



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 AM UTC

PDB ID : 2HTY / pdb_00002hty
Title : N1 neuraminidase
Authors : Russell, R.J.; Haire, L.F.; Stevens, D.J.; Collins, P.J.; Lin, Y.P.; Blackburn, G.M.; Hay, A.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2006-07-26
Resolution : 2.50 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

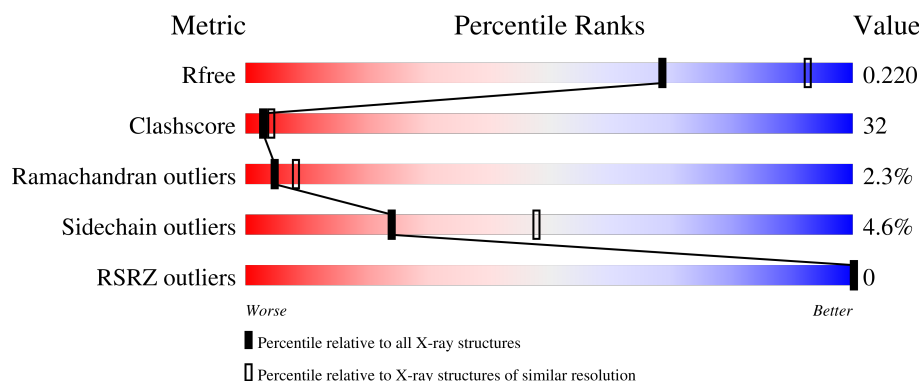
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	387	 55% 37% 7% ..
1	B	387	 52% 40% 7% .
1	C	387	 53% 38% 8% ..
1	D	387	 53% 39% 6% ..
1	E	387	 51% 41% 6% .

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Mol	Chain	Length	Quality of chain
1	F	387	 55% 36% 8% .
1	G	387	 52% 38% 9% .
1	H	387	 51% 41% 7% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24458 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.

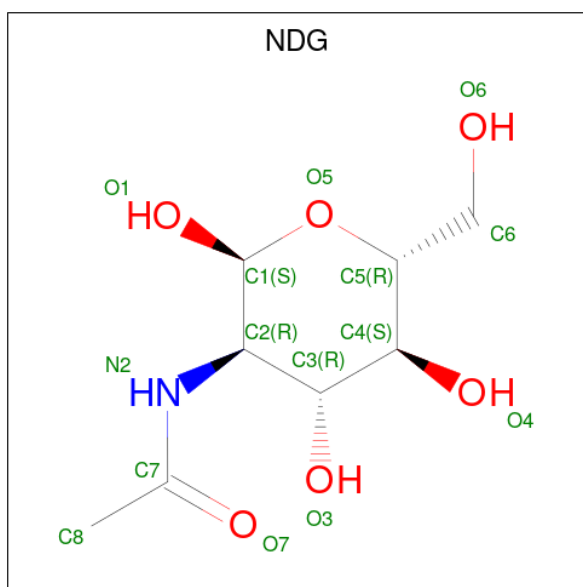
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	B	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	C	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	D	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	E	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	F	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	G	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	H	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
B	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
C	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
D	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
E	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
F	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
G	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
H	169A	TYR	HIS	engineered mutation	UNP Q6DPL2

- Molecule 2 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 15	C 8	N 1	O 6	0	0
2	B	1	Total 15	C 8	N 1	O 6	0	0
2	C	1	Total 15	C 8	N 1	O 6	0	0
2	D	1	Total 15	C 8	N 1	O 6	0	0
2	F	1	Total 15	C 8	N 1	O 6	0	0
2	G	1	Total 15	C 8	N 1	O 6	0	0
2	H	1	Total 15	C 8	N 1	O 6	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is water.

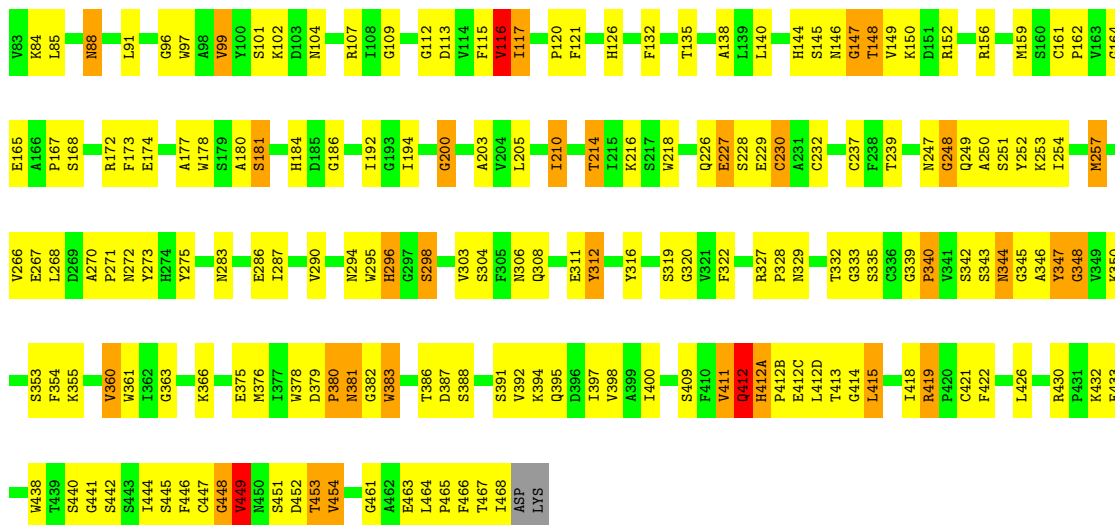
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		
5	B	91	Total	O	0	0
			91	91		
5	C	102	Total	O	0	0
			102	102		
5	D	104	Total	O	0	0
			104	104		
5	E	54	Total	O	0	0
			54	54		

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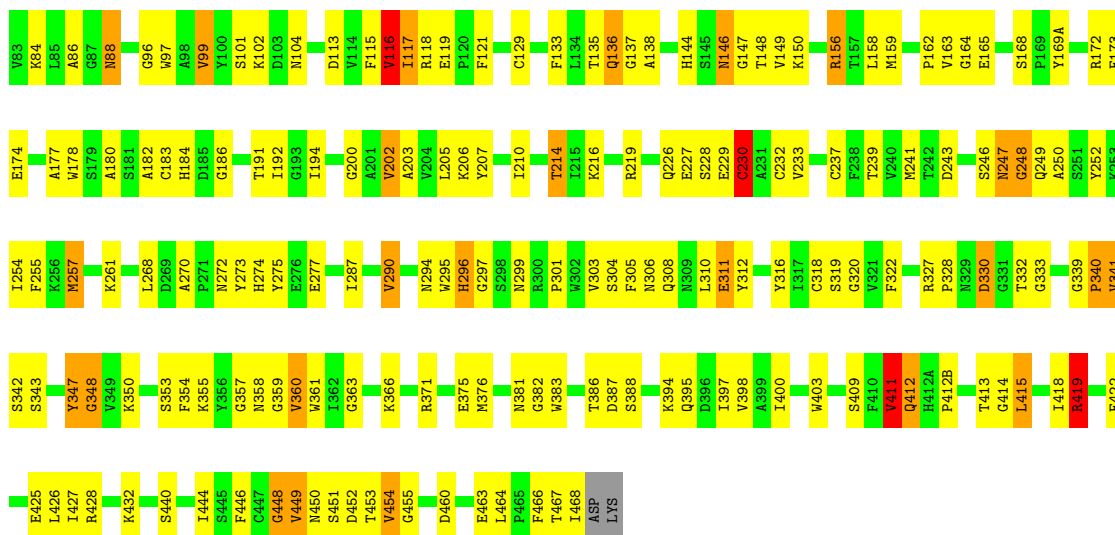
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	46	Total	O	0	0
			46	46		
5	G	86	Total	O	0	0
			86	86		
5	H	40	Total	O	0	0
			40	40		

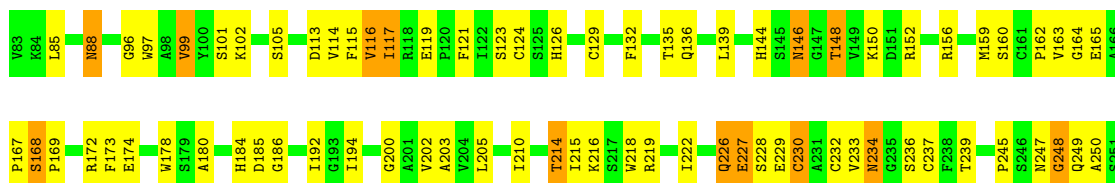
● Molecule 1: Neuraminidase

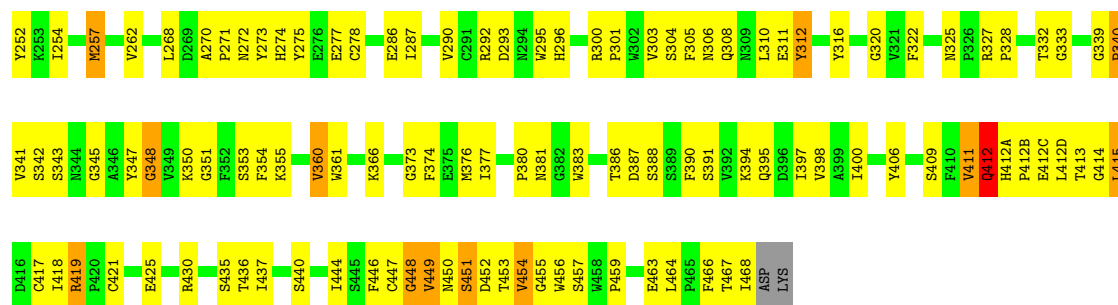
Chain C:  53% 38% 8% ..

● Molecule 1: Neuraminidase

Chain D:  53% 39% 6% ..

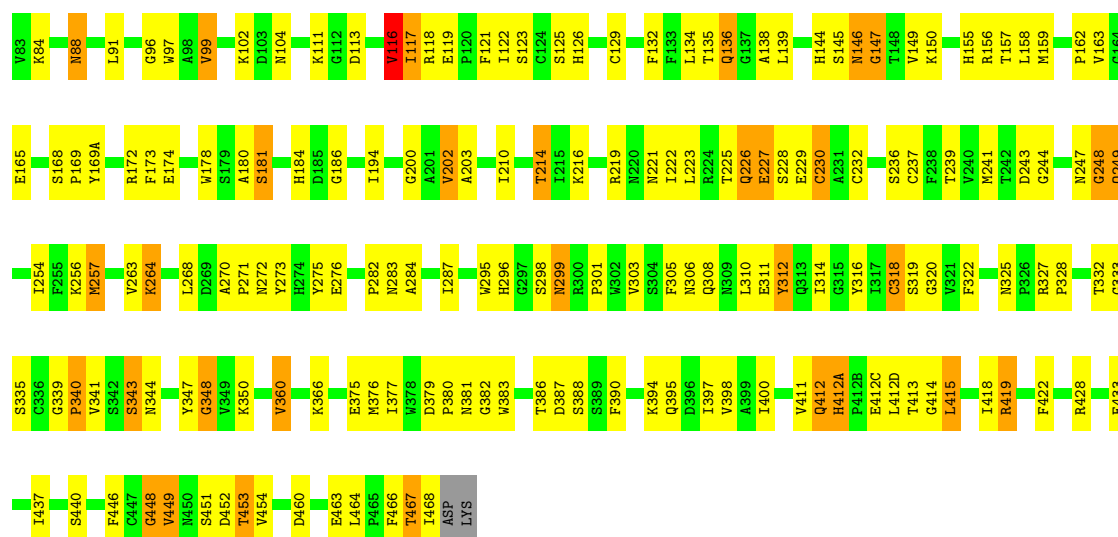
● Molecule 1: Neuraminidase

Chain E:  51% 41% 6% ..



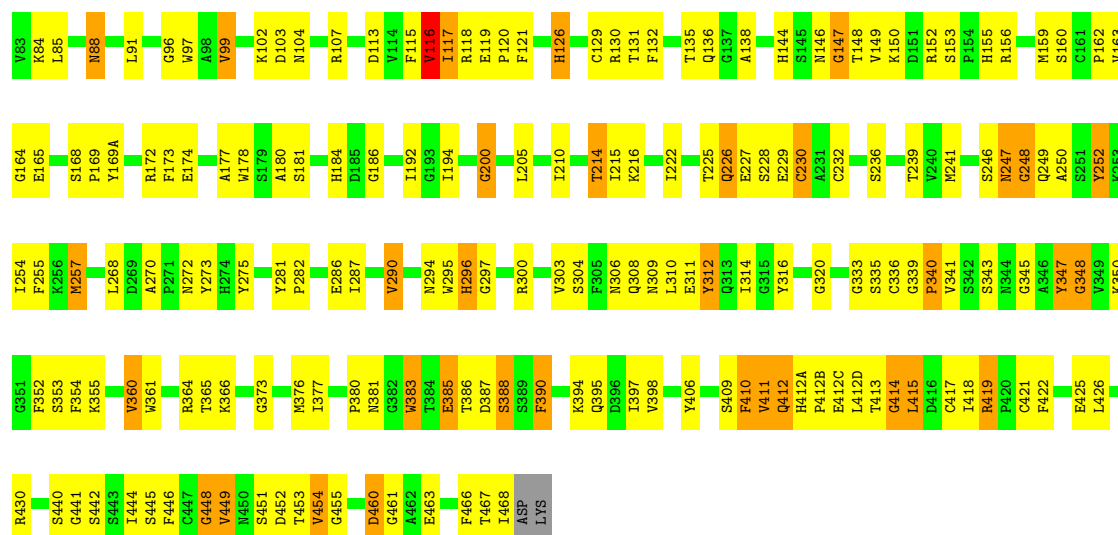
• Molecule 1: Neuraminidase

Chain F: 55% 36% 8% .

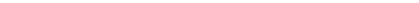


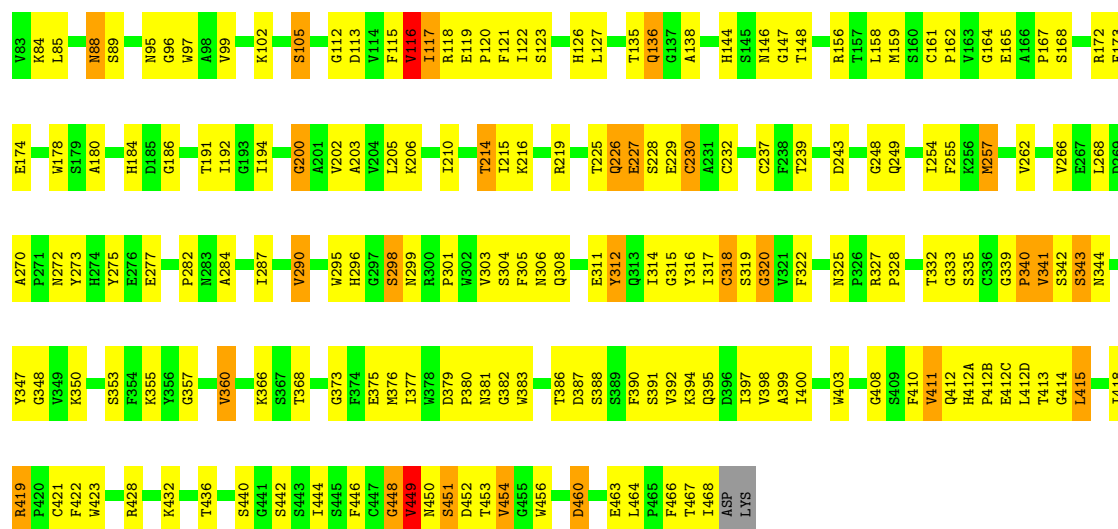
• Molecule 1: Neuraminidase

Chain G: 52% 38% 9% .



• Molecule 1: Neuraminidase

Chain H:  51% 41% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	200.21Å 200.77Å 211.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 97.9 (30.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.262 0.219 , 0.220	Depositor DCC
R_{free} test set	7196 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 7.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.054 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24458	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2128e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NDG, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3045	1.11	26/4141 (0.6%)
1	B	0.61	4/3045 (0.1%)	1.13	20/4141 (0.5%)
1	C	0.62	2/3045 (0.1%)	1.19	25/4141 (0.6%)
1	D	0.57	2/3045 (0.1%)	1.15	32/4141 (0.8%)
1	E	0.55	2/3045 (0.1%)	1.13	23/4141 (0.6%)
1	F	0.45	1/3045 (0.0%)	1.02	14/4141 (0.3%)
1	G	0.52	2/3045 (0.1%)	1.10	27/4141 (0.7%)
1	H	0.42	0/3045	1.04	22/4141 (0.5%)
All	All	0.54	13/24360 (0.1%)	1.11	189/33128 (0.6%)

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	C	0	2
1	D	0	1
1	E	0	2
1	F	0	1
All	All	0	6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	411	VAL	CB-CG2	13.87	1.98	1.52
1	C	412	GLN	C-N	-13.57	1.02	1.34
1	C	411	VAL	CB-CG2	13.22	1.96	1.52
1	B	411	VAL	CB-CG2	13.18	1.96	1.52
1	E	411	VAL	CB-CG2	12.55	1.94	1.52
1	E	412	GLN	C-N	-11.05	1.08	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	412	GLN	CB-CG	9.06	1.79	1.52
1	B	411	VAL	CB-CG1	-9.01	1.22	1.52
1	G	410	PHE	C-N	7.76	1.43	1.33
1	B	412	GLN	C-N	-6.36	1.19	1.34
1	D	412	GLN	CB-CG	5.80	1.69	1.52
1	B	412	GLN	CB-CG	5.54	1.69	1.52
1	F	412(A)	HIS	CA-C	-5.31	1.47	1.53

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	412	GLN	O-C-N	-19.52	91.47	122.70
1	E	412	GLN	O-C-N	-16.21	96.76	122.70
1	B	411	VAL	CA-CB-CG2	-15.25	84.48	110.40
1	E	411	VAL	CA-CB-CG2	-14.14	86.37	110.40
1	D	411	VAL	CA-CB-CG2	-13.55	87.36	110.40
1	C	412	GLN	CA-C-N	13.04	145.88	117.20
1	C	411	VAL	CA-CB-CG2	-12.97	88.34	110.40
1	D	388	SER	N-CA-C	-11.67	100.04	114.75
1	C	412	GLN	C-N-CA	11.54	150.54	121.70
1	E	411	VAL	CG1-CB-CG2	-10.92	86.78	110.80
1	D	226	GLN	N-CA-C	10.57	123.80	111.11
1	C	226	GLN	N-CA-C	10.55	123.77	111.11
1	B	226	GLN	N-CA-C	10.37	123.55	111.11
1	E	412	GLN	CA-C-N	10.35	139.97	117.20
1	G	412	GLN	CA-CB-CG	-10.11	93.89	114.10
1	C	411	VAL	CG1-CB-CG2	-9.95	88.90	110.80
1	C	388	SER	N-CA-C	-9.70	99.89	114.64
1	A	226	GLN	N-CA-C	9.69	122.74	111.11
1	G	226	GLN	N-CA-C	9.67	122.71	111.11
1	E	388	SER	N-CA-C	-9.51	100.60	114.39
1	H	226	GLN	N-CA-C	9.39	122.38	111.11
1	H	411	VAL	N-CA-C	9.19	121.86	108.53
1	A	388	SER	N-CA-C	-9.16	100.72	114.64
1	D	247	ASN	N-CA-C	-9.04	101.37	108.78
1	B	388	SER	N-CA-C	-9.03	100.09	114.09
1	F	226	GLN	N-CA-C	8.86	121.74	111.11
1	G	411	VAL	N-CA-C	8.82	120.52	108.17
1	H	116	VAL	N-CA-C	-8.38	97.83	108.89
1	E	412	GLN	C-N-CA	8.35	142.57	121.70
1	D	348	GLY	N-CA-C	8.34	122.22	110.38
1	A	312	TYR	N-CA-C	8.28	120.94	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	VAL	CA-CB-CG1	8.17	124.28	110.40
1	D	411	VAL	CG1-CB-CG2	-8.08	93.02	110.80
1	E	414	GLY	N-CA-C	-8.06	104.74	115.21
1	C	116	VAL	N-CA-C	-8.02	95.95	108.23
1	E	411	VAL	CA-CB-CG1	-7.80	97.13	110.40
1	H	312	TYR	N-CA-C	7.66	120.06	109.18
1	F	414	GLY	N-CA-C	-7.66	104.96	114.92
1	E	116	VAL	N-CA-C	-7.61	98.84	108.89
1	B	311	GLU	N-CA-C	-7.57	97.72	109.76
1	D	247	ASN	CB-CA-C	-7.43	106.36	117.07
1	F	312	TYR	N-CA-C	7.42	119.71	109.18
1	H	411	VAL	CB-CA-C	-7.42	99.53	110.81
1	G	116	VAL	N-CA-C	-7.40	96.91	108.23
1	D	312	TYR	N-CA-C	7.34	119.61	109.18
1	G	312	TYR	N-CA-C	7.34	120.56	109.41
1	D	414	GLY	N-CA-C	-7.26	105.48	114.92
1	G	412	GLN	N-CA-CB	7.25	122.35	110.39
1	A	413	THR	N-CA-C	7.15	120.49	111.69
1	E	348	GLY	N-CA-C	7.12	120.49	110.38
1	G	117	ILE	N-CA-C	6.99	117.35	108.82
1	E	227	GLU	N-CA-C	-6.98	104.06	112.58
1	A	414	GLY	N-CA-C	-6.86	106.29	115.21
1	A	168	SER	CA-C-N	-6.82	112.78	119.87
1	A	168	SER	C-N-CA	-6.82	112.78	119.87
1	H	311	GLU	N-CA-C	-6.80	98.15	108.96
1	D	296	HIS	N-CA-C	6.78	118.41	110.41
1	E	180	ALA	N-CA-C	6.75	117.49	108.38
1	B	412	GLN	CA-CB-CG	-6.69	100.71	114.10
1	F	116	VAL	N-CA-C	-6.64	98.71	108.54
1	G	455	GLY	N-CA-C	-6.62	102.49	113.02
1	G	411	VAL	CB-CA-C	-6.62	100.97	110.83
1	E	226	GLN	N-CA-C	6.62	122.29	111.37
1	D	116	VAL	N-CA-C	-6.55	98.21	108.23
1	A	117	ILE	N-CA-C	6.54	118.35	108.80
1	H	180	ALA	N-CA-C	6.53	117.20	108.38
1	A	180	ALA	N-CA-C	6.51	117.06	107.88
1	C	348	GLY	N-CA-C	6.51	120.51	110.88
1	F	117	ILE	N-CA-C	6.47	116.71	108.82
1	G	247	ASN	N-CA-C	-6.46	103.48	108.78
1	D	227	GLU	N-CA-C	-6.44	104.72	112.58
1	G	247	ASN	CB-CA-C	-6.44	107.80	117.07
1	H	227	GLU	N-CA-C	-6.42	104.74	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	VAL	N-CA-C	-6.35	98.51	108.23
1	G	311	GLU	N-CA-C	-6.35	98.92	109.46
1	B	227	GLU	N-CA-C	-6.30	104.89	112.58
1	C	227	GLU	N-CA-C	-6.28	104.92	112.58
1	H	320	GLY	N-CA-C	-6.28	106.88	114.66
1	D	412	GLN	CA-CB-CG	-6.26	101.58	114.10
1	F	348	GLY	N-CA-C	6.26	119.08	110.56
1	A	311	GLU	N-CA-C	-6.23	99.11	109.46
1	E	126	HIS	N-CA-C	-6.20	105.57	112.57
1	G	388	SER	N-CA-C	-6.19	97.61	110.80
1	E	455	GLY	N-CA-C	-6.17	104.30	112.82
1	G	414	GLY	N-CA-C	-6.15	106.92	114.92
1	F	311	GLU	N-CA-C	-6.15	99.99	109.76
1	B	432	LYS	N-CA-C	6.10	118.90	111.82
1	E	312	TYR	N-CA-C	6.10	118.68	109.41
1	D	455	GLY	N-CA-C	-6.06	103.39	113.02
1	B	414	GLY	N-CA-C	-6.01	107.39	115.21
1	G	412	GLN	CA-C-O	-6.00	114.36	120.84
1	C	311	GLU	N-CA-C	-5.99	99.44	108.96
1	A	145	SER	N-CA-C	-5.98	106.24	112.93
1	H	317	ILE	N-CA-C	-5.93	101.88	109.30
1	B	348	GLY	N-CA-C	5.92	119.10	110.63
1	C	312	TYR	N-CA-C	5.91	118.86	109.81
1	D	341	VAL	N-CA-C	-5.88	99.23	108.23
1	F	180	ALA	N-CA-C	5.87	116.16	107.88
1	B	247	ASN	CB-CA-C	-5.87	107.97	116.54
1	A	348	GLY	N-CA-C	5.86	118.53	110.56
1	C	329	ASN	N-CA-C	-5.86	101.61	110.28
1	D	250	ALA	N-CA-C	-5.86	100.86	109.18
1	D	361	TRP	N-CA-C	-5.85	98.20	108.20
1	A	427	ILE	N-CA-C	5.83	117.17	108.54
1	C	411	VAL	CA-CB-CG1	-5.83	100.50	110.40
1	F	227	GLU	N-CA-C	-5.82	104.84	113.40
1	H	105	SER	N-CA-C	5.82	118.09	111.11
1	C	148	THR	N-CA-C	-5.81	106.04	113.01
1	B	148	THR	N-CA-C	-5.79	106.07	113.01
1	G	341	VAL	N-CA-C	-5.77	100.00	108.54
1	E	136	GLN	N-CA-C	-5.77	106.10	113.02
1	D	363	GLY	N-CA-C	-5.76	100.94	111.25
1	A	136	GLN	N-CA-C	-5.71	106.30	113.20
1	G	180	ALA	N-CA-C	5.70	116.61	108.74
1	H	117	ILE	N-CA-C	5.68	116.89	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	GLU	N-CA-C	-5.67	99.94	108.96
1	C	346	ALA	N-CA-C	5.64	118.95	112.97
1	D	419	ARG	CA-C-N	-5.64	113.90	119.99
1	D	419	ARG	C-N-CA	-5.64	113.90	119.99
1	D	290	VAL	N-CA-C	-5.63	99.64	107.80
1	G	126	HIS	N-CA-C	-5.62	106.27	113.02
1	E	148	THR	N-CA-C	-5.62	106.39	113.18
1	A	177	ALA	N-CA-C	5.61	117.05	108.52
1	C	180	ALA	N-CA-C	5.61	115.95	108.38
1	C	117	ILE	N-CA-C	5.59	115.64	108.82
1	E	311	GLU	N-CA-C	-5.58	100.72	109.25
1	C	177	ALA	N-CA-C	5.56	116.97	108.52
1	A	296	HIS	N-CA-C	5.56	116.97	110.41
1	G	390	PHE	N-CA-C	-5.55	100.49	108.60
1	H	414	GLY	N-CA-C	-5.55	107.58	115.30
1	A	341	VAL	N-CA-C	-5.55	100.33	108.54
1	F	136	GLN	N-CA-C	-5.53	106.50	113.20
1	H	136	GLN	N-CA-C	-5.53	106.51	113.20
1	B	116	VAL	N-CA-C	-5.52	100.37	108.54
1	D	247	ASN	CA-C-O	5.50	121.13	117.94
1	A	449	VAL	N-CA-C	5.48	120.74	109.34
1	B	342	SER	N-CA-C	5.48	117.33	111.36
1	C	383	TRP	N-CA-C	-5.47	105.73	112.90
1	D	246	SER	N-CA-C	-5.47	106.19	112.92
1	G	177	ALA	N-CA-C	5.44	116.67	108.46
1	G	290	VAL	N-CA-C	-5.43	100.57	108.17
1	A	363	GLY	N-CA-C	-5.41	101.57	111.25
1	B	455	GLY	N-CA-C	-5.40	102.87	112.54
1	A	444	ILE	N-CA-C	-5.38	100.72	108.42
1	D	117	ILE	N-CA-C	5.38	116.65	108.80
1	A	455	GLY	N-CA-C	-5.37	104.48	113.02
1	F	467	THR	N-CA-C	-5.37	106.43	112.87
1	H	341	VAL	N-CA-C	-5.35	100.63	108.54
1	G	246	SER	N-CA-C	-5.33	106.55	113.16
1	D	148	THR	N-CA-C	-5.33	106.28	112.89
1	D	371	ARG	N-CA-C	-5.31	103.29	110.68
1	B	411	VAL	CA-C-O	-5.30	116.05	121.67
1	A	383	TRP	N-CA-C	-5.30	105.95	112.90
1	H	148	THR	N-CA-C	-5.29	106.66	113.01
1	B	177	ALA	N-CA-C	5.28	116.43	108.46
1	D	180	ALA	N-CA-C	5.26	116.14	108.14
1	D	136	GLN	N-CA-C	-5.25	106.90	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	348	GLY	N-CA-C	5.25	118.64	110.88
1	G	361	TRP	N-CA-C	-5.24	98.71	107.99
1	G	442	SER	N-CA-C	-5.24	102.23	110.36
1	B	412	GLN	N-CA-CB	5.21	118.95	110.77
1	F	339	GLY	CA-C-N	5.20	126.34	119.84
1	F	339	GLY	C-N-CA	5.20	126.34	119.84
1	E	341	VAL	N-CA-C	-5.18	100.88	108.54
1	F	299	ASN	N-CA-C	-5.17	103.09	110.59
1	A	437	ILE	N-CA-C	-5.17	107.94	112.90
1	D	230	CYS	N-CA-C	-5.17	103.10	110.59
1	B	392	VAL	N-CA-C	5.15	116.14	108.46
1	C	363	GLY	N-CA-C	-5.15	102.03	111.25
1	B	442	SER	N-CA-C	-5.14	102.85	110.46
1	H	392	VAL	N-CA-C	5.14	116.12	108.46
1	H	342	SER	N-CA-C	5.13	118.00	111.69
1	C	145	SER	N-CA-C	-5.12	106.88	113.02
1	D	432	LYS	N-CA-C	5.12	117.76	111.82
1	E	361	TRP	N-CA-C	-5.08	98.99	107.99
1	G	411	VAL	CA-C-O	5.06	125.85	120.48
1	H	225	THR	N-CA-C	5.06	114.97	108.34
1	E	278	CYS	N-CA-C	5.05	117.76	110.28
1	A	339	GLY	CA-C-N	5.04	126.14	119.84
1	A	339	GLY	C-N-CA	5.04	126.14	119.84
1	C	361	TRP	N-CA-C	-5.03	99.59	108.20
1	C	380	PRO	N-CA-C	-5.03	104.13	111.33
1	C	449	VAL	N-CA-C	5.03	119.81	109.34
1	E	117	ILE	N-CA-C	5.03	115.95	108.65
1	D	207	TYR	N-CA-C	-5.03	101.04	109.24
1	G	383	TRP	N-CA-C	-5.01	107.02	113.23
1	H	449	VAL	N-CA-C	5.01	119.76	109.34
1	H	290	VAL	N-CA-C	-5.00	100.55	107.80
1	H	388	SER	N-CA-C	-5.00	100.15	110.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	412	GLN	Peptide,Mainchain
1	D	411	VAL	Mainchain
1	E	412	GLN	Peptide,Mainchain
1	F	412	GLN	Mainchain

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	2962	0	2783	190	0
1	B	2962	0	2783	203	0
1	C	2962	0	2782	227	1
1	D	2962	0	2783	203	0
1	E	2962	0	2781	204	0
1	F	2962	0	2783	187	0
1	G	2962	0	2783	209	0
1	H	2962	0	2783	202	0
2	A	15	0	12	2	0
2	B	15	0	12	2	0
2	C	15	0	12	4	0
2	D	15	0	12	4	0
2	F	15	0	12	3	0
2	G	15	0	12	3	0
2	H	15	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	E	15	0	15	2	0
5	A	111	0	0	24	0
5	B	91	0	0	31	0
5	C	102	0	0	41	0
5	D	104	0	0	26	1
5	E	54	0	0	16	0
5	F	46	0	0	17	0
5	G	86	0	0	26	0
5	H	40	0	0	27	0
All	All	24458	0	22360	1496	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1496) 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:G:412:GLN:CG	1:G:412:GLN:CB	1.79	1.51
1:C:411:VAL:CG2	1:C:411:VAL:CB	1.96	1.44
1:E:411:VAL:CG2	1:E:411:VAL:CB	1.94	1.43
1:B:411:VAL:CB	1:B:411:VAL:CG2	1.96	1.42
1:D:411:VAL:CB	1:D:411:VAL:CG2	1.98	1.42
1:E:412:GLN:NE2	1:E:421:CYS:SG	1.97	1.37
1:B:412(C):GLU:HG2	5:B:1151:HOH:O	1.37	1.20
1:E:412:GLN:HG3	1:E:419:ARG:CB	1.78	1.14
1:C:412:GLN:NE2	1:C:421:CYS:SG	2.20	1.14
1:H:328:PRO:HD3	5:H:1154:HOH:O	1.46	1.13
1:E:412:GLN:CG	1:E:419:ARG:HB3	1.78	1.13
1:E:412:GLN:HG3	1:E:419:ARG:HB3	1.24	1.12
1:A:216:LYS:HD3	1:D:452:ASP:HB3	1.30	1.10
1:G:85:LEU:HD12	1:G:412(C):GLU:HG3	1.32	1.07
1:E:413:THR:HG21	1:E:415:LEU:HD22	1.34	1.05
1:H:376:MET:HG2	1:H:397:ILE:HD11	1.37	1.05
1:F:216:LYS:HD3	1:G:452:ASP:HB3	1.38	1.05
1:E:412(D):LEU:HA	5:E:1154:HOH:O	1.56	1.04
1:A:413:THR:HG21	1:A:415:LEU:HD22	1.36	1.03
1:E:452:ASP:HB3	1:G:216:LYS:HD3	1.40	1.03
1:E:412:GLN:HB2	1:E:419:ARG:HB2	1.37	1.03
1:D:97:TRP:O	1:D:453:THR:HG21	1.57	1.02
1:E:412:GLN:CG	1:E:419:ARG:CB	2.35	1.02
1:B:413:THR:HG21	1:B:415:LEU:HD22	1.38	1.02
1:C:412:GLN:CG	1:C:419:ARG:HB3	1.90	1.02
1:D:453:THR:HG22	1:D:454:VAL:H	1.26	1.01
1:A:453:THR:HG22	1:A:454:VAL:H	1.26	1.01
1:B:411:VAL:CG2	1:B:411:VAL:CA	2.39	1.01
1:C:328:PRO:HD3	5:C:1147:HOH:O	1.58	1.00
1:A:97:TRP:O	1:A:453:THR:HG21	1.59	1.00
1:D:413:THR:HG21	1:D:415:LEU:HD22	1.41	0.99
1:E:411:VAL:CG2	1:E:411:VAL:CA	2.40	0.98
1:E:412:GLN:CB	1:E:419:ARG:HB2	1.93	0.98
1:G:412(B):PRO:HA	5:G:1148:HOH:O	1.62	0.98
1:G:85:LEU:CD1	1:G:412(C):GLU:HG3	1.92	0.98
1:C:412:GLN:HG3	1:C:419:ARG:HB3	1.46	0.97
1:B:85:LEU:HD12	1:B:412(C):GLU:HG3	1.45	0.97
1:G:84:LYS:HG2	5:G:1163:HOH:O	1.61	0.97
1:E:88:ASN:HD22	1:E:88:ASN:H	1.06	0.97
1:E:249:GLN:NE2	1:E:272:ASN:H	1.62	0.97
1:B:97:TRP:O	1:B:453:THR:HG21	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:THR:HG21	1:C:415:LEU:HD22	1.47	0.96
1:A:144:HIS:HE1	1:D:463:GLU:H	1.01	0.96
1:C:249:GLN:NE2	1:C:272:ASN:H	1.63	0.95
1:G:412:GLN:CG	1:G:412:GLN:CA	2.44	0.95
1:G:453:THR:HG22	1:G:454:VAL:H	1.30	0.95
1:E:85:LEU:HD12	1:E:412(C):GLU:HG3	1.48	0.95
1:D:411:VAL:CG2	1:D:411:VAL:CA	2.45	0.94
1:F:376:MET:HG2	1:F:397:ILE:HD11	1.49	0.94
1:B:144:HIS:HE1	1:C:463:GLU:H	1.01	0.94
1:C:411:VAL:CG2	1:C:411:VAL:CA	2.46	0.93
1:F:463:GLU:H	1:H:144:HIS:HE1	1.11	0.93
1:G:412:GLN:HB2	1:G:419:ARG:CB	1.98	0.93
1:H:320:GLY:HA3	1:H:387:ASP:O	1.68	0.93
1:C:412:GLN:HB2	1:C:419:ARG:HB2	1.50	0.93
1:C:249:GLN:HE21	1:C:272:ASN:H	0.99	0.92
1:G:282:PRO:HD2	1:G:411:VAL:HG21	1.49	0.92
1:C:343:SER:HB2	5:C:1151:HOH:O	1.70	0.92
1:B:463:GLU:H	1:D:144:HIS:HE1	1.10	0.92
1:A:463:GLU:H	1:C:144:HIS:HE1	0.99	0.91
1:B:452:ASP:HB3	1:D:216:LYS:HD3	1.50	0.91
1:D:411:VAL:CG2	1:D:411:VAL:CG1	2.47	0.91
1:E:411:VAL:CG2	1:E:411:VAL:CG1	2.48	0.91
1:F:413:THR:HG21	1:F:415:LEU:HD22	1.50	0.91
1:C:84:LYS:HG2	5:C:1159:HOH:O	1.71	0.90
1:B:411:VAL:CG2	1:B:411:VAL:CG1	2.49	0.90
1:D:249:GLN:HE21	1:D:272:ASN:H	1.15	0.89
1:D:358:ASN:O	1:D:381:ASN:HA	1.72	0.89
1:F:184:HIS:HD2	1:F:186:GLY:H	1.17	0.89
1:E:113:ASP:O	1:E:168:SER:HB2	1.72	0.89
1:H:97:TRP:O	1:H:453:THR:HG21	1.71	0.89
1:D:320:GLY:HA3	1:D:387:ASP:O	1.73	0.89
1:G:320:GLY:HA3	1:G:387:ASP:O	1.73	0.88
1:A:309:ASN:HB3	5:A:1160:HOH:O	1.71	0.88
1:C:97:TRP:O	1:C:453:THR:HG21	1.73	0.88
1:G:412(B):PRO:O	5:G:1171:HOH:O	1.90	0.88
1:C:146:ASN:HD21	2:C:1146:NDG:C1	1.86	0.87
1:F:144:HIS:HE1	1:G:463:GLU:H	1.19	0.87
1:G:97:TRP:O	1:G:453:THR:HG21	1.73	0.87
1:A:463:GLU:H	1:C:144:HIS:CE1	1.91	0.87
1:D:376:MET:HG2	1:D:397:ILE:HD11	1.56	0.87
1:F:452:ASP:HB3	1:H:216:LYS:HD3	1.53	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:SER:C	5:B:1150:HOH:O	2.18	0.87
1:D:343:SER:C	5:D:1150:HOH:O	2.15	0.87
1:G:413:THR:HB	5:G:1148:HOH:O	1.73	0.87
1:B:249:GLN:HE21	1:B:272:ASN:H	1.16	0.86
1:C:411:VAL:CG2	1:C:411:VAL:CG1	2.52	0.86
1:E:306:ASN:HB3	5:E:1152:HOH:O	1.74	0.86
1:E:463:GLU:H	1:G:144:HIS:HE1	1.23	0.86
1:G:306:ASN:HB3	5:G:1158:HOH:O	1.74	0.86
1:G:412(D):LEU:HD13	5:G:1173:HOH:O	1.76	0.86
1:B:360:VAL:HG22	1:B:383:TRP:HB2	1.56	0.86
1:F:214:THR:HB	1:G:451:SER:OG	1.76	0.86
1:E:453:THR:HG22	1:E:454:VAL:H	1.40	0.85
1:H:146:ASN:HD21	2:H:1146:NDG:C1	1.89	0.85
1:B:452:ASP:O	1:D:214:THR:HG21	1.76	0.85
1:E:376:MET:HG2	1:E:397:ILE:HD11	1.59	0.85
1:H:306:ASN:HB3	5:H:1147:HOH:O	1.75	0.85
1:H:412(B):PRO:HA	5:H:1148:HOH:O	1.76	0.85
1:A:88:ASN:H	1:A:88:ASN:HD22	1.19	0.84
1:A:216:LYS:CD	1:D:452:ASP:HB3	2.05	0.84
1:D:248:GLY:HA2	1:D:295:TRP:CE2	2.11	0.84
1:B:411:VAL:CG2	1:B:411:VAL:HA	2.06	0.84
1:E:411:VAL:CG2	1:E:411:VAL:HA	2.06	0.84
1:B:249:GLN:NE2	1:B:272:ASN:H	1.75	0.84
1:D:146:ASN:HD21	2:D:1146:NDG:C1	1.90	0.84
1:G:169(A):TYR:HB2	5:G:1151:HOH:O	1.77	0.84
1:E:452:ASP:HB3	1:G:216:LYS:CD	2.07	0.83
1:F:97:TRP:O	1:F:453:THR:HG21	1.77	0.83
1:D:249:GLN:NE2	1:D:272:ASN:H	1.76	0.83
1:C:453:THR:HG22	1:C:454:VAL:H	1.43	0.83
1:G:412:GLN:HB2	1:G:419:ARG:HB2	1.57	0.83
1:A:249:GLN:NE2	1:A:272:ASN:H	1.75	0.83
1:H:126:HIS:HA	5:H:1149:HOH:O	1.78	0.83
1:D:306:ASN:HB3	5:D:1156:HOH:O	1.75	0.83
1:E:144:HIS:HE1	1:H:463:GLU:H	1.25	0.83
1:D:316:TYR:CE1	1:D:340:PRO:HD3	2.14	0.83
1:A:210:ILE:HD11	5:D:1160:HOH:O	1.77	0.82
1:A:214:THR:HG21	1:D:452:ASP:O	1.78	0.82
1:E:184:HIS:HD2	1:E:186:GLY:H	1.26	0.82
1:B:170:ASN:HB3	5:B:1147:HOH:O	1.80	0.82
1:E:192:ILE:HG12	1:E:205:LEU:HD22	1.62	0.82
1:B:333:GLY:H	1:B:386:THR:HG23	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:PHE:C	1:B:468:ILE:H	1.88	0.82
1:F:117:ILE:HG22	1:F:135:THR:HG22	1.61	0.82
1:E:254:ILE:HD11	1:E:268:LEU:HD21	1.61	0.81
1:H:413:THR:HG21	1:H:415:LEU:HD22	1.59	0.81
1:A:452:ASP:HB3	1:C:216:LYS:HD3	1.59	0.81
1:B:146:ASN:HD21	2:B:1146:NDG:C1	1.91	0.81
1:B:216:LYS:HD3	1:C:452:ASP:HB3	1.61	0.81
1:A:320:GLY:HA3	1:A:387:ASP:O	1.81	0.81
1:G:343:SER:O	5:G:1152:HOH:O	1.99	0.80
1:H:84:LYS:HG2	5:H:1176:HOH:O	1.81	0.80
1:C:112:GLY:HA3	5:C:1149:HOH:O	1.81	0.80
1:G:146:ASN:HD21	2:G:1146:NDG:C1	1.94	0.80
1:E:169:PRO:HG3	5:E:1153:HOH:O	1.81	0.80
1:C:411:VAL:CG2	1:C:411:VAL:HA	2.11	0.80
1:B:85:LEU:CD1	1:B:412(C):GLU:HG3	2.12	0.80
1:H:376:MET:HG2	1:H:397:ILE:CD1	2.11	0.80
1:A:249:GLN:HE21	1:A:272:ASN:H	1.29	0.80
1:B:448:GLY:O	1:B:449:VAL:HB	1.80	0.80
1:A:144:HIS:CE1	1:D:463:GLU:H	1.94	0.79
1:D:412:GLN:HB2	1:D:419:ARG:HB2	1.64	0.79
1:E:412(C):GLU:OE2	5:E:1155:HOH:O	1.99	0.79
1:F:184:HIS:CD2	1:F:186:GLY:H	1.98	0.79
1:B:144:HIS:CE1	1:C:463:GLU:H	1.94	0.79
1:G:275:TYR:CE2	1:G:303:VAL:HG23	2.18	0.79
1:E:249:GLN:HE21	1:E:272:ASN:H	1.31	0.79
1:F:216:LYS:CD	1:G:452:ASP:HB3	2.12	0.79
1:D:359:GLY:CA	1:D:381:ASN:H	1.95	0.79
1:H:412:GLN:HB2	1:H:419:ARG:CB	2.12	0.79
1:A:386:THR:HB	5:A:1216:HOH:O	1.82	0.79
1:A:216:LYS:NZ	1:D:452:ASP:HB2	1.98	0.78
1:B:135:THR:HB	5:B:1202:HOH:O	1.82	0.78
1:E:214:THR:HG21	1:H:452:ASP:O	1.84	0.78
1:E:88:ASN:HD22	1:E:88:ASN:N	1.77	0.78
1:G:117:ILE:HG22	1:G:135:THR:HG22	1.65	0.78
1:B:376:MET:HG2	1:B:397:ILE:HD11	1.65	0.78
1:G:412(C):GLU:OE2	5:G:1154:HOH:O	2.02	0.78
1:H:228:SER:HB3	1:H:350:LYS:HE2	1.64	0.78
1:C:249:GLN:NE2	1:C:272:ASN:N	2.31	0.78
1:E:97:TRP:O	1:E:453:THR:HG21	1.83	0.78
1:G:228:SER:HB3	1:G:350:LYS:HE2	1.65	0.78
1:E:85:LEU:CD1	1:E:412(C):GLU:HG3	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:THR:HG22	1:F:454:VAL:H	1.49	0.77
1:B:306:ASN:HB3	5:B:1158:HOH:O	1.84	0.77
1:C:426:LEU:HB2	5:C:1228:HOH:O	1.84	0.77
1:A:146:ASN:HD21	2:A:1146:NDG:C1	1.98	0.77
1:D:333:GLY:H	1:D:386:THR:HG23	1.48	0.77
1:G:249:GLN:NE2	1:G:272:ASN:H	1.82	0.77
1:C:162:PRO:HG2	1:C:165:GLU:CD	2.10	0.77
1:F:214:THR:HG21	1:G:452:ASP:O	1.84	0.77
1:C:413:THR:HB	5:C:1152:HOH:O	1.85	0.77
1:A:248:GLY:HA2	1:A:295:TRP:CE2	2.20	0.76
1:B:156:ARG:HG2	1:B:178:TRP:HA	1.68	0.76
1:C:228:SER:HB3	1:C:350:LYS:HE2	1.67	0.76
1:D:97:TRP:H	1:D:395:GLN:HE22	1.33	0.76
1:F:249:GLN:NE2	1:F:272:ASN:H	1.84	0.76
1:C:88:ASN:H	1:C:88:ASN:HD22	1.32	0.76
1:G:412:GLN:HB2	1:G:419:ARG:HB3	1.67	0.76
1:G:248:GLY:HA2	1:G:295:TRP:CE2	2.21	0.76
1:A:452:ASP:O	1:C:214:THR:HG21	1.84	0.76
1:C:184:HIS:CD2	1:C:186:GLY:H	2.03	0.76
1:D:192:ILE:HG12	1:D:205:LEU:HD22	1.68	0.76
1:E:412:GLN:CG	1:E:419:ARG:HB2	2.11	0.76
1:D:343:SER:O	5:D:1150:HOH:O	2.01	0.76
1:A:116:VAL:HG23	1:A:440:SER:HB2	1.66	0.76
1:E:184:HIS:CD2	1:E:186:GLY:H	2.03	0.76
1:F:320:GLY:HA3	1:F:387:ASP:O	1.86	0.75
1:H:442:SER:HB3	5:H:1173:HOH:O	1.87	0.75
1:H:343:SER:O	5:H:1154:HOH:O	2.04	0.75
1:A:451:SER:OG	1:C:214:THR:HB	1.85	0.75
1:G:88:ASN:HD22	1:G:88:ASN:H	1.32	0.75
1:E:412:GLN:NE2	1:E:447:CYS:SG	2.58	0.75
1:G:376:MET:HG2	1:G:397:ILE:HD11	1.69	0.75
1:C:412(B):PRO:C	5:C:1150:HOH:O	2.28	0.75
1:E:400:ILE:HG13	5:E:1174:HOH:O	1.84	0.75
1:E:412:GLN:HG2	1:E:419:ARG:HB3	1.69	0.75
1:F:412(C):GLU:HG3	5:F:1148:HOH:O	1.87	0.75
1:F:452:ASP:O	1:H:214:THR:HG21	1.86	0.75
1:H:387:ASP:HB2	5:H:1150:HOH:O	1.86	0.75
1:H:411:VAL:CG1	1:H:418:ILE:HG23	2.17	0.75
1:C:412:GLN:CG	1:C:419:ARG:CB	2.65	0.74
1:H:316:TYR:CE1	1:H:340:PRO:HD3	2.22	0.74
1:C:275:TYR:CE2	1:C:303:VAL:HG23	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:VAL:HG21	1:H:353:SER:HB2	1.70	0.74
1:H:412:GLN:HB2	1:H:419:ARG:HB3	1.69	0.74
1:A:192:ILE:HG12	1:A:205:LEU:HD22	1.69	0.74
1:B:192:ILE:HG12	1:B:205:LEU:HD22	1.69	0.74
1:B:248:GLY:HA2	1:B:295:TRP:CE2	2.22	0.74
1:C:412:GLN:HG3	1:C:419:ARG:CB	2.17	0.74
1:E:121:PHE:CG	1:E:228:SER:HA	2.22	0.74
1:E:316:TYR:CE1	1:E:340:PRO:HD3	2.23	0.74
1:F:144:HIS:CE1	1:G:463:GLU:H	2.04	0.74
1:F:84:LYS:HG2	5:F:1169:HOH:O	1.87	0.74
1:B:214:THR:HG21	1:C:452:ASP:O	1.87	0.74
1:D:216:LYS:HE3	5:D:1220:HOH:O	1.86	0.74
1:D:359:GLY:HA2	1:D:381:ASN:N	2.02	0.74
1:F:88:ASN:H	1:F:88:ASN:HD22	1.35	0.74
1:D:466:PHE:C	1:D:468:ILE:H	1.96	0.73
1:F:412:GLN:HB2	1:F:419:ARG:CB	2.17	0.73
1:H:116:VAL:HG23	1:H:440:SER:HB2	1.70	0.73
1:H:184:HIS:CD2	1:H:186:GLY:H	2.06	0.73
1:H:184:HIS:HD2	1:H:186:GLY:H	1.35	0.73
1:C:228:SER:HB3	1:C:350:LYS:CE	2.18	0.73
1:F:316:TYR:CE1	1:F:340:PRO:HD3	2.24	0.73
1:H:248:GLY:HA2	1:H:295:TRP:CE2	2.22	0.73
1:D:184:HIS:CD2	1:D:186:GLY:H	2.06	0.73
5:F:1154:HOH:O	1:G:451:SER:HB2	1.88	0.73
1:G:316:TYR:CE1	1:G:340:PRO:HD3	2.23	0.73
1:B:109:GLY:HA3	1:B:140:LEU:HD12	1.69	0.73
1:F:463:GLU:H	1:H:144:HIS:CE1	2.01	0.73
1:A:184:HIS:CD2	1:A:186:GLY:H	2.07	0.73
1:F:412:GLN:HB2	1:F:419:ARG:HB3	1.71	0.73
1:F:126:HIS:HA	5:F:1149:HOH:O	1.88	0.73
1:G:88:ASN:HD22	1:G:88:ASN:N	1.86	0.73
1:A:184:HIS:HD2	1:A:186:GLY:H	1.36	0.72
1:E:452:ASP:O	1:G:214:THR:HG21	1.87	0.72
1:F:248:GLY:HA2	1:F:295:TRP:CE2	2.23	0.72
1:G:412:GLN:CG	1:G:412:GLN:HA	2.19	0.72
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.69	0.72
1:B:452:ASP:HB3	1:D:216:LYS:CD	2.18	0.72
1:G:412(D):LEU:HB2	5:G:1173:HOH:O	1.89	0.72
1:B:117:ILE:HG22	1:B:135:THR:HG22	1.70	0.72
1:D:116:VAL:HG12	1:D:138:ALA:O	1.88	0.72
1:B:113:ASP:O	1:B:168:SER:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:SER:HB2	5:A:1147:HOH:O	1.90	0.72
1:B:453:THR:HG22	1:B:454:VAL:H	1.53	0.72
1:G:121:PHE:CG	1:G:228:SER:HA	2.24	0.72
1:H:453:THR:HG22	1:H:454:VAL:H	1.54	0.72
1:A:376:MET:HG2	1:A:397:ILE:HD11	1.72	0.72
1:G:184:HIS:CD2	1:G:186:GLY:H	2.08	0.72
1:C:327:ARG:HA	5:C:1147:HOH:O	1.89	0.72
1:D:228:SER:HB3	1:D:350:LYS:HE2	1.72	0.71
1:E:116:VAL:HG23	1:E:440:SER:HB2	1.72	0.71
1:G:413:THR:HG21	1:G:415:LEU:HD22	1.71	0.71
1:C:113:ASP:O	1:C:168:SER:HB2	1.90	0.71
1:A:463:GLU:N	1:C:144:HIS:HE1	1.83	0.71
1:D:113:ASP:O	1:D:168:SER:HB2	1.91	0.71
1:F:210:ILE:HD12	1:G:413:THR:HG23	1.73	0.71
1:G:453:THR:HG22	1:G:454:VAL:N	2.06	0.71
1:A:121:PHE:CG	1:A:228:SER:HA	2.26	0.71
1:B:376:MET:HG2	1:B:397:ILE:CD1	2.20	0.71
1:B:380:PRO:O	1:B:381:ASN:C	2.33	0.71
1:C:412(C):GLU:O	5:C:1148:HOH:O	2.08	0.71
1:E:228:SER:HB3	1:E:350:LYS:HE2	1.71	0.71
1:F:113:ASP:HB3	1:F:139:LEU:HD13	1.73	0.71
1:B:214:THR:HB	1:C:451:SER:OG	1.91	0.71
1:B:466:PHE:C	1:B:468:ILE:N	2.47	0.71
1:D:411:VAL:CG2	1:D:411:VAL:HG13	2.19	0.71
1:E:248:GLY:HA2	1:E:295:TRP:CE2	2.25	0.71
1:A:168:SER:CB	5:A:1147:HOH:O	2.39	0.70
1:G:448:GLY:O	1:G:449:VAL:HB	1.91	0.70
1:A:448:GLY:O	1:A:449:VAL:HB	1.90	0.70
1:A:452:ASP:HB2	1:C:216:LYS:NZ	2.06	0.70
1:C:298:SER:HB3	5:C:1147:HOH:O	1.91	0.70
1:F:156:ARG:HG2	1:F:178:TRP:HA	1.73	0.70
1:F:282:PRO:HD2	1:F:411:VAL:HG21	1.73	0.70
1:E:454:VAL:HG21	1:G:200:GLY:O	1.92	0.70
1:F:275:TYR:CE2	1:F:303:VAL:HG23	2.26	0.70
1:H:156:ARG:HG2	1:H:178:TRP:HA	1.74	0.70
1:B:116:VAL:HG23	1:B:440:SER:HB2	1.72	0.70
1:F:299:ASN:ND2	1:F:316:TYR:HB3	2.06	0.70
1:F:454:VAL:HG21	1:H:200:GLY:O	1.91	0.70
1:B:264:LYS:HG2	1:B:310:LEU:HD22	1.74	0.70
1:D:411:VAL:CG2	1:D:411:VAL:HA	2.20	0.70
1:E:239:THR:HG22	1:E:257:MET:HE1	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLY:HA2	1:C:295:TRP:CE2	2.26	0.70
1:A:229:GLU:OE1	1:A:410:PHE:HA	1.92	0.70
1:A:290:VAL:HG21	1:A:353:SER:HB2	1.73	0.70
1:B:162:PRO:HG2	1:B:165:GLU:CD	2.16	0.70
1:D:376:MET:HG2	1:D:397:ILE:CD1	2.22	0.70
1:H:466:PHE:C	1:H:468:ILE:H	2.00	0.70
1:E:412(B):PRO:HB3	1:E:415:LEU:O	1.91	0.69
1:C:412:GLN:HB2	1:C:419:ARG:CB	2.21	0.69
1:H:448:GLY:O	1:H:449:VAL:HB	1.91	0.69
1:C:380:PRO:O	1:C:381:ASN:C	2.34	0.69
1:D:448:GLY:O	1:D:449:VAL:HB	1.91	0.69
1:F:341:VAL:CG1	5:F:1156:HOH:O	2.40	0.69
1:C:376:MET:HG2	1:C:397:ILE:CD1	2.22	0.69
1:B:320:GLY:HA3	1:B:387:ASP:O	1.93	0.69
1:E:117:ILE:HG22	1:E:135:THR:HG22	1.74	0.69
1:E:320:GLY:HA3	1:E:387:ASP:O	1.93	0.69
1:H:85:LEU:HA	1:H:412(C):GLU:OE1	1.92	0.69
1:E:210:ILE:HD12	1:H:413:THR:HG23	1.72	0.69
1:F:228:SER:HB3	1:F:350:LYS:HE2	1.72	0.69
1:D:162:PRO:HG2	1:D:165:GLU:CD	2.17	0.69
1:E:411:VAL:HG12	1:E:412:GLN:N	2.08	0.69
1:F:254:ILE:HD11	1:F:268:LEU:HD21	1.74	0.69
1:B:228:SER:HB3	1:B:350:LYS:HE2	1.75	0.68
1:C:412:GLN:CB	1:C:419:ARG:HB2	2.23	0.68
1:B:316:TYR:CE1	1:B:340:PRO:HD3	2.28	0.68
1:B:463:GLU:H	1:D:144:HIS:CE1	2.02	0.68
1:H:113:ASP:O	1:H:168:SER:HB2	1.92	0.68
1:A:135:THR:HB	5:A:1255:HOH:O	1.93	0.68
1:C:117:ILE:HG22	1:C:135:THR:HG22	1.74	0.68
1:D:466:PHE:C	1:D:468:ILE:N	2.50	0.68
1:C:239:THR:HG22	1:C:257:MET:HE1	1.76	0.68
1:B:249:GLN:HE21	1:B:272:ASN:N	1.91	0.68
1:G:380:PRO:O	1:G:381:ASN:C	2.37	0.68
1:D:358:ASN:C	1:D:381:ASN:HA	2.20	0.67
1:F:88:ASN:HD22	1:F:88:ASN:N	1.90	0.67
1:E:290:VAL:HG21	1:E:353:SER:HB2	1.76	0.67
1:E:463:GLU:H	1:G:144:HIS:CE1	2.09	0.67
1:B:309:ASN:HB3	5:B:1224:HOH:O	1.93	0.67
1:B:343:SER:O	1:B:344:ASN:CB	2.41	0.67
1:D:254:ILE:HD11	1:D:268:LEU:HD21	1.77	0.67
1:E:411:VAL:CG2	1:E:411:VAL:HG13	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:ARG:HG2	1:G:178:TRP:HA	1.77	0.67
1:C:150:LYS:HD3	1:C:152:ARG:O	1.94	0.67
1:E:397:ILE:HG22	1:E:398:VAL:HG23	1.77	0.67
1:F:376:MET:HG2	1:F:397:ILE:CD1	2.23	0.67
1:D:249:GLN:NE2	1:D:272:ASN:N	2.42	0.67
1:D:254:ILE:CD1	1:D:268:LEU:HD21	2.24	0.67
1:H:97:TRP:H	1:H:395:GLN:HE22	1.43	0.67
1:H:412(D):LEU:HA	5:H:1149:HOH:O	1.95	0.67
1:F:463:GLU:N	1:H:144:HIS:HE1	1.89	0.67
1:A:294:ASN:HA	1:A:347:TYR:O	1.95	0.67
1:B:228:SER:HB3	1:B:350:LYS:CE	2.25	0.67
1:B:333:GLY:H	1:B:386:THR:CG2	2.07	0.67
1:H:299:ASN:ND2	1:H:316:TYR:HB3	2.10	0.67
1:B:83:VAL:N	5:B:1174:HOH:O	2.27	0.67
1:F:448:GLY:O	1:F:449:VAL:HB	1.94	0.67
1:G:270:ALA:HB1	1:G:273:TYR:HB2	1.77	0.67
1:H:275:TYR:CE2	1:H:303:VAL:HG23	2.30	0.67
1:C:184:HIS:HD2	1:C:186:GLY:H	1.43	0.66
1:F:146:ASN:HD21	2:F:1146:NDG:C1	2.08	0.66
1:B:116:VAL:HG12	1:B:138:ALA:O	1.96	0.66
1:E:88:ASN:H	1:E:88:ASN:ND2	1.83	0.66
1:A:162:PRO:HG2	1:A:165:GLU:CD	2.21	0.66
1:A:216:LYS:HE3	5:A:1204:HOH:O	1.95	0.66
1:A:380:PRO:O	1:A:381:ASN:C	2.37	0.66
1:D:116:VAL:HG23	1:D:440:SER:HB2	1.76	0.66
1:E:325:ASN:O	1:E:348:GLY:HA2	1.96	0.66
1:E:376:MET:HG2	1:E:397:ILE:CD1	2.24	0.66
1:A:117:ILE:HG22	1:A:135:THR:HG22	1.76	0.66
1:E:239:THR:CG2	1:E:257:MET:HE1	2.24	0.66
1:G:466:PHE:C	1:G:468:ILE:H	2.03	0.66
1:G:116:VAL:HG23	1:G:440:SER:HB2	1.77	0.66
1:A:113:ASP:O	1:A:168:SER:HB2	1.95	0.66
1:A:156:ARG:HG2	1:A:178:TRP:HA	1.77	0.66
1:B:249:GLN:NE2	1:B:272:ASN:N	2.41	0.66
1:A:214:THR:HB	1:D:451:SER:OG	1.96	0.66
1:B:216:LYS:CD	1:C:452:ASP:HB3	2.24	0.66
1:A:249:GLN:NE2	1:A:272:ASN:N	2.43	0.66
1:F:375:GLU:OE1	1:F:394:LYS:HE3	1.96	0.66
1:G:229:GLU:HG2	1:G:230:CYS:O	1.95	0.66
1:E:332:THR:HG23	1:E:386:THR:HG21	1.77	0.66
1:B:270:ALA:HB1	1:B:273:TYR:HB2	1.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ILE:N	1:B:287:ILE:HD12	2.11	0.65
1:C:320:GLY:HA3	1:C:387:ASP:O	1.97	0.65
1:A:88:ASN:H	1:A:88:ASN:ND2	1.91	0.65
1:D:210:ILE:O	1:D:210:ILE:HG13	1.94	0.65
1:D:453:THR:HG22	1:D:454:VAL:N	2.06	0.65
1:F:411:VAL:HG11	1:F:412(A):HIS:CD2	2.31	0.65
1:H:249:GLN:NE2	1:H:272:ASN:H	1.93	0.65
1:H:412(A):HIS:O	5:H:1148:HOH:O	2.12	0.65
1:A:316:TYR:CE1	1:A:340:PRO:HD3	2.31	0.65
1:C:88:ASN:HD22	1:C:88:ASN:N	1.93	0.65
1:D:249:GLN:HE21	1:D:272:ASN:N	1.93	0.65
1:A:88:ASN:HD22	1:A:88:ASN:N	1.82	0.65
1:H:412(D):LEU:CA	5:H:1149:HOH:O	2.45	0.65
1:B:411:VAL:CG2	1:B:411:VAL:HG13	2.26	0.65
1:H:228:SER:HB3	1:H:350:LYS:CE	2.27	0.65
1:F:366:LYS:HB2	1:F:400:ILE:HG12	1.79	0.65
1:G:184:HIS:HD2	1:G:186:GLY:H	1.42	0.65
1:C:412:GLN:HG2	1:C:419:ARG:HB3	1.79	0.64
5:A:1168:HOH:O	1:C:210:ILE:HD11	1.97	0.64
1:D:146:ASN:ND2	2:D:1146:NDG:C1	2.59	0.64
1:D:261:LYS:HE3	5:D:1182:HOH:O	1.96	0.64
1:D:339:GLY:C	5:D:1152:HOH:O	2.40	0.64
1:E:249:GLN:NE2	1:E:272:ASN:N	2.42	0.64
1:A:216:LYS:HZ2	1:D:452:ASP:HB2	1.61	0.64
1:B:360:VAL:CG2	1:B:383:TRP:HB2	2.24	0.64
1:C:411:VAL:CG2	1:C:411:VAL:HG13	2.27	0.64
1:E:342:SER:C	5:E:1148:HOH:O	2.41	0.64
1:D:375:GLU:OE1	1:D:394:LYS:HE3	1.97	0.64
1:E:144:HIS:CE1	1:H:463:GLU:H	2.13	0.64
1:B:333:GLY:N	1:B:386:THR:HG23	2.13	0.64
1:C:287:ILE:HD12	1:C:287:ILE:N	2.13	0.64
1:D:360:VAL:HG13	1:D:383:TRP:HE3	1.63	0.64
1:E:287:ILE:HD12	1:E:287:ILE:N	2.12	0.64
1:H:412(B):PRO:CA	5:H:1148:HOH:O	2.40	0.64
1:A:97:TRP:H	1:A:395:GLN:HE22	1.45	0.64
1:D:333:GLY:N	1:D:386:THR:HG23	2.12	0.64
1:G:85:LEU:HD12	1:G:412(C):GLU:CG	2.20	0.64
1:E:448:GLY:O	1:E:449:VAL:HB	1.98	0.64
1:E:466:PHE:C	1:E:468:ILE:H	2.06	0.64
1:G:88:ASN:H	1:G:88:ASN:ND2	1.96	0.64
1:H:266:VAL:HB	5:H:1166:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:THR:CG2	1:C:257:MET:HE1	2.28	0.64
1:C:412:GLN:NE2	1:C:447:CYS:SG	2.71	0.64
1:E:162:PRO:HG2	1:E:165:GLU:CD	2.22	0.64
1:G:113:ASP:O	1:G:168:SER:HB2	1.97	0.64
1:C:414:GLY:N	5:C:1150:HOH:O	2.02	0.63
1:E:216:LYS:HD3	1:H:452:ASP:HB3	1.80	0.63
1:F:169(A):TYR:OH	5:F:1147:HOH:O	2.13	0.63
1:F:451:SER:OG	1:H:214:THR:HB	1.98	0.63
1:A:376:MET:HG2	1:A:397:ILE:CD1	2.27	0.63
1:E:412(D):LEU:HD12	5:E:1154:HOH:O	1.98	0.63
1:F:249:GLN:HE21	1:F:272:ASN:H	1.46	0.63
1:G:287:ILE:HD12	1:G:287:ILE:N	2.14	0.63
1:C:413:THR:HG22	1:C:415:LEU:H	1.64	0.63
1:F:239:THR:CG2	1:F:257:MET:HE1	2.29	0.63
1:H:355:LYS:HD2	1:H:383:TRP:CE2	2.34	0.63
1:D:97:TRP:N	1:D:395:GLN:HE22	1.96	0.63
1:F:377:ILE:HG23	1:F:390:PHE:CD1	2.34	0.63
1:F:380:PRO:O	1:F:381:ASN:C	2.41	0.63
1:E:216:LYS:NZ	1:H:452:ASP:HB3	2.13	0.63
1:G:135:THR:O	1:G:156:ARG:HA	1.99	0.63
1:H:282:PRO:HD2	1:H:411:VAL:HG21	1.81	0.63
1:D:299:ASN:ND2	5:D:1152:HOH:O	2.21	0.63
1:E:411:VAL:HG13	1:E:411:VAL:HG22	1.81	0.63
1:F:88:ASN:H	1:F:88:ASN:ND2	1.97	0.63
1:B:97:TRP:H	1:B:395:GLN:HE22	1.46	0.63
1:F:316:TYR:CZ	1:F:340:PRO:HD3	2.34	0.63
1:G:412:GLN:HA	1:G:412:GLN:HG2	1.80	0.63
1:H:202:VAL:CG2	1:H:214:THR:HG23	2.28	0.63
1:B:214:THR:HB	1:C:451:SER:CB	2.28	0.62
1:B:454:VAL:HG21	1:D:200:GLY:O	1.99	0.62
1:A:205:LEU:HG	5:A:1209:HOH:O	1.99	0.62
1:D:411:VAL:HG13	1:D:418:ILE:HG23	1.81	0.62
1:E:322:PHE:HB2	1:E:327:ARG:HD2	1.81	0.62
1:F:162:PRO:HG2	1:F:165:GLU:CD	2.24	0.62
1:H:162:PRO:HG2	1:H:165:GLU:CD	2.23	0.62
1:A:102:LYS:HG3	1:A:444:ILE:HG22	1.81	0.62
1:B:247:ASN:O	1:B:248:GLY:O	2.17	0.62
1:F:202:VAL:HG23	1:F:214:THR:HG23	1.81	0.62
1:H:88:ASN:N	1:H:88:ASN:HD22	1.97	0.62
1:H:333:GLY:H	1:H:386:THR:HG23	1.64	0.62
1:C:360:VAL:HG22	1:C:383:TRP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:412:GLN:HB2	1:H:419:ARG:HB2	1.79	0.62
1:C:333:GLY:H	1:C:386:THR:HG23	1.64	0.62
1:G:249:GLN:NE2	1:G:272:ASN:N	2.47	0.62
1:E:275:TYR:CE2	1:E:303:VAL:HG23	2.35	0.62
1:A:453:THR:CG2	5:A:1166:HOH:O	2.48	0.62
1:G:466:PHE:C	1:G:468:ILE:N	2.58	0.62
1:C:192:ILE:HG23	1:C:205:LEU:CD2	2.30	0.62
1:D:84:LYS:HG2	5:D:1159:HOH:O	2.00	0.62
1:D:366:LYS:HD2	1:D:398:VAL:O	2.00	0.62
1:F:228:SER:HB3	1:F:350:LYS:CE	2.28	0.61
1:E:332:THR:HG23	1:E:386:THR:CG2	2.28	0.61
1:A:116:VAL:HG12	1:A:138:ALA:O	2.00	0.61
1:C:266:VAL:HB	5:C:1247:HOH:O	1.98	0.61
1:G:333:GLY:H	1:G:386:THR:HG23	1.63	0.61
1:H:254:ILE:HD11	1:H:268:LEU:HD21	1.82	0.61
1:F:113:ASP:O	1:F:168:SER:HB2	2.00	0.61
1:G:168:SER:HB2	1:G:169:PRO:HD2	1.83	0.61
1:D:332:THR:HG22	1:D:386:THR:HG21	1.80	0.61
1:E:328:PRO:HD3	1:E:343:SER:O	1.99	0.61
1:C:146:ASN:ND2	2:C:1146:NDG:C1	2.60	0.61
1:F:413:THR:HG23	1:H:210:ILE:HD12	1.82	0.61
1:D:387:ASP:HB2	5:D:1236:HOH:O	1.99	0.61
1:G:290:VAL:HG21	1:G:353:SER:HB2	1.82	0.61
1:G:309:ASN:HB3	5:G:1156:HOH:O	2.00	0.61
1:D:102:LYS:HZ2	1:D:104:ASN:HD21	1.48	0.61
1:F:91:LEU:HG	1:F:283:ASN:ND2	2.16	0.61
1:G:360:VAL:HG13	1:G:383:TRP:HE3	1.65	0.61
1:A:216:LYS:NZ	1:D:452:ASP:CB	2.63	0.61
1:C:466:PHE:C	1:C:468:ILE:H	2.08	0.61
1:H:344:ASN:HB3	5:H:1154:HOH:O	2.01	0.61
1:C:230:CYS:N	5:C:1178:HOH:O	2.34	0.60
1:C:344:ASN:HB3	5:C:1147:HOH:O	2.00	0.60
1:D:467:THR:O	1:D:468:ILE:HB	1.98	0.60
1:F:322:PHE:HB2	1:F:327:ARG:HD2	1.82	0.60
1:H:411:VAL:HG13	1:H:418:ILE:CG2	2.31	0.60
1:B:87:GLY:N	5:B:1156:HOH:O	2.23	0.60
1:H:339:GLY:C	5:H:1153:HOH:O	2.44	0.60
1:H:411:VAL:CG1	1:H:418:ILE:CG2	2.79	0.60
1:C:96:GLY:O	1:C:448:GLY:O	2.20	0.60
1:A:136:GLN:HE21	1:A:156:ARG:CD	2.14	0.60
1:A:275:TYR:CE2	1:A:303:VAL:HG23	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASP:HB2	1:C:216:LYS:HZ3	1.65	0.60
1:E:360:VAL:HG22	1:E:383:TRP:HB2	1.82	0.60
1:A:162:PRO:HG2	1:A:165:GLU:OE1	2.00	0.60
1:A:287:ILE:N	1:A:287:ILE:HD12	2.17	0.60
1:B:202:VAL:CG2	1:B:214:THR:HG23	2.31	0.60
1:B:364:ARG:HG3	1:B:365:THR:O	2.02	0.60
1:H:333:GLY:N	1:H:386:THR:HG23	2.16	0.60
1:A:95:ASN:ND2	1:A:450:ASN:O	2.34	0.60
1:A:336:CYS:HB3	5:A:1224:HOH:O	2.00	0.60
1:B:355:LYS:HE3	5:B:1236:HOH:O	2.00	0.60
1:F:466:PHE:C	1:F:468:ILE:H	2.10	0.60
1:G:254:ILE:HD11	1:G:268:LEU:HD21	1.83	0.60
1:G:411:VAL:HG13	1:G:418:ILE:HG23	1.82	0.60
1:H:102:LYS:HG3	1:H:444:ILE:HG22	1.84	0.60
1:C:335:SER:OG	1:C:339:GLY:O	2.20	0.60
1:D:184:HIS:HD2	1:D:186:GLY:H	1.48	0.60
1:H:397:ILE:HG22	1:H:398:VAL:HG23	1.84	0.60
1:C:270:ALA:HB1	1:C:273:TYR:HB2	1.83	0.60
1:C:411:VAL:HG13	1:C:418:ILE:HG23	1.84	0.60
1:H:116:VAL:HG12	1:H:138:ALA:O	2.02	0.60
1:A:299:ASN:ND2	1:A:316:TYR:HB3	2.16	0.60
1:A:454:VAL:HG21	1:C:200:GLY:O	2.01	0.60
1:C:413:THR:N	5:C:1150:HOH:O	2.34	0.59
1:D:121:PHE:CG	1:D:228:SER:HA	2.36	0.59
1:B:330:ASP:O	5:B:1218:HOH:O	2.16	0.59
1:D:297:GLY:HA2	1:D:341:VAL:O	2.03	0.59
1:E:96:GLY:HA3	5:E:1178:HOH:O	2.01	0.59
1:E:214:THR:HB	1:H:451:SER:OG	2.02	0.59
1:F:254:ILE:CD1	1:F:268:LEU:HD21	2.31	0.59
1:H:411:VAL:HG13	1:H:418:ILE:HG23	1.84	0.59
1:C:333:GLY:N	1:C:386:THR:HG23	2.18	0.59
1:D:400:ILE:HG13	5:D:1200:HOH:O	2.02	0.59
1:E:173:PHE:CG	1:H:164:GLY:HA3	2.37	0.59
1:E:320:GLY:CA	1:E:387:ASP:O	2.51	0.59
1:C:116:VAL:HG23	1:C:440:SER:HB2	1.84	0.59
1:C:121:PHE:CG	1:C:228:SER:HA	2.37	0.59
1:E:413:THR:HG23	1:G:210:ILE:HD12	1.84	0.59
1:E:466:PHE:C	1:E:468:ILE:N	2.57	0.59
1:F:428:ARG:NH2	1:F:460:ASP:OD1	2.35	0.59
1:A:150:LYS:HD3	1:A:152:ARG:O	2.02	0.59
1:A:228:SER:HB3	1:A:350:LYS:CE	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.84	0.59
1:E:146:ASN:ND2	4:E:1146:NAG:O1	2.36	0.59
1:B:84:LYS:HE3	5:B:1196:HOH:O	2.02	0.59
1:D:397:ILE:HD13	1:D:422:PHE:HZ	1.68	0.59
1:F:116:VAL:HG23	1:F:440:SER:HB2	1.84	0.59
1:H:411:VAL:HG11	1:H:418:ILE:HG23	1.85	0.59
1:A:180:ALA:HB1	1:A:192:ILE:O	2.03	0.59
1:C:192:ILE:HG12	1:C:205:LEU:HD22	1.85	0.59
1:F:173:PHE:CG	1:G:164:GLY:HA3	2.38	0.59
1:C:115:PHE:CZ	1:C:159:MET:HE1	2.37	0.59
1:E:216:LYS:NZ	1:H:452:ASP:CB	2.66	0.59
1:E:254:ILE:CD1	1:E:268:LEU:HD21	2.33	0.59
1:F:452:ASP:HA	5:F:1163:HOH:O	2.03	0.59
1:A:452:ASP:CB	1:C:216:LYS:NZ	2.66	0.58
1:B:184:HIS:HD2	1:B:186:GLY:H	1.50	0.58
1:H:322:PHE:HB2	1:H:327:ARG:HD2	1.85	0.58
1:C:88:ASN:H	1:C:88:ASN:ND2	2.00	0.58
1:C:397:ILE:HD13	1:C:422:PHE:HZ	1.69	0.58
1:G:333:GLY:N	1:G:386:THR:HG23	2.18	0.58
1:B:413:THR:HB	5:B:1149:HOH:O	2.03	0.58
1:E:194:ILE:HG12	1:E:203:ALA:HB2	1.85	0.58
1:F:412:GLN:HB2	1:F:419:ARG:HB2	1.85	0.58
1:G:192:ILE:HG23	1:G:205:LEU:CD2	2.34	0.58
1:H:379:ASP:OD2	1:H:382:GLY:HA3	2.03	0.58
1:C:156:ARG:HG2	1:C:178:TRP:HA	1.85	0.58
1:E:227:GLU:HA	1:E:227:GLU:OE1	2.03	0.58
1:G:303:VAL:HG22	1:G:314:ILE:HG22	1.84	0.58
1:H:316:TYR:CZ	1:H:340:PRO:HD3	2.37	0.58
1:F:466:PHE:C	1:F:468:ILE:N	2.60	0.58
1:H:254:ILE:CD1	1:H:268:LEU:HD21	2.34	0.58
1:A:270:ALA:HB1	1:A:273:TYR:HB2	1.85	0.58
1:B:86:ALA:HA	5:B:1156:HOH:O	2.04	0.58
1:B:184:HIS:CD2	1:B:186:GLY:H	2.21	0.58
1:B:466:PHE:O	1:B:468:ILE:N	2.37	0.58
1:H:249:GLN:HE21	1:H:272:ASN:H	1.49	0.58
1:H:277:GLU:OE1	1:H:350:LYS:HB2	2.03	0.58
1:A:129:CYS:O	1:A:163:VAL:HG23	2.04	0.58
1:B:413:THR:CG2	1:B:415:LEU:HD22	2.23	0.58
1:D:287:ILE:O	1:D:304:SER:HA	2.04	0.58
1:B:113:ASP:HB3	1:B:139:LEU:HD13	1.86	0.57
1:C:328:PRO:HB3	5:C:1151:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:SER:HB2	1:F:382:GLY:O	2.04	0.57
1:G:119:GLU:OE1	1:G:227:GLU:OE1	2.22	0.57
1:G:162:PRO:HG2	1:G:165:GLU:CD	2.29	0.57
1:H:468:ILE:CG2	2:H:1146:NDG:H8C3	2.34	0.57
1:B:219:ARG:HB2	1:B:243:ASP:CG	2.29	0.57
1:B:343:SER:O	1:B:344:ASN:HB2	2.02	0.57
5:B:1153:HOH:O	1:D:216:LYS:HG2	2.03	0.57
5:F:1147:HOH:O	1:G:113:ASP:N	2.34	0.57
1:H:88:ASN:HD22	1:H:88:ASN:H	1.52	0.57
1:A:344:ASN:CA	5:A:1149:HOH:O	2.52	0.57
1:B:411:VAL:HG13	1:B:418:ILE:HG23	1.85	0.57
1:C:376:MET:HG2	1:C:397:ILE:HD11	1.86	0.57
1:C:412:GLN:CB	1:C:419:ARG:CB	2.82	0.57
1:E:156:ARG:HG2	1:E:178:TRP:HA	1.85	0.57
1:E:210:ILE:HG13	1:E:210:ILE:O	2.03	0.57
1:D:102:LYS:HZ2	1:D:104:ASN:ND2	2.03	0.57
1:H:229:GLU:OE1	1:H:410:PHE:HA	2.03	0.57
1:A:451:SER:HB2	5:C:1185:HOH:O	2.04	0.57
1:B:88:ASN:N	1:B:88:ASN:HD22	2.00	0.57
1:D:343:SER:N	5:D:1150:HOH:O	2.37	0.57
1:A:467:THR:O	1:A:468:ILE:HB	2.04	0.57
1:F:347:TYR:CG	1:F:348:GLY:N	2.71	0.57
1:B:322:PHE:HB2	1:B:327:ARG:HD2	1.87	0.57
1:E:184:HIS:HD2	1:E:186:GLY:N	2.01	0.57
1:F:390:PHE:HE1	1:F:394:LYS:HB2	1.69	0.57
1:H:466:PHE:C	1:H:468:ILE:N	2.61	0.57
1:F:194:ILE:HG12	1:F:203:ALA:HB2	1.87	0.57
1:F:230:CYS:N	5:F:1153:HOH:O	2.37	0.57
1:F:366:LYS:CB	1:F:400:ILE:HG12	2.35	0.57
1:G:306:ASN:CG	1:G:308:GLN:N	2.63	0.57
1:G:333:GLY:N	1:G:386:THR:CG2	2.68	0.57
1:G:366:LYS:HD2	1:G:398:VAL:O	2.04	0.57
1:A:216:LYS:CE	1:D:452:ASP:HB3	2.34	0.57
1:B:129:CYS:O	1:B:163:VAL:HG23	2.05	0.57
1:C:216:LYS:HE3	5:C:1208:HOH:O	2.03	0.57
1:C:249:GLN:NE2	1:C:271:PRO:HA	2.19	0.57
1:C:412(C):GLU:C	5:C:1148:HOH:O	2.46	0.57
1:D:342:SER:C	5:D:1150:HOH:O	2.48	0.57
1:E:316:TYR:CZ	1:E:340:PRO:HD3	2.39	0.57
1:F:121:PHE:CG	1:F:228:SER:HA	2.40	0.57
1:G:99:VAL:HG22	5:G:1218:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:TYR:CE1	1:C:340:PRO:HD3	2.40	0.56
1:E:250:ALA:HB3	1:E:252:TYR:CE2	2.39	0.56
1:E:411:VAL:CG1	1:E:412:GLN:N	2.67	0.56
1:F:239:THR:HG22	1:F:257:MET:HE1	1.86	0.56
5:A:1151:HOH:O	1:C:216:LYS:HG2	2.04	0.56
1:B:370:SER:HB2	1:B:372:SER:OG	2.05	0.56
1:H:270:ALA:HB1	1:H:273:TYR:HB2	1.87	0.56
1:B:210:ILE:HD13	1:C:413:THR:HA	1.87	0.56
1:B:275:TYR:CE2	1:B:303:VAL:CG2	2.89	0.56
5:B:1147:HOH:O	1:D:169(A):TYR:HA	2.04	0.56
1:E:452:ASP:HB3	1:G:216:LYS:CE	2.34	0.56
1:F:136:GLN:HE21	1:F:156:ARG:CD	2.18	0.56
1:F:282:PRO:HD2	1:F:411:VAL:CG2	2.34	0.56
1:G:355:LYS:HD2	1:G:383:TRP:CE2	2.40	0.56
1:H:88:ASN:H	1:H:88:ASN:ND2	2.03	0.56
1:H:126:HIS:CA	5:H:1149:HOH:O	2.44	0.56
1:H:226:GLN:NE2	1:H:239:THR:OG1	2.30	0.56
1:A:249:GLN:HE21	1:A:272:ASN:N	2.01	0.56
1:F:216:LYS:NZ	1:G:452:ASP:HB2	2.21	0.56
1:F:419:ARG:HH11	1:F:419:ARG:HG3	1.69	0.56
1:H:298:SER:HB3	5:H:1154:HOH:O	2.03	0.56
1:C:468:ILE:CG2	2:C:1146:NDG:H8C3	2.36	0.56
1:B:333:GLY:N	1:B:386:THR:CG2	2.68	0.56
1:F:366:LYS:HD2	1:F:398:VAL:O	2.06	0.56
1:G:150:LYS:HD3	1:G:152:ARG:O	2.04	0.56
1:B:228:SER:HB3	1:B:350:LYS:NZ	2.20	0.56
1:B:355:LYS:NZ	1:B:357:GLY:O	2.39	0.56
1:C:275:TYR:CE2	1:C:303:VAL:CG2	2.88	0.56
1:D:117:ILE:HG22	1:D:135:THR:HG22	1.87	0.56
1:H:320:GLY:CA	1:H:387:ASP:O	2.49	0.56
1:D:102:LYS:HG3	1:D:444:ILE:HG22	1.87	0.56
1:D:115:PHE:CZ	1:D:159:MET:HE1	2.40	0.56
1:D:247:ASN:O	1:D:248:GLY:O	2.24	0.56
1:E:377:ILE:HG23	1:E:390:PHE:CD1	2.41	0.56
1:H:318:CYS:HA	1:H:335:SER:O	2.05	0.56
1:A:96:GLY:O	1:A:448:GLY:O	2.24	0.56
1:C:227:GLU:O	1:C:350:LYS:HE2	2.06	0.56
1:F:287:ILE:N	1:F:287:ILE:HD12	2.20	0.56
1:F:411:VAL:HG13	1:F:418:ILE:HG23	1.88	0.56
1:A:466:PHE:C	1:A:468:ILE:N	2.61	0.56
1:B:452:ASP:HB2	1:D:216:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:PHE:C	1:C:468:ILE:N	2.63	0.56
1:E:129:CYS:O	1:E:163:VAL:HG23	2.05	0.56
1:C:161:CYS:HB2	1:C:162:PRO:HD2	1.88	0.55
1:C:366:LYS:HD2	1:C:398:VAL:O	2.05	0.55
1:F:172:ARG:HD2	1:F:174:GLU:OE1	2.06	0.55
1:A:342:SER:C	5:A:1148:HOH:O	2.49	0.55
1:G:297:GLY:N	1:G:345:GLY:O	2.39	0.55
1:A:453:THR:HG22	1:A:454:VAL:N	2.06	0.55
1:A:466:PHE:C	1:A:468:ILE:H	2.13	0.55
1:E:202:VAL:CG2	1:E:214:THR:HG23	2.37	0.55
1:E:354:PHE:CZ	1:E:409:SER:HB2	2.41	0.55
1:H:254:ILE:HB	5:H:1166:HOH:O	2.05	0.55
1:B:332:THR:HG23	1:B:386:THR:HG21	1.88	0.55
1:C:412(B):PRO:HA	5:C:1152:HOH:O	2.07	0.55
1:D:413:THR:HG22	1:D:415:LEU:HD13	1.89	0.55
1:E:411:VAL:HG13	1:E:418:ILE:CG2	2.36	0.55
1:F:379:ASP:OD2	1:F:382:GLY:HA3	2.07	0.55
1:B:88:ASN:HD22	1:B:88:ASN:H	1.55	0.55
1:C:467:THR:O	1:C:468:ILE:HB	2.05	0.55
1:E:216:LYS:HZ2	1:H:452:ASP:HB3	1.72	0.55
1:F:327:ARG:HB2	1:F:328:PRO:HD2	1.88	0.55
1:A:135:THR:O	1:A:156:ARG:HA	2.07	0.55
1:A:333:GLY:N	1:A:386:THR:HG23	2.22	0.55
1:G:247:ASN:HB2	5:G:1221:HOH:O	2.06	0.55
1:H:88:ASN:O	1:H:284:ALA:HA	2.07	0.55
1:H:135:THR:O	1:H:156:ARG:HA	2.07	0.55
1:H:360:VAL:HG22	1:H:383:TRP:HB2	1.89	0.55
1:D:182:ALA:O	1:D:229:GLU:HA	2.07	0.55
1:E:412:GLN:HB2	1:E:419:ARG:CB	2.24	0.55
1:A:400:ILE:HG13	5:A:1215:HOH:O	2.05	0.55
1:B:102:LYS:HZ2	1:B:104:ASN:HD21	1.54	0.55
1:D:118:ARG:HB3	5:D:1206:HOH:O	2.07	0.55
1:E:453:THR:HG22	1:E:454:VAL:N	2.18	0.55
1:A:413:THR:HG21	1:A:415:LEU:CD2	2.24	0.54
1:C:254:ILE:HD11	1:C:268:LEU:HD21	1.90	0.54
1:G:247:ASN:O	1:G:248:GLY:O	2.25	0.54
1:G:412(B):PRO:HD3	1:G:417:CYS:O	2.07	0.54
1:B:117:ILE:HG22	1:B:135:THR:CG2	2.36	0.54
1:B:343:SER:N	5:B:1150:HOH:O	2.40	0.54
1:C:375:GLU:OE1	1:C:394:LYS:HE3	2.07	0.54
1:C:247:ASN:O	1:C:295:TRP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ASN:HA	1:D:347:TYR:O	2.07	0.54
1:E:146:ASN:O	1:E:437:ILE:O	2.24	0.54
1:H:97:TRP:N	1:H:395:GLN:HE22	2.05	0.54
1:H:146:ASN:ND2	2:H:1146:NDG:C1	2.65	0.54
1:A:413:THR:HA	1:C:210:ILE:HD13	1.90	0.54
1:D:468:ILE:HG21	2:D:1146:NDG:H8C3	1.89	0.54
1:F:299:ASN:OD1	1:F:341:VAL:HG23	2.08	0.54
1:G:306:ASN:CG	1:G:308:GLN:H	2.14	0.54
1:G:333:GLY:H	1:G:386:THR:CG2	2.20	0.54
1:G:336:CYS:HB2	5:G:1184:HOH:O	2.07	0.54
1:H:355:LYS:NZ	1:H:357:GLY:O	2.38	0.54
1:A:333:GLY:H	1:A:386:THR:HG23	1.73	0.54
1:E:96:GLY:O	1:E:448:GLY:O	2.26	0.54
1:F:136:GLN:NE2	1:F:156:ARG:HD3	2.23	0.54
1:F:194:ILE:HD11	1:F:241:MET:HE2	1.89	0.54
1:C:412(B):PRO:HA	5:C:1150:HOH:O	2.07	0.54
1:G:194:ILE:HD11	1:G:241:MET:HE2	1.90	0.54
1:H:172:ARG:HD2	1:H:174:GLU:OE1	2.08	0.54
1:B:332:THR:CG2	1:B:386:THR:HG21	2.37	0.54
1:C:411:VAL:HG12	1:C:412:GLN:N	2.21	0.54
1:C:229:GLU:HG2	1:C:230:CYS:O	2.08	0.54
1:D:311:GLU:HG3	5:D:1156:HOH:O	2.08	0.54
1:E:229:GLU:HG2	1:E:230:CYS:O	2.08	0.54
1:C:411:VAL:HG13	1:C:411:VAL:HG22	1.91	0.54
1:D:328:PRO:HD3	1:D:343:SER:O	2.07	0.53
1:H:375:GLU:OE1	1:H:394:LYS:HE3	2.08	0.53
1:B:96:GLY:O	1:B:448:GLY:O	2.26	0.53
1:D:219:ARG:NH2	5:D:1246:HOH:O	2.41	0.53
1:F:467:THR:O	1:F:468:ILE:HB	2.08	0.53
1:H:436:THR:HG21	1:H:464:LEU:HD13	1.90	0.53
1:B:102:LYS:HG3	1:B:444:ILE:HG22	1.90	0.53
1:B:452:ASP:HB3	1:D:216:LYS:CE	2.39	0.53
1:G:172:ARG:HD2	1:G:174:GLU:OE1	2.08	0.53
1:B:119:GLU:HG3	1:B:119:GLU:O	2.07	0.53
1:H:229:GLU:HG2	1:H:230:CYS:O	2.07	0.53
1:F:97:TRP:H	1:F:395:GLN:HE22	1.56	0.53
1:H:412(B):PRO:C	5:H:1148:HOH:O	2.51	0.53
1:C:379:ASP:OD2	1:C:382:GLY:HA3	2.09	0.53
1:F:249:GLN:NE2	1:F:272:ASN:N	2.56	0.53
1:B:452:ASP:CB	1:D:216:LYS:NZ	2.71	0.53
1:D:412:GLN:HB2	1:D:419:ARG:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:397:ILE:HG22	1:G:398:VAL:HG23	1.90	0.53
1:H:390:PHE:HE1	1:H:394:LYS:HB2	1.73	0.53
1:A:344:ASN:C	5:A:1149:HOH:O	2.51	0.53
1:E:412:GLN:O	1:E:412(D):LEU:HD23	2.09	0.53
1:A:216:LYS:HZ3	1:D:452:ASP:HB2	1.74	0.53
1:B:343:SER:O	5:B:1150:HOH:O	2.18	0.52
1:G:148:THR:HG22	1:G:430:ARG:HH22	1.72	0.52
1:H:219:ARG:HB2	1:H:243:ASP:CG	2.34	0.52
1:D:156:ARG:HG2	1:D:178:TRP:HA	1.91	0.52
1:D:316:TYR:CZ	1:D:340:PRO:HD3	2.44	0.52
1:E:463:GLU:N	1:G:144:HIS:HE1	2.01	0.52
1:F:144:HIS:HE1	1:G:463:GLU:N	1.98	0.52
1:G:97:TRP:H	1:G:395:GLN:HE22	1.55	0.52
1:H:306:ASN:CG	1:H:308:GLN:N	2.66	0.52
1:E:117:ILE:HD13	1:E:167:PRO:HG3	1.91	0.52
1:B:146:ASN:ND2	2:B:1146:NDG:C1	2.68	0.52
1:F:318:CYS:HA	1:F:335:SER:O	2.09	0.52
1:G:275:TYR:CE2	1:G:303:VAL:CG2	2.92	0.52
1:H:366:LYS:HD2	1:H:398:VAL:O	2.09	0.52
1:A:316:TYR:CZ	1:A:340:PRO:HD3	2.44	0.52
1:D:319:SER:HB2	1:D:382:GLY:O	2.10	0.52
1:E:274:HIS:HB3	1:E:293:ASP:OD2	2.09	0.52
1:F:96:GLY:O	1:F:448:GLY:O	2.27	0.52
1:F:270:ALA:HB1	1:F:273:TYR:HB2	1.92	0.52
1:A:120:PRO:HA	1:A:132:PHE:O	2.10	0.52
1:A:452:ASP:HB3	1:C:216:LYS:CD	2.34	0.52
1:C:254:ILE:CD1	1:C:268:LEU:HD21	2.40	0.52
1:C:468:ILE:HG21	2:C:1146:NDG:H8C3	1.92	0.52
1:D:88:ASN:HD22	1:D:88:ASN:N	2.07	0.52
1:D:290:VAL:HG21	1:D:353:SER:HB2	1.91	0.52
1:E:467:THR:O	1:E:468:ILE:HB	2.09	0.52
1:H:377:ILE:HG23	1:H:390:PHE:CD1	2.44	0.52
1:B:121:PHE:CG	1:B:228:SER:HA	2.45	0.52
1:F:412(C):GLU:CG	5:F:1148:HOH:O	2.53	0.52
1:F:419:ARG:HG3	1:F:419:ARG:NH1	2.25	0.52
1:F:452:ASP:HB3	1:H:216:LYS:CD	2.33	0.52
1:G:453:THR:CG2	1:G:454:VAL:N	2.71	0.52
1:C:397:ILE:HG22	1:C:398:VAL:HG23	1.91	0.52
1:E:380:PRO:O	1:E:381:ASN:C	2.52	0.52
1:A:144:HIS:HE1	1:D:463:GLU:N	1.86	0.52
1:A:215:ILE:HG13	5:A:1209:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:HZ2	1:B:104:ASN:ND2	2.08	0.52
1:C:102:LYS:HG3	1:C:444:ILE:HG22	1.90	0.52
1:A:332:THR:HG23	1:A:386:THR:HG21	1.92	0.51
1:B:214:THR:HB	1:C:451:SER:HB2	1.91	0.51
1:D:275:TYR:CE2	1:D:303:VAL:CG2	2.93	0.51
1:D:355:LYS:NZ	1:D:357:GLY:O	2.41	0.51
1:F:102:LYS:HZ2	1:F:104:ASN:ND2	2.08	0.51
1:G:286:GLU:C	1:G:287:ILE:HD12	2.35	0.51
1:H:287:ILE:O	1:H:304:SER:HA	2.10	0.51
1:A:335:SER:OG	1:A:339:GLY:O	2.28	0.51
1:F:468:ILE:HG12	5:F:1151:HOH:O	2.10	0.51
1:B:88:ASN:H	1:B:88:ASN:ND2	2.09	0.51
1:B:229:GLU:OE1	1:B:410:PHE:HA	2.10	0.51
1:C:376:MET:HG2	1:C:397:ILE:HD12	1.92	0.51
1:D:101:SER:O	1:D:444:ILE:HA	2.10	0.51
1:F:216:LYS:NZ	1:G:452:ASP:CB	2.73	0.51
1:H:121:PHE:CG	1:H:228:SER:HA	2.46	0.51
1:H:333:GLY:N	1:H:386:THR:CG2	2.74	0.51
1:B:411:VAL:HA	1:B:411:VAL:HG22	1.92	0.51
1:C:135:THR:O	1:C:156:ARG:HA	2.11	0.51
1:E:347:TYR:CG	1:E:348:GLY:N	2.79	0.51
1:F:232:CYS:HA	1:F:237:CYS:HA	1.91	0.51
1:C:411:VAL:CG1	1:C:412:GLN:N	2.73	0.51
1:F:451:SER:CB	1:H:214:THR:HB	2.41	0.51
1:G:96:GLY:O	1:G:448:GLY:O	2.29	0.51
1:G:347:TYR:CG	1:G:348:GLY:N	2.79	0.51
1:F:184:HIS:HD2	1:F:186:GLY:N	1.96	0.51
1:G:249:GLN:HE21	1:G:272:ASN:H	1.56	0.51
1:C:333:GLY:H	1:C:386:THR:CG2	2.24	0.51
1:E:412(C):GLU:HG2	5:E:1155:HOH:O	2.10	0.51
1:F:116:VAL:HG12	1:F:138:ALA:O	2.10	0.51
1:F:360:VAL:HG22	1:F:383:TRP:HB2	1.93	0.51
1:H:115:PHE:CZ	1:H:159:MET:HE1	2.46	0.51
1:F:263:VAL:O	1:F:264:LYS:HB2	2.10	0.51
1:G:169(A):TYR:O	5:G:1150:HOH:O	2.19	0.51
1:D:287:ILE:N	1:D:287:ILE:HD12	2.25	0.51
1:D:333:GLY:H	1:D:386:THR:CG2	2.20	0.51
1:F:219:ARG:HB2	1:F:243:ASP:CG	2.36	0.51
1:G:96:GLY:HA3	5:G:1188:HOH:O	2.10	0.51
1:G:414:GLY:N	5:G:1171:HOH:O	2.43	0.51
1:H:428:ARG:NH2	1:H:460:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HD11	1:A:268:LEU:HD21	1.93	0.51
1:B:101:SER:HA	1:D:173:PHE:CZ	2.45	0.51
1:C:366:LYS:HD3	1:C:400:ILE:HG12	1.93	0.51
5:E:1194:HOH:O	1:H:165:GLU:HG2	2.10	0.51
1:A:413:THR:HG22	1:A:415:LEU:HD13	1.93	0.50
1:C:250:ALA:HB3	1:C:252:TYR:CE2	2.46	0.50
1:F:136:GLN:O	1:G:107:ARG:NH1	2.44	0.50
1:A:164:GLY:HA3	1:C:173:PHE:CG	2.45	0.50
1:C:343:SER:O	1:C:345:GLY:N	2.44	0.50
1:H:339:GLY:O	1:H:340:PRO:C	2.53	0.50
1:B:261:LYS:HE3	5:B:1223:HOH:O	2.11	0.50
1:B:397:ILE:HG23	1:B:446:PHE:CZ	2.47	0.50
1:B:451:SER:OG	1:D:214:THR:HB	2.12	0.50
1:E:101:SER:HA	1:G:173:PHE:CZ	2.47	0.50
1:G:294:ASN:HA	1:G:347:TYR:O	2.11	0.50
1:C:249:GLN:HE21	1:C:272:ASN:N	1.82	0.50
1:C:448:GLY:O	1:C:449:VAL:HB	2.10	0.50
1:B:135:THR:O	1:B:156:ARG:HA	2.11	0.50
1:E:355:LYS:HD2	1:E:383:TRP:CE2	2.47	0.50
1:F:222:ILE:HG22	1:F:222:ILE:O	2.11	0.50
1:G:411:VAL:CG1	1:G:418:ILE:HG23	2.41	0.50
1:E:210:ILE:CD1	1:H:413:THR:HG23	2.42	0.50
1:F:254:ILE:HD13	1:F:305:PHE:CD2	2.47	0.50
1:B:347:TYR:CG	1:B:348:GLY:N	2.80	0.50
1:C:433:GLU:CD	1:C:464:LEU:HD12	2.36	0.50
1:F:216:LYS:CE	1:G:452:ASP:HB3	2.41	0.50
1:G:184:HIS:HD2	1:G:186:GLY:N	2.10	0.50
1:H:332:THR:HG23	1:H:386:THR:HG21	1.93	0.50
1:B:366:LYS:CB	1:B:400:ILE:HG12	2.42	0.50
1:C:214:THR:HG22	5:C:1185:HOH:O	2.12	0.50
1:E:452:ASP:CB	1:G:216:LYS:NZ	2.75	0.50
1:F:136:GLN:NE2	1:F:156:ARG:CD	2.74	0.50
1:F:298:SER:HB2	5:F:1156:HOH:O	2.12	0.50
1:G:376:MET:HG2	1:G:397:ILE:CD1	2.41	0.50
1:A:360:VAL:HG13	1:A:383:TRP:HE3	1.75	0.50
1:B:332:THR:HG23	1:B:386:THR:CG2	2.42	0.50
1:C:397:ILE:HD13	1:C:422:PHE:CZ	2.47	0.50
1:D:412(B):PRO:HD2	5:D:1157:HOH:O	2.12	0.50
1:A:210:ILE:HD12	1:D:413:THR:HG23	1.93	0.49
1:A:328:PRO:HD3	1:A:343:SER:O	2.12	0.49
1:B:216:LYS:CE	1:C:452:ASP:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ARG:HB2	1:D:243:ASP:CG	2.37	0.49
1:D:252:TYR:OH	1:D:274:HIS:HA	2.11	0.49
1:E:216:LYS:CD	1:H:452:ASP:HB3	2.40	0.49
1:B:102:LYS:NZ	1:B:104:ASN:ND2	2.60	0.49
1:D:413:THR:CG2	1:D:415:LEU:HD13	2.41	0.49
1:E:286:GLU:C	1:E:287:ILE:HD12	2.37	0.49
1:F:129:CYS:O	1:F:163:VAL:HG23	2.12	0.49
1:G:181:SER:OG	1:G:192:ILE:HD12	2.13	0.49
1:B:366:LYS:HB3	1:B:400:ILE:HG12	1.95	0.49
1:C:228:SER:HB3	1:C:350:LYS:NZ	2.27	0.49
1:E:451:SER:OG	1:G:214:THR:HB	2.13	0.49
1:D:290:VAL:HG11	1:D:353:SER:HB2	1.94	0.49
1:D:450:ASN:ND2	5:D:1154:HOH:O	2.45	0.49
1:H:298:SER:OG	1:H:341:VAL:HB	2.12	0.49
1:C:322:PHE:CD1	1:C:328:PRO:HG2	2.48	0.49
1:E:406:TYR:HB2	1:E:425:GLU:OE1	2.12	0.49
1:A:115:PHE:CZ	1:A:159:MET:HE1	2.48	0.49
1:E:300:ARG:CZ	1:E:351:GLY:HA3	2.42	0.49
1:F:229:GLU:HG2	1:F:230:CYS:O	2.12	0.49
1:H:380:PRO:O	1:H:381:ASN:C	2.55	0.49
1:B:173:PHE:CG	1:C:164:GLY:HA3	2.47	0.49
1:C:116:VAL:O	1:C:116:VAL:HG13	2.12	0.49
1:D:119:GLU:O	1:D:119:GLU:HG3	2.13	0.49
1:D:229:GLU:HG2	1:D:230:CYS:O	2.13	0.49
1:D:413:THR:HG21	1:D:415:LEU:CD2	2.28	0.49
1:F:360:VAL:HG13	1:F:383:TRP:HE3	1.78	0.49
1:B:85:LEU:HD12	1:B:412(C):GLU:CG	2.31	0.49
1:C:117:ILE:HD13	1:C:167:PRO:HG3	1.95	0.49
1:E:216:LYS:HZ2	1:H:452:ASP:CB	2.25	0.49
1:F:341:VAL:HG12	5:F:1156:HOH:O	2.08	0.49
1:G:411:VAL:HG13	1:G:418:ILE:CG2	2.43	0.49
1:D:194:ILE:HG12	1:D:203:ALA:HB2	1.93	0.49
1:H:215:ILE:HD13	1:H:255:PHE:CE2	2.48	0.49
1:H:467:THR:HG22	1:H:467:THR:O	2.13	0.49
1:C:99:VAL:HG22	5:C:1172:HOH:O	2.12	0.49
1:F:102:LYS:HZ2	1:F:104:ASN:HD21	1.60	0.49
1:F:275:TYR:CE2	1:F:303:VAL:CG2	2.96	0.49
1:F:299:ASN:HD22	1:F:316:TYR:HB3	1.76	0.49
1:A:172:ARG:HD2	1:A:174:GLU:OE1	2.13	0.48
1:B:400:ILE:HG13	5:B:1219:HOH:O	2.12	0.48
1:B:454:VAL:HG23	1:D:202:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:GLY:CA	5:C:1149:HOH:O	2.51	0.48
1:G:129:CYS:O	1:G:163:VAL:HG23	2.13	0.48
1:G:366:LYS:HE3	5:G:1199:HOH:O	2.12	0.48
1:H:316:TYR:CD1	1:H:340:PRO:HD3	2.48	0.48
1:D:466:PHE:O	1:D:468:ILE:N	2.45	0.48
1:E:172:ARG:HD2	1:E:174:GLU:OE1	2.13	0.48
1:G:355:LYS:HB2	1:G:383:TRP:CZ3	2.48	0.48
1:H:126:HIS:O	1:H:127:LEU:HD23	2.13	0.48
1:E:332:THR:CG2	1:E:386:THR:HG21	2.42	0.48
1:F:275:TYR:O	1:F:276:GLU:HG3	2.13	0.48
1:G:120:PRO:HA	1:G:132:PHE:O	2.13	0.48
1:B:173:PHE:CZ	1:C:101:SER:HA	2.49	0.48
1:C:294:ASN:HA	1:C:347:TYR:O	2.12	0.48
1:C:452:ASP:HA	5:C:1180:HOH:O	2.14	0.48
1:D:96:GLY:O	1:D:448:GLY:O	2.30	0.48
1:D:354:PHE:CZ	1:D:409:SER:HB2	2.49	0.48
1:D:359:GLY:HA2	1:D:381:ASN:H	1.59	0.48
1:E:226:GLN:O	1:E:227:GLU:HB2	2.14	0.48
1:G:147:GLY:C	1:G:149:VAL:H	2.20	0.48
1:G:406:TYR:HB2	1:G:425:GLU:OE1	2.14	0.48
1:C:109:GLY:HA3	1:C:140:LEU:HD12	1.94	0.48
1:C:411:VAL:HG13	1:C:418:ILE:CG2	2.43	0.48
1:E:306:ASN:CG	1:E:308:GLN:N	2.71	0.48
1:A:330:ASP:C	5:A:1254:HOH:O	2.57	0.48
1:C:442:SER:HB2	5:C:1228:HOH:O	2.13	0.48
1:E:226:GLN:HE22	1:E:230:CYS:HA	1.79	0.48
1:E:228:SER:HB3	1:E:350:LYS:CE	2.41	0.48
1:A:180:ALA:CB	1:A:192:ILE:O	2.62	0.48
1:A:451:SER:CB	1:C:214:THR:HB	2.42	0.48
1:B:218:TRP:CE2	1:B:253:LYS:HE3	2.49	0.48
1:C:413:THR:CA	5:C:1150:HOH:O	2.62	0.48
1:D:97:TRP:CE2	1:D:376:MET:HE2	2.48	0.48
1:E:287:ILE:O	1:E:304:SER:HA	2.14	0.48
1:F:303:VAL:HG22	1:F:314:ILE:HG22	1.94	0.48
1:G:146:ASN:ND2	2:G:1146:NDG:C1	2.72	0.48
1:C:412(D):LEU:HA	5:C:1148:HOH:O	2.13	0.48
1:E:210:ILE:HD13	1:H:413:THR:HA	1.95	0.48
1:E:373:GLY:HA2	1:E:398:VAL:O	2.14	0.48
1:G:412(B):PRO:CA	5:G:1148:HOH:O	2.39	0.48
1:B:343:SER:CA	5:B:1150:HOH:O	2.55	0.48
1:E:320:GLY:N	1:E:387:ASP:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232:CYS:HA	1:H:237:CYS:HA	1.94	0.48
1:H:468:ILE:HG21	2:H:1146:NDG:H8C3	1.95	0.48
1:A:85:LEU:HD12	1:A:412(C):GLU:HG3	1.95	0.48
1:A:247:ASN:O	1:A:295:TRP:HB2	2.14	0.48
1:A:345:GLY:N	5:A:1149:HOH:O	2.47	0.48
1:B:216:LYS:NZ	1:C:452:ASP:HB3	2.29	0.47
1:B:227:GLU:OE1	1:B:227:GLU:HA	2.13	0.47
1:B:321:VAL:HG13	1:B:364:ARG:NH2	2.29	0.47
1:C:320:GLY:CA	1:C:387:ASP:O	2.62	0.47
1:D:425:GLU:OE1	1:D:427:ILE:HD11	2.13	0.47
1:E:333:GLY:N	1:E:386:THR:HG23	2.28	0.47
1:G:385:GLU:HB3	5:G:1165:HOH:O	2.13	0.47
1:H:412(D):LEU:HB2	5:H:1149:HOH:O	2.14	0.47
1:A:226:GLN:O	1:A:227:GLU:HB2	2.14	0.47
1:C:85:LEU:HD12	1:C:412(C):GLU:HG3	1.95	0.47
1:C:162:PRO:CG	1:C:165:GLU:CD	2.85	0.47
1:C:347:TYR:CG	1:C:348:GLY:N	2.77	0.47
1:F:118:ARG:O	1:F:119:GLU:HG3	2.14	0.47
1:A:320:GLY:CA	1:A:387:ASP:O	2.57	0.47
1:A:433:GLU:OE2	1:A:464:LEU:HD12	2.13	0.47
1:D:248:GLY:HA2	1:D:295:TRP:CD2	2.49	0.47
1:D:452:ASP:HA	5:D:1186:HOH:O	2.14	0.47
1:E:271:PRO:O	1:E:272:ASN:CB	2.61	0.47
1:F:412(D):LEU:HB2	5:F:1149:HOH:O	2.13	0.47
1:G:466:PHE:O	1:G:468:ILE:N	2.47	0.47
1:H:254:ILE:HD13	1:H:305:PHE:CD2	2.49	0.47
1:A:254:ILE:HD13	1:A:305:PHE:CD2	2.49	0.47
1:F:122:ILE:HG22	1:F:123:SER:N	2.29	0.47
1:G:113:ASP:O	1:G:168:SER:CB	2.63	0.47
1:G:355:LYS:HB2	1:G:383:TRP:CE3	2.50	0.47
1:G:467:THR:O	1:G:468:ILE:HB	2.14	0.47
1:A:210:ILE:HD13	1:D:413:THR:HA	1.97	0.47
1:A:325:ASN:HA	1:A:326:PRO:C	2.39	0.47
1:B:86:ALA:O	5:B:1160:HOH:O	2.20	0.47
1:D:270:ALA:HB1	1:D:273:TYR:HB2	1.95	0.47
1:H:299:ASN:ND2	5:H:1153:HOH:O	2.47	0.47
1:H:411:VAL:HG11	1:H:418:ILE:CG2	2.44	0.47
1:H:421:CYS:HB3	1:H:446:PHE:O	2.14	0.47
1:B:354:PHE:CZ	1:B:409:SER:HB2	2.50	0.47
1:B:448:GLY:O	1:B:449:VAL:CB	2.56	0.47
1:D:86:ALA:O	5:D:1157:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:PRO:HB3	1:E:316:TYR:CZ	2.50	0.47
1:G:215:ILE:HD13	1:G:255:PHE:CE2	2.49	0.47
1:A:250:ALA:HB3	1:A:252:TYR:CE2	2.49	0.47
1:A:343:SER:O	1:A:344:ASN:CB	2.62	0.47
1:A:355:LYS:HD2	1:A:383:TRP:CE2	2.50	0.47
1:C:254:ILE:HD12	5:C:1247:HOH:O	2.15	0.47
1:C:327:ARG:HB2	1:C:328:PRO:HD2	1.97	0.47
1:D:156:ARG:HB3	1:D:177:ALA:O	2.14	0.47
1:D:228:SER:HB3	1:D:350:LYS:CE	2.43	0.47
1:D:301:PRO:HB3	1:D:316:TYR:CZ	2.50	0.47
1:D:347:TYR:CG	1:D:348:GLY:N	2.75	0.47
1:E:245:PRO:HG2	1:E:249:GLN:O	2.15	0.47
1:E:306:ASN:CG	1:E:308:GLN:H	2.23	0.47
1:E:411:VAL:HG13	1:E:418:ILE:HG23	1.96	0.47
1:G:131:THR:O	1:G:160:SER:HA	2.15	0.47
1:H:105:SER:HB3	1:H:167:PRO:HD2	1.96	0.47
1:H:239:THR:CG2	1:H:257:MET:HE1	2.45	0.47
1:B:150:LYS:HD3	1:B:152:ARG:O	2.15	0.47
1:B:210:ILE:HD11	5:C:1213:HOH:O	2.15	0.47
1:D:232:CYS:HA	1:D:237:CYS:HA	1.96	0.47
1:E:85:LEU:HD12	1:E:412(C):GLU:CG	2.34	0.47
1:F:135:THR:OG1	1:F:159:MET:HE2	2.15	0.47
1:F:226:GLN:HE22	1:F:230:CYS:HB3	1.80	0.47
1:H:159:MET:HG2	1:H:173:PHE:HA	1.96	0.47
1:A:146:ASN:ND2	2:A:1146:NDG:C1	2.74	0.47
1:A:303:VAL:HG22	1:A:314:ILE:HG22	1.96	0.47
1:B:320:GLY:CA	1:B:387:ASP:O	2.62	0.47
1:C:91:LEU:HG	1:C:283:ASN:ND2	2.30	0.47
1:D:97:TRP:HD1	1:D:395:GLN:NE2	2.13	0.47
1:E:99:VAL:HG13	1:E:446:PHE:CE2	2.49	0.47
1:E:390:PHE:HE1	1:E:394:LYS:HB2	1.80	0.47
1:A:275:TYR:CE2	1:A:303:VAL:CG2	2.98	0.47
1:C:333:GLY:N	1:C:386:THR:CG2	2.78	0.47
1:D:468:ILE:CG2	2:D:1146:NDG:H8C3	2.44	0.47
1:A:466:PHE:O	1:A:468:ILE:N	2.48	0.46
1:B:413:THR:HG22	1:B:415:LEU:H	1.79	0.46
1:C:97:TRP:H	1:C:395:GLN:HE22	1.62	0.46
1:F:155:HIS:NE2	1:G:461:GLY:HA3	2.31	0.46
1:H:96:GLY:O	1:H:448:GLY:O	2.32	0.46
1:C:147:GLY:C	1:C:149:VAL:N	2.72	0.46
1:D:387:ASP:N	5:D:1236:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:GLY:N	5:E:1148:HOH:O	2.31	0.46
1:H:343:SER:O	1:H:344:ASN:CB	2.63	0.46
1:C:120:PRO:HA	1:C:132:PHE:O	2.16	0.46
1:C:194:ILE:HG12	1:C:203:ALA:HB2	1.97	0.46
1:E:164:GLY:HA3	1:G:173:PHE:CG	2.50	0.46
1:F:202:VAL:CG2	1:F:214:THR:HG23	2.46	0.46
1:F:256:LYS:HB2	1:F:310:LEU:HD11	1.97	0.46
1:G:126:HIS:C	5:G:1173:HOH:O	2.59	0.46
1:G:226:GLN:O	1:G:227:GLU:HB2	2.16	0.46
1:G:228:SER:HB3	1:G:350:LYS:CE	2.41	0.46
1:H:117:ILE:HG22	1:H:135:THR:HG22	1.97	0.46
1:A:347:TYR:CG	1:A:348:GLY:N	2.83	0.46
1:C:343:SER:C	1:C:345:GLY:H	2.23	0.46
1:D:299:ASN:ND2	1:D:316:TYR:HB3	2.31	0.46
1:H:158:LEU:O	1:H:174:GLU:HB2	2.15	0.46
1:A:332:THR:CG2	1:A:386:THR:HG21	2.46	0.46
1:B:114:VAL:HG13	1:B:167:PRO:O	2.16	0.46
1:B:131:THR:O	1:B:160:SER:HA	2.15	0.46
1:B:275:TYR:CE2	1:B:303:VAL:HG23	2.50	0.46
1:B:347:TYR:N	5:B:1157:HOH:O	2.48	0.46
1:C:342:SER:O	1:C:343:SER:C	2.57	0.46
1:G:287:ILE:O	1:G:304:SER:HA	2.14	0.46
1:B:216:LYS:NZ	1:C:452:ASP:CB	2.79	0.46
1:C:126:HIS:HB2	5:C:1148:HOH:O	2.15	0.46
1:D:360:VAL:CG1	1:D:383:TRP:HE3	2.29	0.46
1:F:397:ILE:HG23	1:F:446:PHE:CZ	2.51	0.46
1:A:216:LYS:CE	1:D:452:ASP:CB	2.94	0.46
1:A:332:THR:HG23	1:A:386:THR:CG2	2.45	0.46
1:B:426:LEU:HD13	1:B:460:ASP:N	2.31	0.46
1:H:327:ARG:O	1:H:368:THR:HB	2.16	0.46
1:A:306:ASN:CG	1:A:308:GLN:N	2.74	0.46
1:A:343:SER:O	1:A:344:ASN:HB3	2.16	0.46
1:A:413:THR:CG2	1:A:415:LEU:HB2	2.46	0.46
1:C:239:THR:HG22	1:C:257:MET:CE	2.45	0.46
1:C:413:THR:HB	5:C:1150:HOH:O	2.16	0.46
1:D:332:THR:CG2	1:D:386:THR:HG21	2.44	0.46
1:H:360:VAL:HG13	1:H:383:TRP:HE3	1.80	0.46
1:A:184:HIS:HD2	1:A:186:GLY:N	2.08	0.46
1:B:450:ASN:HA	5:B:1154:HOH:O	2.16	0.46
1:D:241:MET:HB2	1:D:255:PHE:HE1	1.80	0.46
1:D:397:ILE:CD1	1:D:422:PHE:HZ	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLY:O	1:H:454:VAL:HG21	2.15	0.46
1:F:306:ASN:CG	1:F:308:GLN:N	2.74	0.46
1:G:102:LYS:HG3	1:G:444:ILE:HG22	1.96	0.46
1:G:377:ILE:HG23	1:G:390:PHE:CD1	2.50	0.46
1:B:322:PHE:CE1	1:B:328:PRO:HG2	2.50	0.45
1:D:339:GLY:O	5:D:1152:HOH:O	2.21	0.45
1:E:85:LEU:HB2	1:E:185:ASP:O	2.17	0.45
1:E:105:SER:HB3	1:E:167:PRO:HD2	1.97	0.45
1:F:411:VAL:HG12	1:F:412:GLN:N	2.30	0.45
1:G:136:GLN:HE21	1:G:156:ARG:CD	2.29	0.45
1:H:97:TRP:HD1	1:H:395:GLN:NE2	2.14	0.45
1:C:116:VAL:HG12	1:C:138:ALA:O	2.17	0.45
1:D:333:GLY:N	1:D:386:THR:CG2	2.79	0.45
1:E:216:LYS:CE	1:H:452:ASP:HB3	2.45	0.45
1:A:219:ARG:HB2	1:A:243:ASP:CG	2.41	0.45
1:A:413:THR:HG23	1:C:210:ILE:CD1	2.46	0.45
1:D:102:LYS:NZ	1:D:104:ASN:ND2	2.64	0.45
1:E:222:ILE:O	1:E:222:ILE:HG22	2.15	0.45
1:E:305:PHE:HB3	1:E:312:TYR:HB3	1.98	0.45
1:F:136:GLN:HE21	1:F:156:ARG:HD3	1.80	0.45
1:H:305:PHE:HB3	1:H:312:TYR:HB3	1.99	0.45
1:A:247:ASN:O	1:A:248:GLY:O	2.34	0.45
1:B:232:CYS:HA	1:B:237:CYS:HA	1.97	0.45
1:C:232:CYS:HA	1:C:237:CYS:HA	1.97	0.45
1:C:319:SER:HB2	1:C:382:GLY:O	2.16	0.45
1:D:322:PHE:CE1	1:D:328:PRO:HG2	2.51	0.45
1:G:116:VAL:HG12	1:G:138:ALA:O	2.15	0.45
1:A:136:GLN:HE21	1:A:156:ARG:HD2	1.80	0.45
1:A:397:ILE:CD1	1:A:422:PHE:HZ	2.28	0.45
1:D:133:PHE:O	1:D:158:LEU:HD12	2.17	0.45
1:E:218:TRP:CD1	1:E:219:ARG:HG2	2.52	0.45
1:G:130:ARG:HG2	1:G:130:ARG:HH21	1.81	0.45
1:H:126:HIS:C	5:H:1149:HOH:O	2.60	0.45
1:A:113:ASP:O	5:A:1147:HOH:O	2.21	0.45
1:A:452:ASP:HB2	1:C:216:LYS:HZ2	1.80	0.45
1:C:148:THR:HG23	1:C:430:ARG:HH12	1.80	0.45
1:D:184:HIS:HD2	1:D:186:GLY:N	2.14	0.45
1:E:333:GLY:H	1:E:386:THR:HG23	1.80	0.45
1:F:325:ASN:O	1:F:348:GLY:HA2	2.17	0.45
1:H:226:GLN:O	1:H:227:GLU:HB2	2.15	0.45
1:A:117:ILE:HD13	1:A:167:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169(A):TYR:CD2	1:B:169(A):TYR:N	2.84	0.45
1:B:306:ASN:CG	1:B:308:GLN:N	2.74	0.45
1:B:412(C):GLU:CG	5:B:1151:HOH:O	2.23	0.45
1:D:88:ASN:H	1:D:88:ASN:ND2	2.14	0.45
1:D:135:THR:C	1:D:137:GLY:H	2.24	0.45
1:D:403:TRP:HB3	5:D:1245:HOH:O	2.15	0.45
1:E:325:ASN:O	1:E:348:GLY:CA	2.64	0.45
1:G:103:ASP:O	1:G:104:ASN:HB2	2.17	0.45
1:H:254:ILE:HD11	1:H:303:VAL:HG11	1.98	0.45
1:H:325:ASN:O	1:H:348:GLY:HA2	2.17	0.45
1:C:412(B):PRO:O	5:C:1150:HOH:O	2.20	0.45
1:D:339:GLY:O	1:D:340:PRO:C	2.60	0.45
1:G:91:LEU:HD11	1:G:281:TYR:CE2	2.52	0.45
1:H:192:ILE:HG23	1:H:205:LEU:CD2	2.47	0.45
1:H:239:THR:HG22	1:H:257:MET:HE1	1.98	0.45
1:A:413:THR:CG2	1:A:415:LEU:HD13	2.46	0.45
1:B:239:THR:CG2	1:B:257:MET:HE1	2.47	0.45
1:C:112:GLY:C	5:C:1149:HOH:O	2.59	0.45
1:C:290:VAL:HG11	1:C:353:SER:HB2	1.99	0.45
1:D:397:ILE:HG23	1:D:446:PHE:CZ	2.52	0.45
1:F:118:ARG:C	1:F:119:GLU:CG	2.90	0.45
1:H:273:TYR:OH	1:H:315:GLY:HA2	2.16	0.45
1:A:101:SER:HA	1:C:173:PHE:CZ	2.52	0.45
1:C:147:GLY:C	1:C:149:VAL:H	2.25	0.45
1:E:135:THR:O	1:E:156:ARG:HA	2.16	0.45
1:E:300:ARG:NH1	1:E:351:GLY:HA3	2.32	0.45
1:E:366:LYS:HD2	1:E:398:VAL:O	2.17	0.45
1:F:316:TYR:CD1	1:F:340:PRO:HD3	2.52	0.45
1:H:136:GLN:NE2	1:H:156:ARG:HD3	2.32	0.45
1:B:86:ALA:CA	5:B:1156:HOH:O	2.62	0.44
1:B:316:TYR:CZ	1:B:340:PRO:HD3	2.51	0.44
1:B:413:THR:CG2	1:B:415:LEU:HB2	2.47	0.44
1:H:306:ASN:CG	1:H:308:GLN:H	2.24	0.44
1:H:341:VAL:HG12	5:H:1155:HOH:O	2.16	0.44
1:H:343:SER:N	5:H:1155:HOH:O	2.49	0.44
1:H:355:LYS:HB2	1:H:383:TRP:CZ3	2.52	0.44
1:A:253:LYS:HG2	1:A:267:GLU:HA	1.99	0.44
1:A:391:SER:HB2	5:A:1247:HOH:O	2.18	0.44
1:A:397:ILE:HG22	1:A:398:VAL:HG23	1.97	0.44
1:A:456:TRP:CG	1:A:457:SER:H	2.35	0.44
1:B:346:ALA:C	5:B:1157:HOH:O	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLU:C	1:C:287:ILE:HD12	2.41	0.44
1:E:115:PHE:CZ	1:E:159:MET:HE1	2.52	0.44
1:G:412(D):LEU:CB	5:G:1173:HOH:O	2.58	0.44
1:H:161:CYS:HB2	1:H:162:PRO:HD2	2.00	0.44
1:B:129:CYS:C	1:B:163:VAL:HG23	2.42	0.44
1:B:467:THR:O	1:B:468:ILE:HB	2.17	0.44
1:C:290:VAL:HG21	1:C:353:SER:HB2	1.98	0.44
1:E:232:CYS:HA	1:E:236:SER:O	2.17	0.44
1:G:115:PHE:CZ	1:G:159:MET:HE1	2.53	0.44
1:G:147:GLY:C	1:G:149:VAL:N	2.75	0.44
1:G:354:PHE:CZ	1:G:409:SER:HB2	2.51	0.44
1:B:115:PHE:CE1	1:B:159:MET:HE1	2.52	0.44
1:C:181:SER:CB	5:C:1178:HOH:O	2.65	0.44
1:C:412(A):HIS:C	5:C:1152:HOH:O	2.60	0.44
1:C:453:THR:HG22	1:C:454:VAL:N	2.22	0.44
1:D:397:ILE:HD13	1:D:422:PHE:CZ	2.48	0.44
1:E:150:LYS:HD3	1:E:152:ARG:O	2.18	0.44
1:F:366:LYS:HD3	1:F:400:ILE:HG12	2.00	0.44
1:H:347:TYR:CG	1:H:348:GLY:N	2.86	0.44
1:A:229:GLU:HG2	1:A:230:CYS:O	2.18	0.44
1:B:117:ILE:HD11	5:B:1183:HOH:O	2.17	0.44
1:B:207:TYR:HB3	1:B:212:THR:HG21	2.00	0.44
1:B:412:GLN:HB2	1:B:419:ARG:CB	2.47	0.44
1:E:339:GLY:O	1:E:340:PRO:C	2.60	0.44
1:F:210:ILE:CD1	1:G:413:THR:HA	2.47	0.44
1:G:468:ILE:CG2	2:G:1146:NDG:H8C3	2.47	0.44
1:H:301:PRO:HB3	1:H:316:TYR:CZ	2.52	0.44
1:B:135:THR:OG1	1:B:159:MET:HE2	2.17	0.44
1:D:136:GLN:HE21	1:D:156:ARG:HD2	1.82	0.44
1:D:330:ASP:O	5:D:1214:HOH:O	2.21	0.44
1:E:115:PHE:O	1:E:117:ILE:HG23	2.17	0.44
1:E:233:VAL:O	1:E:234:ASN:C	2.61	0.44
1:E:270:ALA:HB1	1:E:273:TYR:HB2	2.00	0.44
1:E:277:GLU:OE1	1:E:292:ARG:NH2	2.50	0.44
1:F:247:ASN:O	1:F:248:GLY:O	2.36	0.44
1:G:316:TYR:CD1	1:G:340:PRO:HD3	2.53	0.44
1:G:390:PHE:HE1	1:G:394:LYS:HB2	1.83	0.44
1:H:117:ILE:HD12	1:H:120:PRO:HB3	1.99	0.44
1:A:131:THR:O	1:A:160:SER:HA	2.17	0.44
1:B:146:ASN:O	1:B:437:ILE:O	2.36	0.44
1:B:218:TRP:CD1	1:B:219:ARG:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:LYS:NZ	1:F:104:ASN:ND2	2.65	0.44
1:G:287:ILE:N	1:G:287:ILE:CD1	2.81	0.44
1:G:397:ILE:CD1	1:G:422:PHE:HZ	2.31	0.44
1:G:421:CYS:HB3	1:G:446:PHE:O	2.17	0.44
1:G:426:LEU:HD13	1:G:460:ASP:N	2.32	0.44
1:H:254:ILE:HD12	5:H:1166:HOH:O	2.16	0.44
1:A:99:VAL:HG12	1:A:446:PHE:CE2	2.53	0.44
1:A:397:ILE:HD13	1:A:422:PHE:HZ	1.83	0.44
1:E:102:LYS:HG3	1:E:444:ILE:HG22	1.99	0.44
1:E:387:ASP:HB2	5:E:1150:HOH:O	2.17	0.44
1:F:397:ILE:HD13	1:F:422:PHE:CZ	2.53	0.44
1:A:148:THR:HG22	1:A:430:ARG:HH22	1.83	0.44
1:E:232:CYS:HA	1:E:237:CYS:HA	1.99	0.44
1:E:412(B):PRO:HD3	1:E:417:CYS:O	2.18	0.44
1:E:453:THR:CG2	1:E:454:VAL:H	2.13	0.44
1:F:88:ASN:O	1:F:284:ALA:HA	2.18	0.44
1:F:411:VAL:CG1	1:F:412:GLN:N	2.81	0.44
1:A:208:ASN:ND2	5:A:1157:HOH:O	2.51	0.43
1:B:172:ARG:HD2	1:B:174:GLU:OE1	2.17	0.43
1:G:247:ASN:O	1:G:295:TRP:HB2	2.18	0.43
1:G:412:GLN:CB	1:G:419:ARG:HB2	2.40	0.43
1:A:413:THR:HG23	1:C:210:ILE:HD12	2.00	0.43
1:D:358:ASN:HB2	1:D:381:ASN:OD1	2.18	0.43
1:F:226:GLN:O	1:F:227:GLU:HB2	2.18	0.43
1:F:333:GLY:H	1:F:386:THR:HG23	1.83	0.43
1:F:343:SER:O	1:F:344:ASN:CB	2.65	0.43
1:G:296:HIS:HA	1:G:345:GLY:O	2.18	0.43
1:G:445:SER:C	1:G:446:PHE:CD1	2.95	0.43
1:H:333:GLY:H	1:H:386:THR:CG2	2.28	0.43
1:H:390:PHE:CE1	1:H:394:LYS:HB2	2.53	0.43
1:B:254:ILE:HD11	1:B:268:LEU:HD21	1.99	0.43
1:F:125:SER:HA	1:F:184:HIS:HB3	1.99	0.43
1:G:192:ILE:HG12	1:G:205:LEU:HD22	2.00	0.43
1:G:222:ILE:HG22	1:G:222:ILE:O	2.18	0.43
1:G:364:ARG:HG3	1:G:365:THR:O	2.19	0.43
1:H:118:ARG:O	1:H:119:GLU:HG3	2.19	0.43
1:H:397:ILE:HG23	1:H:446:PHE:CZ	2.53	0.43
1:B:99:VAL:HG13	1:B:446:PHE:CE2	2.53	0.43
1:B:464:LEU:HB3	1:B:465:PRO:HA	2.00	0.43
1:C:287:ILE:O	1:C:304:SER:HA	2.19	0.43
1:C:397:ILE:HG23	1:C:446:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:THR:HG22	1:C:415:LEU:N	2.31	0.43
1:C:438:TRP:CD1	1:C:438:TRP:H	2.35	0.43
1:D:239:THR:CG2	1:D:257:MET:HE1	2.47	0.43
1:F:225:THR:OG1	1:F:226:GLN:N	2.50	0.43
1:F:390:PHE:CD2	1:F:390:PHE:N	2.86	0.43
1:H:88:ASN:HD22	1:H:89:SER:H	1.65	0.43
1:A:375:GLU:OE1	1:A:394:LYS:HE3	2.17	0.43
1:D:136:GLN:HE21	1:D:156:ARG:CD	2.31	0.43
1:E:97:TRP:H	1:E:395:GLN:HE22	1.66	0.43
1:E:413:THR:CG2	1:E:415:LEU:HB2	2.47	0.43
1:F:146:ASN:ND2	2:F:1146:NDG:C1	2.80	0.43
1:A:169:PRO:HD2	5:A:1147:HOH:O	2.17	0.43
1:A:360:VAL:HG22	1:A:383:TRP:HB2	2.00	0.43
1:B:412(B):PRO:HB3	1:B:415:LEU:O	2.18	0.43
1:C:312:TYR:CD1	1:C:312:TYR:C	2.97	0.43
1:H:339:GLY:HA2	1:H:340:PRO:HD2	1.79	0.43
1:H:413:THR:CB	5:H:1148:HOH:O	2.67	0.43
1:B:155:HIS:CE1	1:C:461:GLY:HA3	2.54	0.43
1:B:202:VAL:HG23	1:B:214:THR:HG23	2.01	0.43
1:B:365:THR:HG23	5:B:1189:HOH:O	2.19	0.43
1:C:113:ASP:N	5:C:1149:HOH:O	2.51	0.43
1:E:123:SER:OG	1:E:229:GLU:HG3	2.18	0.43
1:E:366:LYS:HG3	1:E:374:PHE:N	2.34	0.43
1:E:457:SER:OG	1:E:459:PRO:HD3	2.18	0.43
1:A:216:LYS:HZ2	1:D:452:ASP:CB	2.29	0.43
1:A:286:GLU:C	1:A:287:ILE:HD12	2.44	0.43
1:A:377:ILE:HG23	1:A:390:PHE:CD1	2.54	0.43
1:A:390:PHE:HE1	1:A:394:LYS:HB2	1.83	0.43
1:B:249:GLN:NE2	1:B:271:PRO:HA	2.33	0.43
1:B:306:ASN:CG	1:B:308:GLN:H	2.27	0.43
1:C:115:PHE:CE1	1:C:159:MET:HE1	2.54	0.43
1:D:88:ASN:N	1:D:88:ASN:ND2	2.66	0.43
1:E:146:ASN:HD21	4:E:1146:NAG:C1	2.32	0.43
1:H:122:ILE:HG22	1:H:123:SER:N	2.34	0.43
1:H:215:ILE:HD11	1:H:262:VAL:HG21	2.01	0.43
1:A:226:GLN:NE2	1:A:239:THR:OG1	2.46	0.43
1:C:445:SER:C	1:C:446:PHE:CD1	2.96	0.43
1:E:254:ILE:HD13	1:E:305:PHE:CD2	2.53	0.43
1:F:202:VAL:CG1	1:G:454:VAL:HG23	2.48	0.43
1:H:413:THR:HB	5:H:1148:HOH:O	2.18	0.43
1:B:200:GLY:O	1:C:454:VAL:HG21	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:CYS:HA	1:E:129:CYS:HA	2.00	0.43
1:G:248:GLY:HA2	1:G:295:TRP:CD2	2.53	0.43
1:G:309:ASN:CB	5:G:1156:HOH:O	2.65	0.43
1:C:251:SER:OG	1:C:267:GLU:OE2	2.36	0.42
1:D:411:VAL:HG13	1:D:411:VAL:HG22	1.97	0.42
1:E:139:LEU:HD11	5:E:1153:HOH:O	2.19	0.42
1:E:436:THR:HG21	1:E:464:LEU:HD13	2.00	0.42
1:E:466:PHE:O	1:E:468:ILE:N	2.52	0.42
1:F:121:PHE:CZ	1:F:132:PHE:HB2	2.54	0.42
1:F:397:ILE:HD13	1:F:422:PHE:HZ	1.83	0.42
1:A:397:ILE:HG23	1:A:446:PHE:CZ	2.55	0.42
1:B:132:PHE:HB3	1:B:158:LEU:HD11	2.01	0.42
1:B:259:LYS:HE3	5:B:1210:HOH:O	2.19	0.42
1:C:172:ARG:HD2	1:C:174:GLU:OE1	2.18	0.42
1:D:136:GLN:NE2	1:D:156:ARG:HD2	2.34	0.42
1:D:426:LEU:HD13	1:D:460:ASP:N	2.34	0.42
1:E:412(B):PRO:HD2	1:E:418:ILE:HG12	2.01	0.42
1:E:452:ASP:HB3	1:G:216:LYS:NZ	2.32	0.42
1:F:335:SER:HB2	5:F:1188:HOH:O	2.18	0.42
1:G:270:ALA:HB1	1:G:273:TYR:CB	2.49	0.42
1:A:136:GLN:HE21	1:A:156:ARG:HD3	1.83	0.42
1:D:413:THR:CG2	1:D:415:LEU:HB2	2.49	0.42
1:F:210:ILE:HD13	1:G:413:THR:HA	2.00	0.42
1:F:468:ILE:CG2	2:F:1146:NDG:H8C3	2.50	0.42
1:H:287:ILE:N	1:H:287:ILE:HD12	2.34	0.42
1:H:408:GLY:HA3	1:H:423:TRP:CZ2	2.54	0.42
1:B:403:TRP:CZ3	1:B:432:LYS:HG3	2.54	0.42
1:F:135:THR:O	1:F:156:ARG:HA	2.19	0.42
1:A:301:PRO:HB3	1:A:316:TYR:CZ	2.54	0.42
1:B:113:ASP:N	5:D:1149:HOH:O	2.52	0.42
1:C:296:HIS:HB2	5:C:1173:HOH:O	2.19	0.42
1:C:355:LYS:HD2	1:C:383:TRP:CE2	2.55	0.42
1:C:415:LEU:HD23	5:C:1227:HOH:O	2.20	0.42
1:C:442:SER:CB	5:C:1228:HOH:O	2.67	0.42
1:D:306:ASN:CG	1:D:308:GLN:N	2.78	0.42
1:D:397:ILE:HG22	1:D:398:VAL:HG23	2.00	0.42
1:G:229:GLU:OE1	1:G:410:PHE:HA	2.20	0.42
1:G:397:ILE:HG23	1:G:446:PHE:CZ	2.55	0.42
1:H:248:GLY:HA2	1:H:295:TRP:NE1	2.33	0.42
1:A:144:HIS:C	1:A:146:ASN:H	2.26	0.42
1:B:319:SER:HB2	1:B:382:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:HA	1:B:326:PRO:C	2.43	0.42
1:C:248:GLY:HA2	1:C:295:TRP:NE1	2.35	0.42
1:D:355:LYS:HD2	1:D:383:TRP:CE2	2.54	0.42
1:F:119:GLU:OE1	1:F:227:GLU:OE1	2.37	0.42
1:G:97:TRP:N	1:G:395:GLN:HE22	2.16	0.42
1:G:118:ARG:C	1:G:119:GLU:HG2	2.45	0.42
1:G:412(D):LEU:CD1	5:G:1173:HOH:O	2.51	0.42
1:A:173:PHE:CG	1:D:164:GLY:HA3	2.54	0.42
1:A:173:PHE:CZ	1:D:101:SER:HA	2.54	0.42
1:B:210:ILE:CD1	1:C:413:THR:HA	2.49	0.42
1:C:218:TRP:CE2	1:C:253:LYS:HE3	2.55	0.42
1:C:306:ASN:CG	1:C:308:GLN:N	2.77	0.42
1:C:453:THR:CG2	1:C:454:VAL:H	2.17	0.42
1:C:464:LEU:HB3	1:C:465:PRO:HA	2.01	0.42
1:D:375:GLU:OE1	1:D:394:LYS:CE	2.66	0.42
1:F:158:LEU:O	1:F:174:GLU:HB2	2.20	0.42
1:F:453:THR:CG2	1:F:454:VAL:H	2.20	0.42
1:G:300:ARG:HG2	1:G:300:ARG:NH2	2.34	0.42
1:G:387:ASP:HB3	1:G:388:SER:H	1.62	0.42
1:H:332:THR:CG2	1:H:386:THR:HG21	2.50	0.42
1:A:433:GLU:CD	1:A:464:LEU:HD12	2.45	0.42
1:A:453:THR:HG22	5:A:1166:HOH:O	2.18	0.42
1:B:133:PHE:O	1:B:158:LEU:HD12	2.20	0.42
1:D:275:TYR:CE2	1:D:303:VAL:HG23	2.54	0.42
1:E:88:ASN:N	1:E:88:ASN:ND2	2.50	0.42
1:F:333:GLY:N	1:F:386:THR:HG23	2.34	0.42
1:F:411:VAL:HG13	1:F:418:ILE:CG2	2.49	0.42
1:G:192:ILE:HG23	1:G:205:LEU:HD22	2.01	0.42
1:D:232:CYS:C	1:D:233:VAL:HG23	2.44	0.42
1:D:450:ASN:CG	5:D:1154:HOH:O	2.62	0.42
1:E:105:SER:CB	1:E:167:PRO:HD2	2.50	0.42
1:E:450:ASN:HA	5:E:1185:HOH:O	2.19	0.42
1:G:413:THR:CB	5:G:1148:HOH:O	2.47	0.42
1:H:210:ILE:O	1:H:210:ILE:HG13	2.20	0.42
1:H:319:SER:HB2	1:H:382:GLY:O	2.20	0.42
1:A:97:TRP:N	1:A:395:GLN:HE22	2.16	0.42
1:A:412(B):PRO:HB3	1:A:415:LEU:O	2.20	0.42
1:B:229:GLU:HG2	1:B:230:CYS:O	2.19	0.42
1:C:354:PHE:CZ	1:C:409:SER:HB2	2.55	0.42
1:C:426:LEU:O	1:C:441:GLY:HA2	2.20	0.42
1:D:413:THR:HG22	1:D:415:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:PRO:O	1:E:272:ASN:HB3	2.19	0.42
1:E:412:GLN:HG3	1:E:419:ARG:CG	2.45	0.42
1:F:173:PHE:CB	1:G:164:GLY:HA3	2.50	0.42
1:F:332:THR:HG23	1:F:386:THR:CG2	2.50	0.42
1:G:412(A):HIS:C	1:G:412(C):GLU:N	2.78	0.42
1:H:303:VAL:HG22	1:H:314:ILE:HG22	2.02	0.42
1:A:158:LEU:O	1:A:174:GLU:HB2	2.20	0.41
1:A:397:ILE:HD13	1:A:422:PHE:CZ	2.54	0.41
1:C:102:LYS:NZ	1:C:104:ASN:ND2	2.68	0.41
1:C:322:PHE:HB2	1:C:327:ARG:HD2	2.01	0.41
1:C:432:LYS:HA	1:C:432:LYS:HD3	1.91	0.41
1:F:134:LEU:HA	1:F:157:THR:O	2.20	0.41
1:G:85:LEU:HD11	1:G:412(C):GLU:HG3	1.92	0.41
1:G:320:GLY:CA	1:G:387:ASP:O	2.58	0.41
1:G:339:GLY:O	1:G:340:PRO:C	2.63	0.41
1:G:365:THR:HA	1:G:373:GLY:O	2.20	0.41
1:B:158:LEU:O	1:B:174:GLU:HB2	2.19	0.41
1:B:412:GLN:HB2	1:B:419:ARG:HB2	2.00	0.41
1:C:287:ILE:N	1:C:287:ILE:CD1	2.82	0.41
1:C:339:GLY:O	1:C:340:PRO:C	2.63	0.41
1:E:148:THR:HG23	1:E:430:ARG:HH12	1.85	0.41
1:E:174:GLU:HA	1:E:174:GLU:OE2	2.19	0.41
1:E:412(D):LEU:CA	5:E:1154:HOH:O	2.37	0.41
1:F:145:SER:O	1:F:147:GLY:N	2.54	0.41
1:F:194:ILE:HD13	1:F:223:LEU:HG	2.02	0.41
1:H:118:ARG:HB2	1:H:156:ARG:HH11	1.85	0.41
1:H:249:GLN:NE2	1:H:272:ASN:N	2.63	0.41
1:B:110:SER:CB	1:D:144:HIS:HD2	2.33	0.41
1:B:250:ALA:HB3	1:B:252:TYR:CE2	2.55	0.41
1:B:254:ILE:HD13	1:B:305:PHE:CD2	2.56	0.41
1:D:172:ARG:HD2	1:D:174:GLU:OE1	2.20	0.41
1:E:202:VAL:HG23	1:E:214:THR:HG23	2.01	0.41
1:F:433:GLU:CD	1:F:464:LEU:HD12	2.45	0.41
1:G:226:GLN:NE2	1:G:239:THR:OG1	2.47	0.41
1:G:232:CYS:HA	1:G:236:SER:O	2.21	0.41
1:G:300:ARG:HG2	1:G:300:ARG:HH21	1.84	0.41
1:H:376:MET:CG	1:H:397:ILE:HD11	2.27	0.41
1:A:101:SER:O	1:A:444:ILE:HA	2.20	0.41
1:B:164:GLY:HA3	1:D:173:PHE:CG	2.55	0.41
1:B:287:ILE:N	1:B:287:ILE:CD1	2.81	0.41
1:D:99:VAL:HG13	1:D:446:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:VAL:CG1	1:E:418:ILE:HG23	2.50	0.41
1:F:221:ASN:ND2	1:F:244:GLY:C	2.79	0.41
1:F:360:VAL:CG1	1:F:383:TRP:HE3	2.33	0.41
1:G:144:HIS:C	1:G:146:ASN:H	2.28	0.41
1:H:397:ILE:HD13	1:H:422:PHE:CZ	2.55	0.41
1:B:181:SER:OG	1:B:192:ILE:HD12	2.20	0.41
1:D:149:VAL:HG12	1:D:150:LYS:N	2.35	0.41
1:D:183:CYS:HB3	1:D:230:CYS:O	2.21	0.41
1:D:191:THR:OG1	1:D:206:LYS:HB2	2.21	0.41
1:E:411:VAL:HA	1:E:411:VAL:HG22	1.92	0.41
1:F:146:ASN:O	1:F:437:ILE:O	2.39	0.41
1:H:403:TRP:CH2	1:H:432:LYS:HB3	2.56	0.41
1:C:332:THR:CG2	1:C:386:THR:HG21	2.50	0.41
1:C:446:PHE:CD1	1:C:446:PHE:N	2.89	0.41
1:E:129:CYS:C	1:E:163:VAL:HG23	2.45	0.41
1:E:132:PHE:CD2	1:E:160:SER:HB3	2.56	0.41
1:F:248:GLY:O	1:F:249:GLN:C	2.64	0.41
1:F:275:TYR:OH	1:F:314:ILE:HB	2.21	0.41
1:H:95:ASN:ND2	1:H:450:ASN:O	2.50	0.41
1:H:332:THR:HG23	1:H:386:THR:CG2	2.50	0.41
1:A:85:LEU:CD1	1:A:412(C):GLU:HG3	2.50	0.41
1:A:297:GLY:HA2	1:A:341:VAL:O	2.20	0.41
1:A:299:ASN:HD22	1:A:316:TYR:HB3	1.83	0.41
1:B:219:ARG:HE	1:B:251:SER:HB2	1.86	0.41
1:D:129:CYS:O	1:D:163:VAL:HG23	2.20	0.41
1:D:254:ILE:HD13	1:D:305:PHE:CD2	2.55	0.41
1:E:316:TYR:CD1	1:E:340:PRO:HD3	2.55	0.41
1:F:149:VAL:HG12	1:F:150:LYS:N	2.36	0.41
1:F:232:CYS:HA	1:F:236:SER:O	2.20	0.41
1:H:184:HIS:HD2	1:H:186:GLY:N	2.10	0.41
1:A:322:PHE:CE2	1:A:341:VAL:HG21	2.55	0.41
1:B:136:GLN:N	5:B:1202:HOH:O	2.54	0.41
1:B:136:GLN:O	1:C:107:ARG:NH1	2.49	0.41
1:B:366:LYS:HD3	1:B:400:ILE:HG12	2.02	0.41
1:G:129:CYS:C	1:G:163:VAL:HG23	2.45	0.41
1:G:250:ALA:HB3	1:G:252:TYR:CE2	2.56	0.41
1:G:352:PHE:HB2	5:G:1157:HOH:O	2.21	0.41
1:G:426:LEU:O	1:G:441:GLY:HA2	2.19	0.41
1:G:453:THR:C	1:G:454:VAL:CG2	2.94	0.41
1:H:453:THR:HG22	1:H:454:VAL:N	2.28	0.41
1:A:215:ILE:HD13	1:A:255:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TRP:CE2	1:A:253:LYS:HE3	2.56	0.41
1:A:293:ASP:C	1:A:293:ASP:OD2	2.63	0.41
1:A:297:GLY:N	1:A:345:GLY:O	2.54	0.41
1:A:411:VAL:HG13	1:A:412:GLN:N	2.36	0.41
1:A:452:ASP:HB3	1:C:216:LYS:CE	2.51	0.41
1:B:117:ILE:HD12	1:B:120:PRO:HB3	2.02	0.41
1:C:84:LYS:H	1:C:84:LYS:HG3	1.66	0.41
1:D:411:VAL:CG1	1:D:418:ILE:HG23	2.48	0.41
1:E:287:ILE:N	1:E:287:ILE:CD1	2.80	0.41
1:F:181:SER:CB	5:F:1153:HOH:O	2.68	0.41
1:F:298:SER:CB	5:F:1156:HOH:O	2.69	0.41
1:G:225:THR:HB	1:G:241:MET:HE2	2.03	0.41
1:G:335:SER:OG	1:G:339:GLY:O	2.37	0.41
1:H:194:ILE:HG12	1:H:203:ALA:HB2	2.03	0.41
1:H:227:GLU:OE1	1:H:227:GLU:HA	2.20	0.41
1:H:373:GLY:HA2	1:H:399:ALA:O	2.21	0.41
1:A:227:GLU:OE1	1:A:227:GLU:HA	2.19	0.41
1:A:346:ALA:N	5:A:1152:HOH:O	2.49	0.41
1:B:218:TRP:CZ2	1:B:253:LYS:HG3	2.56	0.41
1:B:411:VAL:HG13	1:B:418:ILE:CG2	2.51	0.41
1:E:114:VAL:HG13	1:E:167:PRO:O	2.21	0.41
1:F:99:VAL:HG13	1:F:446:PHE:CE2	2.56	0.41
1:G:153:SER:C	1:G:155:HIS:H	2.28	0.41
1:D:184:HIS:CD2	1:D:186:GLY:N	2.83	0.40
1:F:168:SER:HB2	1:F:169:PRO:HD2	2.03	0.40
1:F:366:LYS:HD3	1:F:400:ILE:CG1	2.51	0.40
1:G:312:TYR:CD1	1:G:312:TYR:C	2.99	0.40
1:C:378:TRP:HB3	1:C:392:VAL:HB	2.03	0.40
1:E:119:GLU:OE1	1:E:227:GLU:OE1	2.38	0.40
1:F:271:PRO:O	1:F:272:ASN:HB3	2.22	0.40
1:A:129:CYS:C	1:A:163:VAL:HG23	2.45	0.40
1:B:248:GLY:O	1:B:249:GLN:C	2.62	0.40
1:B:381:ASN:C	5:B:1162:HOH:O	2.64	0.40
1:C:97:TRP:CZ2	1:C:376:MET:HE2	2.56	0.40
1:C:438:TRP:CD1	1:C:438:TRP:N	2.89	0.40
1:D:428:ARG:HB3	1:D:464:LEU:HD11	2.02	0.40
1:G:121:PHE:CB	1:G:228:SER:HA	2.51	0.40
1:G:152:ARG:CZ	1:G:222:ILE:HD13	2.50	0.40
1:H:191:THR:OG1	1:H:206:LYS:HB2	2.22	0.40
1:H:366:LYS:CB	1:H:400:ILE:HG12	2.50	0.40
1:H:466:PHE:O	1:H:468:ILE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:O	1:A:438:TRP:HB3	2.21	0.40
1:A:413:THR:HG22	1:A:415:LEU:H	1.86	0.40
1:B:277:GLU:OE1	1:B:350:LYS:HB2	2.21	0.40
1:D:88:ASN:HD22	1:D:88:ASN:H	1.68	0.40
1:D:306:ASN:CG	1:D:308:GLN:H	2.29	0.40
1:D:359:GLY:HA3	1:D:381:ASN:H	1.78	0.40
1:E:152:ARG:HH21	1:E:152:ARG:HG3	1.86	0.40
1:E:215:ILE:HD11	1:E:262:VAL:CG2	2.50	0.40
1:F:301:PRO:HB3	1:F:316:TYR:CZ	2.56	0.40
1:F:305:PHE:HB3	1:F:312:TYR:HB3	2.02	0.40
1:H:366:LYS:HB3	1:H:400:ILE:HG12	2.03	0.40
1:B:463:GLU:N	1:D:144:HIS:HE1	1.94	0.40
1:C:254:ILE:HB	5:C:1247:HOH:O	2.22	0.40
1:D:277:GLU:OE1	1:D:350:LYS:HB2	2.21	0.40
1:E:247:ASN:O	1:E:295:TRP:HB2	2.22	0.40
1:E:300:ARG:HD2	5:E:1167:HOH:O	2.21	0.40
1:F:111:LYS:NZ	1:H:112:GLY:O	2.55	0.40
1:G:162:PRO:HG2	1:G:165:GLU:OE1	2.21	0.40
1:G:239:THR:CG2	1:G:257:MET:HE1	2.51	0.40
1:H:216:LYS:HE3	1:H:216:LYS:HB2	2.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:SER:OG	5:D:1242:HOH:O[8_456]	2.13	0.07

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	383/387 (99%)	342 (89%)	32 (8%)	9 (2%)	5 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	383/387 (99%)	341 (89%)	32 (8%)	10 (3%)	4	7
1	C	383/387 (99%)	338 (88%)	35 (9%)	10 (3%)	4	7
1	D	383/387 (99%)	344 (90%)	31 (8%)	8 (2%)	5	9
1	E	383/387 (99%)	342 (89%)	32 (8%)	9 (2%)	5	8
1	F	383/387 (99%)	335 (88%)	37 (10%)	11 (3%)	3	5
1	G	383/387 (99%)	346 (90%)	30 (8%)	7 (2%)	6	12
1	H	383/387 (99%)	344 (90%)	31 (8%)	8 (2%)	5	9
All	All	3064/3096 (99%)	2732 (89%)	260 (8%)	72 (2%)	5	8

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	SER
1	B	448	GLY
1	D	340	PRO
1	E	340	PRO
1	E	412(A)	HIS
1	F	340	PRO
1	G	340	PRO
1	H	340	PRO
1	A	248	GLY
1	A	340	PRO
1	A	448	GLY
1	A	449	VAL
1	B	146	ASN
1	B	248	GLY
1	B	449	VAL
1	C	147	GLY
1	C	248	GLY
1	C	448	GLY
1	D	146	ASN
1	D	248	GLY
1	D	448	GLY
1	D	449	VAL
1	E	234	ASN
1	E	448	GLY
1	E	449	VAL
1	F	146	ASN
1	F	248	GLY
1	F	448	GLY

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Mol	Chain	Res	Type
1	F	449	VAL
1	G	147	GLY
1	G	248	GLY
1	G	448	GLY
1	H	343	SER
1	H	448	GLY
1	A	330	ASP
1	B	330	ASP
1	B	340	PRO
1	C	340	PRO
1	C	449	VAL
1	D	347	TYR
1	F	343	SER
1	G	449	VAL
1	H	449	VAL
1	H	451	SER
1	H	456	TRP
1	A	451	SER
1	B	467	THR
1	C	381	ASN
1	C	412(A)	HIS
1	E	248	GLY
1	F	249	GLN
1	F	388	SER
1	H	147	GLY
1	A	147	GLY
1	A	347	TYR
1	B	200	GLY
1	D	330	ASP
1	E	146	ASN
1	E	456	TRP
1	F	264	LYS
1	G	347	TYR
1	C	344	ASN
1	C	347	TYR
1	E	435	SER
1	A	200	GLY
1	D	147	GLY
1	B	222	ILE
1	H	200	GLY
1	G	200	GLY
1	C	200	GLY

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Mol	Chain	Res	Type
1	F	147	GLY
1	F	200	GLY

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	329/331 (99%)	312 (95%)	17 (5%)	21	42
1	B	329/331 (99%)	314 (95%)	15 (5%)	24	48
1	C	329/331 (99%)	313 (95%)	16 (5%)	22	45
1	D	329/331 (99%)	314 (95%)	15 (5%)	24	48
1	E	329/331 (99%)	315 (96%)	14 (4%)	26	51
1	F	329/331 (99%)	315 (96%)	14 (4%)	26	51
1	G	329/331 (99%)	314 (95%)	15 (5%)	24	48
1	H	329/331 (99%)	314 (95%)	15 (5%)	24	48
All	All	2632/2648 (99%)	2511 (95%)	121 (5%)	24	48

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	116	VAL
1	A	168	SER
1	A	210	ILE
1	A	214	THR
1	A	230	CYS
1	A	257	MET
1	A	296	HIS
1	A	310	LEU
1	A	318	CYS
1	A	360	VAL
1	A	391	SER
1	A	411	VAL

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Mol	Chain	Res	Type
1	A	415	LEU
1	A	419	ARG
1	A	454	VAL
1	A	460	ASP
1	B	88	ASN
1	B	99	VAL
1	B	116	VAL
1	B	210	ILE
1	B	230	CYS
1	B	257	MET
1	B	296	HIS
1	B	360	VAL
1	B	372	SER
1	B	391	SER
1	B	415	LEU
1	B	419	ARG
1	B	451	SER
1	B	453	THR
1	B	454	VAL
1	C	88	ASN
1	C	99	VAL
1	C	116	VAL
1	C	181	SER
1	C	210	ILE
1	C	214	THR
1	C	230	CYS
1	C	257	MET
1	C	296	HIS
1	C	298	SER
1	C	360	VAL
1	C	391	SER
1	C	415	LEU
1	C	419	ARG
1	C	453	THR
1	C	454	VAL
1	D	88	ASN
1	D	99	VAL
1	D	116	VAL
1	D	156	ARG
1	D	202	VAL
1	D	214	THR
1	D	230	CYS

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Mol	Chain	Res	Type
1	D	257	MET
1	D	296	HIS
1	D	310	LEU
1	D	318	CYS
1	D	360	VAL
1	D	415	LEU
1	D	419	ARG
1	D	454	VAL
1	E	88	ASN
1	E	99	VAL
1	E	168	SER
1	E	214	THR
1	E	230	CYS
1	E	257	MET
1	E	296	HIS
1	E	310	LEU
1	E	360	VAL
1	E	391	SER
1	E	415	LEU
1	E	419	ARG
1	E	451	SER
1	E	454	VAL
1	F	88	ASN
1	F	99	VAL
1	F	116	VAL
1	F	181	SER
1	F	202	VAL
1	F	214	THR
1	F	230	CYS
1	F	257	MET
1	F	296	HIS
1	F	318	CYS
1	F	360	VAL
1	F	415	LEU
1	F	419	ARG
1	F	453	THR
1	G	88	ASN
1	G	99	VAL
1	G	116	VAL
1	G	214	THR
1	G	230	CYS
1	G	252	TYR

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Mol	Chain	Res	Type
1	G	257	MET
1	G	296	HIS
1	G	310	LEU
1	G	360	VAL
1	G	385	GLU
1	G	415	LEU
1	G	419	ARG
1	G	454	VAL
1	G	460	ASP
1	H	88	ASN
1	H	99	VAL
1	H	116	VAL
1	H	214	THR
1	H	230	CYS
1	H	257	MET
1	H	296	HIS
1	H	298	SER
1	H	318	CYS
1	H	360	VAL
1	H	391	SER
1	H	415	LEU
1	H	419	ARG
1	H	454	VAL
1	H	460	ASP

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	88	ASN
1	A	104	ASN
1	A	136	GLN
1	A	144	HIS
1	A	146	ASN
1	A	155	HIS
1	A	184	HIS
1	A	208	ASN
1	A	226	GLN
1	A	249	GLN
1	A	296	HIS
1	A	313	GLN
1	A	358	ASN
1	A	395	GLN

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Mol	Chain	Res	Type
1	B	88	ASN
1	B	104	ASN
1	B	144	HIS
1	B	146	ASN
1	B	155	HIS
1	B	184	HIS
1	B	226	GLN
1	B	249	GLN
1	B	313	GLN
1	B	358	ASN
1	B	395	GLN
1	C	88	ASN
1	C	104	ASN
1	C	136	GLN
1	C	144	HIS
1	C	146	ASN
1	C	155	HIS
1	C	184	HIS
1	C	226	GLN
1	C	249	GLN
1	C	313	GLN
1	C	381	ASN
1	C	395	GLN
1	D	88	ASN
1	D	104	ASN
1	D	136	GLN
1	D	144	HIS
1	D	146	ASN
1	D	184	HIS
1	D	208	ASN
1	D	226	GLN
1	D	249	GLN
1	D	313	GLN
1	D	325	ASN
1	D	344	ASN
1	D	395	GLN
1	D	450	ASN
1	E	88	ASN
1	E	104	ASN
1	E	136	GLN
1	E	144	HIS
1	E	146	ASN

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Mol	Chain	Res	Type
1	E	184	HIS
1	E	208	ASN
1	E	220	ASN
1	E	226	GLN
1	E	249	GLN
1	E	313	GLN
1	E	344	ASN
1	E	395	GLN
1	F	88	ASN
1	F	104	ASN
1	F	136	GLN
1	F	144	HIS
1	F	146	ASN
1	F	155	HIS
1	F	184	HIS
1	F	226	GLN
1	F	249	GLN
1	F	272	ASN
1	F	296	HIS
1	F	313	GLN
1	F	329	ASN
1	F	358	ASN
1	F	369	ASN
1	F	395	GLN
1	F	412(A)	HIS
1	G	88	ASN
1	G	95	ASN
1	G	104	ASN
1	G	136	GLN
1	G	144	HIS
1	G	146	ASN
1	G	184	HIS
1	G	249	GLN
1	G	313	GLN
1	G	344	ASN
1	G	358	ASN
1	G	395	GLN
1	H	88	ASN
1	H	104	ASN
1	H	144	HIS
1	H	146	ASN
1	H	155	HIS

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Mol	Chain	Res	Type
1	H	184	HIS
1	H	226	GLN
1	H	249	GLN
1	H	313	GLN
1	H	358	ASN
1	H	395	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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDG	F	1146	-	15,15,15	0.71	0	21,21,21	0.61	0
2	NDG	G	1146	-	15,15,15	0.82	1 (6%)	21,21,21	0.68	0
2	NDG	H	1146	-	15,15,15	0.58	0	21,21,21	0.75	0
2	NDG	D	1146	-	15,15,15	0.62	0	21,21,21	0.88	1 (4%)
4	NAG	E	1146	-	15,15,15	0.90	1 (6%)	21,21,21	0.94	0
2	NDG	B	1146	-	15,15,15	0.69	0	21,21,21	0.73	0
2	NDG	A	1146	-	15,15,15	0.73	0	21,21,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDG	C	1146	-	15,15,15	0.68	0	21,21,21	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	F	1146	-	-	2/6/26/26	0/1/1/1
2	NDG	G	1146	-	-	4/6/26/26	0/1/1/1
2	NDG	H	1146	-	-	4/6/26/26	0/1/1/1
2	NDG	D	1146	-	-	4/6/26/26	0/1/1/1
4	NAG	E	1146	-	-	2/6/26/26	0/1/1/1
2	NDG	B	1146	-	-	4/6/26/26	0/1/1/1
2	NDG	A	1146	-	-	4/6/26/26	0/1/1/1
2	NDG	C	1146	-	-	4/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1146	NAG	C1-C2	2.68	1.56	1.52
2	G	1146	NDG	C1-C2	2.00	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1146	NDG	C1-C2-N2	-2.45	107.89	110.73

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1146	NDG	O5-C5-C6-O6
4	E	1146	NAG	O5-C5-C6-O6
2	F	1146	NDG	O5-C5-C6-O6
2	C	1146	NDG	O5-C5-C6-O6
2	B	1146	NDG	O5-C5-C6-O6
2	G	1146	NDG	O5-C5-C6-O6
2	C	1146	NDG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	1146	NDG	C4-C5-C6-O6
4	E	1146	NAG	C4-C5-C6-O6
2	B	1146	NDG	C4-C5-C6-O6
2	G	1146	NDG	C4-C5-C6-O6
2	H	1146	NDG	O5-C5-C6-O6
2	H	1146	NDG	C4-C5-C6-O6
2	A	1146	NDG	O5-C5-C6-O6
2	F	1146	NDG	C4-C5-C6-O6
2	D	1146	NDG	C8-C7-N2-C2
2	D	1146	NDG	O7-C7-N2-C2
2	G	1146	NDG	C8-C7-N2-C2
2	H	1146	NDG	C8-C7-N2-C2
2	A	1146	NDG	C4-C5-C6-O6
2	G	1146	NDG	O7-C7-N2-C2
2	H	1146	NDG	O7-C7-N2-C2
2	B	1146	NDG	C8-C7-N2-C2
2	A	1146	NDG	C8-C7-N2-C2
2	B	1146	NDG	O7-C7-N2-C2
2	C	1146	NDG	C8-C7-N2-C2
2	A	1146	NDG	O7-C7-N2-C2
2	C	1146	NDG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1146	NDG	3	0
2	G	1146	NDG	3	0
2	H	1146	NDG	4	0
2	D	1146	NDG	4	0
4	E	1146	NAG	2	0
2	B	1146	NDG	2	0
2	A	1146	NDG	2	0
2	C	1146	NDG	4	0

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	B	1
1	E	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	412:GLN	C	412(A):HIS	N	1.19
1	E	412:GLN	C	412(A):HIS	N	1.08
1	C	412:GLN	C	412(A):HIS	N	1.02

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	385/387 (99%)	-1.76	0 100 100	9, 20, 36, 50	0
1	B	385/387 (99%)	-1.73	0 100 100	8, 22, 36, 58	0
1	C	385/387 (99%)	-1.74	0 100 100	10, 21, 35, 58	0
1	D	385/387 (99%)	-1.76	0 100 100	8, 20, 33, 55	0
1	E	385/387 (99%)	-1.67	0 100 100	17, 32, 44, 69	0
1	F	385/387 (99%)	-1.65	0 100 100	22, 35, 50, 64	0
1	G	385/387 (99%)	-1.71	0 100 100	14, 27, 41, 63	0
1	H	385/387 (99%)	-1.62	0 100 100	23, 37, 51, 68	0
All	All	3080/3096 (99%)	-1.71	0 100 100	8, 27, 45, 69	0

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDG	A	1146	15/15	0.98	0.08	66,69,73,74	0
2	NDG	C	1146	15/15	0.98	0.08	64,69,73,75	0
2	NDG	D	1146	15/15	0.98	0.06	60,64,65,66	0
2	NDG	F	1146	15/15	0.98	0.07	74,77,79,80	0
2	NDG	G	1146	15/15	0.98	0.06	65,67,68,69	0
2	NDG	H	1146	15/15	0.98	0.06	64,68,71,72	0
2	NDG	B	1146	15/15	0.99	0.06	65,69,71,71	0
4	NAG	E	1146	15/15	0.99	0.05	57,62,65,65	0
3	CA	B	992	1/1	1.00	0.01	21,21,21,21	0
3	CA	C	993	1/1	1.00	0.01	22,22,22,22	0
3	CA	D	994	1/1	1.00	0.01	23,23,23,23	0
3	CA	E	995	1/1	1.00	0.01	28,28,28,28	0
3	CA	F	996	1/1	1.00	0.03	46,46,46,46	0
3	CA	G	997	1/1	1.00	0.01	29,29,29,29	0
3	CA	H	998	1/1	1.00	0.01	40,40,40,40	0
3	CA	A	991	1/1	1.00	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.