



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:04 AM GMT

PDB ID : 2VPW
Title : POLYSULFIDE REDUCTASE WITH BOUND MENAQUINONE
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Deposited on : 2008-03-09
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

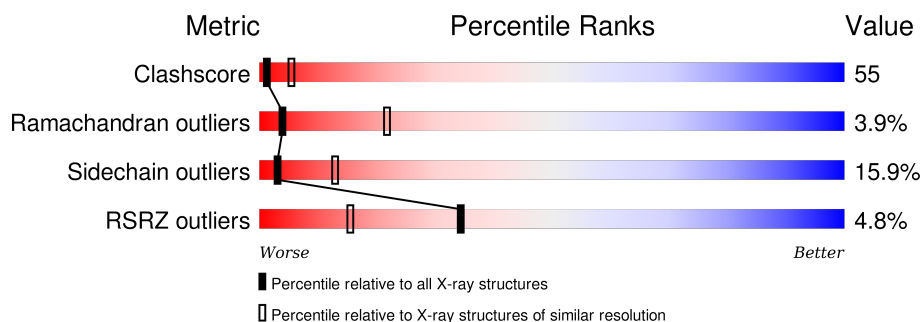
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	765	<div> <div>6%</div> <div> <div>34%</div> <div>45%</div> <div>14%</div> <div>• •</div> </div> </div>
1	E	765	<div> <div>4%</div> <div> <div>35%</div> <div>43%</div> <div>14%</div> <div>• •</div> </div> </div>
2	B	195	<div> <div>3%</div> <div> <div>42%</div> <div>44%</div> <div>12%</div> <div>• •</div> </div> </div>
2	F	195	<div> <div>2%</div> <div> <div>42%</div> <div>44%</div> <div>12%</div> <div>• •</div> </div> </div>
3	C	253	<div> <div>5%</div> <div> <div>52%</div> <div>37%</div> <div>10%</div> <div>• •</div> </div> </div>
3	G	253	<div> <div>7%</div> <div> <div>47%</div> <div>42%</div> <div>9%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	B	1194	-	-	X	-
4	SF4	B	1195	-	-	X	-
4	SF4	B	1196	-	-	X	-
4	SF4	F	1194	-	-	X	-
4	SF4	F	1195	-	-	X	-
7	MQ7	C	1252	-	-	-	X
7	MQ7	G	1251	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20223 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 THIOSULFATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			
1	E	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			

- Molecule 2 is a protein called NRFC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			
2	F	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			

- Molecule 3 is a protein called HYPOTHETICAL MEMBRANE SPANNING PROTEIN.

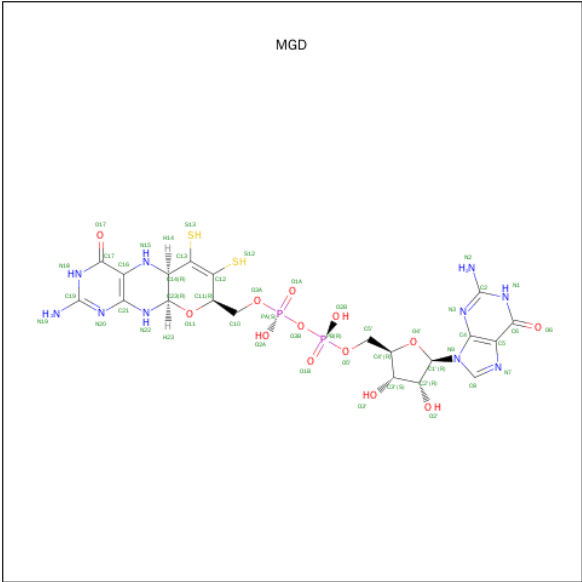
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			
3	G	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

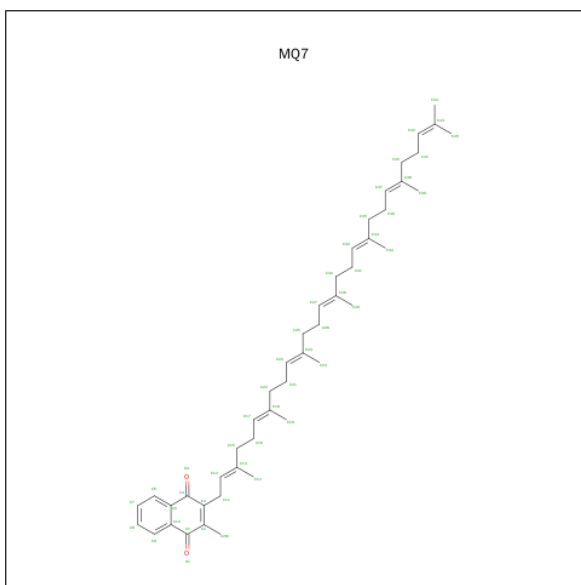


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	E	1	Total	Mo	0	0
			1	1		

- Molecule 7 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C₄₆H₆₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			15	13	2		
7	G	1	Total	C	O	0	0
			15	13	2		

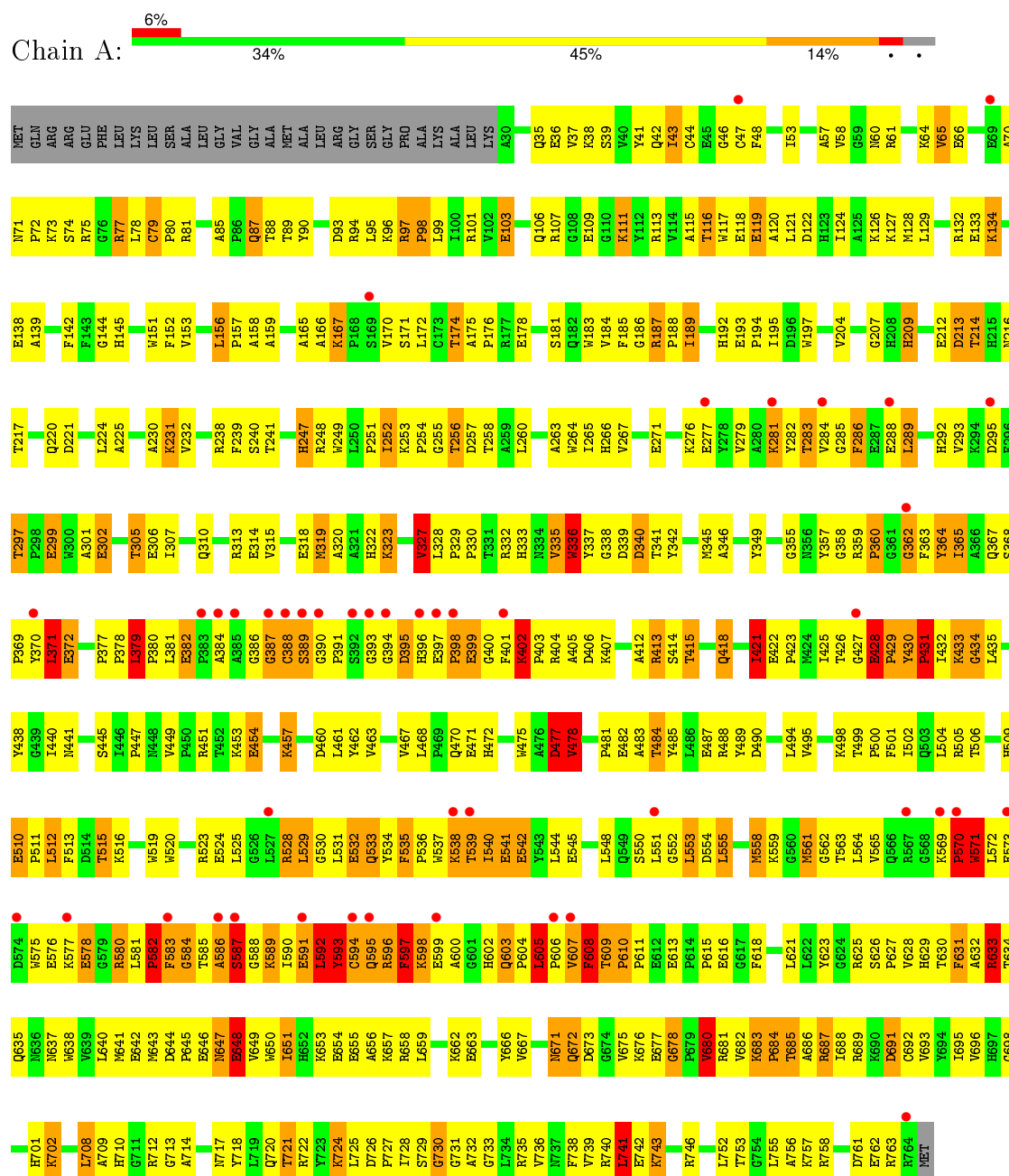
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	386	Total	O	0	0
			386	386		
8	B	149	Total	O	0	0
			149	149		
8	C	90	Total	O	0	0
			90	90		
8	E	453	Total	O	0	0
			453	453		
8	F	129	Total	O	0	0
			129	129		
8	G	78	Total	O	0	0
			78	78		

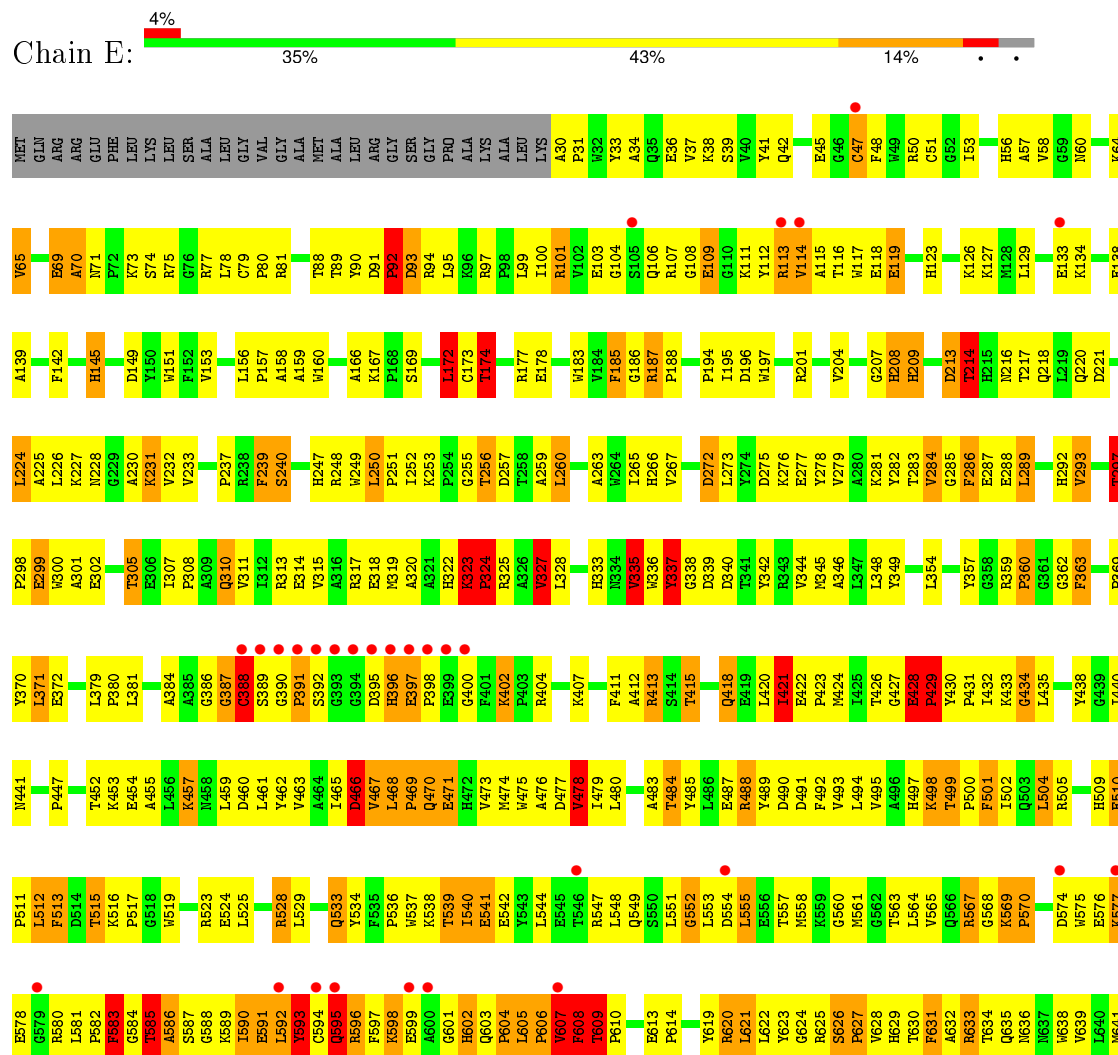
3 Residue-property plots

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

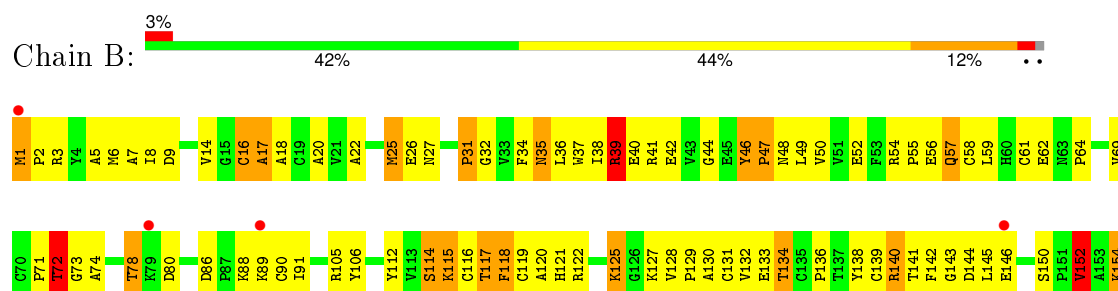
• Molecule 1: THIOSULFATE REDUCTASE



- Molecule 1: THIOSULFATE REDUCTASE



- Molecule 2: NRFC PROTEIN

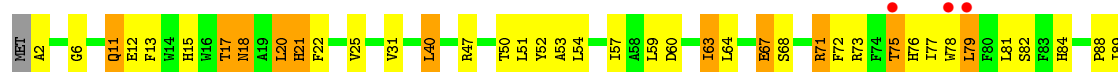




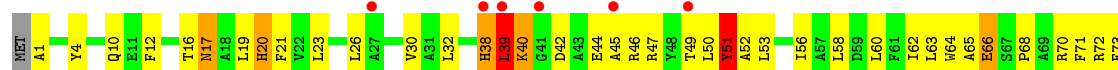
• Molecule 2: NRFC PROTEIN



• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.38Å 163.58Å 238.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.82 – 3.10 39.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.82-3.10) 96.1 (39.82-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.271 , 0.275 0.260 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 87524 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20223	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MO, SF4, MQ7, MGD

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	0.86	3/6079 (0.0%)	1.20	38/8267 (0.5%)
1	E	0.98	9/6079 (0.1%)	1.48	86/8267 (1.0%)
2	B	0.96	2/1512 (0.1%)	1.29	14/2058 (0.7%)
2	F	0.99	2/1512 (0.1%)	1.30	21/2058 (1.0%)
3	C	0.72	0/2016	0.99	9/2764 (0.3%)
3	G	0.86	2/2016 (0.1%)	1.19	14/2764 (0.5%)
All	All	0.91	18/19214 (0.1%)	1.29	182/26178 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	E	1	5
3	G	0	1
All	All	2	8

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	387	GLY	C-N	-29.46	0.66	1.34
1	A	583	PHE	C-N	21.25	1.71	1.33
1	E	323	LYS	C-N	17.11	1.66	1.34
3	G	109	LYS	C-N	-15.26	1.05	1.33
2	F	135	CYS	CB-SG	14.35	2.06	1.82
2	F	16	CYS	CB-SG	8.24	1.96	1.82
1	E	692	CYS	CB-SG	-7.57	1.69	1.82
2	B	16	CYS	CB-SG	6.93	1.94	1.82
1	E	388	CYS	C-N	6.72	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	47	CYS	CB-SG	-6.09	1.71	1.82
3	G	247	TRP	CB-CG	-5.98	1.39	1.50
2	B	90	CYS	CB-SG	-5.68	1.72	1.81
1	A	372	GLU	CB-CG	-5.41	1.41	1.52
1	E	324	PRO	N-CA	5.28	1.56	1.47
1	A	365	ILE	N-CA	5.11	1.56	1.46
1	E	685	THR	CA-C	5.10	1.66	1.52
1	E	421	ILE	C-N	-5.08	1.22	1.34
1	E	585	THR	C-N	-5.04	1.22	1.34

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	240	SER	N-CA-CB	-32.15	62.28	110.50
1	E	595	GLN	N-CA-CB	-20.28	74.10	110.60
1	E	387	GLY	O-C-N	-19.71	91.16	122.70
1	E	231	LYS	N-CA-CB	-18.54	77.23	110.60
1	E	583	PHE	N-CA-CB	-16.79	80.37	110.60
1	A	401	PHE	N-CA-C	16.58	155.76	111.00
1	E	323	LYS	C-N-CD	-15.39	86.74	120.60
1	E	593	TYR	CB-CA-C	-15.07	80.26	110.40
1	A	571	TRP	N-CA-CB	-14.90	83.78	110.60
1	E	594	CYS	N-CA-CB	-14.66	84.20	110.60
1	E	363	PHE	N-CA-CB	-13.88	85.61	110.60
1	E	421	ILE	N-CA-CB	-12.79	81.38	110.80
1	E	585	THR	CB-CA-C	12.53	145.43	111.60
3	G	109	LYS	C-N-CA	11.64	146.75	122.30
1	E	185	PHE	N-CA-C	-11.63	79.61	111.00
3	G	249	GLY	N-CA-C	11.54	141.96	113.10
1	E	324	PRO	CA-N-CD	-10.99	96.11	111.50
1	E	582	PRO	N-CA-C	10.92	140.50	112.10
3	G	207	PHE	CB-CG-CD1	-10.86	113.20	120.80
1	E	421	ILE	O-C-N	-10.65	105.66	122.70
1	A	691	ASP	CB-CA-C	-10.56	89.27	110.40
1	A	583	PHE	O-C-N	10.44	140.94	123.20
1	E	586	ALA	N-CA-CB	-10.36	95.60	110.10
1	A	570	PRO	N-CA-C	10.35	139.02	112.10
3	G	207	PHE	CB-CG-CD2	10.20	127.94	120.80
1	E	594	CYS	N-CA-C	9.94	137.84	111.00
1	E	172	LEU	CA-CB-CG	-9.88	92.57	115.30
2	F	171	THR	N-CA-C	9.86	137.62	111.00
1	A	583	PHE	CA-C-N	-9.82	96.57	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	PRO	CA-N-CD	-9.64	98.01	111.50
1	E	585	THR	O-C-N	-9.58	107.37	122.70
1	E	583	PHE	N-CA-C	9.14	135.68	111.00
1	E	478	VAL	CB-CA-C	8.89	128.28	111.40
2	F	39	ARG	NE-CZ-NH2	-8.80	115.90	120.30
3	G	207	PHE	CB-CA-C	-8.76	92.88	110.40
2	F	44	GLY	N-CA-C	8.52	134.39	113.10
3	C	52	TYR	CB-CG-CD1	-8.49	115.91	121.00
1	E	680	VAL	CB-CA-C	-8.49	95.27	111.40
1	A	570	PRO	CA-N-CD	-8.34	99.83	111.50
2	F	54	ARG	NE-CZ-NH2	-8.30	116.15	120.30
2	B	46	TYR	CB-CA-C	-8.17	94.06	110.40
2	B	46	TYR	N-CA-C	8.15	133.01	111.00
1	E	686	ALA	N-CA-C	8.12	132.93	111.00
1	A	402	LYS	O-C-N	-7.84	106.21	121.10
1	E	594	CYS	CB-CA-C	7.82	126.03	110.40
1	E	725	LEU	CA-CB-CG	7.73	133.09	115.30
3	C	88	PRO	CA-N-CD	-7.67	100.76	111.50
1	E	593	TYR	N-CA-C	-7.65	90.35	111.00
1	A	431	PRO	CA-N-CD	-7.61	100.84	111.50
1	E	659	LEU	N-CA-C	-7.57	90.55	111.00
2	B	169	GLN	N-CA-C	-7.57	90.56	111.00
1	E	710	HIS	C-N-CA	-7.56	106.43	122.30
3	G	131	GLY	N-CA-C	-7.42	94.56	113.10
1	E	590	ILE	CB-CA-C	-7.36	96.88	111.60
2	F	54	ARG	NE-CZ-NH1	7.32	123.96	120.30
3	G	114	ALA	N-CA-C	-7.31	91.26	111.00
1	E	390	GLY	N-CA-C	-7.20	95.10	113.10
1	E	327	VAL	CB-CA-C	-7.20	97.73	111.40
1	A	364	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	A	327	VAL	CB-CA-C	-7.17	97.78	111.40
3	G	240	LEU	CA-CB-CG	7.16	131.77	115.30
1	E	712	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	360	PRO	CA-N-CD	-7.01	101.69	111.50
2	B	72	THR	N-CA-C	-7.00	92.09	111.00
1	E	388	CYS	C-N-CA	-7.00	104.20	121.70
2	F	39	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	401	PHE	CB-CA-C	-6.82	96.76	110.40
2	F	152	VAL	CB-CA-C	-6.78	98.51	111.40
3	C	113	GLN	CB-CA-C	-6.71	96.98	110.40
1	E	731	GLY	N-CA-C	6.68	129.79	113.10
1	E	685	THR	C-N-CA	6.67	138.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	GLN	C-N-CA	-6.65	108.34	122.30
3	G	225	LEU	N-CA-C	-6.64	93.08	111.00
1	E	708	LEU	CA-CB-CG	6.59	130.45	115.30
1	A	608	PHE	CB-CG-CD1	-6.57	116.20	120.80
2	F	166	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	648	GLU	CB-CA-C	6.50	123.39	110.40
1	E	34	ALA	C-N-CA	6.49	137.91	121.70
2	B	72	THR	N-CA-CB	-6.48	97.98	110.30
2	F	16	CYS	C-N-CA	-6.45	105.57	121.70
1	E	214	THR	N-CA-CB	-6.44	98.07	110.30
1	A	741	LEU	CA-CB-CG	6.42	130.07	115.30
1	E	213	ASP	CB-CG-OD1	6.36	124.02	118.30
1	E	92	PRO	N-CA-C	-6.33	95.66	112.10
1	A	364	TYR	C-N-CA	6.29	137.41	121.70
2	F	43	VAL	N-CA-C	-6.25	94.14	111.00
2	F	16	CYS	N-CA-C	-6.24	94.16	111.00
1	E	323	LYS	CB-CA-C	6.20	122.80	110.40
1	A	593	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	E	501	PHE	CB-CG-CD2	6.20	125.14	120.80
1	A	648	GLU	N-CA-CB	-6.20	99.45	110.60
2	B	152	VAL	CB-CA-C	-6.16	99.69	111.40
1	E	712	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	G	248	GLN	N-CA-CB	-6.15	99.52	110.60
1	E	323	LYS	C-N-CA	5.95	147.00	122.00
1	E	467	VAL	N-CA-C	5.93	127.02	111.00
1	E	687	ARG	CB-CG-CD	-5.92	96.21	111.60
1	A	597	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	E	489	TYR	CB-CA-C	-5.88	98.64	110.40
3	C	6	GLY	N-CA-C	-5.87	98.42	113.10
2	F	46	TYR	N-CA-C	5.87	126.86	111.00
1	A	336	TRP	CB-CA-C	-5.86	98.68	110.40
1	E	592	LEU	CB-CA-C	-5.86	99.06	110.20
1	E	185	PHE	C-N-CA	-5.84	110.04	122.30
2	B	57	GLN	CA-CB-CG	-5.82	100.59	113.40
1	E	400	GLY	N-CA-C	-5.82	98.56	113.10
2	F	187	THR	N-CA-CB	-5.80	99.28	110.30
2	F	145	LEU	CA-CB-CG	5.80	128.63	115.30
1	E	619	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	E	692	CYS	CB-CA-C	-5.78	98.84	110.40
1	A	340	ASP	N-CA-C	5.75	126.52	111.00
1	E	608	PHE	CB-CG-CD1	-5.75	116.78	120.80
1	A	185	PHE	C-N-CA	-5.75	110.23	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	429	PRO	CA-N-CD	-5.75	103.46	111.50
1	E	207	GLY	N-CA-C	-5.73	98.78	113.10
1	E	478	VAL	N-CA-C	-5.72	95.55	111.00
1	E	686	ALA	N-CA-CB	-5.70	102.13	110.10
1	E	239	PHE	CB-CA-C	-5.69	99.02	110.40
3	G	4	TYR	N-CA-C	-5.69	95.64	111.00
1	E	741	LEU	CA-CB-CG	5.66	128.32	115.30
1	E	213	ASP	N-CA-C	-5.66	95.71	111.00
1	E	335	VAL	N-CA-CB	-5.66	99.06	111.50
1	A	680	VAL	CB-CA-C	-5.64	100.69	111.40
1	A	379	LEU	CA-CB-CG	5.63	128.25	115.30
1	E	335	VAL	CB-CA-C	5.63	122.10	111.40
3	G	51	TYR	N-CA-C	-5.63	95.80	111.00
1	A	421	ILE	CB-CA-C	-5.62	100.37	111.60
2	B	39	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	388	CYS	CB-CA-C	-5.62	99.17	110.40
1	A	336	TRP	CB-CG-CD2	-5.61	119.31	126.60
3	C	113	GLN	N-CA-C	5.60	126.12	111.00
3	G	130	PRO	N-CA-C	-5.60	97.55	112.10
1	A	592	LEU	N-CA-C	5.58	126.07	111.00
1	E	173	CYS	CA-CB-SG	5.55	123.99	114.00
1	E	337	TYR	N-CA-C	5.54	125.97	111.00
1	A	597	PHE	CB-CG-CD2	5.54	124.68	120.80
1	E	651	ILE	CB-CA-C	-5.54	100.53	111.60
2	F	140	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	B	134	THR	CB-CA-C	-5.52	96.70	111.60
3	C	249	GLN	C-N-CA	5.51	133.87	122.30
1	E	348	LEU	CB-CG-CD1	-5.50	101.65	111.00
1	E	33	TYR	O-C-N	-5.47	113.94	122.70
3	C	249	GLN	CB-CA-C	-5.46	99.47	110.40
1	A	582	PRO	C-N-CA	5.44	135.31	121.70
1	E	421	ILE	CA-C-N	5.42	129.13	117.20
2	F	188	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	E	736	VAL	N-CA-CB	-5.38	99.67	111.50
2	B	166	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	E	174	THR	N-CA-CB	-5.32	100.18	110.30
3	G	109	LYS	O-C-N	-5.30	114.19	123.20
1	A	371	LEU	N-CA-C	-5.29	96.70	111.00
1	E	608	PHE	C-N-CA	5.28	134.91	121.70
1	E	729	SER	C-N-CA	-5.28	111.21	122.30
1	E	710	HIS	N-CA-C	5.28	125.25	111.00
1	E	297	THR	N-CA-CB	-5.28	100.28	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	323	LYS	CA-C-N	-5.27	102.33	117.10
2	F	166	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	706	MET	N-CA-C	-5.26	96.81	111.00
1	A	319	MET	CA-CB-CG	5.25	122.23	113.30
1	E	710	HIS	CA-C-N	5.25	126.70	116.20
2	B	16	CYS	N-CA-C	-5.24	96.86	111.00
1	E	379	LEU	CA-CB-CG	5.23	127.33	115.30
2	B	35	ASN	CB-CA-C	-5.20	100.00	110.40
1	E	388	CYS	N-CA-C	5.19	125.02	111.00
2	F	188	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	364	TYR	CB-CG-CD1	5.19	124.11	121.00
2	F	16	CYS	CA-C-N	5.17	128.57	117.20
2	F	169	GLN	C-N-CA	-5.14	111.50	122.30
1	E	420	LEU	CA-C-N	5.14	128.50	117.20
1	E	335	VAL	CG1-CB-CG2	5.13	119.12	110.90
1	A	477	ASP	N-CA-C	-5.13	97.15	111.00
1	A	282	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	247	HIS	CA-CB-CG	-5.12	104.90	113.60
1	E	260	LEU	CA-CB-CG	5.10	127.03	115.30
2	F	178	LEU	CA-CB-CG	-5.07	103.64	115.30
2	B	31	PRO	C-N-CA	-5.05	111.69	122.30
1	E	429	PRO	N-CA-CB	5.04	109.35	103.30
3	C	52	TYR	CB-CG-CD2	5.04	124.03	121.00
1	E	658	ARG	NE-CZ-NH1	-5.03	117.78	120.30
3	C	84	HIS	CA-CB-CG	-5.03	105.05	113.60
1	E	363	PHE	CB-CA-C	-5.02	100.35	110.40
1	A	741	LEU	CB-CG-CD1	-5.00	102.50	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	401	PHE	CA
1	E	585	THR	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	LYS	Mainchain
1	A	571	TRP	Mainchain
1	E	185	PHE	Mainchain
1	E	387	GLY	Mainchain
1	E	388	CYS	Mainchain

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Mol	Chain	Res	Type	Group
1	E	421	ILE	Mainchain
1	E	585	THR	Mainchain
3	G	109	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5896	0	5813	769	3
1	E	5896	0	5813	694	3
2	B	1475	0	1453	168	0
2	F	1475	0	1454	145	0
3	C	1948	0	2001	164	0
3	G	1948	0	2003	182	0
4	A	8	0	0	0	0
4	B	32	0	0	7	0
4	E	8	0	0	1	0
4	F	32	0	0	6	0
5	A	94	0	44	11	0
5	E	94	0	43	18	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	C	15	0	9	18	0
7	G	15	0	9	19	0
8	A	386	0	0	96	0
8	B	149	0	0	44	0
8	C	90	0	0	10	0
8	E	453	0	0	137	0
8	F	129	0	0	33	0
8	G	78	0	0	34	0
All	All	20223	0	18642	2069	3

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 55.

All (2069) 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:A:602:HIS:CE1	1:A:606:PRO:HG3	1.28	1.63
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.45	1.45
1:A:186:GLY:HA3	1:A:583:PHE:C	1.15	1.44
2:F:135:CYS:SG	2:F:135:CYS:CB	2.06	1.43
1:A:583:PHE:C	1:A:584:GLY:N	1.71	1.43
7:C:1252:MQ7:C12	7:C:1252:MQ7:H2M1	1.36	1.40
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.08	1.39
1:E:605:LEU:CD2	1:E:605:LEU:H	1.01	1.38
3:C:171:TRP:CE3	3:C:171:TRP:O	1.79	1.34
1:E:36:GLU:O	1:E:58:VAL:CG2	1.75	1.34
1:E:602:HIS:CE1	1:E:606:PRO:HG3	1.64	1.32
1:E:477:ASP:O	1:E:478:VAL:HG23	1.16	1.32
1:A:583:PHE:CE2	1:A:588:GLY:N	1.98	1.32
3:G:207:PHE:CE2	3:G:211:LEU:HD13	1.64	1.30
1:A:591:GLU:OE2	1:A:604:PRO:HG3	1.13	1.30
1:A:604:PRO:O	1:A:606:PRO:CD	1.80	1.29
1:E:591:GLU:OE1	1:E:604:PRO:CB	1.81	1.28
1:A:604:PRO:O	1:A:606:PRO:HD2	1.25	1.28
1:E:592:LEU:CA	1:E:603:GLN:HE21	1.44	1.27
2:B:41:ARG:HH11	2:B:187:THR:CG2	1.46	1.27
1:E:477:ASP:O	1:E:478:VAL:CG2	1.80	1.27
2:B:134:THR:O	2:B:134:THR:CG2	1.76	1.27
1:E:388:CYS:HB2	1:E:593:TYR:OH	1.23	1.26
1:A:395:ASP:O	1:A:399:GLU:HB2	1.32	1.26
1:A:582:PRO:HB2	8:A:2274:HOH:O	1.08	1.24
1:A:42:GLN:O	1:A:53:ILE:HG13	1.33	1.24
1:A:602:HIS:CE1	1:A:606:PRO:CG	2.20	1.23
1:A:395:ASP:HA	1:A:399:GLU:CG	1.67	1.23
1:A:97:ARG:HH21	1:A:763:ARG:NH2	1.36	1.23
1:E:607:VAL:O	1:E:607:VAL:CG1	1.83	1.22
1:E:591:GLU:CD	1:E:604:PRO:HB3	1.57	1.22
1:A:583:PHE:HB3	1:A:584:GLY:N	1.56	1.21
1:A:184:VAL:HG23	1:A:592:LEU:CD2	1.70	1.21
1:A:186:GLY:CA	1:A:583:PHE:C	2.07	1.20
2:F:57:GLN:NE2	2:F:140:ARG:HH22	1.38	1.20
1:E:323:LYS:HD3	1:E:354:LEU:CA	1.71	1.20
1:A:284:VAL:O	1:A:590:ILE:HG22	1.35	1.20
1:E:591:GLU:OE1	1:E:604:PRO:HB3	1.04	1.20
2:B:46:TYR:HB2	8:B:2028:HOH:O	1.04	1.20
1:A:569:LYS:O	8:A:2269:HOH:O	1.60	1.20
3:G:1:ALA:HB1	8:G:2001:HOH:O	1.43	1.19
1:A:591:GLU:OE2	1:A:604:PRO:CG	1.90	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:LEU:CA	1:E:603:GLN:NE2	2.03	1.18
1:E:590:ILE:HG13	8:E:2177:HOH:O	1.45	1.16
1:E:116:THR:HG22	1:E:119:GLU:HB3	1.21	1.16
1:A:583:PHE:CB	1:A:584:GLY:N	2.06	1.16
3:C:22:PHE:O	3:C:239:ARG:NH1	1.77	1.16
1:E:605:LEU:N	1:E:605:LEU:CD2	1.72	1.16
1:A:77:ARG:NH1	2:B:138:TYR:HE2	1.43	1.16
7:C:1252:MQ7:C12	7:C:1252:MQ7:C2M	2.22	1.15
1:A:395:ASP:CA	1:A:399:GLU:HG3	1.73	1.15
2:B:46:TYR:CD1	8:B:2028:HOH:O	1.84	1.15
1:E:97:ARG:HG3	8:E:2191:HOH:O	1.43	1.15
1:E:626:SER:HB2	8:E:2348:HOH:O	1.44	1.14
1:E:608:PHE:O	8:E:2335:HOH:O	1.64	1.14
1:E:95:LEU:HD12	1:E:466:ASP:O	1.47	1.14
1:A:288:GLU:HB3	1:A:591:GLU:HG3	1.30	1.13
1:E:602:HIS:CD2	1:E:604:PRO:HD2	1.82	1.13
1:E:602:HIS:NE2	1:E:604:PRO:HD2	1.64	1.13
1:A:632:ALA:O	1:A:635:GLN:HG2	1.47	1.13
1:A:632:ALA:O	1:A:635:GLN:CG	1.96	1.13
1:E:602:HIS:HE1	1:E:606:PRO:CG	1.62	1.13
1:A:467:VAL:HB	8:A:2226:HOH:O	1.49	1.13
2:B:46:TYR:CE2	8:B:2032:HOH:O	2.01	1.13
1:E:763:ARG:HG2	8:E:2442:HOH:O	1.48	1.12
1:A:42:GLN:O	1:A:53:ILE:CG1	1.97	1.11
2:F:57:GLN:HE22	2:F:140:ARG:NH2	1.46	1.11
1:A:97:ARG:NH2	1:A:763:ARG:HH22	1.46	1.11
3:C:171:TRP:CD2	3:C:171:TRP:O	2.04	1.10
1:A:43:ILE:HG13	1:A:505:ARG:HB3	1.14	1.10
1:E:230:ALA:O	8:E:2136:HOH:O	1.66	1.10
1:A:397:GLU:HB3	1:A:398:PRO:HD3	1.11	1.10
1:E:413:ARG:HD3	8:E:2247:HOH:O	1.52	1.09
3:G:63:LEU:HD13	7:G:1251:MQ7:C2M	1.82	1.09
1:A:608:PHE:CD1	1:A:608:PHE:O	2.06	1.09
1:E:598:LYS:HD2	8:E:2329:HOH:O	1.52	1.09
1:A:583:PHE:HE2	1:A:588:GLY:N	1.39	1.08
1:E:339:ASP:HB2	1:E:607:VAL:HG11	1.32	1.08
1:A:165:ALA:O	1:A:415:THR:HG21	1.51	1.08
3:G:154:THR:CG2	3:G:238:ARG:HE	1.66	1.08
1:A:592:LEU:O	1:A:593:TYR:HB2	1.46	1.08
1:A:170:VAL:O	1:A:175:ALA:HB2	1.49	1.08
1:A:279:VAL:HG13	1:A:283:THR:HG21	1.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:THR:CG2	3:C:67:GLU:HG3	1.83	1.07
1:E:511:PRO:HB3	1:E:515:THR:HG22	1.37	1.07
2:B:134:THR:HG23	2:B:134:THR:O	1.25	1.07
3:G:63:LEU:CD1	7:G:1251:MQ7:H2M2	1.85	1.06
1:A:428:GLU:HB3	1:A:429:PRO:HD2	1.33	1.06
1:A:172:LEU:HD13	1:A:445:SER:O	1.54	1.06
1:A:763:ARG:HG2	8:A:2378:HOH:O	1.54	1.06
1:A:186:GLY:HA3	1:A:583:PHE:O	1.53	1.06
1:E:224:LEU:HD12	8:E:2130:HOH:O	1.54	1.06
1:E:112:TYR:OH	1:E:474:MET:O	1.74	1.05
1:A:599:GLU:O	8:A:2281:HOH:O	1.73	1.05
1:A:685:THR:HB	2:B:42:GLU:OE2	1.57	1.05
2:B:41:ARG:HD2	2:B:187:THR:CG2	1.85	1.05
1:E:607:VAL:O	1:E:607:VAL:HG12	1.32	1.05
2:B:41:ARG:HH11	2:B:187:THR:HG22	1.19	1.05
3:G:38:HIS:HD2	3:G:45:ALA:HB1	1.19	1.05
1:E:605:LEU:N	1:E:605:LEU:HD22	1.67	1.05
1:E:764:ARG:N	8:E:2446:HOH:O	1.89	1.05
1:E:429:PRO:HD2	8:E:2256:HOH:O	1.57	1.04
3:C:155:THR:HG22	3:C:239:ARG:HE	1.21	1.04
1:A:604:PRO:C	1:A:606:PRO:HD3	1.77	1.04
1:E:605:LEU:HD23	1:E:605:LEU:N	1.27	1.04
2:B:41:ARG:HD2	2:B:187:THR:HG21	1.35	1.04
2:F:57:GLN:NE2	2:F:140:ARG:NH2	2.05	1.04
1:E:116:THR:CG2	1:E:119:GLU:H	1.70	1.04
1:E:635:GLN:O	1:E:641:MET:CG	2.05	1.04
1:E:95:LEU:CD1	1:E:466:ASP:O	2.06	1.03
1:A:360:PRO:HD3	1:A:571:TRP:CE3	1.94	1.03
3:G:206:GLY:O	3:G:209:TYR:N	1.91	1.03
1:E:653:LYS:HD2	1:E:686:ALA:HB2	1.39	1.03
1:A:604:PRO:C	1:A:606:PRO:CD	2.28	1.02
1:A:603:GLN:HB3	1:A:604:PRO:HD3	1.34	1.02
1:E:478:VAL:HG23	8:E:2280:HOH:O	1.58	1.02
1:E:323:LYS:CD	1:E:354:LEU:HA	1.89	1.02
1:E:47:CYS:HB2	8:E:2452:HOH:O	1.57	1.02
2:B:192:VAL:HG21	8:B:2019:HOH:O	1.60	1.02
1:A:651:ILE:HD11	1:A:682:VAL:HG13	1.39	1.02
1:A:349:TYR:OH	1:A:591:GLU:O	1.78	1.02
1:A:585:THR:O	1:A:586:ALA:HB3	1.59	1.02
1:E:342:TYR:CD1	1:E:607:VAL:HB	1.93	1.02
1:A:531:LEU:O	1:A:534:TYR:O	1.76	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:207:PHE:HE2	3:G:211:LEU:HD13	0.99	1.01
1:E:428:GLU:O	1:E:430:TYR:N	1.92	1.01
1:A:580:ARG:HH11	1:A:580:ARG:CB	1.74	1.01
1:E:551:LEU:O	1:E:553:LEU:N	1.93	1.01
3:G:221:TRP:HE3	3:G:225:LEU:HD22	1.20	1.01
1:E:635:GLN:O	1:E:641:MET:HG3	1.61	1.00
3:G:111:SER:HB3	8:G:2033:HOH:O	1.60	1.00
1:A:116:THR:HG22	1:A:119:GLU:H	1.17	1.00
3:C:207:GLY:O	3:C:210:TYR:N	1.94	1.00
1:A:335:VAL:CG1	1:A:732:ALA:O	2.10	1.00
2:F:46:TYR:HB3	8:F:2035:HOH:O	1.60	1.00
1:A:591:GLU:CD	1:A:604:PRO:HG3	1.81	1.00
1:E:569:LYS:HD2	8:E:2320:HOH:O	1.60	0.99
1:E:349:TYR:OH	1:E:591:GLU:HA	1.63	0.99
1:A:400:GLY:HA3	8:A:2193:HOH:O	1.64	0.98
1:A:729:SER:O	1:A:731:GLY:N	1.97	0.97
1:A:591:GLU:HB3	1:A:603:GLN:NE2	1.79	0.97
2:B:146:GLU:HG2	8:B:2109:HOH:O	1.64	0.97
2:B:160:GLU:H	2:B:179:ASN:HD21	1.10	0.97
1:E:533:GLN:HE21	1:E:533:GLN:H	1.12	0.97
1:A:116:THR:CG2	1:A:119:GLU:H	1.76	0.97
1:E:606:PRO:O	1:E:608:PHE:N	1.97	0.97
1:A:763:ARG:HB2	8:A:2380:HOH:O	1.64	0.97
1:A:680:VAL:HG11	8:A:2310:HOH:O	1.63	0.97
1:E:36:GLU:O	1:E:58:VAL:HG22	0.79	0.97
2:F:41:ARG:HD2	2:F:187:THR:HG23	1.43	0.97
3:G:221:TRP:CE3	3:G:225:LEU:HD22	2.00	0.96
2:F:41:ARG:HD2	2:F:187:THR:CG2	1.95	0.96
1:A:397:GLU:HB3	1:A:398:PRO:CD	1.95	0.96
1:E:209:HIS:HE1	1:E:625:ARG:H	1.11	0.96
1:A:434:GLY:HA2	1:A:461:LEU:O	1.65	0.96
1:E:608:PHE:CD1	1:E:608:PHE:O	2.18	0.96
1:E:297:THR:HG22	1:E:300:TRP:H	1.30	0.96
1:A:276:LYS:HA	8:A:2148:HOH:O	1.65	0.96
2:B:72:THR:HG22	2:B:74:ALA:H	1.28	0.95
3:C:17:THR:HG21	3:C:67:GLU:HG3	1.47	0.95
1:A:184:VAL:CG2	1:A:592:LEU:CD2	2.37	0.95
1:A:653:LYS:HG3	1:A:684:PRO:O	1.66	0.95
1:A:629:HIS:ND1	1:A:634:THR:HG23	1.80	0.95
1:E:604:PRO:O	1:E:606:PRO:HD3	1.65	0.95
1:E:92:PRO:O	1:E:94:ARG:N	1.99	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:ARG:HH11	2:F:187:THR:CG2	1.80	0.94
3:G:38:HIS:CD2	3:G:45:ALA:HB1	2.01	0.94
3:C:168:LYS:HE2	8:C:2064:HOH:O	1.66	0.94
3:G:206:GLY:O	3:G:210:GLY:N	1.99	0.94
1:A:395:ASP:O	1:A:399:GLU:CB	2.16	0.94
1:E:592:LEU:HD23	1:E:603:GLN:HE22	1.30	0.94
2:F:160:GLU:H	2:F:179:ASN:HD21	1.12	0.94
1:A:42:GLN:NE2	1:A:505:ARG:HD3	1.82	0.94
1:A:519:TRP:CE2	1:A:540:ILE:HG12	2.03	0.94
2:B:25:MET:CE	2:B:25:MET:HA	1.98	0.94
3:C:108:LEU:O	3:C:110:LYS:HG2	1.66	0.94
2:B:159:ALA:O	2:F:183:LYS:HE2	1.68	0.93
1:A:77:ARG:NH1	2:B:138:TYR:CE2	2.28	0.93
1:A:335:VAL:HG11	1:A:732:ALA:O	1.66	0.93
1:E:493:VAL:HG13	8:E:2013:HOH:O	1.68	0.93
1:A:607:VAL:HG12	1:A:607:VAL:O	1.69	0.93
2:B:41:ARG:NH1	2:B:187:THR:CG2	2.32	0.93
1:E:388:CYS:SG	1:E:413:ARG:NE	2.42	0.93
2:F:65:PRO:HD2	4:F:1196:SF4:S4	2.08	0.93
3:C:140:ASN:H	3:C:140:ASN:HD22	1.16	0.93
3:C:128:LEU:HB3	8:C:2062:HOH:O	1.66	0.93
1:A:602:HIS:ND1	1:A:606:PRO:HG3	1.82	0.92
1:A:314:GLU:O	1:A:318:GLU:HG3	1.68	0.92
1:A:335:VAL:O	1:A:733:GLY:HA2	1.67	0.92
1:E:397:GLU:HB3	1:E:398:PRO:HD3	1.51	0.92
2:B:46:TYR:HD1	8:B:2028:HOH:O	1.34	0.92
1:E:323:LYS:HD3	1:E:354:LEU:HA	0.93	0.92
2:B:46:TYR:HE2	8:B:2032:HOH:O	1.43	0.92
3:G:196:GLU:HG2	8:G:2057:HOH:O	1.68	0.92
1:E:428:GLU:O	1:E:429:PRO:C	2.05	0.91
2:F:2:PRO:HD2	2:F:80:ASP:OD2	1.71	0.91
1:E:388:CYS:CB	1:E:593:TYR:OH	2.17	0.91
1:A:93:ASP:OD1	1:A:758:ARG:NH2	2.02	0.91
2:F:47:PRO:HD2	8:F:2035:HOH:O	1.70	0.91
1:E:301:ALA:O	1:E:305:THR:HB	1.71	0.91
1:A:602:HIS:ND1	1:A:606:PRO:CG	2.34	0.91
1:A:207:GLY:O	5:A:1766:MGD:O5'	1.89	0.91
1:A:42:GLN:NE2	1:A:485:TYR:O	2.04	0.91
3:G:139:ASN:HD22	3:G:139:ASN:H	1.18	0.91
1:A:429:PRO:O	1:A:430:TYR:CD2	2.23	0.91
1:E:116:THR:HG23	1:E:119:GLU:H	1.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLU:CB	1:A:398:PRO:HD3	2.01	0.90
1:E:81:ARG:HG2	1:E:628:VAL:O	1.71	0.90
3:C:53:ALA:O	3:C:57:ILE:HG13	1.71	0.89
3:G:154:THR:HG22	3:G:238:ARG:HE	1.34	0.89
2:F:146:GLU:HG2	8:F:2004:HOH:O	1.71	0.89
1:A:97:ARG:NH2	1:A:763:ARG:NH2	2.09	0.89
1:E:590:ILE:CG1	8:E:2177:HOH:O	2.06	0.89
1:E:608:PHE:CD1	1:E:608:PHE:C	2.39	0.89
3:C:172:ALA:HA	3:C:175:PRO:HG2	1.53	0.89
1:E:477:ASP:C	1:E:478:VAL:HG23	1.93	0.89
1:E:614:PRO:HG2	8:E:2341:HOH:O	1.71	0.89
1:A:70:ALA:O	8:A:2036:HOH:O	1.88	0.89
3:C:155:THR:HG21	3:C:239:ARG:HG2	1.55	0.88
1:A:632:ALA:O	1:A:635:GLN:HG3	1.73	0.88
1:A:183:TRP:CH2	1:A:596:ARG:HD3	2.06	0.88
1:E:498:LYS:HE2	8:E:2294:HOH:O	1.73	0.88
1:A:256:THR:HG21	1:A:305:THR:HA	1.56	0.88
1:A:686:ALA:HB3	8:A:2330:HOH:O	1.72	0.88
2:B:117:THR:HG21	8:B:2094:HOH:O	1.74	0.88
1:E:305:THR:HG22	1:E:307:ILE:H	1.38	0.88
1:A:183:TRP:HE1	1:A:413:ARG:HH22	1.22	0.88
1:A:97:ARG:HH21	1:A:763:ARG:HH22	0.93	0.88
1:E:116:THR:CG2	1:E:119:GLU:HB3	2.04	0.88
2:B:16:CYS:SG	2:B:16:CYS:O	2.32	0.88
1:A:284:VAL:HG23	1:A:587:SER:HB3	1.56	0.87
1:E:342:TYR:HD1	1:E:607:VAL:HB	1.36	0.87
1:A:740:ARG:NH1	8:A:2360:HOH:O	2.05	0.87
3:C:155:THR:CG2	3:C:239:ARG:HE	1.87	0.87
1:E:324:PRO:HD3	8:E:2166:HOH:O	1.73	0.87
1:E:283:THR:HG22	8:E:2178:HOH:O	1.72	0.87
1:A:580:ARG:HH11	1:A:580:ARG:HB3	1.36	0.87
1:E:510:GLU:HG3	8:E:2299:HOH:O	1.73	0.87
1:E:109:GLU:HG3	8:E:2065:HOH:O	1.73	0.87
1:A:585:THR:O	1:A:586:ALA:CB	2.21	0.87
1:A:48:PHE:CE1	1:A:145:HIS:CE1	2.63	0.87
1:A:279:VAL:HG13	1:A:283:THR:CG2	2.04	0.86
1:A:647:ASN:C	1:A:648:GLU:HG3	1.95	0.86
1:A:629:HIS:HA	1:A:634:THR:HG21	1.56	0.86
8:B:2144:HOH:O	3:C:251:LEU:HD11	1.74	0.86
1:E:116:THR:HG22	1:E:119:GLU:CB	2.04	0.86
2:F:72:THR:HG22	2:F:74:ALA:H	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HD2	1:A:220:GLN:HE22	1.38	0.86
1:A:591:GLU:O	1:A:592:LEU:HD12	1.75	0.86
1:A:183:TRP:HH2	1:A:596:ARG:HD3	1.40	0.86
2:B:41:ARG:NH1	2:B:187:THR:HG22	1.90	0.86
1:E:305:THR:CG2	1:E:307:ILE:H	1.88	0.86
1:E:421:ILE:O	1:E:421:ILE:CG2	2.22	0.86
3:G:63:LEU:HD13	7:G:1251:MQ7:C2	2.05	0.86
1:E:629:HIS:ND1	1:E:634:THR:HG23	1.91	0.86
3:C:207:GLY:O	3:C:209:TRP:N	2.09	0.86
3:C:155:THR:HG21	3:C:239:ARG:CG	2.06	0.86
1:E:494:LEU:HD22	1:E:502:ILE:HG12	1.58	0.86
1:E:453:LYS:HG2	1:E:475:TRP:CH2	2.11	0.85
1:E:488:ARG:HD3	1:E:490:ASP:OD2	1.76	0.85
1:E:388:CYS:HB2	1:E:593:TYR:HH	1.37	0.85
1:A:591:GLU:HB3	1:A:603:GLN:HE22	1.39	0.85
1:E:109:GLU:CG	8:E:2065:HOH:O	2.23	0.85
1:E:648:GLU:HG2	1:E:681:ARG:HH12	1.39	0.85
1:A:75:ARG:HH11	1:A:220:GLN:NE2	1.74	0.85
1:E:95:LEU:HD21	8:E:2275:HOH:O	1.77	0.84
1:A:393:GLY:HA3	1:A:407:LYS:CE	2.07	0.84
1:A:413:ARG:CD	1:A:413:ARG:H	1.90	0.84
2:B:57:GLN:HE22	2:B:140:ARG:HH22	1.21	0.84
1:A:138:GLU:OE2	1:A:402:LYS:HB2	1.77	0.84
1:E:89:THR:OG1	1:E:484:THR:HG21	1.77	0.84
1:A:583:PHE:HE2	1:A:588:GLY:H	1.04	0.84
1:A:170:VAL:O	1:A:175:ALA:CB	2.26	0.84
3:G:111:SER:O	3:G:115:LEU:HD12	1.77	0.84
1:A:232:VAL:H	1:A:247:HIS:HD2	1.20	0.84
3:G:207:PHE:HE2	3:G:211:LEU:CD1	1.89	0.84
1:E:256:THR:HG21	1:E:305:THR:HA	1.59	0.84
1:A:184:VAL:HG22	1:A:592:LEU:HD23	1.60	0.84
3:G:206:GLY:HA2	3:G:209:TYR:HB3	1.58	0.84
1:A:428:GLU:HB3	1:A:429:PRO:CD	2.08	0.84
1:E:277:GLU:O	1:E:281:LYS:HG2	1.77	0.84
1:A:153:VAL:HG11	1:A:167:LYS:HE2	1.60	0.84
1:A:607:VAL:HG13	1:A:609:THR:OG1	1.78	0.83
1:E:592:LEU:HA	1:E:603:GLN:HE22	1.39	0.83
1:A:651:ILE:HD11	1:A:682:VAL:CG1	2.08	0.83
3:G:63:LEU:HD11	7:G:1251:MQ7:H2M2	1.60	0.83
2:F:1:MET:HA	8:F:2001:HOH:O	1.79	0.83
1:A:393:GLY:HA3	1:A:407:LYS:HE3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:PRO:O	1:E:706:MET:HG3	1.78	0.83
1:E:438:TYR:HD2	8:E:2091:HOH:O	1.61	0.83
1:A:284:VAL:O	1:A:590:ILE:CG2	2.24	0.83
1:A:583:PHE:CA	1:A:584:GLY:N	2.42	0.83
1:A:677:GLU:O	1:A:678:GLY:O	1.97	0.83
1:E:339:ASP:CB	1:E:607:VAL:HG11	2.09	0.82
1:A:209:HIS:HE1	1:A:625:ARG:H	1.28	0.82
1:A:633:ARG:HD2	5:A:1765:MGD:O2B	1.78	0.82
1:A:595:GLN:CG	1:A:595:GLN:O	2.27	0.82
1:A:320:ALA:O	1:A:323:LYS:HG2	1.80	0.82
1:A:608:PHE:C	1:A:608:PHE:CD1	2.47	0.82
1:E:602:HIS:HE1	1:E:606:PRO:HG3	0.72	0.82
1:E:100:ILE:HG23	1:E:478:VAL:HG22	1.61	0.82
1:A:42:GLN:HE22	1:A:505:ARG:HD3	1.42	0.82
1:E:539:THR:HG22	1:E:542:GLU:CB	2.10	0.82
2:B:46:TYR:CE2	8:B:2033:HOH:O	2.33	0.82
3:C:140:ASN:H	3:C:140:ASN:ND2	1.73	0.82
1:E:75:ARG:HH11	1:E:220:GLN:HE21	1.26	0.82
3:C:173:LEU:HG	3:C:173:LEU:O	1.79	0.82
1:A:186:GLY:CA	1:A:583:PHE:O	2.22	0.81
1:A:721:THR:HG22	1:A:722:ARG:HG3	1.61	0.81
2:F:57:GLN:HE22	2:F:140:ARG:HH22	1.06	0.81
3:C:235:ALA:O	3:C:239:ARG:HG3	1.80	0.81
3:G:21:PHE:O	3:G:238:ARG:NH1	2.14	0.81
3:G:234:ALA:O	3:G:238:ARG:HG3	1.78	0.81
1:A:116:THR:HG22	1:A:119:GLU:HB3	1.59	0.81
1:A:231:LYS:HA	1:A:247:HIS:CD2	2.15	0.81
1:E:75:ARG:HH11	1:E:220:GLN:NE2	1.77	0.81
1:E:604:PRO:O	1:E:606:PRO:CD	2.28	0.81
1:E:209:HIS:HE1	1:E:625:ARG:N	1.78	0.81
1:A:629:HIS:CA	1:A:634:THR:HG21	2.10	0.81
1:A:285:GLY:O	1:A:590:ILE:HG23	1.81	0.81
1:A:395:ASP:C	1:A:399:GLU:HB2	2.00	0.81
2:B:46:TYR:CB	8:B:2028:HOH:O	1.69	0.81
3:G:206:GLY:HA2	3:G:209:TYR:CB	2.11	0.81
1:A:672:GLN:NE2	1:A:738:PHE:H	1.79	0.81
2:B:41:ARG:HH11	2:B:187:THR:HG23	1.45	0.81
1:E:311:VAL:HB	8:E:2195:HOH:O	1.79	0.81
2:B:134:THR:HG22	2:B:134:THR:O	1.76	0.80
2:B:160:GLU:H	2:B:179:ASN:ND2	1.77	0.80
1:A:595:GLN:HG3	1:A:595:GLN:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:GLU:O	1:E:70:ALA:HB3	1.79	0.80
1:A:592:LEU:O	1:A:593:TYR:CB	2.27	0.80
1:E:602:HIS:CD2	1:E:604:PRO:CD	2.64	0.80
1:E:539:THR:HG23	1:E:542:GLU:H	1.45	0.80
1:A:604:PRO:O	1:A:606:PRO:HD3	1.70	0.80
1:A:377:PRO:HG2	1:A:533:GLN:HG3	1.64	0.80
2:B:16:CYS:O	2:B:18:ALA:N	2.14	0.80
1:E:38:LYS:HG3	8:E:2020:HOH:O	1.82	0.80
1:E:685:THR:HG22	2:F:42:GLU:CD	2.02	0.80
1:A:152:PHE:O	1:A:157:PRO:HD3	1.81	0.80
3:G:222:GLN:OE1	3:G:222:GLN:HA	1.82	0.80
3:C:108:LEU:O	3:C:110:LYS:CG	2.30	0.80
1:A:605:LEU:H	1:A:605:LEU:CD2	1.95	0.80
1:E:297:THR:CG2	1:E:299:GLU:H	1.94	0.80
1:E:297:THR:HG23	1:E:299:GLU:H	1.44	0.80
1:A:519:TRP:NE1	1:A:540:ILE:HG12	1.95	0.79
1:A:427:GLY:O	1:A:428:GLU:O	1.99	0.79
1:E:592:LEU:CD2	1:E:603:GLN:HE22	1.95	0.79
1:E:88:THR:HG23	1:E:468:LEU:HD21	1.63	0.79
3:G:139:ASN:ND2	3:G:139:ASN:H	1.81	0.79
1:A:605:LEU:HD23	1:A:605:LEU:H	1.46	0.79
2:B:47:PRO:O	2:B:48:ASN:OD1	2.01	0.79
1:A:358:GLY:O	1:A:571:TRP:HA	1.81	0.79
1:A:393:GLY:HA3	1:A:407:LYS:NZ	1.96	0.79
1:A:232:VAL:H	1:A:247:HIS:CD2	1.99	0.79
2:F:117:THR:HG23	2:F:120:ALA:H	1.47	0.79
1:A:395:ASP:HA	1:A:399:GLU:HG3	0.85	0.79
2:B:25:MET:HA	2:B:25:MET:HE3	1.62	0.79
3:C:241:LEU:C	3:C:241:LEU:HD12	2.02	0.79
1:E:308:PRO:HB2	8:E:2195:HOH:O	1.83	0.79
1:A:209:HIS:O	1:A:213:ASP:HB3	1.82	0.79
1:E:717:ASN:HD22	5:E:1765:MGD:H192	1.30	0.79
1:E:511:PRO:HB3	1:E:515:THR:CG2	2.12	0.79
2:F:72:THR:HG23	2:F:89:LYS:HB3	1.65	0.78
1:E:100:ILE:HG23	1:E:478:VAL:CG2	2.13	0.78
2:F:67:VAL:HB	2:F:68:PRO:HD3	1.63	0.78
1:A:390:GLY:H	1:A:595:GLN:HE22	1.31	0.78
1:A:651:ILE:HD13	1:A:656:ALA:HB2	1.62	0.78
1:A:653:LYS:HD2	1:A:686:ALA:H	1.47	0.78
1:E:113:ARG:NH1	1:E:114:VAL:HG13	1.97	0.78
3:G:63:LEU:CD1	7:G:1251:MQ7:C2M	2.51	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:TRP:HE3	3:C:171:TRP:O	1.66	0.78
1:E:431:PRO:HD2	8:E:2259:HOH:O	1.84	0.78
2:B:47:PRO:HD3	8:B:2031:HOH:O	1.84	0.78
1:A:400:GLY:CA	8:A:2193:HOH:O	2.24	0.78
1:E:397:GLU:HB3	1:E:398:PRO:CD	2.14	0.78
1:A:186:GLY:HA3	1:A:584:GLY:N	1.99	0.78
1:A:467:VAL:HG13	8:A:2049:HOH:O	1.84	0.78
2:F:41:ARG:HH11	2:F:187:THR:HG23	1.48	0.78
1:A:390:GLY:N	1:A:595:GLN:HE22	1.82	0.77
3:C:21:HIS:HE1	3:C:64:LEU:HD11	1.49	0.77
1:A:729:SER:OG	1:A:729:SER:O	1.93	0.77
1:A:152:PHE:O	1:A:157:PRO:CD	2.33	0.77
3:C:101:LEU:O	3:C:105:LEU:HD12	1.84	0.77
3:C:21:HIS:CE1	3:C:64:LEU:HD21	2.20	0.77
2:F:40:GLU:HB2	8:F:2021:HOH:O	1.85	0.77
1:E:608:PHE:C	8:E:2335:HOH:O	2.13	0.77
1:A:429:PRO:O	1:A:430:TYR:CG	2.37	0.77
1:A:642:GLU:HG2	2:B:34:PHE:HZ	1.50	0.77
1:E:635:GLN:NE2	1:E:635:GLN:H	1.83	0.77
2:B:190:SER:HB3	3:C:252:GLY:N	1.98	0.77
1:E:589:LYS:HB3	1:E:592:LEU:HB2	1.65	0.77
1:E:589:LYS:HG2	1:E:592:LEU:HD12	1.67	0.77
1:A:360:PRO:HD3	1:A:571:TRP:CZ3	2.20	0.77
1:E:116:THR:HG21	8:E:2071:HOH:O	1.84	0.77
3:G:107:LEU:O	3:G:109:LYS:N	2.17	0.77
1:A:625:ARG:HH22	5:A:1765:MGD:H15	1.33	0.76
1:E:397:GLU:CB	1:E:398:PRO:HD3	2.15	0.76
1:A:116:THR:HG22	1:A:119:GLU:N	1.98	0.76
1:A:413:ARG:HD2	1:A:413:ARG:H	1.50	0.76
1:A:388:CYS:HA	1:A:593:TYR:OH	1.84	0.76
1:A:301:ALA:O	1:A:305:THR:HB	1.86	0.76
1:E:671:ASN:C	1:E:671:ASN:HD22	1.88	0.76
2:F:169:GLN:NE2	8:F:2106:HOH:O	2.18	0.76
1:E:551:LEU:O	1:E:553:LEU:HB2	1.86	0.76
1:E:648:GLU:HG2	1:E:681:ARG:NH1	2.00	0.76
1:E:297:THR:CG2	1:E:299:GLU:HG2	2.16	0.76
1:E:490:ASP:O	8:E:2288:HOH:O	2.03	0.76
1:A:673:ASP:OD2	1:A:721:THR:HG21	1.85	0.76
2:F:3:ARG:HG2	8:F:2003:HOH:O	1.85	0.76
3:G:76:ILE:O	3:G:80:LEU:HG	1.86	0.76
2:F:47:PRO:CD	8:F:2035:HOH:O	2.29	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:ILE:O	1:E:421:ILE:HG22	1.86	0.76
3:C:197:GLU:HG2	8:C:2074:HOH:O	1.84	0.76
1:A:174:THR:HG23	1:A:178:GLU:HG2	1.68	0.76
1:E:483:ALA:N	1:E:516:LYS:O	2.17	0.76
1:A:73:LYS:NZ	1:A:192:HIS:HD2	1.83	0.76
1:A:349:TYR:CE2	1:A:590:ILE:O	2.39	0.76
1:E:71:ASN:HD22	1:E:74:SER:H	1.31	0.75
3:C:171:TRP:O	3:C:172:ALA:HB2	1.87	0.75
1:A:510:GLU:HG3	8:A:2023:HOH:O	1.87	0.75
1:A:346:ALA:HB2	1:A:605:LEU:CD1	2.15	0.75
1:A:342:TYR:CD1	1:A:607:VAL:HB	2.22	0.75
1:E:424:MET:HG2	1:E:459:LEU:HD21	1.68	0.75
1:E:118:GLU:HG3	8:E:2305:HOH:O	1.86	0.75
1:E:139:ALA:O	1:E:433:LYS:O	2.04	0.75
3:C:21:HIS:ND1	3:C:64:LEU:HG	2.00	0.75
1:E:465:ILE:O	1:E:466:ASP:HB3	1.86	0.75
1:A:95:LEU:HD11	1:A:468:LEU:O	1.85	0.75
1:A:457:LYS:HA	8:A:2219:HOH:O	1.85	0.75
1:E:232:VAL:H	1:E:247:HIS:CD2	2.04	0.75
3:C:64:LEU:HD22	7:C:1252:MQ7:C2	2.15	0.75
1:E:591:GLU:O	1:E:591:GLU:HG3	1.85	0.75
1:E:632:ALA:O	1:E:635:GLN:NE2	2.19	0.75
1:A:166:ALA:HB2	1:A:415:THR:HG23	1.67	0.75
1:A:561:MET:O	1:A:563:THR:N	2.19	0.75
1:A:606:PRO:O	1:A:608:PHE:N	2.19	0.75
1:E:473:VAL:HG11	8:E:2275:HOH:O	1.86	0.75
1:A:388:CYS:HA	1:A:593:TYR:CE1	2.21	0.75
3:G:150:LEU:O	3:G:154:THR:HB	1.87	0.75
2:B:41:ARG:HD2	2:B:187:THR:HG23	1.68	0.75
1:E:438:TYR:CD2	8:E:2091:HOH:O	2.38	0.75
1:E:69:GLU:O	1:E:70:ALA:CB	2.34	0.75
1:A:382:GLU:HA	8:A:2184:HOH:O	1.86	0.75
1:A:184:VAL:HG23	1:A:592:LEU:HD23	0.77	0.74
1:E:607:VAL:O	1:E:607:VAL:HG13	1.83	0.74
1:E:686:ALA:HB1	8:E:2385:HOH:O	1.86	0.74
1:E:577:LYS:HE2	8:E:2321:HOH:O	1.87	0.74
1:E:762:GLU:HB2	8:E:2445:HOH:O	1.85	0.74
1:E:153:VAL:HG11	1:E:167:LYS:HE2	1.69	0.74
1:A:89:THR:OG1	1:A:484:THR:HG21	1.87	0.74
1:E:95:LEU:HD11	8:E:2275:HOH:O	1.85	0.74
2:B:44:GLY:O	2:B:49:LEU:HD13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:642:GLU:OE2	2:F:32:GLY:N	2.16	0.74
2:F:57:GLN:HE21	2:F:140:ARG:HH22	1.36	0.74
1:E:592:LEU:HD23	1:E:603:GLN:NE2	2.02	0.74
1:E:673:ASP:OD2	1:E:721:THR:CG2	2.36	0.74
2:B:44:GLY:O	2:B:49:LEU:CD1	2.35	0.74
1:E:209:HIS:CE1	1:E:625:ARG:H	2.02	0.74
3:G:63:LEU:HB3	7:G:1251:MQ7:C12	2.18	0.74
1:E:591:GLU:CD	1:E:604:PRO:CB	2.45	0.74
1:E:488:ARG:HB2	1:E:517:PRO:HB3	1.68	0.74
1:E:183:TRP:HH2	1:E:596:ARG:HD3	1.51	0.74
2:F:55:PRO:HG2	4:F:1194:SF4:S2	2.27	0.74
2:F:3:ARG:HD2	2:F:62:GLU:OE2	1.87	0.74
1:E:586:ALA:HB3	8:E:2324:HOH:O	1.87	0.74
1:A:519:TRP:CE2	1:A:540:ILE:CG1	2.70	0.74
1:E:708:LEU:HA	8:E:2407:HOH:O	1.87	0.74
3:C:18:ASN:OD1	3:C:67:GLU:OE2	2.05	0.74
1:E:386:GLY:O	1:E:388:CYS:SG	2.42	0.74
3:G:154:THR:CG2	3:G:238:ARG:NE	2.47	0.74
1:A:653:LYS:CG	1:A:684:PRO:O	2.35	0.74
1:A:578:GLU:HB3	1:A:580:ARG:HD3	1.70	0.74
1:E:186:GLY:H	1:E:583:PHE:HA	1.51	0.74
1:A:186:GLY:H	1:A:583:PHE:HA	1.53	0.74
1:E:97:ARG:NH2	1:E:763:ARG:HD2	2.02	0.74
1:E:346:ALA:N	1:E:605:LEU:HD12	2.03	0.73
3:C:222:TRP:CG	3:C:223:GLN:N	2.52	0.73
1:A:710:HIS:O	8:A:2344:HOH:O	2.06	0.73
1:E:183:TRP:CH2	1:E:596:ARG:HD3	2.23	0.73
1:A:483:ALA:HA	1:A:515:THR:CG2	2.17	0.73
3:G:154:THR:HG21	3:G:238:ARG:HG2	1.70	0.73
1:E:734:LEU:HD22	8:E:2419:HOH:O	1.87	0.73
1:A:367:GLN:HG3	8:A:2268:HOH:O	1.88	0.73
1:A:286:PHE:HA	1:A:590:ILE:HG21	1.70	0.73
1:A:183:TRP:CB	1:A:592:LEU:HD22	2.19	0.73
1:A:488:ARG:NH2	5:A:1765:MGD:O6	2.21	0.73
1:A:42:GLN:O	1:A:53:ILE:HG12	1.88	0.73
2:F:43:VAL:HG23	8:F:2121:HOH:O	1.89	0.73
1:A:581:LEU:CD1	8:A:2271:HOH:O	2.36	0.73
1:E:589:LYS:HG2	1:E:592:LEU:CD1	2.19	0.73
1:E:591:GLU:OE2	1:E:604:PRO:HG3	1.88	0.73
2:F:160:GLU:H	2:F:179:ASN:ND2	1.86	0.73
1:A:611:PRO:HB3	8:A:2136:HOH:O	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ARG:CB	1:A:580:ARG:NH1	2.49	0.73
2:F:117:THR:HG22	2:F:119:CYS:H	1.53	0.73
1:A:422:GLU:HB3	1:A:423:PRO:HD3	1.70	0.73
3:G:12:PHE:CZ	3:G:246:GLN:HG2	2.23	0.73
1:E:591:GLU:OE1	1:E:604:PRO:CA	2.37	0.73
2:B:25:MET:HE2	2:B:25:MET:HA	1.71	0.73
1:A:71:ASN:HD22	1:A:74:SER:H	1.33	0.73
3:G:51:TYR:N	8:G:2015:HOH:O	2.22	0.73
1:A:134:LYS:HE2	8:A:2077:HOH:O	1.87	0.73
1:A:581:LEU:HD11	8:A:2271:HOH:O	1.89	0.72
1:E:635:GLN:O	1:E:641:MET:HG2	1.89	0.72
1:A:672:GLN:HE22	1:A:738:PHE:H	1.34	0.72
1:E:232:VAL:H	1:E:247:HIS:HD2	1.36	0.72
3:G:206:GLY:O	3:G:209:TYR:CA	2.36	0.72
1:E:470:GLN:HG2	1:E:706:MET:SD	2.29	0.72
3:G:115:LEU:HD13	8:G:2031:HOH:O	1.89	0.72
2:F:117:THR:HG21	8:F:2076:HOH:O	1.88	0.72
1:A:339:ASP:HB3	1:A:607:VAL:HG11	1.70	0.72
1:A:153:VAL:CG1	1:A:167:LYS:HE2	2.20	0.72
1:E:575:TRP:O	1:E:578:GLU:HB2	1.87	0.72
3:C:145:ASN:HD22	3:C:145:ASN:C	1.89	0.72
1:A:484:THR:HG22	1:A:487:GLU:HG3	1.72	0.72
1:A:36:GLU:O	1:A:58:VAL:HG22	1.90	0.72
1:E:569:LYS:CD	8:E:2320:HOH:O	2.26	0.72
1:E:259:ALA:HB3	8:E:2193:HOH:O	1.89	0.72
1:A:583:PHE:CE2	1:A:587:SER:C	2.63	0.72
1:A:387:GLY:O	1:A:593:TYR:CE1	2.43	0.72
1:E:75:ARG:HD2	1:E:220:GLN:HE22	1.55	0.72
1:E:539:THR:CG2	1:E:542:GLU:H	2.03	0.72
1:A:642:GLU:HG2	2:B:34:PHE:CZ	2.24	0.72
1:A:330:PRO:HD2	8:A:2164:HOH:O	1.89	0.72
1:A:338:GLY:O	1:A:726:ASP:HA	1.90	0.72
1:A:195:ILE:HA	1:A:362:GLY:O	1.89	0.72
3:C:64:LEU:HD22	7:C:1252:MQ7:C3	2.20	0.72
2:B:46:TYR:O	8:B:2029:HOH:O	2.08	0.72
2:B:117:THR:HG22	2:B:119:CYS:N	2.04	0.72
1:E:239:PHE:HB3	1:E:687:ARG:HB3	1.71	0.72
1:E:477:ASP:O	1:E:478:VAL:HG22	1.88	0.71
3:G:206:GLY:O	3:G:207:PHE:C	2.28	0.71
1:E:116:THR:CG2	1:E:119:GLU:N	2.51	0.71
1:A:75:ARG:HH11	1:A:220:GLN:HE21	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:VAL:CB	8:E:2195:HOH:O	2.37	0.71
1:E:434:GLY:HA2	1:E:461:LEU:O	1.89	0.71
1:A:139:ALA:O	1:A:433:LYS:O	2.08	0.71
1:A:364:TYR:HB2	1:A:570:PRO:HB3	1.72	0.71
7:C:1252:MQ7:O1	8:C:2090:HOH:O	2.08	0.71
1:E:253:LYS:O	1:E:256:THR:HB	1.90	0.71
2:B:47:PRO:CD	8:B:2031:HOH:O	2.37	0.71
1:A:335:VAL:HG13	1:A:732:ALA:O	1.89	0.71
1:E:30:ALA:HB3	8:E:2002:HOH:O	1.88	0.71
1:A:305:THR:HG22	1:A:307:ILE:H	1.56	0.71
1:A:305:THR:O	1:A:306:GLU:HB2	1.89	0.71
1:A:631:PHE:O	1:A:698:GLY:HA3	1.89	0.71
1:E:81:ARG:NH1	1:E:630:THR:OG1	2.23	0.71
1:A:238:ARG:HG3	1:A:688:ILE:HD12	1.70	0.71
1:E:495:VAL:CG2	8:E:2296:HOH:O	2.39	0.71
1:E:589:LYS:NZ	8:E:2324:HOH:O	2.22	0.71
1:A:95:LEU:HD12	1:A:467:VAL:C	2.10	0.71
8:A:2014:HOH:O	2:B:25:MET:HE1	1.90	0.71
1:E:282:TYR:O	1:E:587:SER:HB3	1.91	0.71
1:A:349:TYR:HE1	1:A:605:LEU:HD21	1.56	0.71
1:E:465:ILE:O	1:E:466:ASP:CB	2.39	0.71
1:A:231:LYS:HA	1:A:247:HIS:NE2	2.05	0.71
1:E:673:ASP:OD2	1:E:721:THR:HG21	1.91	0.71
1:E:320:ALA:O	1:E:323:LYS:HB2	1.91	0.71
1:E:91:ASP:O	1:E:92:PRO:O	2.09	0.71
1:A:396:HIS:HB3	1:A:403:PRO:HB3	1.71	0.71
1:E:391:PRO:O	1:E:413:ARG:HG2	1.90	0.70
1:A:37:VAL:HG12	1:A:38:LYS:N	2.06	0.70
2:B:192:VAL:HG12	2:B:193:HIS:N	2.06	0.70
1:E:639:VAL:HG11	2:F:25:MET:HE3	1.72	0.70
1:A:183:TRP:HB2	1:A:592:LEU:HD22	1.74	0.70
1:A:292:HIS:NE2	1:A:604:PRO:HB2	2.07	0.70
1:A:603:GLN:HB3	1:A:604:PRO:CD	2.17	0.70
1:E:720:GLN:HB3	8:E:2419:HOH:O	1.92	0.70
1:A:605:LEU:HD23	1:A:605:LEU:N	2.06	0.70
1:A:583:PHE:HE2	1:A:588:GLY:CA	2.04	0.70
3:G:221:TRP:HZ3	3:G:225:LEU:HD13	1.55	0.70
1:A:336:TRP:HD1	1:A:336:TRP:H	1.35	0.70
1:E:651:ILE:HD11	1:E:682:VAL:CG1	2.22	0.70
2:F:72:THR:HG21	2:F:89:LYS:O	1.90	0.70
1:A:511:PRO:HB3	1:A:515:THR:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:HD1	1:A:607:VAL:HB	1.56	0.70
1:A:391:PRO:O	1:A:413:ARG:HB3	1.92	0.70
1:A:43:ILE:CG1	1:A:505:ARG:HB3	2.08	0.70
1:E:97:ARG:HH21	1:E:763:ARG:NH1	1.88	0.70
1:A:687:ARG:NH2	2:B:40:GLU:OE2	2.24	0.70
1:A:345:MET:HE1	1:A:605:LEU:HD22	1.73	0.69
1:E:670:VAL:HG22	1:E:676:LYS:HG3	1.73	0.69
3:G:129:TYR:CD2	3:G:130:PRO:HD3	2.26	0.69
2:F:78:THR:HG22	2:F:80:ASP:H	1.55	0.69
1:E:708:LEU:O	1:E:712:ARG:HD2	1.93	0.69
1:A:239:PHE:HB3	1:A:687:ARG:HB3	1.75	0.69
1:A:428:GLU:O	1:A:430:TYR:O	2.11	0.69
2:F:45:GLU:HB2	8:F:2028:HOH:O	1.91	0.69
1:A:293:VAL:O	1:A:293:VAL:HG13	1.92	0.69
1:E:622:LEU:HD22	5:E:1766:MGD:H8	1.73	0.69
1:A:335:VAL:HG13	1:A:732:ALA:C	2.12	0.69
1:E:267:VAL:HG22	8:E:2197:HOH:O	1.91	0.69
1:A:166:ALA:HB2	1:A:415:THR:CG2	2.21	0.69
1:A:428:GLU:O	1:A:429:PRO:C	2.27	0.69
2:B:72:THR:HG21	2:B:89:LYS:O	1.92	0.69
1:A:99:LEU:O	1:A:478:VAL:HA	1.93	0.69
1:A:635:GLN:O	1:A:709:ALA:HB2	1.92	0.69
2:F:78:THR:HG21	8:F:2058:HOH:O	1.93	0.69
1:A:127:LYS:HE2	8:A:2223:HOH:O	1.93	0.69
2:B:17:ALA:HB1	2:B:20:ALA:HB3	1.75	0.69
1:E:297:THR:HG23	1:E:299:GLU:HG2	1.75	0.69
1:E:39:SER:HG	1:E:56:HIS:HD1	1.36	0.69
1:A:53:ILE:HD12	1:A:65:VAL:HG22	1.75	0.69
1:E:511:PRO:CB	1:E:515:THR:HG22	2.19	0.69
1:A:427:GLY:O	1:A:430:TYR:O	2.10	0.69
1:E:539:THR:HG22	1:E:542:GLU:HB3	1.73	0.69
1:A:539:THR:CG2	1:A:541:GLU:HG2	2.23	0.69
1:E:174:THR:HG23	1:E:178:GLU:HG2	1.74	0.69
1:A:755:LEU:O	1:A:758:ARG:HD3	1.93	0.69
1:E:746:ARG:HG3	1:E:746:ARG:HH11	1.58	0.69
2:B:121:HIS:O	2:B:125:LYS:HE2	1.93	0.68
1:E:585:THR:OG1	1:E:589:LYS:HE3	1.92	0.68
1:E:553:LEU:HD21	1:E:557:THR:HG21	1.75	0.68
3:G:225:LEU:HB3	8:G:2069:HOH:O	1.92	0.68
1:E:305:THR:HG23	1:E:307:ILE:HG12	1.75	0.68
1:E:418:GLN:H	1:E:418:GLN:NE2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:O	1:A:648:GLU:OE2	2.12	0.68
1:A:79:CYS:HB2	1:A:80:PRO:HD2	1.74	0.68
3:C:47:ARG:NH1	3:C:107:TYR:O	2.26	0.68
2:F:88:LYS:O	3:G:74:THR:HG22	1.93	0.68
3:C:155:THR:HG22	3:C:239:ARG:NE	2.04	0.68
3:C:155:THR:CG2	3:C:239:ARG:NE	2.56	0.68
1:E:297:THR:HG21	8:E:2188:HOH:O	1.93	0.68
1:E:740:ARG:NH1	8:E:2427:HOH:O	2.26	0.68
1:A:582:PRO:C	8:A:2274:HOH:O	2.31	0.68
1:A:685:THR:HB	2:B:42:GLU:CD	2.14	0.68
3:C:64:LEU:CD2	7:C:1252:MQ7:C5	2.72	0.68
2:B:6:MET:HE3	8:B:2044:HOH:O	1.94	0.68
2:F:43:VAL:CG2	8:F:2121:HOH:O	2.42	0.68
3:C:130:TYR:CD2	3:C:131:PRO:HD3	2.29	0.68
1:E:672:GLN:NE2	1:E:738:PHE:H	1.91	0.68
1:A:256:THR:CG2	1:A:305:THR:HA	2.23	0.67
1:A:642:GLU:OE2	2:B:31:PRO:O	2.12	0.67
1:A:580:ARG:HH11	1:A:580:ARG:HB2	1.56	0.67
2:F:41:ARG:HH11	2:F:187:THR:HG22	1.59	0.67
2:B:78:THR:HG21	8:B:2068:HOH:O	1.94	0.67
1:A:121:LEU:HD13	1:A:524:GLU:HB3	1.76	0.67
1:A:293:VAL:O	1:A:293:VAL:CG1	2.41	0.67
3:C:64:LEU:HD22	7:C:1252:MQ7:C1	2.24	0.67
1:E:633:ARG:HD2	5:E:1765:MGD:O2B	1.94	0.67
3:G:38:HIS:CE1	8:G:2011:HOH:O	2.46	0.67
1:A:349:TYR:CE1	1:A:605:LEU:HD21	2.30	0.67
2:B:166:ARG:HH22	3:C:249:GLN:NE2	1.92	0.67
1:A:495:VAL:HG13	8:A:2019:HOH:O	1.94	0.67
2:B:72:THR:HG23	2:B:89:LYS:HB3	1.76	0.67
1:A:721:THR:OG1	8:A:2351:HOH:O	2.12	0.67
1:E:345:MET:HB2	1:E:605:LEU:HD13	1.76	0.67
1:E:606:PRO:CD	1:E:607:VAL:H	2.07	0.67
8:E:2385:HOH:O	2:F:49:LEU:HD11	1.95	0.67
2:F:194:HIS:N	8:F:2128:HOH:O	2.26	0.67
3:G:63:LEU:CD1	7:G:1251:MQ7:C2	2.73	0.67
1:A:314:GLU:HG2	8:A:2161:HOH:O	1.95	0.67
1:A:345:MET:HE1	1:A:605:LEU:CD2	2.25	0.67
1:E:318:GLU:O	1:E:322:HIS:HD2	1.79	0.67
1:E:539:THR:HG22	1:E:542:GLU:HB2	1.77	0.67
1:A:647:ASN:H	1:A:647:ASN:HD22	1.42	0.66
1:A:75:ARG:NH1	1:A:220:GLN:NE2	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:TYR:OH	1:E:509:HIS:HE1	1.78	0.66
1:E:116:THR:HG22	1:E:119:GLU:H	1.50	0.66
2:B:166:ARG:NH2	3:C:249:GLN:NE2	2.43	0.66
3:C:17:THR:CG2	3:C:67:GLU:CG	2.68	0.66
1:A:346:ALA:HB2	1:A:605:LEU:HD13	1.75	0.66
3:C:171:TRP:CG	3:C:171:TRP:O	2.47	0.66
1:A:471:GLU:HG2	1:A:471:GLU:O	1.96	0.66
3:G:208:TRP:HA	3:G:208:TRP:CE3	2.31	0.66
1:A:603:GLN:CB	1:A:604:PRO:HD3	2.19	0.66
1:A:607:VAL:O	1:A:607:VAL:CG1	2.41	0.66
1:A:204:VAL:HB	1:A:328:LEU:HG	1.78	0.66
1:E:679:PRO:HG2	1:E:747:PRO:HB3	1.78	0.66
1:A:708:LEU:HD22	1:A:755:LEU:HB3	1.77	0.66
8:B:2027:HOH:O	3:C:2:ALA:HB1	1.95	0.66
1:A:630:THR:H	1:A:634:THR:HG21	1.60	0.66
2:F:193:HIS:HB2	8:F:2129:HOH:O	1.95	0.66
2:B:57:GLN:HE22	2:B:140:ARG:NH2	1.92	0.65
3:C:241:LEU:C	3:C:241:LEU:CD1	2.63	0.65
1:A:413:ARG:NE	1:A:413:ARG:H	1.93	0.65
3:G:105:LEU:HB3	8:G:2011:HOH:O	1.96	0.65
1:E:642:GLU:HG3	8:E:2436:HOH:O	1.96	0.65
1:A:594:CYS:O	1:A:598:LYS:HG3	1.95	0.65
1:E:604:PRO:C	1:E:605:LEU:CD2	2.62	0.65
3:C:59:LEU:O	3:C:63:ILE:HG23	1.96	0.65
1:E:479:ILE:O	1:E:480:LEU:HD23	1.97	0.65
2:B:3:ARG:HG2	8:B:2001:HOH:O	1.96	0.65
1:A:558:MET:HE2	1:A:558:MET:HA	1.78	0.65
1:A:37:VAL:HG13	1:A:57:ALA:O	1.97	0.65
1:E:588:GLY:HA3	8:E:2173:HOH:O	1.96	0.65
1:A:345:MET:HG2	1:A:592:LEU:HD21	1.79	0.65
1:A:602:HIS:HE1	1:A:606:PRO:HG3	0.87	0.65
2:B:2:PRO:HB3	2:B:144:ASP:CG	2.16	0.65
3:G:39:LEU:HD13	3:G:116:ALA:HB3	1.79	0.65
2:B:91:ILE:HD12	7:C:1252:MQ7:H2M2	1.79	0.65
1:A:467:VAL:CG2	8:A:2226:HOH:O	2.44	0.65
3:G:105:LEU:HG	8:G:2031:HOH:O	1.94	0.65
1:A:107:ARG:HG2	1:A:475:TRP:O	1.96	0.65
1:E:669:LEU:CD2	1:E:741:LEU:HD22	2.26	0.65
2:B:88:LYS:O	3:C:75:THR:HG22	1.95	0.65
2:F:164:VAL:HG22	2:F:173:PRO:HB2	1.79	0.65
1:A:689:ARG:NH2	1:A:691:ASP:OD2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:GLN:NE2	1:E:314:GLU:OE2	2.30	0.65
1:A:39:SER:HB2	8:A:2005:HOH:O	1.97	0.65
3:G:189:TYR:O	3:G:192:THR:HB	1.97	0.65
1:A:252:ILE:CD1	1:A:256:THR:HG22	2.26	0.65
2:B:27:ASN:HD21	2:B:121:HIS:CE1	2.15	0.65
1:A:540:ILE:O	1:A:544:LEU:HG	1.97	0.64
1:E:647:ASN:HD21	1:E:714:ALA:H	1.45	0.64
1:A:319:MET:CE	1:A:328:LEU:HD11	2.26	0.64
1:A:428:GLU:O	1:A:430:TYR:N	2.31	0.64
3:G:115:LEU:HB3	8:G:2031:HOH:O	1.97	0.64
2:B:117:THR:CG2	2:B:120:ALA:H	2.10	0.64
2:B:117:THR:HB	8:B:2010:HOH:O	1.96	0.64
1:A:120:ALA:HB3	8:A:2067:HOH:O	1.97	0.64
1:A:602:HIS:HE1	1:A:606:PRO:CG	1.81	0.64
1:E:345:MET:CB	1:E:605:LEU:HD13	2.27	0.64
2:B:57:GLN:NE2	2:B:140:ARG:HH22	1.92	0.64
1:A:382:GLU:HB3	8:A:2185:HOH:O	1.97	0.64
1:A:519:TRP:CZ2	1:A:540:ILE:HG13	2.32	0.64
1:E:649:VAL:HG13	1:E:695:ILE:CG2	2.27	0.64
1:A:81:ARG:HH21	1:A:214:THR:HG22	1.61	0.64
1:A:558:MET:CE	1:A:561:MET:SD	2.86	0.64
1:A:109:GLU:OE2	1:A:111:LYS:HE2	1.97	0.64
1:E:100:ILE:HG12	1:E:478:VAL:HG22	1.78	0.64
1:A:152:PHE:O	1:A:157:PRO:CG	2.45	0.64
1:A:39:SER:OG	8:A:2004:HOH:O	2.15	0.64
1:A:635:GLN:HG3	1:A:701:HIS:NE2	2.13	0.64
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.12	0.64
1:E:591:GLU:O	1:E:603:GLN:NE2	2.31	0.64
3:G:63:LEU:CD2	7:G:1251:MQ7:C1	2.76	0.64
2:B:36:LEU:HD11	8:B:2103:HOH:O	1.98	0.64
1:A:53:ILE:HD12	1:A:65:VAL:CG2	2.28	0.64
3:C:207:GLY:HA2	3:C:210:TYR:HB3	1.80	0.64
1:E:204:VAL:HB	1:E:328:LEU:HG	1.79	0.64
2:F:166:ARG:HH22	3:G:248:GLN:HE21	1.46	0.64
1:E:391:PRO:HG3	1:E:411:PHE:CZ	2.33	0.64
1:E:77:ARG:NE	8:E:2044:HOH:O	2.31	0.63
1:E:418:GLN:H	1:E:418:GLN:HE21	1.44	0.63
3:G:206:GLY:CA	3:G:209:TYR:CB	2.76	0.63
1:E:671:ASN:ND2	1:E:673:ASP:H	1.96	0.63
2:B:142:PHE:C	2:B:152:VAL:HG22	2.18	0.63
1:A:583:PHE:CE2	1:A:588:GLY:CA	2.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:VAL:HG12	2:B:193:HIS:H	1.62	0.63
1:E:687:ARG:NH2	2:F:40:GLU:OE2	2.31	0.63
1:A:122:ASP:OD1	1:A:528:ARG:NH1	2.31	0.63
3:C:64:LEU:HD21	7:C:1252:MQ7:C5	2.28	0.63
1:E:279:VAL:O	1:E:283:THR:HB	1.97	0.63
1:A:336:TRP:O	1:A:735:ARG:HB2	1.97	0.63
2:B:57:GLN:O	2:B:58:CYS:C	2.36	0.63
1:E:311:VAL:CG2	8:E:2195:HOH:O	2.46	0.63
1:E:339:ASP:HB2	1:E:607:VAL:CG1	2.19	0.63
2:B:114:SER:O	2:B:115:LYS:HB3	1.98	0.63
3:G:196:GLU:CD	3:G:196:GLU:H	2.00	0.63
1:E:108:GLY:HA3	8:E:2063:HOH:O	1.98	0.63
3:G:207:PHE:O	3:G:211:LEU:N	2.32	0.63
1:E:323:LYS:CD	1:E:354:LEU:CA	2.64	0.63
1:E:428:GLU:OE1	1:E:428:GLU:HA	1.97	0.63
3:C:140:ASN:HD22	3:C:140:ASN:N	1.93	0.63
1:A:384:ALA:N	8:A:2186:HOH:O	2.22	0.63
3:G:206:GLY:C	3:G:209:TYR:H	2.01	0.63
3:C:128:LEU:HD22	8:C:2062:HOH:O	1.99	0.63
1:A:633:ARG:CD	5:A:1765:MGD:O2B	2.47	0.62
3:C:239:ARG:NH2	8:C:2083:HOH:O	2.29	0.62
1:E:632:ALA:C	1:E:635:GLN:NE2	2.51	0.62
1:E:297:THR:HG22	1:E:300:TRP:N	2.10	0.62
1:A:81:ARG:HE	1:A:214:THR:HG22	1.64	0.62
2:B:117:THR:HG22	2:B:119:CYS:H	1.64	0.62
1:E:539:THR:HG23	1:E:541:GLU:HG2	1.81	0.62
1:E:605:LEU:HD23	1:E:605:LEU:H	0.45	0.62
1:A:519:TRP:CD1	1:A:540:ILE:HG21	2.34	0.62
1:A:286:PHE:CA	1:A:590:ILE:HG21	2.29	0.62
1:E:256:THR:CG2	1:E:305:THR:HA	2.30	0.62
1:E:590:ILE:O	1:E:592:LEU:HG	2.00	0.62
1:E:591:GLU:OE2	1:E:604:PRO:HB3	1.99	0.62
1:E:553:LEU:CD2	1:E:557:THR:HG21	2.29	0.62
1:A:426:THR:HG23	8:A:2051:HOH:O	1.98	0.62
3:G:63:LEU:HD22	7:G:1251:MQ7:C4	2.30	0.62
3:C:197:GLU:CD	3:C:197:GLU:H	2.03	0.62
1:A:483:ALA:CA	1:A:515:THR:HG23	2.30	0.62
1:E:549:GLN:HG3	8:E:2311:HOH:O	2.00	0.62
1:A:609:THR:O	1:A:610:PRO:C	2.38	0.62
3:C:172:ALA:CA	3:C:175:PRO:HG2	2.29	0.62
1:E:116:THR:HG23	1:E:119:GLU:N	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:ILE:O	1:E:421:ILE:HG23	2.00	0.62
1:E:598:LYS:HB3	1:E:599:GLU:OE1	2.00	0.61
2:F:41:ARG:HD2	2:F:187:THR:HG21	1.78	0.61
1:A:630:THR:N	1:A:634:THR:HG21	2.15	0.61
1:E:396:HIS:CE1	1:E:404:ARG:H	2.18	0.61
1:A:186:GLY:C	1:A:583:PHE:O	2.38	0.61
1:E:470:GLN:NE2	8:E:2276:HOH:O	2.33	0.61
3:G:63:LEU:HD22	7:G:1251:MQ7:C5	2.30	0.61
1:E:651:ILE:HD13	1:E:656:ALA:HB2	1.81	0.61
2:B:46:TYR:CD2	8:B:2033:HOH:O	2.52	0.61
1:A:151:TRP:O	1:A:156:LEU:HB2	1.99	0.61
1:E:208:HIS:HE1	1:E:218:GLN:NE2	1.98	0.61
1:A:388:CYS:HA	1:A:593:TYR:CZ	2.35	0.61
1:A:380:PRO:HD3	1:A:534:TYR:OH	2.00	0.61
1:A:534:TYR:O	1:A:535:PHE:HB2	1.99	0.61
2:F:72:THR:HG22	2:F:74:ALA:N	2.11	0.61
1:A:299:GLU:OE2	1:A:313:ARG:NH2	2.22	0.61
1:E:81:ARG:HE	1:E:214:THR:HG22	1.65	0.61
1:A:81:ARG:HE	1:A:214:THR:CG2	2.14	0.61
1:E:724:LYS:HG2	8:E:2424:HOH:O	1.99	0.61
1:E:647:ASN:H	1:E:647:ASN:HD22	1.46	0.61
1:A:483:ALA:HA	1:A:515:THR:HG21	1.82	0.61
1:E:194:PRO:O	1:E:363:PHE:HA	2.00	0.61
1:E:346:ALA:H	1:E:605:LEU:HD12	1.64	0.61
1:E:345:MET:HB3	1:E:605:LEU:CD1	2.31	0.61
2:B:2:PRO:HB3	2:B:144:ASP:HB2	1.83	0.61
3:G:220:PHE:HD1	8:G:2065:HOH:O	1.84	0.61
3:G:207:PHE:CD2	3:G:207:PHE:C	2.73	0.61
3:G:221:TRP:HD1	8:G:2032:HOH:O	1.84	0.61
1:E:109:GLU:HG2	8:E:2065:HOH:O	1.94	0.61
1:E:396:HIS:HB3	1:E:407:LYS:HE3	1.83	0.61
1:E:79:CYS:HB2	1:E:80:PRO:HD2	1.83	0.61
1:A:421:ILE:HG22	1:A:421:ILE:O	2.00	0.61
1:E:93:ASP:OD1	1:E:758:ARG:NH2	2.34	0.61
1:E:299:GLU:OE2	1:E:313:ARG:NH2	2.22	0.61
1:A:658:ARG:C	1:A:659:LEU:O	2.33	0.61
1:E:129:LEU:O	1:E:133:GLU:HG2	2.00	0.61
1:E:519:TRP:CE2	1:E:540:ILE:CG1	2.84	0.61
1:A:336:TRP:CD1	1:A:336:TRP:N	2.60	0.60
1:A:79:CYS:CB	1:A:80:PRO:HD2	2.31	0.60
2:B:57:GLN:NE2	8:B:2044:HOH:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:NH2	1:A:367:GLN:NE2	2.49	0.60
1:A:36:GLU:HG2	1:A:36:GLU:O	2.01	0.60
3:G:156:LEU:HD12	3:G:178:LEU:HD13	1.83	0.60
1:A:558:MET:HE2	1:A:561:MET:SD	2.41	0.60
1:E:622:LEU:HD22	8:E:2426:HOH:O	2.00	0.60
1:E:474:MET:HE2	8:E:2068:HOH:O	2.00	0.60
1:A:523:ARG:HG3	1:A:535:PHE:HB3	1.83	0.60
1:A:232:VAL:N	1:A:247:HIS:HD2	1.95	0.60
1:A:319:MET:HE1	1:A:328:LEU:HD11	1.81	0.60
3:C:67:GLU:O	3:C:67:GLU:HG2	2.01	0.60
1:A:193:GLU:HG2	8:A:2118:HOH:O	2.02	0.60
1:E:88:THR:HG21	1:E:467:VAL:HG11	1.81	0.60
1:A:519:TRP:CZ2	1:A:540:ILE:CG1	2.85	0.60
1:A:422:GLU:HB2	8:A:2201:HOH:O	2.00	0.60
2:B:32:GLY:N	8:B:2011:HOH:O	2.33	0.60
3:G:206:GLY:CA	3:G:209:TYR:HB3	2.31	0.60
1:A:678:GLY:HA3	8:A:2328:HOH:O	2.01	0.60
1:A:134:LYS:CE	8:A:2077:HOH:O	2.46	0.60
1:A:364:TYR:HB2	1:A:570:PRO:CB	2.32	0.60
1:A:295:ASP:HB2	8:A:2156:HOH:O	2.01	0.60
2:B:140:ARG:NH2	8:B:2044:HOH:O	2.34	0.60
1:A:320:ALA:O	1:A:323:LYS:CG	2.49	0.60
1:E:568:GLY:O	1:E:570:PRO:HD3	2.01	0.60
1:A:671:ASN:HD21	1:A:675:VAL:H	1.50	0.60
3:C:207:GLY:C	3:C:209:TRP:N	2.54	0.60
3:C:21:HIS:CE1	3:C:64:LEU:HD11	2.36	0.60
1:A:42:GLN:CD	1:A:505:ARG:HB2	2.22	0.60
3:G:30:VAL:HG12	3:G:52:ALA:HB2	1.84	0.60
1:E:512:LEU:O	1:E:515:THR:HB	2.02	0.59
1:A:427:GLY:C	1:A:428:GLU:O	2.41	0.59
1:A:602:HIS:ND1	1:A:606:PRO:HG2	2.15	0.59
1:E:635:GLN:NE2	1:E:635:GLN:N	2.48	0.59
1:A:415:THR:HG22	8:A:2200:HOH:O	2.03	0.59
1:A:239:PHE:O	1:A:687:ARG:HD2	2.02	0.59
1:E:239:PHE:CB	1:E:687:ARG:HB3	2.32	0.59
1:E:608:PHE:HD1	1:E:608:PHE:O	1.81	0.59
1:A:629:HIS:NE2	1:A:644:ASP:O	2.29	0.59
1:E:689:ARG:NH2	1:E:691:ASP:OD2	2.23	0.59
3:C:151:LEU:O	3:C:155:THR:HB	2.03	0.59
1:E:281:LYS:HG3	1:E:282:TYR:CE1	2.38	0.59
2:B:121:HIS:O	2:B:125:LYS:CE	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:2074:HOH:O	3:C:82:SER:HB3	2.02	0.59
1:A:536:PRO:HG2	1:A:537:TRP:H	1.68	0.59
1:E:551:LEU:O	1:E:552:GLY:C	2.41	0.59
1:A:285:GLY:C	1:A:590:ILE:HG23	2.23	0.59
1:E:391:PRO:HG2	1:E:392:SER:H	1.66	0.59
1:E:467:VAL:HG12	1:E:468:LEU:HG	1.83	0.59
1:E:632:ALA:C	1:E:635:GLN:HE22	2.06	0.59
2:F:41:ARG:CD	2:F:187:THR:HG23	2.27	0.59
1:E:359:ARG:HD3	8:E:2220:HOH:O	2.02	0.59
1:A:346:ALA:HB2	1:A:605:LEU:HD12	1.85	0.59
1:A:608:PHE:HD1	1:A:608:PHE:O	1.82	0.59
1:E:342:TYR:HD1	1:E:607:VAL:CB	2.11	0.59
2:B:72:THR:CG2	2:B:74:ALA:H	2.09	0.59
2:B:2:PRO:HB3	2:B:144:ASP:CB	2.32	0.59
1:E:315:VAL:HG12	1:E:319:MET:HE3	1.85	0.59
2:F:166:ARG:HH22	3:G:248:GLN:NE2	2.00	0.59
1:E:81:ARG:HE	1:E:214:THR:CG2	2.16	0.59
1:E:112:TYR:CZ	1:E:474:MET:O	2.55	0.59
3:C:171:TRP:O	3:C:172:ALA:CB	2.49	0.59
1:E:81:ARG:HD2	1:E:630:THR:OG1	2.03	0.59
2:F:2:PRO:HB3	2:F:144:ASP:CG	2.22	0.59
1:A:73:LYS:NZ	1:A:192:HIS:CD2	2.68	0.59
3:G:226:ALA:HB3	3:G:227:PRO:HD3	1.85	0.59
3:C:64:LEU:HD22	7:C:1252:MQ7:C4	2.33	0.59
1:E:273:LEU:O	1:E:323:LYS:NZ	2.26	0.59
2:B:86:ASP:OD1	2:B:88:LYS:HB2	2.03	0.59
3:G:132:LEU:O	3:G:136:VAL:HB	2.03	0.59
1:A:357:TYR:HA	1:A:363:PHE:HB2	1.85	0.58
1:E:397:GLU:CG	1:E:398:PRO:HD3	2.33	0.58
3:G:66:GLU:HG2	3:G:66:GLU:O	2.03	0.58
1:A:519:TRP:CG	1:A:540:ILE:HG21	2.37	0.58
1:A:335:VAL:HG13	1:A:733:GLY:HA2	1.84	0.58
1:A:367:GLN:O	1:A:500:PRO:HG3	2.02	0.58
1:A:604:PRO:C	1:A:606:PRO:HD2	2.01	0.58
3:C:155:THR:CG2	3:C:239:ARG:CG	2.79	0.58
3:G:46:ARG:HG3	8:G:2014:HOH:O	2.02	0.58
3:C:64:LEU:CD2	7:C:1252:MQ7:C4	2.80	0.58
1:E:81:ARG:NE	1:E:214:THR:HG22	2.18	0.58
1:A:48:PHE:HE1	1:A:145:HIS:CE1	2.21	0.58
3:G:144:ASN:OD1	3:G:192:THR:CG2	2.52	0.58
1:E:345:MET:CB	1:E:605:LEU:CD1	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:ILE:HA	1:E:424:MET:SD	2.44	0.58
1:A:457:LYS:HD3	8:A:2221:HOH:O	2.03	0.58
3:C:112:SER:O	3:C:113:GLN:HG2	2.03	0.58
1:E:209:HIS:CG	5:E:1766:MGD:H5'1	2.39	0.58
1:A:428:GLU:OE2	1:A:428:GLU:HA	1.96	0.58
3:C:68:SER:O	3:C:71:ARG:HB3	2.04	0.58
1:A:591:GLU:CB	1:A:603:GLN:HE22	2.13	0.58
1:E:153:VAL:CG1	1:E:167:LYS:HE2	2.34	0.58
1:A:483:ALA:HA	1:A:515:THR:HG23	1.84	0.58
3:C:248:TRP:CE2	3:C:250:GLY:HA3	2.38	0.58
3:C:207:GLY:O	3:C:208:PHE:C	2.39	0.58
1:A:605:LEU:N	1:A:606:PRO:CD	2.62	0.58
1:A:708:LEU:N	1:A:708:LEU:HD23	2.19	0.58
3:G:49:THR:HG21	8:G:2011:HOH:O	2.03	0.58
3:C:140:ASN:ND2	3:C:140:ASN:N	2.48	0.58
1:A:512:LEU:O	1:A:515:THR:HB	2.04	0.58
1:A:525:LEU:O	1:A:529:LEU:HG	2.04	0.58
2:B:122:ARG:HB3	2:B:127:LYS:HB2	1.84	0.58
1:E:454:GLU:HG2	8:E:2271:HOH:O	2.04	0.58
1:A:583:PHE:CZ	1:A:587:SER:HA	2.39	0.57
3:C:89:ILE:HD12	7:C:1252:MQ7:C6	2.34	0.57
3:G:63:LEU:HD22	7:G:1251:MQ7:C10	2.34	0.57
1:A:80:PRO:HD3	2:B:18:ALA:HB2	1.85	0.57
1:E:684:PRO:O	1:E:685:THR:C	2.41	0.57
1:A:388:CYS:O	1:A:391:PRO:HD3	2.04	0.57
1:A:583:PHE:HB2	1:A:584:GLY:N	2.13	0.57
2:B:160:GLU:N	2:B:179:ASN:HD21	1.92	0.57
1:A:75:ARG:HD2	1:A:220:GLN:NE2	2.13	0.57
1:A:96:LYS:HB3	1:A:513:PHE:HB3	1.86	0.57
1:A:519:TRP:CD2	1:A:540:ILE:HG23	2.38	0.57
1:E:95:LEU:CD2	8:E:2275:HOH:O	2.45	0.57
3:G:76:ILE:HG12	3:G:80:LEU:HD11	1.86	0.57
1:A:388:CYS:HA	1:A:593:TYR:HE1	1.65	0.57
1:A:345:MET:CE	1:A:592:LEU:HD11	2.34	0.57
1:A:607:VAL:HG13	1:A:609:THR:CB	2.33	0.57
2:F:67:VAL:CB	2:F:68:PRO:HD3	2.34	0.57
1:E:519:TRP:NE1	1:E:540:ILE:HG12	2.19	0.57
2:F:115:LYS:HG3	2:F:116:CYS:O	2.05	0.57
1:E:601:GLY:HA2	8:E:2332:HOH:O	2.04	0.57
1:E:93:ASP:O	1:E:469:PRO:HD3	2.04	0.57
2:F:117:THR:HG22	2:F:119:CYS:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:VAL:O	1:A:453:LYS:HG3	2.04	0.57
2:F:39:ARG:HD2	2:F:56:GLU:OE2	2.03	0.57
1:A:454:GLU:HG2	8:A:2099:HOH:O	2.04	0.57
2:B:47:PRO:CG	8:B:2031:HOH:O	2.53	0.57
1:A:558:MET:HE1	1:A:561:MET:SD	2.45	0.57
1:A:595:GLN:HA	1:A:598:LYS:HD2	1.87	0.57
1:E:285:GLY:HA3	1:E:592:LEU:HD11	1.85	0.57
3:C:140:ASN:O	3:C:142:PRO:HD3	2.04	0.57
1:E:519:TRP:CE2	1:E:540:ILE:HG13	2.39	0.57
3:G:172:LEU:O	3:G:176:ARG:HG3	2.05	0.57
1:A:183:TRP:HB3	1:A:592:LEU:O	2.05	0.57
1:E:342:TYR:CE1	1:E:607:VAL:HB	2.38	0.57
1:E:533:GLN:HE21	1:E:533:GLN:N	1.93	0.57
3:C:17:THR:HG22	3:C:18:ASN:N	2.20	0.57
1:E:686:ALA:CB	8:E:2385:HOH:O	2.47	0.57
1:A:113:ARG:NH2	8:A:2065:HOH:O	2.37	0.57
1:A:627:PRO:HB2	2:B:16:CYS:HA	1.87	0.57
1:A:548:LEU:HD13	1:A:558:MET:HB2	1.87	0.57
3:C:21:HIS:CE1	3:C:64:LEU:CD2	2.88	0.56
1:E:466:ASP:HA	5:E:1765:MGD:N2	2.20	0.56
1:E:630:THR:HG23	8:E:2452:HOH:O	2.04	0.56
1:E:41:TYR:HE1	1:E:560:GLY:O	1.88	0.56
1:A:93:ASP:CG	1:A:758:ARG:HH22	2.08	0.56
1:E:519:TRP:CE2	1:E:540:ILE:HG12	2.39	0.56
1:A:277:GLU:HB3	1:A:281:LYS:HZ2	1.70	0.56
1:E:604:PRO:C	1:E:606:PRO:HD3	2.26	0.56
1:E:607:VAL:HG23	8:E:2144:HOH:O	2.05	0.56
1:E:623:TYR:HA	1:E:695:ILE:O	2.05	0.56
1:E:755:LEU:O	1:E:758:ARG:HD3	2.05	0.56
3:G:139:ASN:N	3:G:139:ASN:HD22	1.97	0.56
1:E:620:ARG:HB3	8:E:2391:HOH:O	2.04	0.56
8:B:2079:HOH:O	3:C:251:LEU:HD11	2.04	0.56
1:A:483:ALA:CA	1:A:515:THR:CG2	2.83	0.56
2:B:2:PRO:HD2	2:B:80:ASP:OD2	2.05	0.56
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.05	0.56
1:E:658:ARG:C	1:E:659:LEU:O	2.33	0.56
1:A:183:TRP:HB3	1:A:592:LEU:HD22	1.86	0.56
1:A:209:HIS:CE1	1:A:625:ARG:H	2.16	0.56
1:E:671:ASN:ND2	1:E:671:ASN:C	2.58	0.56
1:A:64:LYS:CE	2:B:26:GLU:HB2	2.35	0.56
1:A:285:GLY:C	1:A:590:ILE:CG2	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:LEU:CD2	7:C:1252:MQ7:C10	2.83	0.56
1:A:429:PRO:C	1:A:430:TYR:CD2	2.78	0.56
1:A:673:ASP:OD2	1:A:721:THR:CG2	2.52	0.56
1:A:64:LYS:HE2	2:B:26:GLU:HB2	1.87	0.56
3:G:70:ARG:HG2	3:G:71:PHE:H	1.70	0.56
1:E:214:THR:HG21	1:E:627:PRO:O	2.05	0.56
3:G:63:LEU:HD21	7:G:1251:MQ7:C1	2.36	0.56
1:A:276:LYS:CA	8:A:2148:HOH:O	2.39	0.56
1:E:231:LYS:HA	1:E:247:HIS:CD2	2.41	0.56
1:A:183:TRP:HE1	1:A:413:ARG:NH2	1.98	0.56
2:B:183:LYS:HE3	8:B:2141:HOH:O	2.06	0.56
1:E:116:THR:HG22	1:E:119:GLU:N	2.20	0.56
3:C:145:ASN:ND2	3:C:145:ASN:C	2.57	0.56
1:A:195:ILE:HG12	1:A:329:PRO:HB3	1.88	0.56
3:G:227:PRO:O	3:G:231:LEU:HB2	2.05	0.56
1:A:132:ARG:CD	8:A:2075:HOH:O	2.52	0.56
1:E:265:ILE:HD11	1:E:349:TYR:HB2	1.88	0.56
3:G:206:GLY:HA2	3:G:209:TYR:HB2	1.87	0.56
1:A:519:TRP:CG	1:A:540:ILE:CG2	2.88	0.56
1:E:397:GLU:HB3	8:E:2239:HOH:O	2.05	0.56
1:E:497:HIS:O	1:E:498:LYS:C	2.43	0.56
1:A:305:THR:CG2	1:A:307:ILE:H	2.19	0.56
2:B:117:THR:CG2	2:B:117:THR:O	2.53	0.56
1:A:75:ARG:NH1	1:A:220:GLN:HE21	1.99	0.56
1:A:231:LYS:CA	1:A:247:HIS:CD2	2.88	0.56
1:A:231:LYS:HB2	1:A:247:HIS:CD2	2.41	0.56
1:A:404:ARG:HG3	1:A:406:ASP:OD2	2.06	0.56
3:C:89:ILE:CD1	7:C:1252:MQ7:C6	2.84	0.56
3:G:225:LEU:CB	8:G:2069:HOH:O	2.52	0.56
1:E:620:ARG:CG	1:E:620:ARG:O	2.53	0.56
1:A:284:VAL:CG2	1:A:587:SER:HB3	2.30	0.56
3:C:174:PHE:H	3:C:175:PRO:HD2	1.71	0.56
1:E:621:LEU:HD22	1:E:622:LEU:O	2.06	0.56
3:G:38:HIS:CE1	3:G:105:LEU:HD22	2.40	0.56
1:E:371:LEU:HD13	1:E:547:ARG:CZ	2.35	0.56
1:A:71:ASN:HD21	1:A:73:LYS:HB2	1.70	0.56
1:E:45:GLU:HG3	8:E:2011:HOH:O	2.05	0.56
1:A:184:VAL:HG22	1:A:592:LEU:CB	2.36	0.55
1:A:602:HIS:CD2	1:A:604:PRO:HD2	2.42	0.55
3:C:21:HIS:CE1	3:C:64:LEU:CG	2.89	0.55
1:A:422:GLU:HB3	1:A:423:PRO:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:190:SER:O	2:F:194:HIS:N	2.38	0.55
1:A:85:ALA:HA	8:A:2042:HOH:O	2.05	0.55
1:E:160:TRP:O	1:E:160:TRP:CG	2.59	0.55
1:A:591:GLU:OE2	1:A:604:PRO:HG2	1.98	0.55
2:B:117:THR:O	2:B:117:THR:HG23	2.06	0.55
2:B:36:LEU:CD1	8:B:2103:HOH:O	2.54	0.55
3:C:20:LEU:HD13	3:C:63:ILE:HD13	1.88	0.55
1:A:81:ARG:NH2	1:A:214:THR:HG22	2.20	0.55
1:E:311:VAL:HG23	8:E:2195:HOH:O	2.05	0.55
1:E:201:ARG:HD3	8:E:2121:HOH:O	2.05	0.55
3:G:240:LEU:C	3:G:240:LEU:HD12	2.26	0.55
1:E:36:GLU:HB3	8:E:2005:HOH:O	2.06	0.55
1:E:119:GLU:HG2	8:E:2075:HOH:O	2.07	0.55
1:A:647:ASN:HD21	1:A:714:ALA:H	1.54	0.55
1:A:187:ARG:HH22	1:A:367:GLN:NE2	2.04	0.55
8:A:2040:HOH:O	2:B:133:GLU:HG3	2.07	0.55
1:E:97:ARG:HH22	1:E:763:ARG:HD2	1.70	0.55
1:E:75:ARG:NH1	1:E:220:GLN:HE21	1.99	0.55
1:A:342:TYR:CD2	1:A:605:LEU:HA	2.42	0.55
1:A:413:ARG:N	1:A:413:ARG:HD2	2.14	0.55
1:A:214:THR:HG23	1:A:214:THR:O	2.07	0.55
1:E:495:VAL:HG21	8:E:2296:HOH:O	2.05	0.55
2:F:44:GLY:O	2:F:45:GLU:HB2	2.07	0.55
1:A:555:LEU:O	1:A:559:LYS:HG3	2.05	0.55
1:E:724:LYS:CG	8:E:2424:HOH:O	2.54	0.55
1:E:604:PRO:C	1:E:605:LEU:HD23	2.18	0.55
3:G:63:LEU:CD2	7:G:1251:MQ7:C10	2.84	0.55
1:A:533:GLN:HG2	1:A:534:TYR:N	2.20	0.55
1:A:575:TRP:O	1:A:580:ARG:HG2	2.07	0.55
1:A:483:ALA:HB2	1:A:515:THR:CG2	2.37	0.55
1:E:397:GLU:CB	1:E:398:PRO:CD	2.82	0.55
2:F:88:LYS:O	3:G:74:THR:CG2	2.54	0.55
1:E:469:PRO:O	1:E:706:MET:CG	2.51	0.55
1:E:622:LEU:HB2	1:E:693:VAL:O	2.07	0.55
1:A:81:ARG:HH21	1:A:214:THR:CG2	2.20	0.55
1:A:345:MET:CE	1:A:605:LEU:HD22	2.38	0.54
1:E:100:ILE:CG2	1:E:478:VAL:HG22	2.36	0.54
1:E:635:GLN:HE21	1:E:635:GLN:H	1.54	0.54
1:A:194:PRO:O	1:A:363:PHE:HA	2.07	0.54
2:B:139:CYS:SG	4:B:1194:SF4:S3	3.04	0.54
1:A:396:HIS:CB	1:A:403:PRO:HB3	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:ASN:ND2	2:F:106:TYR:HE2	2.06	0.54
1:A:599:GLU:HB2	8:A:2279:HOH:O	2.07	0.54
1:A:379:LEU:O	1:A:380:PRO:C	2.46	0.54
1:A:255:GLY:HA2	1:A:337:TYR:CE1	2.42	0.54
1:A:183:TRP:HH2	1:A:596:ARG:CD	2.18	0.54
1:A:289:LEU:HD12	1:A:590:ILE:HD11	1.90	0.54
1:E:590:ILE:HB	8:E:2177:HOH:O	2.05	0.54
3:G:206:GLY:CA	3:G:209:TYR:HB2	2.37	0.54
1:A:395:ASP:CA	1:A:399:GLU:CG	2.54	0.54
1:E:433:LYS:HB3	1:E:460:ASP:HB2	1.88	0.54
3:G:100:LEU:HB3	8:G:2030:HOH:O	2.07	0.54
1:A:310:GLN:HG3	8:A:2160:HOH:O	2.07	0.54
1:A:635:GLN:C	1:A:709:ALA:HB2	2.27	0.54
1:E:453:LYS:HG2	1:E:475:TRP:CZ2	2.42	0.54
1:E:247:HIS:CE1	8:E:2145:HOH:O	2.60	0.54
2:F:35:ASN:HD22	2:F:106:TYR:HE2	1.55	0.54
1:E:380:PRO:HD3	1:E:534:TYR:OH	2.07	0.54
1:E:536:PRO:O	8:E:2308:HOH:O	2.17	0.54
1:E:701:HIS:O	1:E:710:HIS:O	2.24	0.54
1:A:184:VAL:HG22	1:A:592:LEU:CG	2.37	0.54
1:A:589:LYS:O	1:A:592:LEU:CA	2.55	0.54
1:E:412:ALA:HB1	1:E:413:ARG:NH1	2.22	0.54
1:E:209:HIS:CD2	5:E:1766:MGD:H5'1	2.43	0.54
1:E:428:GLU:O	1:E:430:TYR:CA	2.55	0.54
1:E:149:ASP:CB	8:E:2091:HOH:O	2.54	0.54
1:A:37:VAL:CG1	1:A:38:LYS:N	2.69	0.54
1:E:142:PHE:CG	1:E:157:PRO:HG3	2.42	0.54
1:A:391:PRO:O	1:A:413:ARG:CB	2.55	0.54
2:F:78:THR:CG2	2:F:79:LYS:N	2.71	0.54
3:G:52:ALA:O	3:G:56:ILE:HG13	2.08	0.54
3:G:63:LEU:HD22	7:G:1251:MQ7:C1	2.38	0.54
1:E:169:SER:O	1:E:174:THR:HB	2.08	0.54
2:B:27:ASN:HD21	2:B:121:HIS:HE1	1.54	0.54
1:E:336:TRP:O	1:E:340:ASP:OD1	2.26	0.54
3:C:50:THR:O	3:C:54:LEU:HG	2.08	0.54
1:E:591:GLU:OE2	1:E:604:PRO:CG	2.55	0.54
3:G:63:LEU:HD22	7:G:1251:MQ7:C3	2.37	0.54
1:E:553:LEU:HD21	1:E:557:THR:CG2	2.38	0.54
1:A:116:THR:HG23	1:A:118:GLU:N	2.23	0.54
1:A:462:TYR:OH	1:A:472:HIS:O	2.21	0.54
1:A:554:ASP:N	1:A:554:ASP:OD2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ALA:HB1	1:E:413:ARG:HH12	1.72	0.54
1:E:97:ARG:NH2	1:E:763:ARG:NH1	2.56	0.54
3:G:17:ASN:O	3:G:21:PHE:HD1	1.91	0.54
3:C:108:LEU:HB3	3:C:110:LYS:HG3	1.90	0.54
1:E:302:GLU:O	1:E:302:GLU:HG2	2.08	0.54
1:A:124:ILE:HD11	1:A:478:VAL:HG11	1.90	0.54
1:E:197:TRP:CG	1:E:221:ASP:HB3	2.43	0.54
1:E:627:PRO:HB2	2:F:16:CYS:HA	1.90	0.53
8:E:2164:HOH:O	2:F:46:TYR:HB2	2.07	0.53
1:E:305:THR:HG23	1:E:307:ILE:H	1.70	0.53
1:E:651:ILE:HD11	1:E:682:VAL:HG12	1.90	0.53
1:E:186:GLY:HA3	1:E:584:GLY:N	2.23	0.53
1:E:37:VAL:HA	1:E:57:ALA:O	2.09	0.53
3:C:77:ILE:HG12	3:C:81:LEU:HD11	1.90	0.53
1:E:609:THR:HG23	8:E:2336:HOH:O	2.08	0.53
1:A:490:ASP:OD2	1:A:505:ARG:NH1	2.40	0.53
1:A:305:THR:HG23	1:A:307:ILE:HD12	1.90	0.53
1:E:683:LYS:HE2	1:E:685:THR:HB	1.88	0.53
1:E:638:TRP:O	1:E:642:GLU:HB2	2.08	0.53
1:A:671:ASN:ND2	1:A:675:VAL:H	2.05	0.53
1:E:100:ILE:HG12	1:E:478:VAL:CG2	2.38	0.53
1:E:97:ARG:HH21	1:E:763:ARG:CZ	2.22	0.53
1:E:346:ALA:N	1:E:605:LEU:CD1	2.70	0.53
1:E:604:PRO:C	1:E:605:LEU:HD22	2.25	0.53
1:E:717:ASN:ND2	5:E:1765:MGD:H192	2.02	0.53
1:E:252:ILE:HG12	1:E:256:THR:HG22	1.90	0.53
2:B:55:PRO:HB2	8:B:2103:HOH:O	2.07	0.53
1:A:535:PHE:N	1:A:536:PRO:CD	2.71	0.53
3:C:208:PHE:CD2	3:C:208:PHE:C	2.80	0.53
1:A:341:THR:OG1	1:A:729:SER:HB3	2.08	0.53
2:B:57:GLN:CD	8:B:2044:HOH:O	2.47	0.53
1:A:124:ILE:O	1:A:128:MET:HG3	2.08	0.53
1:A:654:GLU:HG3	8:A:2315:HOH:O	2.08	0.53
1:A:592:LEU:HD13	1:A:592:LEU:C	2.28	0.53
1:A:279:VAL:HA	1:A:283:THR:HB	1.91	0.53
3:G:40:LYS:O	3:G:40:LYS:HG3	2.08	0.53
1:E:519:TRP:CZ2	1:E:540:ILE:HG13	2.44	0.53
1:E:336:TRP:O	1:E:338:GLY:N	2.42	0.53
2:F:63:ASN:HB2	8:F:2109:HOH:O	2.07	0.53
1:A:284:VAL:HG12	1:A:285:GLY:N	2.23	0.53
1:A:572:LEU:HD22	8:A:2271:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:591:GLU:O	1:E:591:GLU:CG	2.55	0.53
2:B:155:ALA:HB1	8:B:2113:HOH:O	2.09	0.53
1:A:488:ARG:HD3	1:A:490:ASP:OD2	2.09	0.53
3:C:143:LEU:CD2	3:C:198:ALA:HB1	2.39	0.53
1:A:623:TYR:HA	1:A:695:ILE:O	2.09	0.53
1:A:585:THR:HG22	1:A:585:THR:O	2.08	0.53
1:A:428:GLU:CB	1:A:429:PRO:CD	2.85	0.53
1:A:118:GLU:CD	1:A:118:GLU:H	2.11	0.53
1:E:447:PRO:HB3	8:E:2419:HOH:O	2.08	0.53
1:E:315:VAL:HG12	1:E:319:MET:CE	2.39	0.53
3:G:205:ALA:HB1	3:G:240:LEU:CD2	2.39	0.53
3:C:229:TRP:O	3:C:233:LEU:HG	2.08	0.53
2:F:46:TYR:C	2:F:46:TYR:CD1	2.81	0.53
3:G:46:ARG:CG	8:G:2014:HOH:O	2.57	0.53
1:A:284:VAL:HG23	1:A:587:SER:CB	2.35	0.52
1:A:369:PRO:HG2	1:A:494:LEU:HB3	1.91	0.52
1:A:122:ASP:HB2	8:A:2069:HOH:O	2.08	0.52
1:E:424:MET:CE	1:E:455:ALA:HB1	2.39	0.52
1:A:231:LYS:HB2	1:A:247:HIS:CG	2.44	0.52
1:E:606:PRO:CG	1:E:607:VAL:N	2.72	0.52
1:E:99:LEU:O	1:E:478:VAL:HA	2.09	0.52
1:E:81:ARG:HB2	4:E:1764:SF4:S3	2.49	0.52
1:A:651:ILE:HG23	1:A:693:VAL:HG23	1.90	0.52
3:C:57:ILE:HG21	3:C:100:PHE:HB2	1.91	0.52
1:E:672:GLN:H	1:E:672:GLN:NE2	2.07	0.52
1:A:72:PRO:HG2	1:A:501:PHE:CD2	2.44	0.52
1:A:295:ASP:O	1:A:297:THR:HG22	2.10	0.52
1:A:676:LYS:NZ	1:A:742:GLU:OE1	2.41	0.52
1:A:286:PHE:HA	1:A:590:ILE:CG2	2.37	0.52
1:E:286:PHE:CB	8:E:2177:HOH:O	2.57	0.52
1:A:207:GLY:O	5:A:1766:MGD:PB	2.68	0.52
2:F:57:GLN:HE22	2:F:140:ARG:HH21	1.50	0.52
3:C:155:THR:CG2	3:C:239:ARG:CD	2.87	0.52
1:E:91:ASP:C	1:E:92:PRO:O	2.48	0.52
1:A:115:ALA:HB1	1:A:119:GLU:HG2	1.91	0.52
1:E:69:GLU:HA	8:E:2037:HOH:O	2.08	0.52
1:A:548:LEU:O	1:A:553:LEU:O	2.28	0.52
3:G:70:ARG:CG	3:G:71:PHE:N	2.72	0.52
1:A:686:ALA:CB	8:A:2330:HOH:O	2.44	0.52
1:A:335:VAL:HG13	1:A:733:GLY:CA	2.39	0.52
1:A:680:VAL:HG22	1:A:714:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:THR:HG22	2:B:80:ASP:H	1.75	0.52
2:B:129:PRO:HB3	4:B:1195:SF4:S3	2.50	0.52
1:E:397:GLU:CB	8:E:2239:HOH:O	2.57	0.52
1:E:421:ILE:HD11	1:E:452:THR:HG23	1.92	0.52
2:F:44:GLY:HA3	8:F:2025:HOH:O	2.08	0.52
3:G:189:TYR:HB3	3:G:190:PRO:HD3	1.92	0.52
1:A:592:LEU:O	1:A:592:LEU:HD13	2.09	0.52
1:E:583:PHE:CD2	1:E:583:PHE:N	2.68	0.52
3:C:222:TRP:CD1	3:C:223:GLN:N	2.78	0.52
1:A:483:ALA:CB	1:A:515:THR:CG2	2.88	0.52
1:A:101:ARG:HB2	1:A:477:ASP:HA	1.92	0.52
1:A:107:ARG:HB2	8:A:2219:HOH:O	2.09	0.52
2:B:112:TYR:HB3	3:C:73:ARG:NH2	2.24	0.52
3:G:160:LEU:HB3	3:G:175:LEU:HB2	1.91	0.52
1:A:499:THR:HB	1:A:565:VAL:CG1	2.40	0.52
1:E:591:GLU:OE2	1:E:604:PRO:CB	2.57	0.52
3:G:222:GLN:C	8:G:2069:HOH:O	2.47	0.52
1:E:313:ARG:HD3	1:E:317:ARG:NH2	2.25	0.52
1:A:212:GLU:OE1	1:A:240:SER:HB2	2.10	0.52
1:E:286:PHE:C	1:E:288:GLU:H	2.12	0.51
1:A:254:PRO:HG2	1:A:692:CYS:SG	2.50	0.51
1:E:48:PHE:CZ	1:E:145:HIS:CE1	2.98	0.51
1:A:583:PHE:CZ	1:A:587:SER:CA	2.93	0.51
3:C:185:LEU:O	3:C:189:LEU:HG	2.09	0.51
1:E:492:PHE:HZ	1:E:548:LEU:HG	1.74	0.51
3:C:64:LEU:HD22	7:C:1252:MQ7:C10	2.40	0.51
1:E:604:PRO:CA	1:E:605:LEU:CD2	2.87	0.51
1:E:606:PRO:CD	1:E:607:VAL:N	2.73	0.51
1:A:209:HIS:HD2	5:A:1766:MGD:O2A	1.93	0.51
1:E:248:ARG:NH1	1:E:318:GLU:OE2	2.44	0.51
1:A:81:ARG:NE	1:A:214:THR:HG22	2.24	0.51
1:E:647:ASN:HD22	1:E:647:ASN:N	2.03	0.51
1:E:685:THR:HG22	2:F:42:GLU:OE2	2.10	0.51
1:A:156:LEU:HB3	1:A:157:PRO:HD3	1.93	0.51
1:E:574:ASP:HA	1:E:577:LYS:HD3	1.91	0.51
3:C:145:ASN:OD1	3:C:193:THR:CG2	2.57	0.51
3:G:16:THR:HG21	3:G:66:GLU:HB2	1.93	0.51
1:A:591:GLU:O	1:A:592:LEU:CD1	2.53	0.51
2:B:46:TYR:HE2	8:B:2033:HOH:O	1.82	0.51
1:E:142:PHE:CD1	1:E:157:PRO:HB3	2.45	0.51
1:E:272:ASP:OD2	1:E:276:LYS:NZ	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ALA:HB1	1:A:381:LEU:O	2.10	0.51
1:E:100:ILE:HA	1:E:478:VAL:HG22	1.92	0.51
1:A:159:ALA:HA	1:A:380:PRO:HD2	1.92	0.51
2:B:88:LYS:O	3:C:75:THR:CG2	2.58	0.51
2:B:5:ALA:HB3	2:B:145:LEU:HD13	1.93	0.51
1:A:288:GLU:HB3	1:A:591:GLU:CG	2.22	0.51
1:A:42:GLN:OE1	1:A:506:THR:N	2.43	0.51
2:B:192:VAL:CG1	2:B:193:HIS:H	2.23	0.51
1:E:553:LEU:CD2	1:E:557:THR:CG2	2.88	0.51
3:G:139:ASN:ND2	8:G:2040:HOH:O	2.43	0.51
1:E:275:ASP:N	1:E:323:LYS:HE3	2.25	0.51
3:G:63:LEU:HD22	7:G:1251:MQ7:C2	2.40	0.51
2:B:132:VAL:HA	2:B:140:ARG:HG3	1.93	0.51
1:E:158:ALA:HB1	1:E:381:LEU:O	2.10	0.51
1:A:166:ALA:CB	1:A:415:THR:CG2	2.88	0.51
1:A:170:VAL:HG12	1:A:171:SER:N	2.25	0.51
1:E:499:THR:HA	1:E:567:ARG:O	2.11	0.51
1:A:305:THR:CG2	1:A:307:ILE:HB	2.41	0.51
1:A:73:LYS:HZ1	1:A:192:HIS:HD2	1.55	0.51
3:G:205:ALA:HB1	3:G:240:LEU:HD22	1.92	0.51
3:G:249:GLY:HA2	8:G:2078:HOH:O	2.11	0.51
2:B:61:CYS:HB2	4:B:1196:SF4:S3	2.51	0.51
1:E:166:ALA:HB2	1:E:415:THR:CG2	2.40	0.51
1:A:589:LYS:O	1:A:592:LEU:HA	2.11	0.51
1:A:43:ILE:HB	1:A:505:ARG:HH21	1.76	0.51
1:A:534:TYR:O	1:A:535:PHE:CB	2.59	0.51
2:B:25:MET:CE	2:B:25:MET:CA	2.80	0.51
1:E:484:THR:HB	1:E:487:GLU:OE1	2.10	0.51
2:F:67:VAL:HB	2:F:68:PRO:CD	2.39	0.51
1:A:548:LEU:C	1:A:553:LEU:O	2.50	0.51
3:G:39:LEU:HD13	3:G:116:ALA:CB	2.41	0.51
2:B:64:PRO:HB3	4:B:1196:SF4:S3	2.51	0.51
3:G:42:ASP:OD1	3:G:44:GLU:HG3	2.11	0.51
1:A:596:ARG:NH1	1:A:600:ALA:CB	2.73	0.51
1:E:708:LEU:HD22	1:E:755:LEU:HB3	1.93	0.51
1:E:149:ASP:HA	8:E:2091:HOH:O	2.11	0.51
1:E:651:ILE:HD11	1:E:682:VAL:HG13	1.92	0.51
1:A:90:TYR:OH	1:A:509:HIS:HE1	1.93	0.51
1:A:195:ILE:N	1:A:195:ILE:HD12	2.25	0.51
3:G:70:ARG:HG2	3:G:71:PHE:N	2.25	0.51
1:E:48:PHE:CE1	1:E:145:HIS:CE1	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:2029:HOH:O	3:G:250:LEU:HD12	2.09	0.51
2:B:191:GLU:HG3	8:B:2143:HOH:O	2.10	0.51
1:A:65:VAL:HG13	1:A:78:LEU:HD21	1.93	0.50
2:F:172:ARG:N	2:F:173:PRO:HD3	2.26	0.50
3:G:44:GLU:OE1	3:G:47:ARG:NH1	2.43	0.50
3:C:133:LEU:O	3:C:137:VAL:HG22	2.11	0.50
1:A:390:GLY:H	1:A:595:GLN:NE2	2.05	0.50
1:A:587:SER:O	1:A:589:LYS:HE2	2.11	0.50
1:E:100:ILE:HG12	1:E:478:VAL:HG13	1.93	0.50
1:E:101:ARG:HB2	1:E:477:ASP:HA	1.93	0.50
1:E:595:GLN:HA	1:E:598:LYS:HB2	1.93	0.50
1:A:647:ASN:HD22	1:A:647:ASN:N	2.03	0.50
3:C:173:LEU:CG	3:C:173:LEU:O	2.55	0.50
1:A:712:ARG:NH2	8:A:2346:HOH:O	2.43	0.50
1:A:488:ARG:CD	1:A:490:ASP:OD2	2.59	0.50
1:E:708:LEU:HD22	8:E:2407:HOH:O	2.11	0.50
1:E:88:THR:CG2	1:E:467:VAL:HG11	2.41	0.50
1:A:252:ILE:HG13	1:A:307:ILE:HD11	1.92	0.50
1:A:501:PHE:HA	1:A:564:LEU:O	2.11	0.50
1:E:201:ARG:CD	8:E:2121:HOH:O	2.58	0.50
1:A:42:GLN:NE2	1:A:505:ARG:CD	2.66	0.50
1:E:630:THR:HA	5:E:1766:MGD:N18	2.26	0.50
2:F:55:PRO:CG	4:F:1194:SF4:S2	2.98	0.50
1:E:335:VAL:HG13	1:E:732:ALA:O	2.12	0.50
2:F:147:ASP:O	2:F:150:SER:HB2	2.10	0.50
3:C:190:TYR:HB3	3:C:191:PRO:HD3	1.93	0.50
2:F:16:CYS:O	2:F:16:CYS:SG	2.69	0.50
1:E:575:TRP:HB3	1:E:580:ARG:O	2.11	0.50
1:A:422:GLU:N	1:A:423:PRO:HD2	2.26	0.50
3:G:144:ASN:HD22	3:G:144:ASN:C	2.14	0.50
2:F:166:ARG:HD2	8:F:2104:HOH:O	2.11	0.50
1:A:628:VAL:HG13	1:A:640:LEU:HD22	1.93	0.50
3:G:148:ALA:HA	8:G:2047:HOH:O	2.12	0.50
2:B:160:GLU:N	2:B:179:ASN:ND2	2.55	0.50
1:E:263:ALA:HB2	1:E:301:ALA:HB2	1.94	0.50
1:A:193:GLU:CG	8:A:2118:HOH:O	2.57	0.50
1:E:639:VAL:HG21	2:F:25:MET:HE3	1.93	0.50
1:A:655:GLU:CD	1:A:658:ARG:HH22	2.14	0.50
2:F:35:ASN:ND2	2:F:106:TYR:CE2	2.78	0.50
1:E:95:LEU:HD11	1:E:466:ASP:O	2.04	0.50
8:E:2130:HOH:O	2:F:138:TYR:CD1	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:THR:HG22	1:E:299:GLU:H	1.75	0.50
1:E:488:ARG:HG3	8:E:2287:HOH:O	2.11	0.50
1:E:651:ILE:HD12	1:E:684:PRO:HA	1.93	0.50
2:B:190:SER:CB	3:C:252:GLY:N	2.71	0.50
1:A:702:LYS:HG3	8:A:2231:HOH:O	2.11	0.50
1:E:669:LEU:HD23	1:E:741:LEU:HD22	1.92	0.50
1:E:630:THR:HA	5:E:1766:MGD:C17	2.41	0.50
1:E:423:PRO:HB2	1:E:432:ILE:HG13	1.93	0.50
1:E:369:PRO:HG2	1:E:494:LEU:HB3	1.94	0.50
1:E:647:ASN:C	1:E:648:GLU:HG3	2.33	0.50
1:E:734:LEU:CD2	8:E:2419:HOH:O	2.54	0.50
3:C:228:PRO:O	3:C:232:LEU:HD12	2.12	0.50
3:G:91:GLY:O	3:G:95:LEU:HD12	2.11	0.50
2:B:52:GLU:OE2	2:B:187:THR:HB	2.12	0.50
8:E:2130:HOH:O	2:F:138:TYR:CE1	2.65	0.50
2:F:117:THR:HB	8:F:2012:HOH:O	2.10	0.50
1:A:73:LYS:HZ3	1:A:192:HIS:CD2	2.30	0.50
3:G:206:GLY:O	3:G:209:TYR:CB	2.60	0.49
3:G:129:TYR:OH	7:G:1251:MQ7:O1	2.22	0.49
1:A:629:HIS:ND1	1:A:634:THR:CG2	2.65	0.49
1:A:232:VAL:N	1:A:247:HIS:CD2	2.74	0.49
3:C:222:TRP:CD1	3:C:222:TRP:C	2.85	0.49
1:E:204:VAL:HG21	1:E:319:MET:CE	2.42	0.49
3:G:65:ALA:O	3:G:70:ARG:NH1	2.45	0.49
2:F:125:LYS:HE2	8:F:2077:HOH:O	2.12	0.49
1:A:284:VAL:N	1:A:588:GLY:O	2.28	0.49
1:E:345:MET:HB3	1:E:605:LEU:HD11	1.94	0.49
1:A:405:ALA:HB2	1:A:430:TYR:CZ	2.48	0.49
1:E:524:GLU:OE1	1:E:528:ARG:NH2	2.45	0.49
2:F:129:PRO:HB3	4:F:1195:SF4:S2	2.52	0.49
1:E:287:GLU:N	1:E:287:GLU:OE1	2.45	0.49
1:E:323:LYS:HD3	1:E:354:LEU:C	2.30	0.49
1:A:116:THR:HG23	1:A:118:GLU:H	1.76	0.49
1:A:193:GLU:HB2	1:A:195:ILE:CD1	2.42	0.49
2:B:106:TYR:CE1	2:B:114:SER:HB3	2.46	0.49
1:A:184:VAL:HG22	1:A:592:LEU:CD2	2.28	0.49
1:A:77:ARG:NH2	8:A:2040:HOH:O	2.34	0.49
8:B:2079:HOH:O	3:C:251:LEU:CD1	2.59	0.49
1:E:371:LEU:HD12	1:E:494:LEU:HD21	1.95	0.49
2:F:117:THR:CG2	2:F:119:CYS:N	2.74	0.49
3:C:143:LEU:HD23	3:C:198:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:548:LEU:CD1	1:E:555:LEU:HA	2.42	0.49
1:A:530:GLY:HA2	1:A:532:GLU:OE2	2.12	0.49
2:F:107:LEU:HD21	3:G:68:PRO:HG2	1.94	0.49
1:A:666:TYR:CZ	1:A:681:ARG:HG3	2.47	0.49
1:A:65:VAL:CG1	1:A:78:LEU:HD21	2.42	0.49
1:E:627:PRO:CB	2:F:16:CYS:HA	2.42	0.49
1:E:95:LEU:CD1	8:E:2275:HOH:O	2.54	0.49
2:B:192:VAL:CG1	2:B:193:HIS:N	2.73	0.49
1:A:682:VAL:HG12	1:A:684:PRO:HD3	1.95	0.49
1:E:647:ASN:H	1:E:647:ASN:ND2	2.11	0.49
3:C:161:LEU:CD1	3:C:179:LEU:HD12	2.43	0.49
1:E:504:LEU:HD22	1:E:505:ARG:N	2.28	0.49
2:B:41:ARG:CD	2:B:187:THR:HG23	2.41	0.49
2:B:22:ALA:HB2	2:B:134:THR:HG21	1.95	0.49
1:A:506:THR:CG2	8:A:2244:HOH:O	2.60	0.49
1:A:489:TYR:CD1	1:A:540:ILE:HD13	2.48	0.49
1:A:689:ARG:NE	1:A:691:ASP:OD2	2.43	0.49
1:E:53:ILE:HG22	1:E:78:LEU:HD11	1.95	0.49
1:A:186:GLY:N	1:A:583:PHE:HA	2.22	0.49
1:A:586:ALA:O	1:A:587:SER:CB	2.60	0.49
3:C:21:HIS:C	3:C:21:HIS:CD2	2.86	0.49
1:A:42:GLN:OE1	1:A:506:THR:O	2.31	0.49
2:F:190:SER:N	3:G:251:GLY:N	2.61	0.49
1:A:96:LYS:HB3	1:A:513:PHE:CB	2.42	0.49
1:E:384:ALA:HB1	8:E:2237:HOH:O	2.13	0.49
1:E:606:PRO:CG	1:E:607:VAL:H	2.26	0.49
1:E:225:ALA:O	1:E:230:ALA:HB3	2.13	0.49
1:A:393:GLY:HA3	1:A:407:LYS:HZ1	1.72	0.49
1:E:113:ARG:HB3	8:E:2042:HOH:O	2.13	0.49
3:C:76:HIS:O	3:C:79:LEU:HB2	2.13	0.49
1:A:116:THR:HG22	1:A:119:GLU:CB	2.37	0.49
1:A:256:THR:O	1:A:256:THR:HG23	2.11	0.49
1:E:539:THR:CG2	1:E:541:GLU:HG2	2.42	0.49
1:A:482:GLU:HG2	1:A:483:ALA:H	1.78	0.49
1:A:122:ASP:CB	8:A:2069:HOH:O	2.60	0.49
1:A:394:GLY:CA	8:A:2189:HOH:O	2.61	0.49
1:E:540:ILE:O	1:E:544:LEU:HG	2.13	0.49
2:B:164:VAL:HG22	2:B:173:PRO:HB2	1.94	0.49
2:F:160:GLU:N	2:F:179:ASN:HD21	1.96	0.48
2:B:166:ARG:HH22	3:C:249:GLN:HE21	1.59	0.48
1:A:113:ARG:NE	8:A:2065:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:MET:O	1:A:563:THR:O	2.31	0.48
1:E:677:GLU:O	1:E:678:GLY:O	2.30	0.48
2:F:9:ASP:HA	2:F:178:LEU:HB2	1.94	0.48
1:E:227:LYS:HE2	2:F:12:LEU:HD11	1.94	0.48
3:C:21:HIS:ND1	3:C:64:LEU:CG	2.74	0.48
1:A:43:ILE:HB	1:A:505:ARG:NH2	2.28	0.48
1:E:650:TRP:HB2	1:E:694:TYR:HB3	1.95	0.48
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.95	0.48
1:A:647:ASN:ND2	1:A:713:GLY:HA3	2.27	0.48
2:F:117:THR:HG23	2:F:117:THR:O	2.12	0.48
2:B:71:PRO:HB2	3:C:79:LEU:CD1	2.43	0.48
1:E:233:VAL:HG13	1:E:248:ARG:HB2	1.95	0.48
3:G:222:GLN:CA	3:G:222:GLN:OE1	2.57	0.48
2:B:159:ALA:O	2:F:183:LYS:CE	2.53	0.48
3:G:47:ARG:O	3:G:50:LEU:O	2.31	0.48
2:F:122:ARG:HG2	2:F:127:LYS:HE3	1.95	0.48
1:E:50:ARG:HD2	8:E:2013:HOH:O	2.12	0.48
1:A:371:LEU:HD23	1:A:551:LEU:CD1	2.44	0.48
1:E:730:GLY:HA3	8:E:2250:HOH:O	2.13	0.48
1:E:325:ARG:NH1	8:E:2211:HOH:O	2.26	0.48
3:C:64:LEU:HD21	7:C:1252:MQ7:C4	2.43	0.48
1:A:761:ASP:C	1:A:763:ARG:H	2.16	0.48
1:E:112:TYR:OH	1:E:476:ALA:O	2.32	0.48
3:G:112:GLN:N	8:G:2033:HOH:O	2.45	0.48
1:E:250:LEU:HD13	1:E:307:ILE:HG21	1.95	0.48
1:E:670:VAL:HB	1:E:740:ARG:HG3	1.94	0.48
1:E:588:GLY:HA3	8:E:2106:HOH:O	2.13	0.48
1:A:628:VAL:HG11	1:A:643:MET:HB2	1.95	0.48
1:A:435:LEU:O	1:A:462:TYR:HA	2.13	0.48
1:E:297:THR:HG21	1:E:299:GLU:HG2	1.94	0.48
1:A:349:TYR:OH	1:A:592:LEU:HG	2.13	0.48
1:E:256:THR:HG23	8:E:2193:HOH:O	2.13	0.48
1:E:247:HIS:N	1:E:247:HIS:CD2	2.80	0.48
1:E:79:CYS:CB	1:E:80:PRO:HD2	2.43	0.48
1:A:753:THR:CG2	1:A:757:LYS:HE2	2.44	0.48
2:F:27:ASN:HD21	2:F:121:HIS:HE1	1.62	0.48
1:A:596:ARG:CZ	1:A:600:ALA:HB1	2.44	0.48
2:B:117:THR:HG23	2:B:120:ALA:H	1.78	0.48
2:B:57:GLN:O	2:B:59:LEU:HD23	2.14	0.48
1:A:722:ARG:NE	8:A:2353:HOH:O	2.47	0.48
1:E:576:GLU:C	1:E:578:GLU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:VAL:HG21	1:E:319:MET:HE1	1.96	0.48
1:E:123:HIS:CE1	8:E:2079:HOH:O	2.67	0.48
2:F:135:CYS:HA	2:F:136:PRO:HD3	1.73	0.47
1:A:509:HIS:HD2	1:A:510:GLU:O	1.97	0.47
1:A:541:GLU:HB2	1:A:555:LEU:HD12	1.95	0.47
1:E:491:ASP:OD1	1:E:492:PHE:N	2.47	0.47
3:G:195:PRO:HD2	3:G:196:GLU:OE2	2.14	0.47
2:F:164:VAL:CG2	2:F:173:PRO:HB2	2.43	0.47
1:E:53:ILE:HD12	1:E:65:VAL:HG22	1.96	0.47
2:B:157:LYS:HD3	8:F:2039:HOH:O	2.14	0.47
1:A:743:LYS:HG3	8:A:2364:HOH:O	2.14	0.47
1:E:292:HIS:HD2	8:E:2083:HOH:O	1.96	0.47
1:E:590:ILE:HG22	1:E:591:GLU:N	2.28	0.47
1:A:253:LYS:O	1:A:256:THR:HB	2.14	0.47
1:E:370:TYR:OH	1:E:372:GLU:HG3	2.14	0.47
1:A:345:MET:HE3	1:A:592:LEU:HD11	1.95	0.47
1:E:346:ALA:HB2	1:E:605:LEU:HD12	1.96	0.47
1:E:602:HIS:CE1	1:E:606:PRO:CG	2.53	0.47
1:A:252:ILE:HD11	1:A:256:THR:HG22	1.95	0.47
1:E:308:PRO:CB	8:E:2195:HOH:O	2.51	0.47
1:A:193:GLU:OE2	1:A:332:ARG:NH1	2.47	0.47
1:A:319:MET:CE	1:A:328:LEU:CD1	2.93	0.47
1:E:289:LEU:HD12	1:E:590:ILE:HG21	1.96	0.47
1:E:589:LYS:CB	1:E:592:LEU:HB2	2.42	0.47
1:A:393:GLY:CA	1:A:407:LYS:HE3	2.39	0.47
1:E:314:GLU:HG3	8:E:2199:HOH:O	2.13	0.47
1:A:277:GLU:HB3	1:A:281:LYS:NZ	2.29	0.47
1:A:66:GLU:HG3	8:A:2039:HOH:O	2.15	0.47
2:F:99:ALA:HB2	3:G:137:ASN:ND2	2.29	0.47
1:A:596:ARG:O	1:A:600:ALA:N	2.34	0.47
1:E:606:PRO:HG2	1:E:607:VAL:N	2.30	0.47
1:A:209:HIS:H	1:A:209:HIS:CD2	2.32	0.47
1:E:761:ASP:C	1:E:763:ARG:H	2.17	0.47
1:A:536:PRO:O	8:A:2256:HOH:O	2.20	0.47
1:E:324:PRO:HD2	8:E:2210:HOH:O	2.08	0.47
3:G:208:TRP:HE3	3:G:208:TRP:HA	1.76	0.47
1:E:107:ARG:O	1:E:108:GLY:C	2.50	0.47
1:E:492:PHE:CZ	1:E:548:LEU:HG	2.50	0.47
1:A:284:VAL:HB	1:A:589:LYS:HA	1.96	0.47
2:B:41:ARG:NH1	2:B:187:THR:HG23	2.15	0.47
1:E:47:CYS:HB3	1:E:81:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:17:ASN:HB2	8:G:2010:HOH:O	2.14	0.47
3:C:108:LEU:O	3:C:109:GLY:C	2.53	0.47
1:A:615:PRO:O	1:A:618:PHE:HB2	2.15	0.47
2:F:166:ARG:NH2	3:G:248:GLN:NE2	2.62	0.47
2:F:23:CYS:SG	2:F:35:ASN:HB2	2.53	0.47
1:E:197:TRP:CB	1:E:221:ASP:HB3	2.44	0.47
1:E:422:GLU:HG3	8:E:2103:HOH:O	2.13	0.47
1:E:51:CYS:SG	1:E:216:ASN:HB3	2.55	0.47
1:A:390:GLY:N	1:A:391:PRO:HD3	2.30	0.47
1:E:391:PRO:HD3	1:E:595:GLN:CD	2.35	0.47
1:E:500:PRO:CD	1:E:567:ARG:O	2.63	0.47
3:G:19:LEU:O	3:G:19:LEU:HD23	2.14	0.47
1:A:651:ILE:HG23	1:A:693:VAL:CG2	2.45	0.47
1:A:434:GLY:CA	1:A:461:LEU:O	2.52	0.47
1:A:433:LYS:HD3	1:A:460:ASP:OD2	2.15	0.47
1:A:113:ARG:CZ	8:A:2065:HOH:O	2.63	0.47
1:E:177:ARG:HA	1:E:344:VAL:HG11	1.96	0.47
1:A:266:HIS:HB2	1:A:293:VAL:HG13	1.95	0.47
1:A:118:GLU:HG3	8:A:2252:HOH:O	2.14	0.47
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.55	0.47
1:A:494:LEU:HD22	1:A:502:ILE:HG12	1.96	0.47
1:E:166:ALA:HB2	1:E:415:THR:HG21	1.97	0.47
3:G:26:LEU:HG	3:G:158:LEU:HB3	1.97	0.47
1:A:263:ALA:O	1:A:267:VAL:HG23	2.15	0.46
1:E:239:PHE:O	1:E:687:ARG:HD2	2.15	0.46
1:A:370:TYR:CD2	1:A:551:LEU:HD21	2.50	0.46
1:E:53:ILE:HD12	1:E:65:VAL:CG2	2.45	0.46
1:E:753:THR:HG22	1:E:757:LYS:HE3	1.96	0.46
2:B:168:GLU:C	2:B:169:GLN:O	2.50	0.46
1:A:339:ASP:HB3	1:A:607:VAL:CG1	2.42	0.46
1:E:621:LEU:HD22	1:E:622:LEU:N	2.30	0.46
1:E:636:ASN:HA	1:E:708:LEU:HB2	1.96	0.46
1:E:95:LEU:HG	1:E:468:LEU:O	2.15	0.46
2:F:16:CYS:O	4:F:1194:SF4:S3	2.74	0.46
2:B:190:SER:CA	3:C:252:GLY:N	2.78	0.46
1:A:541:GLU:O	1:A:545:GLU:HG2	2.14	0.46
2:B:3:ARG:HD2	2:B:62:GLU:OE2	2.15	0.46
1:E:201:ARG:NH2	1:E:228:ASN:O	2.37	0.46
1:E:523:ARG:HG2	1:E:523:ARG:HH11	1.81	0.46
2:B:118:PHE:HD1	2:B:118:PHE:HA	1.65	0.46
1:A:583:PHE:N	8:A:2274:HOH:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ASP:CB	1:E:607:VAL:CG1	2.87	0.46
1:E:606:PRO:HD2	1:E:607:VAL:H	1.79	0.46
3:G:206:GLY:O	3:G:209:TYR:C	2.54	0.46
1:E:209:HIS:CE1	1:E:625:ARG:N	2.70	0.46
1:E:634:THR:H	1:E:635:GLN:NE2	2.13	0.46
1:A:683:LYS:HA	1:A:684:PRO:HD2	1.58	0.46
3:C:207:GLY:HA2	3:C:210:TYR:CB	2.43	0.46
1:E:620:ARG:HA	1:E:738:PHE:HD2	1.80	0.46
2:B:117:THR:HG22	2:B:119:CYS:CA	2.45	0.46
3:C:241:LEU:CD1	3:C:241:LEU:O	2.63	0.46
1:A:174:THR:HG23	1:A:178:GLU:CG	2.42	0.46
1:A:41:TYR:HD1	1:A:559:LYS:O	1.97	0.46
3:G:249:GLY:O	8:G:2076:HOH:O	2.21	0.46
1:A:248:ARG:HB3	8:A:2133:HOH:O	2.14	0.46
1:A:581:LEU:HD23	1:A:583:PHE:HE1	1.81	0.46
1:E:342:TYR:CD1	1:E:607:VAL:CB	2.83	0.46
1:A:65:VAL:CG1	1:A:78:LEU:CD2	2.92	0.46
1:E:468:LEU:HB3	1:E:469:PRO:HD2	1.97	0.46
3:C:17:THR:HG21	8:C:2015:HOH:O	2.14	0.46
1:A:686:ALA:O	1:A:687:ARG:HG2	2.15	0.46
2:B:161:ARG:HG2	2:B:179:ASN:HA	1.95	0.46
1:A:138:GLU:CD	1:A:402:LYS:HB2	2.35	0.46
1:E:597:PHE:HB3	8:E:2325:HOH:O	2.16	0.46
8:F:2074:HOH:O	3:G:72:ARG:HD3	2.15	0.46
1:E:591:GLU:O	1:E:603:GLN:HG2	2.14	0.46
8:F:2031:HOH:O	3:G:1:ALA:CB	2.63	0.46
1:A:647:ASN:H	1:A:647:ASN:ND2	2.09	0.46
2:F:79:LYS:HD2	2:F:79:LYS:HA	1.77	0.46
2:B:57:GLN:OE1	8:B:2044:HOH:O	2.20	0.46
1:E:60:ASN:ND2	8:E:2021:HOH:O	2.47	0.46
1:A:253:LYS:NZ	1:A:613:GLU:OE2	2.36	0.46
1:A:73:LYS:HZ1	1:A:192:HIS:CD2	2.33	0.46
1:A:483:ALA:HB2	1:A:515:THR:HG22	1.97	0.46
1:E:45:GLU:HB2	1:E:485:TYR:HB3	1.96	0.46
1:E:106:GLN:NE2	8:E:2061:HOH:O	2.49	0.46
1:E:138:GLU:CD	1:E:402:LYS:HB2	2.36	0.46
1:E:288:GLU:HG3	8:E:2182:HOH:O	2.15	0.46
3:C:174:PHE:N	3:C:175:PRO:HD2	2.31	0.46
1:A:267:VAL:O	1:A:271:GLU:HB2	2.15	0.46
1:A:371:LEU:HG	1:A:502:ILE:HD13	1.97	0.46
3:G:214:LEU:O	3:G:217:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:LEU:HD22	4:F:1195:SF4:S4	2.56	0.46
1:E:187:ARG:HB3	1:E:188:PRO:HD2	1.97	0.46
1:E:625:ARG:HD2	5:E:1766:MGD:C17	2.46	0.46
3:G:20:HIS:CE1	3:G:63:LEU:HD21	2.51	0.46
1:E:672:GLN:HE22	1:E:738:PHE:H	1.64	0.46
1:E:424:MET:HE2	1:E:455:ALA:HB1	1.97	0.46
3:C:166:LEU:HD21	3:C:228:PRO:HB2	1.97	0.46
1:A:538:LYS:HE2	1:A:538:LYS:N	2.30	0.46
1:A:129:LEU:O	1:A:133:GLU:HG2	2.16	0.46
1:A:349:TYR:CZ	1:A:590:ILE:O	2.68	0.46
1:A:589:LYS:H	1:A:589:LYS:HG2	1.54	0.46
1:E:630:THR:HA	5:E:1766:MGD:H18	1.81	0.46
1:E:30:ALA:N	1:E:31:PRO:CD	2.79	0.46
1:A:121:LEU:HD22	1:A:525:LEU:HG	1.97	0.46
1:E:664:GLY:N	8:E:2374:HOH:O	2.45	0.46
5:E:1766:MGD:H8	8:E:2426:HOH:O	2.16	0.46
1:A:618:PHE:CZ	1:A:740:ARG:HD3	2.51	0.46
1:A:220:GLN:HG2	2:B:136:PRO:O	2.15	0.46
2:B:169:GLN:NE2	8:B:2127:HOH:O	2.32	0.46
1:E:501:PHE:HB3	1:E:565:VAL:HG13	1.97	0.46
1:A:447:PRO:HD3	8:A:2212:HOH:O	2.16	0.46
1:E:249:TRP:CZ2	1:E:251:PRO:HB3	2.50	0.46
1:A:186:GLY:CA	1:A:584:GLY:N	2.75	0.45
1:E:494:LEU:HD23	1:E:502:ILE:HG23	1.98	0.45
1:E:648:GLU:CG	1:E:681:ARG:NH1	2.76	0.45
1:E:117:TRP:CE2	1:E:516:LYS:HG3	2.51	0.45
3:C:145:ASN:OD1	3:C:193:THR:HG23	2.16	0.45
3:G:208:TRP:O	3:G:212:PHE:CD2	2.69	0.45
2:B:35:ASN:HB3	2:B:116:CYS:HB2	1.99	0.45
1:A:241:THR:HG21	2:B:14:VAL:HB	1.98	0.45
1:E:413:ARG:H	1:E:413:ARG:NH1	2.14	0.45
3:G:60:LEU:HD23	3:G:63:LEU:HD12	1.96	0.45
1:E:462:TYR:CE1	1:E:463:VAL:O	2.69	0.45
1:E:435:LEU:HB3	1:E:459:LEU:CD1	2.46	0.45
1:E:369:PRO:CG	1:E:494:LEU:HB3	2.46	0.45
1:E:75:ARG:NH1	1:E:220:GLN:NE2	2.55	0.45
1:E:160:TRP:CD1	1:E:160:TRP:O	2.70	0.45
2:F:19:CYS:HB2	2:F:131:CYS:HB2	1.98	0.45
1:A:430:TYR:HB2	1:A:431:PRO:CD	2.46	0.45
1:E:426:THR:C	1:E:428:GLU:N	2.70	0.45
1:E:614:PRO:HB3	1:E:738:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:VAL:CG1	1:A:453:LYS:HE3	2.47	0.45
1:A:743:LYS:CG	8:A:2364:HOH:O	2.65	0.45
1:E:457:LYS:HD3	8:E:2064:HOH:O	2.15	0.45
1:A:389:SER:CA	1:A:595:GLN:HE22	2.30	0.45
3:C:64:LEU:HD22	7:C:1252:MQ7:C5	2.45	0.45
1:E:93:ASP:CG	1:E:758:ARG:HH22	2.19	0.45
1:E:427:GLY:O	1:E:428:GLU:O	2.35	0.45
1:E:500:PRO:HD3	1:E:567:ARG:O	2.15	0.45
1:A:422:GLU:N	1:A:423:PRO:CD	2.79	0.45
2:B:50:VAL:HG13	2:B:181:PRO:HB2	1.98	0.45
1:E:537:TRP:O	1:E:537:TRP:CE3	2.69	0.45
1:E:625:ARG:HH22	5:E:1765:MGD:H15	1.63	0.45
2:F:46:TYR:HB2	8:F:2034:HOH:O	2.15	0.45
2:F:184:LYS:HE2	8:F:2120:HOH:O	2.17	0.45
3:G:170:TRP:CE3	3:G:171:ALA:N	2.85	0.45
1:E:127:LYS:HD3	8:E:2082:HOH:O	2.16	0.45
1:A:630:THR:H	1:A:634:THR:CG2	2.27	0.45
2:F:78:THR:HG23	2:F:79:LYS:N	2.31	0.45
1:E:457:LYS:CD	8:E:2064:HOH:O	2.64	0.45
3:G:86:SER:O	3:G:87:PRO:C	2.53	0.45
3:G:73:PHE:HA	8:G:2021:HOH:O	2.17	0.45
1:A:430:TYR:HB2	1:A:431:PRO:HD3	1.98	0.45
1:E:462:TYR:CD2	1:E:476:ALA:HA	2.51	0.45
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.81	0.45
3:C:153:PRO:HB3	8:C:2062:HOH:O	2.15	0.45
1:E:497:HIS:HB3	1:E:499:THR:O	2.17	0.45
2:B:166:ARG:HD2	8:B:2124:HOH:O	2.16	0.45
3:C:193:THR:HG23	3:C:193:THR:O	2.17	0.45
1:A:471:GLU:HB2	1:A:702:LYS:O	2.16	0.45
3:G:240:LEU:C	3:G:240:LEU:CD1	2.84	0.45
1:A:588:GLY:HA3	8:A:2152:HOH:O	2.17	0.45
1:E:717:ASN:ND2	8:E:2415:HOH:O	2.49	0.45
1:E:557:THR:O	1:E:561:MET:HG3	2.17	0.45
1:A:677:GLU:C	1:A:678:GLY:O	2.55	0.45
1:E:113:ARG:CB	8:E:2042:HOH:O	2.64	0.45
1:A:423:PRO:HB2	1:A:432:ILE:HD12	1.97	0.45
3:C:25:VAL:HB	3:C:60:ASP:OD2	2.17	0.45
1:A:302:GLU:HG3	1:A:302:GLU:O	2.15	0.45
1:E:283:THR:HG23	1:E:590:ILE:HG13	1.99	0.45
1:E:604:PRO:CA	1:E:605:LEU:HD23	2.47	0.45
2:F:146:GLU:O	2:F:148:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ARG:HG2	8:B:2144:HOH:O	2.17	0.45
2:F:54:ARG:NH1	2:F:56:GLU:OE2	2.42	0.45
2:B:150:SER:O	2:B:154:LYS:HG2	2.17	0.45
1:E:391:PRO:HD2	1:E:595:GLN:OE1	2.17	0.45
1:A:429:PRO:HD2	8:A:2202:HOH:O	2.17	0.45
1:E:75:ARG:HD2	1:E:220:GLN:NE2	2.26	0.45
1:E:195:ILE:CD1	1:E:363:PHE:CE2	3.00	0.45
2:B:130:ALA:HB3	4:B:1195:SF4:S2	2.57	0.45
1:E:335:VAL:CG1	1:E:335:VAL:O	2.65	0.45
3:C:40:LEU:HD13	3:C:117:ALA:CB	2.47	0.45
1:A:418:GLN:NE2	1:A:730:GLY:O	2.50	0.45
3:G:134:LEU:N	8:G:2035:HOH:O	2.49	0.45
1:E:255:GLY:HA2	1:E:337:TYR:CE1	2.52	0.45
1:E:591:GLU:O	1:E:603:GLN:CD	2.55	0.44
1:E:284:VAL:HG12	1:E:592:LEU:CD1	2.47	0.44
1:A:504:LEU:HD22	1:A:505:ARG:N	2.31	0.44
1:A:653:LYS:HD3	8:B:2025:HOH:O	2.17	0.44
1:E:297:THR:CG2	1:E:299:GLU:N	2.73	0.44
1:E:114:VAL:HG21	8:E:2038:HOH:O	2.17	0.44
1:A:66:GLU:HB3	8:A:2017:HOH:O	2.17	0.44
3:C:25:VAL:HG23	3:C:96:LEU:HD21	2.00	0.44
1:A:727:PRO:HA	8:A:2197:HOH:O	2.16	0.44
1:A:573:GLU:O	1:A:577:LYS:HG3	2.16	0.44
1:A:60:ASN:HB2	8:A:2022:HOH:O	2.16	0.44
2:F:82:LEU:HD12	2:F:84:LEU:HD11	1.98	0.44
1:A:644:ASP:HA	1:A:645:PRO:HD3	1.72	0.44
2:B:35:ASN:ND2	2:B:106:TYR:OH	2.50	0.44
1:E:597:PHE:CD1	1:E:597:PHE:O	2.70	0.44
3:C:13:PHE:CZ	3:C:247:GLN:HG2	2.52	0.44
1:A:602:HIS:CE1	1:A:606:PRO:CD	2.94	0.44
1:E:71:ASN:HD21	1:E:73:LYS:HB2	1.83	0.44
3:C:89:ILE:HD12	7:C:1252:MQ7:C5	2.46	0.44
3:G:206:GLY:H	3:G:209:TYR:HB2	1.83	0.44
1:E:633:ARG:HB2	5:E:1765:MGD:H2'	2.00	0.44
1:E:708:LEU:O	1:E:712:ARG:CD	2.64	0.44
3:C:128:LEU:HA	8:C:2050:HOH:O	2.16	0.44
1:E:502:ILE:O	1:E:563:THR:HA	2.16	0.44
2:B:143:GLY:N	2:B:152:VAL:CG2	2.80	0.44
1:E:196:ASP:OD1	1:E:360:PRO:HA	2.17	0.44
1:A:98:PRO:HD3	1:A:481:PRO:HD2	1.99	0.44
1:E:275:ASP:C	1:E:275:ASP:OD1	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:630:THR:H	1:E:634:THR:HG21	1.81	0.44
1:A:335:VAL:HG13	1:A:733:GLY:N	2.32	0.44
1:A:457:LYS:HD2	8:A:2219:HOH:O	2.17	0.44
3:C:71:ARG:HG2	3:C:72:PHE:N	2.33	0.44
3:C:220:THR:HA	3:C:227:ALA:HA	1.98	0.44
1:A:626:SER:HB2	1:A:696:VAL:HG11	2.00	0.44
3:C:172:ALA:HA	3:C:175:PRO:CG	2.35	0.44
1:A:95:LEU:N	1:A:467:VAL:O	2.41	0.44
3:C:63:ILE:O	3:C:67:GLU:HB3	2.16	0.44
3:C:17:THR:HG22	3:C:67:GLU:HG3	1.89	0.44
1:A:336:TRP:HA	1:A:735:ARG:HG3	1.98	0.44
1:A:647:ASN:HD21	1:A:713:GLY:CA	2.30	0.44
1:E:45:GLU:HB2	1:E:485:TYR:CB	2.48	0.44
1:A:552:GLY:O	8:A:2261:HOH:O	2.21	0.44
3:C:186:LEU:HD22	3:G:149:GLY:HA2	2.00	0.44
1:A:587:SER:O	1:A:589:LYS:CE	2.65	0.44
1:E:607:VAL:CG2	8:E:2144:HOH:O	2.63	0.44
1:E:297:THR:HG22	1:E:299:GLU:N	2.32	0.44
2:B:72:THR:CG2	2:B:73:GLY:N	2.80	0.44
3:C:31:VAL:HG12	3:C:53:ALA:HB2	1.99	0.44
1:A:558:MET:CE	1:A:558:MET:HA	2.41	0.44
1:E:208:HIS:HE1	1:E:218:GLN:HE22	1.65	0.44
1:A:132:ARG:HD3	8:A:2075:HOH:O	2.14	0.44
3:C:227:ALA:HB3	3:C:228:PRO:HD3	2.00	0.44
1:E:187:ARG:HB3	1:E:188:PRO:CD	2.47	0.44
1:A:605:LEU:N	1:A:606:PRO:HD3	2.28	0.44
1:A:65:VAL:HG13	1:A:78:LEU:CD2	2.48	0.44
1:A:647:ASN:HD21	1:A:713:GLY:HA3	1.83	0.44
2:F:27:ASN:O	2:F:28:GLU:C	2.56	0.44
1:A:249:TRP:O	1:A:251:PRO:HD3	2.18	0.44
1:A:498:LYS:HE3	8:A:2107:HOH:O	2.15	0.44
1:E:257:ASP:OD2	5:E:1766:MGD:N1	2.43	0.44
1:A:358:GLY:N	1:A:363:PHE:O	2.48	0.44
1:A:523:ARG:HG2	1:A:523:ARG:NH1	2.32	0.44
2:F:86:ASP:OD1	2:F:88:LYS:HB2	2.18	0.44
1:A:319:MET:HE1	1:A:328:LEU:CD1	2.46	0.44
1:A:712:ARG:NH1	8:A:2345:HOH:O	2.49	0.44
1:A:596:ARG:CZ	1:A:600:ALA:CB	2.96	0.44
1:E:74:SER:HB2	1:E:77:ARG:O	2.18	0.44
1:E:604:PRO:O	1:E:606:PRO:HD2	2.15	0.44
1:A:488:ARG:HG2	1:A:489:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ASP:OD1	1:E:473:VAL:HG21	2.18	0.44
7:G:1251:MQ7:H2M1	7:G:1251:MQ7:H111	1.66	0.44
3:C:161:LEU:HD12	3:C:179:LEU:HD12	1.99	0.44
1:E:730:GLY:N	8:E:2249:HOH:O	2.42	0.44
1:E:187:ARG:NH1	8:E:2107:HOH:O	2.47	0.44
2:F:6:MET:HG2	2:F:175:LEU:HD22	2.00	0.44
2:B:39:ARG:HD2	2:B:56:GLU:OE2	2.18	0.44
1:E:77:ARG:NH1	2:F:135:CYS:O	2.51	0.43
1:E:292:HIS:HE1	1:E:605:LEU:O	2.01	0.43
1:A:88:THR:HG23	1:A:468:LEU:HD21	1.99	0.43
3:G:223:GLU:C	3:G:225:LEU:H	2.21	0.43
1:E:647:ASN:C	1:E:648:GLU:CG	2.87	0.43
1:A:421:ILE:CG2	1:A:421:ILE:O	2.65	0.43
3:C:111:GLY:O	3:C:116:LEU:HD11	2.18	0.43
1:A:666:TYR:CE1	1:A:681:ARG:HG3	2.53	0.43
2:F:101:PRO:HD2	2:F:102:TYR:CD1	2.53	0.43
1:E:622:LEU:HD23	1:E:622:LEU:HA	1.87	0.43
1:E:622:LEU:O	1:E:623:TYR:HB3	2.18	0.43
1:E:708:LEU:CA	8:E:2407:HOH:O	2.58	0.43
3:G:223:GLU:N	8:G:2069:HOH:O	2.50	0.43
3:C:207:GLY:C	3:C:209:TRP:H	2.21	0.43
2:B:38:ILE:HD12	4:B:1194:SF4:S1	2.58	0.43
2:B:25:MET:HE3	2:B:25:MET:CA	2.42	0.43
1:E:302:GLU:HG3	1:E:307:ILE:O	2.18	0.43
1:A:38:LYS:HG2	8:A:2021:HOH:O	2.18	0.43
2:F:166:ARG:NH2	3:G:248:GLN:HG3	2.33	0.43
2:F:29:VAL:HA	2:F:30:PRO:HD3	1.63	0.43
1:E:745:GLU:HG3	8:E:2431:HOH:O	2.17	0.43
1:A:257:ASP:OD2	8:A:2138:HOH:O	2.21	0.43
1:A:425:ILE:HD11	1:A:451:ARG:HG2	2.00	0.43
1:A:604:PRO:HA	1:A:605:LEU:HD23	2.00	0.43
1:A:81:ARG:HD2	1:A:630:THR:OG1	2.18	0.43
1:A:539:THR:HG21	1:A:541:GLU:HG2	2.00	0.43
1:E:48:PHE:CE1	1:E:631:PHE:CE1	3.06	0.43
1:A:394:GLY:N	8:A:2189:HOH:O	2.52	0.43
2:F:191:GLU:HB2	8:F:2122:HOH:O	2.18	0.43
1:E:423:PRO:O	1:E:427:GLY:HA2	2.19	0.43
1:A:252:ILE:HG13	1:A:307:ILE:CD1	2.48	0.43
2:F:72:THR:HG21	2:F:89:LYS:C	2.38	0.43
1:E:186:GLY:HA3	1:E:584:GLY:CA	2.48	0.43
1:E:328:LEU:N	1:E:328:LEU:HD12	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:TYR:CE1	2:F:114:SER:HB3	2.53	0.43
2:F:35:ASN:ND2	2:F:106:TYR:OH	2.46	0.43
1:A:418:GLN:HG3	1:A:418:GLN:H	1.39	0.43
1:E:602:HIS:NE2	1:E:604:PRO:CD	2.56	0.43
1:E:346:ALA:CA	1:E:605:LEU:HD12	2.49	0.43
1:E:596:ARG:CZ	1:E:601:GLY:HA3	2.49	0.43
1:E:282:TYR:C	1:E:587:SER:HB3	2.38	0.43
1:E:407:LYS:HG3	1:E:407:LYS:O	2.18	0.43
1:A:753:THR:HG22	1:A:757:LYS:HE2	1.99	0.43
1:A:264:TRP:CZ2	1:A:315:VAL:HG11	2.53	0.43
3:C:21:HIS:CE1	3:C:64:LEU:CD1	3.01	0.43
3:G:38:HIS:CE1	3:G:105:LEU:HD13	2.53	0.43
3:G:222:GLN:CB	8:G:2069:HOH:O	2.67	0.43
2:B:1:MET:O	2:B:146:GLU:OE1	2.36	0.43
1:E:239:PHE:HB3	1:E:687:ARG:CD	2.49	0.43
1:E:457:LYS:HE2	8:E:2060:HOH:O	2.18	0.43
1:A:638:TRP:HB2	1:A:756:ALA:HB2	2.01	0.43
2:F:71:PRO:HB2	3:G:78:LEU:HD12	2.01	0.43
1:A:412:ALA:HB2	1:A:728:ILE:O	2.17	0.43
1:A:581:LEU:HD12	1:A:581:LEU:HA	1.91	0.43
1:A:335:VAL:O	1:A:337:TYR:N	2.52	0.43
3:G:247:TRP:CE2	3:G:249:GLY:HA3	2.54	0.43
1:E:422:GLU:HB2	8:E:2252:HOH:O	2.18	0.43
1:E:103:GLU:HG2	1:E:104:GLY:N	2.34	0.43
3:C:11:GLN:NE2	3:C:11:GLN:H	2.17	0.43
1:E:604:PRO:HA	1:E:605:LEU:CD2	2.47	0.43
2:B:183:LYS:NZ	2:F:157:LYS:O	2.52	0.43
1:E:630:THR:HA	5:E:1766:MGD:O17	2.17	0.43
1:E:626:SER:HB3	1:E:696:VAL:HG11	2.01	0.43
1:A:47:CYS:HB3	1:A:81:ARG:HH12	1.83	0.43
2:F:72:THR:CG2	2:F:89:LYS:HB3	2.44	0.43
1:A:477:ASP:C	1:A:478:VAL:HG23	2.39	0.43
1:E:746:ARG:CG	1:E:746:ARG:HH11	2.30	0.43
1:A:87:GLN:HG3	1:A:637:ASN:CG	2.39	0.43
1:E:595:GLN:O	1:E:595:GLN:HG3	2.15	0.43
1:A:519:TRP:CG	1:A:540:ILE:HG23	2.53	0.43
1:E:626:SER:O	1:E:628:VAL:N	2.52	0.43
3:G:112:GLN:O	3:G:114:ALA:N	2.52	0.43
1:A:649:VAL:HA	1:A:695:ILE:HG22	2.00	0.43
1:A:753:THR:HG22	1:A:757:LYS:CE	2.49	0.43
3:C:150:GLY:HA2	3:G:185:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:LEU:HD12	3:G:120:LEU:HD12	2.01	0.43
1:A:386:GLY:HA3	1:A:391:PRO:HB2	2.00	0.43
3:C:171:TRP:CE3	3:C:172:ALA:HB2	2.54	0.43
1:E:100:ILE:HG12	1:E:478:VAL:CG1	2.49	0.43
1:A:717:ASN:HA	1:A:720:GLN:OE1	2.19	0.43
1:E:470:GLN:O	1:E:471:GLU:C	2.57	0.43
1:A:629:HIS:CB	1:A:634:THR:HG21	2.48	0.43
1:A:124:ILE:HG12	1:A:463:VAL:HG21	1.99	0.43
3:G:217:LEU:CD2	8:G:2065:HOH:O	2.66	0.43
1:A:657:LYS:O	1:A:659:LEU:O	2.35	0.43
3:C:40:LEU:HD12	3:C:40:LEU:HA	1.91	0.43
1:A:183:TRP:CH2	1:A:596:ARG:CD	2.90	0.42
1:A:625:ARG:HD2	5:A:1766:MGD:C17	2.49	0.42
1:E:469:PRO:O	1:E:706:MET:SD	2.77	0.42
1:A:536:PRO:HG2	1:A:537:TRP:N	2.32	0.42
1:A:482:GLU:HG2	1:A:483:ALA:N	2.34	0.42
1:A:338:GLY:HA3	1:A:724:LYS:HG2	2.00	0.42
3:G:58:LEU:HD12	3:G:58:LEU:O	2.19	0.42
3:C:21:HIS:CE1	3:C:64:LEU:HG	2.50	0.42
1:A:189:ILE:O	1:A:194:PRO:HD3	2.19	0.42
1:E:281:LYS:HG3	1:E:282:TYR:CD1	2.54	0.42
1:A:73:LYS:HG3	1:A:501:PHE:HZ	1.83	0.42
1:E:186:GLY:N	1:E:583:PHE:HA	2.28	0.42
2:F:164:VAL:HG12	2:F:167:PRO:HB3	2.00	0.42
2:B:36:LEU:HD12	2:B:37:TRP:N	2.34	0.42
1:A:498:LYS:HD2	8:A:2241:HOH:O	2.17	0.42
3:C:215:LEU:O	3:C:216:LEU:C	2.57	0.42
1:A:572:LEU:O	1:A:576:GLU:HB2	2.18	0.42
1:E:349:TYR:CE1	1:E:605:LEU:HD11	2.53	0.42
1:E:172:LEU:HB3	5:E:1765:MGD:H23	2.01	0.42
1:E:574:ASP:O	1:E:578:GLU:HG3	2.19	0.42
1:E:702:LYS:HE3	1:E:718:TYR:CE2	2.54	0.42
1:E:707:ARG:NE	8:E:2404:HOH:O	2.50	0.42
8:F:2052:HOH:O	3:G:88:ILE:HG13	2.18	0.42
3:G:117:TRP:CB	8:G:2034:HOH:O	2.67	0.42
2:F:132:VAL:HA	2:F:140:ARG:HG3	2.01	0.42
1:A:77:ARG:HD2	2:B:138:TYR:CE2	2.55	0.42
1:E:650:TRP:O	1:E:693:VAL:HG22	2.19	0.42
3:C:241:LEU:HD12	3:C:242:LEU:N	2.34	0.42
1:E:239:PHE:HB3	1:E:687:ARG:HD2	2.00	0.42
1:A:471:GLU:OE2	1:A:718:TYR:OH	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:LEU:CD2	1:E:741:LEU:CD2	2.96	0.42
1:A:671:ASN:HD22	1:A:671:ASN:C	2.22	0.42
1:A:132:ARG:HG2	1:A:132:ARG:O	2.20	0.42
1:E:151:TRP:O	1:E:156:LEU:HB3	2.19	0.42
2:F:10:LEU:HD22	2:F:53:PHE:O	2.19	0.42
1:E:183:TRP:CG	1:E:593:TYR:CD1	3.07	0.42
1:E:634:THR:H	1:E:635:GLN:HE22	1.66	0.42
1:E:636:ASN:HB2	1:E:706:MET:HE3	2.01	0.42
1:A:95:LEU:HG	1:A:467:VAL:O	2.19	0.42
1:A:336:TRP:HB3	1:A:337:TYR:CD1	2.53	0.42
1:A:453:LYS:HB3	1:A:475:TRP:CH2	2.54	0.42
3:G:70:ARG:HG3	3:G:71:PHE:CD2	2.54	0.42
1:E:278:TYR:OH	1:E:357:TYR:HB3	2.19	0.42
2:B:172:ARG:HD3	8:F:2126:HOH:O	2.20	0.42
3:G:23:LEU:HD22	3:G:62:ILE:HD12	2.01	0.42
1:A:186:GLY:N	1:A:583:PHE:C	2.68	0.42
3:G:207:PHE:CE2	3:G:211:LEU:CD1	2.61	0.42
1:A:647:ASN:C	1:A:648:GLU:CG	2.73	0.42
1:E:620:ARG:O	1:E:620:ARG:HG2	2.19	0.42
1:E:648:GLU:CG	1:E:681:ARG:HH12	2.21	0.42
3:C:145:ASN:HD21	3:C:147:LEU:HB2	1.84	0.42
1:E:90:TYR:OH	1:E:509:HIS:CE1	2.65	0.42
1:E:669:LEU:HD21	1:E:741:LEU:HD22	1.98	0.42
8:F:2029:HOH:O	3:G:250:LEU:CD1	2.65	0.42
1:A:355:GLY:O	1:A:359:ARG:HG3	2.19	0.42
1:E:327:VAL:HG13	1:E:362:GLY:HA2	2.01	0.42
1:A:589:LYS:O	1:A:592:LEU:CB	2.67	0.42
3:G:154:THR:HG21	3:G:238:ARG:CG	2.45	0.42
1:A:80:PRO:HG2	1:A:627:PRO:O	2.18	0.42
3:C:108:LEU:HB3	3:C:110:LYS:CG	2.50	0.42
1:E:79:CYS:HB2	1:E:80:PRO:CD	2.50	0.42
3:G:165:LEU:HG	3:G:227:PRO:HB2	2.01	0.42
3:G:134:LEU:HG	8:G:2035:HOH:O	2.19	0.42
2:B:7:ALA:HB3	2:B:141:THR:OG1	2.20	0.42
1:E:293:VAL:HG13	1:E:293:VAL:O	2.18	0.42
1:A:265:ILE:CG2	1:A:293:VAL:HG21	2.49	0.42
3:G:206:GLY:N	3:G:209:TYR:HB2	2.35	0.42
1:E:649:VAL:HG13	1:E:695:ILE:HG23	1.99	0.42
1:E:613:GLU:HB3	1:E:614:PRO:HD2	2.01	0.42
1:E:683:LYS:O	1:E:683:LYS:HG2	2.18	0.42
1:A:555:LEU:HA	1:A:555:LEU:HD23	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ALA:HA	1:E:380:PRO:HD2	2.02	0.42
1:A:117:TRP:CE2	1:A:516:LYS:HG3	2.54	0.42
1:A:582:PRO:CB	8:A:2274:HOH:O	1.94	0.42
1:E:602:HIS:CE1	1:E:606:PRO:CD	3.02	0.42
1:E:391:PRO:C	1:E:413:ARG:CG	2.88	0.42
1:A:214:THR:HG21	1:A:627:PRO:O	2.19	0.42
3:C:109:GLY:C	3:C:110:LYS:HG2	2.39	0.42
3:C:241:LEU:HD12	3:C:241:LEU:O	2.17	0.42
1:A:396:HIS:CD2	1:A:403:PRO:CB	3.03	0.42
1:A:37:VAL:HG12	1:A:38:LYS:H	1.82	0.42
1:A:39:SER:CB	8:A:2005:HOH:O	2.64	0.42
1:E:315:VAL:O	1:E:319:MET:HG2	2.20	0.42
3:G:165:LEU:C	3:G:167:LYS:H	2.22	0.42
1:E:525:LEU:O	1:E:529:LEU:HG	2.20	0.42
1:A:186:GLY:N	1:A:583:PHE:CA	2.83	0.42
1:A:519:TRP:CD2	1:A:540:ILE:CG2	3.02	0.42
1:A:533:GLN:HE21	1:A:533:GLN:H	1.68	0.42
1:A:629:HIS:CB	1:A:634:THR:CG2	2.98	0.42
3:C:173:LEU:O	3:C:177:ARG:HG3	2.20	0.42
1:A:187:ARG:HB3	1:A:188:PRO:HD2	2.02	0.42
1:A:64:LYS:HE3	2:B:26:GLU:HB2	2.02	0.42
1:E:138:GLU:OE2	1:E:402:LYS:HB2	2.19	0.42
1:E:183:TRP:CD1	1:E:593:TYR:CE1	3.08	0.41
1:E:708:LEU:CB	8:E:2407:HOH:O	2.68	0.41
1:A:667:VAL:HG11	1:A:741:LEU:HB3	2.01	0.41
1:A:71:ASN:ND2	1:A:74:SER:H	2.08	0.41
1:E:642:GLU:OE2	2:F:31:PRO:HA	2.20	0.41
1:A:310:GLN:CG	8:A:2160:HOH:O	2.67	0.41
1:A:144:GLY:HA2	1:A:438:TYR:O	2.20	0.41
3:G:81:SER:HB2	3:G:83:HIS:CD2	2.55	0.41
1:A:342:TYR:CG	1:A:605:LEU:HA	2.56	0.41
3:G:206:GLY:O	3:G:209:TYR:HB3	2.20	0.41
1:E:252:ILE:CG1	1:E:256:THR:HG22	2.49	0.41
1:A:502:ILE:N	1:A:564:LEU:O	2.49	0.41
1:E:237:PRO:CB	1:E:689:ARG:HD3	2.50	0.41
2:B:71:PRO:HB2	3:C:79:LEU:HD11	2.01	0.41
1:A:224:LEU:HB3	8:A:2124:HOH:O	2.20	0.41
1:A:583:PHE:C	1:A:584:GLY:CA	2.77	0.41
1:A:292:HIS:CD2	1:A:604:PRO:HB2	2.55	0.41
2:B:47:PRO:C	2:B:48:ASN:OD1	2.57	0.41
1:A:77:ARG:HH12	2:B:138:TYR:HE2	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:CYS:CB	8:E:2452:HOH:O	2.37	0.41
1:E:430:TYR:HB2	1:E:431:PRO:CD	2.50	0.41
1:A:534:TYR:O	1:A:535:PHE:CD1	2.73	0.41
1:E:553:LEU:HD23	1:E:553:LEU:HA	1.76	0.41
8:B:2074:HOH:O	3:C:78:TRP:HE3	2.02	0.41
1:E:42:GLN:CB	1:E:53:ILE:HG13	2.51	0.41
1:E:64:LYS:HD2	8:E:2046:HOH:O	2.19	0.41
3:G:142:LEU:HD23	3:G:197:ALA:HB1	2.02	0.41
2:F:135:CYS:SG	2:F:135:CYS:CA	3.00	0.41
1:E:607:VAL:HG22	1:E:609:THR:OG1	2.20	0.41
1:A:717:ASN:HD22	5:A:1765:MGD:H192	1.68	0.41
1:E:112:TYR:CE1	1:E:474:MET:O	2.73	0.41
3:C:251:LEU:HD23	8:C:2087:HOH:O	2.20	0.41
1:A:510:GLU:H	1:A:510:GLU:HG3	1.62	0.41
1:A:520:TRP:O	1:A:524:GLU:HG2	2.20	0.41
3:C:111:GLY:O	3:C:112:SER:HB3	2.20	0.41
1:E:548:LEU:HD23	1:E:548:LEU:HA	1.81	0.41
3:C:92:GLY:O	3:C:96:LEU:HD12	2.20	0.41
2:F:175:LEU:HD12	2:F:175:LEU:C	2.40	0.41
3:C:180:ALA:O	3:C:184:LEU:HG	2.21	0.41
1:E:629:HIS:HA	1:E:634:THR:HG21	2.01	0.41
1:A:685:THR:CG2	8:B:2026:HOH:O	2.67	0.41
1:A:693:VAL:HG21	1:A:741:LEU:HD21	2.01	0.41
1:A:70:ALA:C	8:A:2036:HOH:O	2.49	0.41
1:E:69:GLU:H	1:E:69:GLU:HG2	1.62	0.41
1:A:655:GLU:OE2	1:A:658:ARG:NH2	2.53	0.41
3:G:178:LEU:HA	3:G:178:LEU:HD23	1.84	0.41
2:B:46:TYR:HB2	2:B:47:PRO:HD3	2.03	0.41
1:E:512:LEU:O	1:E:513:PHE:HB2	2.21	0.41
2:F:46:TYR:N	8:F:2035:HOH:O	2.53	0.41
1:A:708:LEU:HB3	1:A:752:LEU:HD23	2.01	0.41
1:E:39:SER:OG	1:E:56:HIS:ND1	2.31	0.41
1:E:667:VAL:HG11	1:E:741:LEU:HD13	2.02	0.41
1:A:532:GLU:HB3	8:A:2253:HOH:O	2.20	0.41
1:A:394:GLY:HA2	8:A:2188:HOH:O	2.20	0.41
2:F:7:ALA:HB1	2:F:178:LEU:HD11	2.03	0.41
2:F:109:PRO:HG3	8:F:2015:HOH:O	2.19	0.41
2:F:96:CYS:SG	2:F:113:VAL:HG11	2.61	0.41
3:G:63:LEU:CD2	7:G:1251:MQ7:C2	2.98	0.41
1:A:318:GLU:O	1:A:322:HIS:HD2	2.03	0.41
1:E:510:GLU:HG3	1:E:510:GLU:H	1.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:CG1	1:A:38:LYS:H	2.33	0.41
1:E:79:CYS:CB	1:E:80:PRO:CD	2.99	0.41
2:B:61:CYS:HB3	2:B:171:THR:O	2.19	0.41
3:G:83:HIS:HA	3:G:84:PRO:HD2	1.85	0.41
1:A:44:CYS:SG	1:A:46:GLY:N	2.90	0.41
2:B:128:VAL:HG11	8:B:2069:HOH:O	2.19	0.41
1:A:596:ARG:NH1	1:A:600:ALA:HB1	2.34	0.41
1:A:717:ASN:ND2	5:A:1765:MGD:H192	2.19	0.41
2:B:48:ASN:ND2	2:F:157:LYS:HE2	2.36	0.41
1:A:181:SER:HB2	1:A:189:ILE:HD12	2.03	0.41
1:A:650:TRP:O	1:A:693:VAL:HA	2.20	0.41
1:A:116:THR:CG2	1:A:119:GLU:N	2.61	0.41
2:B:18:ALA:HB3	4:B:1194:SF4:S2	2.61	0.41
1:E:680:VAL:HG22	1:E:714:ALA:HB2	2.03	0.41
2:F:71:PRO:HB2	3:G:78:LEU:CD1	2.51	0.41
3:G:23:LEU:CD2	3:G:62:ILE:HD12	2.51	0.41
2:F:174:LYS:HE2	8:F:2046:HOH:O	2.21	0.41
2:F:59:LEU:O	2:F:60:HIS:C	2.59	0.41
1:A:225:ALA:C	1:A:230:ALA:HB3	2.41	0.41
1:A:258:THR:HB	1:A:608:PHE:HA	2.03	0.41
1:A:266:HIS:C	1:A:266:HIS:CD2	2.94	0.41
1:A:289:LEU:O	1:A:293:VAL:HB	2.21	0.41
1:E:621:LEU:HD22	1:E:622:LEU:H	1.84	0.41
1:E:512:LEU:HD12	1:E:512:LEU:HA	1.79	0.41
3:G:221:TRP:CZ3	3:G:225:LEU:HD13	2.45	0.41
1:A:333:HIS:O	1:A:336:TRP:NE1	2.52	0.41
1:A:263:ALA:HB2	1:A:301:ALA:HB2	2.02	0.41
2:F:72:THR:CG2	2:F:89:LYS:O	2.64	0.41
2:F:67:VAL:CB	2:F:68:PRO:CD	2.98	0.41
1:A:327:VAL:HG13	1:A:362:GLY:HA3	2.03	0.41
1:E:174:THR:HG23	1:E:178:GLU:CG	2.48	0.41
2:B:8:ILE:HD13	2:B:55:PRO:HG2	2.02	0.41
3:G:46:ARG:NH1	3:G:106:TYR:O	2.54	0.41
3:G:100:LEU:O	3:G:103:GLY:N	2.51	0.41
3:G:47:ARG:HH21	3:G:166:LEU:HB3	1.84	0.41
3:C:157:LEU:HB3	3:C:179:LEU:HD13	2.02	0.41
1:E:64:LYS:HE3	2:F:26:GLU:HB2	2.03	0.41
3:C:201:HIS:CE1	3:C:205:GLU:HG3	2.56	0.41
2:F:118:PHE:HA	2:F:118:PHE:HD1	1.53	0.41
3:G:153:LEU:HA	3:G:153:LEU:HD23	1.93	0.41
1:A:286:PHE:CG	1:A:286:PHE:O	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:O	5:A:1766:MGD:O2B	2.39	0.41
1:E:322:HIS:O	1:E:323:LYS:O	2.39	0.41
1:E:115:ALA:HB1	1:E:119:GLU:CG	2.51	0.41
1:E:333:HIS:HB2	5:E:1766:MGD:S12	2.60	0.41
1:A:95:LEU:CG	1:A:467:VAL:O	2.68	0.41
1:A:641:MET:CE	1:A:645:PRO:HA	2.51	0.41
1:E:620:ARG:HD3	1:E:735:ARG:O	2.20	0.41
1:E:308:PRO:HD2	8:E:2195:HOH:O	2.20	0.41
2:F:3:ARG:O	2:F:145:LEU:HB2	2.20	0.41
1:A:539:THR:HG23	1:A:541:GLU:H	1.85	0.41
2:B:78:THR:CG2	8:B:2068:HOH:O	2.61	0.41
1:E:133:GLU:HB2	8:E:2086:HOH:O	2.20	0.41
1:E:340:ASP:O	1:E:344:VAL:HG23	2.20	0.41
3:G:117:TRP:HB3	8:G:2034:HOH:O	2.21	0.41
3:C:169:SER:HA	3:C:170:PRO:HD3	1.81	0.41
1:A:591:GLU:HB3	1:A:603:GLN:HE21	1.77	0.40
1:A:399:GLU:OE1	1:A:399:GLU:HA	2.22	0.40
1:E:551:LEU:O	1:E:553:LEU:CB	2.64	0.40
2:F:46:TYR:CD2	2:F:47:PRO:HD3	2.56	0.40
1:A:435:LEU:N	1:A:461:LEU:O	2.53	0.40
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.94	0.40
2:B:9:ASP:HA	2:B:178:LEU:HB2	2.03	0.40
3:C:12:GLU:OE1	3:C:15:HIS:ND1	2.43	0.40
1:A:389:SER:HA	1:A:595:GLN:NE2	2.36	0.40
1:A:608:PHE:CE1	1:A:608:PHE:O	2.67	0.40
1:E:391:PRO:O	1:E:413:ARG:CG	2.66	0.40
1:A:239:PHE:HB3	1:A:687:ARG:CB	2.49	0.40
1:A:116:THR:HG23	1:A:118:GLU:OE1	2.21	0.40
3:C:128:LEU:HD23	3:C:156:ALA:CB	2.51	0.40
1:E:671:ASN:ND2	1:E:673:ASP:N	2.65	0.40
2:B:78:THR:CG2	2:B:80:ASP:H	2.33	0.40
1:E:80:PRO:HD3	2:F:18:ALA:HB2	2.04	0.40
1:A:94:ARG:O	1:A:94:ARG:HG3	2.22	0.40
2:B:54:ARG:NH2	2:B:187:THR:O	2.51	0.40
1:A:142:PHE:O	1:A:165:ALA:HA	2.21	0.40
1:E:494:LEU:CD2	1:E:502:ILE:HG23	2.52	0.40
1:A:477:ASP:O	1:A:478:VAL:HG23	2.20	0.40
1:A:539:THR:HG22	1:A:542:GLU:H	1.86	0.40
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.97	0.40
3:G:217:LEU:HD22	8:G:2065:HOH:O	2.21	0.40
1:E:159:ALA:O	1:E:380:PRO:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:CYS:SG	2:F:20:ALA:N	2.95	0.40
1:A:638:TRP:HB2	1:A:756:ALA:CB	2.51	0.40
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.90	0.40
1:E:413:ARG:HH11	1:E:413:ARG:HD2	1.72	0.40
1:A:42:GLN:OE1	1:A:505:ARG:HB2	2.22	0.40
3:G:38:HIS:O	3:G:40:LYS:N	2.55	0.40
1:A:107:ARG:O	1:A:457:LYS:HE3	2.22	0.40
3:G:53:LEU:O	3:G:99:PHE:HE1	2.04	0.40
1:A:213:ASP:C	1:A:213:ASP:OD1	2.59	0.40
1:E:466:ASP:OD1	1:E:473:VAL:CG2	2.69	0.40
1:E:624:GLY:HA3	1:E:694:TYR:OH	2.22	0.40
3:G:222:GLN:HB2	8:G:2069:HOH:O	2.21	0.40
1:E:510:GLU:CG	8:E:2299:HOH:O	2.51	0.40
3:G:165:LEU:HD22	3:G:224:ARG:HH11	1.85	0.40
3:C:51:LEU:O	3:C:54:LEU:HB2	2.22	0.40
1:A:532:GLU:HG2	1:A:532:GLU:H	1.48	0.40
1:E:266:HIS:HB2	1:E:293:VAL:HG13	2.04	0.40
1:A:197:TRP:HB2	1:A:221:ASP:HB3	2.02	0.40

All (3) 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:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.32	0.88
1:A:399:GLU:OE2	1:E:134:LYS:N[2_674]	1.51	0.69
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	1.91	0.29

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	733/765 (96%)	651 (89%)	46 (6%)	36 (5%)	3 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	733/765 (96%)	634 (86%)	65 (9%)	34 (5%)	3	17
2	B	192/195 (98%)	176 (92%)	12 (6%)	4 (2%)	9	37
2	F	192/195 (98%)	181 (94%)	7 (4%)	4 (2%)	9	37
3	C	249/253 (98%)	232 (93%)	12 (5%)	5 (2%)	9	38
3	G	249/253 (98%)	220 (88%)	20 (8%)	9 (4%)	4	24
All	All	2348/2426 (97%)	2094 (89%)	162 (7%)	92 (4%)	4	22

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TRP
1	A	340	ASP
1	A	428	GLU
1	A	429	PRO
1	A	430	TYR
1	A	431	PRO
1	A	535	PHE
1	A	562	GLY
1	A	570	PRO
1	A	586	ALA
1	A	587	SER
1	A	592	LEU
1	A	593	TYR
1	A	605	LEU
1	A	678	GLY
1	A	687	ARG
1	A	730	GLY
2	B	193	HIS
3	C	208	PHE
3	C	250	GLY
1	E	92	PRO
1	E	93	ASP
1	E	109	GLU
1	E	324	PRO
1	E	396	HIS
1	E	397	GLU
1	E	428	GLU
1	E	429	PRO
1	E	552	GLY
1	E	567	ARG

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Mol	Chain	Res	Type
1	E	583	PHE
1	E	593	TYR
1	E	607	VAL
1	E	631	PHE
1	E	678	GLY
1	E	686	ALA
2	F	46	TYR
3	G	108	GLY
3	G	110	GLY
3	G	222	GLN
1	A	365	ILE
1	A	399	GLU
1	A	434	GLY
1	A	582	PRO
1	A	631	PHE
2	B	17	ALA
3	C	112	SER
3	C	172	ALA
1	E	337	TYR
1	E	391	PRO
1	E	570	PRO
1	E	606	PRO
1	E	685	THR
3	G	39	LEU
3	G	51	TYR
3	G	113	ARG
1	A	398	PRO
1	A	633	ARG
2	B	115	LYS
3	C	113	GLN
1	E	466	ASP
1	E	469	PRO
1	E	471	GLU
1	E	513	PHE
1	E	763	ARG
2	F	45	GLU
2	F	178	LEU
2	F	179	ASN
1	A	389	SER
1	A	478	VAL
1	A	607	VAL
1	E	478	VAL

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Mol	Chain	Res	Type
1	E	627	PRO
3	G	38	HIS
1	A	216	ASN
1	A	387	GLY
1	A	597	PHE
1	A	598	LYS
1	A	610	PRO
1	E	70	ALA
1	E	604	PRO
3	G	167	LYS
3	G	207	PHE
1	A	609	THR
1	E	468	LEU
2	B	47	PRO
1	E	610	PRO
1	A	584	GLY
1	A	684	PRO
1	E	434	GLY
1	E	609	THR
1	A	362	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	610/632 (96%)	494 (81%)	116 (19%)	2	8
1	E	610/632 (96%)	502 (82%)	108 (18%)	2	10
2	B	162/163 (99%)	144 (89%)	18 (11%)	8	29
2	F	162/163 (99%)	146 (90%)	16 (10%)	10	34
3	C	185/187 (99%)	161 (87%)	24 (13%)	5	21
3	G	185/187 (99%)	163 (88%)	22 (12%)	6	25
All	All	1914/1964 (98%)	1610 (84%)	304 (16%)	3	13

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	43	ILE
1	A	61	ARG
1	A	65	VAL
1	A	77	ARG
1	A	79	CYS
1	A	87	GLN
1	A	97	ARG
1	A	103	GLU
1	A	106	GLN
1	A	111	LYS
1	A	116	THR
1	A	119	GLU
1	A	126	LYS
1	A	134	LYS
1	A	156	LEU
1	A	167	LYS
1	A	174	THR
1	A	187	ARG
1	A	189	ILE
1	A	209	HIS
1	A	213	ASP
1	A	214	THR
1	A	217	THR
1	A	231	LYS
1	A	252	ILE
1	A	256	THR
1	A	260	LEU
1	A	281	LYS
1	A	283	THR
1	A	286	PHE
1	A	289	LEU
1	A	297	THR
1	A	299	GLU
1	A	302	GLU
1	A	305	THR
1	A	323	LYS
1	A	327	VAL
1	A	335	VAL
1	A	368	SER
1	A	371	LEU
1	A	372	GLU
1	A	378	PRO

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Mol	Chain	Res	Type
1	A	379	LEU
1	A	382	GLU
1	A	388	CYS
1	A	395	ASP
1	A	413	ARG
1	A	414	SER
1	A	415	THR
1	A	418	GLN
1	A	421	ILE
1	A	428	GLU
1	A	433	LYS
1	A	440	ILE
1	A	441	ASN
1	A	454	GLU
1	A	457	LYS
1	A	470	GLN
1	A	477	ASP
1	A	478	VAL
1	A	484	THR
1	A	510	GLU
1	A	512	LEU
1	A	515	THR
1	A	528	ARG
1	A	529	LEU
1	A	532	GLU
1	A	533	GLN
1	A	538	LYS
1	A	539	THR
1	A	540	ILE
1	A	541	GLU
1	A	542	GLU
1	A	550	SER
1	A	553	LEU
1	A	555	LEU
1	A	558	MET
1	A	561	MET
1	A	578	GLU
1	A	580	ARG
1	A	587	SER
1	A	589	LYS
1	A	591	GLU
1	A	592	LEU

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Mol	Chain	Res	Type
1	A	594	CYS
1	A	595	GLN
1	A	596	ARG
1	A	597	PHE
1	A	603	GLN
1	A	605	LEU
1	A	608	PHE
1	A	616	GLU
1	A	621	LEU
1	A	633	ARG
1	A	647	ASN
1	A	648	GLU
1	A	651	ILE
1	A	662	LYS
1	A	663	GLU
1	A	671	ASN
1	A	672	GLN
1	A	680	VAL
1	A	683	LYS
1	A	685	THR
1	A	702	LYS
1	A	708	LEU
1	A	721	THR
1	A	724	LYS
1	A	725	LEU
1	A	736	VAL
1	A	739	VAL
1	A	741	LEU
1	A	743	LYS
1	A	746	ARG
1	A	762	GLU
2	B	1	MET
2	B	25	MET
2	B	39	ARG
2	B	69	VAL
2	B	72	THR
2	B	78	THR
2	B	105	ARG
2	B	114	SER
2	B	117	THR
2	B	118	PHE
2	B	125	LYS

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Mol	Chain	Res	Type
2	B	131	CYS
2	B	140	ARG
2	B	152	VAL
2	B	154	LYS
2	B	164	VAL
2	B	175	LEU
2	B	187	THR
3	C	11	GLN
3	C	17	THR
3	C	18	ASN
3	C	20	LEU
3	C	21	HIS
3	C	40	LEU
3	C	63	ILE
3	C	67	GLU
3	C	71	ARG
3	C	75	THR
3	C	79	LEU
3	C	110	LYS
3	C	130	TYR
3	C	140	ASN
3	C	145	ASN
3	C	147	LEU
3	C	155	THR
3	C	163	LEU
3	C	193	THR
3	C	216	LEU
3	C	225	ARG
3	C	232	LEU
3	C	241	LEU
3	C	249	GLN
1	E	65	VAL
1	E	69	GLU
1	E	101	ARG
1	E	111	LYS
1	E	113	ARG
1	E	114	VAL
1	E	119	GLU
1	E	126	LYS
1	E	145	HIS
1	E	172	LEU
1	E	174	THR

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Mol	Chain	Res	Type
1	E	187	ARG
1	E	208	HIS
1	E	209	HIS
1	E	213	ASP
1	E	214	THR
1	E	217	THR
1	E	224	LEU
1	E	240	SER
1	E	250	LEU
1	E	256	THR
1	E	260	LEU
1	E	272	ASP
1	E	284	VAL
1	E	286	PHE
1	E	289	LEU
1	E	293	VAL
1	E	297	THR
1	E	298	PRO
1	E	299	GLU
1	E	305	THR
1	E	310	GLN
1	E	323	LYS
1	E	327	VAL
1	E	335	VAL
1	E	360	PRO
1	E	371	LEU
1	E	389	SER
1	E	395	ASP
1	E	402	LYS
1	E	413	ARG
1	E	415	THR
1	E	418	GLN
1	E	421	ILE
1	E	428	GLU
1	E	440	ILE
1	E	441	ASN
1	E	457	LYS
1	E	466	ASP
1	E	470	GLN
1	E	484	THR
1	E	488	ARG
1	E	498	LYS

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Mol	Chain	Res	Type
1	E	499	THR
1	E	504	LEU
1	E	510	GLU
1	E	512	LEU
1	E	515	THR
1	E	528	ARG
1	E	533	GLN
1	E	538	LYS
1	E	539	THR
1	E	540	ILE
1	E	541	GLU
1	E	554	ASP
1	E	555	LEU
1	E	558	MET
1	E	564	LEU
1	E	569	LYS
1	E	577	LYS
1	E	581	LEU
1	E	585	THR
1	E	591	GLU
1	E	595	GLN
1	E	596	ARG
1	E	598	LYS
1	E	602	HIS
1	E	605	LEU
1	E	607	VAL
1	E	608	PHE
1	E	609	THR
1	E	620	ARG
1	E	621	LEU
1	E	626	SER
1	E	633	ARG
1	E	647	ASN
1	E	649	VAL
1	E	651	ILE
1	E	657	LYS
1	E	667	VAL
1	E	671	ASN
1	E	672	GLN
1	E	676	LYS
1	E	680	VAL
1	E	685	THR

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Mol	Chain	Res	Type
1	E	691	ASP
1	E	693	VAL
1	E	702	LYS
1	E	708	LEU
1	E	721	THR
1	E	725	LEU
1	E	736	VAL
1	E	739	VAL
1	E	740	ARG
1	E	746	ARG
1	E	748	ARG
1	E	751	SER
1	E	752	LEU
2	F	49	LEU
2	F	68	PRO
2	F	69	VAL
2	F	72	THR
2	F	88	LYS
2	F	114	SER
2	F	117	THR
2	F	118	PHE
2	F	133	GLU
2	F	145	LEU
2	F	150	SER
2	F	152	VAL
2	F	164	VAL
2	F	171	THR
2	F	175	LEU
2	F	187	THR
3	G	10	GLN
3	G	17	ASN
3	G	20	HIS
3	G	39	LEU
3	G	40	LYS
3	G	64	TRP
3	G	66	GLU
3	G	74	THR
3	G	88	ILE
3	G	113	ARG
3	G	129	TYR
3	G	136	VAL
3	G	139	ASN

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Mol	Chain	Res	Type
3	G	144	ASN
3	G	154	THR
3	G	162	LEU
3	G	167	LYS
3	G	192	THR
3	G	196	GLU
3	G	204	GLU
3	G	215	LEU
3	G	240	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	71	ASN
1	A	83	GLN
1	A	192	HIS
1	A	209	HIS
1	A	220	GLN
1	A	247	HIS
1	A	322	HIS
1	A	367	GLN
1	A	441	ASN
1	A	470	GLN
1	A	509	HIS
1	A	533	GLN
1	A	595	GLN
1	A	602	HIS
1	A	603	GLN
1	A	647	ASN
1	A	671	ASN
1	A	672	GLN
1	A	717	ASN
2	B	27	ASN
2	B	35	ASN
2	B	48	ASN
2	B	57	GLN
2	B	77	GLN
2	B	179	ASN
3	C	9	ASN
3	C	11	GLN
3	C	21	HIS

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Mol	Chain	Res	Type
3	C	39	HIS
3	C	84	HIS
3	C	113	GLN
3	C	140	ASN
3	C	145	ASN
3	C	201	HIS
3	C	249	GLN
1	E	60	ASN
1	E	71	ASN
1	E	83	GLN
1	E	192	HIS
1	E	208	HIS
1	E	209	HIS
1	E	218	GLN
1	E	220	GLN
1	E	247	HIS
1	E	292	HIS
1	E	322	HIS
1	E	396	HIS
1	E	418	GLN
1	E	441	ASN
1	E	444	HIS
1	E	470	GLN
1	E	509	HIS
1	E	533	GLN
1	E	602	HIS
1	E	603	GLN
1	E	635	GLN
1	E	647	ASN
1	E	671	ASN
1	E	672	GLN
1	E	717	ASN
2	F	27	ASN
2	F	35	ASN
2	F	57	GLN
2	F	77	GLN
2	F	179	ASN
3	G	8	ASN
3	G	38	HIS
3	G	137	ASN
3	G	139	ASN
3	G	248	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
4	SF4	A	1764	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	A	1765	6	38,52,52	2.37	14 (36%)	43,81,81	3.12	17 (39%)
5	MGD	A	1766	6	38,52,52	2.25	11 (28%)	43,81,81	2.78	11 (25%)
4	SF4	B	1194	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1195	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1196	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1197	2	0,12,12	0.00	-	0,24,24	0.00	-
7	MQ7	C	1252	-	16,16,49	0.27	0	23,23,63	1.55	4 (17%)
4	SF4	E	1764	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	E	1765	6	38,52,52	2.12	13 (34%)	43,81,81	2.66	18 (41%)
5	MGD	E	1766	6	38,52,52	2.44	14 (36%)	43,81,81	2.47	14 (32%)
4	SF4	F	1194	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1195	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1196	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	1197	2	0,12,12	0.00	-	0,24,24	0.00	-
7	MQ7	G	1251	-	16,16,49	0.32	0	23,23,63	1.57	4 (17%)

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
4	SF4	A	1764	1	-	0/0/48/48	0/6/5/5
5	MGD	A	1765	6	-	0/18/66/66	0/6/6/6
5	MGD	A	1766	6	-	0/18/66/66	0/6/6/6
4	SF4	B	1194	2	-	0/0/48/48	0/6/5/5
4	SF4	B	1195	2	-	0/0/48/48	0/6/5/5
4	SF4	B	1196	2	-	0/0/48/48	0/6/5/5
4	SF4	B	1197	2	-	0/0/48/48	0/6/5/5
7	MQ7	C	1252	-	-	0/2/22/61	0/2/2/2
4	SF4	E	1764	1	-	0/0/48/48	0/6/5/5
5	MGD	E	1765	6	-	0/18/66/66	0/6/6/6
5	MGD	E	1766	6	-	0/18/66/66	0/6/6/6
4	SF4	F	1194	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1195	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1196	2	-	0/0/48/48	0/6/5/5
4	SF4	F	1197	2	-	0/0/48/48	0/6/5/5
7	MQ7	G	1251	-	-	0/2/22/61	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1765	MGD	C23-C14	-10.33	1.45	1.53
5	A	1766	MGD	C23-C14	-8.09	1.47	1.53
5	E	1765	MGD	C23-C14	-7.59	1.48	1.53
5	E	1766	MGD	C23-C14	-7.34	1.48	1.53
5	A	1766	MGD	C14-N15	-4.98	1.38	1.45
5	E	1766	MGD	C21-N22	-4.96	1.25	1.35
5	E	1766	MGD	C19-N18	-4.26	1.27	1.35
5	E	1766	MGD	C14-N15	-4.15	1.39	1.45
5	E	1766	MGD	C19-N19	-4.14	1.25	1.34
5	E	1766	MGD	C16-N15	-3.81	1.29	1.38
5	E	1766	MGD	O11-C11	-3.44	1.38	1.43
5	E	1765	MGD	C19-N18	-3.24	1.29	1.35
5	A	1766	MGD	PB-O2B	-3.23	1.41	1.54
5	E	1765	MGD	C19-N20	-3.07	1.29	1.35
5	A	1766	MGD	C21-N22	-3.05	1.29	1.35
5	A	1766	MGD	PA-O2A	-3.00	1.42	1.54
5	E	1765	MGD	C3'-C4'	-2.99	1.44	1.53
5	A	1765	MGD	C19-N20	-2.98	1.30	1.35
5	E	1766	MGD	O4'-C4'	-2.93	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1766	MGD	C4-N3	-2.81	1.31	1.35
5	E	1765	MGD	C2-N1	-2.71	1.30	1.35
5	E	1765	MGD	O3'-C3'	-2.62	1.36	1.43
5	A	1765	MGD	C21-N22	-2.57	1.30	1.35
5	A	1766	MGD	C19-N19	-2.50	1.28	1.34
5	A	1766	MGD	PA-O1A	-2.50	1.42	1.51
5	A	1765	MGD	O2'-C2'	-2.44	1.37	1.43
5	A	1766	MGD	O4'-C4'	-2.43	1.39	1.45
5	A	1766	MGD	C23-N22	-2.42	1.39	1.44
5	A	1765	MGD	C23-N22	-2.41	1.39	1.44
5	A	1765	MGD	O11-C23	-2.34	1.40	1.43
5	E	1766	MGD	O17-C17	-2.33	1.19	1.24
5	A	1765	MGD	O4'-C4'	-2.32	1.39	1.45
5	A	1765	MGD	O11-C11	-2.30	1.40	1.43
5	E	1765	MGD	C4-N3	-2.28	1.32	1.35
5	E	1765	MGD	O11-C11	-2.24	1.40	1.43
5	E	1766	MGD	PA-O1A	-2.22	1.43	1.51
5	E	1765	MGD	O3A-C10	-2.19	1.35	1.44
5	A	1765	MGD	PA-O2A	-2.17	1.45	1.54
5	A	1765	MGD	C19-N18	-2.13	1.31	1.35
5	A	1765	MGD	C3'-C4'	-2.13	1.47	1.53
5	E	1765	MGD	O2'-C2'	-2.11	1.37	1.43
5	E	1766	MGD	C23-N22	-2.11	1.40	1.44
5	E	1765	MGD	PA-O2A	-2.08	1.46	1.54
5	A	1765	MGD	C21-N20	-2.01	1.30	1.34
5	A	1766	MGD	O11-C23	2.16	1.46	1.43
5	E	1765	MGD	C16-C21	2.23	1.46	1.41
5	E	1766	MGD	O3'-C3'	2.48	1.48	1.43
5	E	1765	MGD	C5-C4	2.51	1.46	1.40
5	A	1766	MGD	C5-C4	2.62	1.46	1.40
5	A	1765	MGD	C5-C4	2.69	1.46	1.40
5	E	1766	MGD	C5-C4	3.62	1.48	1.40
5	A	1765	MGD	C6-C5	4.16	1.49	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1765	MGD	O11-C23-C14	-7.85	103.60	108.96
5	A	1765	MGD	C5-C6-N1	-6.25	115.04	123.59
5	E	1765	MGD	C4-C5-N7	-6.09	103.88	109.48
5	A	1765	MGD	C4-C5-N7	-5.09	104.80	109.48
5	E	1765	MGD	C5-C6-N1	-4.59	117.32	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1766	MGD	C5-C6-N1	-4.42	117.55	123.59
5	A	1765	MGD	N3-C2-N1	-4.31	120.89	127.44
7	C	1252	MQ7	C11-C3-C2	-4.22	119.48	124.30
5	E	1766	MGD	C4'-O4'-C1'	-4.18	105.12	109.72
7	G	1251	MQ7	C11-C3-C2	-4.17	119.54	124.30
5	E	1765	MGD	C1'-N9-C4	-3.70	121.37	126.94
5	A	1766	MGD	C5-C6-N1	-3.56	118.71	123.59
5	E	1765	MGD	C6-C5-C4	-3.51	116.70	120.90
5	E	1765	MGD	N3-C2-N1	-3.40	122.27	127.44
5	A	1765	MGD	N18-C19-N20	-3.37	120.01	125.53
5	A	1766	MGD	C6-C5-C4	-3.28	116.97	120.90
5	A	1766	MGD	N3-C2-N1	-3.28	122.44	127.44
5	E	1766	MGD	C4-C5-N7	-2.95	106.77	109.48
5	E	1765	MGD	O3'-C3'-C4'	-2.62	103.18	111.05
5	A	1766	MGD	O5'-C5'-C4'	-2.60	99.52	109.12
5	E	1765	MGD	C16-N15-C14	-2.56	111.76	118.65
5	A	1765	MGD	O4'-C4'-C5'	-2.52	100.29	109.32
5	A	1765	MGD	C6-C5-C4	-2.33	118.12	120.90
5	A	1766	MGD	C16-C21-N22	-2.14	116.10	118.34
7	G	1251	MQ7	C2M-C2-C3	-2.11	119.58	124.10
7	C	1252	MQ7	C2M-C2-C3	-2.11	119.59	124.10
5	E	1765	MGD	N18-C19-N20	-2.10	122.10	125.53
5	E	1765	MGD	O2A-PA-O1A	2.01	123.44	112.53
7	G	1251	MQ7	C2M-C2-C1	2.04	119.58	116.27
7	C	1252	MQ7	C2M-C2-C1	2.05	119.60	116.27
5	E	1766	MGD	O3B-PB-O5'	2.16	108.68	102.94
5	E	1765	MGD	O2B-PB-O1B	2.18	124.32	112.53
5	A	1766	MGD	O2B-PB-O3B	2.40	115.98	105.09
5	E	1766	MGD	O3'-C3'-C4'	2.49	118.52	111.05
5	E	1765	MGD	N2-C2-N1	2.52	121.37	117.20
5	E	1766	MGD	N19-C19-N20	2.52	121.38	117.20
5	E	1766	MGD	O2A-PA-O1A	2.55	126.32	112.53
5	A	1765	MGD	O2B-PB-O3B	2.55	116.67	105.09
5	A	1765	MGD	N22-C21-N20	2.57	120.71	116.62
5	A	1765	MGD	C4'-O4'-C1'	2.59	112.57	109.72
5	E	1766	MGD	C19-N20-C21	2.69	120.58	114.54
5	A	1765	MGD	PA-O3B-PB	2.92	140.93	132.73
5	E	1765	MGD	O3B-PA-O3A	3.06	111.05	102.94
5	A	1766	MGD	C2'-C1'-N9	3.07	118.97	114.29
5	A	1765	MGD	N19-C19-N18	3.14	122.40	117.20
5	E	1766	MGD	C17-N18-C19	3.15	120.32	115.94
5	A	1765	MGD	C2'-C1'-N9	3.23	119.23	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1766	MGD	C6-N1-C2	3.29	120.51	115.94
5	E	1765	MGD	N22-C21-N20	3.31	121.89	116.62
5	E	1765	MGD	O3B-PB-O5'	3.34	111.80	102.94
5	E	1766	MGD	C21-C16-N15	3.49	123.25	118.85
5	A	1766	MGD	N22-C21-N20	3.62	122.38	116.62
5	A	1765	MGD	C19-N20-C21	3.85	123.20	114.54
5	E	1765	MGD	C17-N18-C19	3.87	121.31	115.94
5	A	1765	MGD	N2-C2-N1	3.88	123.62	117.20
5	E	1766	MGD	O4'-C1'-N9	3.90	116.26	108.10
5	E	1765	MGD	C19-N20-C21	4.20	123.97	114.54
7	G	1251	MQ7	C11-C3-C4	4.48	119.53	115.53
7	C	1252	MQ7	C11-C3-C4	4.55	119.60	115.53
5	A	1766	MGD	C6-N1-C2	4.63	122.36	115.94
5	E	1766	MGD	N22-C21-N20	4.93	124.47	116.62
5	E	1765	MGD	C6-N1-C2	5.17	123.11	115.94
5	A	1765	MGD	C17-N18-C19	5.68	123.82	115.94
5	A	1766	MGD	O4'-C1'-N9	5.71	120.05	108.10
5	A	1765	MGD	C6-N1-C2	6.27	124.64	115.94
5	E	1766	MGD	O11-C23-C14	9.44	115.42	108.96
5	A	1765	MGD	O11-C23-C14	11.58	116.88	108.96
5	A	1766	MGD	O11-C23-C14	12.87	117.76	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1765	MGD	6	0
5	A	1766	MGD	5	0
4	B	1194	SF4	3	0
4	B	1195	SF4	2	0
4	B	1196	SF4	2	0
7	C	1252	MQ7	18	0
4	E	1764	SF4	1	0
5	E	1765	MGD	7	0
5	E	1766	MGD	11	0
4	F	1194	SF4	3	0
4	F	1195	SF4	2	0
4	F	1196	SF4	1	0
7	G	1251	MQ7	19	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	735/765 (96%)	0.31	45 (6%)	25	10	48, 71, 103, 158	0
1	E	735/765 (96%)	0.23	30 (4%)	41	19	46, 70, 101, 161	0
2	B	194/195 (99%)	0.08	6 (3%)	52	28	50, 66, 88, 115	0
2	F	194/195 (99%)	0.25	4 (2%)	67	44	53, 71, 91, 114	0
3	C	251/253 (99%)	0.17	12 (4%)	34	15	55, 78, 105, 123	0
3	G	251/253 (99%)	0.48	17 (6%)	20	7	57, 86, 116, 131	0
All	All	2360/2426 (97%)	0.27	114 (4%)	34	15	46, 72, 105, 161	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	111	GLY	10.5
2	F	194	HIS	9.2
1	A	389	SER	7.7
1	A	764	ARG	7.1
1	A	392	SER	6.8
1	E	394	GLY	6.4
1	E	398	PRO	6.2
3	G	111	SER	5.9
1	E	397	GLU	5.8
2	F	1	MET	5.6
1	A	397	GLU	5.6
2	B	1	MET	5.3
1	E	396	HIS	5.2
1	A	384	ALA	5.2
1	A	393	GLY	5.1
1	E	389	SER	5.1
1	A	388	CYS	5.1
3	G	104	LEU	5.0
1	A	396	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
3	C	252	GLY	4.9
3	G	221	TRP	4.8
1	E	390	GLY	4.8
1	E	393	GLY	4.7
3	G	251	GLY	4.6
1	E	600	ALA	4.4
3	C	223	GLN	4.4
3	C	110	LYS	4.2
1	E	592	LEU	4.1
2	F	193	HIS	4.0
3	G	224	ARG	3.9
3	G	110	GLY	3.8
3	G	49	THR	3.8
1	E	392	SER	3.7
1	E	114	VAL	3.7
1	E	594	CYS	3.6
3	C	75	THR	3.5
1	E	388	CYS	3.5
3	G	101	THR	3.5
1	E	764	ARG	3.5
1	A	385	ALA	3.5
1	E	395	ASP	3.4
1	E	105	SER	3.3
3	G	74	THR	3.3
3	G	112	GLN	3.3
1	A	607	VAL	3.3
1	E	599	GLU	3.3
1	E	595	GLN	3.2
1	E	607	VAL	3.2
2	B	193	HIS	3.2
1	A	398	PRO	3.2
1	A	401	PHE	3.1
1	A	606	PRO	2.9
1	E	133	GLU	2.9
1	A	281	LYS	2.9
2	F	2	PRO	2.8
3	C	222	TRP	2.8
1	E	391	PRO	2.8
1	A	394	GLY	2.7
1	E	400	GLY	2.7
1	A	586	ALA	2.7
1	A	577	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	277	GLU	2.7
1	E	113	ARG	2.7
1	A	383	PRO	2.7
1	A	573	GLU	2.7
3	G	225	LEU	2.7
1	E	399	GLU	2.7
1	A	538	LYS	2.6
1	A	295	ASP	2.6
1	A	390	GLY	2.6
3	C	109	GLY	2.6
3	G	45	ALA	2.6
1	E	579	GLY	2.5
1	A	362	GLY	2.5
1	A	427	GLY	2.5
1	E	574	ASP	2.5
1	A	47	CYS	2.5
1	A	527	LEU	2.5
1	A	539	THR	2.5
3	C	112	SER	2.5
1	E	47	CYS	2.4
1	A	551	LEU	2.4
3	G	107	LEU	2.3
2	B	146	GLU	2.3
1	A	583	PHE	2.3
3	G	41	GLY	2.3
3	C	224	GLU	2.3
1	A	567	ARG	2.3
3	G	27	ALA	2.3
2	B	194	HIS	2.3
1	A	599	GLU	2.3
1	A	169	SER	2.3
1	A	69	GLU	2.2
1	A	387	GLY	2.2
1	A	595	GLN	2.2
3	C	95	GLY	2.2
3	G	38	HIS	2.2
3	C	79	LEU	2.2
2	B	89	LYS	2.2
1	A	591	GLU	2.2
1	A	570	PRO	2.2
3	C	78	TRP	2.2
1	A	569	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	79	LYS	2.2
1	E	554	ASP	2.2
1	A	587	SER	2.2
1	A	594	CYS	2.1
1	E	546	THR	2.1
1	A	288	GLU	2.1
1	E	577	LYS	2.1
1	A	370	TYR	2.1
3	G	39	LEU	2.1
1	A	284	VAL	2.0
1	A	574	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	MQ7	G	1251	15/48	0.84	0.56	4.24	27,31,36,42	0
7	MQ7	C	1252	15/48	0.81	0.57	3.80	26,27,28,29	0
5	MGD	A	1765	47/47	0.96	0.24	-0.48	48,52,55,58	0
5	MGD	E	1765	47/47	0.96	0.24	-0.48	46,53,56,56	0
5	MGD	E	1766	47/47	0.95	0.22	-0.64	41,46,48,50	0
4	SF4	B	1197	8/8	0.99	0.11	-1.13	57,60,61,63	0
4	SF4	B	1196	8/8	0.92	0.15	-1.58	55,59,62,65	0
5	MGD	A	1766	47/47	0.97	0.18	-1.60	37,46,48,52	0
4	SF4	E	1764	8/8	0.99	0.17	-1.78	45,49,52,52	0
4	SF4	F	1196	8/8	0.95	0.15	-1.79	60,65,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SF4	A	1764	8/8	0.99	0.15	-1.83	44,46,48,49	0
4	SF4	F	1197	8/8	0.93	0.14	-1.88	68,72,73,75	0
4	SF4	F	1195	8/8	0.96	0.14	-2.49	70,71,74,75	0
4	SF4	B	1195	8/8	0.98	0.09	-2.67	65,66,68,68	0
4	SF4	B	1194	8/8	0.95	0.09	-2.85	78,79,80,81	0
4	SF4	F	1194	8/8	0.95	0.10	-2.94	81,83,84,87	0
6	MO	E	1767	1/1	0.98	0.18	-	60,60,60,60	0
6	MO	A	1767	1/1	0.97	0.18	-	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.