:B:222:GLN:C	2.30	0.56
1:A:0:HIS:CE1	1:A:206:VAL:HG11	2.40	0.56
1:A:475:SER:OG	1:A:520:MSE:HE1	2.05	0.56
1:B:385:GLN:HB2	1:B:424:TYR:CE1	2.41	0.56
1:B:465:LEU:CD1	1:B:500:ILE:HG23	2.35	0.56
1:A:14:LYS:CD	1:A:176:LEU:HB2	2.29	0.56
1:A:221:GLN:HG3	2:A:648:HOH:O	2.05	0.56
1:A:447:MSE:O	1:A:448:PHE:CD1	2.58	0.56
1:A:563:VAL:O	1:A:564:GLY:C	2.48	0.56
1:B:15:LEU:HD23	1:B:173:SER:HB3	1.82	0.56
1:A:335:GLU:O	1:A:335:GLU:CG	2.52	0.56
1:A:381:ASN:HB3	1:A:383:GLU:H	1.69	0.56
1:B:466:ASN:CB	1:B:504:GLU:HB2	2.21	0.56
1:B:288:PHE:HA	1:B:594:GLY:O	2.05	0.56
1:B:196:ASP:OD2	1:B:196:ASP:N	2.37	0.56
1:A:229:GLY:O	1:A:230:THR:C	2.49	0.56
1:B:36:GLU:HA	1:B:129:ARG:CZ	2.36	0.56
1:B:291:THR:HG1	1:B:324:ASN:H	1.52	0.56
1:A:309:VAL:HG21	1:B:302:ARG:HE	1.70	0.55
1:B:82:GLN:CD	1:B:82:GLN:H	2.14	0.55
1:B:94:TYR:HD2	1:B:135:ASN:HB2	1.72	0.55
1:B:218:ASP:HB2	1:B:248:TYR:OH	2.05	0.55
1:B:315:HIS:CE1	1:B:336:GLU:OE1	2.54	0.55
1:B:388:HIS:O	1:B:392:ILE:HG13	2.06	0.55
1:B:402:HIS:CB	2:B:654:HOH:O	2.53	0.55
1:B:415:ASP:N	2:B:679:HOH:O	1.92	0.55
1:B:41:GLU:HA	2:B:623:HOH:O	2.04	0.55
1:A:337:MSE:O	1:A:341:ALA:HB3	2.06	0.55
1:B:282:LEU:HA	1:B:286:LYS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:ASN:CB	1:B:568:LYS:HD2	2.24	0.55
1:B:570:ILE:CD1	1:B:584:LEU:HD22	2.37	0.55
1:B:216:LEU:C	1:B:216:LEU:HD12	2.32	0.55
1:B:467:ARG:C	1:B:468:TYR:CD2	2.84	0.55
1:A:450:ASP:CG	2:A:671:HOH:O	2.48	0.55
1:A:456:ILE:CB	1:A:459:LEU:HD12	2.36	0.55
1:B:377:GLU:HA	1:B:380:VAL:HG13	1.89	0.55
1:A:101:ASN:OD1	1:A:101:ASN:N	2.39	0.55
1:A:107:HIS:CD2	1:A:109:GLY:O	2.59	0.55
1:A:454:ASP:N	1:A:454:ASP:OD1	2.38	0.55
1:B:299:ALA:HB2	1:B:310:LEU:CD1	2.31	0.55
1:A:102:GLN:CG	1:A:121:TYR:CD1	2.90	0.55
1:B:187:ILE:HA	1:B:204:TRP:CB	2.37	0.55
1:B:402:HIS:HB3	2:B:654:HOH:O	2.06	0.55
1:A:73:VAL:O	1:A:127:SER:HA	2.07	0.55
1:A:372:LYS:C	1:A:373:GLU:HG3	2.31	0.55
1:A:475:SER:OG	1:A:520:MSE:CE	2.55	0.55
1:B:94:TYR:HD2	1:B:135:ASN:CB	2.20	0.55
1:B:99:VAL:CG1	1:B:100:ASN:H	2.20	0.55
1:B:249:LEU:HD21	1:B:268:ARG:HH11	1.71	0.55
1:B:455:THR:HG23	1:B:456:ILE:HG13	1.89	0.55
1:B:174:VAL:O	1:B:174:VAL:HG13	2.08	0.54
1:B:447:MSE:CE	1:B:467:ARG:HB3	2.23	0.54
1:A:12:ILE:CG2	1:A:79:TRP:HH2	2.20	0.54
1:A:315:HIS:CD2	1:A:318:MSE:HE3	2.42	0.54
1:A:562:ARG:HH11	1:A:566:ASN:HD22	1.53	0.54
1:B:18:LEU:H	1:B:46:ALA:HA	1.72	0.54
1:B:156:LYS:HD2	2:B:604:HOH:O	2.07	0.54
1:B:351:GLU:HG2	1:B:409:SER:CB	2.37	0.54
1:A:216:LEU:CD2	1:A:250:TYR:HB3	2.37	0.54
1:B:562:ARG:HB2	1:B:562:ARG:NH1	2.23	0.54
1:A:311:MSE:HE3	1:A:340:TRP:CE3	2.43	0.54
1:A:377:GLU:OE2	1:A:377:GLU:CA	2.55	0.54
1:A:417:ARG:NH2	2:A:625:HOH:O	2.40	0.54
1:B:25:ARG:C	1:B:27:ASN:N	2.63	0.54
1:A:17:GLY:CA	1:A:47:VAL:H	2.17	0.54
1:A:230:THR:C	1:A:231:SER:OG	2.50	0.54
1:A:456:ILE:CG1	1:A:459:LEU:CB	2.59	0.54
1:B:407:MSE:SE	1:B:442:THR:HG21	2.58	0.54
1:A:20:ALA:HB1	1:A:42:SER:HB2	1.90	0.54
1:A:100:ASN:C	1:A:101:ASN:OD1	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:CG2	1:A:234:LEU:HD22	2.38	0.54
1:B:359:LEU:HD12	1:B:372:LYS:HZ3	1.67	0.54
1:A:308:ASN:O	1:A:312:VAL:HG23	2.07	0.54
1:B:114:PHE:N	1:B:114:PHE:CD2	2.76	0.54
1:B:184:VAL:CG1	1:B:185:ASP:N	2.70	0.54
1:B:295:ARG:HG3	1:B:326:TYR:CD1	2.42	0.54
1:A:12:ILE:CG2	1:A:176:LEU:HB3	2.38	0.54
1:A:216:LEU:C	1:A:216:LEU:HD22	2.33	0.54
1:A:469:TYR:HD2	1:A:533:TYR:OH	1.91	0.54
1:A:535:ARG:HA	2:A:650:HOH:O	2.07	0.54
1:B:51:PHE:CE2	1:B:168:ALA:HB3	2.43	0.54
1:A:0:HIS:CD2	1:A:186:ASP:OD2	2.60	0.53
1:B:144:PRO:HD3	1:B:353:ALA:O	2.04	0.53
1:A:12:ILE:HG23	1:A:12:ILE:O	2.09	0.53
1:A:242:TRP:HZ2	1:A:345:GLY:HA2	1.74	0.53
1:A:548:VAL:CG1	1:A:570:ILE:CD1	2.84	0.53
1:B:52:ASN:ND2	1:B:167:TYR:HA	2.23	0.53
1:B:15:LEU:CD2	1:B:173:SER:CA	2.80	0.53
1:B:122:VAL:HG23	1:B:123:ILE:CD1	2.37	0.53
1:B:138:LEU:HD13	1:B:144:PRO:O	2.08	0.53
1:B:293:PHE:CE1	1:B:570:ILE:HD12	2.43	0.53
1:A:39:LEU:HB2	1:A:70:GLN:HE21	1.73	0.53
1:A:147:MSE:HE3	1:A:161:PHE:HZ	1.74	0.53
1:A:479:GLU:OE1	1:A:479:GLU:N	2.30	0.53
1:B:217:ARG:NH1	1:B:223:VAL:HG22	2.24	0.53
1:B:398:ARG:HG2	1:B:399:ASP:OD1	2.08	0.53
1:B:469:TYR:CD2	1:B:485:LEU:HD13	2.43	0.53
1:B:407:MSE:SE	1:B:442:THR:CG2	3.06	0.53
1:B:445:ASN:ND2	1:B:465:LEU:HB3	2.24	0.53
1:A:86:LEU:HB2	1:A:176:LEU:HD22	1.89	0.53
1:A:224:VAL:HG22	1:A:237:VAL:HG21	1.91	0.53
1:B:96:LYS:CE	1:B:103:GLU:OE2	2.50	0.53
1:B:450:ASP:N	1:B:452:HIS:HB2	2.23	0.53
1:A:81:GLY:C	1:A:82:GLN:HE21	2.15	0.53
1:A:205:GLN:HG3	1:A:212:VAL:HG21	1.89	0.53
1:A:297:GLU:O	1:A:304:LYS:HA	2.08	0.53
1:B:183:TRP:HE3	1:B:184:VAL:O	1.92	0.53
1:B:241:LEU:O	1:B:243:GLN:NE2	2.41	0.53
1:B:276:VAL:HG21	1:B:461:ASP:HB3	1.90	0.53
1:B:375:TYR:CD1	1:B:379:ALA:CB	2.92	0.53
1:B:467:ARG:HH21	1:B:492:TRP:HE1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:VAL:HA	1:A:255:THR:O	2.09	0.53
1:B:193:VAL:HG11	1:B:271:ILE:CG2	2.39	0.53
1:B:202:VAL:HG23	1:B:234:LEU:HD22	1.90	0.53
1:B:495:LYS:HG2	1:B:496:LEU:HG	1.91	0.53
1:A:140:TRP:HB3	1:A:379:ALA:O	2.09	0.53
1:A:292:GLY:HA3	1:A:325:SER:O	2.09	0.53
1:B:114:PHE:N	1:B:114:PHE:HD2	2.07	0.53
1:A:494:GLU:O	1:A:497:HIS:CE1	2.62	0.52
1:B:339:ASP:O	1:B:343:GLU:HG3	2.09	0.52
1:A:73:VAL:HG22	1:A:74:PHE:N	2.24	0.52
1:A:230:THR:C	1:A:231:SER:HG	2.18	0.52
1:B:248:TYR:CD1	1:B:248:TYR:C	2.87	0.52
1:A:180:PRO:HB2	1:A:261:GLU:HG2	1.91	0.52
1:A:33:ARG:NH1	1:A:36:GLU:OE2	2.42	0.52
1:A:139:ASN:H	1:A:142:THR:CG2	2.22	0.52
1:A:377:GLU:OE2	1:A:377:GLU:HA	2.10	0.52
1:B:396:ILE:HG23	1:B:408:TRP:CZ2	2.44	0.52
1:B:562:ARG:HA	1:B:566:ASN:OD1	2.09	0.52
1:A:39:LEU:HD13	1:A:70:GLN:NE2	2.24	0.52
1:A:515:SER:HB3	1:A:517:TYR:O	2.08	0.52
1:B:151:ASP:HB3	1:B:155:LYS:HB2	1.91	0.52
1:B:465:LEU:HD13	1:B:500:ILE:HG23	1.91	0.52
1:A:21:PHE:CE2	1:A:23:LEU:HD23	2.44	0.52
1:A:302:ARG:HH22	1:B:307:ASP:CG	2.18	0.52
1:A:344:HIS:ND1	1:A:344:HIS:N	2.57	0.52
1:B:107:HIS:HE1	1:B:394:GLU:OE1	1.92	0.52
1:B:19:TRP:CE3	1:B:71:ARG:HB3	2.44	0.52
1:A:289:TYR:OH	1:A:546:GLU:OE1	2.19	0.52
1:A:340:TRP:CA	2:A:695:HOH:O	2.56	0.52
1:A:71:ARG:NH1	1:A:72:GLU:O	2.43	0.52
1:A:452:HIS:C	1:A:453:THR:OG1	2.53	0.52
1:A:482:GLU:OE2	1:A:539:ARG:NH2	2.42	0.52
1:A:504:GLU:HG2	1:A:549:TRP:HB2	1.92	0.52
1:B:92:THR:HG22	1:B:93:HIS:H	1.75	0.52
1:A:16:ASP:OD2	1:A:18:LEU:HD12	2.10	0.52
1:A:456:ILE:HG13	1:A:459:LEU:CD1	2.39	0.52
1:A:259:GLN:HE21	1:A:259:GLN:HA	1.75	0.51
1:A:469:TYR:HB2	1:A:533:TYR:OH	2.10	0.51
1:B:379:ALA:HB3	2:B:684:HOH:O	2.09	0.51
1:A:311:MSE:HE3	1:A:340:TRP:HE3	1.75	0.51
1:A:453:THR:HA	2:A:707:HOH:O	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASN:OD1	1:A:551:PHE:N	2.43	0.51
1:B:6:GLU:O	1:B:7:THR:HB	2.10	0.51
1:B:82:GLN:HB3	1:B:179:THR:O	2.10	0.51
1:B:338:LEU:O	1:B:342:ASP:HB2	2.10	0.51
1:B:414:PRO:HD3	1:B:444:VAL:O	2.10	0.51
1:A:205:GLN:OE1	1:A:206:VAL:N	2.41	0.51
1:A:297:GLU:HG3	1:A:331:TYR:HE1	1.76	0.51
1:B:33:ARG:HG3	1:B:35:TRP:CZ2	2.45	0.51
1:B:99:VAL:O	1:B:101:ASN:N	2.43	0.51
1:B:438:THR:HG23	1:B:439:ARG:HG3	1.91	0.51
1:A:180:PRO:HG3	1:A:262:CYS:O	2.09	0.51
1:B:110:GLY:N	2:B:688:HOH:O	2.42	0.51
1:B:380:VAL:HG12	2:B:684:HOH:O	2.09	0.51
1:B:482:GLU:HG3	1:B:536:VAL:CG2	2.40	0.51
1:A:98:TRP:CZ3	1:A:103:GLU:HB3	2.46	0.51
1:A:381:ASN:HB2	1:A:384:THR:H	1.76	0.51
1:B:396:ILE:HA	1:B:408:TRP:CH2	2.45	0.51
1:B:548:VAL:HG21	1:B:584:LEU:CD2	2.40	0.51
1:B:141:GLN:HA	1:B:384:THR:HG22	1.93	0.51
1:B:538:ASP:HB2	1:B:597:PRO:HG2	1.93	0.51
1:B:202:VAL:O	1:B:231:SER:HA	2.10	0.51
1:B:302:ARG:O	1:B:302:ARG:HG2	2.10	0.51
1:B:352:THR:HG22	1:B:353:ALA:N	2.26	0.51
1:A:337:MSE:HE1	1:A:348:VAL:HG11	1.92	0.51
1:A:198:ASN:O	1:A:199:HIS:CD2	2.64	0.51
1:B:187:ILE:CG2	1:B:188:THR:N	2.74	0.51
1:A:20:ALA:HB1	1:A:42:SER:CB	2.41	0.50
1:A:216:LEU:HD13	1:A:216:LEU:O	2.12	0.50
1:B:83:ARG:NH2	1:B:183:TRP:CE3	2.79	0.50
1:A:33:ARG:C	1:A:36:GLU:OE1	2.54	0.50
1:B:91:VAL:HG11	1:B:134:VAL:HG13	1.94	0.50
1:B:372:LYS:HB2	1:B:372:LYS:HZ2	1.75	0.50
1:B:493:GLN:HG2	1:B:494:GLU:N	2.26	0.50
1:B:76:PRO:O	1:B:79:TRP:HB2	2.12	0.50
1:B:171:HIS:CG	1:B:304:LYS:O	2.64	0.50
1:B:553:ASP:OD1	1:B:578:LYS:NZ	2.43	0.50
1:A:198:ASN:HB3	1:A:199:HIS:CD2	2.42	0.50
1:A:340:TRP:CH2	1:B:44:ALA:HB3	2.46	0.50
1:A:453:THR:O	2:A:707:HOH:O	2.19	0.50
1:B:176:LEU:C	1:B:176:LEU:HD12	2.36	0.50
1:B:244:PRO:HG2	1:B:593:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:THR:OG1	1:B:324:ASN:CG	2.55	0.50
1:B:469:TYR:HD2	1:B:533:TYR:HH	1.60	0.50
1:B:560:ILE:O	1:B:561:LEU:C	2.54	0.50
1:A:560:ILE:C	1:A:562:ARG:N	2.69	0.50
1:A:-1:SER:O	1:A:0:HIS:HB2	2.06	0.50
1:B:101:ASN:N	1:B:101:ASN:ND2	2.45	0.50
1:B:476:GLY:HA2	1:B:525:TYR:OH	2.11	0.50
1:B:499:PRO:HA	2:B:665:HOH:O	2.11	0.50
1:A:92:THR:HA	1:A:110:GLY:O	2.12	0.50
1:A:116:ALA:HB1	2:A:655:HOH:O	2.11	0.50
1:A:455:THR:C	1:A:456:ILE:CG2	2.83	0.50
1:A:565:GLY:O	1:A:567:LYS:HD3	2.11	0.50
1:B:549:TRP:HZ3	1:B:568:LYS:HZ3	0.75	0.50
1:A:392:ILE:HD13	1:A:432:THR:HG22	1.91	0.50
1:A:452:HIS:ND1	1:A:453:THR:O	2.45	0.50
1:A:453:THR:N	2:A:707:HOH:O	2.43	0.50
1:A:552:ALA:HA	1:A:571:PHE:O	2.11	0.50
1:B:102:GLN:O	1:B:102:GLN:NE2	2.45	0.50
1:B:242:TRP:CE2	1:B:403:PRO:HB2	2.47	0.50
1:B:337:MSE:HE1	1:B:348:VAL:CG2	2.29	0.50
1:A:21:PHE:HE2	1:A:23:LEU:CD2	2.25	0.50
1:A:248:TYR:HB3	2:A:689:HOH:O	2.10	0.50
1:A:381:ASN:HB2	1:A:383:GLU:H	1.77	0.50
1:B:267:LEU:CD1	1:B:269:VAL:HG13	2.42	0.50
1:A:83:ARG:CB	1:A:179:THR:O	2.44	0.49
1:A:214:VAL:O	1:A:227:GLY:N	2.45	0.49
1:B:372:LYS:HZ3	1:B:372:LYS:HB2	1.76	0.49
1:B:469:TYR:HD2	1:B:533:TYR:OH	1.95	0.49
1:B:566:ASN:N	2:B:682:HOH:O	2.18	0.49
1:A:15:LEU:CD2	1:A:48:PRO:HD3	2.40	0.49
1:A:312:VAL:HG11	1:B:54:GLN:NE2	2.27	0.49
1:A:337:MSE:HB2	2:A:614:HOH:O	2.13	0.49
1:A:342:ASP:CG	2:A:673:HOH:O	2.48	0.49
1:B:51:PHE:HE2	1:B:168:ALA:HB3	1.76	0.49
1:B:92:THR:HG21	1:B:168:ALA:CB	2.42	0.49
1:B:96:LYS:HE3	1:B:106:GLU:OE2	2.12	0.49
1:B:558:GLN:OE1	1:B:559:GLY:N	2.46	0.49
1:A:242:TRP:HA	2:A:689:HOH:O	2.10	0.49
1:B:379:ALA:C	2:B:684:HOH:O	2.54	0.49
1:B:433:ARG:HA	2:B:627:HOH:O	2.11	0.49
1:B:490:LEU:O	1:B:493:GLN:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:C	1:A:17:GLY:N	2.68	0.49
1:A:69:TYR:CE2	1:A:170:ILE:HG13	2.47	0.49
1:A:197:CYS:CB	1:A:198:ASN:OD1	2.53	0.49
1:A:238:ASN:HB3	1:A:239:PRO:CD	2.43	0.49
2:A:662:HOH:O	1:B:12:ILE:CD1	2.56	0.49
1:B:122:VAL:HG22	1:B:123:ILE:HD12	1.93	0.49
1:A:83:ARG:NH2	1:A:183:TRP:CH2	2.80	0.49
1:A:222:GLN:HG2	2:A:645:HOH:O	2.12	0.49
1:A:381:ASN:C	1:A:383:GLU:N	2.68	0.49
1:A:422:ARG:NH1	1:A:454:ASP:O	2.46	0.49
1:A:532:MSE:O	1:A:533:TYR:C	2.54	0.49
1:B:11:GLU:OE1	1:B:11:GLU:N	2.45	0.49
1:B:295:ARG:HB2	1:B:333:TYR:OH	2.12	0.49
1:B:556:THR:HG23	1:B:565:GLY:HA2	1.95	0.49
1:A:254:VAL:O	1:A:264:ILE:HA	2.13	0.49
1:B:14:LYS:C	1:B:16:ASP:N	2.69	0.49
1:B:93:HIS:CD2	1:B:138:LEU:HD21	2.48	0.49
1:B:171:HIS:HB3	1:B:304:LYS:O	2.13	0.49
1:B:392:ILE:HG21	1:B:432:THR:CG2	2.43	0.49
1:A:288:PHE:CZ	1:A:347:VAL:HG11	2.48	0.49
1:A:314:ASP:OD1	1:A:551:PHE:HE2	1.95	0.49
1:A:456:ILE:HA	1:A:459:LEU:H	1.77	0.49
1:A:392:ILE:CG2	1:A:432:THR:HG22	2.42	0.49
1:A:470:GLY:N	1:A:529:TRP:CH2	2.80	0.49
1:A:555:ALA:HA	1:A:565:GLY:HA2	1.94	0.49
1:B:410:ILE:HD12	1:B:460:PHE:HE1	1.78	0.49
1:B:488:GLU:O	1:B:488:GLU:HG3	2.13	0.49
1:B:532:MSE:C	1:B:532:MSE:SE	3.06	0.49
1:A:16:ASP:OD2	1:A:18:LEU:CD1	2.61	0.49
1:A:10:ARG:NH1	1:A:10:ARG:CB	2.76	0.48
1:A:32:GLN:HB2	1:A:34:TRP:HE1	1.78	0.48
1:A:35:TRP:CE2	1:A:36:GLU:OE2	2.66	0.48
1:A:35:TRP:CE2	1:A:36:GLU:CD	2.91	0.48
1:A:273:SER:O	1:A:283:ILE:HA	2.14	0.48
1:A:373:GLU:OE2	1:A:373:GLU:N	2.46	0.48
1:A:407:MSE:SE	1:A:462:VAL:CG1	3.11	0.48
1:B:328:THR:O	1:B:351:GLU:HB2	2.13	0.48
1:B:341:ALA:HB1	1:B:346:ILE:O	2.13	0.48
1:A:21:PHE:CE2	1:A:23:LEU:CD2	2.96	0.48
1:A:197:CYS:C	1:A:198:ASN:OD1	2.56	0.48
1:B:35:TRP:CE2	1:B:98:TRP:CZ3	3.00	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:CG	1:B:179:THR:HG23	2.43	0.48
1:B:102:GLN:N	1:B:102:GLN:HE21	2.11	0.48
1:B:392:ILE:HG21	1:B:432:THR:HG22	1.95	0.48
1:B:467:ARG:NH2	1:B:492:TRP:HE1	2.11	0.48
1:A:20:ALA:HB1	1:A:42:SER:OG	2.12	0.48
1:A:337:MSE:HE2	1:A:337:MSE:HA	1.95	0.48
1:A:376:SER:O	1:A:377:GLU:OE2	2.31	0.48
1:A:401:ASN:HB2	2:A:676:HOH:O	2.12	0.48
1:A:504:GLU:HG2	1:A:549:TRP:CG	2.47	0.48
1:B:12:ILE:HG22	1:B:176:LEU:HG	1.95	0.48
1:B:138:LEU:HB2	1:B:158:GLN:HE22	1.78	0.48
1:A:183:TRP:CE2	1:A:208:ALA:CB	2.96	0.48
1:A:362:GLY:O	1:A:363:ILE:CB	2.62	0.48
1:A:529:TRP:CE2	1:A:533:TYR:HE1	2.32	0.48
1:B:199:HIS:O	1:B:199:HIS:CD2	2.66	0.48
1:A:187:ILE:CG2	1:A:188:THR:H	2.26	0.48
1:A:92:THR:C	1:A:110:GLY:HA2	2.35	0.48
1:A:249:LEU:HD22	1:A:268:ARG:HB3	1.96	0.48
1:A:330:HIS:O	2:A:701:HOH:O	2.20	0.48
1:B:76:PRO:HD2	1:B:79:TRP:CE3	2.48	0.48
1:B:213:SER:HB3	1:B:255:THR:CB	2.23	0.48
1:A:456:ILE:HG13	1:A:459:LEU:HD12	1.96	0.48
1:B:27:ASN:O	1:B:28:CYS:SG	2.72	0.48
1:B:183:TRP:CE3	1:B:185:ASP:HB2	2.48	0.48
1:B:248:TYR:C	1:B:248:TYR:HD1	2.20	0.48
1:B:286:LYS:HE3	1:B:286:LYS:HB2	1.77	0.48
1:B:162:HIS:CD2	1:B:164:PHE:CZ	3.01	0.48
1:B:375:TYR:CE2	1:B:379:ALA:N	2.81	0.48
1:A:107:HIS:CE1	1:A:394:GLU:OE1	2.65	0.48
1:A:327:ARG:HA	1:A:349:ILE:O	2.14	0.48
1:B:424:TYR:HB2	2:B:626:HOH:O	2.14	0.48
1:A:230:THR:HG22	1:A:231:SER:OG	2.14	0.48
1:A:449:CYS:HA	1:A:452:HIS:HB2	1.96	0.48
1:B:481:ALA:O	1:B:485:LEU:HB2	2.14	0.48
1:B:531:ASP:OD1	1:B:531:ASP:C	2.57	0.48
1:A:119:THR:N	1:A:120:PRO:CD	2.77	0.47
1:A:255:THR:HG23	1:A:264:ILE:HG23	1.95	0.47
1:B:142:THR:HG22	1:B:145:PRO:HA	1.96	0.47
1:B:471:TRP:CZ3	1:B:520:MSE:HG2	2.35	0.47
1:A:116:ALA:CB	2:A:655:HOH:O	2.62	0.47
1:A:140:TRP:HE1	1:A:147:MSE:HE2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:O	1:A:321:ILE:CG2	2.55	0.47
1:A:335:GLU:N	2:A:614:HOH:O	2.25	0.47
1:B:48:PRO:O	2:B:645:HOH:O	2.20	0.47
1:B:194:ALA:HB3	1:B:196:ASP:OD2	2.14	0.47
1:A:17:GLY:HA3	1:A:47:VAL:N	2.21	0.47
1:A:183:TRP:HZ3	1:A:185:ASP:OD1	1.97	0.47
1:A:273:SER:HB3	1:A:284:ASN:HA	1.96	0.47
1:A:341:ALA:HA	1:A:346:ILE:HB	1.96	0.47
1:A:550:ASN:O	1:A:551:PHE:C	2.54	0.47
1:A:10:ARG:HB3	1:A:10:ARG:NH1	2.30	0.47
1:A:19:TRP:CZ2	1:A:71:ARG:HD2	2.49	0.47
1:A:162:HIS:HB3	1:A:355:VAL:HB	1.97	0.47
1:A:540:VAL:O	1:A:596:LYS:NZ	2.47	0.47
1:B:1:MSE:SE	1:B:113:PRO:HB2	2.64	0.47
1:B:189:VAL:O	1:B:190:VAL:HB	2.13	0.47
1:B:293:PHE:CD2	1:B:551:PHE:HD1	2.32	0.47
1:A:52:ASN:HD21	1:A:168:ALA:H	1.63	0.47
1:A:183:TRP:CZ3	1:A:185:ASP:CG	2.92	0.47
1:A:205:GLN:HB2	1:A:231:SER:HA	1.96	0.47
1:A:327:ARG:HB2	1:A:349:ILE:HB	1.96	0.47
1:A:342:ASP:OD1	1:A:404:SER:OG	2.33	0.47
1:B:67:VAL:O	1:B:134:VAL:HG23	2.14	0.47
1:A:19:TRP:CE3	1:A:69:TYR:HB3	2.49	0.47
1:A:321:ILE:CG2	1:A:588:TRP:CE3	2.97	0.47
1:A:397:ALA:O	1:A:400:LYS:HD2	2.14	0.47
1:B:83:ARG:HA	1:B:119:THR:HG1	1.77	0.47
1:B:212:VAL:HG21	1:B:230:THR:CG2	2.44	0.47
1:B:399:ASP:HB3	1:B:405:VAL:HG21	1.95	0.47
1:A:29:GLY:HA2	1:A:34:TRP:CD2	2.50	0.47
1:A:241:LEU:O	1:A:248:TYR:HB3	2.15	0.47
1:A:320:TRP:CZ3	1:A:321:ILE:HG13	2.49	0.47
1:B:2:LEU:HD11	1:B:187:ILE:H	1.80	0.47
1:B:33:ARG:HH11	1:B:36:GLU:HB3	1.80	0.47
1:B:73:VAL:O	1:B:127:SER:HA	2.15	0.47
1:B:189:VAL:HG12	1:B:190:VAL:N	2.29	0.47
1:B:280:GLN:NE2	2:B:633:HOH:O	2.45	0.47
1:B:295:ARG:HE	1:B:295:ARG:HB3	1.48	0.47
1:A:15:LEU:HD21	1:A:173:SER:OG	2.14	0.47
1:A:309:VAL:HG21	1:B:302:ARG:HB3	1.96	0.47
1:A:507:VAL:CG1	1:A:529:TRP:CD1	2.98	0.47
1:B:268:ARG:O	1:B:269:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PHE:HB2	2:B:679:HOH:O	2.14	0.47
1:A:10:ARG:CZ	1:A:10:ARG:CB	2.92	0.47
1:A:295:ARG:N	1:A:329:SER:OG	2.47	0.47
1:A:547:GLN:NE2	2:A:663:HOH:O	2.48	0.47
1:B:191:THR:OG1	1:B:271:ILE:HA	2.15	0.47
1:B:468:TYR:OH	1:B:504:GLU:HB3	2.14	0.47
1:A:4:PRO:HD3	1:A:87:ARG:NH1	2.30	0.47
1:A:186:ASP:OD1	1:A:400:LYS:NZ	2.40	0.47
1:A:344:HIS:O	1:A:345:GLY:C	2.57	0.47
1:A:468:TYR:O	1:A:472:TYR:CD2	2.68	0.47
1:A:513:LEU:O	1:A:522:SER:HA	2.15	0.47
1:B:252:LEU:HD22	1:B:269:VAL:HG21	1.97	0.47
1:B:315:HIS:HB3	1:B:340:TRP:CZ3	2.50	0.47
1:B:570:ILE:CD1	1:B:584:LEU:CD2	2.93	0.47
1:A:24:ASP:OD2	1:A:29:GLY:HA3	2.15	0.46
1:A:35:TRP:CD2	1:A:36:GLU:OE1	2.68	0.46
1:A:119:THR:N	1:A:120:PRO:HD2	2.30	0.46
1:A:340:TRP:HA	1:A:344:HIS:CE1	2.49	0.46
1:B:18:LEU:HA	1:B:45:ILE:O	2.16	0.46
1:B:375:TYR:CG	1:B:379:ALA:HB3	2.50	0.46
1:A:74:PHE:CE1	1:B:7:THR:HA	2.47	0.46
1:A:141:GLN:NE2	1:A:381:ASN:OD1	2.47	0.46
1:A:471:TRP:HZ2	1:A:521:TRP:CZ2	2.34	0.46
1:A:474:GLN:HE21	1:A:480:THR:HG22	1.80	0.46
1:B:155:LYS:HD2	1:B:155:LYS:HA	1.82	0.46
1:A:218:ASP:HA	2:A:686:HOH:O	2.15	0.46
1:B:217:ARG:N	1:B:251:GLU:O	2.44	0.46
1:A:207:VAL:HG13	1:A:210:GLY:H	1.79	0.46
1:A:381:ASN:HB2	1:A:383:GLU:N	2.31	0.46
1:A:480:THR:O	1:A:484:VAL:HG13	2.15	0.46
1:B:273:SER:CB	1:B:284:ASN:N	2.65	0.46
1:B:533:TYR:HB3	1:B:537:PHE:CE1	2.50	0.46
1:B:562:ARG:HG3	1:B:562:ARG:NH1	2.29	0.46
1:B:43:ARG:HG2	1:B:44:ALA:N	2.27	0.46
1:B:172:ARG:HH12	1:B:334:ALA:N	2.13	0.46
1:B:272:ARG:HD2	1:B:274:VAL:HG21	1.97	0.46
1:B:293:PHE:CZ	1:B:321:ILE:HD13	2.48	0.46
1:B:531:ASP:HA	1:B:534:HIS:ND1	2.31	0.46
1:A:468:TYR:O	1:A:472:TYR:HD2	1.99	0.46
1:B:47:VAL:HG13	1:B:170:ILE:HG22	1.97	0.46
1:B:183:TRP:CZ3	1:B:185:ASP:CG	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:C	1:A:120:PRO:HD2	2.41	0.46
1:B:83:ARG:HH11	1:B:118:VAL:CG1	2.28	0.46
1:B:219:ALA:O	1:B:220:ASP:OD2	2.34	0.46
1:B:242:TRP:CD1	1:B:270:GLY:HA3	2.51	0.46
1:B:304:LYS:HE3	1:B:331:TYR:CE2	2.50	0.46
1:B:470:GLY:HA2	1:B:474:GLN:HB2	1.98	0.46
1:A:29:GLY:HA3	1:A:68:TRP:CZ2	2.51	0.46
1:A:33:ARG:O	1:A:36:GLU:OE1	2.34	0.46
1:A:51:PHE:C	1:A:51:PHE:HD1	2.24	0.46
1:A:187:ILE:CG2	1:A:188:THR:N	2.79	0.46
1:A:329:SER:HB2	2:A:678:HOH:O	2.15	0.46
1:A:588:TRP:HA	1:A:591:MSE:HE3	1.98	0.46
1:B:15:LEU:HD13	1:B:48:PRO:CD	2.44	0.46
1:B:293:PHE:HA	1:B:548:VAL:O	2.15	0.46
1:B:306:PHE:HE1	1:B:311:MSE:HE3	1.81	0.46
1:B:341:ALA:CB	1:B:404:SER:CB	2.93	0.46
1:B:432:THR:HB	1:B:441:ILE:HD11	1.98	0.46
1:A:309:VAL:HG21	1:B:302:ARG:NE	2.31	0.45
1:A:514:HIS:HA	1:A:524:GLU:OE2	2.16	0.45
1:B:318:MSE:HA	1:B:321:ILE:HG22	1.98	0.45
1:A:139:ASN:N	1:A:142:THR:HG21	2.31	0.45
1:B:66:ASN:HA	1:B:134:VAL:O	2.16	0.45
1:B:138:LEU:HB3	1:B:142:THR:HG21	1.97	0.45
1:B:570:ILE:HD11	1:B:584:LEU:CD2	2.46	0.45
1:A:295:ARG:O	1:A:329:SER:CB	2.62	0.45
1:A:381:ASN:HB2	1:A:383:GLU:CB	2.45	0.45
1:A:550:ASN:HD22	1:A:554:PHE:HE2	1.62	0.45
1:B:94:TYR:O	1:B:134:VAL:HA	2.16	0.45
1:B:184:VAL:CG2	1:B:254:VAL:HG12	2.41	0.45
1:B:213:SER:OG	1:B:228:GLN:NE2	2.48	0.45
1:B:469:TYR:CD2	1:B:533:TYR:OH	2.68	0.45
1:B:504:GLU:HG2	1:B:549:TRP:CD1	2.51	0.45
1:A:225:ALA:HB1	1:A:235:GLN:HG2	1.99	0.45
1:A:442:THR:CA	1:A:460:PHE:CD1	2.99	0.45
1:A:457:SER:CB	1:A:496:LEU:HD11	2.46	0.45
1:B:197:CYS:CB	1:B:198:ASN:HD22	2.28	0.45
1:B:465:LEU:N	1:B:465:LEU:CD1	2.69	0.45
1:A:39:LEU:HD13	1:A:70:GLN:HE21	1.81	0.45
1:A:139:ASN:H	1:A:142:THR:HG21	1.81	0.45
1:A:442:THR:HA	1:A:460:PHE:CD1	2.51	0.45
1:A:453:THR:O	1:A:455:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASP:HB3	1:B:155:LYS:CB	2.46	0.45
1:B:217:ARG:HG2	2:B:628:HOH:O	2.17	0.45
1:B:257:LYS:HA	1:B:262:CYS:HB3	1.97	0.45
1:B:311:MSE:HE2	1:B:336:GLU:CG	2.38	0.45
1:A:248:TYR:CB	2:A:689:HOH:O	2.64	0.45
1:A:18:LEU:C	1:A:19:TRP:HD1	2.23	0.45
1:A:384:THR:O	1:A:385:GLN:C	2.60	0.45
1:B:47:VAL:CG1	1:B:170:ILE:HG22	2.47	0.45
1:B:197:CYS:HB3	1:B:198:ASN:HD22	1.76	0.45
1:B:377:GLU:HB2	1:B:419:GLN:OE1	2.16	0.45
1:B:422:ARG:HB3	1:B:454:ASP:OD2	2.17	0.45
1:B:453:THR:CB	1:B:456:ILE:HB	2.46	0.45
1:A:51:PHE:CD2	1:A:168:ALA:O	2.69	0.45
1:A:385:GLN:HE22	1:A:427:PRO:HG2	1.80	0.45
1:A:295:ARG:HB3	1:A:295:ARG:HH11	1.82	0.45
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.81	0.45
1:A:420:GLY:N	2:A:697:HOH:O	2.49	0.45
1:A:474:GLN:HE22	1:A:484:VAL:HG13	1.82	0.45
1:B:14:LYS:O	1:B:16:ASP:N	2.49	0.45
1:B:36:GLU:CB	1:B:101:ASN:HD21	2.15	0.45
1:A:32:GLN:O	1:A:33:ARG:C	2.60	0.45
1:A:259:GLN:HA	1:A:259:GLN:NE2	2.32	0.45
1:A:312:VAL:HG11	1:B:54:GLN:HE21	1.81	0.45
1:B:83:ARG:HG2	1:B:179:THR:HG23	1.98	0.45
1:B:358:ASN:OD1	1:B:358:ASN:N	2.48	0.45
1:B:463:LEU:CD2	1:B:492:TRP:CZ3	2.99	0.45
1:B:564:GLY:O	1:B:567:LYS:HE3	2.17	0.45
1:A:205:GLN:HB2	1:A:231:SER:N	2.30	0.44
1:A:293:PHE:HE1	1:A:570:ILE:HD13	1.81	0.44
1:B:24:ASP:OD1	1:B:27:ASN:O	2.35	0.44
1:A:87:ARG:HB3	1:A:115:GLU:CB	2.48	0.44
1:A:377:GLU:OE1	2:A:691:HOH:O	2.21	0.44
1:A:400:LYS:O	1:A:439:ARG:NH2	2.46	0.44
1:B:23:LEU:HD13	1:B:63:TYR:CD1	2.52	0.44
1:B:101:ASN:HD21	1:B:129:ARG:HH12	1.65	0.44
1:B:241:LEU:CD2	1:B:241:LEU:N	2.79	0.44
1:A:138:LEU:CA	1:A:142:THR:HG21	2.46	0.44
1:A:151:ASP:HB3	1:A:155:LYS:HB3	1.87	0.44
1:A:7:THR:HB	1:A:8:PRO:HD2	1.98	0.44
1:A:82:GLN:NE2	1:A:82:GLN:CA	2.80	0.44
1:B:10:ARG:CB	1:B:10:ARG:NH1	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:CG1	1:B:170:ILE:CG2	2.96	0.44
1:B:83:ARG:NH2	1:B:183:TRP:CD2	2.85	0.44
1:B:183:TRP:CZ3	1:B:185:ASP:HB2	2.53	0.44
1:B:242:TRP:NE1	1:B:403:PRO:HB2	2.32	0.44
1:A:462:VAL:HG23	1:A:499:PRO:HB2	1.99	0.44
1:B:5:VAL:HG11	1:B:266:PRO:HG2	2.00	0.44
1:B:33:ARG:HH11	1:B:33:ARG:HG2	1.82	0.44
1:B:203:ASP:OD2	1:B:203:ASP:C	2.60	0.44
1:B:498:GLN:HB2	1:B:499:PRO:CD	2.40	0.44
1:A:6:GLU:C	1:A:7:THR:HG23	2.42	0.44
1:A:455:THR:O	1:A:456:ILE:CG2	2.66	0.44
1:A:469:TYR:O	1:A:473:VAL:HG23	2.18	0.44
1:A:511:ALA:O	1:A:523:GLU:OE2	2.35	0.44
1:B:21:PHE:HE2	1:B:69:TYR:HE2	1.66	0.44
1:B:212:VAL:HG11	1:B:229:GLY:C	2.42	0.44
1:A:268:ARG:NH2	1:A:343:GLU:HG3	2.33	0.44
1:A:313:HIS:CG	1:B:301:LEU:HD22	2.52	0.44
1:A:376:SER:C	1:A:377:GLU:OE2	2.61	0.44
1:B:390:GLN:O	1:B:394:GLU:HG3	2.17	0.44
1:B:467:ARG:HG3	1:B:469:TYR:OH	2.17	0.44
1:B:592:ASN:HB2	1:B:595:GLU:HG2	2.00	0.44
1:A:2:LEU:HD11	1:A:187:ILE:HG13	2.00	0.44
1:A:314:ASP:OD1	1:A:551:PHE:CE2	2.71	0.44
1:B:448:PHE:O	1:B:448:PHE:CD1	2.65	0.44
1:A:23:LEU:HD22	1:A:67:VAL:HG12	2.00	0.44
1:A:377:GLU:C	1:A:379:ALA:H	2.26	0.44
1:B:10:ARG:H	1:B:178:THR:CG2	2.15	0.44
1:B:183:TRP:O	1:B:206:VAL:HG23	2.17	0.44
1:B:236:VAL:HG23	1:B:236:VAL:O	2.17	0.44
1:B:379:ALA:O	1:B:380:VAL:CG1	2.66	0.44
1:B:556:THR:HB	1:B:562:ARG:HD2	1.99	0.44
1:A:92:THR:OG1	1:A:168:ALA:HA	2.18	0.43
1:A:4:PRO:HG2	1:A:87:ARG:HD3	2.00	0.43
1:A:32:GLN:HB2	1:A:34:TRP:NE1	2.33	0.43
1:A:183:TRP:N	1:A:183:TRP:CD1	2.86	0.43
1:A:202:VAL:CG2	1:A:234:LEU:CD2	2.90	0.43
1:A:476:GLY:CA	1:A:520:MSE:HE2	2.49	0.43
1:A:534:HIS:CE1	1:A:587:ARG:HD2	2.54	0.43
1:B:184:VAL:O	1:B:185:ASP:HB2	2.17	0.43
1:B:562:ARG:CG	1:B:562:ARG:NH1	2.70	0.43
1:A:407:MSE:SE	1:A:462:VAL:HG11	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:THR:OG1	2:B:690:HOH:O	2.21	0.43
1:B:33:ARG:HG3	1:B:35:TRP:CE2	2.52	0.43
1:B:47:VAL:HG11	1:B:170:ILE:HG21	2.00	0.43
1:A:202:VAL:HG13	1:A:204:TRP:CZ3	2.53	0.43
1:B:21:PHE:HB2	1:B:45:ILE:HB	2.01	0.43
1:B:75:ILE:HD11	1:B:128:VAL:CG2	2.48	0.43
1:B:110:GLY:CA	2:B:688:HOH:O	2.67	0.43
1:B:208:ALA:C	1:B:210:GLY:H	2.24	0.43
1:B:214:VAL:O	1:B:214:VAL:HG12	2.18	0.43
1:B:244:PRO:HG2	1:B:593:PHE:HE1	1.83	0.43
1:B:349:ILE:HG22	1:B:349:ILE:O	2.17	0.43
1:B:375:TYR:CZ	1:B:379:ALA:HB2	2.54	0.43
1:B:240:HIS:CD2	1:B:250:TYR:OH	2.71	0.43
1:B:583:LEU:C	1:B:585:GLN:H	2.25	0.43
1:B:21:PHE:CZ	1:B:51:PHE:HB2	2.54	0.43
1:B:186:ASP:HB3	1:B:205:GLN:HB3	2.00	0.43
1:B:559:GLY:C	1:B:562:ARG:HH12	2.26	0.43
1:A:144:PRO:HD3	1:A:353:ALA:HB1	2.01	0.43
1:A:295:ARG:HB3	1:A:295:ARG:NH1	2.33	0.43
1:B:203:ASP:O	1:B:204:TRP:HB3	2.18	0.43
1:B:583:LEU:O	1:B:585:GLN:N	2.52	0.43
1:A:105:MSE:HE1	1:A:115:GLU:CA	2.42	0.43
1:A:187:ILE:O	1:A:400:LYS:HE2	2.19	0.43
1:A:351:GLU:O	1:A:395:LEU:HD11	2.19	0.43
1:B:315:HIS:CD2	1:B:340:TRP:CE3	3.07	0.43
1:B:602:LYS:C	1:B:603:GLN:HG2	2.44	0.43
1:A:24:ASP:OD1	1:A:26:GLU:O	2.37	0.43
1:A:160:TYR:CD2	1:A:160:TYR:N	2.86	0.43
1:A:330:HIS:CE1	1:A:412:ASN:CG	2.97	0.43
1:A:451:ALA:O	1:A:453:THR:OG1	2.37	0.43
1:A:534:HIS:O	1:A:535:ARG:C	2.62	0.43
1:B:193:VAL:HG23	1:B:194:ALA:O	2.19	0.43
1:B:267:LEU:C	1:B:267:LEU:HD13	2.44	0.43
1:B:318:MSE:O	1:B:319:ASP:C	2.62	0.43
1:B:489:LEU:O	1:B:493:GLN:N	2.49	0.43
1:A:193:VAL:CG2	1:A:285:HIS:NE2	2.82	0.43
1:A:469:TYR:HB2	1:A:529:TRP:HZ2	1.83	0.43
1:B:105:MSE:SE	1:B:114:PHE:HB2	2.68	0.43
1:B:358:ASN:HB3	1:B:360:SER:HB3	2.01	0.43
1:B:453:THR:OG1	1:B:457:SER:N	2.39	0.43
1:A:150:THR:HA	1:A:155:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:O	1:A:566:ASN:ND2	2.51	0.42
1:B:265:TYR:HD2	2:B:655:HOH:O	2.01	0.42
1:B:486:GLU:O	1:B:489:LEU:N	2.52	0.42
1:A:14:LYS:HZ2	1:A:14:LYS:HB2	1.81	0.42
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.34	0.42
1:A:525:TYR:HD2	2:A:708:HOH:O	2.02	0.42
1:A:203:ASP:OD2	1:A:203:ASP:C	2.61	0.42
1:A:413:GLU:HG3	1:A:466:ASN:HD22	1.84	0.42
1:A:453:THR:O	1:A:454:ASP:C	2.62	0.42
1:B:187:ILE:HG22	1:B:188:THR:N	2.33	0.42
1:B:293:PHE:HE1	1:B:570:ILE:HD12	1.83	0.42
1:B:414:PRO:CD	1:B:444:VAL:O	2.67	0.42
1:A:102:GLN:OE1	1:A:102:GLN:CA	2.54	0.42
1:A:171:HIS:NE2	1:A:304:LYS:HB2	2.35	0.42
1:B:101:ASN:ND2	1:B:129:ARG:HH12	2.17	0.42
1:A:12:ILE:CD1	2:A:698:HOH:O	2.63	0.42
1:A:426:ALA:HA	1:A:459:LEU:HD13	2.01	0.42
1:A:477:ASP:OD1	1:A:480:THR:HB	2.20	0.42
1:A:507:VAL:HG13	1:A:529:TRP:CD1	2.55	0.42
1:B:243:GLN:O	1:B:247:GLY:N	2.42	0.42
1:B:291:THR:O	1:B:588:TRP:CH2	2.72	0.42
1:B:359:LEU:HG	1:B:359:LEU:O	2.20	0.42
1:A:19:TRP:HE3	1:A:69:TYR:HB3	1.83	0.42
1:A:28:CYS:O	1:A:29:GLY:C	2.62	0.42
1:A:160:TYR:CD1	1:A:162:HIS:CD2	3.07	0.42
1:B:1:MSE:HE3	1:B:1:MSE:HB3	1.72	0.42
1:B:12:ILE:O	1:B:12:ILE:CG2	2.65	0.42
1:B:12:ILE:O	1:B:13:LYS:C	2.63	0.42
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.71	0.42
1:B:88:PHE:N	1:B:88:PHE:CD2	2.87	0.42
1:B:94:TYR:CD2	1:B:135:ASN:HB2	2.53	0.42
1:B:189:VAL:HG11	1:B:269:VAL:HG11	2.01	0.42
1:B:549:TRP:HZ3	1:B:568:LYS:CE	2.28	0.42
1:A:31:ASP:C	1:A:33:ARG:H	2.28	0.42
1:A:192:HIS:HB2	1:A:200:ALA:HB3	2.00	0.42
1:A:329:SER:C	2:A:711:HOH:O	2.61	0.42
1:A:330:HIS:N	2:A:678:HOH:O	2.31	0.42
1:A:426:ALA:O	1:A:429:ALA:HB3	2.19	0.42
1:A:502:ILE:HD12	1:A:537:PHE:CE2	2.48	0.42
1:B:354:ALA:HB3	1:B:411:ALA:HA	2.02	0.42
1:B:400:LYS:HA	1:B:439:ARG:NH1	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:O	1:A:400:LYS:HB3	2.20	0.42
1:A:426:ALA:HB3	1:A:427:PRO:HD3	2.02	0.42
1:A:498:GLN:HB2	1:A:499:PRO:CD	2.49	0.42
1:B:352:THR:C	1:B:354:ALA:H	2.27	0.42
1:B:449:CYS:HG	1:B:488:GLU:CD	2.19	0.42
1:B:456:ILE:O	1:B:457:SER:C	2.62	0.42
1:A:138:LEU:HA	1:A:142:THR:HG21	2.01	0.42
1:A:351:GLU:CG	1:A:409:SER:OG	2.68	0.42
1:B:143:ILE:HD11	1:B:388:HIS:CA	2.41	0.42
1:B:175:MSE:HE2	1:B:175:MSE:H	1.85	0.42
1:B:292:GLY:N	2:B:691:HOH:O	2.52	0.42
1:A:248:TYR:N	2:A:689:HOH:O	2.53	0.42
1:A:306:PHE:CD2	1:A:306:PHE:C	2.98	0.42
1:B:213:SER:CB	1:B:255:THR:HB	2.23	0.42
1:B:449:CYS:SG	1:B:488:GLU:OE2	2.78	0.42
1:A:315:HIS:CD2	1:A:318:MSE:CE	3.03	0.41
1:B:6:GLU:HA	1:B:9:THR:O	2.19	0.41
1:B:92:THR:HG21	1:B:168:ALA:HB1	2.01	0.41
1:B:137:GLU:HG2	1:B:148:VAL:HG11	2.01	0.41
1:B:272:ARG:HG3	1:B:274:VAL:CG2	2.36	0.41
1:B:83:ARG:HE	1:B:179:THR:HG23	1.85	0.41
1:B:194:ALA:CB	1:B:196:ASP:OD2	2.69	0.41
1:B:540:VAL:O	1:B:541:SER:C	2.63	0.41
1:A:505:TYR:CZ	1:A:548:VAL:HG22	2.55	0.41
1:A:507:VAL:HG22	1:A:526:GLN:HG3	2.02	0.41
1:B:142:THR:O	1:B:142:THR:CG2	2.66	0.41
1:B:276:VAL:CG1	1:B:499:PRO:HG3	2.50	0.41
1:B:432:THR:OG1	1:B:441:ILE:CD1	2.65	0.41
1:A:199:HIS:CE1	1:A:236:VAL:HB	2.55	0.41
1:B:104:VAL:HG12	1:B:105:MSE:HG2	2.02	0.41
1:B:388:HIS:O	1:B:392:ILE:CG1	2.68	0.41
1:A:417:ARG:HE	1:A:417:ARG:HB2	1.57	0.41
1:B:425:PHE:CD2	1:B:455:THR:HG21	2.55	0.41
1:B:474:GLN:HE22	1:B:484:VAL:HG21	1.86	0.41
1:A:348:VAL:HG12	1:A:349:ILE:N	2.35	0.41
1:B:212:VAL:CG2	1:B:230:THR:CG2	2.99	0.41
1:A:199:HIS:CE1	1:A:236:VAL:CB	3.04	0.41
1:A:372:LYS:C	1:A:373:GLU:CG	2.93	0.41
1:A:381:ASN:C	1:A:383:GLU:H	2.27	0.41
1:A:463:LEU:HD21	1:A:492:TRP:CE3	2.56	0.41
1:B:47:VAL:CG1	1:B:48:PRO:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:PRO:HB3	1:B:172:ARG:C	2.46	0.41
1:B:172:ARG:HH22	1:B:333:TYR:HA	1.85	0.41
1:B:538:ASP:HA	1:B:596:LYS:NZ	2.36	0.41
1:B:560:ILE:C	1:B:562:ARG:N	2.78	0.41
1:A:333:TYR:O	1:A:398:ARG:NH2	2.54	0.41
1:A:375:TYR:O	1:A:377:GLU:N	2.53	0.41
1:B:450:ASP:C	1:B:450:ASP:OD2	2.63	0.41
1:B:531:ASP:HA	1:B:534:HIS:HB2	2.02	0.41
1:B:562:ARG:HG2	1:B:566:ASN:HD22	1.83	0.41
1:A:11:GLU:HB2	1:A:177:TYR:HB2	2.03	0.41
1:A:163:ASP:HB3	2:A:706:HOH:O	2.20	0.41
1:A:193:VAL:HG22	1:A:273:SER:HB2	2.03	0.41
1:A:358:ASN:O	1:A:359:LEU:HD13	2.21	0.41
1:A:397:ALA:O	1:A:400:LYS:CD	2.68	0.41
1:A:421:ALA:HB1	1:A:455:THR:OG1	2.21	0.41
1:A:479:GLU:H	1:A:479:GLU:CD	2.22	0.41
1:A:531:ASP:OD1	1:A:583:LEU:HD21	2.20	0.41
1:B:180:PRO:HB2	1:B:261:GLU:HG3	2.03	0.41
1:B:273:SER:HB3	1:B:284:ASN:HA	2.03	0.41
1:B:342:ASP:OD1	1:B:404:SER:OG	2.38	0.41
1:B:363:ILE:C	1:B:561:LEU:HD13	2.46	0.41
1:B:459:LEU:H	1:B:459:LEU:HG	1.52	0.41
1:B:538:ASP:CB	1:B:597:PRO:HG2	2.51	0.41
1:A:95:GLY:O	1:A:106:GLU:HA	2.21	0.41
1:A:160:TYR:HD1	1:A:162:HIS:CD2	2.39	0.41
1:A:233:THR:O	1:A:234:LEU:CD2	2.52	0.41
1:A:413:GLU:CG	1:A:466:ASN:HD22	2.34	0.41
1:A:508:ASP:OD2	1:A:568:LYS:HD3	2.20	0.41
1:B:15:LEU:O	1:B:15:LEU:CD1	2.64	0.41
1:B:35:TRP:CD1	1:B:98:TRP:CE3	3.09	0.41
1:B:275:ALA:O	1:B:282:LEU:HD13	2.20	0.41
1:B:380:VAL:HG22	1:B:380:VAL:O	2.20	0.41
1:A:18:LEU:C	1:A:19:TRP:CD1	2.99	0.40
1:A:176:LEU:HD13	1:A:177:TYR:N	2.36	0.40
1:A:179:THR:CB	2:A:715:HOH:O	2.38	0.40
1:B:83:ARG:HH11	1:B:118:VAL:HG12	1.87	0.40
1:B:113:PRO:C	1:B:114:PHE:HD2	2.29	0.40
1:B:328:THR:CA	1:B:333:TYR:CZ	2.97	0.40
1:B:358:ASN:OD1	1:B:415:ASP:HB2	2.21	0.40
1:B:437:PRO:HA	2:B:627:HOH:O	2.19	0.40
1:A:238:ASN:ND2	1:A:239:PRO:HD3	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ILE:O	1:A:561:LEU:C	2.65	0.40
1:A:578:LYS:O	1:A:579:SER:C	2.62	0.40
1:B:217:ARG:HD2	1:B:221:GLN:HA	2.02	0.40
1:B:242:TRP:NE1	1:B:403:PRO:CB	2.84	0.40
1:B:538:ASP:O	1:B:596:LYS:NZ	2.54	0.40
1:A:50:SER:OG	1:A:171:HIS:NE2	2.54	0.40
1:A:97:VAL:HG22	1:A:132:VAL:HG22	2.03	0.40
1:A:218:ASP:HB2	1:A:221:GLN:CA	2.42	0.40
1:B:352:THR:C	1:B:354:ALA:N	2.78	0.40
1:B:524:GLU:OE1	1:B:524:GLU:N	2.49	0.40
1:A:13:LYS:HE3	1:A:175:MSE:HE2	2.02	0.40
1:A:283:ILE:O	1:A:284:ASN:C	2.64	0.40
1:A:321:ILE:CG2	1:A:588:TRP:HE3	2.33	0.40
1:A:361:LEU:O	1:A:362:GLY:C	2.65	0.40
1:B:119:THR:N	1:B:120:PRO:CD	2.83	0.40
1:B:335:GLU:O	1:B:335:GLU:CG	2.67	0.40
1:A:85:VAL:HA	1:A:117:ASP:O	2.21	0.40
1:B:75:ILE:HD11	1:B:128:VAL:HG21	2.04	0.40
1:B:139:ASN:O	1:B:145:PRO:HA	2.22	0.40
1:B:297:GLU:O	1:B:304:LYS:HA	2.21	0.40
1:B:392:ILE:CD1	1:B:410:ILE:HG23	2.48	0.40
1:B:420:GLY:HA3	2:B:671:HOH:O	2.21	0.40
1:B:432:THR:O	1:B:433:ARG:C	2.64	0.40
1:B:463:LEU:HB3	1:B:500:ILE:HG12	2.02	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLU:OE2	2:A:685:HOH:O[2_554]	1.03	1.17
1:B:152:GLU:CD	2:A:685:HOH:O[2_554]	1.50	0.70
1:B:152:GLU:OE1	2:A:685:HOH:O[2_554]	1.83	0.37
1:A:599:GLN:O	1:B:603:GLN:C[2_564]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/605 (98%)	522 (88%)	58 (10%)	13 (2%)	5	20
1	B	593/605 (98%)	494 (83%)	76 (13%)	23 (4%)	2	10
All	All	1186/1210 (98%)	1016 (86%)	134 (11%)	36 (3%)	3	14

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	B	7	THR
1	B	119	THR
1	B	123	ILE
1	B	144	PRO
1	B	209	ASN
1	B	561	LEU
1	A	237	VAL
1	B	137	GLU
1	B	198	ASN
1	B	335	GLU
1	B	560	ILE
1	A	0	HIS
1	A	378	GLU
1	B	337	MSE
1	B	339	ASP
1	B	453	THR
1	B	518	THR
1	A	7	THR
1	A	199	HIS
1	A	550	ASN
1	B	109	GLY
1	B	239	PRO
1	B	541	SER
1	A	230	THR
1	B	27	ASN
1	B	100	ASN
1	B	230	THR
1	A	152	GLU
1	A	65	GLY
1	A	154	GLY

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Mol	Chain	Res	Type
1	A	266	PRO
1	B	190	VAL
1	B	266	PRO
1	B	446	VAL
1	A	224	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	505/501 (101%)	408 (81%)	97 (19%)	1	5
1	B	502/501 (100%)	381 (76%)	121 (24%)	1	2
All	All	1007/1002 (100%)	789 (78%)	218 (22%)	1	3

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	1	MSE
1	A	11	GLU
1	A	12	ILE
1	A	14	LYS
1	A	15	LEU
1	A	33	ARG
1	A	47	VAL
1	A	59	ASP
1	A	71	ARG
1	A	74	PHE
1	A	75	ILE
1	A	76	PRO
1	A	82	GLN
1	A	85	VAL
1	A	96	LYS
1	A	101	ASN
1	A	102	GLN

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Mol	Chain	Res	Type
1	A	103	GLU
1	A	105	MSE
1	A	108	GLN
1	A	112	THR
1	A	120	PRO
1	A	122	VAL
1	A	128	VAL
1	A	136	ASN
1	A	143	ILE
1	A	148	VAL
1	A	151	ASP
1	A	153	ASN
1	A	155	LYS
1	A	160	TYR
1	A	170	ILE
1	A	174	VAL
1	A	176	LEU
1	A	178	THR
1	A	182	THR
1	A	184	VAL
1	A	193	VAL
1	A	195	GLN
1	A	203	ASP
1	A	206	VAL
1	A	207	VAL
1	A	212	VAL
1	A	214	VAL
1	A	215	GLU
1	A	216	LEU
1	A	217	ARG
1	A	218	ASP
1	A	221	GLN
1	A	226	THR
1	A	228	GLN
1	A	233	THR
1	A	234	LEU
1	A	236	VAL
1	A	249	LEU
1	A	251	GLU
1	A	259	GLN
1	A	261	GLU
1	A	262	CYS

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Mol	Chain	Res	Type
1	A	264	ILE
1	A	277	LYS
1	A	298	ASP
1	A	300	ASP
1	A	321	ILE
1	A	328	THR
1	A	335	GLU
1	A	338	LEU
1	A	344	HIS
1	A	347	VAL
1	A	355	VAL
1	A	359	LEU
1	A	373	GLU
1	A	375	TYR
1	A	377	GLU
1	A	396	ILE
1	A	398	ARG
1	A	400	LYS
1	A	446	VAL
1	A	450	ASP
1	A	456	ILE
1	A	469	TYR
1	A	473	VAL
1	A	479	GLU
1	A	484	VAL
1	A	487	LYS
1	A	488	GLU
1	A	494	GLU
1	A	507	VAL
1	A	530	LEU
1	A	536	VAL
1	A	558	GLN
1	A	561	LEU
1	A	563	VAL
1	A	570	ILE
1	A	598	GLN
1	A	603	GLN
1	B	0	HIS
1	B	1	MSE
1	B	8	PRO
1	B	10	ARG
1	B	12	ILE

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Mol	Chain	Res	Type
1	B	14	LYS
1	B	16	ASP
1	B	18	LEU
1	B	26	GLU
1	B	28	CYS
1	B	31	ASP
1	B	37	SER
1	B	39	LEU
1	B	40	GLN
1	B	43	ARG
1	B	45	ILE
1	B	67	VAL
1	B	72	GLU
1	B	85	VAL
1	B	92	THR
1	B	101	ASN
1	B	102	GLN
1	B	104	VAL
1	B	114	PHE
1	B	115	GLU
1	B	119	THR
1	B	122	VAL
1	B	123	ILE
1	B	127	SER
1	B	134	VAL
1	B	143	ILE
1	B	144	PRO
1	B	147	MSE
1	B	148	VAL
1	B	149	ILE
1	B	152	GLU
1	B	163	ASP
1	B	176	LEU
1	B	178	THR
1	B	179	THR
1	B	182	THR
1	B	190	VAL
1	B	192	HIS
1	B	193	VAL
1	B	196	ASP
1	B	198	ASN
1	B	199	HIS

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Mol	Chain	Res	Type
1	B	207	VAL
1	B	209	ASN
1	B	214	VAL
1	B	216	LEU
1	B	223	VAL
1	B	224	VAL
1	B	234	LEU
1	B	235	GLN
1	B	240	HIS
1	B	241	LEU
1	B	243	GLN
1	B	246	GLU
1	B	248	TYR
1	B	249	LEU
1	B	252	LEU
1	B	254	VAL
1	B	255	THR
1	B	259	GLN
1	B	260	THR
1	B	262	CYS
1	B	267	LEU
1	B	268	ARG
1	B	269	VAL
1	B	272	ARG
1	B	276	VAL
1	B	282	LEU
1	B	283	ILE
1	B	288	PHE
1	B	318	MSE
1	B	319	ASP
1	B	321	ILE
1	B	327	ARG
1	B	328	THR
1	B	330	HIS
1	B	335	GLU
1	B	348	VAL
1	B	350	ASP
1	B	361	LEU
1	B	372	LYS
1	B	373	GLU
1	B	375	TYR
1	B	392	ILE

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Mol	Chain	Res	Type
1	B	395	LEU
1	B	396	ILE
1	B	416	THR
1	B	422	ARG
1	B	434	LYS
1	B	441	ILE
1	B	445	ASN
1	B	446	VAL
1	B	448	PHE
1	B	449	CYS
1	B	452	HIS
1	B	455	THR
1	B	458	ASP
1	B	459	LEU
1	B	463	LEU
1	B	465	LEU
1	B	466	ASN
1	B	467	ARG
1	B	472	TYR
1	B	473	VAL
1	B	500	ILE
1	B	509	THR
1	B	513	LEU
1	B	517	TYR
1	B	520	MSE
1	B	530	LEU
1	B	537	PHE
1	B	558	GLN
1	B	562	ARG
1	B	584	LEU
1	B	598	GLN
1	B	599	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	40	GLN
1	A	52	ASN
1	A	66	ASN
1	A	70	GLN
1	A	82	GLN

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Mol	Chain	Res	Type
1	A	107	HIS
1	A	136	ASN
1	A	141	GLN
1	A	199	HIS
1	A	228	GLN
1	A	259	GLN
1	A	313	HIS
1	A	402	HIS
1	A	412	ASN
1	A	445	ASN
1	A	466	ASN
1	A	474	GLN
1	A	493	GLN
1	A	497	HIS
1	A	547	GLN
1	B	32	GLN
1	B	52	ASN
1	B	54	GLN
1	B	93	HIS
1	B	101	ASN
1	B	102	GLN
1	B	107	HIS
1	B	192	HIS
1	B	199	HIS
1	B	205	GLN
1	B	222	GLN
1	B	228	GLN
1	B	238	ASN
1	B	240	HIS
1	B	259	GLN
1	B	280	GLN
1	B	315	HIS
1	B	386	GLN
1	B	466	ASN
1	B	497	HIS
1	B	498	GLN
1	B	514	HIS
1	B	550	ASN
1	B	592	ASN
1	B	598	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	584/605 (96%)	0.28	27 (4%) 37 29	18, 45, 78, 103	0
1	B	584/605 (96%)	0.74	38 (6%) 25 20	39, 70, 89, 99	0
All	All	1168/1210 (96%)	0.51	65 (5%) 30 23	18, 61, 86, 103	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	ASP	5.5
1	B	206	VAL	5.1
1	B	227	GLY	4.3
1	B	204	TRP	4.2
1	A	456	ILE	4.2
1	B	97	VAL	4.0
1	B	84	ILE	4.0
1	A	117	ASP	4.0
1	A	470	GLY	3.8
1	A	601	GLY	3.7
1	B	469	TYR	3.7
1	A	564	GLY	3.6
1	A	471	TRP	3.6
1	B	266	PRO	3.5
1	A	97	VAL	3.3
1	A	455	THR	3.3
1	B	207	VAL	3.2
1	A	214	VAL	3.1
1	B	410	ILE	3.1
1	B	560	ILE	3.1
1	A	98	TRP	2.9
1	A	224	VAL	2.9
1	B	18	LEU	2.9
1	B	468	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	357	PHE	2.8
1	A	476	GLY	2.7
1	A	205	GLN	2.7
1	B	465	LEU	2.7
1	B	363	ILE	2.6
1	B	339	ASP	2.6
1	B	451	ALA	2.6
1	B	19	TRP	2.5
1	B	187	ILE	2.5
1	B	463	LEU	2.5
1	B	561	LEU	2.5
1	B	122	VAL	2.5
1	A	92	THR	2.5
1	B	104	VAL	2.4
1	B	223	VAL	2.4
1	B	116	ALA	2.3
1	A	207	VAL	2.3
1	A	235	GLN	2.3
1	B	443	CYS	2.3
1	B	111	TYR	2.3
1	A	449	CYS	2.2
1	B	31	ASP	2.2
1	A	100	ASN	2.2
1	B	130	ILE	2.2
1	A	254	VAL	2.2
1	B	442	THR	2.2
1	B	356	GLY	2.2
1	A	472	TYR	2.2
1	A	17	GLY	2.1
1	B	441	ILE	2.1
1	A	38	ALA	2.1
1	B	456	ILE	2.1
1	A	558	GLN	2.1
1	B	228	GLN	2.1
1	A	209	ASN	2.1
1	B	209	ASN	2.1
1	A	453	THR	2.1
1	A	236	VAL	2.1
1	B	30	ILE	2.0
1	B	328	THR	2.0
1	B	411	ALA	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.