



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:16 AM UTC

PDB ID : 5ECL / pdb_00005ecl
Title : Crystal Structure of FIN219-FIP1 complex with JA, Ile and Mg
Authors : Chen, C.Y.; Cheng, Y.S.
Deposited on : 2015-10-20
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

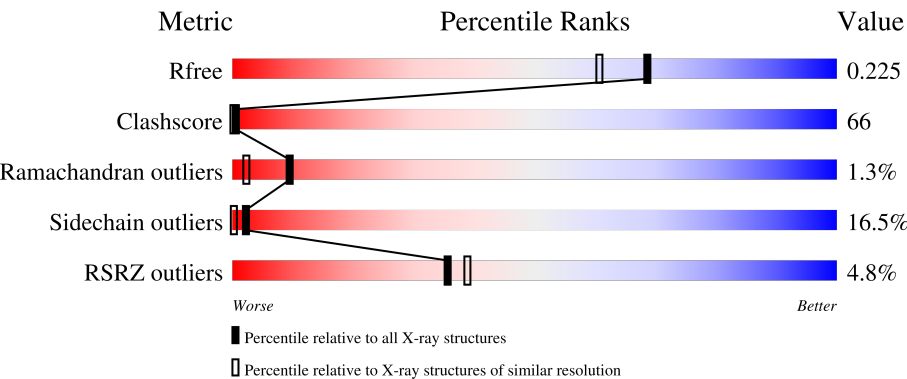
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	575	
1	D	575	
2	B	223	
2	C	223	
2	E	223	

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Mol	Chain	Length	Quality of chain
2	F	223	4% 27% 54% 14% • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17172 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 Jasmonic acid-amido synthetase JAR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4479	2859	748	850	22			
1	D	569	Total	C	N	O	S	0	0	0
			4479	2859	748	850	22			

- Molecule 2 is a protein called Glutathione S-transferase U20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	C	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	E	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	F	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			

There are 24 discrepancies between the modelled and reference sequences:

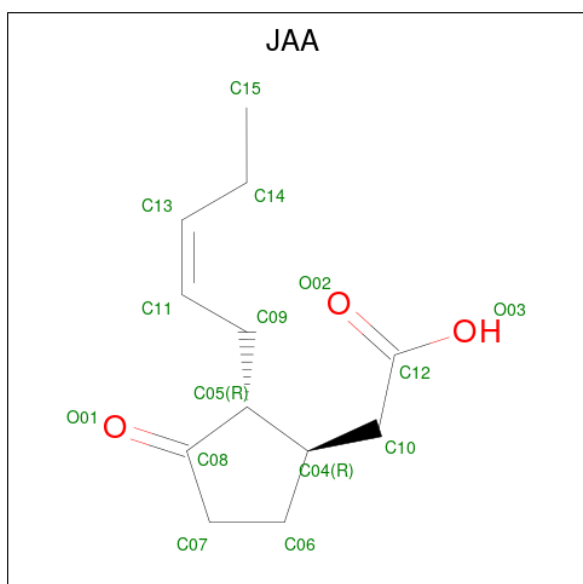
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9
C	-4	HIS	-	expression tag	UNP Q8L7C9
C	-3	HIS	-	expression tag	UNP Q8L7C9
C	-2	HIS	-	expression tag	UNP Q8L7C9
C	-1	HIS	-	expression tag	UNP Q8L7C9
C	0	HIS	-	expression tag	UNP Q8L7C9

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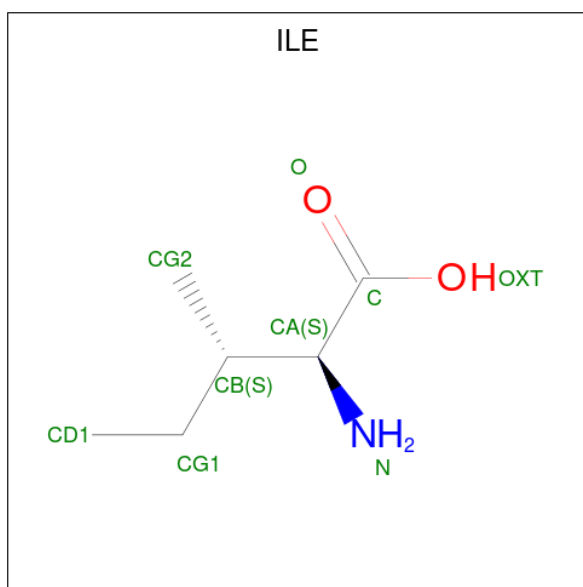
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9
F	-4	HIS	-	expression tag	UNP Q8L7C9
F	-3	HIS	-	expression tag	UNP Q8L7C9
F	-2	HIS	-	expression tag	UNP Q8L7C9
F	-1	HIS	-	expression tag	UNP Q8L7C9
F	0	HIS	-	expression tag	UNP Q8L7C9

- Molecule 3 is {(1R,2R)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetic acid (CCD ID: JAA) (formula: C₁₂H₁₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is ISOLEUCINE (CCD ID: ILE) (formula: C₆H₁₃NO₂).

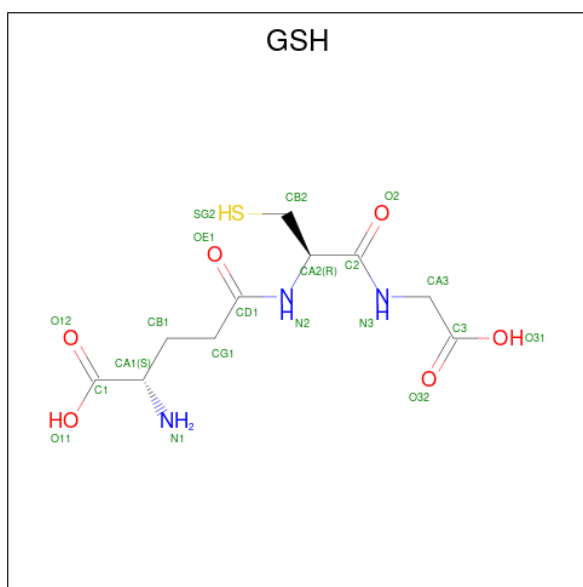


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	1	2		
4	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	3	Total	Mg	0	0
			3	3		

- Molecule 6 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

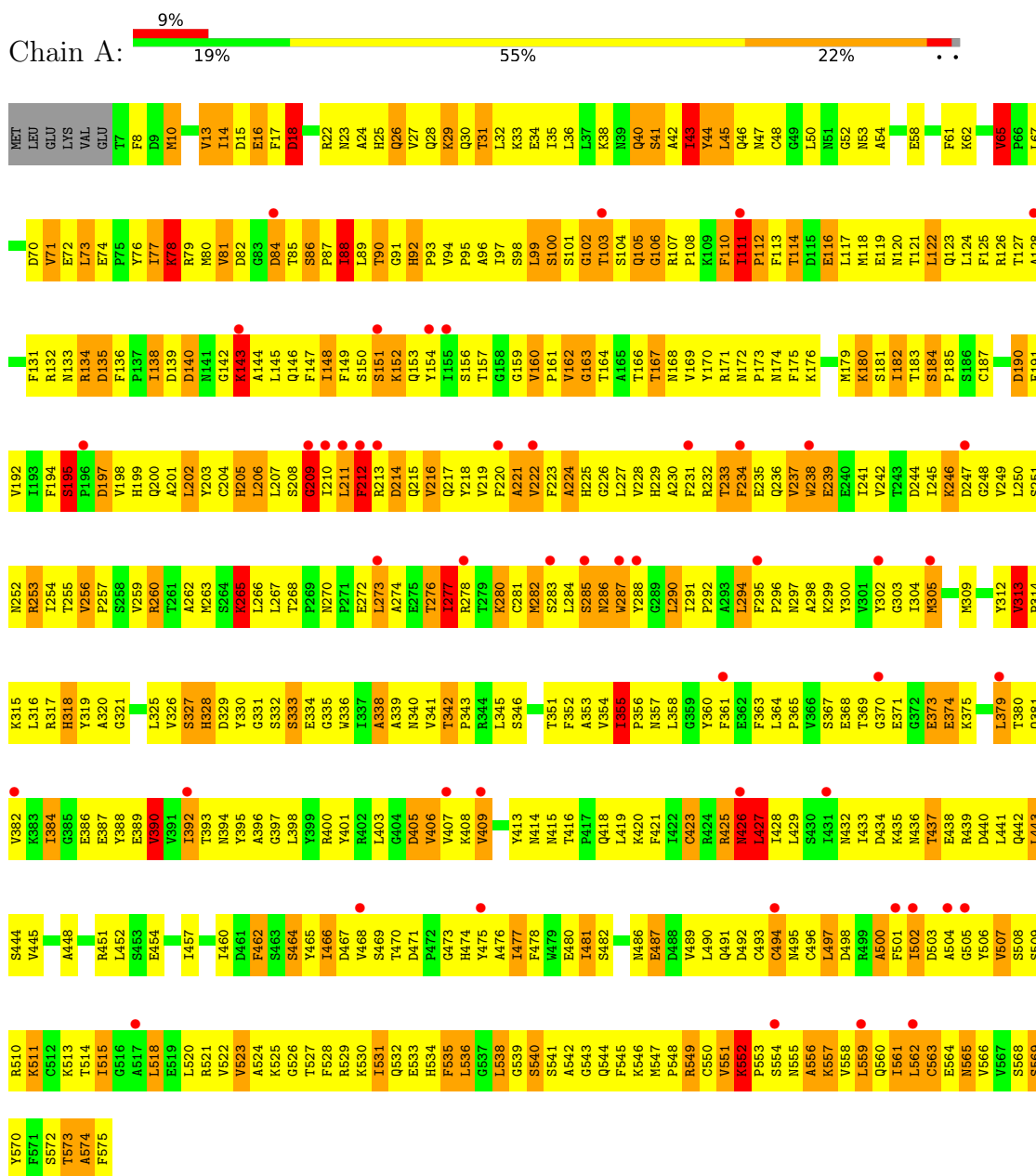
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	260	Total	O	0	0
			260	260		
7	B	162	Total	O	0	0
			162	162		
7	C	130	Total	O	0	0
			130	130		
7	D	276	Total	O	0	0
			276	276		
7	E	121	Total	O	0	0
			121	121		
7	F	141	Total	O	0	0
			141	141		

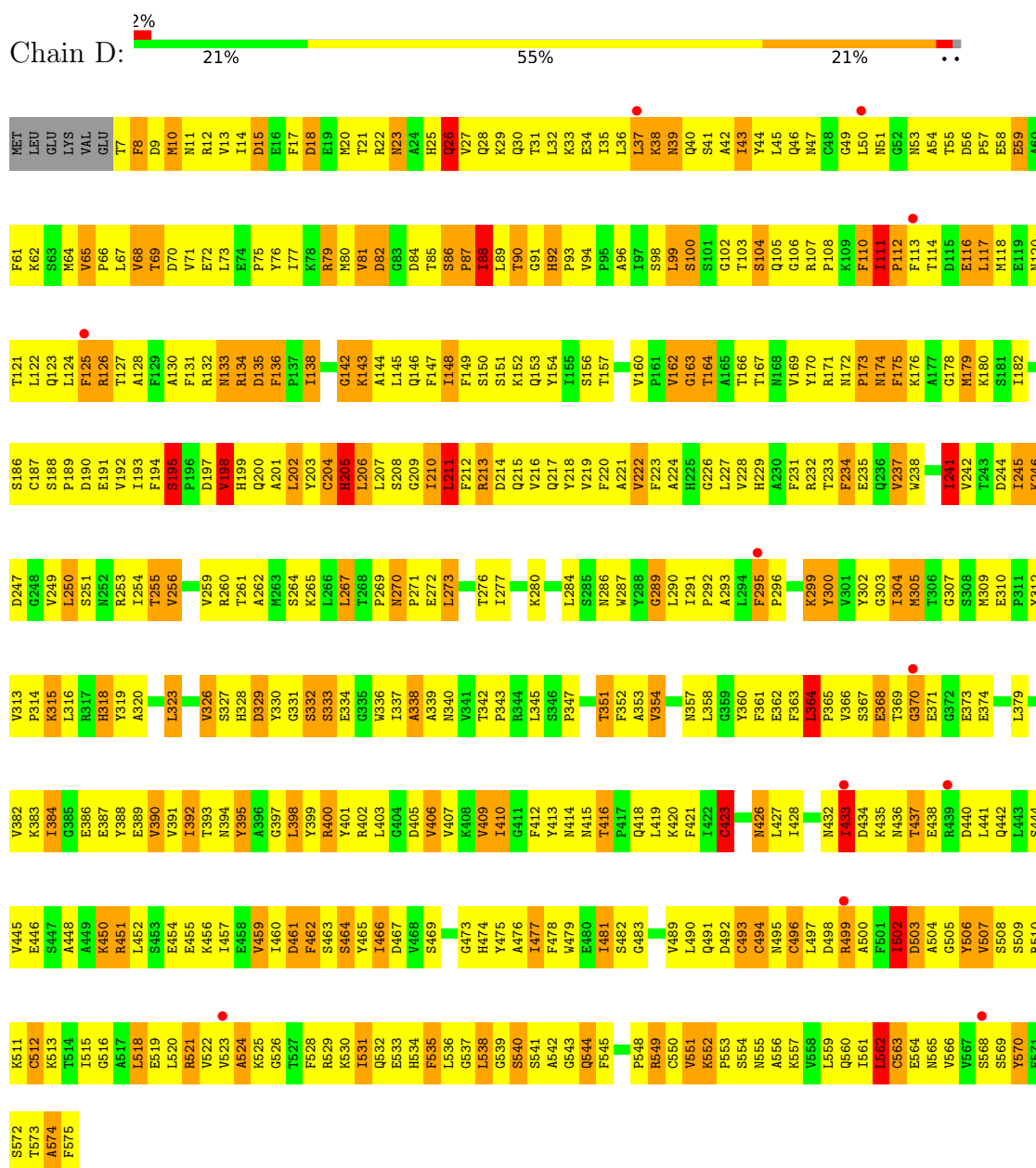
3 Residue-property plots

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

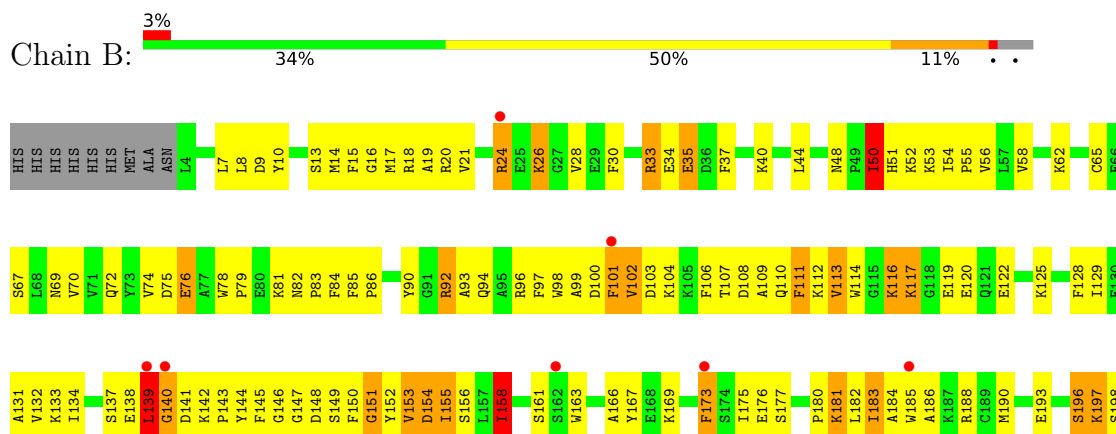
- Molecule 1: Jasmonic acid-amido synthetase JAR1



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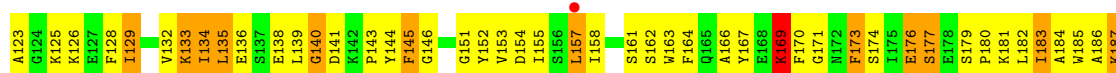


• Molecule 2: Glutathione S-transferase U20

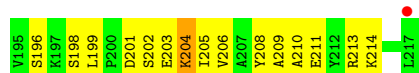
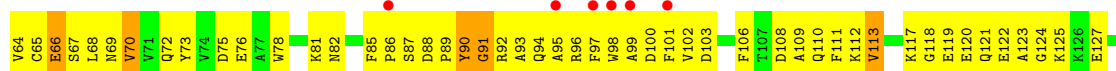
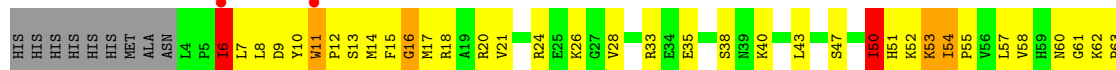




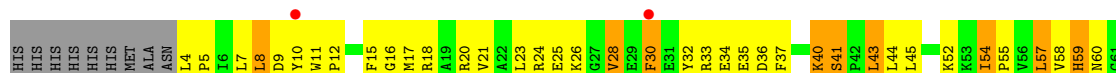
• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.80Å 53.88Å 193.16Å 90.07° 90.03° 66.39°	Depositor
Resolution (Å)	24.15 – 1.85 24.15 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.15-1.85) 97.4 (24.15-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.219 (Not available) , 0.225	Depositor DCC
R_{free} test set	16564 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	0.6	Xtriage
Anisotropy	2.777	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.53 , 121.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.095 for -h,-k,l 0.095 for k,h,-l 0.088 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	17172	wwPDB-VP
Average B, all atoms (Å ²)	4.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3658e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, MG, JAA

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	0.83	5/4581 (0.1%)	1.45	87/6219 (1.4%)
1	D	0.79	3/4581 (0.1%)	1.47	89/6219 (1.4%)
2	B	0.65	0/1799	1.21	15/2428 (0.6%)
2	C	0.69	0/1799	1.30	20/2428 (0.8%)
2	E	0.67	0/1799	1.20	20/2428 (0.8%)
2	F	0.70	0/1799	1.31	19/2428 (0.8%)
All	All	0.75	8/16358 (0.0%)	1.37	250/22150 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	LYS	CG-CD	-5.80	1.35	1.52
1	D	524	ALA	CA-CB	-5.78	1.43	1.53
1	A	277	ILE	C-O	5.62	1.30	1.24
1	A	313	VAL	CA-CB	5.51	1.57	1.53
1	D	198	VAL	C-O	-5.20	1.18	1.24
1	A	277	ILE	CA-C	-5.17	1.46	1.52
1	D	241	ILE	C-O	5.13	1.29	1.24
1	A	392	ILE	C-O	5.08	1.29	1.24

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	VAL	N-CA-C	13.77	124.17	110.82
1	D	563	CYS	N-CA-C	12.82	127.78	111.24
1	D	210	ILE	CA-CB-CG1	12.12	131.00	110.40
2	F	175	ILE	N-CA-C	11.98	129.24	112.35
2	F	145	PHE	N-CA-C	11.59	123.99	111.36
1	D	86	SER	CA-C-N	11.51	131.59	120.31
1	D	86	SER	C-N-CA	11.51	131.59	120.31
1	A	163	GLY	N-CA-C	10.31	127.79	111.08
2	B	158	ILE	CB-CA-C	-9.88	98.80	112.14
2	B	50	ILE	N-CA-C	9.49	119.45	110.53
2	E	50	ILE	N-CA-C	9.34	119.38	110.42
1	A	559	LEU	N-CA-C	9.28	121.40	111.28
1	D	246	LYS	N-CA-C	8.82	120.59	110.97
1	D	255	THR	N-CA-C	8.81	126.36	114.12
2	F	85	PHE	N-CA-C	8.73	122.05	110.36
1	D	505	GLY	N-CA-C	8.49	122.35	112.50
1	A	427	LEU	N-CA-C	8.43	123.22	108.56
1	A	237	VAL	N-CA-C	8.39	126.78	109.34
2	B	158	ILE	N-CA-C	8.35	119.14	110.62
2	B	76	GLU	N-CA-C	8.25	120.36	111.36
1	D	562	LEU	N-CA-C	8.11	119.90	111.14
1	D	270	ASN	CA-C-N	8.09	128.03	119.05
1	D	270	ASN	C-N-CA	8.09	128.03	119.05
1	D	206	LEU	N-CA-C	-8.01	102.14	111.03
1	D	65	VAL	N-CA-C	7.99	116.71	107.77
1	A	563	CYS	N-CA-C	7.96	127.74	110.80
1	D	392	ILE	N-CA-C	7.92	119.20	108.11
1	A	509	SER	N-CA-C	7.90	119.58	110.97
2	C	50	ILE	N-CA-C	7.85	118.75	111.45
2	B	185	TRP	N-CA-C	-7.84	102.73	111.28
1	A	392	ILE	CG1-CB-CG2	-7.80	87.30	110.70
1	A	211	LEU	N-CA-C	7.79	122.79	113.28
1	D	47	ASN	N-CA-C	-7.79	102.74	111.07
1	D	102	GLY	N-CA-C	-7.78	98.05	112.37
2	F	178	GLU	N-CA-C	-7.76	102.82	111.28
1	D	384	ILE	N-CA-C	7.73	119.56	109.58
1	D	535	PHE	N-CA-C	7.72	119.48	111.14
1	A	500	ALA	N-CA-C	7.62	119.37	111.14
2	C	208	TYR	N-CA-C	-7.59	103.00	111.28
1	A	280	LYS	N-CA-C	7.58	119.32	111.14
1	A	406	VAL	N-CA-C	7.58	119.20	108.36
1	A	18	ASP	N-CA-C	-7.50	103.10	111.28
2	F	198	SER	N-CA-C	7.50	119.54	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ALA	N-CA-C	-7.41	103.14	111.07
1	D	300	TYR	N-CA-C	7.39	119.39	108.60
2	C	18	ARG	N-CA-C	-7.30	103.25	111.07
1	A	134	ARG	N-CA-C	-7.29	103.27	111.14
1	A	342	THR	CA-C-N	7.17	127.16	119.28
1	A	342	THR	C-N-CA	7.17	127.16	119.28
1	A	106	GLY	N-CA-C	-7.14	106.58	115.08
1	D	433	ILE	CA-C-O	7.14	125.03	119.46
1	A	318	HIS	N-CA-C	-7.12	103.52	111.28
1	A	535	PHE	N-CA-C	7.07	118.78	111.14
1	D	237	VAL	N-CA-C	7.07	119.37	111.88
2	F	175	ILE	CB-CA-C	-7.05	101.72	111.65
1	D	271	PRO	N-CA-C	7.04	123.31	113.53
1	D	494	CYS	N-CA-C	-7.02	103.63	111.28
1	A	82	ASP	N-CA-C	6.94	120.33	110.68
2	E	53	LYS	N-CA-C	6.93	120.75	109.59
2	F	174	SER	N-CA-C	6.92	119.81	108.52
1	D	117	LEU	N-CA-C	-6.91	103.75	111.28
1	D	82	ASP	N-CA-C	6.89	119.96	109.62
2	E	142	LYS	N-CA-C	6.88	120.37	109.64
1	D	506	TYR	N-CA-C	-6.86	103.81	111.28
2	F	67	SER	N-CA-C	6.85	118.44	110.97
1	D	211	LEU	N-CA-C	6.83	118.42	110.97
1	D	163	GLY	N-CA-C	6.79	129.28	113.18
1	A	182	ILE	N-CA-C	6.78	118.66	112.29
1	A	549	ARG	N-CA-C	6.76	118.73	111.36
1	D	549	ARG	N-CA-C	6.76	119.67	111.82
1	A	111	ILE	CA-C-N	6.74	126.72	119.78
1	A	111	ILE	C-N-CA	6.74	126.72	119.78
1	D	112	PRO	N-CA-C	6.66	120.54	111.22
1	A	390	VAL	N-CA-C	6.65	117.49	108.17
2	F	36	ASP	N-CA-C	-6.64	97.72	108.41
2	B	140	GLY	N-CA-C	-6.64	97.45	113.18
1	D	531	ILE	N-CA-C	6.63	116.79	110.42
1	A	102	GLY	N-CA-C	-6.62	100.18	112.37
1	D	111	ILE	CA-C-N	6.62	126.56	120.21
1	D	111	ILE	C-N-CA	6.62	126.56	120.21
1	A	562	LEU	N-CA-C	6.61	119.31	111.71
1	D	10	MET	N-CA-C	6.60	118.14	111.07
2	F	154	ASP	N-CA-C	-6.60	104.00	111.07
1	A	221	ALA	N-CA-C	-6.56	98.39	108.76
2	F	123	ALA	N-CA-C	-6.52	104.17	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	SER	CB-CA-C	-6.51	100.94	110.96
1	D	175	PHE	N-CA-C	6.47	118.13	111.14
2	F	188	ARG	N-CA-C	-6.47	104.22	111.28
1	A	44	TYR	N-CA-C	-6.44	104.27	111.28
2	E	6	ILE	N-CA-C	6.42	117.32	109.30
1	D	570	TYR	N-CA-C	6.42	118.87	108.41
2	C	179	SER	CA-C-N	6.39	125.82	118.85
2	C	179	SER	C-N-CA	6.39	125.82	118.85
1	D	86	SER	N-CA-C	6.38	117.93	109.83
2	B	215	ASN	N-CA-C	6.34	120.28	112.54
1	D	173	PRO	N-CA-C	6.33	122.20	113.65
1	D	256	VAL	N-CA-C	6.31	114.06	108.63
1	D	189	PRO	N-CA-C	-6.24	101.47	111.38
1	D	88	ILE	N-CA-C	6.23	122.29	109.34
1	D	367	SER	N-CA-C	6.22	118.42	108.41
1	A	481	ILE	N-CA-C	6.20	117.64	108.65
1	D	410	ILE	N-CA-C	6.20	116.98	110.72
1	D	421	PHE	N-CA-C	6.19	118.99	108.90
2	F	199	LEU	CA-C-N	6.18	126.14	120.03
2	F	199	LEU	C-N-CA	6.18	126.14	120.03
1	A	246	LYS	N-CA-C	6.17	117.67	111.07
1	A	272	GLU	N-CA-C	6.15	117.99	111.28
1	A	212	PHE	CA-CB-CG	6.13	119.94	113.80
1	D	459	VAL	CB-CA-C	-6.13	104.60	111.23
2	E	209	ALA	N-CA-C	-6.11	104.70	111.36
2	C	169	LYS	N-CA-C	6.08	117.98	111.36
2	E	158	ILE	CB-CA-C	-6.08	102.74	112.16
1	A	65	VAL	N-CA-C	6.07	114.50	107.89
1	A	81	VAL	N-CA-C	6.06	120.89	112.35
2	B	116	LYS	N-CA-C	6.05	118.16	109.14
1	A	206	LEU	N-CA-C	-6.05	104.60	111.07
1	D	370	GLY	N-CA-C	-6.04	98.86	113.18
2	E	154	ASP	N-CA-C	-6.04	104.61	111.07
1	D	354	VAL	N-CA-C	6.03	117.41	109.21
1	D	39	ASN	N-CA-C	6.03	118.68	110.06
1	D	80	MET	N-CA-C	6.01	117.83	111.28
1	D	483	GLY	N-CA-C	5.97	120.03	110.90
2	E	169	LYS	N-CA-C	5.97	117.58	111.14
2	C	115	GLY	N-CA-C	5.96	119.70	112.49
1	A	487	GLU	N-CA-C	5.96	117.78	111.28
1	D	8	PHE	N-CA-C	5.96	118.95	109.24
1	A	152	LYS	N-CA-C	5.95	118.11	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	LYS	N-CA-C	-5.95	106.03	113.28
1	A	297	ASN	N-CA-C	5.94	120.54	112.88
1	D	222	VAL	N-CA-C	-5.93	104.73	110.72
1	A	256	VAL	CA-C-N	5.92	125.62	119.05
1	A	256	VAL	C-N-CA	5.92	125.62	119.05
1	A	43	ILE	N-CA-C	5.91	116.65	110.62
1	D	462	PHE	N-CA-C	5.89	117.81	108.79
1	D	390	VAL	N-CA-C	5.88	116.40	108.17
1	A	502	ILE	N-CA-C	5.88	121.06	113.07
1	D	205	HIS	N-CA-C	-5.85	104.50	111.69
2	E	90	TYR	N-CA-C	5.85	117.73	111.36
2	E	185	TRP	N-CA-C	-5.83	104.92	111.28
2	F	103	ASP	N-CA-C	5.83	117.63	111.28
1	A	8	PHE	N-CA-C	5.79	118.85	110.28
1	A	209	GLY	N-CA-C	-5.79	105.78	112.73
1	A	265	LYS	CD-CE-NZ	5.79	130.42	111.90
1	D	142	GLY	N-CA-C	5.77	122.00	112.30
1	A	255	THR	N-CA-C	5.73	119.86	112.41
2	C	67	SER	N-CA-C	5.73	117.21	110.97
2	E	162	SER	N-CA-C	-5.73	105.04	111.28
1	A	238	TRP	CA-CB-CG	5.72	124.47	113.60
2	C	35	GLU	N-CA-C	5.71	118.20	108.90
1	D	211	LEU	CA-CB-CG	5.69	136.23	116.30
2	B	151	GLY	N-CA-C	5.69	119.45	111.14
2	C	36	ASP	N-CA-C	-5.69	98.44	108.23
1	D	195	SER	CA-C-N	5.68	125.36	119.56
1	D	195	SER	C-N-CA	5.68	125.36	119.56
2	E	188	ARG	N-CA-C	-5.67	105.09	111.28
1	A	552	LYS	CA-C-N	-5.67	113.04	119.28
1	A	552	LYS	C-N-CA	-5.67	113.04	119.28
1	A	462	PHE	N-CA-C	5.65	116.85	108.60
1	A	88	ILE	N-CA-C	5.65	121.09	109.34
2	E	72	GLN	N-CA-C	-5.65	105.12	111.28
2	B	139	LEU	CA-CB-CG	-5.65	96.54	116.30
2	B	92	ARG	N-CA-C	-5.64	105.22	111.71
2	E	145	PHE	N-CA-C	5.64	119.68	112.12
1	A	111	ILE	CB-CG1-CD1	5.63	125.62	113.80
1	D	256	VAL	CA-C-N	5.62	125.73	119.32
1	D	256	VAL	C-N-CA	5.62	125.73	119.32
1	A	561	ILE	N-CA-C	5.62	118.07	111.05
1	D	332	SER	N-CA-C	5.62	115.66	108.24
2	E	111	PHE	N-CA-C	-5.59	105.19	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	ILE	CA-CB-CG2	-5.58	101.02	110.50
1	D	213	ARG	N-CA-C	5.58	117.36	111.28
1	D	364	LEU	CA-C-N	5.56	125.32	119.76
1	D	364	LEU	C-N-CA	5.56	125.32	119.76
1	D	461	ASP	N-CA-C	5.56	117.25	108.96
1	A	355	ILE	CA-C-N	5.55	125.21	119.05
1	A	355	ILE	C-N-CA	5.55	125.21	119.05
1	A	212	PHE	N-CA-CB	5.54	119.57	111.54
1	D	477	ILE	N-CA-C	5.53	115.86	108.11
1	D	357	ASN	N-CA-C	5.53	119.29	112.54
2	B	111	PHE	N-CA-C	-5.53	105.26	111.28
1	D	176	LYS	N-CA-C	-5.52	105.16	111.07
1	A	556	ALA	N-CA-C	5.49	120.49	113.18
1	D	289	GLY	N-CA-C	5.46	121.45	113.48
1	D	574	ALA	N-CA-C	-5.44	103.72	110.41
1	A	216	VAL	CB-CA-C	-5.43	103.00	111.26
1	D	366	VAL	N-CA-C	5.43	119.35	113.43
1	A	270	ASN	CA-C-N	5.43	124.77	118.85
1	A	270	ASN	C-N-CA	5.43	124.77	118.85
1	D	26	GLN	N-CA-C	-5.42	105.27	111.07
1	D	18	ASP	N-CA-C	-5.42	105.38	111.28
1	D	174	ASN	N-CA-C	5.42	119.52	113.02
1	A	367	SER	N-CA-C	5.41	117.93	108.52
1	D	267	LEU	N-CA-C	5.41	118.07	110.23
2	C	41	SER	N-CA-C	5.40	117.53	110.08
1	D	136	PHE	CA-C-N	5.40	125.34	119.78
1	D	136	PHE	C-N-CA	5.40	125.34	119.78
1	A	423	CYS	N-CA-C	5.38	117.03	110.41
1	A	277	ILE	CA-CB-CG1	5.37	119.53	110.40
2	C	201	ASP	N-CA-C	5.36	117.64	110.35
1	A	41	SER	N-CA-C	5.34	119.54	113.19
1	D	423	CYS	N-CA-C	5.33	118.18	109.59
2	E	118	GLY	N-CA-C	5.33	120.67	110.86
1	D	138	ILE	N-CA-C	5.33	117.44	108.81
1	A	234	PHE	N-CA-C	-5.32	105.48	111.28
2	C	216	ASN	N-CA-C	5.32	117.60	109.62
1	A	86	SER	N-CA-C	5.32	118.81	107.91
2	E	16	GLY	N-CA-C	-5.31	106.36	112.73
1	A	151	SER	N-CA-C	5.30	119.38	113.02
1	D	563	CYS	CA-CB-SG	-5.29	102.23	114.40
1	D	338	ALA	N-CA-C	5.27	118.15	109.72
1	D	234	PHE	N-CA-C	-5.26	105.66	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	GLU	N-CA-C	5.25	117.38	109.23
2	F	184	ALA	N-CA-C	-5.25	107.25	113.97
1	A	112	PRO	N-CA-C	5.24	119.55	111.21
1	A	24	ALA	N-CA-C	5.24	116.68	111.07
2	F	76	GLU	N-CA-C	5.23	117.06	111.36
1	A	373	GLU	N-CA-C	5.23	118.60	107.67
2	C	50	ILE	CB-CA-C	-5.21	105.09	111.92
1	A	105	GLN	N-CA-C	-5.21	106.87	113.23
2	F	147	GLY	N-CA-C	-5.20	104.17	111.09
2	C	81	LYS	N-CA-C	5.20	119.26	112.13
1	A	328	HIS	N-CA-C	5.20	117.83	110.50
1	A	214	ASP	N-CA-C	-5.18	105.63	111.28
2	C	188	ARG	N-CA-C	-5.18	105.55	111.14
1	A	148	ILE	CB-CA-C	-5.18	103.68	110.98
1	A	338	ALA	N-CA-C	5.17	117.67	109.50
1	A	195	SER	CA-C-N	5.17	125.25	119.87
1	A	195	SER	C-N-CA	5.17	125.25	119.87
1	A	162	VAL	N-CA-C	5.17	115.42	107.77
2	C	177	SER	N-CA-C	5.17	116.91	111.28
1	A	31	THR	N-CA-C	-5.16	105.65	111.28
2	E	91	GLY	N-CA-C	-5.15	106.55	112.73
2	E	139	LEU	CA-CB-CG	-5.13	98.34	116.30
1	D	496	CYS	N-CA-C	5.12	116.86	111.28
1	A	78	LYS	N-CA-C	-5.11	105.71	111.28
2	C	129	ILE	N-CA-CB	5.11	117.49	110.54
1	A	290	LEU	CA-CB-CG	-5.11	98.43	116.30
1	D	502	ILE	N-CA-C	5.10	119.64	113.00
1	A	239	GLU	N-CA-C	-5.09	105.62	111.07
2	E	6	ILE	CB-CA-C	-5.08	103.76	111.33
1	A	233	THR	N-CA-C	-5.08	105.74	111.28
2	C	53	LYS	N-CA-C	5.08	117.67	109.40
2	C	161	SER	N-CA-C	5.07	117.54	111.71
1	D	428	ILE	N-CA-C	-5.07	100.35	107.75
1	A	273	LEU	CA-CB-CG	-5.06	98.58	116.30
1	A	265	LYS	CB-CG-CD	-5.04	99.70	111.30
2	B	48	ASN	CA-C-N	5.04	124.21	118.97
2	B	48	ASN	C-N-CA	5.04	124.21	118.97
2	F	164	PHE	N-CA-C	-5.02	105.81	111.28
1	D	451	ARG	N-CA-C	-5.01	105.95	111.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	GLY	Mainchain
1	A	426	ASN	Sidechain

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	4479	0	4434	663	2
1	D	4479	0	4434	711	0
2	B	1748	0	1704	190	0
2	C	1748	0	1704	217	0
2	E	1748	0	1704	229	1
2	F	1748	0	1704	217	2
3	A	15	0	0	1	0
3	D	15	0	0	1	0
4	A	9	0	10	4	0
4	D	9	0	10	1	0
5	A	1	0	0	0	0
5	D	3	0	0	0	0
6	B	20	0	15	3	0
6	C	20	0	15	1	0
6	E	20	0	15	2	0
6	F	20	0	15	0	0
7	A	260	0	0	46	2
7	B	162	0	0	17	1
7	C	130	0	0	21	1
7	D	276	0	0	47	2
7	E	121	0	0	27	0
7	F	141	0	0	19	1
All	All	17172	0	15764	2108	8

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 66.

All (2108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:NZ	7:D:701:HOH:O	1.72	1.21
1:A:163:GLY:HA3	1:A:560:GLN:HG3	1.24	1.17
1:A:213:ARG:NH1	1:A:294:LEU:HD13	1.66	1.10
2:B:20:ARG:HB3	2:B:24:ARG:HH22	1.23	1.04
2:E:143:PRO:O	2:E:188:ARG:NH1	1.90	1.04
2:C:188:ARG:HB2	1:D:499:ARG:NH2	1.76	1.01
2:E:185:TRP:HD1	2:E:188:ARG:NH1	1.59	1.00
2:E:145:PHE:HB3	2:E:153:VAL:HG13	1.44	1.00
1:D:498:ASP:OD2	7:D:702:HOH:O	1.77	1.00
1:A:42:ALA:HB3	1:A:45:LEU:HD12	1.44	1.00
1:D:451:ARG:NH1	1:D:489:VAL:O	1.95	0.99
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.42	0.98
1:A:426:ASN:H	1:A:426:ASN:ND2	1.61	0.97
2:F:176:GLU:HB2	2:F:183:ILE:HG12	1.46	0.97
2:F:17:MET:HE2	2:F:200:PRO:HD2	1.45	0.95
2:E:53:LYS:HD3	6:E:301:GSH:HA1	1.49	0.95
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.46	0.95
1:D:199:HIS:H	1:D:524:ALA:HB1	1.31	0.95
1:A:164:THR:HG21	1:A:561:ILE:HG13	1.48	0.95
1:D:534:HIS:CE1	1:D:557:LYS:HG2	2.02	0.95
1:D:94:VAL:HG11	1:D:112:PRO:HB3	1.47	0.95
2:B:145:PHE:N	2:B:154:ASP:OD2	2.01	0.94
1:D:200:GLN:HB3	1:D:254:ILE:HG23	1.50	0.93
1:D:499:ARG:NH1	7:D:704:HOH:O	1.97	0.93
1:A:213:ARG:HA	1:A:216:VAL:HG23	1.48	0.93
1:D:150:SER:HB2	1:D:167:THR:HA	1.51	0.92
1:A:238:TRP:HZ3	1:A:277:ILE:HG12	1.32	0.92
2:F:98:TRP:CD1	2:F:153:VAL:HG21	2.03	0.92
1:A:157:THR:HG22	1:A:469:SER:HB3	1.49	0.92
2:C:132:VAL:HG23	2:C:182:LEU:HD13	1.51	0.92
1:D:206:LEU:O	1:D:210:ILE:HG22	1.70	0.92
2:B:112:LYS:HD2	2:B:116:LYS:HZ1	1.34	0.91
1:A:213:ARG:HH12	1:A:294:LEU:HD13	1.30	0.91
1:A:211:LEU:O	7:A:701:HOH:O	1.89	0.91
1:A:238:TRP:CZ3	1:A:277:ILE:HG12	2.06	0.90
1:D:551:VAL:HB	1:D:555:ASN:HB2	1.53	0.90
1:A:143:LYS:HZ1	1:A:212:PHE:C	1.79	0.90
2:C:10:TYR:HB3	2:C:13:SER:HB2	1.55	0.89
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.53	0.89
2:B:18:ARG:NH1	2:B:103:ASP:OD2	2.06	0.89
1:D:164:THR:HG23	1:D:557:LYS:HG3	1.55	0.89
1:A:135:ASP:OD2	1:A:343:PRO:HD2	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:HIS:HB3	2:B:53:LYS:HG2	1.54	0.89
1:A:432:ASN:HB3	1:A:435:LYS:HD2	1.55	0.88
1:A:426:ASN:HD22	1:A:426:ASN:N	1.70	0.88
2:E:95:ALA:O	7:E:401:HOH:O	1.90	0.88
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.07	0.88
1:D:143:LYS:HD3	1:D:216:VAL:HG12	1.53	0.88
1:D:198:VAL:HG23	1:D:524:ALA:HB3	1.53	0.88
1:A:444:SER:HB3	1:A:497:LEU:HG	1.55	0.88
1:A:41:SER:HB2	2:B:142:LYS:HG2	1.56	0.87
1:A:327:SER:HB2	1:A:352:PHE:HZ	1.38	0.87
1:A:99:LEU:HB3	1:A:557:LYS:H	1.38	0.87
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.39	0.87
1:D:405:ASP:OD2	7:D:703:HOH:O	1.92	0.87
2:F:57:LEU:HG	2:F:64:VAL:HG22	1.58	0.86
1:D:93:PRO:HD2	2:E:181:LYS:HA	1.58	0.86
2:F:26:LYS:HG3	2:F:74:VAL:HG12	1.57	0.86
1:A:454:GLU:OE2	7:A:702:HOH:O	1.93	0.86
1:A:150:SER:HB2	1:A:167:THR:HA	1.56	0.85
1:D:540:SER:OG	1:D:544:GLN:NE2	2.09	0.85
2:F:57:LEU:HD23	2:F:70:VAL:HG13	1.58	0.85
1:D:403:LEU:HD13	1:D:540:SER:HB3	1.57	0.85
2:E:18:ARG:NH2	7:E:406:HOH:O	2.09	0.85
2:E:17:MET:O	7:E:402:HOH:O	1.94	0.85
1:D:247:ASP:HB2	1:D:249:VAL:HG12	1.59	0.85
2:F:135:LEU:HD22	2:F:182:LEU:HD12	1.59	0.85
1:D:93:PRO:HD3	2:E:188:ARG:HH21	1.42	0.84
1:D:93:PRO:HG2	2:E:184:ALA:HB3	1.60	0.84
1:D:147:PHE:HA	1:D:205:HIS:CD2	2.11	0.84
2:F:98:TRP:HZ2	2:F:135:LEU:HG	1.40	0.84
2:B:20:ARG:HB3	2:B:24:ARG:NH2	1.93	0.83
2:C:176:GLU:OE2	1:D:573:THR:OG1	1.95	0.83
1:A:392:ILE:HG22	1:A:401:TYR:CE1	2.14	0.83
2:E:185:TRP:CD1	2:E:188:ARG:NH1	2.46	0.83
1:A:426:ASN:H	1:A:426:ASN:HD22	0.85	0.83
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.60	0.83
1:A:143:LYS:NZ	1:A:212:PHE:C	2.36	0.83
1:A:118:MET:HE1	1:A:169:VAL:HA	1.60	0.82
1:D:208:SER:O	7:D:701:HOH:O	1.97	0.82
2:B:20:ARG:NH2	2:B:198:SER:O	2.12	0.82
1:D:133:ASN:HD21	1:D:138:ILE:HG13	1.43	0.82
1:D:519:GLU:OE2	1:D:569:SER:OG	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:TRP:CH2	1:A:281:CYS:HB2	2.14	0.82
1:D:226:GLY:HA2	1:D:529:ARG:HD3	1.61	0.82
1:A:143:LYS:NZ	1:A:212:PHE:O	2.11	0.82
1:A:43:ILE:O	1:A:46:GLN:HG2	1.80	0.81
1:A:405:ASP:HB2	1:A:541:SER:HB3	1.60	0.81
1:A:477:ILE:HD13	1:A:497:LEU:HD22	1.62	0.81
1:D:96:ALA:HB1	1:D:163:GLY:H	1.45	0.81
1:A:226:GLY:O	1:A:229:HIS:ND1	2.12	0.81
1:D:81:VAL:HG21	1:D:110:PHE:CE2	2.15	0.81
2:C:209:ALA:HA	2:C:212:TYR:HE2	1.46	0.80
1:A:242:VAL:HG22	1:A:277:ILE:HD13	1.62	0.80
1:D:494:CYS:HB3	1:D:520:LEU:HB2	1.64	0.80
1:D:42:ALA:HB3	1:D:45:LEU:HD13	1.62	0.80
1:D:451:ARG:NH1	1:D:490:LEU:HA	1.95	0.80
1:A:334:GLU:O	1:A:394:ASN:ND2	2.15	0.80
1:D:99:LEU:HD11	1:D:548:PRO:HG3	1.62	0.80
2:B:85:PHE:HB2	2:B:92:ARG:HG2	1.64	0.80
2:F:98:TRP:CZ2	2:F:135:LEU:HG	2.17	0.80
1:A:138:ILE:HB	1:A:217:GLN:HG3	1.64	0.80
2:C:135:LEU:HD13	2:C:182:LEU:HD11	1.64	0.80
1:A:434:ASP:HB2	1:A:550:CYS:HB3	1.61	0.80
2:B:169:LYS:HZ1	2:B:206:VAL:HG11	1.47	0.79
2:B:116:LYS:NZ	2:B:120:GLU:HB3	1.97	0.79
1:D:384:ILE:HA	1:D:409:VAL:HG13	1.64	0.79
1:A:92:HIS:O	7:A:703:HOH:O	1.99	0.79
1:A:282:MET:N	1:A:282:MET:SD	2.55	0.79
2:F:10:TYR:O	2:F:20:ARG:NH2	2.15	0.79
1:A:238:TRP:HA	1:A:241:ILE:HB	1.65	0.79
1:D:455:GLU:OE2	7:D:705:HOH:O	2.00	0.79
1:D:107:ARG:HG2	1:D:433:ILE:HG22	1.63	0.79
1:D:332:SER:HB2	1:D:538:LEU:HA	1.63	0.78
1:D:405:ASP:HB2	1:D:541:SER:HB3	1.65	0.78
2:E:96:ARG:NH1	2:F:72:GLN:HB2	1.97	0.78
1:D:507:VAL:HG23	1:D:511:LYS:HE2	1.65	0.78
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.65	0.78
1:D:451:ARG:NH1	1:D:493:CYS:HB3	1.97	0.78
1:D:451:ARG:HH12	1:D:490:LEU:HA	1.49	0.78
2:B:26:LYS:HZ2	2:B:78:TRP:CG	2.02	0.78
1:D:76:TYR:HA	1:D:79:ARG:HD3	1.66	0.78
2:C:209:ALA:HA	2:C:212:TYR:CE2	2.19	0.78
1:D:22:ARG:HA	1:D:415:ASN:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:LEU:HD23	1:D:481:ILE:HG21	1.66	0.78
2:B:116:LYS:HZ2	2:B:120:GLU:HB3	1.49	0.78
2:E:139:LEU:HD21	2:E:145:PHE:CE1	2.19	0.78
1:A:489:VAL:O	7:A:704:HOH:O	2.01	0.77
1:D:401:TYR:CE2	1:D:403:LEU:HG	2.18	0.77
2:B:76:GLU:OE2	2:C:92:ARG:NH2	2.16	0.77
1:D:143:LYS:HD2	1:D:212:PHE:CB	2.13	0.77
1:A:132:ARG:O	1:A:136:PHE:N	2.18	0.77
1:A:405:ASP:OD2	7:A:705:HOH:O	2.02	0.77
2:B:33:ARG:NH1	7:B:408:HOH:O	2.17	0.77
1:D:440:ASP:O	7:D:706:HOH:O	2.02	0.77
2:C:54:ILE:HB	2:C:55:PRO:HA	1.67	0.77
2:F:18:ARG:NH2	2:F:159:THR:OG1	2.18	0.77
1:A:42:ALA:HA	2:B:143:PRO:HG3	1.66	0.77
1:A:393:THR:O	7:A:706:HOH:O	2.03	0.76
2:C:7:LEU:HD21	2:C:23:LEU:HD12	1.67	0.76
1:D:38:LYS:C	2:E:142:LYS:HZ2	1.93	0.76
1:D:38:LYS:NZ	2:E:138:GLU:OE1	2.16	0.76
1:D:138:ILE:HB	1:D:217:GLN:HG3	1.68	0.76
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.66	0.76
1:D:242:VAL:HG22	1:D:277:ILE:HD13	1.68	0.76
2:E:106:PHE:CE2	2:E:131:ALA:HB1	2.20	0.76
2:E:145:PHE:HD2	2:E:153:VAL:HG22	1.50	0.76
2:F:85:PHE:HE1	2:F:95:ALA:HB3	1.49	0.75
1:A:435:LYS:HE3	1:A:438:GLU:HG2	1.67	0.75
1:A:197:ASP:OD2	1:A:200:GLN:NE2	2.18	0.75
1:A:153:GLN:H	1:A:564:GLU:HB2	1.50	0.75
1:A:563:CYS:SG	1:A:564:GLU:N	2.60	0.75
1:D:223:PHE:CZ	1:D:536:LEU:HB2	2.20	0.75
1:D:401:TYR:HE2	1:D:403:LEU:HG	1.50	0.75
1:D:223:PHE:CE2	1:D:545:PHE:HZ	2.05	0.75
1:A:199:HIS:H	1:A:524:ALA:HB1	1.52	0.75
2:F:179:SER:OG	2:F:182:LEU:HB3	1.86	0.75
1:A:122:LEU:O	1:A:126:ARG:HG3	1.87	0.75
1:A:140:ASP:OD1	7:A:707:HOH:O	2.05	0.75
1:D:364:LEU:HD23	1:D:389:GLU:OE2	1.87	0.75
2:F:23:LEU:HA	2:F:74:VAL:HG11	1.67	0.75
1:A:204:CYS:SG	7:A:891:HOH:O	2.45	0.74
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.21	0.74
2:B:24:ARG:HD3	2:B:197:LYS:HZ2	1.52	0.74
1:D:394:ASN:O	7:D:707:HOH:O	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:LYS:HA	2:E:82:ASN:HD21	1.51	0.74
2:E:94:GLN:HA	2:E:97:PHE:HD2	1.51	0.74
2:F:168:GLU:OE2	2:F:175:ILE:HG12	1.87	0.74
1:A:97:ILE:HD12	1:A:162:VAL:HG22	1.68	0.74
1:A:457:ILE:HB	1:A:482:SER:HB3	1.67	0.74
1:A:504:ALA:O	1:A:507:VAL:HG22	1.87	0.74
1:D:369:THR:OG1	1:D:370:GLY:N	2.11	0.74
1:A:152:LYS:HA	1:A:564:GLU:HB3	1.68	0.74
1:A:152:LYS:NZ	1:A:527:THR:HG22	2.03	0.74
2:C:145:PHE:HB2	2:C:153:VAL:HG21	1.68	0.74
1:A:102:GLY:HA2	1:A:546:LYS:HG3	1.69	0.74
1:D:87:PRO:HB3	1:D:91:GLY:O	1.88	0.74
1:D:496:CYS:HA	1:D:499:ARG:NH1	2.02	0.74
1:A:111:ILE:HD12	1:A:334:GLU:OE2	1.88	0.74
1:D:521:ARG:HA	1:D:569:SER:HA	1.70	0.74
2:F:37:PHE:HZ	2:F:54:ILE:HG12	1.51	0.74
1:A:441:LEU:HD23	1:A:549:ARG:HB3	1.68	0.74
1:D:352:PHE:O	7:D:708:HOH:O	2.05	0.74
1:A:18:ASP:O	1:A:22:ARG:HG3	1.88	0.73
1:A:477:ILE:HD12	1:A:520:LEU:HD13	1.67	0.73
2:C:60:ASN:ND2	7:C:409:HOH:O	2.19	0.73
1:A:238:TRP:O	1:A:242:VAL:HG23	1.87	0.73
2:B:9:ASP:OD2	2:B:20:ARG:HD3	1.88	0.73
1:D:87:PRO:HG2	2:E:188:ARG:NE	2.04	0.73
1:D:138:ILE:HA	1:D:217:GLN:HE21	1.54	0.73
1:A:451:ARG:NH1	1:A:454:GLU:OE1	2.21	0.73
1:D:42:ALA:HA	2:E:143:PRO:HG3	1.69	0.73
1:A:364:LEU:HB3	1:A:389:GLU:HG2	1.70	0.73
1:D:339:ALA:N	1:D:353:ALA:O	2.19	0.73
1:D:387:GLU:HG2	1:D:406:VAL:HB	1.71	0.73
1:D:392:ILE:HB	1:D:401:TYR:CE1	2.23	0.73
1:D:143:LYS:HE3	1:D:187:CYS:HA	1.71	0.73
1:A:551:VAL:HG12	1:A:555:ASN:HD22	1.54	0.73
2:F:144:TYR:OH	7:F:401:HOH:O	2.05	0.73
1:D:460:ILE:HG22	1:D:461:ASP:OD2	1.89	0.72
1:D:510:ARG:HG2	1:D:515:ILE:HD11	1.71	0.72
2:B:53:LYS:HD3	6:B:301:GSH:HG12	1.68	0.72
2:B:21:VAL:HG11	2:B:158:ILE:HD11	1.71	0.72
1:D:99:LEU:HB3	1:D:557:LYS:HB2	1.71	0.72
1:D:563:CYS:SG	1:D:564:GLU:N	2.60	0.72
2:E:198:SER:HB3	7:E:402:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:THR:H	1:D:117:LEU:HD23	1.54	0.72
1:D:451:ARG:HH12	1:D:490:LEU:CA	2.03	0.72
2:E:100:ASP:OD2	7:E:404:HOH:O	2.07	0.72
1:D:302:TYR:HH	1:D:328:HIS:HD1	1.29	0.72
1:A:108:PRO:HD2	1:A:552:LYS:HD2	1.70	0.72
1:A:492:ASP:OD1	7:A:709:HOH:O	2.08	0.72
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.70	0.72
1:D:390:VAL:HG11	1:D:540:SER:HA	1.71	0.72
1:D:498:ASP:HB3	1:D:510:ARG:NH2	2.04	0.72
1:A:521:ARG:NH2	7:A:726:HOH:O	2.22	0.72
1:D:152:LYS:HA	1:D:564:GLU:HB3	1.72	0.71
2:E:146:GLY:H	2:E:151:GLY:HA3	1.53	0.71
1:A:200:GLN:HB3	1:A:254:ILE:HG13	1.70	0.71
1:A:390:VAL:O	7:A:708:HOH:O	2.08	0.71
1:A:401:TYR:HE2	1:A:403:LEU:HD13	1.55	0.71
2:F:98:TRP:CE2	2:F:138:GLU:OE2	2.43	0.71
2:B:112:LYS:HD2	2:B:116:LYS:NZ	2.05	0.71
2:C:26:LYS:NZ	2:C:82:ASN:O	2.21	0.71
1:D:326:VAL:HG21	1:D:343:PRO:HB3	1.72	0.71
1:D:451:ARG:CZ	1:D:493:CYS:HB3	2.19	0.71
1:A:92:HIS:CG	2:B:181:LYS:HG2	2.25	0.71
1:A:226:GLY:HA2	1:A:529:ARG:HD3	1.71	0.71
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.26	0.71
1:D:199:HIS:N	1:D:524:ALA:HB1	2.06	0.71
2:F:213:ARG:NH2	7:F:411:HOH:O	2.23	0.71
1:D:448:ALA:O	1:D:451:ARG:HG2	1.91	0.71
1:A:552:LYS:HB2	1:A:553:PRO:HD2	1.72	0.70
2:B:26:LYS:NZ	2:B:28:VAL:HB	2.06	0.70
1:D:232:ARG:NH2	7:D:724:HOH:O	2.23	0.70
2:E:63:PRO:O	7:E:405:HOH:O	2.08	0.70
1:A:40:GLN:O	7:A:710:HOH:O	2.09	0.70
1:A:94:VAL:HG11	1:A:112:PRO:HB3	1.74	0.70
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.73	0.70
1:A:534:HIS:CE1	1:A:557:LYS:HG2	2.26	0.70
2:C:114:TRP:O	2:C:212:TYR:OH	2.09	0.70
1:D:45:LEU:O	1:D:49:GLY:N	2.23	0.70
2:E:95:ALA:HA	2:E:98:TRP:CE3	2.26	0.70
1:A:465:TYR:HD1	1:A:551:VAL:HG23	1.55	0.70
2:F:92:ARG:O	7:F:402:HOH:O	2.08	0.70
1:A:98:SER:HB3	1:A:113:PHE:CZ	2.26	0.70
1:A:126:ARG:NH1	7:A:728:HOH:O	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:N	1:A:371:GLU:OE2	2.24	0.70
1:A:551:VAL:HG11	1:A:558:VAL:HG11	1.72	0.70
1:D:44:TYR:HB2	1:D:89:LEU:HD22	1.72	0.70
1:D:253:ARG:NH2	7:D:726:HOH:O	2.24	0.70
2:E:40:LYS:NZ	2:E:52:LYS:HD2	2.06	0.70
1:A:551:VAL:HB	1:A:555:ASN:HB2	1.74	0.70
1:D:126:ARG:HH11	1:D:126:ARG:HG3	1.56	0.70
1:D:198:VAL:CG2	1:D:524:ALA:HB3	2.22	0.70
2:E:94:GLN:OE1	7:E:407:HOH:O	2.10	0.70
2:C:33:ARG:NH1	2:C:41:SER:OG	2.25	0.70
2:C:125:LYS:NZ	2:C:171:GLY:HA3	2.06	0.70
1:D:333:SER:OG	1:D:557:LYS:NZ	2.24	0.70
1:D:99:LEU:HD13	1:D:555:ASN:OD1	1.92	0.70
1:D:494:CYS:HB3	1:D:520:LEU:CB	2.21	0.70
1:A:145:LEU:HD22	1:A:213:ARG:NH2	2.07	0.70
1:A:207:LEU:HD21	1:A:245:ILE:HD11	1.73	0.70
1:A:238:TRP:HZ2	1:A:282:MET:HE1	1.56	0.70
1:D:451:ARG:HE	1:D:452:LEU:HD13	1.56	0.70
1:D:533:GLU:O	7:D:709:HOH:O	2.09	0.70
1:A:87:PRO:HB3	2:B:143:PRO:HA	1.74	0.70
1:A:262:ALA:O	1:A:265:LYS:HE3	1.91	0.70
1:D:392:ILE:HB	1:D:401:TYR:HE1	1.56	0.70
1:A:84:ASP:OD1	1:A:84:ASP:N	2.23	0.69
1:A:108:PRO:HD3	1:A:434:ASP:OD2	1.92	0.69
2:C:26:LYS:HD2	2:C:74:VAL:HG13	1.74	0.69
1:D:208:SER:HA	1:D:211:LEU:HG	1.73	0.69
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.27	0.69
1:D:280:LYS:HE2	1:D:293:ALA:HB1	1.74	0.69
1:A:81:VAL:HB	1:A:110:PHE:HE2	1.57	0.69
1:A:152:LYS:HG3	1:A:565:ASN:HB2	1.72	0.69
1:A:464:SER:HG	1:A:550:CYS:HG	1.25	0.69
1:D:342:THR:O	1:D:345:LEU:HG	1.92	0.69
2:F:8:LEU:HD22	2:F:43:LEU:HD13	1.75	0.69
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.27	0.69
2:E:165:GLN:NE2	7:E:414:HOH:O	2.20	0.69
1:A:520:LEU:O	7:A:711:HOH:O	2.09	0.69
1:D:23:ASN:HB3	1:D:27:VAL:HG23	1.73	0.69
2:F:25:GLU:OE2	2:F:82:ASN:ND2	2.26	0.69
1:A:22:ARG:HH11	1:A:414:ASN:HB3	1.55	0.69
1:A:340:ASN:HB2	1:A:352:PHE:CD1	2.27	0.69
2:B:100:ASP:OD2	7:B:401:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ALA:HA	2:B:169:LYS:HZ3	1.57	0.69
1:D:332:SER:OG	1:D:333:SER:N	2.22	0.69
2:F:128:PHE:CE1	2:F:175:ILE:HG22	2.27	0.69
2:F:154:ASP:HA	2:F:185:TRP:HZ2	1.57	0.69
1:A:77:ILE:HG22	1:A:110:PHE:HD2	1.57	0.69
1:A:154:TYR:HB2	1:A:563:CYS:SG	2.32	0.69
2:B:24:ARG:HH21	2:B:30:PHE:HZ	1.39	0.69
2:B:35:GLU:O	7:B:402:HOH:O	2.11	0.69
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.28	0.69
1:A:87:PRO:HG3	1:A:93:PRO:HD3	1.75	0.69
1:A:163:GLY:CA	1:A:560:GLN:HG3	2.15	0.69
2:C:121:GLN:O	2:C:125:LYS:HG3	1.93	0.69
2:E:154:ASP:O	2:E:158:ILE:HG23	1.93	0.69
1:A:164:THR:HG22	1:A:557:LYS:O	1.92	0.69
1:D:154:TYR:HB3	1:D:563:CYS:SG	2.33	0.69
1:A:152:LYS:HZ1	1:A:198:VAL:HG21	1.58	0.68
2:C:184:ALA:O	7:D:704:HOH:O	2.11	0.68
1:A:41:SER:HA	2:B:148:ASP:HA	1.75	0.68
1:A:41:SER:OG	2:B:147:GLY:O	2.06	0.68
1:A:81:VAL:O	7:A:712:HOH:O	2.11	0.68
2:B:201:ASP:O	7:B:403:HOH:O	2.12	0.68
2:C:146:GLY:O	7:C:403:HOH:O	2.11	0.68
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.28	0.68
2:C:174:SER:O	7:C:402:HOH:O	2.09	0.68
1:D:51:ASN:ND2	2:E:87:SER:OG	2.26	0.68
1:A:108:PRO:HB3	1:A:555:ASN:CG	2.18	0.68
2:F:168:GLU:OE1	7:F:403:HOH:O	2.11	0.68
1:D:202:LEU:HA	1:D:205:HIS:HB2	1.74	0.68
1:D:462:PHE:O	1:D:549:ARG:NH1	2.27	0.68
1:D:544:GLN:NE2	7:D:703:HOH:O	2.17	0.68
2:F:57:LEU:HG	2:F:64:VAL:CG2	2.23	0.68
1:A:48:CYS:SG	1:A:65:VAL:HB	2.33	0.68
1:A:418:GLN:N	7:A:730:HOH:O	2.26	0.68
2:F:191:GLU:OE2	7:F:401:HOH:O	2.12	0.68
1:A:390:VAL:HG11	1:A:540:SER:HA	1.75	0.68
2:C:188:ARG:NH1	1:D:499:ARG:O	2.26	0.68
1:D:477:ILE:HD11	1:D:497:LEU:HD13	1.76	0.68
2:F:139:LEU:O	7:F:404:HOH:O	2.11	0.68
1:A:180:LYS:O	7:A:713:HOH:O	2.11	0.68
1:A:421:PHE:CE1	1:A:541:SER:HA	2.29	0.68
2:C:187:LYS:HE3	1:D:493:CYS:HA	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:ARG:HD2	2:C:67:SER:HB2	1.74	0.67
2:E:182:LEU:O	2:E:185:TRP:HB3	1.94	0.67
2:F:33:ARG:NH1	2:F:35:GLU:OE2	2.27	0.67
2:B:75:ASP:OD2	2:B:85:PHE:HD1	1.78	0.67
1:D:172:ASN:HB3	1:D:175:PHE:CE2	2.30	0.67
2:E:190:MET:SD	7:E:471:HOH:O	2.51	0.67
1:A:114:THR:OG1	2:B:141:ASP:OD2	2.10	0.67
1:A:480:GLU:HG3	1:A:525:LYS:HA	1.74	0.67
1:D:305:MET:HG3	1:D:347:PRO:HB3	1.75	0.67
1:D:423:CYS:SG	1:D:541:SER:OG	2.49	0.67
1:A:38:LYS:O	2:B:142:LYS:HB2	1.94	0.67
1:A:143:LYS:HZ2	1:A:212:PHE:CA	2.07	0.67
1:A:169:VAL:HG13	1:A:170:TYR:CD1	2.29	0.67
1:A:360:TYR:N	7:A:706:HOH:O	2.27	0.67
2:B:26:LYS:HZ2	2:B:78:TRP:CD1	2.12	0.67
2:B:76:GLU:OE1	2:C:92:ARG:NE	2.28	0.67
1:D:435:LYS:NZ	1:D:549:ARG:HB2	2.08	0.67
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.74	0.67
1:A:471:ASP:OD1	7:A:714:HOH:O	2.13	0.67
1:D:39:ASN:HA	2:E:142:LYS:HE3	1.75	0.67
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.29	0.67
1:A:106:GLY:HA3	1:A:432:ASN:HB2	1.77	0.67
2:E:143:PRO:C	2:E:188:ARG:NH1	2.52	0.67
1:A:46:GLN:HB3	2:B:148:ASP:HB3	1.75	0.67
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.29	0.67
1:D:25:HIS:HA	1:D:28:GLN:HG2	1.77	0.67
1:D:135:ASP:OD2	1:D:343:PRO:HB2	1.94	0.67
2:E:185:TRP:HD1	2:E:188:ARG:HH12	1.43	0.67
2:C:98:TRP:HE1	2:C:145:PHE:HD2	1.41	0.67
1:A:108:PRO:HG2	1:A:552:LYS:HG2	1.77	0.67
2:C:144:TYR:HB3	2:C:154:ASP:OD2	1.95	0.67
1:D:331:GLY:HA3	1:D:336:TRP:CE3	2.28	0.67
1:A:166:THR:HA	1:A:169:VAL:HG12	1.77	0.66
1:A:247:ASP:CG	1:A:249:VAL:HG12	2.20	0.66
1:A:363:PHE:HD2	1:A:382:VAL:HG21	1.59	0.66
1:A:409:VAL:HG13	7:A:730:HOH:O	1.95	0.66
2:B:204:LYS:HB2	7:B:403:HOH:O	1.95	0.66
2:F:125:LYS:HA	2:F:128:PHE:CD2	2.30	0.66
1:D:96:ALA:HA	1:D:162:VAL:HA	1.75	0.66
1:D:199:HIS:H	1:D:524:ALA:CB	2.05	0.66
2:E:150:PHE:CE2	2:E:192:LYS:HG3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG23	1:A:397:GLY:HA2	1.75	0.66
1:D:99:LEU:HB3	1:D:557:LYS:H	1.60	0.66
2:B:142:LYS:O	7:B:405:HOH:O	2.14	0.66
2:C:40:LYS:HD3	2:C:52:LYS:HB3	1.77	0.66
2:F:23:LEU:HD11	2:F:30:PHE:CD2	2.30	0.66
2:B:150:PHE:HZ	2:B:158:ILE:HG21	1.60	0.66
1:A:116:GLU:OE2	1:A:395:TYR:HB3	1.95	0.66
2:C:201:ASP:HB3	1:D:454:GLU:O	1.96	0.66
1:D:224:ALA:HA	1:D:316:LEU:HD22	1.78	0.66
2:E:11:TRP:HZ2	2:E:204:LYS:HB3	1.60	0.66
2:F:98:TRP:NE1	2:F:138:GLU:OE2	2.29	0.66
2:F:162:SER:O	7:F:405:HOH:O	2.13	0.66
1:A:143:LYS:NZ	1:A:212:PHE:CB	2.59	0.66
1:D:451:ARG:NH1	1:D:490:LEU:CA	2.58	0.66
1:D:534:HIS:CD2	1:D:557:LYS:HE2	2.30	0.66
1:A:390:VAL:HG11	1:A:540:SER:CA	2.26	0.66
2:C:17:MET:SD	2:C:199:LEU:HG	2.36	0.66
2:E:136:GLU:HG3	2:E:181:LYS:HE2	1.78	0.66
2:E:145:PHE:O	7:E:408:HOH:O	2.14	0.66
1:A:23:ASN:HB3	1:A:27:VAL:HG23	1.77	0.66
1:A:90:THR:HG22	2:B:141:ASP:HB3	1.78	0.66
1:A:126:ARG:HA	1:A:182:ILE:HG21	1.77	0.66
1:A:213:ARG:HH11	1:A:294:LEU:HD13	1.59	0.66
1:A:223:PHE:HD2	1:A:225:HIS:CE1	2.14	0.66
2:E:157:LEU:HD21	2:E:182:LEU:HD11	1.77	0.66
1:A:143:LYS:HZ2	1:A:212:PHE:CB	2.09	0.65
1:A:163:GLY:HA3	1:A:560:GLN:CG	2.16	0.65
1:A:237:VAL:HG11	1:A:253:ARG:NH2	2.11	0.65
1:A:427:LEU:O	7:A:715:HOH:O	2.13	0.65
2:B:33:ARG:O	7:B:404:HOH:O	2.13	0.65
2:E:99:ALA:N	7:E:401:HOH:O	2.28	0.65
1:A:116:GLU:O	1:A:119:GLU:HG2	1.96	0.65
2:C:60:ASN:O	7:C:406:HOH:O	2.15	0.65
1:D:273:LEU:H	1:D:273:LEU:HD12	1.61	0.65
2:F:98:TRP:CZ3	2:F:101:PHE:HB2	2.31	0.65
2:E:13:SER:O	2:E:17:MET:HG3	1.96	0.65
2:E:211:GLU:HA	2:E:214:LYS:HG3	1.78	0.65
1:A:239:GLU:OE1	7:A:716:HOH:O	2.13	0.65
1:A:475:TYR:O	1:A:518:LEU:HD23	1.96	0.65
2:B:24:ARG:NH1	2:B:198:SER:OG	2.29	0.65
2:F:215:ASN:OD1	7:F:406:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLY:C	1:A:213:ARG:HE	2.05	0.65
1:D:116:GLU:OE2	1:D:395:TYR:HB2	1.96	0.65
1:D:478:PHE:HZ	1:D:562:LEU:HD12	1.61	0.65
2:E:26:LYS:HZ1	2:E:81:LYS:H	1.43	0.65
2:F:158:ILE:HG12	2:F:195:VAL:HG11	1.79	0.65
1:A:97:ILE:HG21	1:A:110:PHE:CD2	2.32	0.65
1:A:575:PHE:O	7:A:718:HOH:O	2.14	0.65
1:D:69:THR:OG1	1:D:72:GLU:OE2	2.15	0.65
2:F:201:ASP:HB2	2:F:204:LYS:HE3	1.79	0.65
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.31	0.65
1:A:551:VAL:HB	1:A:555:ASN:CB	2.27	0.65
2:C:196:SER:O	7:C:404:HOH:O	2.14	0.65
2:E:21:VAL:HG11	2:E:158:ILE:HD11	1.79	0.65
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.31	0.65
1:A:87:PRO:HD3	1:A:93:PRO:HG3	1.78	0.65
1:A:152:LYS:NZ	1:A:198:VAL:HG21	2.11	0.65
2:C:152:TYR:O	7:C:407:HOH:O	2.15	0.65
1:A:108:PRO:HG2	1:A:552:LYS:H	1.61	0.64
1:D:132:ARG:O	1:D:136:PHE:N	2.20	0.64
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.32	0.64
2:F:63:PRO:O	7:F:407:HOH:O	2.14	0.64
1:A:211:LEU:HD12	1:A:212:PHE:CD2	2.32	0.64
2:B:24:ARG:HD3	2:B:197:LYS:NZ	2.12	0.64
2:B:193:GLU:HA	2:B:196:SER:HB3	1.80	0.64
2:B:40:LYS:NZ	2:B:52:LYS:HD2	2.13	0.64
2:C:177:SER:HA	1:D:573:THR:HG21	1.78	0.64
1:D:17:PHE:HA	1:D:20:MET:HG2	1.79	0.64
2:F:10:TYR:CG	2:F:12:PRO:HD2	2.33	0.64
1:A:149:PHE:HB2	1:A:530:LYS:NZ	2.13	0.64
1:A:246:LYS:HG3	1:A:274:ALA:HB2	1.80	0.64
2:C:24:ARG:HB3	2:C:194:SER:HA	1.79	0.64
2:C:109:ALA:HB1	2:C:128:PHE:HB3	1.78	0.64
2:C:203:GLU:OE2	7:C:405:HOH:O	2.14	0.64
2:F:208:TYR:O	7:F:408:HOH:O	2.15	0.64
1:A:96:ALA:O	1:A:113:PHE:HB2	1.98	0.64
1:A:435:LYS:HB3	1:A:436:ASN:C	2.23	0.64
1:A:498:ASP:HB3	1:A:510:ARG:NH2	2.13	0.64
2:B:110:GLN:O	2:B:113:VAL:HG12	1.98	0.64
1:D:254:ILE:O	7:D:714:HOH:O	2.15	0.64
1:D:492:ASP:O	1:D:495:ASN:HB2	1.98	0.64
2:E:166:ALA:HB2	2:E:206:VAL:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:CD2	2:B:181:LYS:HG2	2.32	0.64
1:A:336:TRP:HB3	1:A:358:LEU:HD13	1.80	0.64
1:A:364:LEU:HD23	1:A:389:GLU:OE2	1.97	0.64
2:B:125:LYS:HB2	2:B:173:PHE:CE2	2.32	0.64
1:D:18:ASP:O	1:D:22:ARG:HG3	1.96	0.64
1:D:29:LYS:NZ	1:D:58:GLU:OE2	2.31	0.64
1:A:81:VAL:HB	1:A:110:PHE:CE2	2.32	0.64
2:C:180:PRO:HB3	1:D:573:THR:HG22	1.80	0.64
1:D:40:GLN:NE2	1:D:51:ASN:O	2.31	0.64
1:D:73:LEU:HD23	1:D:89:LEU:HD12	1.79	0.64
2:E:142:LYS:HD3	2:E:143:PRO:HD2	1.78	0.64
2:B:9:ASP:N	7:B:404:HOH:O	2.26	0.64
2:C:125:LYS:HZ2	2:C:171:GLY:HA3	1.61	0.63
2:B:9:ASP:OD1	2:B:10:TYR:N	2.30	0.63
1:D:42:ALA:N	7:D:739:HOH:O	2.32	0.63
1:A:77:ILE:HG23	1:A:80:MET:HE3	1.79	0.63
1:A:164:THR:OG1	1:A:167:THR:OG1	2.10	0.63
1:A:392:ILE:HG22	1:A:401:TYR:HE1	1.64	0.63
1:D:504:ALA:O	1:D:507:VAL:HG13	1.99	0.63
2:E:145:PHE:CD2	2:E:153:VAL:HG22	2.32	0.63
1:A:40:GLN:HE21	1:A:52:GLY:HA3	1.62	0.63
1:A:191:GLU:O	1:A:195:SER:N	2.32	0.63
1:A:407:VAL:HG21	1:A:419:LEU:HD23	1.80	0.63
2:C:12:PRO:O	2:C:163:TRP:HZ2	1.81	0.63
1:D:172:ASN:HB3	1:D:175:PHE:CZ	2.32	0.63
1:D:423:CYS:HG	1:D:541:SER:HG	1.45	0.63
1:A:197:ASP:N	1:A:197:ASP:OD1	2.30	0.63
1:A:219:VAL:HB	1:A:295:PHE:CE2	2.33	0.63
1:A:250:LEU:HD22	1:A:260:ARG:HE	1.63	0.63
1:A:486:ASN:ND2	7:A:739:HOH:O	2.30	0.63
2:E:26:LYS:NZ	2:E:81:LYS:H	1.95	0.63
2:E:62:LYS:HB3	2:F:90:TYR:CZ	2.34	0.63
2:E:103:ASP:OD2	7:E:409:HOH:O	2.14	0.63
2:E:132:VAL:HG21	2:E:175:ILE:HG23	1.79	0.63
1:A:252:ASN:HA	1:A:260:ARG:HH22	1.63	0.63
1:A:494:CYS:SG	1:A:495:ASN:N	2.72	0.63
2:B:215:ASN:O	7:B:407:HOH:O	2.16	0.63
1:D:93:PRO:HD2	2:E:181:LYS:CA	2.27	0.63
2:F:167:TYR:HB2	2:F:168:GLU:OE1	1.99	0.63
1:A:218:TYR:HA	1:A:298:ALA:HB1	1.79	0.63
1:A:315:LYS:HA	1:A:318:HIS:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LEU:O	7:D:715:HOH:O	2.16	0.63
1:D:146:GLN:O	1:D:205:HIS:NE2	2.31	0.63
2:C:14:MET:HG3	2:C:163:TRP:CH2	2.33	0.63
2:C:98:TRP:CH2	2:C:135:LEU:HG	2.33	0.63
1:D:87:PRO:HG2	2:E:188:ARG:CZ	2.28	0.63
1:D:383:LYS:O	1:D:386:GLU:HG2	1.98	0.63
2:E:6:ILE:HD12	2:E:6:ILE:H	1.63	0.63
1:A:190:ASP:O	1:A:194:PHE:HD2	1.81	0.62
1:D:473:GLY:O	1:D:516:GLY:N	2.29	0.62
2:F:21:VAL:HG12	2:F:155:ILE:HG12	1.80	0.62
1:A:503:ASP:OD1	1:A:504:ALA:N	2.32	0.62
1:D:228:VAL:HG11	1:D:315:LYS:HD3	1.79	0.62
2:F:4:LEU:HD12	2:F:5:PRO:HD2	1.79	0.62
1:D:146:GLN:NE2	7:D:720:HOH:O	2.19	0.62
1:D:371:GLU:N	1:D:371:GLU:OE2	2.32	0.62
2:E:66:GLU:OE2	2:F:97:PHE:HD1	1.82	0.62
1:D:20:MET:HA	1:D:23:ASN:HB2	1.80	0.62
1:D:153:GLN:NE2	1:D:171:ARG:HG3	2.14	0.62
1:D:212:PHE:N	7:D:701:HOH:O	2.12	0.62
1:D:433:ILE:O	1:D:433:ILE:HG13	1.98	0.62
2:F:140:GLY:HA2	2:F:181:LYS:NZ	2.15	0.62
1:A:152:LYS:HD3	1:A:561:ILE:HA	1.82	0.62
1:A:238:TRP:CZ2	1:A:281:CYS:HB2	2.35	0.62
1:A:526:GLY:O	1:A:530:LYS:HG2	2.00	0.62
2:F:40:LYS:HD2	2:F:52:LYS:HD2	1.80	0.62
2:C:117:LYS:HE3	2:C:213:ARG:HH11	1.65	0.62
1:D:150:SER:HB2	1:D:167:THR:CA	2.28	0.62
1:D:198:VAL:HG22	1:D:565:ASN:HD22	1.62	0.62
2:F:35:GLU:OE2	2:F:41:SER:HB2	1.99	0.62
2:F:112:LYS:O	7:F:409:HOH:O	2.16	0.62
1:A:118:MET:HG2	1:A:174:ASN:ND2	2.15	0.62
2:B:119:GLU:N	2:B:119:GLU:OE1	2.33	0.62
1:D:315:LYS:HA	1:D:318:HIS:HB3	1.82	0.62
1:D:442:GLN:HA	1:D:462:PHE:CZ	2.34	0.62
2:E:24:ARG:HG3	2:E:194:SER:HA	1.79	0.62
1:A:315:LYS:O	1:A:318:HIS:HB3	2.00	0.62
1:A:507:VAL:O	1:A:511:LYS:HB2	2.00	0.62
1:A:523:VAL:HG22	1:A:524:ALA:H	1.64	0.62
2:C:194:SER:O	2:C:198:SER:OG	2.18	0.62
1:A:242:VAL:O	1:A:246:LYS:HB2	2.00	0.61
2:E:163:TRP:HB3	2:E:167:TYR:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.35	0.61
2:F:166:ALA:HB2	2:F:206:VAL:HA	1.82	0.61
2:B:65:CYS:SG	7:B:458:HOH:O	2.53	0.61
2:B:75:ASP:OD2	2:B:85:PHE:CD1	2.53	0.61
2:B:205:ILE:HA	2:B:208:TYR:CE2	2.35	0.61
1:D:105:GLN:NE2	7:D:736:HOH:O	2.28	0.61
1:D:566:VAL:HG21	1:D:569:SER:HB2	1.81	0.61
2:F:40:LYS:NZ	2:F:40:LYS:H	1.98	0.61
1:D:226:GLY:CA	1:D:529:ARG:HD3	2.29	0.61
1:D:292:PRO:HB3	1:D:323:LEU:HD12	1.82	0.61
1:D:463:SER:HB3	1:D:478:PHE:HD2	1.65	0.61
2:E:11:TRP:HZ2	2:E:204:LYS:CB	2.13	0.61
2:F:133:LYS:O	2:F:136:GLU:HG3	2.00	0.61
1:A:274:ALA:O	1:A:278:ARG:HD2	2.00	0.61
1:A:398:LEU:HB3	1:A:401:TYR:CD1	2.36	0.61
2:B:86:PRO:HD3	2:B:146:GLY:O	2.00	0.61
1:D:435:LYS:HZ3	1:D:549:ARG:HB2	1.65	0.61
1:A:338:ALA:HA	1:A:354:VAL:HA	1.80	0.61
2:B:109:ALA:HA	2:B:112:LYS:HG2	1.81	0.61
2:C:98:TRP:CZ2	2:C:157:LEU:HD22	2.35	0.61
1:D:108:PRO:HB2	1:D:554:SER:HB2	1.80	0.61
2:E:18:ARG:HD3	2:E:156:SER:HA	1.82	0.61
2:C:84:PHE:HB2	2:C:152:TYR:N	2.16	0.61
2:C:145:PHE:N	2:C:145:PHE:CD1	2.64	0.61
1:D:93:PRO:HD3	2:E:188:ARG:NH2	2.14	0.61
1:D:464:SER:HB2	1:D:477:ILE:HG22	1.83	0.61
2:B:40:LYS:HZ2	2:B:52:LYS:HD2	1.64	0.61
2:B:90:TYR:O	2:B:93:ALA:HB3	2.01	0.61
2:C:176:GLU:OE2	1:D:491:GLN:HG2	2.01	0.61
1:D:59:GLU:HA	1:D:62:LYS:HZ3	1.65	0.61
1:D:172:ASN:CG	1:D:173:PRO:HD2	2.25	0.61
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.81	0.61
1:A:153:GLN:HE22	1:A:171:ARG:HG2	1.66	0.61
1:D:38:LYS:HB3	2:E:140:GLY:HA3	1.82	0.61
1:D:330:TYR:O	1:D:338:ALA:N	2.32	0.61
1:A:38:LYS:HB3	2:B:140:GLY:HA3	1.82	0.61
1:D:108:PRO:HG2	1:D:552:LYS:HG2	1.82	0.61
1:D:149:PHE:CE2	1:D:202:LEU:HD22	2.35	0.60
1:D:509:SER:OG	1:D:515:ILE:HG12	2.00	0.60
2:F:60:ASN:ND2	7:F:418:HOH:O	2.26	0.60
2:C:17:MET:HE2	2:C:200:PRO:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:SER:HA	1:D:573:THR:CG2	2.31	0.60
1:D:8:PHE:HA	1:D:126:ARG:CZ	2.31	0.60
1:A:278:ARG:O	1:A:282:MET:HG2	2.00	0.60
1:A:305:MET:SD	1:A:325:LEU:HB3	2.41	0.60
2:B:20:ARG:HH22	2:B:200:PRO:HD3	1.67	0.60
1:D:363:PHE:HE1	1:D:390:VAL:HG23	1.65	0.60
1:D:394:ASN:ND2	7:D:744:HOH:O	2.33	0.60
2:E:144:TYR:HB3	2:E:154:ASP:OD2	2.02	0.60
2:C:98:TRP:O	2:C:101:PHE:HB2	2.01	0.60
2:C:108:ASP:O	2:C:112:LYS:HG2	2.02	0.60
1:D:351:THR:HG21	1:D:410:ILE:HG12	1.83	0.60
1:A:274:ALA:HB1	1:A:278:ARG:NH2	2.16	0.60
1:A:365:PRO:HG3	1:A:374:GLU:HG2	1.82	0.60
1:D:87:PRO:HD3	1:D:93:PRO:HG3	1.82	0.60
2:F:163:TRP:HB3	2:F:167:TYR:CZ	2.37	0.60
1:A:312:TYR:CD2	1:A:315:LYS:HE2	2.36	0.60
1:D:273:LEU:HD12	1:D:273:LEU:N	2.16	0.60
2:C:188:ARG:HE	1:D:499:ARG:HH21	1.50	0.60
1:A:13:VAL:HG22	1:A:17:PHE:CZ	2.37	0.60
1:A:114:THR:HB	1:A:116:GLU:CD	2.27	0.60
2:B:96:ARG:HA	2:B:152:TYR:HE2	1.66	0.60
1:D:526:GLY:HA2	1:D:529:ARG:NH1	2.17	0.60
1:A:42:ALA:HB1	1:A:44:TYR:CE1	2.37	0.60
1:A:435:LYS:HG2	1:A:438:GLU:OE2	2.01	0.60
1:D:118:MET:HE3	1:D:175:PHE:CE1	2.37	0.60
1:D:432:ASN:OD1	1:D:433:ILE:N	2.35	0.60
1:D:498:ASP:HB3	1:D:510:ARG:HH21	1.67	0.60
2:E:119:GLU:HA	2:E:122:GLU:HG2	1.83	0.60
2:F:114:TRP:HZ3	2:F:212:TYR:HD2	1.50	0.60
1:D:79:ARG:NH2	1:D:87:PRO:O	2.35	0.60
1:D:93:PRO:HG2	2:E:184:ALA:CB	2.30	0.60
1:A:29:LYS:HG3	1:A:30:GLN:H	1.67	0.59
1:D:46:GLN:HB2	2:E:148:ASP:HB2	1.84	0.59
1:D:46:GLN:HE21	2:E:148:ASP:HB2	1.66	0.59
1:D:87:PRO:HG2	2:E:188:ARG:HE	1.65	0.59
1:D:234:PHE:CD2	1:D:287:TRP:HH2	2.20	0.59
1:A:451:ARG:NH1	1:A:489:VAL:HG12	2.17	0.59
1:D:451:ARG:HH12	1:D:490:LEU:C	2.09	0.59
2:F:169:LYS:HG3	2:F:170:PHE:H	1.67	0.59
1:A:58:GLU:O	1:A:61:PHE:HB2	2.02	0.59
1:A:531:ILE:HA	1:A:534:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:TRP:NE1	2:C:145:PHE:HD2	2.01	0.59
1:D:104:SER:O	1:D:107:ARG:HB2	2.02	0.59
2:E:65:CYS:O	2:E:66:GLU:HB2	2.02	0.59
1:A:532:GLN:HG2	1:A:547:MET:HE3	1.84	0.59
2:B:112:LYS:CD	2:B:116:LYS:HZ1	2.10	0.59
2:B:146:GLY:HA3	2:B:151:GLY:HA3	1.84	0.59
2:B:202:SER:O	2:B:206:VAL:HG13	2.01	0.59
1:D:273:LEU:H	1:D:273:LEU:CD1	2.15	0.59
1:D:276:THR:OG1	1:D:277:ILE:N	2.33	0.59
1:A:46:GLN:OE1	2:B:149:SER:OG	2.20	0.59
1:A:292:PRO:O	1:A:296:PRO:HA	2.02	0.59
1:A:506:TYR:CE1	1:A:510:ARG:HD3	2.37	0.59
2:B:13:SER:O	2:B:17:MET:HG3	2.03	0.59
2:C:20:ARG:HB3	2:C:198:SER:HB3	1.85	0.59
1:D:87:PRO:HG2	2:E:188:ARG:NH2	2.17	0.59
1:A:247:ASP:OD2	1:A:249:VAL:HG12	2.03	0.59
2:B:17:MET:HG2	2:B:20:ARG:NH2	2.18	0.59
1:D:92:HIS:HE1	2:E:185:TRP:HB2	1.68	0.59
1:D:108:PRO:HG2	1:D:552:LYS:H	1.68	0.59
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.83	0.59
1:A:53:ASN:OD1	1:A:54:ALA:N	2.36	0.59
1:A:225:HIS:CD2	1:A:529:ARG:HE	2.21	0.59
1:D:504:ALA:C	1:D:507:VAL:HG13	2.27	0.59
1:A:22:ARG:NH1	1:A:414:ASN:HB3	2.18	0.59
1:D:149:PHE:CZ	1:D:202:LEU:HD22	2.38	0.59
1:D:229:HIS:O	1:D:233:THR:HG23	2.02	0.59
1:D:328:HIS:CG	1:D:329:ASP:N	2.71	0.59
1:A:99:LEU:HD11	1:A:548:PRO:HG2	1.85	0.59
1:D:451:ARG:O	1:D:454:GLU:HG2	2.02	0.59
1:D:92:HIS:CG	2:E:181:LYS:HB2	2.38	0.58
1:A:143:LYS:HB2	1:A:185:PRO:O	2.02	0.58
1:A:159:GLY:N	7:A:725:HOH:O	2.36	0.58
1:A:282:MET:HA	1:A:282:MET:HE3	1.85	0.58
1:A:316:LEU:O	1:A:320:ALA:N	2.24	0.58
1:D:38:LYS:HE3	2:E:138:GLU:O	2.02	0.58
1:D:178:GLY:O	7:D:713:HOH:O	2.15	0.58
1:D:451:ARG:HG3	1:D:452:LEU:N	2.19	0.58
1:D:572:SER:OG	7:D:702:HOH:O	2.09	0.58
2:E:57:LEU:O	7:E:412:HOH:O	2.17	0.58
2:F:98:TRP:HZ3	2:F:101:PHE:HB2	1.68	0.58
2:B:176:GLU:HG3	2:B:180:PRO:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:153:VAL:HB	7:E:401:HOH:O	2.03	0.58
2:F:54:ILE:HB	2:F:55:PRO:HA	1.84	0.58
1:D:368:GLU:OE2	7:D:716:HOH:O	2.16	0.58
1:D:228:VAL:HA	1:D:319:TYR:CE2	2.38	0.58
2:F:203:GLU:HA	2:F:206:VAL:HG22	1.86	0.58
1:A:327:SER:HB2	1:A:352:PHE:CZ	2.29	0.58
1:D:29:LYS:NZ	1:D:58:GLU:CD	2.61	0.58
1:D:146:GLN:NE2	7:D:738:HOH:O	2.31	0.58
1:D:195:SER:OG	1:D:197:ASP:OD1	2.22	0.58
1:D:465:TYR:HD1	1:D:551:VAL:HG23	1.69	0.58
1:A:284:LEU:HD13	1:A:287:TRP:N	2.19	0.58
1:A:342:THR:HB	1:A:345:LEU:HD13	1.84	0.58
1:D:204:CYS:HA	1:D:207:LEU:HB3	1.85	0.58
2:F:135:LEU:HD22	2:F:182:LEU:HB2	1.84	0.58
1:A:207:LEU:HD11	1:A:245:ILE:HG13	1.84	0.58
1:A:331:GLY:HA2	1:A:539:GLY:N	2.18	0.58
2:C:176:GLU:CD	1:D:491:GLN:HG2	2.28	0.58
1:D:153:GLN:HE21	1:D:171:ARG:HG3	1.68	0.58
1:D:503:ASP:OD1	1:D:504:ALA:N	2.36	0.58
2:C:14:MET:HB3	7:C:401:HOH:O	2.03	0.58
2:C:84:PHE:HD1	2:C:85:PHE:N	2.02	0.58
1:D:148:ILE:HB	1:D:170:TYR:CE2	2.39	0.58
1:D:231:PHE:CZ	1:D:291:ILE:HG12	2.39	0.58
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.38	0.58
1:A:32:LEU:HD22	1:A:61:PHE:CE2	2.39	0.58
1:A:276:THR:OG1	1:A:277:ILE:N	2.35	0.58
2:B:35:GLU:HG2	7:B:404:HOH:O	2.04	0.58
2:B:153:VAL:O	2:B:156:SER:OG	2.19	0.58
1:D:10:MET:O	1:D:14:ILE:HG23	2.04	0.58
1:D:197:ASP:OD2	1:D:256:VAL:HB	2.04	0.58
1:D:510:ARG:HH11	1:D:510:ARG:HG3	1.69	0.58
2:E:62:LYS:HB3	2:F:90:TYR:CE1	2.39	0.58
1:A:143:LYS:NZ	1:A:212:PHE:CG	2.72	0.57
1:D:244:ASP:OD1	1:D:251:SER:HB3	2.03	0.57
2:E:169:LYS:O	7:E:411:HOH:O	2.17	0.57
2:B:122:GLU:O	2:B:125:LYS:HG3	2.04	0.57
1:D:153:GLN:H	1:D:564:GLU:HB2	1.69	0.57
1:D:506:TYR:CE1	1:D:510:ARG:HD3	2.39	0.57
1:D:562:LEU:HD23	1:D:563:CYS:N	2.19	0.57
1:A:152:LYS:HZ1	1:A:527:THR:HG22	1.69	0.57
2:C:84:PHE:HB2	2:C:151:GLY:C	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:HA	1:D:217:GLN:NE2	2.18	0.57
2:F:166:ALA:HA	2:F:169:LYS:HG2	1.85	0.57
1:A:96:ALA:C	1:A:97:ILE:HG13	2.28	0.57
2:B:81:LYS:O	2:B:83:PRO:HD3	2.03	0.57
1:D:31:THR:HA	1:D:34:GLU:HG2	1.86	0.57
2:B:21:VAL:HG11	2:B:158:ILE:CD1	2.33	0.57
1:D:172:ASN:H	1:D:175:PHE:HE2	1.52	0.57
1:D:520:LEU:HG	1:D:522:VAL:HG23	1.85	0.57
2:E:169:LYS:NZ	2:E:206:VAL:HG21	2.18	0.57
1:A:225:HIS:HB3	1:A:309:MET:SD	2.45	0.57
2:C:110:GLN:O	2:C:114:TRP:HD1	1.87	0.57
1:D:451:ARG:NE	1:D:452:LEU:HD13	2.18	0.57
1:D:518:LEU:N	7:D:702:HOH:O	2.31	0.57
2:E:68:LEU:HD11	2:E:152:TYR:CE1	2.40	0.57
2:E:180:PRO:HD2	2:E:181:LYS:HG2	1.85	0.57
7:E:404:HOH:O	2:F:68:LEU:HD11	2.04	0.57
2:B:112:LYS:HD2	2:B:116:LYS:CE	2.34	0.57
2:C:164:PHE:CD2	2:C:183:ILE:HG22	2.40	0.57
1:D:56:ASP:O	1:D:59:GLU:HG2	2.05	0.57
2:E:26:LYS:NZ	2:E:78:TRP:O	2.34	0.57
2:F:43:LEU:HD12	2:F:44:LEU:H	1.69	0.57
1:A:95:PRO:O	1:A:161:PRO:HG2	2.04	0.57
1:A:148:ILE:HB	1:A:170:TYR:CE2	2.40	0.57
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.68	0.57
1:A:86:SER:HB2	2:B:188:ARG:HH21	1.68	0.57
1:A:361:PHE:CZ	1:A:379:LEU:HD13	2.40	0.57
1:A:528:PHE:O	1:A:532:GLN:HG3	2.05	0.57
4:A:602:ILE:O	4:A:602:ILE:HG23	2.04	0.57
1:D:77:ILE:O	1:D:81:VAL:HG23	2.05	0.57
1:D:330:TYR:HB3	1:D:338:ALA:HB3	1.87	0.57
2:E:16:GLY:HA2	2:E:55:PRO:HB3	1.86	0.57
1:A:423:CYS:HG	1:A:541:SER:HG	1.53	0.57
2:C:112:LYS:HB3	7:C:421:HOH:O	2.03	0.57
1:D:29:LYS:HZ1	1:D:58:GLU:CD	2.13	0.57
1:D:118:MET:HE1	1:D:121:THR:HG21	1.87	0.57
1:D:250:LEU:HD21	1:D:254:ILE:HB	1.86	0.57
2:E:121:GLN:O	2:E:125:LYS:HG2	2.04	0.57
2:F:70:VAL:O	2:F:74:VAL:HG23	2.05	0.57
2:F:187:LYS:HA	2:F:190:MET:HB2	1.87	0.57
2:F:110:GLN:O	2:F:114:TRP:HD1	1.88	0.56
2:F:154:ASP:HA	2:F:185:TRP:CZ2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:N	2:B:142:LYS:HE3	2.20	0.56
1:A:228:VAL:HG12	1:A:232:ARG:NH1	2.20	0.56
2:B:202:SER:O	2:B:205:ILE:HG13	2.06	0.56
2:C:35:GLU:HB3	7:C:451:HOH:O	2.04	0.56
2:C:121:GLN:HA	7:C:421:HOH:O	2.05	0.56
1:D:76:TYR:HB3	1:D:88:ILE:HB	1.87	0.56
1:D:528:PHE:HE2	1:D:549:ARG:HH12	1.53	0.56
1:A:99:LEU:HD13	1:A:555:ASN:OD1	2.04	0.56
1:A:222:VAL:O	1:A:223:PHE:HD1	1.89	0.56
1:A:361:PHE:CE1	1:A:379:LEU:HB2	2.41	0.56
1:A:478:PHE:CE1	1:A:521:ARG:HB2	2.40	0.56
2:C:64:VAL:HG13	2:C:73:TYR:HD2	1.70	0.56
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.40	0.56
1:D:65:VAL:HG11	1:D:400:ARG:NH1	2.20	0.56
1:D:416:THR:N	7:D:722:HOH:O	2.37	0.56
2:E:130:GLU:O	2:E:134:ILE:HG12	2.05	0.56
2:F:125:LYS:NZ	2:F:129:ILE:HG21	2.21	0.56
2:F:135:LEU:CD2	2:F:182:LEU:HD12	2.34	0.56
2:E:68:LEU:HD11	2:E:152:TYR:OH	2.05	0.56
1:A:25:HIS:HA	1:A:28:GLN:HG2	1.86	0.56
1:A:112:PRO:HG2	1:A:397:GLY:HA3	1.86	0.56
1:A:153:GLN:NE2	1:A:171:ARG:HG2	2.19	0.56
1:A:219:VAL:HG21	1:A:231:PHE:CZ	2.41	0.56
1:D:92:HIS:CE1	2:E:185:TRP:HB2	2.41	0.56
1:D:309:MET:HE3	1:D:545:PHE:CE2	2.41	0.56
2:E:85:PHE:HB2	2:E:92:ARG:HG2	1.87	0.56
2:E:150:PHE:HE2	2:E:192:LYS:HG3	1.70	0.56
1:A:522:VAL:HB	1:A:568:SER:OG	2.06	0.56
1:D:32:LEU:HD22	1:D:61:PHE:CE2	2.41	0.56
1:D:96:ALA:HB3	1:D:113:PHE:CD2	2.41	0.56
1:D:203:TYR:HA	1:D:206:LEU:HD12	1.88	0.56
1:D:364:LEU:HB3	1:D:389:GLU:HG2	1.87	0.56
1:A:150:SER:OG	1:A:170:TYR:HB2	2.06	0.56
2:B:169:LYS:NZ	2:B:206:VAL:HG11	2.18	0.56
1:D:111:ILE:HD11	1:D:334:GLU:OE2	2.06	0.56
1:D:213:ARG:HA	1:D:216:VAL:HG13	1.86	0.56
2:F:84:PHE:HE1	2:F:85:PHE:CE2	2.23	0.56
1:A:13:VAL:HA	1:A:16:GLU:OE2	2.04	0.56
1:A:228:VAL:HA	1:A:319:TYR:CE2	2.41	0.56
2:E:26:LYS:HE2	2:E:78:TRP:HB3	1.88	0.56
1:A:286:ASN:O	1:A:287:TRP:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:GLU:O	2:B:206:VAL:HG22	2.06	0.56
2:C:40:LYS:HA	7:C:451:HOH:O	2.05	0.56
2:C:85:PHE:CD2	2:C:92:ARG:HG2	2.41	0.56
1:D:90:THR:HG23	1:D:397:GLY:HA2	1.88	0.56
1:D:151:SER:HB2	1:D:194:PHE:HA	1.87	0.56
1:D:365:PRO:HB2	1:D:374:GLU:HG2	1.88	0.56
1:A:87:PRO:HD2	2:B:188:ARG:CB	2.35	0.56
1:A:199:HIS:HB2	1:A:525:LYS:HE3	1.88	0.56
1:D:46:GLN:HB2	2:E:148:ASP:CB	2.36	0.56
1:D:150:SER:OG	1:D:170:TYR:HB2	2.06	0.56
1:D:540:SER:HG	1:D:544:GLN:HE22	1.49	0.56
1:A:111:ILE:HG21	1:A:398:LEU:HD21	1.87	0.55
1:A:116:GLU:CD	1:A:395:TYR:HB3	2.31	0.55
1:A:152:LYS:HE3	1:A:565:ASN:HB2	1.88	0.55
2:C:176:GLU:HG2	1:D:573:THR:HG21	1.88	0.55
1:D:9:ASP:OD1	7:D:717:HOH:O	2.18	0.55
1:D:238:TRP:O	1:D:242:VAL:HG23	2.06	0.55
1:D:361:PHE:HD1	1:D:392:ILE:HG12	1.71	0.55
1:A:203:TYR:CE1	1:A:241:ILE:HG13	2.42	0.55
1:A:222:VAL:HA	1:A:328:HIS:NE2	2.22	0.55
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.41	0.55
1:A:555:ASN:O	1:A:559:LEU:HD22	2.05	0.55
2:C:110:GLN:O	2:C:114:TRP:CD1	2.59	0.55
1:D:446:GLU:O	1:D:450:LYS:NZ	2.35	0.55
1:D:574:ALA:O	1:D:575:PHE:HB2	2.06	0.55
2:C:188:ARG:HB2	1:D:499:ARG:HH22	1.68	0.55
2:B:62:LYS:HD3	2:C:90:TYR:CD2	2.41	0.55
1:D:26:GLN:HG3	1:D:27:VAL:N	2.22	0.55
1:D:228:VAL:HA	1:D:319:TYR:HE2	1.72	0.55
1:D:563:CYS:O	1:D:566:VAL:HG12	2.05	0.55
1:A:22:ARG:HA	1:A:415:ASN:CB	2.35	0.55
1:A:29:LYS:HG3	1:A:30:GLN:N	2.21	0.55
1:A:361:PHE:HZ	1:A:379:LEU:HD13	1.70	0.55
2:B:116:LYS:O	2:B:213:ARG:NH2	2.40	0.55
2:C:139:LEU:HG	2:C:145:PHE:CE1	2.42	0.55
1:D:15:ASP:HA	1:D:18:ASP:OD2	2.06	0.55
1:D:105:GLN:HB2	1:D:107:ARG:NH1	2.21	0.55
1:D:368:GLU:HG3	1:D:369:THR:HG23	1.89	0.55
2:E:89:PRO:HB3	2:F:76:GLU:HG2	1.87	0.55
1:A:223:PHE:HZ	1:A:536:LEU:HB2	1.69	0.55
2:B:150:PHE:CZ	2:B:158:ILE:HG21	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:LEU:HG	2:C:56:VAL:HB	1.88	0.55
2:C:28:VAL:HG21	2:C:78:TRP:CZ3	2.41	0.55
1:D:128:ALA:HA	1:D:131:PHE:CE2	2.41	0.55
1:D:338:ALA:HA	1:D:354:VAL:HA	1.89	0.55
2:E:40:LYS:HZ2	2:E:52:LYS:HD2	1.70	0.55
2:F:33:ARG:HH12	2:F:35:GLU:CD	2.15	0.55
2:F:81:LYS:HG3	2:F:82:ASN:H	1.71	0.55
2:F:195:VAL:O	2:F:199:LEU:HG	2.06	0.55
1:A:41:SER:H	2:B:142:LYS:HE3	1.71	0.55
1:D:519:GLU:OE2	1:D:521:ARG:NH2	2.37	0.55
1:D:551:VAL:HG12	1:D:555:ASN:HD22	1.71	0.55
2:B:19:ALA:HB2	2:B:70:VAL:HG11	1.89	0.55
2:F:32:TYR:HD2	2:F:34:GLU:OE2	1.90	0.55
1:A:152:LYS:CG	1:A:565:ASN:HB2	2.35	0.55
1:A:478:PHE:HE1	1:A:521:ARG:HB2	1.72	0.55
1:D:55:THR:C	1:D:57:PRO:HD3	2.32	0.55
1:D:234:PHE:HD2	1:D:287:TRP:HH2	1.54	0.55
1:D:269:PRO:O	1:D:270:ASN:ND2	2.40	0.55
1:D:569:SER:C	1:D:570:TYR:HD1	2.14	0.55
1:D:199:HIS:HB2	1:D:525:LYS:HE3	1.89	0.55
1:D:223:PHE:CE2	1:D:533:GLU:HA	2.42	0.55
2:F:37:PHE:CZ	2:F:54:ILE:HG12	2.39	0.55
2:F:96:ARG:NH2	7:F:424:HOH:O	2.38	0.55
2:F:151:GLY:N	2:F:154:ASP:OD2	2.40	0.55
2:C:5:PRO:HG2	2:C:30:PHE:HB3	1.89	0.54
1:D:22:ARG:HG2	1:D:414:ASN:HB3	1.88	0.54
1:D:132:ARG:HA	1:D:343:PRO:HG2	1.88	0.54
2:F:132:VAL:HG22	2:F:179:SER:HB3	1.89	0.54
1:A:250:LEU:HD21	1:A:254:ILE:HB	1.89	0.54
1:A:281:CYS:O	1:A:284:LEU:HG	2.06	0.54
1:D:76:TYR:HB3	1:D:88:ILE:CG2	2.38	0.54
1:D:223:PHE:CE1	1:D:536:LEU:HB2	2.41	0.54
1:D:336:TRP:HB2	1:D:358:LEU:HD13	1.90	0.54
2:E:11:TRP:HH2	2:E:208:TYR:CD1	2.25	0.54
1:A:152:LYS:HZ3	1:A:527:THR:HG22	1.72	0.54
1:A:224:ALA:O	1:A:228:VAL:HG23	2.07	0.54
1:A:445:VAL:HG21	1:A:462:PHE:CD1	2.43	0.54
2:B:18:ARG:HH12	2:B:103:ASP:CG	2.08	0.54
2:B:108:ASP:O	2:B:111:PHE:HB3	2.06	0.54
1:D:8:PHE:HE1	1:D:130:ALA:HB2	1.72	0.54
1:D:164:THR:OG1	1:D:557:LYS:O	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:O	1:A:124:LEU:HG	2.08	0.54
1:D:34:GLU:O	1:D:38:LYS:HG2	2.05	0.54
1:D:154:TYR:OH	1:D:162:VAL:HG22	2.07	0.54
1:D:405:ASP:OD2	1:D:540:SER:HB2	2.08	0.54
1:A:211:LEU:HD12	1:A:212:PHE:HD2	1.72	0.54
2:B:139:LEU:O	2:B:141:ASP:N	2.41	0.54
2:C:188:ARG:HE	1:D:499:ARG:NH2	2.04	0.54
2:C:212:TYR:CZ	2:C:213:ARG:HG3	2.43	0.54
1:D:8:PHE:CE1	1:D:130:ALA:HB2	2.41	0.54
1:D:171:ARG:HH21	1:D:194:PHE:HB3	1.73	0.54
1:D:179:MET:SD	7:D:811:HOH:O	2.58	0.54
1:D:506:TYR:CZ	1:D:510:ARG:HD3	2.41	0.54
2:E:122:GLU:HG3	2:E:123:ALA:N	2.23	0.54
1:A:317:ARG:O	1:A:321:GLY:N	2.37	0.54
2:B:176:GLU:HB2	2:B:183:ILE:HG21	1.89	0.54
1:D:332:SER:CB	1:D:538:LEU:HA	2.35	0.54
1:D:365:PRO:HG2	1:D:374:GLU:HG2	1.89	0.54
1:D:365:PRO:HG3	1:D:388:TYR:CE2	2.42	0.54
1:D:475:TYR:CE1	1:D:515:ILE:HD12	2.43	0.54
2:F:66:GLU:O	2:F:70:VAL:HG23	2.08	0.54
1:A:104:SER:O	1:A:104:SER:OG	2.22	0.54
1:A:200:GLN:HE21	1:A:254:ILE:HG23	1.72	0.54
1:A:444:SER:HA	1:A:500:ALA:HB1	1.90	0.54
1:A:464:SER:OG	7:A:720:HOH:O	2.18	0.54
1:D:152:LYS:HB3	1:D:560:GLN:O	2.07	0.54
1:D:224:ALA:O	1:D:228:VAL:HG23	2.08	0.54
1:D:445:VAL:HG21	1:D:462:PHE:CB	2.37	0.54
1:D:465:TYR:HB2	1:D:551:VAL:HG22	1.90	0.54
2:E:75:ASP:OD2	2:E:85:PHE:CD2	2.61	0.54
2:E:169:LYS:HZ1	2:E:206:VAL:HG21	1.73	0.54
1:A:160:VAL:N	7:A:725:HOH:O	2.20	0.54
1:D:41:SER:H	2:E:142:LYS:HE2	1.72	0.54
1:D:151:SER:O	1:D:151:SER:OG	2.25	0.54
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.42	0.54
2:B:110:GLN:HB2	2:B:167:TYR:CZ	2.43	0.54
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.42	0.54
2:F:16:GLY:HA2	2:F:55:PRO:HG3	1.89	0.54
1:A:265:LYS:NZ	1:A:266:LEU:HG	2.22	0.54
1:A:541:SER:O	1:A:544:GLN:NE2	2.41	0.54
2:C:140:GLY:O	2:C:181:LYS:NZ	2.40	0.54
2:C:206:VAL:O	2:C:209:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:HE3	1:D:187:CYS:CA	2.38	0.54
1:D:186:SER:HA	7:D:720:HOH:O	2.08	0.54
1:D:477:ILE:HD13	1:D:497:LEU:HD22	1.89	0.54
1:D:563:CYS:HG	1:D:564:GLU:H	1.56	0.54
2:E:185:TRP:O	2:E:188:ARG:HG2	2.08	0.54
2:B:133:LYS:O	2:B:137:SER:N	2.39	0.53
1:D:198:VAL:HG23	1:D:524:ALA:CB	2.33	0.53
1:D:212:PHE:HD2	1:D:215:GLN:CD	2.16	0.53
1:D:213:ARG:HG3	1:D:214:ASP:N	2.23	0.53
1:D:493:CYS:SG	1:D:520:LEU:HD22	2.48	0.53
2:F:125:LYS:O	2:F:129:ILE:HG23	2.07	0.53
1:A:403:LEU:HD21	1:A:538:LEU:HD21	1.89	0.53
2:B:150:PHE:CZ	2:B:158:ILE:HD13	2.43	0.53
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.43	0.53
2:C:21:VAL:HG12	2:C:155:ILE:HG12	1.89	0.53
1:D:200:GLN:OE1	1:D:255:THR:N	2.40	0.53
1:D:221:ALA:HB2	1:D:227:LEU:HG	1.91	0.53
1:A:10:MET:O	1:A:14:ILE:HG22	2.07	0.53
1:A:104:SER:O	1:A:107:ARG:HB2	2.09	0.53
1:A:143:LYS:NZ	1:A:212:PHE:CA	2.69	0.53
1:A:223:PHE:CZ	1:A:536:LEU:HB2	2.43	0.53
1:A:508:SER:HB2	7:A:831:HOH:O	2.07	0.53
2:B:15:PHE:HB3	2:B:67:SER:HB3	1.90	0.53
1:D:114:THR:OG1	2:E:141:ASP:OD2	2.18	0.53
1:D:536:LEU:HG	1:D:545:PHE:CE1	2.43	0.53
1:A:425:ARG:HE	1:A:546:LYS:HD2	1.73	0.53
2:C:66:GLU:HB2	2:C:69:ASN:HB2	1.89	0.53
1:D:198:VAL:HB	1:D:202:LEU:HD21	1.89	0.53
2:E:15:PHE:HB3	2:E:67:SER:HB3	1.90	0.53
1:A:31:THR:OG1	1:A:357:ASN:HA	2.08	0.53
2:C:81:LYS:HG3	2:C:82:ASN:H	1.74	0.53
2:C:133:LYS:O	2:C:136:GLU:HB3	2.08	0.53
2:E:110:GLN:OE1	2:E:167:TYR:OH	2.26	0.53
1:A:142:GLY:O	1:A:185:PRO:HD2	2.09	0.53
1:A:219:VAL:HG21	1:A:231:PHE:HZ	1.72	0.53
1:D:235:GLU:HG2	1:D:287:TRP:CD2	2.43	0.53
1:D:496:CYS:CA	1:D:499:ARG:NH1	2.72	0.53
1:A:86:SER:HA	2:B:188:ARG:HB2	1.89	0.53
1:A:441:LEU:HA	1:A:501:PHE:HE1	1.72	0.53
1:A:448:ALA:CB	1:A:496:CYS:HB3	2.39	0.53
2:C:70:VAL:O	2:C:73:TYR:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ILE:HG21	1:D:134:ARG:NH1	2.24	0.53
1:D:233:THR:O	1:D:237:VAL:HG22	2.08	0.53
1:D:329:ASP:N	1:D:329:ASP:OD1	2.42	0.53
1:D:451:ARG:CZ	1:D:490:LEU:HA	2.39	0.53
1:D:509:SER:O	1:D:513:LYS:N	2.42	0.53
2:E:88:ASP:OD1	2:E:91:GLY:N	2.36	0.53
2:E:142:LYS:HD2	2:E:144:TYR:O	2.08	0.53
2:F:10:TYR:CG	2:F:37:PHE:HE1	2.27	0.53
2:F:183:ILE:O	2:F:183:ILE:HG13	2.09	0.53
1:A:79:ARG:HG2	1:A:86:SER:OG	2.09	0.53
1:A:179:MET:HE3	1:A:183:THR:HG21	1.91	0.53
1:A:413:TYR:CD2	1:A:418:GLN:HG2	2.44	0.53
1:A:435:LYS:HE2	1:A:437:THR:HA	1.91	0.53
1:A:440:ASP:HA	1:A:443:LEU:HB2	1.90	0.53
1:D:37:LEU:O	7:E:403:HOH:O	2.19	0.53
1:D:365:PRO:HA	1:D:388:TYR:CD1	2.42	0.53
1:D:526:GLY:HA2	1:D:529:ARG:CZ	2.39	0.53
1:D:538:LEU:HD23	1:D:544:GLN:HG2	1.90	0.53
1:A:47:ASN:O	7:A:721:HOH:O	2.18	0.53
1:A:199:HIS:N	1:A:524:ALA:HB1	2.21	0.53
1:A:466:ILE:CG1	1:A:552:LYS:HA	2.38	0.53
1:D:92:HIS:ND1	2:E:188:ARG:NH2	2.56	0.53
1:D:110:PHE:HE1	1:D:556:ALA:HB2	1.74	0.53
2:E:73:TYR:HE1	2:F:90:TYR:HA	1.73	0.53
1:A:231:PHE:O	1:A:235:GLU:HG3	2.08	0.53
1:A:386:GLU:N	7:A:733:HOH:O	2.42	0.53
2:B:96:ARG:NH1	2:C:76:GLU:OE2	2.41	0.53
1:D:152:LYS:HD3	1:D:561:ILE:HA	1.91	0.53
1:D:154:TYR:HE2	1:D:162:VAL:O	1.92	0.53
1:D:211:LEU:HD13	1:D:212:PHE:HD1	1.74	0.53
1:D:365:PRO:HG3	1:D:388:TYR:CZ	2.44	0.53
2:E:130:GLU:HA	2:E:133:LYS:HE3	1.90	0.53
2:E:155:ILE:HA	2:E:158:ILE:HG12	1.91	0.53
2:F:40:LYS:HB2	2:F:45:LEU:HD11	1.90	0.53
2:F:128:PHE:HE1	2:F:175:ILE:HG22	1.71	0.53
2:F:165:GLN:HG3	2:F:202:SER:OG	2.09	0.53
1:A:143:LYS:CA	1:A:184:SER:HB2	2.40	0.52
1:A:164:THR:HG23	1:A:560:GLN:HB2	1.91	0.52
2:B:67:SER:O	2:B:70:VAL:HG12	2.09	0.52
1:D:91:GLY:HA3	2:E:141:ASP:O	2.08	0.52
1:D:162:VAL:HG23	1:D:556:ALA:HB1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:THR:C	1:D:265:LYS:HZ3	2.17	0.52
1:D:312:TYR:CD1	1:D:315:LYS:HD2	2.44	0.52
2:E:20:ARG:HB2	7:E:402:HOH:O	2.08	0.52
2:F:140:GLY:HA2	2:F:181:LYS:HZ1	1.74	0.52
1:A:41:SER:HB2	2:B:142:LYS:CG	2.35	0.52
1:A:451:ARG:O	1:A:454:GLU:HG2	2.09	0.52
1:A:534:HIS:HB3	4:A:602:ILE:C	2.34	0.52
1:D:12:ARG:HH12	1:D:126:ARG:HH21	1.57	0.52
1:A:224:ALA:HA	1:A:316:LEU:HD22	1.91	0.52
1:A:437:THR:O	1:A:440:ASP:N	2.42	0.52
1:A:521:ARG:HG2	1:A:569:SER:OG	2.09	0.52
2:B:18:ARG:NE	2:B:156:SER:O	2.42	0.52
2:C:8:LEU:HD13	2:C:44:LEU:HB2	1.91	0.52
1:D:199:HIS:HB3	1:D:525:LYS:H	1.74	0.52
1:D:217:GLN:OE1	1:D:217:GLN:HA	2.08	0.52
1:D:234:PHE:HD2	1:D:287:TRP:CH2	2.28	0.52
1:D:493:CYS:O	1:D:497:LEU:HD12	2.10	0.52
1:D:531:ILE:HA	1:D:534:HIS:ND1	2.25	0.52
2:E:97:PHE:HE1	2:F:65:CYS:O	1.93	0.52
2:E:122:GLU:HG3	2:E:123:ALA:H	1.74	0.52
2:F:168:GLU:CD	2:F:175:ILE:HG12	2.35	0.52
1:A:294:LEU:HD12	1:A:295:PHE:N	2.24	0.52
1:A:303:GLY:O	1:A:327:SER:HA	2.09	0.52
2:C:140:GLY:C	2:C:181:LYS:HZ1	2.17	0.52
1:D:87:PRO:CD	1:D:93:PRO:HG3	2.40	0.52
1:D:118:MET:HE1	1:D:169:VAL:HG23	1.92	0.52
1:D:435:LYS:HA	1:D:436:ASN:HB2	1.92	0.52
2:E:86:PRO:HD3	2:E:146:GLY:O	2.09	0.52
1:A:86:SER:HB2	2:B:188:ARG:NH2	2.25	0.52
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.72	0.52
2:E:99:ALA:HA	2:E:102:VAL:HG12	1.92	0.52
2:E:150:PHE:HE2	2:E:192:LYS:CG	2.21	0.52
6:E:301:GSH:OE1	7:E:413:HOH:O	2.19	0.52
1:A:26:GLN:O	1:A:29:LYS:HG3	2.10	0.52
1:A:192:VAL:HG22	1:A:259:VAL:HG23	1.91	0.52
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.45	0.52
2:C:187:LYS:HD3	1:D:492:ASP:HB3	1.91	0.52
1:D:32:LEU:HD22	1:D:61:PHE:HE2	1.74	0.52
1:D:126:ARG:HG3	1:D:126:ARG:NH1	2.24	0.52
1:D:149:PHE:HB2	1:D:530:LYS:HE3	1.92	0.52
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:GLY:O	1:D:310:GLU:HG3	2.10	0.52
2:F:9:ASP:OD1	2:F:9:ASP:N	2.42	0.52
2:F:110:GLN:O	2:F:114:TRP:CD1	2.63	0.52
1:A:71:VAL:HG23	1:A:107:ARG:HH22	1.74	0.52
1:A:138:ILE:O	7:A:723:HOH:O	2.19	0.52
2:C:88:ASP:HB2	7:C:457:HOH:O	2.09	0.52
2:C:139:LEU:O	2:C:141:ASP:N	2.43	0.52
2:C:191:GLU:HA	1:D:450:LYS:CE	2.40	0.52
1:D:7:THR:OG1	7:D:718:HOH:O	2.19	0.52
1:D:30:GLN:OE1	1:D:30:GLN:HA	2.09	0.52
1:D:163:GLY:HA3	1:D:560:GLN:HB2	1.91	0.52
1:D:213:ARG:HH21	1:D:296:PRO:HD3	1.74	0.52
2:E:64:VAL:HG13	2:F:93:ALA:HB1	1.92	0.52
2:E:185:TRP:HA	2:E:188:ARG:CZ	2.39	0.52
4:A:602:ILE:O	7:A:722:HOH:O	2.19	0.52
2:B:98:TRP:CE2	2:B:138:GLU:HG2	2.45	0.52
2:B:107:THR:HA	2:B:110:GLN:HE21	1.73	0.52
2:C:10:TYR:CG	2:C:12:PRO:HD2	2.44	0.52
2:C:111:PHE:HA	2:C:114:TRP:NE1	2.25	0.52
1:D:45:LEU:HB3	1:D:50:LEU:HB2	1.90	0.52
1:D:51:ASN:N	1:D:51:ASN:OD1	2.41	0.52
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.75	0.52
2:E:8:LEU:HD22	2:E:35:GLU:OE2	2.09	0.52
2:E:51:HIS:HB3	2:E:53:LYS:HE3	1.91	0.52
2:E:67:SER:HA	2:E:70:VAL:HG12	1.92	0.52
2:E:125:LYS:HB2	2:E:173:PHE:CE2	2.44	0.52
1:A:143:LYS:HA	1:A:184:SER:HB2	1.91	0.52
1:A:445:VAL:HG11	1:A:462:PHE:CD2	2.45	0.52
2:B:106:PHE:O	2:B:110:GLN:HG2	2.10	0.52
1:D:8:PHE:CD1	1:D:126:ARG:NH1	2.77	0.52
1:D:57:PRO:HD2	1:D:58:GLU:OE2	2.10	0.52
2:E:164:PHE:O	2:E:168:GLU:HG2	2.10	0.52
2:E:201:ASP:OD2	2:E:204:LYS:HE2	2.10	0.52
2:F:8:LEU:HD22	2:F:33:ARG:HD3	1.92	0.52
1:A:315:LYS:O	1:A:319:TYR:N	2.40	0.52
2:B:17:MET:HE2	2:B:200:PRO:HD2	1.93	0.52
1:D:174:ASN:OD1	7:D:719:HOH:O	2.19	0.52
1:D:405:ASP:CG	1:D:540:SER:HB2	2.35	0.52
1:D:476:ALA:HB1	1:D:521:ARG:HD2	1.92	0.52
1:D:523:VAL:HG12	1:D:566:VAL:HA	1.92	0.52
1:D:526:GLY:O	1:D:530:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:LEU:O	1:D:562:LEU:HB3	2.09	0.52
2:F:158:ILE:HG23	2:F:159:THR:HG23	1.92	0.52
1:A:77:ILE:HG22	1:A:110:PHE:CD2	2.42	0.51
2:B:26:LYS:HZ3	2:B:28:VAL:HB	1.74	0.51
2:B:54:ILE:HB	2:B:55:PRO:HA	1.92	0.51
2:C:64:VAL:HG13	2:C:73:TYR:CD2	2.45	0.51
2:C:185:TRP:NE1	2:C:189:CYS:HG	2.08	0.51
1:D:105:GLN:HB2	1:D:107:ARG:HH12	1.75	0.51
1:D:478:PHE:O	1:D:479:TRP:HD1	1.93	0.51
1:D:142:GLY:HA2	1:D:215:GLN:HB2	1.90	0.51
1:D:451:ARG:NH1	1:D:489:VAL:C	2.66	0.51
1:D:506:TYR:CD2	1:D:510:ARG:NH1	2.78	0.51
1:D:506:TYR:O	1:D:510:ARG:HG3	2.09	0.51
1:A:229:HIS:CG	1:A:230:ALA:N	2.77	0.51
1:D:13:VAL:HB	1:D:126:ARG:CZ	2.41	0.51
1:D:448:ALA:HB1	1:D:493:CYS:HB2	1.91	0.51
2:F:24:ARG:HB3	2:F:194:SER:HA	1.92	0.51
2:F:131:ALA:HA	2:F:134:ILE:HG12	1.92	0.51
2:F:163:TRP:HB3	2:F:167:TYR:CE1	2.46	0.51
1:A:38:LYS:HD2	2:B:138:GLU:O	2.11	0.51
1:A:168:ASN:O	1:A:172:ASN:HB2	2.10	0.51
1:A:503:ASP:CG	1:A:505:GLY:H	2.18	0.51
2:C:196:SER:OG	7:C:408:HOH:O	2.18	0.51
1:D:147:PHE:HA	1:D:205:HIS:HD2	1.70	0.51
1:D:363:PHE:HD1	1:D:390:VAL:HA	1.74	0.51
2:F:33:ARG:HH12	2:F:35:GLU:CG	2.23	0.51
1:A:251:SER:O	1:A:260:ARG:NH2	2.34	0.51
1:D:133:ASN:HB3	7:D:845:HOH:O	2.10	0.51
1:D:166:THR:O	1:D:169:VAL:HG12	2.11	0.51
1:D:535:PHE:O	1:D:538:LEU:HB3	2.10	0.51
2:E:69:ASN:OD1	2:F:96:ARG:NE	2.38	0.51
1:A:118:MET:HG2	1:A:174:ASN:CG	2.36	0.51
1:A:219:VAL:HB	1:A:295:PHE:HZ	1.71	0.51
1:A:316:LEU:HD12	1:A:319:TYR:HB2	1.92	0.51
2:C:75:ASP:HB2	2:C:84:PHE:CZ	2.45	0.51
1:D:92:HIS:H	2:E:142:LYS:N	2.09	0.51
1:D:187:CYS:O	1:D:208:SER:HB3	2.10	0.51
1:D:228:VAL:O	1:D:232:ARG:HG2	2.10	0.51
2:E:94:GLN:HB3	2:E:98:TRP:CZ2	2.46	0.51
1:A:156:SER:OG	1:A:157:THR:N	2.43	0.51
1:A:212:PHE:HD1	1:A:215:GLN:HE21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:GLU:HG3	2:B:44:LEU:HD21	1.92	0.51
1:A:234:PHE:C	1:A:234:PHE:CD2	2.88	0.51
1:A:334:GLU:HG3	1:A:538:LEU:HD13	1.92	0.51
1:A:466:ILE:HG13	1:A:552:LYS:HA	1.92	0.51
1:A:556:ALA:HA	1:A:559:LEU:HB2	1.93	0.51
2:C:90:TYR:O	2:C:94:GLN:HG3	2.10	0.51
1:D:77:ILE:HG21	1:D:110:PHE:HB3	1.93	0.51
1:D:255:THR:HA	1:D:260:ARG:HD2	1.92	0.51
2:E:183:ILE:HG13	2:E:187:LYS:HZ1	1.74	0.51
2:E:210:ALA:O	2:E:213:ARG:HB3	2.11	0.51
2:F:17:MET:HE1	2:F:163:TRP:CH2	2.46	0.51
2:F:43:LEU:HD12	2:F:44:LEU:N	2.25	0.51
1:A:341:VAL:C	1:A:343:PRO:HD3	2.35	0.51
1:D:33:LYS:O	1:D:37:LEU:HB2	2.11	0.51
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.31	0.51
2:F:125:LYS:HZ3	2:F:129:ILE:HG21	1.76	0.51
1:A:32:LEU:HB3	1:A:61:PHE:HE2	1.76	0.51
1:A:287:TRP:NE1	1:A:319:TYR:CD1	2.79	0.51
1:A:448:ALA:HB2	1:A:496:CYS:HB3	1.92	0.51
2:B:72:GLN:O	2:B:76:GLU:HG3	2.11	0.51
2:B:97:PHE:CE2	2:B:101:PHE:HE2	2.29	0.51
1:D:164:THR:OG1	1:D:561:ILE:HG12	2.11	0.51
2:F:7:LEU:HD22	2:F:30:PHE:CD1	2.46	0.51
1:A:77:ILE:CG2	1:A:110:PHE:HB3	2.41	0.50
1:A:149:PHE:HD2	1:A:530:LYS:HE2	1.77	0.50
1:A:172:ASN:OD1	1:A:173:PRO:HD2	2.09	0.50
2:C:8:LEU:HD22	2:C:33:ARG:NH2	2.26	0.50
2:C:57:LEU:HB3	2:C:64:VAL:HG12	1.93	0.50
2:C:170:PHE:HD1	2:C:213:ARG:HH21	1.59	0.50
1:D:124:LEU:HD13	1:D:336:TRP:CE3	2.45	0.50
2:E:54:ILE:HB	2:E:55:PRO:HA	1.93	0.50
2:E:109:ALA:HB3	7:E:416:HOH:O	2.11	0.50
2:E:163:TRP:HA	2:E:205:ILE:CD1	2.42	0.50
2:E:185:TRP:HA	2:E:188:ARG:NE	2.26	0.50
1:A:203:TYR:HD1	1:A:237:VAL:HG21	1.74	0.50
1:A:406:VAL:O	1:A:541:SER:OG	2.27	0.50
2:B:24:ARG:HG2	2:B:197:LYS:HZ1	1.76	0.50
1:D:70:ASP:OD1	1:D:71:VAL:N	2.44	0.50
1:A:42:ALA:O	1:A:45:LEU:HB2	2.11	0.50
1:A:97:ILE:HG21	1:A:110:PHE:CE2	2.46	0.50
1:A:103:THR:HB	1:A:106:GLY:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:O	1:A:210:ILE:HG13	2.11	0.50
2:C:92:ARG:O	2:C:96:ARG:HG3	2.11	0.50
2:C:185:TRP:NE1	2:C:189:CYS:SG	2.85	0.50
1:A:76:TYR:O	1:A:79:ARG:HB3	2.11	0.50
2:C:190:MET:C	1:D:450:LYS:HD2	2.36	0.50
1:D:90:THR:OG1	1:D:112:PRO:HG2	2.10	0.50
1:D:328:HIS:CG	1:D:329:ASP:H	2.28	0.50
2:E:75:ASP:OD2	2:E:85:PHE:HD2	1.94	0.50
2:F:110:GLN:HA	2:F:113:VAL:HG12	1.93	0.50
1:A:146:GLN:HB2	1:A:148:ILE:HG23	1.93	0.50
1:A:341:VAL:O	1:A:343:PRO:HD3	2.11	0.50
1:A:398:LEU:HD22	1:A:401:TYR:CZ	2.45	0.50
2:B:117:LYS:HG3	2:B:213:ARG:NH1	2.27	0.50
2:C:99:ALA:CB	2:C:152:TYR:HE1	2.24	0.50
2:C:111:PHE:O	2:C:115:GLY:HA3	2.11	0.50
1:D:41:SER:HB2	2:E:147:GLY:O	2.12	0.50
1:D:69:THR:HB	1:D:71:VAL:HG12	1.93	0.50
1:D:174:ASN:N	7:D:719:HOH:O	2.37	0.50
2:F:133:LYS:HA	2:F:136:GLU:HG2	1.94	0.50
2:F:135:LEU:O	2:F:138:GLU:HG3	2.11	0.50
1:A:91:GLY:HA3	2:B:141:ASP:C	2.36	0.50
1:A:252:ASN:HA	1:A:260:ARG:NH2	2.25	0.50
1:A:340:ASN:HB2	1:A:352:PHE:CE1	2.46	0.50
2:B:96:ARG:HH12	2:C:76:GLU:CD	2.20	0.50
2:C:34:GLU:N	2:C:34:GLU:CD	2.69	0.50
2:C:73:TYR:HD1	2:C:76:GLU:OE2	1.94	0.50
1:D:12:ARG:HH12	1:D:126:ARG:NH2	2.09	0.50
1:D:59:GLU:HA	1:D:62:LYS:NZ	2.26	0.50
1:D:118:MET:SD	1:D:175:PHE:HE1	2.34	0.50
1:D:148:ILE:HB	1:D:170:TYR:HE2	1.77	0.50
1:D:227:LEU:HB3	1:D:316:LEU:HD11	1.93	0.50
1:D:434:ASP:O	1:D:550:CYS:HB3	2.11	0.50
2:F:17:MET:SD	2:F:163:TRP:HZ3	2.35	0.50
2:F:169:LYS:HG3	2:F:170:PHE:N	2.26	0.50
1:A:393:THR:HG22	1:A:400:ARG:H	1.76	0.50
1:A:563:CYS:O	1:A:566:VAL:HG12	2.12	0.50
1:D:94:VAL:HG21	1:D:112:PRO:HA	1.94	0.50
1:D:99:LEU:HD12	1:D:100:SER:N	2.27	0.50
1:D:154:TYR:OH	1:D:559:LEU:HD13	2.11	0.50
1:D:541:SER:O	1:D:543:GLY:N	2.44	0.50
2:E:96:ARG:NE	2:F:69:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:THR:HB	1:A:116:GLU:OE2	2.10	0.50
1:A:562:LEU:HD12	1:A:563:CYS:N	2.27	0.50
1:D:82:ASP:OD2	1:D:553:PRO:HB3	2.12	0.50
1:D:191:GLU:O	1:D:195:SER:N	2.45	0.50
2:E:142:LYS:NZ	7:E:403:HOH:O	2.05	0.50
2:F:139:LEU:HB2	2:F:145:PHE:CZ	2.47	0.50
1:A:17:PHE:CE2	1:A:127:THR:HG23	2.47	0.50
1:A:143:LYS:C	1:A:184:SER:HB2	2.37	0.50
1:A:352:PHE:N	1:A:352:PHE:CD2	2.80	0.50
2:C:169:LYS:HG3	2:C:170:PHE:N	2.27	0.50
2:C:183:ILE:HD13	1:D:492:ASP:OD1	2.12	0.50
1:A:77:ILE:O	1:A:80:MET:HG2	2.11	0.49
1:A:304:ILE:HG13	1:A:328:HIS:CD2	2.47	0.49
2:B:150:PHE:CE2	2:B:158:ILE:HD13	2.47	0.49
1:D:148:ILE:HG23	1:D:220:PHE:HE2	1.77	0.49
1:D:313:VAL:N	1:D:314:PRO:HD2	2.27	0.49
1:D:441:LEU:HD23	1:D:549:ARG:HB3	1.94	0.49
2:E:106:PHE:CE2	2:E:135:LEU:HD11	2.47	0.49
2:E:202:SER:O	2:E:206:VAL:HG13	2.11	0.49
2:B:139:LEU:HD11	2:B:145:PHE:CE1	2.47	0.49
1:D:13:VAL:HB	1:D:126:ARG:NH2	2.27	0.49
1:D:135:ASP:OD1	1:D:136:PHE:N	2.44	0.49
1:D:138:ILE:CB	1:D:217:GLN:HG3	2.40	0.49
2:E:143:PRO:O	2:E:188:ARG:HD2	2.13	0.49
1:A:85:THR:HB	2:B:184:ALA:HB1	1.94	0.49
1:A:121:THR:HG23	3:A:601:JAA:C14	2.42	0.49
1:A:534:HIS:HB3	4:A:602:ILE:O	2.12	0.49
2:B:166:ALA:HB2	2:B:206:VAL:HG12	1.93	0.49
1:D:118:MET:HE2	1:D:118:MET:HA	1.93	0.49
1:D:462:PHE:C	1:D:528:PHE:HZ	2.20	0.49
1:A:176:LYS:HE3	1:A:190:ASP:OD2	2.12	0.49
1:A:244:ASP:OD1	1:A:251:SER:HB3	2.11	0.49
1:A:285:SER:O	1:A:286:ASN:CB	2.59	0.49
1:D:56:ASP:HA	1:D:59:GLU:OE2	2.13	0.49
1:D:98:SER:HG	1:D:113:PHE:HE1	1.56	0.49
1:A:27:VAL:HB	1:A:356:PRO:HB2	1.93	0.49
1:A:294:LEU:HD12	1:A:295:PHE:H	1.76	0.49
1:D:143:LYS:HG2	1:D:144:ALA:H	1.77	0.49
1:D:445:VAL:HG21	1:D:462:PHE:HB2	1.95	0.49
2:F:23:LEU:HD11	2:F:30:PHE:CE2	2.47	0.49
2:F:125:LYS:HD2	2:F:128:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:HB3	1:A:525:LYS:H	1.76	0.49
1:A:309:MET:SD	1:A:312:TYR:HB2	2.53	0.49
2:B:15:PHE:CD2	6:B:301:GSH:HB12	2.46	0.49
2:B:145:PHE:HB2	2:B:153:VAL:HG13	1.93	0.49
1:D:241:ILE:O	1:D:245:ILE:HG12	2.13	0.49
1:D:312:TYR:HD1	1:D:315:LYS:HD2	1.78	0.49
1:D:363:PHE:CE1	1:D:390:VAL:HG23	2.46	0.49
1:D:507:VAL:O	1:D:511:LYS:HG3	2.12	0.49
2:F:20:ARG:O	2:F:24:ARG:HB2	2.13	0.49
2:F:33:ARG:NH2	7:F:428:HOH:O	2.43	0.49
2:F:44:LEU:HD21	2:F:52:LYS:C	2.37	0.49
1:A:146:GLN:HA	1:A:220:PHE:HB3	1.94	0.49
1:A:379:LEU:HG	1:A:380:THR:N	2.26	0.49
1:A:534:HIS:HE1	1:A:535:PHE:CE1	2.30	0.49
2:C:7:LEU:HA	2:C:56:VAL:O	2.13	0.49
2:C:139:LEU:HD13	2:C:181:LYS:HE2	1.94	0.49
1:D:126:ARG:HA	1:D:182:ILE:HG21	1.95	0.49
2:E:135:LEU:HD12	2:E:135:LEU:N	2.27	0.49
2:F:41:SER:HB3	2:F:43:LEU:CD1	2.43	0.49
2:F:110:GLN:HB3	2:F:167:TYR:CZ	2.48	0.49
1:A:210:ILE:HA	1:A:213:ARG:NE	2.28	0.49
2:C:110:GLN:HB3	2:C:167:TYR:CZ	2.48	0.49
1:D:231:PHE:HD1	1:D:287:TRP:HZ2	1.60	0.49
2:E:14:MET:O	2:E:17:MET:HB2	2.12	0.49
2:E:188:ARG:HG3	2:E:189:CYS:N	2.27	0.49
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.48	0.49
1:A:126:ARG:HG2	1:A:182:ILE:HD12	1.95	0.49
1:A:143:LYS:HD3	1:A:212:PHE:CD1	2.48	0.49
1:A:315:LYS:HA	1:A:318:HIS:CB	2.43	0.49
2:B:8:LEU:HD13	2:B:44:LEU:HG	1.95	0.49
2:C:5:PRO:HB3	2:C:59:HIS:CE1	2.48	0.49
2:C:136:GLU:HG3	2:C:181:LYS:CD	2.33	0.49
2:C:184:ALA:HA	2:C:187:LYS:NZ	2.27	0.49
1:A:119:GLU:O	1:A:123:GLN:HG2	2.12	0.49
1:A:143:LYS:NZ	1:A:212:PHE:CD1	2.80	0.49
1:A:265:LYS:HZ2	1:A:266:LEU:HG	1.76	0.49
1:A:302:TYR:HA	1:A:326:VAL:HG13	1.95	0.49
1:A:420:LYS:HG2	1:A:421:PHE:N	2.28	0.49
1:A:444:SER:HA	1:A:500:ALA:CB	2.42	0.49
2:B:13:SER:CB	2:B:54:ILE:HD11	2.43	0.49
2:B:16:GLY:O	2:B:20:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ALA:CB	2:B:70:VAL:HG11	2.43	0.49
2:C:98:TRP:CE3	2:C:138:GLU:OE2	2.66	0.49
1:D:445:VAL:HG13	1:D:479:TRP:CE2	2.48	0.49
2:E:24:ARG:NH1	2:E:198:SER:OG	2.38	0.49
2:E:148:ASP:N	2:E:148:ASP:OD1	2.43	0.49
1:A:45:LEU:CD2	1:A:50:LEU:HD23	2.42	0.48
2:B:18:ARG:O	2:B:21:VAL:HG12	2.13	0.48
2:C:32:TYR:CD1	2:C:34:GLU:OE2	2.66	0.48
2:C:184:ALA:HA	2:C:187:LYS:HZ1	1.78	0.48
2:C:187:LYS:HE3	1:D:492:ASP:C	2.38	0.48
1:D:76:TYR:HB3	1:D:88:ILE:CB	2.43	0.48
1:D:108:PRO:CG	1:D:552:LYS:H	2.26	0.48
1:D:163:GLY:CA	1:D:560:GLN:HB2	2.43	0.48
1:D:426:ASN:OD1	1:D:426:ASN:N	2.41	0.48
1:A:152:LYS:HA	1:A:564:GLU:CB	2.41	0.48
1:A:295:PHE:CD1	1:A:295:PHE:O	2.66	0.48
2:C:184:ALA:O	1:D:499:ARG:NH1	2.47	0.48
1:D:36:LEU:O	1:D:40:GLN:N	2.46	0.48
1:A:103:THR:HB	1:A:106:GLY:CA	2.44	0.48
2:C:24:ARG:NH2	7:C:420:HOH:O	2.45	0.48
1:D:35:ILE:O	1:D:39:ASN:HB2	2.13	0.48
1:D:331:GLY:N	1:D:537:GLY:O	2.44	0.48
2:E:58:VAL:HG23	7:E:418:HOH:O	2.13	0.48
2:E:66:GLU:HB2	2:E:69:ASN:HB3	1.95	0.48
2:F:15:PHE:HB3	2:F:67:SER:HB2	1.95	0.48
2:F:68:LEU:O	2:F:72:GLN:HG3	2.12	0.48
2:F:125:LYS:HD3	2:F:173:PHE:CG	2.47	0.48
2:F:136:GLU:HB3	2:F:179:SER:OG	2.13	0.48
2:F:143:PRO:HB2	2:F:144:TYR:CD2	2.48	0.48
1:A:22:ARG:HH11	1:A:22:ARG:HG2	1.78	0.48
1:A:192:VAL:HG12	1:A:205:HIS:HD2	1.79	0.48
1:A:273:LEU:HA	1:A:276:THR:HG23	1.95	0.48
1:A:335:GLY:HA3	1:A:394:ASN:HD22	1.79	0.48
1:A:460:ILE:HD12	1:A:481:ILE:C	2.39	0.48
2:B:34:GLU:OE2	7:B:402:HOH:O	2.20	0.48
1:D:121:THR:HG23	3:D:601:JAA:C15	2.43	0.48
1:D:231:PHE:O	1:D:235:GLU:HG3	2.13	0.48
1:D:303:GLY:O	1:D:327:SER:HA	2.13	0.48
1:D:441:LEU:CD2	1:D:549:ARG:HB3	2.43	0.48
1:A:213:ARG:HD3	1:A:216:VAL:HG21	1.94	0.48
2:F:7:LEU:HD11	2:F:57:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HE2	1:A:163:GLY:O	1.97	0.48
2:B:14:MET:O	2:B:17:MET:HB2	2.14	0.48
2:B:34:GLU:HG3	2:B:35:GLU:N	2.28	0.48
1:D:549:ARG:NH2	7:D:725:HOH:O	2.46	0.48
2:E:17:MET:HG2	2:E:20:ARG:HH21	1.79	0.48
2:E:154:ASP:HA	2:E:185:TRP:HZ2	1.78	0.48
2:F:114:TRP:CZ3	2:F:212:TYR:HD2	2.29	0.48
1:A:97:ILE:HD13	1:A:110:PHE:CE2	2.48	0.48
1:A:211:LEU:HD12	1:A:212:PHE:CE2	2.48	0.48
1:A:491:GLN:OE1	1:A:573:THR:N	2.47	0.48
2:B:15:PHE:HA	2:B:18:ARG:HD2	1.96	0.48
1:D:132:ARG:HD3	1:D:300:TYR:CZ	2.49	0.48
1:D:190:ASP:O	1:D:194:PHE:N	2.44	0.48
1:D:191:GLU:OE1	1:D:191:GLU:N	2.47	0.48
1:D:235:GLU:HG2	1:D:287:TRP:CE3	2.49	0.48
1:D:365:PRO:CG	1:D:374:GLU:HG2	2.42	0.48
1:A:96:ALA:HB3	1:A:113:PHE:HD2	1.78	0.48
1:A:169:VAL:O	1:A:175:PHE:HB2	2.13	0.48
1:A:238:TRP:CZ2	1:A:282:MET:SD	3.07	0.48
1:A:510:ARG:HG2	1:A:515:ILE:HG13	1.94	0.48
2:B:117:LYS:HG3	2:B:213:ARG:HH11	1.78	0.48
2:B:120:GLU:HG2	7:B:454:HOH:O	2.14	0.48
2:C:8:LEU:HD21	2:C:43:LEU:HD21	1.95	0.48
1:D:50:LEU:HD13	1:D:61:PHE:HE1	1.77	0.48
1:D:508:SER:O	1:D:512:CYS:HB3	2.13	0.48
2:E:66:GLU:OE2	2:F:97:PHE:CD1	2.65	0.48
2:F:211:GLU:O	2:F:214:LYS:HG2	2.14	0.48
1:A:332:SER:HB2	1:A:538:LEU:HA	1.96	0.48
1:A:354:VAL:HG11	1:A:361:PHE:CZ	2.48	0.48
1:A:432:ASN:OD1	1:A:433:ILE:N	2.46	0.48
1:A:492:ASP:HB2	7:A:704:HOH:O	2.14	0.48
2:C:117:LYS:HE3	2:C:213:ARG:NH1	2.28	0.48
2:C:136:GLU:OE2	2:C:180:PRO:HD2	2.14	0.48
1:D:131:PHE:CD1	1:D:132:ARG:N	2.81	0.48
1:A:238:TRP:HZ2	1:A:282:MET:CE	2.23	0.48
1:A:465:TYR:CE2	1:A:467:ASP:HB3	2.49	0.48
2:B:97:PHE:CE1	2:C:65:CYS:HB2	2.49	0.48
2:C:73:TYR:HA	2:C:76:GLU:HG2	1.96	0.48
1:D:398:LEU:HB3	1:D:401:TYR:CD1	2.49	0.48
1:D:441:LEU:O	1:D:444:SER:HB2	2.14	0.48
2:E:98:TRP:HE3	2:E:153:VAL:HG11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:SER:C	1:A:556:ALA:HB3	2.39	0.47
1:A:340:ASN:ND2	1:A:343:PRO:HA	2.29	0.47
2:B:8:LEU:HB2	2:B:56:VAL:HB	1.96	0.47
1:D:41:SER:H	2:E:142:LYS:CE	2.27	0.47
1:D:122:LEU:HD12	1:D:123:GLN:N	2.28	0.47
1:D:336:TRP:CB	1:D:358:LEU:HD13	2.44	0.47
1:D:337:ILE:HG22	1:D:338:ALA:N	2.29	0.47
1:D:393:THR:HG22	1:D:400:ARG:H	1.79	0.47
1:A:331:GLY:HA2	1:A:539:GLY:CA	2.44	0.47
1:A:421:PHE:CD1	1:A:541:SER:HA	2.49	0.47
1:D:507:VAL:HG23	1:D:511:LYS:CE	2.40	0.47
1:A:152:LYS:HG2	1:A:561:ILE:O	2.15	0.47
1:A:201:ALA:O	1:A:205:HIS:HB2	2.14	0.47
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.69	0.47
1:A:562:LEU:HD12	1:A:563:CYS:HB3	1.96	0.47
2:B:116:LYS:HZ3	2:B:120:GLU:HB3	1.78	0.47
1:D:117:LEU:HB2	7:D:793:HOH:O	2.14	0.47
1:D:525:LYS:NZ	7:D:755:HOH:O	2.42	0.47
1:D:528:PHE:O	1:D:532:GLN:HG2	2.14	0.47
2:E:96:ARG:NH1	2:F:73:TYR:CE1	2.82	0.47
2:C:187:LYS:HE2	2:C:187:LYS:HB2	1.69	0.47
1:D:17:PHE:CD2	1:D:127:THR:HG21	2.50	0.47
2:E:43:LEU:HD21	2:E:58:VAL:HG21	1.96	0.47
1:A:118:MET:HG2	1:A:174:ASN:HD21	1.78	0.47
1:A:149:PHE:HB2	1:A:530:LYS:HZ3	1.79	0.47
1:A:210:ILE:O	1:A:210:ILE:HG22	2.15	0.47
2:B:15:PHE:HB3	2:B:67:SER:CB	2.45	0.47
2:C:10:TYR:H	2:C:20:ARG:NH2	2.12	0.47
1:D:118:MET:HE3	1:D:175:PHE:HE1	1.79	0.47
1:D:223:PHE:CE2	1:D:545:PHE:CZ	2.95	0.47
1:D:412:PHE:N	1:D:418:GLN:HE21	2.12	0.47
2:E:7:LEU:HD13	2:E:9:ASP:HB2	1.97	0.47
2:E:60:ASN:HD21	2:E:62:LYS:HD2	1.79	0.47
2:F:175:ILE:HG13	2:F:176:GLU:N	2.27	0.47
1:A:35:ILE:HA	1:A:395:TYR:CE1	2.50	0.47
1:A:209:GLY:O	1:A:213:ARG:NE	2.34	0.47
1:A:284:LEU:HD23	1:A:290:LEU:HD13	1.97	0.47
1:A:342:THR:OG1	1:A:413:TYR:OH	2.18	0.47
1:A:546:LYS:HG3	1:A:546:LYS:O	2.15	0.47
2:B:50:ILE:HD11	2:C:101:PHE:CZ	2.50	0.47
1:D:329:ASP:HB3	1:D:338:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:LEU:HD22	1:D:479:TRP:HZ3	1.79	0.47
2:F:77:ALA:C	2:F:79:PRO:HD3	2.39	0.47
2:F:152:TYR:O	2:F:155:ILE:HB	2.14	0.47
1:A:93:PRO:HG2	2:B:184:ALA:HB3	1.96	0.47
1:A:97:ILE:O	1:A:556:ALA:HB1	2.15	0.47
1:A:105:GLN:HG3	1:A:107:ARG:HH21	1.80	0.47
1:A:120:ASN:OD1	1:A:121:THR:N	2.47	0.47
1:A:154:TYR:HB2	1:A:563:CYS:CB	2.45	0.47
1:A:223:PHE:HD2	1:A:225:HIS:ND1	2.12	0.47
2:B:144:TYR:OH	2:B:188:ARG:HD2	2.15	0.47
1:D:148:ILE:HG21	1:D:170:TYR:OH	2.15	0.47
1:D:151:SER:HB2	1:D:194:PHE:C	2.40	0.47
1:D:552:LYS:HB2	1:D:553:PRO:HD2	1.95	0.47
2:E:85:PHE:HB2	2:E:92:ARG:CG	2.45	0.47
2:E:202:SER:O	2:E:205:ILE:HG13	2.15	0.47
2:F:148:ASP:O	7:F:410:HOH:O	2.20	0.47
1:A:208:SER:HA	1:A:211:LEU:CD2	2.45	0.47
1:D:340:ASN:HD21	1:D:345:LEU:HD11	1.80	0.47
2:E:11:TRP:CZ2	2:E:204:LYS:HB3	2.44	0.47
2:E:60:ASN:ND2	2:E:62:LYS:HD2	2.30	0.47
2:E:108:ASP:O	2:E:112:LYS:HG2	2.14	0.47
2:F:110:GLN:O	2:F:113:VAL:HG12	2.14	0.47
2:F:180:PRO:HA	2:F:183:ILE:HG22	1.96	0.47
2:F:201:ASP:O	2:F:204:LYS:HG2	2.13	0.47
1:A:139:ASP:OD1	1:A:142:GLY:HA3	2.14	0.47
1:A:228:VAL:HG13	1:A:319:TYR:HE2	1.79	0.47
1:A:280:LYS:O	1:A:283:SER:OG	2.31	0.47
1:A:291:ILE:HB	1:A:320:ALA:HA	1.97	0.47
1:D:438:GLU:HG2	1:D:442:GLN:OE1	2.15	0.47
1:A:171:ARG:O	1:A:171:ARG:HD3	2.15	0.47
2:C:33:ARG:NE	2:C:35:GLU:OE2	2.48	0.47
1:D:67:LEU:HD23	1:D:400:ARG:HB3	1.97	0.47
1:D:246:LYS:HE3	1:D:246:LYS:HB3	1.60	0.47
1:D:326:VAL:CG2	1:D:343:PRO:HB3	2.43	0.47
1:D:444:SER:HA	1:D:500:ALA:HB1	1.96	0.47
2:F:23:LEU:HD21	2:F:30:PHE:CD1	2.50	0.47
1:A:339:ALA:O	1:A:353:ALA:N	2.40	0.46
1:A:543:GLY:C	1:A:544:GLN:HG3	2.40	0.46
2:B:50:ILE:HG21	2:C:134:ILE:HD12	1.97	0.46
2:B:163:TRP:HB3	2:B:167:TYR:CZ	2.49	0.46
2:C:47:SER:HB2	2:C:63:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ASP:OD2	1:D:104:SER:HA	2.15	0.46
1:D:131:PHE:HD1	1:D:132:ARG:N	2.12	0.46
1:D:394:ASN:O	1:D:399:TYR:HE1	1.96	0.46
1:D:434:ASP:HB2	1:D:550:CYS:HB3	1.96	0.46
2:E:70:VAL:O	2:E:73:TYR:HB3	2.15	0.46
1:A:314:PRO:O	1:A:318:HIS:N	2.40	0.46
1:A:434:ASP:CB	1:A:550:CYS:HB3	2.40	0.46
1:A:435:LYS:HB3	1:A:436:ASN:O	2.16	0.46
1:A:440:ASP:OD1	1:A:441:LEU:N	2.48	0.46
2:B:92:ARG:NH1	7:B:412:HOH:O	2.27	0.46
2:C:116:LYS:O	2:C:121:GLN:HG3	2.15	0.46
2:C:195:VAL:HG23	2:C:199:LEU:HD13	1.96	0.46
1:D:36:LEU:C	1:D:39:ASN:H	2.23	0.46
1:D:529:ARG:CZ	1:D:529:ARG:HB2	2.45	0.46
1:D:534:HIS:NE2	1:D:557:LYS:HG2	2.30	0.46
2:E:90:TYR:HE1	7:F:407:HOH:O	1.98	0.46
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.50	0.46
1:A:413:TYR:N	1:A:416:THR:O	2.48	0.46
1:A:549:ARG:HD3	1:A:549:ARG:HA	1.47	0.46
2:C:14:MET:HE3	2:C:14:MET:HB2	1.88	0.46
1:D:304:ILE:HG12	1:D:536:LEU:HD13	1.96	0.46
1:D:405:ASP:CB	1:D:541:SER:HB3	2.39	0.46
2:F:162:SER:O	2:F:165:GLN:HG3	2.15	0.46
1:A:172:ASN:OD1	1:A:174:ASN:ND2	2.49	0.46
1:D:234:PHE:HB3	1:D:287:TRP:CH2	2.50	0.46
1:D:452:LEU:HG	1:D:457:ILE:HD11	1.97	0.46
2:F:84:PHE:CG	2:F:152:TYR:HB2	2.50	0.46
1:A:199:HIS:HA	1:A:525:LYS:HG2	1.97	0.46
1:A:202:LEU:HD13	1:A:229:HIS:NE2	2.31	0.46
1:A:442:GLN:HG2	1:A:462:PHE:HZ	1.81	0.46
1:D:242:VAL:HG22	1:D:277:ILE:CD1	2.42	0.46
1:D:254:ILE:O	1:D:260:ARG:HD2	2.15	0.46
1:D:364:LEU:HB3	1:D:389:GLU:CG	2.45	0.46
2:E:96:ARG:HH11	2:F:69:ASN:HA	1.80	0.46
1:A:206:LEU:HD11	1:A:234:PHE:HD1	1.81	0.46
1:A:330:TYR:CE2	1:A:352:PHE:CD2	3.03	0.46
1:A:436:ASN:HA	1:A:440:ASP:OD2	2.15	0.46
1:D:110:PHE:CE2	1:D:553:PRO:O	2.69	0.46
1:D:125:PHE:HD1	1:D:125:PHE:HA	1.63	0.46
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.50	0.46
1:D:552:LYS:HG3	1:D:553:PRO:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:LYS:NZ	7:D:711:HOH:O	2.13	0.46
2:E:68:LEU:HD12	2:E:68:LEU:HA	1.52	0.46
1:A:143:LYS:NZ	1:A:212:PHE:HB2	2.31	0.46
1:A:215:GLN:O	1:A:217:GLN:NE2	2.43	0.46
1:A:295:PHE:CD1	1:A:298:ALA:HB3	2.51	0.46
1:A:305:MET:HE3	1:A:326:VAL:O	2.15	0.46
2:C:116:LYS:HB2	7:C:436:HOH:O	2.15	0.46
1:D:43:ILE:HD11	1:D:76:TYR:CE2	2.50	0.46
1:D:405:ASP:OD1	1:D:540:SER:HB2	2.15	0.46
1:D:494:CYS:SG	1:D:572:SER:HA	2.56	0.46
1:D:531:ILE:O	1:D:534:HIS:CE1	2.68	0.46
2:E:169:LYS:HG3	2:E:170:PHE:CD1	2.50	0.46
2:C:73:TYR:HA	2:C:76:GLU:CD	2.41	0.46
6:C:301:GSH:O32	7:C:410:HOH:O	2.20	0.46
1:D:154:TYR:HD2	1:D:560:GLN:HA	1.80	0.46
1:D:235:GLU:O	1:D:238:TRP:CD1	2.69	0.46
2:E:9:ASP:OD1	2:E:10:TYR:N	2.49	0.46
2:E:96:ARG:HH12	2:F:72:GLN:HB2	1.79	0.46
1:A:30:GLN:OE1	1:A:30:GLN:HA	2.15	0.46
1:A:181:SER:OG	1:A:182:ILE:HG13	2.16	0.46
1:A:195:SER:O	1:A:565:ASN:ND2	2.45	0.46
2:B:128:PHE:HE2	2:B:175:ILE:HG12	1.81	0.46
2:C:187:LYS:O	7:C:411:HOH:O	2.21	0.46
1:D:207:LEU:O	1:D:210:ILE:HG23	2.15	0.46
1:D:452:LEU:HD21	1:D:481:ILE:HD13	1.97	0.46
1:D:497:LEU:O	1:D:500:ALA:HB3	2.15	0.46
2:F:8:LEU:HA	2:F:33:ARG:HG3	1.98	0.46
2:F:135:LEU:HD13	2:F:182:LEU:HD12	1.98	0.46
1:A:100:SER:HA	1:A:535:PHE:HE1	1.81	0.46
1:A:313:VAL:HG23	1:A:325:LEU:HD12	1.98	0.46
2:C:57:LEU:O	2:C:64:VAL:HB	2.16	0.46
1:D:53:ASN:OD1	1:D:54:ALA:N	2.49	0.46
1:D:503:ASP:CG	1:D:504:ALA:N	2.73	0.46
2:F:57:LEU:HD13	2:F:59:HIS:HD2	1.81	0.46
1:A:28:GLN:HG3	1:A:29:LYS:N	2.31	0.45
1:A:224:ALA:HB3	1:A:309:MET:HG3	1.98	0.45
1:A:248:GLY:O	1:A:267:LEU:HB3	2.16	0.45
1:A:346:SER:N	7:A:749:HOH:O	2.41	0.45
1:A:390:VAL:HG11	1:A:540:SER:C	2.41	0.45
1:A:470:THR:OG1	1:A:473:GLY:HA2	2.17	0.45
2:C:16:GLY:HA3	2:C:20:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:ILE:HG13	2:C:51:HIS:H	1.81	0.45
2:C:166:ALA:CA	2:C:206:VAL:HG22	2.46	0.45
1:D:391:VAL:HA	1:D:401:TYR:O	2.16	0.45
2:E:65:CYS:HB2	2:F:97:PHE:CZ	2.51	0.45
2:E:188:ARG:N	7:E:419:HOH:O	2.49	0.45
2:E:201:ASP:HB2	2:E:204:LYS:HG2	1.98	0.45
1:A:46:GLN:HB3	2:B:148:ASP:CB	2.41	0.45
1:A:73:LEU:HD22	1:A:89:LEU:HD13	1.97	0.45
1:A:355:ILE:HA	1:A:356:PRO:HD3	1.75	0.45
1:A:500:ALA:O	1:A:502:ILE:HG23	2.15	0.45
2:B:34:GLU:HG3	2:B:35:GLU:H	1.81	0.45
2:B:76:GLU:O	2:B:79:PRO:HD3	2.17	0.45
2:C:110:GLN:HA	2:C:113:VAL:HG12	1.98	0.45
2:C:188:ARG:N	7:D:704:HOH:O	2.49	0.45
1:D:41:SER:N	2:E:142:LYS:HE2	2.31	0.45
1:D:76:TYR:C	1:D:88:ILE:HG21	2.42	0.45
1:D:273:LEU:N	1:D:273:LEU:CD1	2.78	0.45
1:D:289:GLY:N	1:D:318:HIS:O	2.35	0.45
1:D:334:GLU:HG3	1:D:538:LEU:HD13	1.98	0.45
1:D:467:ASP:OD2	1:D:474:HIS:CE1	2.69	0.45
2:F:7:LEU:HD22	2:F:30:PHE:CE1	2.52	0.45
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.52	0.45
1:A:99:LEU:HD22	1:A:555:ASN:CG	2.41	0.45
1:A:491:GLN:HE22	1:A:570:TYR:HB3	1.80	0.45
2:C:141:ASP:N	2:C:141:ASP:OD1	2.50	0.45
2:F:98:TRP:CE3	2:F:101:PHE:HB2	2.51	0.45
1:A:14:ILE:HG13	1:A:131:PHE:HE1	1.81	0.45
1:A:145:LEU:O	1:A:220:PHE:N	2.49	0.45
1:A:313:VAL:HG13	1:A:314:PRO:HD3	1.97	0.45
1:A:389:GLU:HA	1:A:405:ASP:O	2.17	0.45
1:A:464:SER:OG	1:A:550:CYS:SG	2.48	0.45
1:A:465:TYR:N	1:A:476:ALA:O	2.47	0.45
2:B:177:SER:OG	7:B:406:HOH:O	2.15	0.45
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.52	0.45
2:C:117:LYS:HA	2:C:121:GLN:HB2	1.98	0.45
1:D:452:LEU:HD22	1:D:479:TRP:CZ3	2.52	0.45
1:A:53:ASN:CG	1:A:54:ALA:H	2.22	0.45
1:A:223:PHE:HB3	1:A:309:MET:HE3	1.99	0.45
2:C:125:LYS:HB3	2:C:125:LYS:HE3	1.62	0.45
1:D:143:LYS:O	1:D:216:VAL:HA	2.17	0.45
1:D:333:SER:HG	1:D:557:LYS:HZ1	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:ILE:HD11	1:D:552:LYS:HB2	1.99	0.45
2:E:106:PHE:CE2	2:E:135:LEU:CD1	2.99	0.45
2:F:18:ARG:HG3	2:F:67:SER:OG	2.16	0.45
1:A:53:ASN:ND2	7:A:760:HOH:O	2.49	0.45
1:A:132:ARG:NH2	1:A:300:TYR:OH	2.50	0.45
1:A:274:ALA:C	1:A:278:ARG:HD2	2.42	0.45
1:A:329:ASP:OD2	7:A:724:HOH:O	2.20	0.45
1:A:493:CYS:N	7:A:704:HOH:O	2.48	0.45
1:A:552:LYS:HB2	1:A:553:PRO:CD	2.45	0.45
2:B:37:PHE:CZ	6:B:301:GSH:HA32	2.52	0.45
2:C:213:ARG:O	2:C:217:LEU:HG	2.16	0.45
1:D:451:ARG:NH2	1:D:490:LEU:HD23	2.31	0.45
2:F:40:LYS:H	2:F:40:LYS:HZ3	1.64	0.45
2:F:135:LEU:HD11	2:F:157:LEU:HD13	1.99	0.45
2:F:188:ARG:O	2:F:191:GLU:HG2	2.17	0.45
1:A:452:LEU:HD13	1:A:493:CYS:SG	2.57	0.45
2:C:157:LEU:CD1	2:C:185:TRP:CH2	2.99	0.45
2:E:122:GLU:HA	2:E:125:LYS:HE3	1.99	0.45
1:A:290:LEU:O	1:A:290:LEU:HG	2.17	0.45
1:A:560:GLN:HG2	7:A:734:HOH:O	2.16	0.45
1:D:29:LYS:HD3	7:D:813:HOH:O	2.17	0.45
2:F:101:PHE:N	2:F:101:PHE:CD1	2.84	0.45
2:F:136:GLU:OE1	2:F:179:SER:HA	2.17	0.45
2:F:144:TYR:HE1	2:F:189:CYS:HG	1.63	0.45
1:A:256:VAL:HA	1:A:257:PRO:HD3	1.83	0.45
1:A:423:CYS:HB2	1:A:542:ALA:C	2.42	0.45
1:A:477:ILE:H	1:A:477:ILE:HG13	1.59	0.45
1:A:538:LEU:HB3	1:A:544:GLN:OE1	2.17	0.45
2:B:97:PHE:CZ	2:B:101:PHE:HE2	2.35	0.45
2:B:106:PHE:C	2:B:110:GLN:HE21	2.25	0.45
2:C:158:ILE:HD11	2:C:186:ALA:O	2.16	0.45
2:C:164:PHE:HD2	2:C:183:ILE:HG22	1.79	0.45
2:C:183:ILE:HD12	2:C:184:ALA:N	2.32	0.45
1:D:152:LYS:CB	1:D:561:ILE:HA	2.46	0.45
1:D:197:ASP:CG	1:D:256:VAL:HB	2.42	0.45
1:D:413:TYR:HD2	1:D:418:GLN:HG2	1.82	0.45
2:E:176:GLU:CD	2:E:183:ILE:HD11	2.42	0.45
2:F:23:LEU:CA	2:F:74:VAL:HG11	2.43	0.45
1:A:79:ARG:HG3	1:A:84:ASP:OD2	2.17	0.45
1:A:104:SER:N	1:A:107:ARG:O	2.49	0.45
1:A:224:ALA:HB3	1:A:309:MET:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:OE2	1:A:287:TRP:CG	2.70	0.45
2:C:16:GLY:HA3	2:C:20:ARG:HH21	1.82	0.45
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.47	0.45
1:D:29:LYS:O	1:D:32:LEU:HB2	2.17	0.45
1:D:58:GLU:CD	1:D:58:GLU:H	2.24	0.45
1:D:393:THR:CG2	1:D:400:ARG:H	2.30	0.45
1:D:500:ALA:HB1	7:D:706:HOH:O	2.17	0.45
2:F:135:LEU:HD23	2:F:145:PHE:HZ	1.82	0.45
1:A:286:ASN:O	1:A:287:TRP:CB	2.63	0.44
1:A:510:ARG:NH1	1:A:518:LEU:H	2.15	0.44
2:B:14:MET:HG3	2:B:163:TRP:NE1	2.32	0.44
2:B:21:VAL:HG21	2:B:158:ILE:HD12	1.99	0.44
2:C:10:TYR:O	2:C:20:ARG:NH2	2.42	0.44
1:D:198:VAL:HG13	1:D:565:ASN:ND2	2.32	0.44
1:D:364:LEU:CD2	1:D:402:ARG:HH12	2.30	0.44
1:D:407:VAL:HG23	1:D:420:LYS:O	2.16	0.44
2:F:41:SER:HB3	2:F:43:LEU:HD11	1.98	0.44
2:F:98:TRP:CE3	2:F:98:TRP:O	2.70	0.44
2:F:136:GLU:HB3	2:F:179:SER:HG	1.81	0.44
1:A:133:ASN:HA	1:A:136:PHE:O	2.17	0.44
1:A:192:VAL:HG12	1:A:205:HIS:CD2	2.53	0.44
1:A:278:ARG:O	1:A:282:MET:SD	2.75	0.44
1:A:507:VAL:CG2	1:A:508:SER:N	2.81	0.44
2:B:161:SER:HB2	2:B:186:ALA:HB1	2.00	0.44
2:C:5:PRO:HB3	2:C:59:HIS:NE2	2.32	0.44
1:D:192:VAL:HG23	1:D:259:VAL:HG21	1.98	0.44
1:D:360:TYR:HB3	1:D:393:THR:OG1	2.17	0.44
2:F:170:PHE:CD1	2:F:170:PHE:C	2.91	0.44
1:A:145:LEU:HD11	1:A:147:PHE:CE1	2.51	0.44
1:A:238:TRP:HE3	1:A:277:ILE:HD11	1.82	0.44
1:D:38:LYS:O	2:E:142:LYS:HG2	2.18	0.44
1:D:86:SER:HA	1:D:87:PRO:HD2	1.86	0.44
1:D:369:THR:HG1	1:D:370:GLY:H	1.53	0.44
1:A:233:THR:O	1:A:237:VAL:HG22	2.17	0.44
1:A:423:CYS:HA	7:A:782:HOH:O	2.16	0.44
1:A:487:GLU:O	1:A:490:LEU:HG	2.17	0.44
1:A:506:TYR:CZ	1:A:510:ARG:HD3	2.53	0.44
2:B:74:VAL:HA	2:B:78:TRP:CE3	2.52	0.44
2:C:10:TYR:HB3	2:C:13:SER:CB	2.36	0.44
2:C:14:MET:HG3	2:C:163:TRP:CZ2	2.52	0.44
1:D:133:ASN:ND2	1:D:138:ILE:HG13	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLY:HA3	1:D:560:GLN:CD	2.43	0.44
1:D:206:LEU:HD22	1:D:234:PHE:HD1	1.82	0.44
1:D:210:ILE:HD12	1:D:234:PHE:CZ	2.52	0.44
1:D:407:VAL:HG21	1:D:419:LEU:HD23	2.00	0.44
2:E:98:TRP:HB2	7:E:401:HOH:O	2.16	0.44
2:F:136:GLU:HG2	2:F:179:SER:HB2	2.00	0.44
1:A:32:LEU:HG	1:A:360:TYR:HB2	2.00	0.44
1:A:90:THR:HB	1:A:91:GLY:H	1.55	0.44
1:A:213:ARG:HD3	1:A:216:VAL:CG2	2.48	0.44
1:A:464:SER:O	1:A:551:VAL:N	2.46	0.44
1:A:534:HIS:CE1	1:A:535:PHE:CE1	3.06	0.44
1:A:545:PHE:HE1	7:A:919:HOH:O	2.00	0.44
2:C:128:PHE:O	2:C:132:VAL:HG12	2.16	0.44
2:C:163:TRP:HB3	2:C:167:TYR:CE2	2.52	0.44
2:C:209:ALA:CA	2:C:212:TYR:HE2	2.26	0.44
1:D:21:THR:HB	1:D:416:THR:HB	2.00	0.44
1:D:310:GLU:O	1:D:313:VAL:HG12	2.18	0.44
2:E:145:PHE:N	2:E:154:ASP:OD2	2.39	0.44
2:F:144:TYR:HB3	2:F:154:ASP:OD2	2.17	0.44
2:F:190:MET:O	2:F:196:SER:HB2	2.17	0.44
1:A:76:TYR:HB2	1:A:89:LEU:HD11	1.99	0.44
1:A:284:LEU:HB2	1:A:287:TRP:H	1.81	0.44
1:A:477:ILE:HG21	1:A:497:LEU:HD23	1.99	0.44
1:A:558:VAL:HG22	7:A:829:HOH:O	2.17	0.44
2:C:114:TRP:CE3	2:C:212:TYR:CE2	3.06	0.44
2:C:209:ALA:HA	2:C:212:TYR:CD2	2.51	0.44
1:D:242:VAL:O	1:D:246:LYS:HG3	2.17	0.44
1:D:360:TYR:OH	1:D:362:GLU:OE2	2.24	0.44
1:D:494:CYS:HB3	1:D:520:LEU:HB3	2.00	0.44
1:A:27:VAL:CG1	1:A:357:ASN:HB3	2.48	0.44
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.98	0.44
2:C:57:LEU:HB3	2:C:64:VAL:CG1	2.47	0.44
2:C:166:ALA:HB2	2:C:206:VAL:HG22	2.00	0.44
1:D:218:TYR:CE1	1:D:220:PHE:HB2	2.52	0.44
1:D:440:ASP:OD1	1:D:441:LEU:N	2.50	0.44
2:E:50:ILE:HD12	2:E:51:HIS:N	2.33	0.44
2:F:113:VAL:HG22	2:F:167:TYR:O	2.17	0.44
1:A:74:GLU:O	1:A:78:LYS:HB2	2.18	0.44
1:A:151:SER:O	1:A:565:ASN:ND2	2.50	0.44
1:A:313:VAL:N	1:A:314:PRO:HD2	2.32	0.44
2:C:98:TRP:CE2	2:C:157:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:SER:HB2	7:C:402:HOH:O	2.16	0.44
2:C:187:LYS:O	2:C:190:MET:HB2	2.18	0.44
1:D:76:TYR:O	1:D:88:ILE:HG21	2.17	0.44
1:D:77:ILE:HG13	1:D:88:ILE:CD1	2.48	0.44
1:D:87:PRO:C	1:D:88:ILE:HG23	2.43	0.44
1:D:120:ASN:CG	1:D:358:LEU:HD22	2.43	0.44
1:D:475:TYR:HB2	1:D:518:LEU:HB2	2.00	0.44
1:D:493:CYS:SG	1:D:497:LEU:HD11	2.58	0.44
1:D:518:LEU:HD12	1:D:519:GLU:N	2.33	0.44
2:E:93:ALA:HA	2:F:73:TYR:CE1	2.53	0.44
2:F:10:TYR:CD1	2:F:12:PRO:HD2	2.52	0.44
1:A:96:ALA:HA	1:A:161:PRO:O	2.18	0.44
1:A:210:ILE:HG21	1:A:210:ILE:HD13	1.55	0.44
1:A:315:LYS:CA	1:A:318:HIS:HB3	2.46	0.44
1:A:332:SER:HB3	1:A:538:LEU:HD12	1.99	0.44
1:A:408:LYS:HE3	1:A:420:LYS:NZ	2.33	0.44
1:A:429:LEU:HD13	1:A:546:LYS:NZ	2.33	0.44
2:C:21:VAL:O	2:C:194:SER:HB2	2.18	0.44
1:D:79:ARG:O	1:D:84:ASP:HB3	2.17	0.44
1:D:104:SER:O	1:D:105:GLN:HB2	2.18	0.44
1:D:154:TYR:CD2	1:D:560:GLN:HA	2.53	0.44
1:D:383:LYS:N	1:D:386:GLU:OE2	2.49	0.44
2:E:165:GLN:HG3	2:E:168:GLU:OE2	2.17	0.44
2:E:192:LYS:O	2:E:196:SER:HB2	2.17	0.44
2:F:77:ALA:HB3	2:F:78:TRP:CE3	2.53	0.44
2:F:89:PRO:O	2:F:92:ARG:HB3	2.17	0.44
1:A:148:ILE:HB	1:A:170:TYR:HE2	1.83	0.43
1:A:198:VAL:HA	1:A:201:ALA:HB3	2.00	0.43
1:A:354:VAL:HG23	1:A:419:LEU:HD13	2.00	0.43
1:A:551:VAL:CG1	1:A:555:ASN:HD22	2.26	0.43
2:B:70:VAL:O	2:B:74:VAL:HG23	2.18	0.43
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.99	0.43
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.77	0.43
2:E:163:TRP:HA	2:E:205:ILE:HD13	1.98	0.43
2:F:182:LEU:HD23	2:F:183:ILE:N	2.32	0.43
1:A:214:ASP:OD1	1:A:214:ASP:N	2.50	0.43
1:A:329:ASP:HA	1:A:352:PHE:HD1	1.82	0.43
1:A:365:PRO:HB3	1:A:388:TYR:CE1	2.53	0.43
2:B:20:ARG:NH2	2:B:200:PRO:HD3	2.32	0.43
1:D:56:ASP:N	1:D:57:PRO:HD3	2.33	0.43
1:D:136:PHE:CD1	1:D:299:LYS:HD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:LEU:O	1:D:277:ILE:HG22	2.18	0.43
2:E:99:ALA:HB3	2:E:152:TYR:OH	2.18	0.43
1:A:87:PRO:HA	1:A:91:GLY:O	2.18	0.43
1:A:295:PHE:CE1	1:A:298:ALA:HB3	2.54	0.43
1:A:379:LEU:HG	1:A:380:THR:HG23	2.01	0.43
1:A:408:LYS:HE3	1:A:420:LYS:HE2	2.00	0.43
2:B:18:ARG:HH22	2:B:103:ASP:CG	2.26	0.43
2:C:129:ILE:HA	2:C:132:VAL:HG12	1.99	0.43
1:D:128:ALA:HA	1:D:131:PHE:CZ	2.53	0.43
1:D:156:SER:OG	1:D:160:VAL:O	2.19	0.43
1:D:261:THR:HB	1:D:265:LYS:HZ1	1.83	0.43
1:A:128:ALA:HB2	1:A:329:ASP:OD2	2.18	0.43
1:A:145:LEU:HD22	1:A:213:ARG:CZ	2.47	0.43
1:A:152:LYS:HE3	1:A:565:ASN:CB	2.49	0.43
1:A:250:LEU:HD11	7:A:891:HOH:O	2.17	0.43
1:A:381:GLN:NE2	7:A:762:HOH:O	2.50	0.43
2:B:94:GLN:O	2:B:98:TRP:HD1	2.01	0.43
2:B:217:LEU:O	7:B:409:HOH:O	2.21	0.43
2:C:103:ASP:HA	2:C:107:THR:HG23	2.00	0.43
1:D:7:THR:O	1:D:126:ARG:NE	2.52	0.43
2:E:102:VAL:HG13	7:E:406:HOH:O	2.18	0.43
1:A:70:ASP:OD2	1:A:104:SER:HA	2.19	0.43
1:A:77:ILE:HG21	1:A:110:PHE:HB3	2.00	0.43
1:A:274:ALA:O	1:A:278:ARG:HB2	2.18	0.43
1:A:302:TYR:CG	1:A:328:HIS:CE1	3.07	0.43
2:B:96:ARG:HA	2:B:152:TYR:CE2	2.51	0.43
2:B:169:LYS:NZ	2:B:206:VAL:CG1	2.82	0.43
2:C:126:LYS:O	2:C:129:ILE:HG13	2.18	0.43
1:D:85:THR:O	1:D:87:PRO:HD3	2.18	0.43
1:D:152:LYS:CG	1:D:565:ASN:HB2	2.48	0.43
1:D:444:SER:HB3	1:D:497:LEU:HD23	1.99	0.43
1:D:502:ILE:H	1:D:502:ILE:HG13	1.56	0.43
1:D:575:PHE:CD1	1:D:575:PHE:N	2.87	0.43
2:F:129:ILE:O	2:F:132:VAL:HG12	2.18	0.43
2:F:170:PHE:CE2	2:F:213:ARG:HD2	2.54	0.43
2:B:93:ALA:HA	2:B:96:ARG:HE	1.83	0.43
2:C:105:LYS:CB	2:C:105:LYS:HZ2	2.31	0.43
1:D:213:ARG:HG3	1:D:214:ASP:H	1.83	0.43
1:D:457:ILE:HD12	1:D:481:ILE:HB	2.00	0.43
1:A:167:THR:O	1:A:171:ARG:HB3	2.19	0.43
1:A:208:SER:O	1:A:211:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ALA:HB1	1:A:521:ARG:HD2	2.00	0.43
1:D:187:CYS:HB2	1:D:209:GLY:HA2	2.00	0.43
1:D:330:TYR:N	1:D:338:ALA:O	2.29	0.43
2:E:8:LEU:HG	7:E:418:HOH:O	2.19	0.43
1:A:149:PHE:CD2	1:A:530:LYS:HE2	2.53	0.43
1:A:238:TRP:CE3	1:A:277:ILE:HG12	2.52	0.43
1:A:384:ILE:H	1:A:384:ILE:HG23	1.58	0.43
2:B:13:SER:HB3	2:B:54:ILE:HD11	2.00	0.43
2:C:81:LYS:HG3	2:C:82:ASN:N	2.33	0.43
1:D:87:PRO:HG2	2:E:188:ARG:HH21	1.83	0.43
1:D:103:THR:HG22	1:D:548:PRO:HB3	2.00	0.43
1:D:193:ILE:HG12	1:D:205:HIS:HE1	1.82	0.43
1:D:207:LEU:HA	1:D:210:ILE:CG2	2.48	0.43
1:D:462:PHE:C	1:D:528:PHE:CZ	2.97	0.43
2:E:135:LEU:O	2:E:139:LEU:HB2	2.19	0.43
2:F:114:TRP:CD1	2:F:167:TYR:CD1	3.06	0.43
1:A:33:LYS:O	1:A:36:LEU:HG	2.19	0.43
1:A:213:ARG:HA	1:A:213:ARG:HD3	1.94	0.43
1:A:423:CYS:HB2	1:A:542:ALA:HB3	2.01	0.43
2:C:15:PHE:O	2:C:18:ARG:HB2	2.19	0.43
2:C:65:CYS:O	2:C:66:GLU:HB2	2.18	0.43
2:C:114:TRP:CD1	2:C:167:TYR:CE1	3.06	0.43
2:C:187:LYS:HD3	1:D:492:ASP:CB	2.49	0.43
2:C:209:ALA:O	2:C:212:TYR:CE2	2.72	0.43
1:D:146:GLN:O	1:D:205:HIS:CD2	2.71	0.43
1:D:170:TYR:HB3	1:D:194:PHE:CZ	2.53	0.43
2:E:26:LYS:HA	2:E:82:ASN:ND2	2.28	0.43
1:A:235:GLU:OE2	1:A:287:TRP:CD1	2.72	0.43
1:A:448:ALA:CB	1:A:497:LEU:HD12	2.49	0.43
1:D:87:PRO:CG	2:E:188:ARG:NE	2.78	0.43
1:D:120:ASN:CB	1:D:358:LEU:HD22	2.49	0.43
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.84	0.43
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.52	0.43
2:E:15:PHE:HB3	2:E:67:SER:CB	2.48	0.43
2:F:81:LYS:O	2:F:83:PRO:HD3	2.19	0.43
2:F:213:ARG:NH1	2:F:217:LEU:HD21	2.34	0.43
1:A:34:GLU:O	1:A:38:LYS:HG2	2.19	0.42
1:A:273:LEU:O	1:A:277:ILE:HG22	2.19	0.42
1:A:336:TRP:CB	1:A:358:LEU:HD13	2.46	0.42
2:B:8:LEU:HD12	2:B:56:VAL:HB	2.00	0.42
2:C:11:TRP:HH2	2:C:204:LYS:C	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:LEU:HD12	1:D:539:GLY:N	2.34	0.42
2:F:190:MET:HA	2:F:195:VAL:CG2	2.48	0.42
1:A:31:THR:O	1:A:34:GLU:HG3	2.19	0.42
1:A:87:PRO:HD2	2:B:188:ARG:HB3	2.00	0.42
1:A:108:PRO:CG	1:A:552:LYS:HG2	2.48	0.42
1:A:111:ILE:HG21	1:A:398:LEU:CD2	2.49	0.42
1:A:152:LYS:O	1:A:167:THR:HG21	2.19	0.42
1:A:365:PRO:CG	1:A:374:GLU:HG2	2.48	0.42
1:A:466:ILE:HG13	1:A:466:ILE:O	2.19	0.42
1:D:20:MET:HG3	1:D:21:THR:N	2.33	0.42
1:D:157:THR:OG1	1:D:469:SER:HB3	2.19	0.42
1:D:218:TYR:HE1	1:D:220:PHE:HB2	1.84	0.42
1:D:222:VAL:HG21	4:D:602:ILE:N	2.34	0.42
1:D:510:ARG:HG3	1:D:510:ARG:NH1	2.34	0.42
1:D:531:ILE:O	1:D:534:HIS:ND1	2.52	0.42
2:E:7:LEU:O	2:E:33:ARG:HB2	2.19	0.42
2:E:151:GLY:O	2:E:154:ASP:HB2	2.19	0.42
1:A:91:GLY:HA2	2:B:143:PRO:N	2.34	0.42
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.48	0.42
1:A:182:ILE:O	1:A:182:ILE:HG22	2.19	0.42
1:A:233:THR:C	1:A:236:GLN:H	2.26	0.42
1:A:242:VAL:HG11	1:A:278:ARG:NE	2.34	0.42
1:A:432:ASN:CB	1:A:435:LYS:HD2	2.38	0.42
2:B:183:ILE:O	2:B:186:ALA:HB3	2.19	0.42
1:D:77:ILE:CG2	1:D:110:PHE:HB3	2.49	0.42
1:D:211:LEU:HD12	7:D:701:HOH:O	2.19	0.42
1:D:365:PRO:CB	1:D:374:GLU:HG2	2.48	0.42
1:D:522:VAL:O	1:D:566:VAL:HG23	2.19	0.42
2:E:65:CYS:HB2	2:F:97:PHE:CE1	2.55	0.42
2:E:124:GLY:HA2	2:E:127:GLU:OE1	2.19	0.42
2:F:20:ARG:HB2	2:F:198:SER:OG	2.19	0.42
2:F:23:LEU:HA	2:F:74:VAL:CG1	2.44	0.42
2:F:126:LYS:O	2:F:129:ILE:HG13	2.18	0.42
2:F:153:VAL:HA	2:F:156:SER:OG	2.19	0.42
1:A:113:PHE:CE1	1:A:333:SER:HB2	2.55	0.42
2:B:40:LYS:HB3	2:B:40:LYS:HE2	1.83	0.42
2:C:185:TRP:O	2:C:188:ARG:HB3	2.19	0.42
1:D:70:ASP:CG	1:D:104:SER:HA	2.44	0.42
1:D:94:VAL:HG11	1:D:112:PRO:CB	2.33	0.42
1:D:199:HIS:HA	1:D:525:LYS:HG2	2.01	0.42
1:D:210:ILE:HD12	1:D:234:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:204:LYS:O	2:E:208:TYR:HD1	2.03	0.42
2:F:17:MET:O	2:F:21:VAL:HG23	2.18	0.42
1:A:23:ASN:O	1:A:27:VAL:HG23	2.19	0.42
1:A:78:LYS:HB3	1:A:78:LYS:HE3	1.74	0.42
1:A:98:SER:HB3	1:A:113:PHE:CE1	2.54	0.42
1:A:232:ARG:HG3	1:A:233:THR:N	2.33	0.42
1:A:245:ILE:HD13	1:A:267:LEU:HD21	2.01	0.42
1:A:302:TYR:HD1	1:A:326:VAL:HG13	1.85	0.42
1:A:328:HIS:O	1:A:352:PHE:CE1	2.72	0.42
1:A:396:ALA:HB2	7:A:808:HOH:O	2.19	0.42
2:B:67:SER:HA	2:B:70:VAL:HG12	2.02	0.42
2:C:81:LYS:HB3	2:C:81:LYS:HE2	1.79	0.42
2:C:122:GLU:HA	2:C:125:LYS:HG3	2.02	0.42
2:C:143:PRO:HB2	2:C:144:TYR:CD2	2.54	0.42
1:D:41:SER:HG	2:E:144:TYR:H	1.67	0.42
1:D:87:PRO:HD2	2:E:188:ARG:HE	1.84	0.42
1:D:166:THR:HA	1:D:169:VAL:HG12	2.02	0.42
1:D:227:LEU:HD23	1:D:227:LEU:HA	1.73	0.42
1:D:256:VAL:O	1:D:260:ARG:HG3	2.19	0.42
1:D:305:MET:CG	1:D:347:PRO:HB3	2.48	0.42
2:E:73:TYR:CE1	2:F:90:TYR:HA	2.54	0.42
2:F:98:TRP:HZ2	2:F:135:LEU:CG	2.21	0.42
1:A:388:TYR:O	1:A:407:VAL:HG12	2.19	0.42
1:A:408:LYS:HE3	1:A:420:LYS:CE	2.50	0.42
1:D:99:LEU:HB3	1:D:557:LYS:CB	2.43	0.42
1:D:143:LYS:C	1:D:216:VAL:HA	2.44	0.42
1:D:152:LYS:HE3	1:D:530:LYS:HE2	2.02	0.42
1:D:197:ASP:OD1	1:D:197:ASP:N	2.43	0.42
1:D:287:TRP:CD1	1:D:319:TYR:CD1	3.07	0.42
1:D:402:ARG:NH2	7:D:731:HOH:O	2.53	0.42
2:E:52:LYS:HE3	2:E:52:LYS:HB2	1.91	0.42
2:E:152:TYR:O	2:E:155:ILE:HG13	2.20	0.42
1:A:161:PRO:HB2	7:A:755:HOH:O	2.20	0.42
1:A:203:TYR:HE1	1:A:237:VAL:HB	1.84	0.42
1:A:420:LYS:HE3	1:A:420:LYS:HB3	1.80	0.42
1:A:477:ILE:HG12	1:A:518:LEU:HD21	2.01	0.42
2:B:7:LEU:HG	7:B:418:HOH:O	2.20	0.42
2:B:99:ALA:O	2:B:102:VAL:HG13	2.20	0.42
2:C:84:PHE:HD1	2:C:84:PHE:C	2.27	0.42
1:D:153:GLN:C	1:D:563:CYS:SG	3.03	0.42
1:D:437:THR:N	1:D:440:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:TYR:N	1:D:475:TYR:CD1	2.88	0.42
2:F:18:ARG:N	2:F:159:THR:HG21	2.34	0.42
1:A:62:LYS:HB3	1:A:62:LYS:HE3	1.87	0.42
1:D:10:MET:HG3	1:D:11:ASN:H	1.85	0.42
1:D:87:PRO:CG	2:E:188:ARG:HE	2.30	0.42
2:E:11:TRP:CE3	2:E:12:PRO:HD3	2.55	0.42
2:F:5:PRO:HB3	2:F:59:HIS:NE2	2.35	0.42
1:A:145:LEU:HD13	1:A:209:GLY:CA	2.48	0.42
1:A:452:LEU:HD23	1:A:481:ILE:HG21	2.02	0.42
2:E:10:TYR:H	2:E:54:ILE:HD13	1.85	0.42
2:E:68:LEU:HD11	2:E:152:TYR:CZ	2.55	0.42
2:F:106:PHE:O	2:F:110:GLN:HG3	2.20	0.42
1:A:42:ALA:HA	2:B:143:PRO:CG	2.43	0.42
2:F:23:LEU:HD13	2:F:28:VAL:HG13	2.02	0.42
1:A:167:THR:HG21	1:A:560:GLN:HB3	2.02	0.41
1:A:227:LEU:HD13	1:A:316:LEU:HD21	2.02	0.41
1:A:295:PHE:O	1:A:295:PHE:HD1	2.02	0.41
1:A:527:THR:HB	1:A:561:ILE:HG21	2.02	0.41
2:C:183:ILE:HD13	1:D:492:ASP:HA	2.02	0.41
1:D:53:ASN:CG	1:D:54:ALA:H	2.27	0.41
1:D:94:VAL:HB	1:D:113:PHE:H	1.84	0.41
1:D:127:THR:O	1:D:130:ALA:HB3	2.20	0.41
2:F:203:GLU:O	2:F:206:VAL:HG22	2.19	0.41
1:A:29:LYS:O	1:A:32:LEU:HB2	2.20	0.41
1:A:136:PHE:HD1	1:A:299:LYS:HE2	1.84	0.41
1:A:339:ALA:N	1:A:353:ALA:O	2.27	0.41
1:A:477:ILE:HG12	1:A:518:LEU:CD2	2.50	0.41
1:A:494:CYS:SG	1:A:572:SER:HA	2.59	0.41
1:A:498:ASP:OD1	1:A:518:LEU:HB3	2.20	0.41
2:C:9:ASP:HB2	2:C:20:ARG:NH2	2.35	0.41
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.85	0.41
2:C:166:ALA:O	2:C:170:PHE:HD2	2.03	0.41
2:C:188:ARG:HB2	2:C:188:ARG:HE	1.68	0.41
1:D:67:LEU:HB2	7:D:878:HOH:O	2.19	0.41
1:D:76:TYR:HB3	1:D:88:ILE:HG21	2.02	0.41
1:D:149:PHE:CD2	1:D:202:LEU:HD22	2.55	0.41
1:D:151:SER:HB2	1:D:194:PHE:CA	2.50	0.41
1:D:358:LEU:H	1:D:358:LEU:HG	1.59	0.41
1:D:382:VAL:HG22	1:D:388:TYR:CD2	2.55	0.41
1:D:451:ARG:NH1	1:D:493:CYS:H	2.18	0.41
2:E:169:LYS:HE2	2:E:169:LYS:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:211:GLU:HA	2:F:214:LYS:HG2	2.01	0.41
1:A:210:ILE:HD12	7:A:847:HOH:O	2.20	0.41
2:B:65:CYS:O	2:B:69:ASN:HB3	2.20	0.41
2:C:17:MET:CE	2:C:200:PRO:HD2	2.48	0.41
2:C:60:ASN:O	2:C:60:ASN:CG	2.63	0.41
2:C:120:GLU:HB3	7:C:436:HOH:O	2.20	0.41
2:C:169:LYS:HE2	2:C:169:LYS:HB2	1.69	0.41
1:D:46:GLN:NE2	2:E:148:ASP:OD2	2.54	0.41
1:D:190:ASP:O	1:D:193:ILE:HB	2.20	0.41
1:D:223:PHE:HZ	1:D:536:LEU:HB2	1.76	0.41
2:E:183:ILE:HG13	2:E:184:ALA:N	2.34	0.41
1:A:103:THR:HB	1:A:106:GLY:HA2	2.02	0.41
1:A:143:LYS:HG3	1:A:144:ALA:N	2.34	0.41
1:A:423:CYS:SG	1:A:541:SER:OG	2.67	0.41
1:A:574:ALA:O	1:A:575:PHE:HB2	2.21	0.41
2:C:123:ALA:HA	7:C:454:HOH:O	2.20	0.41
2:C:144:TYR:HB3	2:C:154:ASP:CG	2.45	0.41
1:D:46:GLN:HE21	2:E:148:ASP:CB	2.33	0.41
1:D:211:LEU:HD13	1:D:212:PHE:CD1	2.55	0.41
1:D:316:LEU:O	1:D:320:ALA:N	2.48	0.41
1:D:318:HIS:ND1	1:D:318:HIS:C	2.78	0.41
1:D:552:LYS:C	1:D:554:SER:H	2.26	0.41
2:F:176:GLU:O	2:F:183:ILE:HG21	2.19	0.41
2:F:213:ARG:HH11	2:F:217:LEU:HD21	1.85	0.41
1:A:263:MET:HE3	1:A:263:MET:HB3	1.97	0.41
1:A:303:GLY:N	1:A:328:HIS:CE1	2.89	0.41
1:D:64:MET:O	1:D:66:PRO:HD3	2.20	0.41
1:D:510:ARG:HB3	1:D:575:PHE:CE2	2.55	0.41
2:E:93:ALA:HA	2:F:73:TYR:HE1	1.86	0.41
2:E:99:ALA:O	2:E:102:VAL:HG12	2.21	0.41
2:E:125:LYS:HD2	2:E:173:PHE:CE2	2.54	0.41
2:F:114:TRP:CD1	2:F:167:TYR:CE1	3.09	0.41
2:F:212:TYR:HD1	2:F:212:TYR:HA	1.78	0.41
1:A:44:TYR:HE1	1:A:89:LEU:C	2.29	0.41
1:A:110:PHE:CD1	1:A:556:ALA:HB2	2.56	0.41
1:A:222:VAL:HB	1:A:533:GLU:HB3	2.02	0.41
2:B:146:GLY:CA	2:B:151:GLY:HA3	2.50	0.41
1:D:39:ASN:OD1	2:E:141:ASP:O	2.38	0.41
1:D:75:PRO:O	1:D:79:ARG:HG3	2.20	0.41
2:E:68:LEU:HD11	2:E:152:TYR:HE1	1.84	0.41
2:E:76:GLU:OE2	2:F:92:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:ILE:O	2:E:186:ALA:HB3	2.20	0.41
1:A:77:ILE:HD12	1:A:112:PRO:HD3	2.03	0.41
1:A:119:GLU:CG	1:A:120:ASN:N	2.83	0.41
1:A:439:ARG:O	1:A:443:LEU:HB2	2.21	0.41
1:A:467:ASP:OD1	1:A:474:HIS:N	2.46	0.41
1:A:491:GLN:NE2	1:A:570:TYR:HB3	2.36	0.41
2:B:151:GLY:O	2:B:154:ASP:HB2	2.20	0.41
2:C:22:ALA:HB1	2:C:74:VAL:HG11	2.03	0.41
2:C:84:PHE:CZ	2:C:152:TYR:HD2	2.38	0.41
1:D:11:ASN:O	1:D:14:ILE:HG13	2.21	0.41
1:D:13:VAL:HG22	1:D:127:THR:HG23	2.03	0.41
1:D:286:ASN:O	1:D:287:TRP:HB3	2.21	0.41
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.71	0.41
2:E:66:GLU:OE2	2:F:100:ASP:CB	2.69	0.41
2:E:144:TYR:C	2:E:145:PHE:HD1	2.27	0.41
2:F:10:TYR:CG	2:F:37:PHE:CE1	3.09	0.41
2:F:23:LEU:HD23	7:F:442:HOH:O	2.21	0.41
1:A:163:GLY:HA2	1:A:556:ALA:O	2.21	0.41
1:A:187:CYS:HB2	1:A:208:SER:O	2.21	0.41
1:A:225:HIS:NE2	1:A:529:ARG:HG3	2.36	0.41
1:A:433:ILE:HG21	1:A:552:LYS:NZ	2.36	0.41
2:B:114:TRP:HD1	2:B:167:TYR:HE1	1.67	0.41
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.56	0.41
1:D:99:LEU:HD12	1:D:100:SER:H	1.86	0.41
1:D:111:ILE:HD12	7:D:815:HOH:O	2.20	0.41
1:D:154:TYR:CZ	1:D:559:LEU:HB3	2.56	0.41
1:D:179:MET:HB3	1:D:179:MET:HE2	1.73	0.41
1:D:227:LEU:HD22	1:D:231:PHE:CE2	2.56	0.41
1:D:510:ARG:HG2	1:D:515:ILE:CD1	2.46	0.41
1:D:528:PHE:O	1:D:531:ILE:HG12	2.20	0.41
2:E:40:LYS:HZ1	2:E:52:LYS:HD2	1.81	0.41
2:E:110:GLN:O	2:E:113:VAL:HG12	2.21	0.41
2:E:180:PRO:HD2	2:E:181:LYS:H	1.85	0.41
2:F:179:SER:HG	2:F:182:LEU:HB3	1.84	0.41
1:A:27:VAL:CG1	1:A:356:PRO:HB2	2.51	0.41
1:A:33:LYS:HA	1:A:36:LEU:CD2	2.51	0.41
1:A:95:PRO:HD2	1:A:113:PHE:O	2.20	0.41
1:A:234:PHE:CD2	1:A:287:TRP:CZ3	3.09	0.41
1:A:374:GLU:HG3	1:A:375:LYS:N	2.35	0.41
1:A:433:ILE:HG21	1:A:552:LYS:HZ1	1.86	0.41
1:A:546:LYS:HE3	1:A:546:LYS:HB2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:TRP:CZ2	2:B:138:GLU:HG2	2.56	0.41
2:B:151:GLY:O	2:B:155:ILE:HG13	2.21	0.41
2:B:158:ILE:H	2:B:158:ILE:HG12	1.64	0.41
2:B:216:ASN:C	2:B:217:LEU:HD12	2.46	0.41
2:C:14:MET:O	2:C:18:ARG:HG3	2.21	0.41
2:C:84:PHE:CD1	2:C:84:PHE:C	2.99	0.41
2:C:125:LYS:HE2	2:C:173:PHE:CE2	2.55	0.41
1:D:8:PHE:CD1	1:D:182:ILE:HG23	2.56	0.41
1:D:68:VAL:HG12	1:D:401:TYR:CB	2.50	0.41
1:D:79:ARG:HE	1:D:79:ARG:HB2	1.65	0.41
1:D:106:GLY:O	1:D:432:ASN:ND2	2.54	0.41
1:D:163:GLY:HA3	1:D:560:GLN:OE1	2.20	0.41
1:D:175:PHE:O	1:D:179:MET:HB2	2.21	0.41
1:D:207:LEU:HD13	1:D:241:ILE:HG23	2.02	0.41
1:D:272:GLU:O	1:D:276:THR:HG23	2.21	0.41
1:D:363:PHE:HB3	1:D:388:TYR:HB3	2.03	0.41
1:D:434:ASP:HB2	1:D:550:CYS:CB	2.50	0.41
1:D:435:LYS:HZ2	1:D:435:LYS:HG3	1.47	0.41
1:D:541:SER:C	1:D:543:GLY:H	2.29	0.41
1:D:575:PHE:N	1:D:575:PHE:HD1	2.19	0.41
2:E:15:PHE:CD1	2:E:15:PHE:N	2.88	0.41
2:F:92:ARG:HG3	7:F:402:HOH:O	2.20	0.41
2:F:135:LEU:HD13	2:F:182:LEU:CD1	2.51	0.41
2:F:144:TYR:HB3	2:F:154:ASP:CG	2.46	0.41
1:A:551:VAL:HG11	1:A:558:VAL:CG1	2.47	0.41
2:B:24:ARG:HH11	2:B:24:ARG:HD2	1.69	0.41
2:B:110:GLN:HB2	2:B:167:TYR:OH	2.20	0.41
2:B:198:SER:O	2:B:200:PRO:HD3	2.21	0.41
2:C:70:VAL:HA	2:C:73:TYR:CD2	2.57	0.41
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.39	0.41
1:D:38:LYS:HE2	7:D:862:HOH:O	2.21	0.41
1:D:154:TYR:CE2	1:D:559:LEU:HB3	2.56	0.41
1:D:284:LEU:HD22	1:D:287:TRP:HA	2.03	0.41
1:D:390:VAL:HG11	1:D:540:SER:CA	2.46	0.41
1:D:398:LEU:N	1:D:398:LEU:HD12	2.36	0.41
1:D:496:CYS:CB	1:D:499:ARG:NH1	2.83	0.41
2:E:62:LYS:HB3	2:F:90:TYR:CE2	2.56	0.41
2:F:23:LEU:C	2:F:23:LEU:HD12	2.45	0.41
2:F:134:ILE:HG13	2:F:135:LEU:N	2.36	0.41
2:F:187:LYS:HB3	2:F:187:LYS:HE3	1.78	0.41
1:A:67:LEU:HD23	1:A:400:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:SER:O	1:A:111:ILE:HG13	2.21	0.40
1:A:203:TYR:OH	1:A:241:ILE:HA	2.22	0.40
1:A:302:TYR:CG	1:A:328:HIS:HE1	2.38	0.40
2:B:24:ARG:CD	2:B:197:LYS:NZ	2.81	0.40
2:B:106:PHE:CZ	2:B:131:ALA:HB1	2.57	0.40
1:D:108:PRO:HG3	1:D:551:VAL:HA	2.03	0.40
1:D:116:GLU:N	7:D:768:HOH:O	2.54	0.40
1:D:192:VAL:HG23	1:D:259:VAL:CG2	2.52	0.40
1:D:262:ALA:O	1:D:265:LYS:HB2	2.21	0.40
2:E:162:SER:HB3	2:E:199:LEU:HD11	2.03	0.40
2:E:173:PHE:HD1	2:E:173:PHE:HA	1.80	0.40
1:A:41:SER:HB3	2:B:144:TYR:H	1.86	0.40
1:A:152:LYS:HB3	1:A:563:CYS:SG	2.61	0.40
1:A:169:VAL:HG13	1:A:170:TYR:CE1	2.56	0.40
2:C:105:LYS:HB2	2:C:105:LYS:HE3	1.84	0.40
1:D:143:LYS:HZ1	1:D:187:CYS:HB2	1.86	0.40
1:D:213:ARG:HA	1:D:216:VAL:CG1	2.51	0.40
2:E:120:GLU:OE1	7:E:415:HOH:O	2.21	0.40
2:E:162:SER:HB3	2:E:199:LEU:CG	2.51	0.40
1:A:44:TYR:CD1	1:A:89:LEU:HA	2.56	0.40
1:A:86:SER:HA	1:A:87:PRO:HD2	1.94	0.40
1:A:208:SER:HA	1:A:211:LEU:HG	2.04	0.40
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.70	0.40
1:A:299:LYS:HB2	1:A:299:LYS:HE3	1.53	0.40
2:B:84:PHE:N	2:B:84:PHE:CD1	2.89	0.40
1:D:87:PRO:CG	1:D:93:PRO:HG3	2.51	0.40
1:D:226:GLY:HA2	1:D:529:ARG:CD	2.43	0.40
1:D:264:SER:HA	1:D:267:LEU:HD12	2.03	0.40
1:D:499:ARG:CZ	1:D:499:ARG:CB	2.98	0.40
1:D:559:LEU:HD23	1:D:559:LEU:HA	1.69	0.40
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.69	0.40
1:A:228:VAL:HG22	1:A:319:TYR:CE2	2.56	0.40
1:A:238:TRP:HZ2	1:A:282:MET:SD	2.43	0.40
1:A:375:LYS:H	1:A:375:LYS:HG2	1.53	0.40
1:A:437:THR:HG21	1:A:439:ARG:NH1	2.36	0.40
1:A:465:TYR:CG	1:A:466:ILE:N	2.89	0.40
1:A:547:MET:HA	1:A:548:PRO:HD3	1.76	0.40
2:B:167:TYR:CD1	2:B:167:TYR:N	2.83	0.40
1:D:87:PRO:HD2	2:E:188:ARG:HB3	2.02	0.40
1:D:132:ARG:HE	1:D:326:VAL:HG21	1.85	0.40
1:D:143:LYS:HZ1	1:D:209:GLY:HA2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:VAL:CG1	1:D:315:LYS:HD3	2.47	0.40
1:D:452:LEU:CG	1:D:457:ILE:HD11	2.52	0.40
1:D:465:TYR:CD1	1:D:551:VAL:HG23	2.53	0.40
2:E:101:PHE:CE2	2:E:135:LEU:HD11	2.56	0.40
2:E:151:GLY:N	2:E:154:ASP:OD2	2.49	0.40
1:A:164:THR:HA	1:A:557:LYS:HG3	2.04	0.40
1:A:329:ASP:HA	1:A:352:PHE:CD1	2.57	0.40
2:B:35:GLU:HG3	2:B:44:LEU:CD2	2.52	0.40
2:B:129:ILE:HD13	2:B:129:ILE:HA	1.89	0.40
2:C:33:ARG:HE	2:C:33:ARG:HB3	1.75	0.40
1:D:43:ILE:H	1:D:43:ILE:HG23	1.64	0.40
1:D:43:ILE:HG13	1:D:44:TYR:N	2.36	0.40
1:D:81:VAL:HG21	1:D:110:PHE:HE2	1.77	0.40
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.50	0.40
2:F:43:LEU:H	2:F:43:LEU:HG	1.45	0.40
2:F:166:ALA:HB2	7:F:453:HOH:O	2.21	0.40

All (8) 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:234:PHE:O	2:F:177:SER:OG[1_554]	1.77	0.43
1:A:214:ASP:OD2	1:A:475:TYR:OH[1_545]	1.90	0.30
7:D:897:HOH:O	7:D:961:HOH:O[1_455]	2.06	0.14
7:A:831:HOH:O	7:A:847:HOH:O[1_565]	2.15	0.05
2:E:61:GLY:N	2:F:211:GLU:OE2[1_565]	2.16	0.04
7:A:822:HOH:O	7:F:486:HOH:O[1_554]	2.17	0.03
7:B:411:HOH:O	7:C:456:HOH:O[1_565]	2.17	0.03
7:D:918:HOH:O	7:D:930:HOH:O[1_455]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/575 (99%)	531 (94%)	27 (5%)	9 (2%)	7	2
1	D	567/575 (99%)	544 (96%)	16 (3%)	7 (1%)	10	2
2	B	212/223 (95%)	198 (93%)	13 (6%)	1 (0%)	24	13
2	C	212/223 (95%)	200 (94%)	9 (4%)	3 (1%)	9	2
2	E	212/223 (95%)	200 (94%)	10 (5%)	2 (1%)	14	4
2	F	212/223 (95%)	198 (93%)	11 (5%)	3 (1%)	9	2
All	All	1982/2042 (97%)	1871 (94%)	86 (4%)	25 (1%)	9	2

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	513	LYS
1	A	540	SER
1	D	180	LYS
1	D	540	SER
1	D	542	ALA
2	E	141	ASP
1	A	287	TRP
2	C	140	GLY
1	D	437	THR
2	F	140	GLY
1	A	552	LYS
1	D	88	ILE
2	F	80	GLU
2	F	180	PRO
1	A	88	ILE
1	A	369	THR
2	C	66	GLU
1	A	574	ALA
1	D	368	GLU
1	D	552	LYS
2	B	82	ASN
2	E	66	GLU
2	C	83	PRO
1	A	523	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	401 (80%)	98 (20%)	1	0
1	D	499/505 (99%)	416 (83%)	83 (17%)	2	0
2	B	187/195 (96%)	161 (86%)	26 (14%)	3	0
2	C	187/195 (96%)	161 (86%)	26 (14%)	3	0
2	E	187/195 (96%)	164 (88%)	23 (12%)	4	0
2	F	187/195 (96%)	156 (83%)	31 (17%)	2	0
All	All	1746/1790 (98%)	1459 (84%)	287 (16%)	2	0

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	13	VAL
1	A	14	ILE
1	A	15	ASP
1	A	16	GLU
1	A	18	ASP
1	A	26	GLN
1	A	29	LYS
1	A	40	GLN
1	A	43	ILE
1	A	45	LEU
1	A	65	VAL
1	A	71	VAL
1	A	72	GLU
1	A	73	LEU
1	A	77	ILE
1	A	78	LYS
1	A	84	ASP
1	A	88	ILE
1	A	90	THR
1	A	92	HIS
1	A	99	LEU

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Mol	Chain	Res	Type
1	A	100	SER
1	A	101	SER
1	A	103	THR
1	A	110	PHE
1	A	111	ILE
1	A	114	THR
1	A	116	GLU
1	A	117	LEU
1	A	122	LEU
1	A	125	PHE
1	A	134	ARG
1	A	135	ASP
1	A	138	ILE
1	A	140	ASP
1	A	143	LYS
1	A	160	VAL
1	A	167	THR
1	A	180	LYS
1	A	184	SER
1	A	190	ASP
1	A	195	SER
1	A	197	ASP
1	A	202	LEU
1	A	205	HIS
1	A	212	PHE
1	A	222	VAL
1	A	253	ARG
1	A	260	ARG
1	A	265	LYS
1	A	268	THR
1	A	276	THR
1	A	277	ILE
1	A	282	MET
1	A	285	SER
1	A	288	TYR
1	A	294	LEU
1	A	305	MET
1	A	313	VAL
1	A	327	SER
1	A	333	SER
1	A	351	THR
1	A	355	ILE

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Mol	Chain	Res	Type
1	A	368	GLU
1	A	373	GLU
1	A	374	GLU
1	A	379	LEU
1	A	384	ILE
1	A	390	VAL
1	A	405	ASP
1	A	409	VAL
1	A	425	ARG
1	A	426	ASN
1	A	427	LEU
1	A	428	ILE
1	A	437	THR
1	A	443	LEU
1	A	464	SER
1	A	466	ILE
1	A	468	VAL
1	A	477	ILE
1	A	494	CYS
1	A	497	LEU
1	A	507	VAL
1	A	511	LYS
1	A	514	THR
1	A	515	ILE
1	A	518	LEU
1	A	531	ILE
1	A	536	LEU
1	A	538	LEU
1	A	551	VAL
1	A	554	SER
1	A	557	LYS
1	A	565	ASN
1	A	569	SER
1	A	573	THR
2	B	24	ARG
2	B	26	LYS
2	B	33	ARG
2	B	50	ILE
2	B	58	VAL
2	B	101	PHE
2	B	102	VAL
2	B	104	LYS

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Mol	Chain	Res	Type
2	B	113	VAL
2	B	117	LYS
2	B	132	VAL
2	B	134	ILE
2	B	139	LEU
2	B	153	VAL
2	B	154	ASP
2	B	155	ILE
2	B	158	ILE
2	B	173	PHE
2	B	181	LYS
2	B	182	LEU
2	B	183	ILE
2	B	190	MET
2	B	196	SER
2	B	197	LYS
2	B	208	TYR
2	B	211	GLU
2	C	14	MET
2	C	24	ARG
2	C	40	LYS
2	C	43	LEU
2	C	59	HIS
2	C	64	VAL
2	C	65	CYS
2	C	74	VAL
2	C	84	PHE
2	C	87	SER
2	C	105	LYS
2	C	121	GLN
2	C	133	LYS
2	C	134	ILE
2	C	135	LEU
2	C	145	PHE
2	C	157	LEU
2	C	162	SER
2	C	169	LYS
2	C	173	PHE
2	C	176	GLU
2	C	183	ILE
2	C	187	LYS
2	C	188	ARG

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Mol	Chain	Res	Type
2	C	195	VAL
2	C	198	SER
1	D	15	ASP
1	D	23	ASN
1	D	26	GLN
1	D	37	LEU
1	D	43	ILE
1	D	59	GLU
1	D	68	VAL
1	D	69	THR
1	D	79	ARG
1	D	87	PRO
1	D	90	THR
1	D	92	HIS
1	D	99	LEU
1	D	100	SER
1	D	104	SER
1	D	110	PHE
1	D	111	ILE
1	D	116	GLU
1	D	125	PHE
1	D	126	ARG
1	D	133	ASN
1	D	134	ARG
1	D	135	ASP
1	D	143	LYS
1	D	162	VAL
1	D	164	THR
1	D	179	MET
1	D	188	SER
1	D	195	SER
1	D	198	VAL
1	D	202	LEU
1	D	204	CYS
1	D	205	HIS
1	D	211	LEU
1	D	241	ILE
1	D	245	ILE
1	D	250	LEU
1	D	273	LEU
1	D	290	LEU
1	D	295	PHE

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Mol	Chain	Res	Type
1	D	299	LYS
1	D	304	ILE
1	D	305	MET
1	D	315	LYS
1	D	318	HIS
1	D	323	LEU
1	D	326	VAL
1	D	329	ASP
1	D	333	SER
1	D	351	THR
1	D	364	LEU
1	D	373	GLU
1	D	379	LEU
1	D	395	TYR
1	D	398	LEU
1	D	400	ARG
1	D	406	VAL
1	D	409	VAL
1	D	416	THR
1	D	423	CYS
1	D	426	ASN
1	D	427	LEU
1	D	433	ILE
1	D	450	LYS
1	D	456	LYS
1	D	459	VAL
1	D	464	SER
1	D	466	ILE
1	D	481	ILE
1	D	482	SER
1	D	493	CYS
1	D	499	ARG
1	D	502	ILE
1	D	503	ASP
1	D	507	VAL
1	D	512	CYS
1	D	518	LEU
1	D	521	ARG
1	D	538	LEU
1	D	544	GLN
1	D	551	VAL
1	D	562	LEU

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Mol	Chain	Res	Type
1	D	568	SER
2	E	6	ILE
2	E	11	TRP
2	E	28	VAL
2	E	38	SER
2	E	47	SER
2	E	50	ILE
2	E	54	ILE
2	E	70	VAL
2	E	113	VAL
2	E	117	LYS
2	E	132	VAL
2	E	139	LEU
2	E	142	LYS
2	E	148	ASP
2	E	150	PHE
2	E	153	VAL
2	E	155	ILE
2	E	173	PHE
2	E	181	LYS
2	E	183	ILE
2	E	187	LYS
2	E	203	GLU
2	E	204	LYS
2	F	8	LEU
2	F	28	VAL
2	F	30	PHE
2	F	40	LYS
2	F	41	SER
2	F	43	LEU
2	F	54	ILE
2	F	57	LEU
2	F	58	VAL
2	F	59	HIS
2	F	62	LYS
2	F	64	VAL
2	F	71	VAL
2	F	76	GLU
2	F	88	ASP
2	F	98	TRP
2	F	101	PHE
2	F	136	GLU

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Mol	Chain	Res	Type
2	F	139	LEU
2	F	153	VAL
2	F	168	GLU
2	F	172	ASN
2	F	175	ILE
2	F	176	GLU
2	F	178	GLU
2	F	181	LYS
2	F	182	LEU
2	F	195	VAL
2	F	202	SER
2	F	203	GLU
2	F	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	153	GLN
1	A	168	ASN
1	A	200	GLN
1	A	215	GLN
1	A	426	ASN
1	A	534	HIS
2	B	110	GLN
2	C	121	GLN
2	C	172	ASN
1	D	28	GLN
1	D	46	GLN
1	D	133	ASN
1	D	153	GLN
1	D	217	GLN
1	D	270	ASN
1	D	340	ASN
1	D	418	GLN
1	D	491	GLN
1	D	544	GLN
1	D	565	ASN
2	E	60	ASN
2	E	82	ASN
2	E	94	GLN
2	F	215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GSH	C	301	-	18,19,19	1.55	4 (22%)	21,24,24	1.41	4 (19%)
4	ILE	D	602	-	8,8,8	1.15	2 (25%)	9,10,10	2.00	3 (33%)
6	GSH	E	301	-	18,19,19	1.44	3 (16%)	21,24,24	1.71	2 (9%)
3	JAA	A	601	-	15,15,15	5.03	7 (46%)	14,19,19	2.76	6 (42%)
6	GSH	F	301	-	18,19,19	1.52	4 (22%)	21,24,24	1.29	2 (9%)
3	JAA	D	601	-	15,15,15	5.28	6 (40%)	14,19,19	2.67	9 (64%)
6	GSH	B	301	-	18,19,19	1.49	2 (11%)	21,24,24	1.18	2 (9%)
4	ILE	A	602	-	8,8,8	0.94	0	9,10,10	1.87	3 (33%)

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
6	GSH	C	301	-	-	5/24/24/24	-
4	ILE	D	602	-	-	6/10/10/10	-
6	GSH	E	301	-	-	4/24/24/24	-
3	JAA	A	601	-	-	6/9/22/22	0/1/1/1
6	GSH	F	301	-	-	2/24/24/24	-
3	JAA	D	601	-	-	4/9/22/22	0/1/1/1
6	GSH	B	301	-	-	7/24/24/24	-
4	ILE	A	602	-	-	1/10/10/10	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	JAA	C05-C08	-14.08	1.29	1.52
3	A	601	JAA	C05-C08	-12.89	1.31	1.52
3	A	601	JAA	C06-C04	-10.49	1.27	1.53
3	D	601	JAA	C06-C04	-10.35	1.27	1.53
3	D	601	JAA	C07-C08	7.58	1.63	1.51
3	A	601	JAA	C07-C08	7.00	1.62	1.51
3	A	601	JAA	C05-C04	5.37	1.67	1.54
3	D	601	JAA	C05-C04	5.28	1.67	1.54
3	D	601	JAA	C10-C04	-3.59	1.47	1.53
6	B	301	GSH	CD1-N2	3.59	1.41	1.34
6	F	301	GSH	CD1-N2	3.38	1.41	1.34
6	B	301	GSH	C2-N3	3.37	1.41	1.33
6	C	301	GSH	CD1-N2	3.34	1.41	1.34
6	E	301	GSH	CD1-N2	3.20	1.40	1.34
3	A	601	JAA	C10-C04	-3.20	1.48	1.53
6	F	301	GSH	C2-N3	3.13	1.41	1.33
6	C	301	GSH	C2-N3	3.01	1.40	1.33
6	E	301	GSH	C2-N3	2.89	1.40	1.33
3	A	601	JAA	C06-C07	2.80	1.59	1.53
3	D	601	JAA	C06-C07	2.75	1.59	1.53
3	A	601	JAA	O03-C12	-2.28	1.23	1.30
6	C	301	GSH	O11-C1	-2.21	1.23	1.30
4	D	602	ILE	CA-C	-2.17	1.48	1.52
6	E	301	GSH	CB2-CA2	-2.17	1.50	1.53
6	C	301	GSH	CB2-CA2	-2.16	1.50	1.53
6	F	301	GSH	O11-C1	-2.09	1.24	1.30
6	F	301	GSH	CB2-CA2	-2.02	1.50	1.53
4	D	602	ILE	CG2-CB	-2.02	1.47	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	301	GSH	CA2-CB2-SG2	-6.12	107.26	114.16
3	A	601	JAA	C04-C10-C12	-6.11	100.95	113.33
3	A	601	JAA	C06-C04-C05	4.81	110.12	103.36
4	D	602	ILE	C-CA-N	4.46	118.87	109.49
3	D	601	JAA	C07-C06-C04	-4.16	100.06	104.45
4	A	602	ILE	C-CA-N	4.05	118.00	109.49
3	D	601	JAA	C04-C10-C12	-3.85	105.53	113.33
3	D	601	JAA	C06-C04-C05	3.83	108.75	103.36
3	D	601	JAA	C09-C11-C13	-3.51	113.30	126.21
3	A	601	JAA	C07-C06-C04	3.43	108.07	104.45
3	D	601	JAA	O03-C12-C10	3.31	124.28	114.00
6	C	301	GSH	CA2-CB2-SG2	-3.10	110.67	114.16
6	C	301	GSH	O2-C2-N3	-2.93	116.78	122.98
6	B	301	GSH	CA2-CB2-SG2	-2.79	111.01	114.16
3	D	601	JAA	C14-C13-C11	-2.70	110.18	126.42
6	C	301	GSH	CA2-C2-N3	2.69	122.30	116.54
3	A	601	JAA	O03-C12-C10	2.66	122.28	114.00
3	A	601	JAA	C09-C11-C13	-2.66	116.44	126.21
6	F	301	GSH	CA2-CB2-SG2	-2.65	111.17	114.16
3	D	601	JAA	O02-C12-C10	-2.61	114.83	122.84
3	D	601	JAA	O01-C08-C05	2.57	128.88	125.60
6	F	301	GSH	O2-C2-N3	-2.56	117.56	122.98
4	A	602	ILE	OXT-C-O	-2.40	118.63	124.08
6	E	301	GSH	CA2-N2-CD1	-2.40	115.67	121.68
6	B	301	GSH	O2-C2-N3	-2.38	117.94	122.98
4	D	602	ILE	CB-CA-C	-2.33	102.30	111.28
3	D	601	JAA	C06-C07-C08	-2.29	103.12	105.39
4	A	602	ILE	OXT-C-CA	2.25	121.90	114.15
6	C	301	GSH	CA3-N3-C2	-2.21	115.80	121.38
4	D	602	ILE	OXT-C-CA	2.16	121.61	114.15
3	A	601	JAA	C06-C04-C10	-2.02	109.66	113.41

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	JAA	C05-C04-C10-C12
3	A	601	JAA	C06-C04-C10-C12
3	A	601	JAA	C08-C05-C09-C11
4	A	602	ILE	OXT-C-CA-N
4	D	602	ILE	C-CA-CB-CG1
4	D	602	ILE	C-CA-CB-CG2
6	B	301	GSH	N1-CA1-CB1-CG1

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Mol	Chain	Res	Type	Atoms
6	B	301	GSH	N2-CA2-CB2-SG2
6	B	301	GSH	C2-CA2-CB2-SG2
6	C	301	GSH	O12-C1-CA1-N1
6	C	301	GSH	N2-CA2-CB2-SG2
6	C	301	GSH	C2-CA2-CB2-SG2
6	E	301	GSH	N1-CA1-CB1-CG1
6	E	301	GSH	C1-CA1-CB1-CG1
6	F	301	GSH	N2-CA2-CB2-SG2
6	F	301	GSH	C2-CA2-CB2-SG2
4	D	602	ILE	N-CA-CB-CG1
6	E	301	GSH	O32-C3-CA3-N3
4	D	602	ILE	CG2-CB-CG1-CD1
3	D	601	JAA	C09-C11-C13-C14
4	D	602	ILE	CA-CB-CG1-CD1
6	C	301	GSH	O11-C1-CA1-N1
3	A	601	JAA	C05-C09-C11-C13
6	E	301	GSH	O31-C3-CA3-N3
6	B	301	GSH	C1-CA1-CB1-CG1
6	C	301	GSH	C1-CA1-CB1-CG1
3	A	601	JAA	C04-C05-C09-C11
3	D	601	JAA	C04-C05-C09-C11
4	D	602	ILE	N-CA-CB-CG2
6	B	301	GSH	O12-C1-CA1-CB1
6	B	301	GSH	O11-C1-CA1-CB1
3	D	601	JAA	C05-C09-C11-C13
6	B	301	GSH	C3-CA3-N3-C2
3	D	601	JAA	C08-C05-C09-C11
3	A	601	JAA	C04-C10-C12-O03

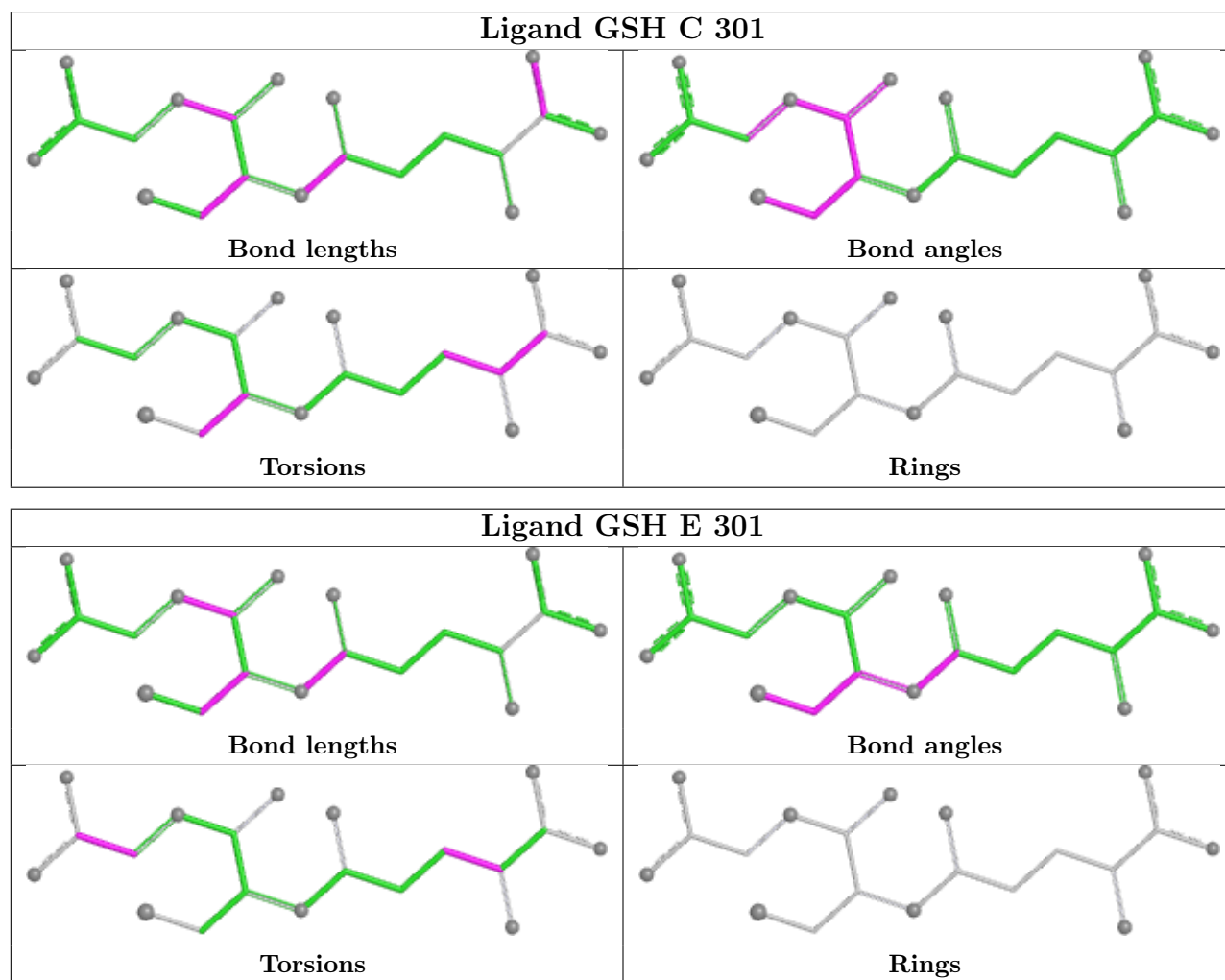
There are no ring outliers.

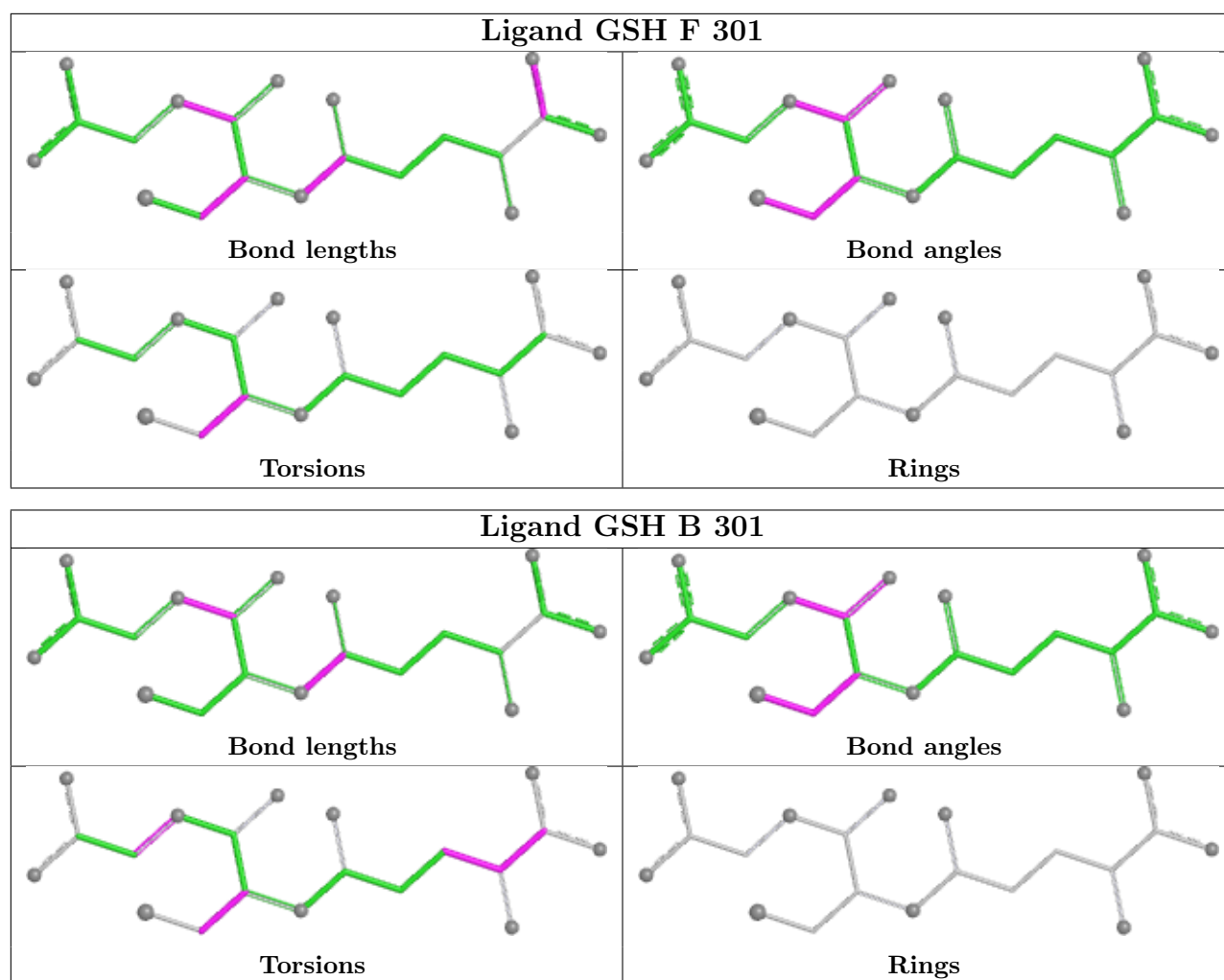
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301	GSH	1	0
4	D	602	ILE	1	0
6	E	301	GSH	2	0
3	A	601	JAA	1	0
3	D	601	JAA	1	0
6	B	301	GSH	3	0
4	A	602	ILE	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	569/575 (98%)	0.81	49 (8%)	16 16	2, 5, 9, 13	0
1	D	569/575 (98%)	0.55	11 (1%)	66 70	2, 4, 7, 13	0
2	B	214/223 (95%)	0.45	7 (3%)	49 53	2, 3, 6, 11	0
2	C	214/223 (95%)	0.46	5 (2%)	61 64	2, 3, 5, 9	0
2	E	214/223 (95%)	0.67	14 (6%)	25 27	2, 5, 8, 13	0
2	F	214/223 (95%)	0.58	9 (4%)	40 44	2, 4, 9, 22	0
All	All	1994/2042 (97%)	0.62	95 (4%)	35 39	2, 4, 8, 22	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	10.5
1	A	247	ASP	5.7
1	A	213	ARG	5.3
2	E	98	TRP	5.3
2	E	150	PHE	5.3
1	A	288	TYR	5.1
2	E	152	TYR	5.0
1	A	210	ILE	5.0
1	A	151	SER	4.9
2	C	212	TYR	4.5
1	A	295	PHE	4.2
1	A	143	LYS	4.2
1	A	209	GLY	4.2
1	A	426	ASN	3.9
2	E	217	LEU	3.9
2	C	157	LEU	3.7
2	C	32	TYR	3.7
2	F	86	PRO	3.6
2	C	209	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	234	PHE	3.5
2	B	24	ARG	3.3
1	A	305	MET	3.3
2	F	177	SER	3.3
1	D	125	PHE	3.2
2	B	185	TRP	3.2
2	E	95	ALA	3.1
1	A	554	SER	3.1
1	A	505	GLY	3.0
2	F	175	ILE	3.0
1	A	559	LEU	2.9
2	B	139	LEU	2.9
2	E	11	TRP	2.8
1	A	409	VAL	2.8
2	B	101	PHE	2.8
2	F	30	PHE	2.8
1	A	155	ILE	2.8
1	A	273	LEU	2.7
1	A	111	ILE	2.7
1	A	103	THR	2.7
1	D	50	LEU	2.7
1	A	287	TRP	2.6
1	A	211	LEU	2.6
2	E	97	PHE	2.6
1	A	392	ILE	2.6
1	A	517	ALA	2.5
1	D	439	ARG	2.5
1	A	504	ALA	2.5
1	A	222	VAL	2.5
1	A	278	ARG	2.4
1	D	568	SER	2.4
1	A	220	PHE	2.4
1	D	433	ILE	2.4
2	E	186	ALA	2.4
1	A	382	VAL	2.4
1	A	468	VAL	2.4
2	E	86	PRO	2.4
1	A	196	PRO	2.3
1	D	370	GLY	2.3
1	A	494	CYS	2.3
1	A	431	ILE	2.3
1	A	502	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	6	ILE	2.3
1	A	370	GLY	2.3
2	E	142	LYS	2.3
1	A	283	SER	2.3
1	D	113	PHE	2.2
2	F	178	GLU	2.2
1	A	285	SER	2.2
1	D	499	ARG	2.2
1	A	128	ALA	2.2
2	B	173	PHE	2.2
1	A	562	LEU	2.2
2	C	109	ALA	2.2
1	A	302	TYR	2.1
1	A	238	TRP	2.1
2	B	140	GLY	2.1
2	F	184	ALA	2.1
1	A	154	TYR	2.1
1	A	501	PHE	2.1
2	E	155	ILE	2.1
1	A	407	VAL	2.1
1	D	37	LEU	2.1
2	E	99	ALA	2.1
2	F	95	ALA	2.1
1	A	84	ASP	2.1
1	A	231	PHE	2.0
1	A	361	PHE	2.0
1	D	295	PHE	2.0
2	E	101	PHE	2.0
2	F	10	TYR	2.0
1	A	379	LEU	2.0
2	B	162	SER	2.0
2	F	128	PHE	2.0
1	A	475	TYR	2.0
1	D	523	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

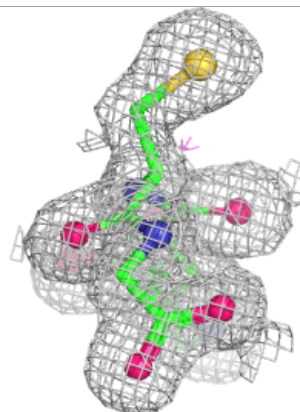
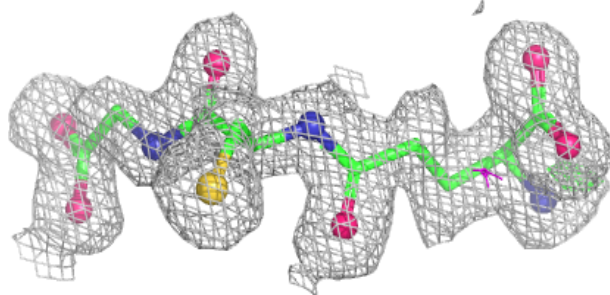
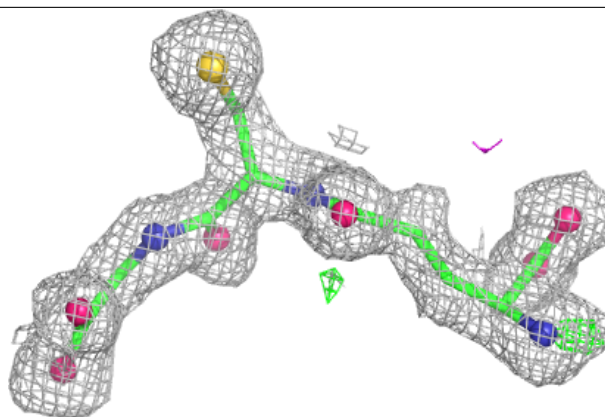
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ILE	D	602	9/9	0.86	0.10	2,2,4,6	0
3	JAA	D	601	15/15	0.87	0.13	2,4,7,9	0
5	MG	A	603	1/1	0.90	0.07	10,10,10,10	0
3	JAA	A	601	15/15	0.92	0.10	2,2,6,7	0
4	ILE	A	602	9/9	0.93	0.09	2,2,4,5	0
6	GSH	C	301	20/20	0.96	0.07	2,2,4,8	0
6	GSH	B	301	20/20	0.97	0.06	2,2,3,5	0
5	MG	D	603	1/1	0.97	0.08	9,9,9,9	0
6	GSH	E	301	20/20	0.97	0.06	2,2,6,9	0
6	GSH	F	301	20/20	0.97	0.06	2,2,2,3	0
5	MG	D	604	1/1	0.98	0.04	10,10,10,10	0
5	MG	D	605	1/1	0.99	0.03	9,9,9,9	0

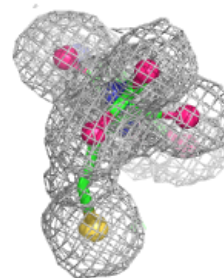
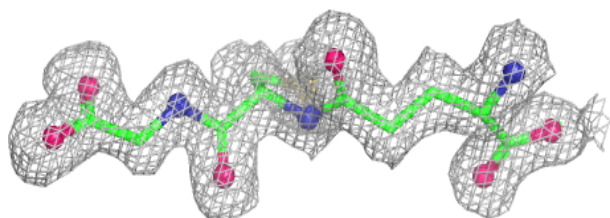
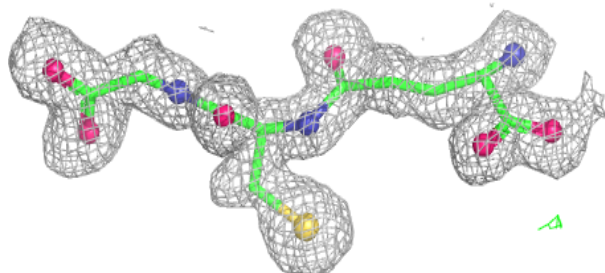
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GSH C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

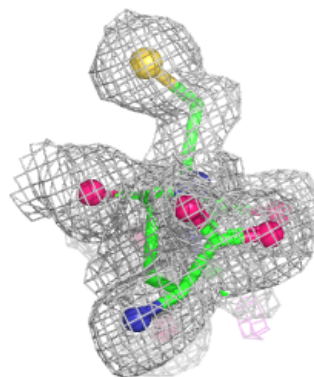
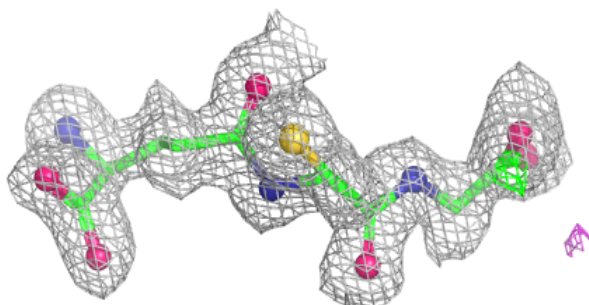
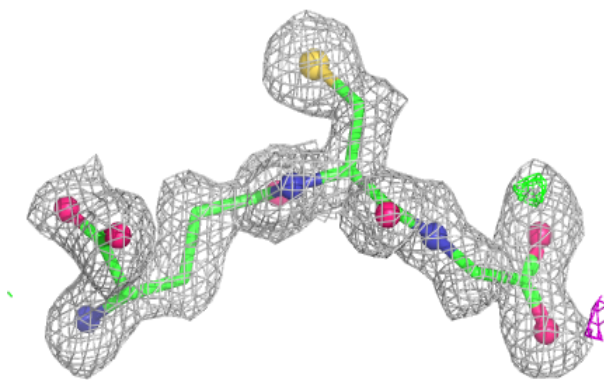
**Electron density around GSH B 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

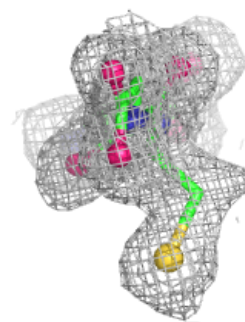
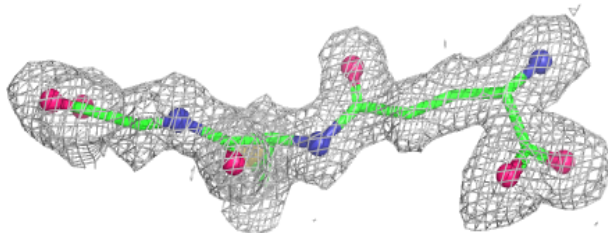
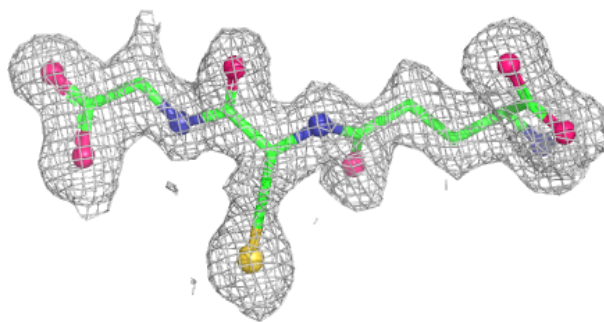


Electron density around GSH E 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GSH F 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.