



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:04 AM UTC

PDB ID : 5ECP / pdb_00005ecp
Title : Crystal Structure of FIN219-FIP1 complex with JA, MET and ATP
Authors : Chen, C.Y.; Cheng, Y.S.
Deposited on : 2015-10-20
Resolution : 2.25 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:

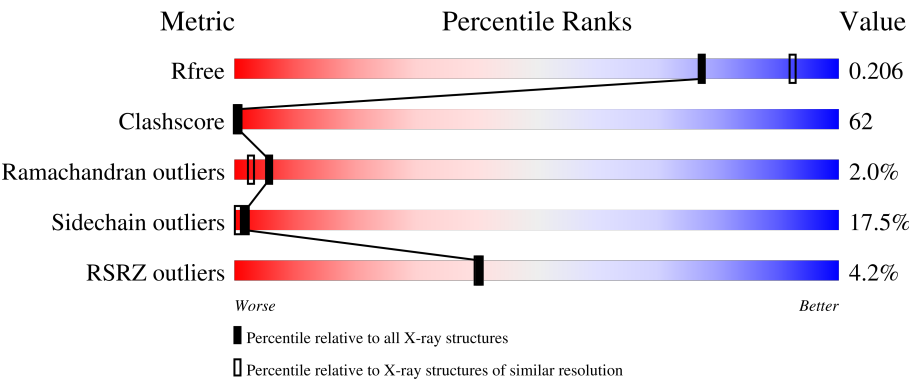
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.25 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.



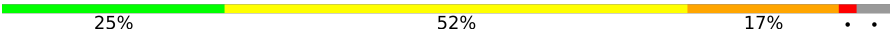
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	6% 23%58%16% ..
1	D	575	5% 21%59%17% ..
2	B	223	4% 35%55%5% ..
2	C	223	% 29%57%10% .
2	E	223	4% 32%54%9% .

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Mol	Chain	Length	Quality of chain
2	F	223	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (25%), yellow (52%), and orange (17%). The segments are labeled with their respective percentages. The bar ends with a small red segment and two dots.

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ATP	A	603	-	X	X	-
5	ATP	D	603	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17707 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:

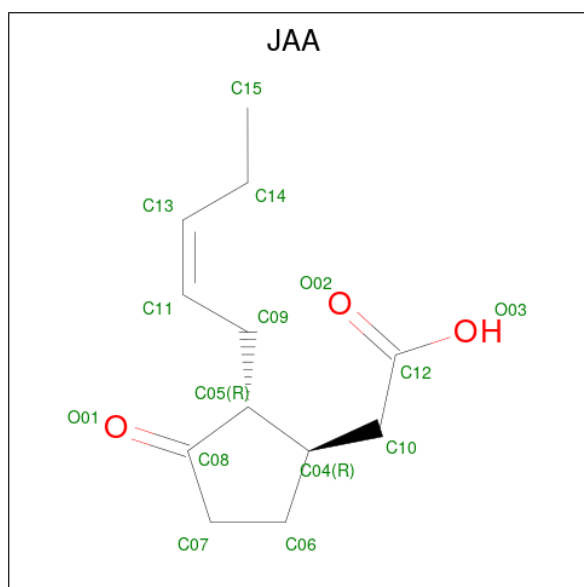
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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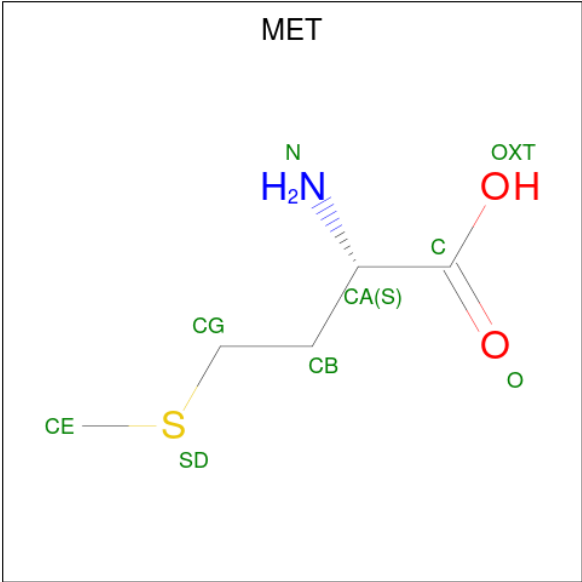
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9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



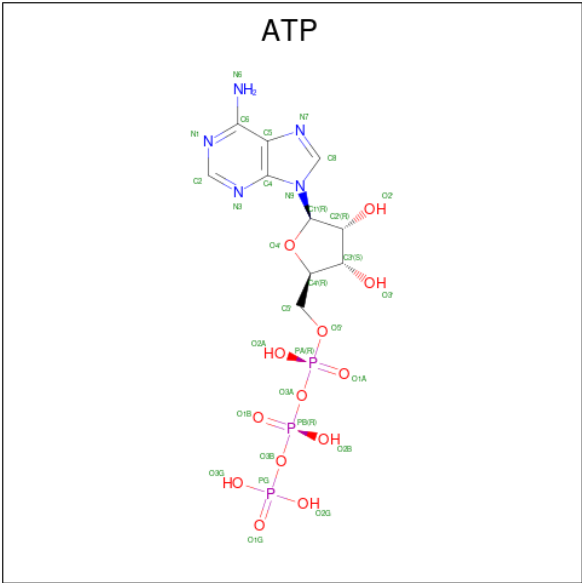
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



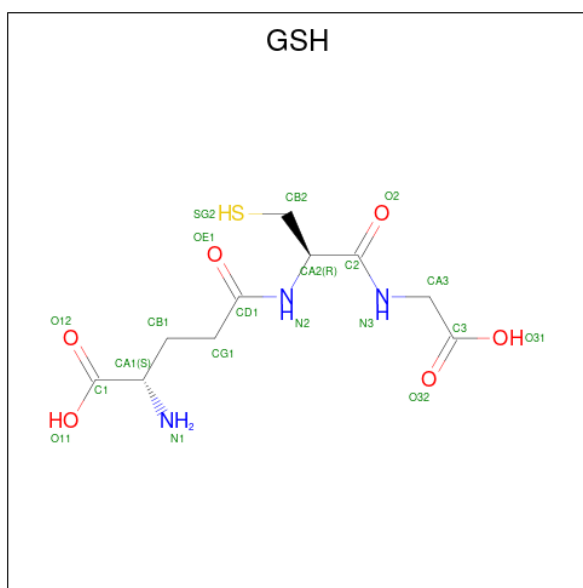
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
4	D	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

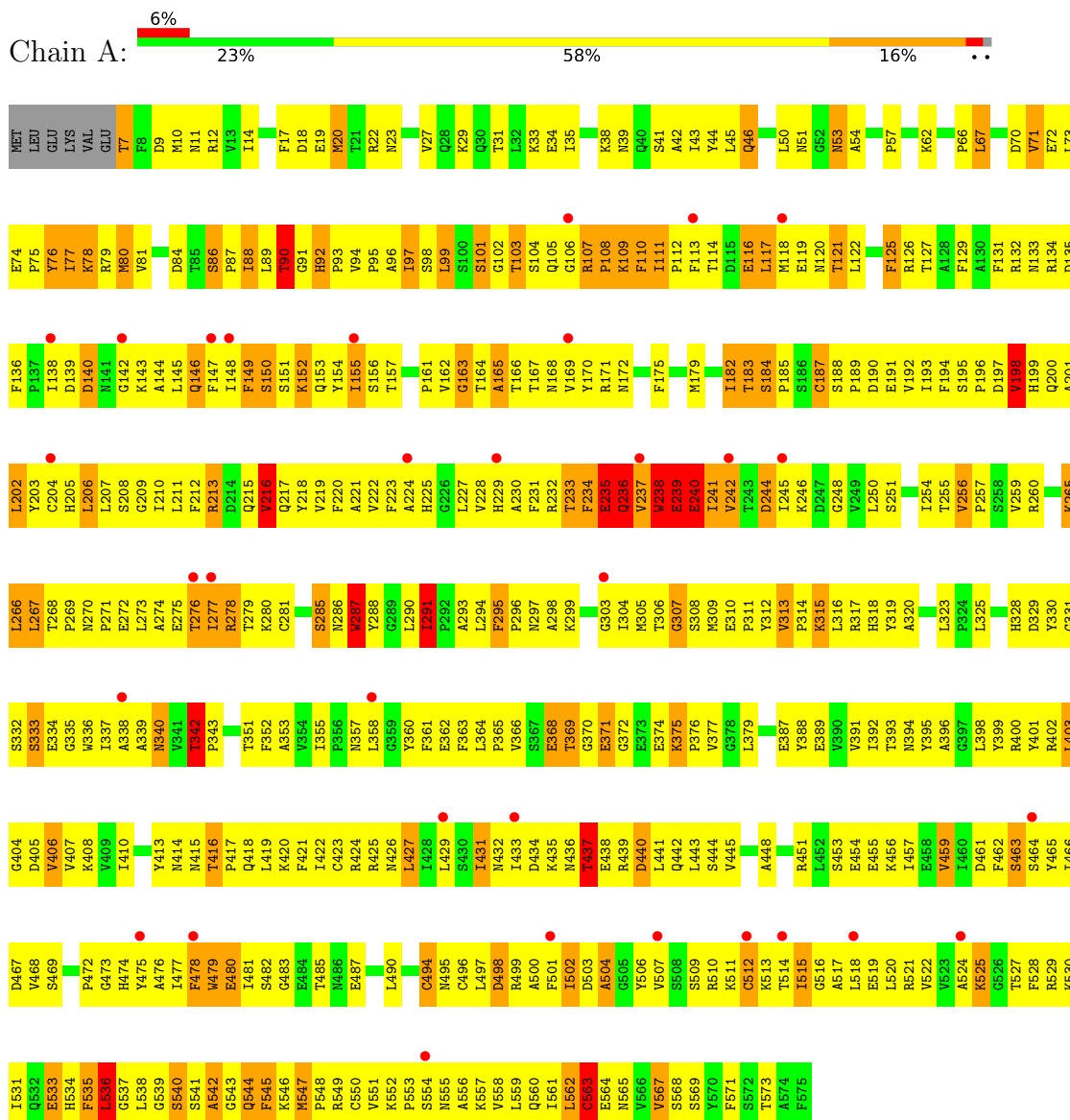
- Molecule 6 is GLUTATHIONE (CCD ID: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



3 Residue-property plots

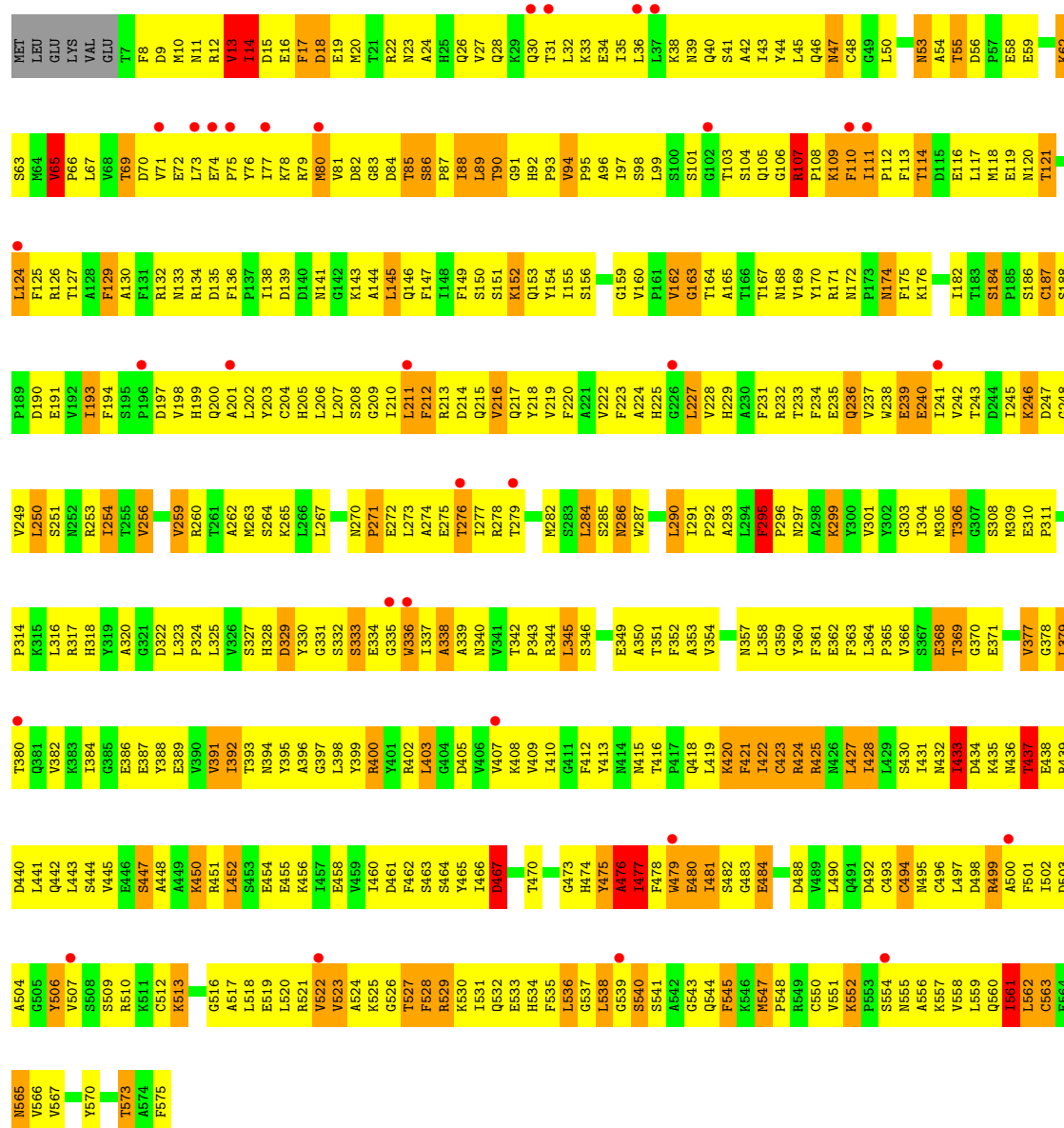
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

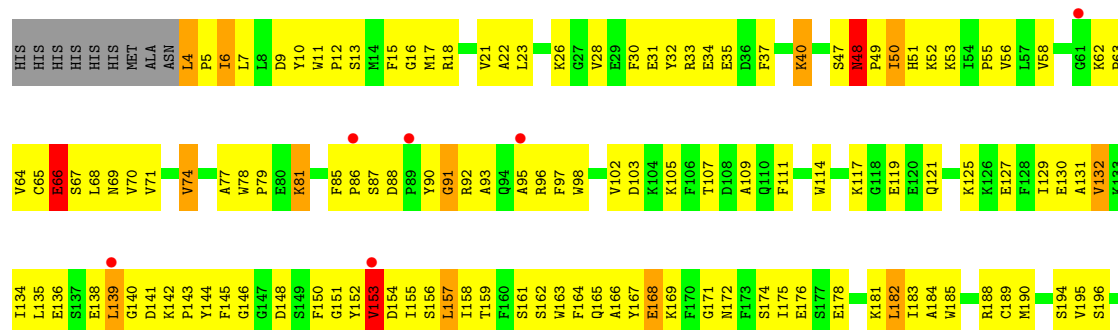


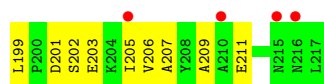
- Molecule 1: Jasmonic acid-amido synthetase JAR1



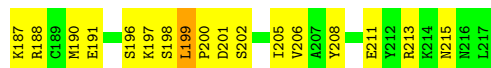
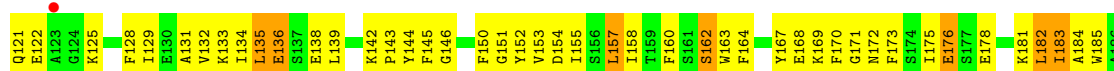
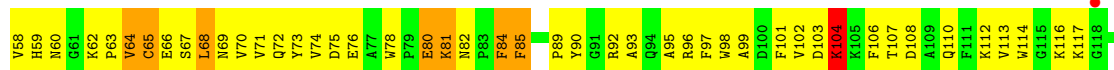
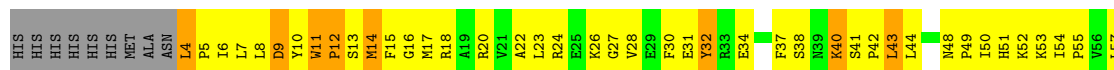


• Molecule 2: Glutathione S-transferase U20

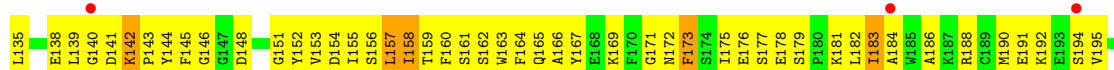
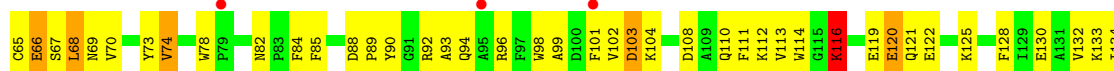
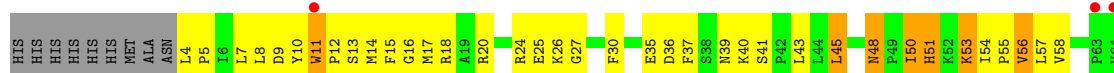




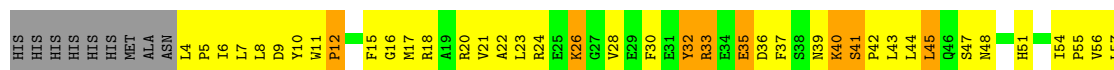
• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20



M190	E191	K192	E193	S194	V195	S196	K197	S198	L199	P200	D201	S202	E203	R204	I205	V206	A207	Y208	A209	A210	E211	Y212	R213	K214	W215	R216	L217
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.71Å 53.70Å 192.03Å 89.96° 90.16° 113.24°	Depositor
Resolution (Å)	23.35 – 2.25 23.35 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.5 (23.35-2.25) 95.4 (23.35-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.208 0.184 , 0.206	Depositor DCC
R_{free} test set	2254 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 197.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l 0.076 for -k,-h,-l 0.076 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	17707	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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 27.70 % 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 2.1005e-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: ATP, JAA, GSH

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	1/4581 (0.0%)	1.22	39/6219 (0.6%)
1	D	0.84	0/4581	1.19	38/6219 (0.6%)
2	B	0.83	1/1799 (0.1%)	1.06	4/2428 (0.2%)
2	C	0.96	0/1799	1.09	4/2428 (0.2%)
2	E	0.85	0/1799	1.11	8/2428 (0.3%)
2	F	1.06	2/1799 (0.1%)	1.27	11/2428 (0.5%)
All	All	0.88	4/16358 (0.0%)	1.18	104/22150 (0.5%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	VAL	CA-CB	5.62	1.61	1.54
2	F	134	ILE	CA-CB	5.23	1.60	1.54
2	F	163	TRP	CA-C	-5.03	1.46	1.52
1	A	216	VAL	CA-CB	5.01	1.59	1.54

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	PHE	CA-C-N	12.35	135.28	119.84
1	A	295	PHE	C-N-CA	12.35	135.28	119.84
2	E	11	TRP	CA-C-N	-9.95	109.00	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	11	TRP	C-N-CA	-9.95	109.00	121.04
1	D	295	PHE	CA-C-N	9.46	129.69	119.28
1	D	295	PHE	C-N-CA	9.46	129.69	119.28
1	D	86	SER	CA-C-N	9.26	131.42	119.84
1	D	86	SER	C-N-CA	9.26	131.42	119.84
1	D	422	ILE	N-CA-C	-9.21	102.12	111.88
2	F	145	PHE	N-CA-C	9.01	120.72	111.07
2	F	179	SER	CA-C-N	8.71	130.72	119.84
2	F	179	SER	C-N-CA	8.71	130.72	119.84
1	A	163	GLY	N-CA-C	8.55	127.03	111.03
2	F	178	GLU	N-CA-C	-8.45	102.42	112.89
1	D	163	GLY	N-CA-C	8.32	123.35	110.96
2	C	199	LEU	CA-C-N	8.11	128.59	119.92
2	C	199	LEU	C-N-CA	8.11	128.59	119.92
1	A	233	THR	N-CA-C	-8.10	103.41	113.38
1	D	529	ARG	N-CA-C	-7.99	102.57	111.28
2	F	185	TRP	N-CA-C	-7.63	103.05	111.36
1	D	475	TYR	N-CA-C	7.43	121.61	109.72
1	A	372	GLY	N-CA-C	-7.36	102.32	112.18
1	D	17	PHE	N-CA-C	-7.34	103.27	111.71
1	D	506	TYR	N-CA-C	-7.29	103.33	111.28
2	B	48	ASN	CA-C-N	7.19	127.19	119.28
2	B	48	ASN	C-N-CA	7.19	127.19	119.28
1	D	18	ASP	N-CA-C	-7.15	103.09	111.03
1	A	536	LEU	N-CA-C	-7.06	103.59	111.71
1	A	86	SER	CA-C-N	7.02	127.01	119.78
1	A	86	SER	C-N-CA	7.02	127.01	119.78
1	A	53	ASN	CB-CA-C	-6.85	108.66	116.54
1	A	86	SER	N-CA-C	6.74	119.38	110.08
1	D	476	ALA	CA-C-N	6.64	133.92	121.97
1	D	476	ALA	C-N-CA	6.64	133.92	121.97
2	F	173	PHE	N-CA-C	-6.57	99.67	108.74
1	A	291	ILE	CA-C-N	-6.49	113.00	119.56
1	A	291	ILE	C-N-CA	-6.49	113.00	119.56
1	D	65	VAL	CA-C-N	6.48	126.39	119.85
1	D	65	VAL	C-N-CA	6.48	126.39	119.85
2	F	132	VAL	N-CA-C	-6.48	103.22	112.35
1	D	256	VAL	N-CA-C	6.45	115.27	108.95
2	E	27	GLY	N-CA-C	-6.37	106.34	115.64
1	D	338	ALA	N-CA-C	6.31	118.77	109.24
1	A	107	ARG	CA-C-N	6.31	126.33	119.90
1	A	107	ARG	C-N-CA	6.31	126.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	SER	CA-C-N	6.25	126.28	119.90
1	D	184	SER	C-N-CA	6.25	126.28	119.90
1	D	475	TYR	CA-CB-CG	-6.18	102.78	113.90
1	D	433	ILE	N-CA-C	6.16	118.41	111.88
1	A	240	GLU	N-CA-C	-6.15	97.71	110.80
1	A	287	TRP	N-CA-C	-6.11	104.42	112.24
1	D	107	ARG	CA-C-N	6.05	127.40	119.84
1	D	107	ARG	C-N-CA	6.05	127.40	119.84
1	A	313	VAL	CB-CA-C	-6.04	106.09	114.00
2	E	88	ASP	CA-C-N	6.01	125.22	118.97
2	E	88	ASP	C-N-CA	6.01	125.22	118.97
2	C	11	TRP	CA-C-N	-5.91	112.45	119.84
2	C	11	TRP	C-N-CA	-5.91	112.45	119.84
1	A	563	CYS	N-CA-C	5.88	117.49	111.14
1	D	392	ILE	N-CA-C	5.80	116.51	107.28
2	E	82	ASN	CA-C-N	5.77	126.26	120.14
2	E	82	ASN	C-N-CA	5.77	126.26	120.14
1	A	198	VAL	CB-CA-C	-5.74	104.31	112.22
2	F	79	PRO	CA-C-O	-5.72	116.98	121.38
2	E	116	LYS	N-CA-C	5.71	118.37	109.52
1	D	477	ILE	N-CA-C	5.66	121.11	109.34
1	D	467	ASP	N-CA-C	-5.63	101.20	109.81
1	A	239	GLU	N-CA-C	-5.62	98.84	110.80
1	A	242	VAL	CB-CA-C	-5.58	104.84	111.81
1	D	567	VAL	N-CA-C	-5.53	104.14	111.05
1	A	71	VAL	N-CA-C	5.50	115.70	110.42
1	D	53	ASN	CB-CA-C	-5.49	110.23	116.54
1	A	342	THR	CA-C-N	5.48	125.31	119.28
1	A	342	THR	C-N-CA	5.48	125.31	119.28
1	A	255	THR	CA-C-N	-5.48	118.00	123.04
1	A	255	THR	C-N-CA	-5.48	118.00	123.04
1	A	92	HIS	CA-C-N	5.48	126.69	119.84
1	A	92	HIS	C-N-CA	5.48	126.69	119.84
1	A	504	ALA	N-CA-C	5.42	117.62	111.11
2	B	91	GLY	N-CA-C	-5.36	106.30	112.73
2	B	71	VAL	N-CA-C	5.36	115.56	110.42
1	A	236	GLN	N-CA-C	5.35	122.20	110.80
1	A	97	ILE	N-CA-C	5.35	116.19	108.48
1	D	336	TRP	CA-C-N	-5.29	117.78	122.97
1	D	336	TRP	C-N-CA	-5.29	117.78	122.97
1	D	256	VAL	CA-C-N	5.28	124.73	119.24
1	D	256	VAL	C-N-CA	5.28	124.73	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	ASN	N-CA-C	-5.27	105.71	111.82
1	A	111	ILE	CA-C-N	5.24	126.39	119.84
1	A	111	ILE	C-N-CA	5.24	126.39	119.84
1	A	256	VAL	CA-C-N	5.24	124.69	119.24
1	A	256	VAL	C-N-CA	5.24	124.69	119.24
1	D	55	THR	CA-C-N	-5.23	117.03	122.89
1	D	55	THR	C-N-CA	-5.23	117.03	122.89
1	D	346	SER	CA-C-N	5.20	124.64	119.24
1	D	346	SER	C-N-CA	5.20	124.64	119.24
2	F	177	SER	N-CA-C	5.20	121.86	110.80
1	A	416	THR	CA-C-N	5.11	125.56	120.14
1	A	416	THR	C-N-CA	5.11	125.56	120.14
1	A	567	VAL	N-CA-C	-5.09	105.43	110.62
1	D	479	TRP	N-CA-C	5.08	117.69	109.06
2	F	35	GLU	N-CA-C	5.06	117.21	109.07
1	A	427	LEU	N-CA-C	5.04	116.51	108.79
2	F	132	VAL	CB-CA-C	5.02	118.72	111.65

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4479	0	4434	636	6
1	D	4479	0	4434	656	5
2	B	1748	0	1704	189	1
2	C	1748	0	1704	197	1
2	E	1748	0	1704	180	1
2	F	1748	0	1704	212	1
3	A	15	0	0	2	0
3	D	15	0	0	2	0
4	A	9	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	9	0	8	5	0
5	A	31	0	8	17	0
5	D	31	0	8	26	0
6	B	20	0	15	1	0
6	C	20	0	15	0	0
6	E	20	0	15	3	0
6	F	20	0	15	0	0
7	A	357	0	0	77	7
7	B	193	0	0	29	2
7	C	214	0	0	30	1
7	D	403	0	0	74	4
7	E	201	0	0	28	1
7	F	199	0	0	34	3
All	All	17707	0	15776	1980	22

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 62.

All (1980) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HG21	1:A:175:PHE:CE1	1.69	1.27
1:A:121:THR:CG2	1:A:175:PHE:HE1	1.56	1.18
1:A:120:ASN:HD21	1:A:358:LEU:HD22	1.17	1.10
1:A:121:THR:HG21	1:A:175:PHE:HE1	0.93	1.05
1:D:334:GLU:O	1:D:394:ASN:ND2	1.93	1.02
1:D:150:SER:HB2	1:D:170:TYR:HD2	1.19	1.02
1:A:233:THR:HA	1:A:236:GLN:HB2	1.38	1.01
2:C:201:ASP:OD2	1:D:456:LYS:NZ	1.92	1.01
1:A:547:MET:SD	7:A:966:HOH:O	2.17	1.01
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.25	1.01
1:D:15:ASP:OD2	7:D:702:HOH:O	1.79	1.00
1:D:480:GLU:OE2	7:D:701:HOH:O	1.79	0.99
1:D:58:GLU:OE2	1:D:62:LYS:NZ	1.97	0.98
1:A:132:ARG:HA	1:A:343:PRO:HG3	1.46	0.97
1:A:152:LYS:HE2	1:A:565:ASN:HB2	1.47	0.96
1:A:169:VAL:HB	5:A:603:ATP:O3'	1.64	0.96
1:A:232:ARG:HA	1:A:235:GLU:HG3	1.46	0.96
1:D:235:GLU:OE2	7:D:703:HOH:O	1.83	0.95
1:A:477:ILE:HG12	1:A:518:LEU:HD11	1.47	0.95
2:C:17:MET:HE2	2:C:200:PRO:HD2	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASN:ND2	1:A:543:GLY:O	2.01	0.94
1:D:199:HIS:HB3	1:D:525:LYS:H	1.32	0.93
1:D:465:TYR:H	1:D:476:ALA:HA	1.32	0.93
1:D:126:ARG:HA	1:D:182:ILE:HG21	1.51	0.93
1:A:199:HIS:HB3	1:A:525:LYS:H	1.33	0.93
1:D:20:MET:SD	1:D:357:ASN:ND2	2.42	0.93
1:A:213:ARG:NH1	7:A:704:HOH:O	1.97	0.93
1:D:143:LYS:HD3	1:D:212:PHE:HB2	1.48	0.93
1:A:439:ARG:NH1	7:A:705:HOH:O	2.02	0.92
1:D:150:SER:HB2	1:D:170:TYR:CD2	2.05	0.92
1:D:432:ASN:ND2	1:D:434:ASP:OD1	2.01	0.92
2:F:139:LEU:HB3	2:F:181:LYS:HD2	1.51	0.92
2:F:139:LEU:HD13	2:F:181:LYS:HB3	1.50	0.92
2:B:18:ARG:HD2	2:B:156:SER:HA	1.52	0.91
1:D:135:ASP:OD2	7:D:704:HOH:O	1.87	0.91
2:F:26:LYS:NZ	2:F:82:ASN:O	2.04	0.91
1:A:99:LEU:HB3	1:A:557:LYS:HB3	1.51	0.91
1:A:152:LYS:HA	1:A:564:GLU:HB3	1.52	0.90
1:D:477:ILE:HD11	1:D:520:LEU:HA	1.53	0.90
2:B:88:ASP:OD2	2:B:91:GLY:N	2.04	0.90
1:A:199:HIS:H	1:A:524:ALA:HB1	1.35	0.90
2:B:165:GLN:NE2	7:B:403:HOH:O	2.04	0.90
1:D:432:ASN:HD22	1:D:434:ASP:H	1.19	0.89
2:C:80:GLU:OE2	7:C:401:HOH:O	1.91	0.89
1:A:332:SER:HB2	1:A:538:LEU:HA	1.53	0.89
1:A:92:HIS:CE1	2:B:139:LEU:HB3	2.08	0.88
1:A:228:VAL:O	1:A:232:ARG:N	2.07	0.88
2:B:166:ALA:HB2	2:B:206:VAL:HG12	1.56	0.88
1:D:87:PRO:HB3	1:D:92:HIS:HA	1.54	0.88
2:E:10:TYR:O	2:E:20:ARG:NH2	2.06	0.88
1:D:557:LYS:NZ	5:D:603:ATP:O2G	2.08	0.87
2:E:122:GLU:HA	2:E:125:LYS:HD2	1.55	0.87
1:D:475:TYR:OH	7:D:705:HOH:O	1.89	0.87
1:D:56:ASP:HB2	1:D:59:GLU:HB2	1.54	0.87
1:A:451:ARG:NH1	1:A:454:GLU:OE1	2.07	0.87
2:B:145:PHE:N	2:B:154:ASP:OD2	2.08	0.86
2:C:135:LEU:HD22	2:C:182:LEU:HD12	1.58	0.86
1:A:231:PHE:HA	1:A:234:PHE:HB2	1.57	0.86
1:D:87:PRO:HD2	2:E:188:ARG:HB2	1.55	0.86
1:A:442:GLN:NE2	7:A:710:HOH:O	2.07	0.86
1:D:9:ASP:HB3	1:D:12:ARG:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:SER:O	7:E:401:HOH:O	1.94	0.85
1:A:556:ALA:O	7:A:702:HOH:O	1.94	0.85
1:D:387:GLU:HG2	1:D:408:LYS:HB2	1.57	0.85
1:A:98:SER:HB3	1:A:111:ILE:HB	1.55	0.85
1:D:333:SER:OG	5:D:603:ATP:O1A	1.95	0.85
1:A:162:VAL:HB	1:A:556:ALA:HB1	1.56	0.85
1:A:467:ASP:OD2	7:A:703:HOH:O	1.95	0.85
2:B:66:GLU:OE2	2:B:69:ASN:ND2	2.10	0.85
1:D:245:ILE:O	7:D:706:HOH:O	1.94	0.85
1:D:464:SER:HA	1:D:477:ILE:H	1.41	0.85
1:A:457:ILE:HD13	1:A:483:GLY:HA3	1.58	0.84
1:A:241:ILE:O	1:A:245:ILE:HG12	1.77	0.84
4:D:602:MET:HA	5:D:603:ATP:H2	1.41	0.84
1:D:434:ASP:OD1	1:D:435:LYS:HD2	1.78	0.84
1:A:285:SER:O	7:A:701:HOH:O	1.93	0.83
1:A:42:ALA:HA	2:B:143:PRO:HG2	1.59	0.83
1:A:90:THR:OG1	1:A:91:GLY:N	2.08	0.83
2:C:188:ARG:NH1	1:D:499:ARG:O	2.11	0.83
2:E:155:ILE:O	7:E:403:HOH:O	1.97	0.83
1:D:477:ILE:HD12	1:D:518:LEU:HD21	1.59	0.82
2:E:89:PRO:O	7:E:402:HOH:O	1.96	0.82
2:E:145:PHE:N	2:E:154:ASP:OD2	2.12	0.82
1:A:482:SER:O	1:A:525:LYS:NZ	2.12	0.82
1:D:330:TYR:CZ	1:D:338:ALA:HB3	2.15	0.82
1:D:528:PHE:HB3	1:D:531:ILE:HD12	1.60	0.81
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.62	0.81
1:D:169:VAL:HB	5:D:603:ATP:H3'	1.63	0.81
1:D:284:LEU:HD21	1:D:290:LEU:HD12	1.61	0.81
1:A:167:THR:OG1	1:A:560:GLN:OE1	1.99	0.81
2:B:37:PHE:O	7:B:401:HOH:O	1.99	0.81
1:A:92:HIS:HE1	2:B:139:LEU:HB3	1.45	0.80
1:A:102:GLY:N	1:A:546:LYS:O	2.11	0.80
1:D:551:VAL:HG13	1:D:555:ASN:HB2	1.63	0.80
2:B:152:TYR:CD1	2:B:153:VAL:HG12	2.16	0.80
1:D:171:ARG:NH2	7:D:721:HOH:O	2.12	0.80
1:D:199:HIS:H	1:D:524:ALA:HB1	1.44	0.80
1:D:22:ARG:HA	1:D:415:ASN:HB2	1.63	0.80
2:B:142:LYS:HD3	2:B:145:PHE:HA	1.62	0.80
1:A:164:THR:OG1	1:A:557:LYS:O	2.00	0.80
1:D:236:GLN:OE1	1:D:482:SER:HB2	1.82	0.80
2:E:73:TYR:OH	7:E:404:HOH:O	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:THR:HG1	1:A:413:TYR:HH	1.01	0.79
1:A:231:PHE:HB3	1:A:290:LEU:HD22	1.64	0.79
2:C:70:VAL:HA	2:C:73:TYR:CD2	2.16	0.79
4:D:602:MET:HA	5:D:603:ATP:C2	2.18	0.79
1:D:87:PRO:HD3	1:D:93:PRO:HD3	1.65	0.79
2:B:178:GLU:OE2	7:B:402:HOH:O	2.01	0.79
1:D:143:LYS:HE2	1:D:216:VAL:HG13	1.64	0.79
1:D:143:LYS:HG2	1:D:215:GLN:HB2	1.65	0.79
1:A:120:ASN:ND2	1:A:358:LEU:HD22	1.94	0.79
1:A:113:PHE:HB2	1:A:117:LEU:HD11	1.65	0.78
1:A:199:HIS:HE1	1:A:567:VAL:HG11	1.46	0.78
1:D:496:CYS:O	1:D:500:ALA:N	2.15	0.78
2:F:69:ASN:HA	2:F:72:GLN:HG3	1.65	0.78
1:D:425:ARG:HB2	1:D:427:LEU:HB2	1.65	0.78
2:F:136:GLU:HG3	2:F:180:PRO:HD2	1.63	0.78
2:F:75:ASP:OD1	7:F:401:HOH:O	2.00	0.78
1:A:512:CYS:SG	1:A:514:THR:OG1	2.40	0.78
2:C:8:LEU:HD21	2:C:43:LEU:HD11	1.66	0.78
2:F:161:SER:HA	2:F:164:PHE:CD2	2.19	0.78
1:A:233:THR:HG22	1:A:237:VAL:HG22	1.64	0.78
1:A:473:GLY:O	1:A:516:GLY:N	2.14	0.78
1:D:540:SER:O	7:D:709:HOH:O	2.02	0.78
2:F:26:LYS:HD3	2:F:78:TRP:HB2	1.63	0.77
1:D:480:GLU:HB2	1:D:528:PHE:CZ	2.19	0.77
2:B:6:ILE:HG12	2:B:31:GLU:OE2	1.85	0.77
1:D:361:PHE:N	7:D:717:HOH:O	2.13	0.77
2:F:169:LYS:HD2	2:F:206:VAL:HG13	1.66	0.77
2:F:184:ALA:HA	2:F:187:LYS:HB2	1.65	0.77
1:D:451:ARG:NH2	7:D:730:HOH:O	2.18	0.77
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.65	0.77
1:D:287:TRP:CE3	1:D:290:LEU:HD13	2.19	0.77
1:D:551:VAL:HG11	1:D:559:LEU:HD13	1.66	0.77
1:D:345:LEU:HD13	1:D:350:ALA:HA	1.65	0.77
2:C:103:ASP:O	2:C:107:THR:OG1	2.02	0.77
1:D:141:ASN:OD1	7:D:707:HOH:O	2.01	0.77
2:E:96:ARG:HH21	2:F:73:TYR:HE1	1.33	0.76
1:A:79:ARG:HB2	1:A:88:ILE:HD11	1.64	0.76
2:B:178:GLU:N	7:B:409:HOH:O	2.16	0.76
1:D:39:ASN:ND2	2:E:141:ASP:O	2.18	0.76
2:E:35:GLU:OE2	7:E:405:HOH:O	2.03	0.76
1:A:143:LYS:HB2	1:A:185:PRO:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LYS:NZ	7:A:728:HOH:O	2.17	0.76
1:A:418:GLN:NE2	7:A:733:HOH:O	2.18	0.76
1:A:560:GLN:NE2	7:A:738:HOH:O	2.19	0.76
2:E:41:SER:OG	7:E:405:HOH:O	2.02	0.76
1:A:121:THR:CG2	1:A:175:PHE:CE1	2.48	0.76
1:D:108:PRO:HG2	1:D:552:LYS:H	1.50	0.76
1:D:154:TYR:HD1	1:D:560:GLN:HA	1.50	0.76
1:D:120:ASN:HB3	1:D:358:LEU:HD23	1.68	0.76
1:D:437:THR:HB	1:D:439:ARG:HH21	1.51	0.76
2:F:184:ALA:O	2:F:188:ARG:N	2.19	0.76
1:A:511:LYS:O	7:A:708:HOH:O	2.05	0.75
1:D:108:PRO:HD2	1:D:552:LYS:HE3	1.68	0.75
1:D:292:PRO:HB3	1:D:323:LEU:HD13	1.67	0.75
2:E:50:ILE:HD12	2:E:51:HIS:H	1.50	0.75
2:E:162:SER:HB3	2:E:199:LEU:HD23	1.66	0.75
1:A:405:ASP:HB2	1:A:541:SER:HB3	1.68	0.75
1:D:331:GLY:N	1:D:537:GLY:O	2.19	0.75
2:F:69:ASN:OD1	7:F:402:HOH:O	2.03	0.75
1:A:465:TYR:HB3	1:A:476:ALA:HB3	1.68	0.75
2:E:192:LYS:HZ1	2:E:194:SER:HB3	1.49	0.75
2:B:16:GLY:HA2	2:B:55:PRO:HG3	1.69	0.75
2:C:15:PHE:HB3	2:C:67:SER:HB3	1.69	0.75
2:C:26:LYS:HD3	2:C:74:VAL:HG12	1.69	0.75
2:C:196:SER:O	7:C:402:HOH:O	2.04	0.75
1:D:497:LEU:O	7:D:710:HOH:O	2.04	0.75
7:E:402:HOH:O	2:F:76:GLU:OE1	2.03	0.75
2:E:166:ALA:HB2	2:E:206:VAL:HG12	1.68	0.75
2:F:165:GLN:HA	2:F:168:GLU:HG3	1.68	0.74
1:A:190:ASP:O	1:A:194:PHE:N	2.19	0.74
1:A:287:TRP:HB3	1:A:290:LEU:HD11	1.68	0.74
1:A:433:ILE:O	1:A:552:LYS:NZ	2.20	0.74
1:D:322:ASP:OD2	7:D:711:HOH:O	2.05	0.74
2:F:9:ASP:HB2	2:F:20:ARG:HH21	1.52	0.74
1:A:234:PHE:CZ	1:A:294:LEU:HD21	2.22	0.74
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.52	0.74
2:F:176:GLU:HB2	2:F:183:ILE:HB	1.69	0.74
1:D:154:TYR:CD1	1:D:560:GLN:HA	2.21	0.74
1:D:464:SER:HB3	1:D:476:ALA:HB1	1.68	0.74
2:E:94:GLN:NE2	7:E:407:HOH:O	2.14	0.74
2:F:68:LEU:HD23	2:F:103:ASP:OD2	1.87	0.74
1:A:67:LEU:O	7:A:709:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HB3	5:A:603:ATP:O2B	1.87	0.73
1:A:291:ILE:HG13	1:A:320:ALA:HA	1.70	0.73
2:B:130:GLU:OE2	7:B:404:HOH:O	2.05	0.73
1:A:234:PHE:HZ	1:A:294:LEU:HD21	1.53	0.73
1:A:355:ILE:O	7:A:711:HOH:O	2.07	0.73
1:D:229:HIS:NE2	7:D:701:HOH:O	2.00	0.73
1:D:239:GLU:OE2	1:D:278:ARG:NH2	2.21	0.73
2:B:7:LEU:O	7:B:405:HOH:O	2.06	0.73
2:F:57:LEU:N	7:F:405:HOH:O	2.11	0.73
1:A:408:LYS:NZ	7:A:727:HOH:O	2.16	0.73
1:D:490:LEU:HD13	1:D:522:VAL:HG21	1.68	0.73
1:A:108:PRO:HB3	1:A:555:ASN:CG	2.14	0.73
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.71	0.73
2:C:108:ASP:OD2	7:C:405:HOH:O	2.06	0.72
2:E:92:ARG:HB2	7:E:402:HOH:O	1.88	0.72
1:D:223:PHE:CZ	1:D:536:LEU:HB3	2.24	0.72
1:D:330:TYR:OH	1:D:419:LEU:HB2	1.88	0.72
2:B:53:LYS:HD3	6:B:301:GSH:HB12	1.71	0.72
2:C:10:TYR:O	2:C:20:ARG:NH2	2.22	0.72
1:A:38:LYS:O	2:B:142:LYS:HB2	1.89	0.72
2:B:169:LYS:O	7:B:406:HOH:O	2.07	0.72
1:A:99:LEU:HB3	1:A:557:LYS:HE3	1.70	0.72
1:D:105:GLN:HA	1:D:430:SER:HB2	1.71	0.72
1:D:461:ASP:O	7:D:712:HOH:O	2.06	0.72
1:D:480:GLU:HB2	1:D:528:PHE:CE1	2.24	0.72
2:F:10:TYR:O	2:F:20:ARG:NH2	2.20	0.72
1:D:432:ASN:ND2	1:D:434:ASP:H	1.87	0.72
1:D:482:SER:HA	1:D:525:LYS:HD2	1.72	0.72
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.72	0.72
2:B:162:SER:O	2:B:165:GLN:NE2	2.19	0.72
1:D:73:LEU:HD22	1:D:89:LEU:HD22	1.70	0.72
1:A:93:PRO:HB2	2:B:181:LYS:HA	1.71	0.72
1:A:290:LEU:N	1:A:319:TYR:O	2.23	0.72
1:D:46:GLN:HB2	2:E:148:ASP:HB3	1.71	0.72
1:D:527:THR:HG23	1:D:561:ILE:HG21	1.70	0.72
2:B:172:ASN:ND2	7:B:413:HOH:O	2.22	0.72
2:B:190:MET:O	2:B:196:SER:OG	2.07	0.72
1:D:213:ARG:NH1	1:D:214:ASP:OD1	2.23	0.72
1:A:39:ASN:ND2	1:A:399:TYR:OH	2.19	0.71
1:A:316:LEU:O	1:A:320:ALA:N	2.22	0.71
2:C:162:SER:OG	7:C:406:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.25	0.71
2:F:135:LEU:HB3	2:F:182:LEU:HD11	1.72	0.71
1:D:99:LEU:HG	1:D:557:LYS:HB2	1.72	0.71
2:F:26:LYS:HE2	2:F:75:ASP:HA	1.72	0.71
2:F:92:ARG:NH2	7:F:415:HOH:O	2.21	0.71
1:A:219:VAL:HG21	1:A:231:PHE:CZ	2.25	0.71
1:A:405:ASP:HB3	1:A:426:ASN:HD22	1.56	0.71
1:A:519:GLU:CD	1:A:521:ARG:HE	1.98	0.71
1:A:304:ILE:HG13	1:A:328:HIS:HB3	1.71	0.71
1:A:509:SER:O	1:A:513:LYS:N	2.22	0.71
1:A:375:LYS:O	7:A:714:HOH:O	2.09	0.71
1:D:22:ARG:O	7:D:714:HOH:O	2.09	0.71
1:D:306:THR:HA	1:D:310:GLU:HG3	1.73	0.71
1:A:98:SER:O	7:A:713:HOH:O	2.08	0.71
1:D:330:TYR:HE1	1:D:352:PHE:HB2	1.56	0.71
1:A:432:ASN:ND2	1:A:434:ASP:OD2	2.17	0.71
1:D:231:PHE:HA	1:D:234:PHE:HD2	1.56	0.71
2:C:40:LYS:H	2:C:40:LYS:HZ3	1.35	0.70
2:C:117:LYS:HA	2:C:121:GLN:HB2	1.73	0.70
1:D:99:LEU:HD21	1:D:558:VAL:HG23	1.73	0.70
2:F:201:ASP:OD2	7:F:403:HOH:O	2.07	0.70
2:C:188:ARG:HB2	1:D:499:ARG:HH21	1.56	0.70
1:D:330:TYR:HD1	1:D:352:PHE:HD2	1.39	0.70
1:D:394:ASN:N	1:D:398:LEU:O	2.24	0.70
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.09	0.70
1:D:444:SER:HA	1:D:500:ALA:HB1	1.72	0.70
1:D:470:THR:HG21	1:D:474:HIS:HD1	1.54	0.70
1:A:162:VAL:O	7:A:702:HOH:O	2.09	0.70
1:A:199:HIS:N	1:A:524:ALA:HB1	2.07	0.70
1:A:239:GLU:O	1:A:241:ILE:N	2.24	0.70
1:D:87:PRO:O	2:E:188:ARG:NH1	2.25	0.70
1:D:519:GLU:O	7:D:708:HOH:O	2.10	0.70
2:E:9:ASP:OD1	2:E:10:TYR:N	2.23	0.70
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.27	0.70
1:A:87:PRO:HD3	1:A:93:PRO:HD3	1.74	0.70
1:A:136:PHE:HD1	1:A:299:LYS:HD2	1.56	0.70
1:A:210:ILE:HG22	1:A:294:LEU:HD13	1.74	0.70
1:A:521:ARG:HH11	1:A:562:LEU:HD11	1.56	0.70
1:D:212:PHE:HB3	1:D:215:GLN:HG3	1.71	0.70
1:D:27:VAL:HA	1:D:30:GLN:HB3	1.74	0.70
1:D:424:ARG:NH2	7:D:749:HOH:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:LYS:NZ	7:C:418:HOH:O	2.23	0.70
2:B:109:ALA:HB2	2:B:127:GLU:HG2	1.73	0.70
2:B:172:ASN:OD1	7:B:406:HOH:O	2.09	0.70
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.74	0.69
1:A:223:PHE:CZ	1:A:536:LEU:HB3	2.27	0.69
1:A:271:PRO:O	7:A:716:HOH:O	2.10	0.69
2:C:92:ARG:HB3	2:C:96:ARG:NH2	2.07	0.69
1:D:96:ALA:HA	1:D:162:VAL:HA	1.75	0.69
1:D:229:HIS:O	1:D:233:THR:OG1	2.06	0.69
1:D:272:GLU:OE1	7:D:716:HOH:O	2.10	0.69
1:D:364:LEU:HB3	1:D:389:GLU:HG3	1.74	0.69
1:D:498:ASP:OD1	1:D:518:LEU:HD22	1.92	0.69
1:A:540:SER:OG	1:A:541:SER:N	2.24	0.69
2:B:136:GLU:HG3	2:B:181:LYS:HD3	1.74	0.69
1:A:240:GLU:O	1:A:244:ASP:N	2.19	0.69
2:B:169:LYS:HZ2	2:B:206:VAL:HG11	1.58	0.69
1:D:85:THR:HB	2:E:184:ALA:HB1	1.73	0.69
2:F:40:LYS:NZ	7:F:420:HOH:O	2.26	0.69
2:F:88:ASP:O	7:F:404:HOH:O	2.10	0.69
2:E:26:LYS:HE2	2:E:78:TRP:HD1	1.57	0.69
1:A:290:LEU:HD13	1:A:319:TYR:CD1	2.28	0.69
2:E:132:VAL:HG13	2:E:182:LEU:HD13	1.74	0.69
1:A:29:LYS:NZ	7:A:732:HOH:O	2.17	0.69
1:A:213:ARG:HA	1:A:216:VAL:HG22	1.75	0.69
1:A:290:LEU:HD13	1:A:319:TYR:HD1	1.57	0.69
1:A:330:TYR:HE2	1:A:540:SER:H	1.40	0.69
1:A:46:GLN:HA	2:B:148:ASP:HB2	1.75	0.69
1:A:74:GLU:O	1:A:78:LYS:HG2	1.93	0.69
1:A:490:LEU:HD22	1:A:522:VAL:HG21	1.72	0.69
2:C:176:GLU:OE2	1:D:573:THR:OG1	2.07	0.69
1:D:470:THR:HG21	1:D:474:HIS:ND1	2.08	0.69
2:F:64:VAL:HG23	2:F:70:VAL:HG22	1.75	0.69
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.75	0.69
1:A:199:HIS:N	7:A:712:HOH:O	2.26	0.69
1:A:475:TYR:OH	1:A:515:ILE:HD12	1.91	0.69
1:A:534:HIS:CE1	1:A:557:LYS:HD2	2.28	0.69
1:D:89:LEU:HD12	1:D:90:THR:HG23	1.75	0.69
1:D:425:ARG:HD3	1:D:427:LEU:HD13	1.75	0.69
2:F:181:LYS:O	2:F:185:TRP:HB3	1.93	0.69
1:A:96:ALA:HB3	1:A:113:PHE:CE2	2.28	0.69
2:B:150:PHE:CE1	2:B:155:ILE:HG13	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LYS:HG2	7:A:720:HOH:O	1.92	0.68
1:A:149:PHE:CZ	1:A:152:LYS:HD2	2.29	0.68
1:A:219:VAL:HG21	1:A:231:PHE:HZ	1.58	0.68
1:D:59:GLU:OE2	7:D:715:HOH:O	2.10	0.68
1:A:108:PRO:HB2	1:A:554:SER:HB2	1.74	0.68
2:B:150:PHE:HE1	2:B:155:ILE:HG13	1.59	0.68
2:E:139:LEU:HG	2:E:142:LYS:HG3	1.76	0.68
1:A:149:PHE:HZ	1:A:152:LYS:HD2	1.59	0.68
1:D:147:PHE:O	1:D:529:ARG:NH2	2.25	0.68
1:D:305:MET:HA	7:D:756:HOH:O	1.92	0.68
1:D:225:HIS:O	1:D:229:HIS:N	2.23	0.68
1:D:461:ASP:HB3	1:D:528:PHE:CD1	2.27	0.68
2:F:201:ASP:OD1	7:F:406:HOH:O	2.11	0.68
1:A:232:ARG:CA	1:A:235:GLU:HG3	2.23	0.68
2:E:18:ARG:NH1	7:E:415:HOH:O	2.26	0.68
1:D:152:LYS:HD3	1:D:561:ILE:HA	1.75	0.68
2:C:24:ARG:HG3	2:C:30:PHE:HE1	1.57	0.68
2:F:135:LEU:HD13	2:F:182:LEU:HD21	1.76	0.68
1:A:163:GLY:HA3	1:A:168:ASN:HD21	1.59	0.68
1:A:223:PHE:CE1	1:A:304:ILE:HB	2.29	0.68
1:A:223:PHE:CE2	1:A:533:GLU:HA	2.28	0.68
1:D:28:GLN:OE1	7:D:717:HOH:O	2.10	0.68
2:F:15:PHE:HB3	2:F:67:SER:HB3	1.76	0.68
1:A:444:SER:HA	1:A:500:ALA:HB1	1.76	0.67
1:A:143:LYS:HD2	1:A:212:PHE:HB2	1.76	0.67
1:A:287:TRP:O	1:A:290:LEU:HD12	1.94	0.67
2:C:187:LYS:HD3	1:D:492:ASP:HB3	1.74	0.67
1:A:31:THR:HA	1:A:34:GLU:HG2	1.74	0.67
1:A:86:SER:HB2	2:B:188:ARG:NE	2.10	0.67
1:A:421:PHE:CE1	1:A:541:SER:HA	2.29	0.67
2:B:189:CYS:HB3	2:B:195:VAL:HG21	1.76	0.67
1:A:99:LEU:HD13	1:A:558:VAL:H	1.58	0.67
1:A:329:ASP:HB3	1:A:339:ALA:HA	1.75	0.67
2:F:188:ARG:HD3	2:F:191:GLU:OE2	1.95	0.67
1:A:179:MET:HA	1:A:182:ILE:HD11	1.77	0.67
1:A:525:LYS:O	7:A:718:HOH:O	2.12	0.67
2:E:139:LEU:HD23	2:E:142:LYS:HB2	1.75	0.67
1:A:238:TRP:CZ3	1:A:281:CYS:HB3	2.30	0.67
2:B:203:GLU:OE1	7:B:408:HOH:O	2.13	0.67
2:C:17:MET:SD	7:C:406:HOH:O	2.52	0.67
2:C:68:LEU:O	2:C:72:GLN:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:HG13	1:A:107:ARG:HH22	1.60	0.67
1:A:154:TYR:CD2	1:A:563:CYS:HB2	2.30	0.67
1:A:478:PHE:CZ	1:A:562:LEU:HD22	2.30	0.67
1:A:494:CYS:HA	1:A:497:LEU:HD12	1.76	0.67
2:C:171:GLY:N	7:C:407:HOH:O	2.13	0.67
1:D:149:PHE:HZ	1:D:202:LEU:HB2	1.59	0.67
1:A:235:GLU:OE1	7:A:719:HOH:O	2.13	0.67
2:C:110:GLN:HA	2:C:113:VAL:HG12	1.76	0.67
1:D:132:ARG:HA	1:D:343:PRO:HG2	1.77	0.67
5:D:603:ATP:N3	5:D:603:ATP:O2'	2.27	0.67
1:D:12:ARG:C	1:D:14:ILE:H	2.03	0.66
2:C:84:PHE:HB2	2:C:152:TYR:N	2.10	0.66
1:D:76:TYR:HB3	1:D:88:ILE:HG21	1.75	0.66
1:A:87:PRO:HD2	2:B:188:ARG:HB2	1.78	0.66
1:D:108:PRO:HG2	1:D:552:LYS:HB2	1.77	0.66
1:A:509:SER:HB3	1:A:515:ILE:HD11	1.75	0.66
1:A:514:THR:OG1	7:A:721:HOH:O	2.13	0.66
1:D:331:GLY:HA3	1:D:336:TRP:CE3	2.30	0.66
1:D:533:GLU:OE1	7:D:720:HOH:O	2.12	0.66
2:F:96:ARG:HD3	7:F:415:HOH:O	1.96	0.66
2:B:114:TRP:CD1	2:B:167:TYR:HE1	2.13	0.66
1:D:169:VAL:HB	5:D:603:ATP:C3'	2.24	0.66
2:B:161:SER:HA	2:B:164:PHE:CD2	2.30	0.66
1:D:331:GLY:O	5:D:603:ATP:N6	2.29	0.66
2:E:145:PHE:H	2:E:154:ASP:CG	2.02	0.66
1:D:407:VAL:HG21	1:D:419:LEU:HB3	1.78	0.66
1:A:391:VAL:HG22	1:A:402:ARG:HG2	1.78	0.66
2:F:85:PHE:CD2	2:F:92:ARG:HG2	2.31	0.66
1:D:121:THR:CG2	1:D:336:TRP:CZ2	2.79	0.66
1:A:212:PHE:O	7:A:720:HOH:O	2.13	0.65
2:E:182:LEU:O	7:E:406:HOH:O	2.13	0.65
1:A:96:ALA:HB3	1:A:113:PHE:HE2	1.60	0.65
1:A:19:GLU:O	1:A:23:ASN:ND2	2.20	0.65
1:A:403:LEU:HB3	1:A:405:ASP:OD1	1.97	0.65
2:C:125:LYS:HE2	2:C:171:GLY:HA2	1.78	0.65
2:E:37:PHE:CZ	6:E:301:GSH:HA32	2.32	0.65
1:A:135:ASP:OD1	7:A:723:HOH:O	2.13	0.65
1:A:229:HIS:O	1:A:233:THR:N	2.30	0.65
2:E:151:GLY:H	2:E:154:ASP:HB2	1.62	0.65
1:A:78:LYS:NZ	1:A:553:PRO:O	2.25	0.65
1:A:395:TYR:HD1	2:B:141:ASP:OD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:CYS:HB2	1:A:520:LEU:HB3	1.78	0.65
2:C:34:GLU:O	7:C:408:HOH:O	2.13	0.65
1:D:76:TYR:HD2	1:D:88:ILE:HD13	1.60	0.65
2:F:48:ASN:HB2	7:F:414:HOH:O	1.95	0.65
2:C:70:VAL:HA	2:C:73:TYR:HD2	1.61	0.65
2:C:92:ARG:HB3	2:C:96:ARG:HH22	1.61	0.65
2:B:145:PHE:CD2	2:B:153:VAL:HG22	2.32	0.65
1:D:164:THR:OG1	1:D:557:LYS:O	2.11	0.65
1:D:570:TYR:O	7:D:723:HOH:O	2.14	0.65
2:E:26:LYS:HG3	2:E:78:TRP:HE1	1.61	0.65
1:A:98:SER:OG	5:A:603:ATP:O2G	2.15	0.65
1:A:432:ASN:OD1	1:A:434:ASP:N	2.29	0.65
5:A:603:ATP:O2B	5:A:603:ATP:O2A	2.12	0.65
2:C:164:PHE:HD2	2:C:183:ILE:HD13	1.61	0.65
1:D:36:LEU:HD11	1:D:50:LEU:HD11	1.79	0.65
1:D:38:LYS:O	2:E:142:LYS:HG2	1.96	0.65
1:D:473:GLY:O	1:D:516:GLY:N	2.29	0.65
2:E:192:LYS:NZ	7:E:420:HOH:O	2.30	0.65
1:A:77:ILE:HD13	1:A:112:PRO:HD3	1.78	0.64
2:B:7:LEU:HD11	2:B:55:PRO:HB2	1.78	0.64
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.31	0.64
1:A:152:LYS:NZ	1:A:561:ILE:HG22	2.11	0.64
1:A:465:TYR:HD1	1:A:551:VAL:HG23	1.61	0.64
1:D:98:SER:HB3	5:D:603:ATP:O2G	1.97	0.64
1:D:445:VAL:HA	1:D:479:TRP:HZ2	1.62	0.64
1:A:236:GLN:OE1	7:A:724:HOH:O	2.15	0.64
1:A:531:ILE:HD13	1:A:558:VAL:HG22	1.78	0.64
1:A:426:ASN:HD21	1:A:544:GLN:NE2	1.96	0.64
1:D:309:MET:HB3	7:D:756:HOH:O	1.96	0.64
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.78	0.64
1:A:77:ILE:HB	1:A:110:PHE:HD2	1.62	0.64
2:B:152:TYR:CE1	2:B:153:VAL:HG12	2.32	0.64
1:A:143:LYS:HD3	1:A:187:CYS:HB3	1.80	0.64
1:A:319:TYR:OH	7:A:707:HOH:O	2.05	0.64
2:C:139:LEU:HB3	2:C:181:LYS:HZ1	1.60	0.64
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.32	0.64
1:D:229:HIS:HA	1:D:232:ARG:HE	1.63	0.64
1:D:535:PHE:O	1:D:538:LEU:HB3	1.97	0.64
1:A:152:LYS:HZ2	1:A:561:ILE:HG22	1.62	0.64
1:D:77:ILE:HG12	1:D:89:LEU:HD11	1.79	0.64
1:D:143:LYS:NZ	1:D:209:GLY:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LEU:HD13	1:D:231:PHE:HE2	1.63	0.64
1:A:200:GLN:HA	1:A:203:TYR:CE2	2.32	0.64
2:B:26:LYS:HB2	2:B:81:LYS:HE3	1.78	0.64
1:A:150:SER:O	1:A:150:SER:OG	2.10	0.64
1:A:464:SER:HB3	1:A:550:CYS:HB2	1.80	0.64
1:A:560:GLN:N	7:A:702:HOH:O	2.16	0.64
2:C:26:LYS:HB3	2:C:78:TRP:HE1	1.62	0.64
2:E:17:MET:HG2	2:E:20:ARG:NH1	2.13	0.64
2:F:165:GLN:HG2	2:F:206:VAL:HG21	1.80	0.64
1:A:462:PHE:N	7:A:752:HOH:O	2.29	0.63
2:C:172:ASN:OD1	7:C:409:HOH:O	2.15	0.63
1:D:330:TYR:CE1	1:D:352:PHE:HB2	2.32	0.63
1:D:476:ALA:O	7:D:708:HOH:O	2.15	0.63
2:F:65:CYS:O	2:F:69:ASN:ND2	2.25	0.63
2:B:145:PHE:H	2:B:154:ASP:CG	2.06	0.63
1:D:38:LYS:HG2	1:D:395:TYR:HE2	1.63	0.63
1:D:316:LEU:O	1:D:320:ALA:N	2.31	0.63
2:C:201:ASP:OD2	1:D:456:LYS:HG3	1.97	0.63
2:F:199:LEU:O	7:F:408:HOH:O	2.15	0.63
2:E:85:PHE:O	7:E:409:HOH:O	2.15	0.63
2:C:24:ARG:HG3	2:C:30:PHE:CE1	2.34	0.63
2:E:183:ILE:HG13	2:E:184:ALA:N	2.14	0.63
1:A:165:ALA:N	5:A:603:ATP:O3G	2.31	0.63
1:D:284:LEU:HD21	1:D:287:TRP:HA	1.80	0.63
1:D:424:ARG:C	1:D:543:GLY:HA2	2.23	0.63
1:A:72:GLU:OE1	1:A:72:GLU:N	2.27	0.63
1:A:98:SER:N	1:A:111:ILE:O	2.20	0.63
1:D:494:CYS:SG	1:D:495:ASN:N	2.71	0.63
1:A:136:PHE:CD1	1:A:299:LYS:HD2	2.34	0.63
1:A:295:PHE:HD2	1:A:298:ALA:HB2	1.62	0.63
1:A:405:ASP:OD1	1:A:540:SER:HB2	1.99	0.63
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.34	0.63
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.34	0.63
2:B:145:PHE:CB	2:B:153:VAL:HG13	2.27	0.62
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.34	0.62
1:D:498:ASP:HB3	1:D:510:ARG:NH1	2.14	0.62
1:A:17:PHE:HA	1:A:20:MET:SD	2.39	0.62
1:D:203:TYR:HA	1:D:206:LEU:HD12	1.81	0.62
2:F:92:ARG:HG3	7:F:404:HOH:O	1.98	0.62
2:B:6:ILE:HG23	2:B:31:GLU:HG2	1.81	0.62
2:E:188:ARG:NE	2:E:191:GLU:OE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:GLY:C	2:F:181:LYS:HE2	2.25	0.62
2:F:153:VAL:O	2:F:157:LEU:HD23	1.99	0.62
1:A:423:CYS:HB2	1:A:542:ALA:HB3	1.81	0.62
1:D:88:ILE:HG22	1:D:89:LEU:N	2.14	0.62
1:D:498:ASP:HB3	1:D:510:ARG:CZ	2.30	0.62
2:C:114:TRP:HA	2:C:170:PHE:HD2	1.64	0.62
1:D:101:SER:HB3	1:D:535:PHE:CD2	2.35	0.62
2:E:36:ASP:HB3	2:E:39:ASN:OD1	2.00	0.62
1:A:92:HIS:CE1	2:B:142:LYS:HB3	2.34	0.62
1:A:276:THR:OG1	1:A:277:ILE:N	2.33	0.62
1:A:440:ASP:O	1:A:444:SER:N	2.33	0.62
2:C:110:GLN:HB3	2:C:167:TYR:CZ	2.35	0.62
1:D:330:TYR:CD1	1:D:352:PHE:HD2	2.18	0.62
1:A:274:ALA:O	1:A:278:ARG:HB2	2.00	0.62
1:D:81:VAL:HG22	1:D:97:ILE:HG13	1.80	0.62
1:D:146:GLN:HB2	1:D:220:PHE:HD2	1.65	0.62
1:D:41:SER:HB2	2:E:142:LYS:HD2	1.81	0.62
1:D:464:SER:O	1:D:551:VAL:N	2.31	0.62
2:F:84:PHE:CG	2:F:152:TYR:HB2	2.34	0.62
1:A:200:GLN:HA	1:A:203:TYR:CZ	2.35	0.62
1:A:238:TRP:CH2	1:A:287:TRP:HZ2	2.16	0.62
1:A:246:LYS:O	1:A:269:PRO:HA	2.00	0.62
2:C:64:VAL:HB	2:C:73:TYR:CE2	2.35	0.62
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.34	0.62
1:A:51:ASN:ND2	2:B:87:SER:OG	2.33	0.61
1:A:333:SER:HB3	5:A:603:ATP:PA	2.39	0.61
1:A:451:ARG:O	1:A:454:GLU:HG2	2.00	0.61
1:D:476:ALA:O	1:D:477:ILE:HD13	2.00	0.61
2:E:148:ASP:OD1	7:E:410:HOH:O	2.16	0.61
2:F:107:THR:HA	2:F:110:GLN:HE21	1.64	0.61
1:A:496:CYS:O	1:A:500:ALA:N	2.33	0.61
3:A:601:JAA:C08	4:A:602:MET:HE2	2.30	0.61
1:D:204:CYS:O	1:D:208:SER:N	2.24	0.61
2:E:202:SER:HA	2:E:205:ILE:HD11	1.82	0.61
2:F:37:PHE:O	2:F:40:LYS:NZ	2.29	0.61
2:F:132:VAL:O	2:F:179:SER:HB3	2.00	0.61
1:A:207:LEU:O	1:A:211:LEU:HG	1.99	0.61
1:D:62:LYS:O	1:D:400:ARG:NH2	2.33	0.61
1:D:377:VAL:O	7:D:725:HOH:O	2.16	0.61
1:A:287:TRP:HB3	1:A:290:LEU:CD1	2.31	0.61
1:A:140:ASP:OD1	1:A:140:ASP:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:THR:CG2	1:D:336:TRP:HZ2	2.14	0.61
1:D:434:ASP:OD2	1:D:550:CYS:HB3	2.00	0.61
1:A:224:ALA:HA	1:A:227:LEU:HD12	1.83	0.61
2:B:6:ILE:HG21	2:B:33:ARG:HD2	1.82	0.61
1:D:344:ARG:N	7:D:704:HOH:O	2.33	0.61
2:E:50:ILE:HG21	2:F:134:ILE:HD12	1.81	0.61
2:F:211:GLU:HA	2:F:214:LYS:HE3	1.83	0.61
2:B:135:LEU:HD13	2:B:157:LEU:HD11	1.82	0.61
1:A:547:MET:HE2	1:A:549:ARG:HH11	1.66	0.61
1:D:93:PRO:O	2:E:181:LYS:HG2	2.00	0.61
1:D:338:ALA:HB2	1:D:354:VAL:HG22	1.83	0.61
1:A:498:ASP:N	1:A:498:ASP:OD1	2.33	0.61
2:B:66:GLU:CD	2:B:69:ASN:HB2	2.26	0.61
2:F:136:GLU:CG	2:F:180:PRO:HD2	2.30	0.61
1:A:154:TYR:O	7:A:726:HOH:O	2.16	0.60
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.36	0.60
2:B:26:LYS:O	2:B:81:LYS:NZ	2.30	0.60
2:F:84:PHE:HB2	2:F:152:TYR:N	2.16	0.60
2:F:132:VAL:HG13	2:F:179:SER:OG	2.00	0.60
2:F:164:PHE:O	2:F:168:GLU:HG3	2.01	0.60
1:A:41:SER:OG	2:B:144:TYR:O	2.12	0.60
1:A:195:SER:OG	1:A:197:ASP:OD1	2.18	0.60
1:A:229:HIS:HB2	1:A:529:ARG:CZ	2.31	0.60
1:A:273:LEU:HA	1:A:276:THR:HG23	1.83	0.60
1:A:404:GLY:O	1:A:426:ASN:HB2	2.02	0.60
1:A:444:SER:HA	1:A:500:ALA:CB	2.31	0.60
1:D:39:ASN:HD21	2:E:143:PRO:HD3	1.65	0.60
1:A:225:HIS:O	1:A:229:HIS:N	2.29	0.60
1:D:285:SER:O	1:D:287:TRP:N	2.35	0.60
1:D:538:LEU:CD2	1:D:540:SER:HB2	2.31	0.60
1:D:202:LEU:O	1:D:206:LEU:HG	2.01	0.60
1:D:278:ARG:NH1	7:D:752:HOH:O	2.25	0.60
1:A:86:SER:HB2	2:B:188:ARG:HE	1.65	0.60
1:A:530:LYS:HA	1:A:533:GLU:HG3	1.83	0.60
2:C:184:ALA:HB1	1:D:499:ARG:HH11	1.65	0.60
1:A:245:ILE:HA	1:A:267:LEU:HD11	1.83	0.60
2:B:64:VAL:HG12	2:C:90:TYR:HD1	1.67	0.60
2:F:33:ARG:NH2	2:F:41:SER:OG	2.26	0.60
2:F:64:VAL:HB	2:F:73:TYR:CD2	2.36	0.60
2:F:165:GLN:HG2	2:F:206:VAL:CG2	2.31	0.60
2:C:168:GLU:OE2	1:D:488:ASP:OD2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:HIS:HB2	1:D:93:PRO:HD2	1.83	0.60
2:F:114:TRP:HA	2:F:170:PHE:HD2	1.67	0.60
1:A:88:ILE:HG22	1:A:89:LEU:N	2.15	0.60
1:D:435:LYS:HE2	1:D:438:GLU:HB3	1.82	0.60
2:E:112:LYS:O	2:E:116:LYS:HB2	2.01	0.60
1:A:20:MET:HA	1:A:23:ASN:HB2	1.84	0.60
1:A:421:PHE:HB3	1:A:542:ALA:HB2	1.83	0.60
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.36	0.60
1:D:461:ASP:HB3	1:D:528:PHE:CE1	2.36	0.60
1:A:213:ARG:HH21	1:A:296:PRO:HD2	1.66	0.59
2:C:4:LEU:O	7:C:411:HOH:O	2.17	0.59
2:C:52:LYS:HA	7:C:413:HOH:O	2.01	0.59
1:D:80:MET:HE1	1:D:88:ILE:HG13	1.84	0.59
2:F:204:LYS:NZ	7:F:409:HOH:O	2.35	0.59
1:A:78:LYS:HE3	1:A:554:SER:HA	1.82	0.59
1:A:223:PHE:CD1	1:A:304:ILE:HB	2.37	0.59
1:A:510:ARG:HH21	1:A:517:ALA:HA	1.67	0.59
2:B:47:SER:OG	2:B:56:VAL:HG21	2.02	0.59
1:D:120:ASN:CB	1:D:358:LEU:HD23	2.32	0.59
1:A:118:MET:HE3	1:A:175:PHE:CE2	2.38	0.59
1:A:151:SER:HB3	1:A:193:ILE:O	2.02	0.59
1:D:231:PHE:CZ	1:D:291:ILE:HG12	2.37	0.59
1:D:287:TRP:HE3	1:D:290:LEU:HD13	1.65	0.59
2:B:96:ARG:HD2	2:C:73:TYR:CE1	2.37	0.59
1:D:8:PHE:CZ	1:D:130:ALA:HB2	2.37	0.59
1:D:41:SER:HA	2:E:148:ASP:HA	1.85	0.59
1:D:82:ASP:O	1:D:84:ASP:N	2.34	0.59
1:D:99:LEU:H	1:D:557:LYS:H	1.50	0.59
1:D:523:VAL:HG12	1:D:565:ASN:HB3	1.83	0.59
2:E:30:PHE:O	7:E:411:HOH:O	2.16	0.59
1:A:42:ALA:HB3	1:A:45:LEU:HB2	1.84	0.59
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.84	0.59
2:B:93:ALA:HA	2:C:73:TYR:HE1	1.66	0.59
2:C:188:ARG:HB2	1:D:499:ARG:NH2	2.17	0.59
1:D:431:ILE:O	7:D:728:HOH:O	2.17	0.59
2:F:169:LYS:NZ	7:F:424:HOH:O	2.35	0.59
1:A:198:VAL:O	1:A:202:LEU:N	2.31	0.59
1:D:14:ILE:HG22	1:D:16:GLU:HB2	1.83	0.59
1:D:504:ALA:O	1:D:507:VAL:HB	2.02	0.59
2:F:70:VAL:HG23	7:F:402:HOH:O	2.01	0.59
2:C:42:PRO:O	7:C:410:HOH:O	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:THR:O	1:D:530:LYS:HB2	2.02	0.59
2:F:110:GLN:HG2	2:F:167:TYR:HE2	1.67	0.59
1:A:31:THR:O	1:A:35:ILE:HG13	2.02	0.59
1:A:116:GLU:O	1:A:119:GLU:HG2	2.02	0.59
1:A:406:VAL:O	1:A:541:SER:OG	2.21	0.59
1:D:286:ASN:O	7:D:726:HOH:O	2.16	0.59
1:A:423:CYS:SG	1:A:541:SER:OG	2.61	0.59
2:E:116:LYS:O	2:E:213:ARG:NH1	2.36	0.59
2:F:141:ASP:N	2:F:141:ASP:OD1	2.33	0.59
2:F:157:LEU:HG	2:F:185:TRP:CH2	2.38	0.59
1:A:27:VAL:O	1:A:31:THR:OG1	2.13	0.59
2:C:27:GLY:O	7:C:412:HOH:O	2.17	0.59
1:A:223:PHE:HE2	1:A:533:GLU:HA	1.67	0.58
1:D:65:VAL:HG21	1:D:399:TYR:HE2	1.66	0.58
1:D:470:THR:N	7:D:705:HOH:O	2.35	0.58
2:E:125:LYS:HD3	2:E:173:PHE:HZ	1.67	0.58
2:F:17:MET:HE2	2:F:200:PRO:HD2	1.85	0.58
1:A:45:LEU:HG	1:A:50:LEU:HB2	1.85	0.58
1:A:465:TYR:N	1:A:476:ALA:O	2.35	0.58
1:D:15:ASP:OD1	7:D:727:HOH:O	2.17	0.58
2:F:23:LEU:HD23	2:F:74:VAL:HG22	1.85	0.58
1:A:197:ASP:OD1	1:A:197:ASP:N	2.37	0.58
1:A:331:GLY:HA3	1:A:336:TRP:HA	1.84	0.58
2:C:37:PHE:O	2:C:40:LYS:NZ	2.36	0.58
1:D:94:VAL:HG21	1:D:113:PHE:H	1.66	0.58
2:E:110:GLN:HB2	2:E:167:TYR:CZ	2.39	0.58
2:F:165:GLN:O	2:F:168:GLU:HB2	2.03	0.58
1:A:216:VAL:N	7:A:720:HOH:O	2.36	0.58
1:A:244:ASP:HB2	1:A:251:SER:N	2.18	0.58
1:D:478:PHE:CZ	1:D:562:LEU:HA	2.38	0.58
1:A:535:PHE:CZ	1:A:557:LYS:HE2	2.37	0.58
2:B:119:GLU:N	7:B:425:HOH:O	2.35	0.58
2:B:169:LYS:NZ	2:B:206:VAL:HG11	2.17	0.58
2:C:84:PHE:HD1	2:C:85:PHE:N	2.01	0.58
2:C:102:VAL:O	2:C:106:PHE:HB3	2.03	0.58
1:D:227:LEU:HD12	1:D:316:LEU:HD21	1.85	0.58
1:D:551:VAL:HG22	1:D:555:ASN:HD22	1.69	0.58
2:F:132:VAL:HG22	2:F:182:LEU:HD13	1.85	0.58
1:A:352:PHE:HA	7:A:856:HOH:O	2.04	0.58
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.39	0.58
1:A:441:LEU:HD23	1:A:549:ARG:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:TRP:HA	2:C:170:PHE:CD2	2.38	0.58
1:D:393:THR:HA	1:D:399:TYR:HA	1.85	0.58
1:D:466:ILE:HD12	1:D:552:LYS:HG3	1.84	0.58
2:E:172:ASN:OD1	7:E:412:HOH:O	2.16	0.58
2:E:183:ILE:O	2:E:186:ALA:HB3	2.03	0.58
2:F:22:ALA:HA	2:F:155:ILE:HD13	1.85	0.58
1:D:99:LEU:HG	1:D:557:LYS:CB	2.32	0.58
2:E:65:CYS:HB3	2:F:97:PHE:CZ	2.38	0.58
1:A:88:ILE:HG22	1:A:89:LEU:HG	1.85	0.58
1:A:222:VAL:HG21	4:A:602:MET:N	2.19	0.58
1:A:233:THR:HA	1:A:236:GLN:CB	2.24	0.58
2:B:163:TRP:CD2	2:B:205:ILE:HD13	2.39	0.58
2:B:165:GLN:O	2:B:169:LYS:HE3	2.03	0.58
2:B:188:ARG:NH1	7:B:426:HOH:O	2.37	0.58
1:D:169:VAL:O	1:D:172:ASN:HB2	2.04	0.58
2:F:85:PHE:CG	2:F:92:ARG:HG2	2.39	0.58
1:A:442:GLN:HG2	1:A:462:PHE:HZ	1.68	0.58
1:A:478:PHE:HB2	1:A:528:PHE:HZ	1.69	0.58
1:A:541:SER:O	1:A:543:GLY:N	2.37	0.58
1:D:78:LYS:HA	1:D:110:PHE:HD2	1.68	0.58
1:D:94:VAL:CG2	1:D:113:PHE:H	2.17	0.58
1:D:98:SER:HB3	1:D:113:PHE:CE2	2.38	0.58
1:A:149:PHE:CE2	1:A:530:LYS:HD3	2.39	0.58
2:B:51:HIS:NE2	7:B:422:HOH:O	2.32	0.58
1:D:194:PHE:O	7:D:721:HOH:O	2.18	0.58
1:D:246:LYS:HB2	7:D:852:HOH:O	2.03	0.58
1:A:457:ILE:HG22	1:A:481:ILE:HG22	1.85	0.57
2:B:155:ILE:HD13	7:B:516:HOH:O	2.02	0.57
2:B:155:ILE:O	2:B:158:ILE:HG22	2.04	0.57
1:D:287:TRP:HA	1:D:290:LEU:HD12	1.85	0.57
2:F:178:GLU:C	2:F:180:PRO:HD3	2.29	0.57
1:A:233:THR:O	1:A:237:VAL:N	2.35	0.57
1:A:552:LYS:HB3	1:A:553:PRO:HD2	1.84	0.57
2:B:85:PHE:CE1	2:B:152:TYR:HB3	2.40	0.57
2:B:130:GLU:O	2:B:134:ILE:HG13	2.05	0.57
1:A:108:PRO:HB2	1:A:554:SER:CB	2.33	0.57
1:A:191:GLU:O	1:A:195:SER:N	2.37	0.57
1:A:223:PHE:HB3	1:A:309:MET:HG3	1.86	0.57
1:A:480:GLU:HB2	1:A:528:PHE:CD2	2.39	0.57
2:C:26:LYS:NZ	2:C:82:ASN:O	2.32	0.57
1:D:203:TYR:HE2	1:D:253:ARG:HD3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:22:ALA:HA	2:C:155:ILE:HD13	1.85	0.57
1:D:121:THR:HG23	1:D:336:TRP:CZ2	2.39	0.57
1:D:199:HIS:N	1:D:524:ALA:HB1	2.17	0.57
2:E:14:MET:HB3	2:E:163:TRP:NE1	2.19	0.57
1:A:71:VAL:O	1:A:75:PRO:HD3	2.03	0.57
1:A:101:SER:OG	1:A:544:GLN:HB3	2.04	0.57
2:B:153:VAL:HA	2:B:156:SER:OG	2.04	0.57
2:C:187:LYS:HA	2:C:190:MET:HG3	1.87	0.57
1:D:199:HIS:H	1:D:524:ALA:CB	2.17	0.57
1:A:365:PRO:HG2	1:A:374:GLU:HG2	1.87	0.57
1:D:114:THR:HB	1:D:395:TYR:HE1	1.70	0.57
1:D:163:GLY:HA2	1:D:560:GLN:CD	2.29	0.57
1:D:201:ALA:O	1:D:205:HIS:N	2.37	0.57
1:D:253:ARG:HG3	1:D:484:GLU:HB3	1.87	0.57
1:A:138:ILE:HB	1:A:217:GLN:HG3	1.87	0.57
1:A:187:CYS:SG	1:A:209:GLY:HA2	2.45	0.57
1:A:291:ILE:CG1	1:A:320:ALA:HA	2.33	0.57
1:A:339:ALA:HB3	1:A:355:ILE:HD11	1.87	0.57
2:C:131:ALA:O	2:C:135:LEU:HB2	2.03	0.57
2:E:26:LYS:HE2	2:E:78:TRP:CD1	2.40	0.57
2:E:208:TYR:O	2:E:212:TYR:N	2.26	0.57
2:C:169:LYS:HG3	2:C:170:PHE:N	2.19	0.57
1:A:332:SER:N	1:A:335:GLY:O	2.37	0.57
2:B:22:ALA:HA	7:B:496:HOH:O	2.05	0.57
1:D:110:PHE:HE1	1:D:556:ALA:HB2	1.69	0.57
1:D:219:VAL:HB	1:D:295:PHE:CE2	2.40	0.57
1:D:338:ALA:CB	1:D:354:VAL:HA	2.34	0.57
1:A:369:THR:N	7:A:739:HOH:O	2.38	0.56
2:B:175:ILE:HB	2:B:183:ILE:HD13	1.87	0.56
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.39	0.56
1:D:47:ASN:OD1	1:D:47:ASN:N	2.33	0.56
1:D:80:MET:SD	1:D:88:ILE:N	2.78	0.56
1:D:223:PHE:HD2	1:D:225:HIS:CE1	2.23	0.56
1:D:354:VAL:O	1:D:416:THR:HG21	2.05	0.56
2:F:68:LEU:HD12	2:F:69:ASN:N	2.20	0.56
1:A:18:ASP:OD1	7:A:729:HOH:O	2.17	0.56
1:A:535:PHE:CE1	1:A:557:LYS:HE2	2.40	0.56
1:A:551:VAL:HB	1:A:555:ASN:HB2	1.87	0.56
1:D:75:PRO:HA	1:D:78:LYS:HG2	1.87	0.56
1:D:445:VAL:HA	1:D:479:TRP:CZ2	2.39	0.56
1:D:474:HIS:HB2	1:D:517:ALA:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:ARG:O	2:E:96:ARG:HG2	2.05	0.56
1:A:97:ILE:HG21	1:A:110:PHE:CZ	2.41	0.56
1:A:107:ARG:HG3	1:A:108:PRO:HD2	1.87	0.56
1:A:463:SER:HB3	1:A:478:PHE:CD2	2.40	0.56
2:B:146:GLY:HA2	2:B:152:TYR:CZ	2.40	0.56
1:D:223:PHE:CE2	1:D:533:GLU:HA	2.40	0.56
1:D:304:ILE:HG12	1:D:328:HIS:O	2.06	0.56
1:D:463:SER:O	1:D:477:ILE:HA	2.05	0.56
1:D:557:LYS:HD2	5:D:603:ATP:O1G	2.05	0.56
1:A:143:LYS:C	1:A:184:SER:HB2	2.30	0.56
2:B:31:GLU:OE1	2:B:31:GLU:N	2.38	0.56
2:B:51:HIS:O	2:B:52:LYS:HG2	2.05	0.56
1:D:169:VAL:HG13	1:D:170:TYR:CD1	2.40	0.56
2:F:23:LEU:HG	7:F:417:HOH:O	2.06	0.56
1:D:421:PHE:CD2	1:D:541:SER:HA	2.40	0.56
2:E:40:LYS:HB3	7:E:401:HOH:O	2.05	0.56
2:B:114:TRP:CD1	2:B:167:TYR:CE1	2.94	0.56
2:B:162:SER:HB3	2:B:199:LEU:HG	1.86	0.56
1:D:149:PHE:CZ	1:D:198:VAL:HB	2.40	0.56
1:D:219:VAL:HG21	1:D:231:PHE:HZ	1.69	0.56
2:E:104:LYS:O	2:E:108:ASP:N	2.37	0.56
2:C:54:ILE:HB	2:C:55:PRO:HA	1.88	0.56
1:D:238:TRP:O	1:D:240:GLU:N	2.39	0.56
1:D:435:LYS:HG2	1:D:438:GLU:N	2.21	0.56
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.38	0.56
2:F:129:ILE:HA	2:F:132:VAL:HG12	1.87	0.56
2:F:214:LYS:NZ	7:F:428:HOH:O	2.39	0.56
1:A:309:MET:SD	1:A:312:TYR:HD2	2.29	0.56
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.41	0.56
1:D:34:GLU:O	1:D:38:LYS:HB2	2.06	0.56
1:A:104:SER:O	1:A:107:ARG:HB3	2.06	0.56
1:A:152:LYS:HD3	1:A:561:ILE:HA	1.88	0.56
2:C:64:VAL:HG23	2:C:70:VAL:HG22	1.87	0.56
1:D:389:GLU:OE1	7:D:729:HOH:O	2.18	0.56
1:D:501:PHE:HD2	1:D:506:TYR:CZ	2.22	0.56
2:E:96:ARG:HD2	2:F:73:TYR:CE1	2.40	0.56
2:C:184:ALA:HB1	1:D:499:ARG:NH1	2.21	0.55
1:D:169:VAL:O	1:D:175:PHE:HB2	2.06	0.55
2:E:85:PHE:HE1	2:E:152:TYR:CG	2.24	0.55
1:A:92:HIS:CE1	2:B:142:LYS:H	2.25	0.55
1:D:36:LEU:O	1:D:40:GLN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:HIS:CE1	2:E:181:LYS:HE3	2.40	0.55
1:D:197:ASP:OD2	1:D:200:GLN:NE2	2.40	0.55
1:D:233:THR:HG23	1:D:525:LYS:HZ3	1.71	0.55
1:D:532:GLN:HB3	1:D:545:PHE:CZ	2.41	0.55
2:E:175:ILE:H	2:E:175:ILE:HD12	1.70	0.55
2:E:176:GLU:HB2	2:E:183:ILE:HG12	1.87	0.55
1:A:126:ARG:HE	1:A:182:ILE:HG21	1.71	0.55
2:B:146:GLY:H	2:B:151:GLY:HA3	1.71	0.55
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.88	0.55
1:D:8:PHE:HZ	1:D:130:ALA:HB2	1.70	0.55
1:D:89:LEU:HD12	1:D:90:THR:CG2	2.36	0.55
1:A:256:VAL:O	1:A:260:ARG:HB2	2.06	0.55
2:B:32:TYR:OH	2:B:34:GLU:OE1	2.24	0.55
1:D:403:LEU:HD21	1:D:544:GLN:HE22	1.71	0.55
1:A:227:LEU:O	1:A:231:PHE:N	2.29	0.55
1:D:206:LEU:HD11	1:D:233:THR:HG22	1.89	0.55
2:F:165:GLN:CA	2:F:168:GLU:HG3	2.37	0.55
2:B:92:ARG:NH1	2:B:96:ARG:HH12	2.04	0.55
2:C:92:ARG:HD2	7:C:488:HOH:O	2.06	0.55
2:C:169:LYS:HG3	2:C:170:PHE:H	1.71	0.55
1:D:357:ASN:ND2	7:D:718:HOH:O	2.11	0.55
1:A:351:THR:N	7:A:774:HOH:O	2.39	0.55
1:A:552:LYS:C	1:A:554:SER:H	2.14	0.55
2:B:96:ARG:NH2	2:C:76:GLU:OE1	2.40	0.55
1:D:107:ARG:HB2	1:D:552:LYS:CE	2.36	0.55
2:E:125:LYS:HD3	2:E:173:PHE:CZ	2.42	0.55
2:F:26:LYS:HG2	2:F:81:LYS:NZ	2.22	0.55
1:A:498:ASP:HB3	1:A:510:ARG:NH1	2.22	0.55
2:B:97:PHE:N	2:C:69:ASN:HD21	2.04	0.55
1:D:466:ILE:N	1:D:551:VAL:O	2.40	0.55
2:F:128:PHE:O	2:F:132:VAL:HG12	2.05	0.55
1:A:156:SER:HB2	1:A:162:VAL:HG13	1.89	0.55
2:B:114:TRP:HD1	2:B:167:TYR:CE1	2.24	0.55
1:D:91:GLY:HA2	2:E:142:LYS:C	2.31	0.55
1:D:97:ILE:HG23	1:D:111:ILE:H	1.70	0.55
1:D:98:SER:HB2	1:D:557:LYS:HD3	1.89	0.55
1:D:271:PRO:HA	7:D:852:HOH:O	2.06	0.55
1:D:439:ARG:NH2	7:D:777:HOH:O	2.39	0.55
1:D:467:ASP:O	1:D:475:TYR:CZ	2.60	0.55
1:A:117:LEU:HD13	5:A:603:ATP:N3	2.21	0.54
2:C:114:TRP:HD1	2:C:167:TYR:CE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:ILE:CD1	1:D:518:LEU:HD21	2.34	0.54
1:D:510:ARG:HB2	7:D:955:HOH:O	2.06	0.54
2:B:69:ASN:ND2	2:C:93:ALA:O	2.31	0.54
2:C:114:TRP:CD1	2:C:167:TYR:CE1	2.94	0.54
1:D:193:ILE:HG22	1:D:205:HIS:NE2	2.23	0.54
1:D:223:PHE:HZ	1:D:536:LEU:HB3	1.71	0.54
2:E:152:TYR:OH	7:E:408:HOH:O	2.14	0.54
2:F:183:ILE:O	2:F:186:ALA:HB3	2.06	0.54
1:A:405:ASP:HB3	1:A:426:ASN:ND2	2.20	0.54
1:A:440:ASP:OD1	1:A:502:ILE:HG13	2.08	0.54
2:B:202:SER:O	2:B:206:VAL:HG13	2.08	0.54
2:C:11:TRP:O	2:C:200:PRO:HG2	2.08	0.54
2:F:7:LEU:HA	2:F:56:VAL:O	2.08	0.54
1:A:287:TRP:HA	1:A:287:TRP:CE3	2.42	0.54
2:B:35:GLU:OE2	7:B:410:HOH:O	2.18	0.54
1:D:94:VAL:HG11	1:D:97:ILE:HG12	1.88	0.54
1:D:445:VAL:HG21	1:D:462:PHE:CD2	2.42	0.54
1:D:479:TRP:HB2	1:D:522:VAL:HG12	1.89	0.54
2:E:18:ARG:NH2	2:E:67:SER:OG	2.39	0.54
2:F:178:GLU:O	2:F:180:PRO:HD3	2.07	0.54
1:D:143:LYS:HB2	7:D:755:HOH:O	2.07	0.54
1:D:519:GLU:HG3	1:D:570:TYR:C	2.32	0.54
1:A:97:ILE:H	1:A:162:VAL:HA	1.70	0.54
1:A:238:TRP:CH2	1:A:281:CYS:HB3	2.43	0.54
2:C:138:GLU:HG3	2:C:145:PHE:HE1	1.72	0.54
1:D:113:PHE:CG	5:D:603:ATP:O1B	2.60	0.54
1:A:76:TYR:HB3	1:A:88:ILE:CG2	2.38	0.54
2:B:93:ALA:HA	2:C:73:TYR:CE1	2.43	0.54
1:D:99:LEU:HB3	1:D:556:ALA:H	1.71	0.54
1:D:498:ASP:O	1:D:510:ARG:NH2	2.41	0.54
2:E:201:ASP:HB3	2:E:203:GLU:HG2	1.90	0.54
2:F:110:GLN:O	2:F:113:VAL:HG12	2.08	0.54
1:A:97:ILE:HG21	1:A:110:PHE:CE2	2.43	0.54
2:B:98:TRP:NE1	7:B:431:HOH:O	2.39	0.54
2:C:26:LYS:HE3	2:C:78:TRP:NE1	2.23	0.54
2:C:98:TRP:CD1	2:C:153:VAL:HG11	2.42	0.54
1:D:191:GLU:OE1	1:D:191:GLU:N	2.41	0.54
1:D:332:SER:HA	5:D:603:ATP:N6	2.23	0.54
1:A:221:ALA:HA	7:A:751:HOH:O	2.07	0.54
1:D:170:TYR:OH	4:D:602:MET:HE3	2.07	0.54
1:D:290:LEU:O	1:D:293:ALA:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PHE:CZ	1:A:294:LEU:HD11	2.43	0.53
1:A:535:PHE:O	1:A:538:LEU:HB3	2.07	0.53
1:A:536:LEU:HD23	1:A:542:ALA:HA	1.90	0.53
2:B:10:TYR:HB3	2:B:13:SER:HB3	1.90	0.53
2:C:139:LEU:HB3	2:C:181:LYS:NZ	2.23	0.53
1:D:130:ALA:HA	1:D:133:ASN:HB2	1.89	0.53
2:F:110:GLN:CG	2:F:167:TYR:HE2	2.21	0.53
1:A:242:VAL:O	1:A:246:LYS:HB2	2.09	0.53
1:A:286:ASN:O	7:A:735:HOH:O	2.19	0.53
1:D:116:GLU:HA	1:D:119:GLU:HG3	1.90	0.53
1:D:225:HIS:HA	1:D:228:VAL:HB	1.90	0.53
1:D:243:THR:HA	1:D:246:LYS:CD	2.38	0.53
1:D:290:LEU:N	7:D:753:HOH:O	2.34	0.53
1:D:409:VAL:HA	1:D:420:LYS:NZ	2.23	0.53
1:D:413:TYR:N	1:D:418:GLN:OE1	2.39	0.53
2:C:98:TRP:HD1	2:C:153:VAL:HG11	1.74	0.53
1:D:172:ASN:HB3	1:D:174:ASN:OD1	2.08	0.53
1:D:239:GLU:O	1:D:243:THR:N	2.30	0.53
1:D:405:ASP:CG	1:D:540:SER:HB3	2.33	0.53
1:A:9:ASP:OD2	1:A:12:ARG:HB3	2.09	0.53
1:A:143:LYS:HD3	1:A:187:CYS:CB	2.39	0.53
2:B:90:TYR:O	2:B:93:ALA:HB3	2.09	0.53
2:B:154:ASP:OD1	2:B:185:TRP:NE1	2.38	0.53
1:D:13:VAL:C	1:D:14:ILE:HG13	2.33	0.53
2:F:169:LYS:HG3	2:F:170:PHE:N	2.24	0.53
1:A:22:ARG:HG2	1:A:414:ASN:HB3	1.89	0.53
2:C:10:TYR:CG	2:C:12:PRO:HD2	2.43	0.53
1:D:78:LYS:HA	1:D:110:PHE:CD2	2.43	0.53
2:F:9:ASP:HA	2:F:54:ILE:HD13	1.91	0.53
1:A:465:TYR:HB2	1:A:478:PHE:CZ	2.44	0.53
1:D:403:LEU:CD2	1:D:544:GLN:HE22	2.21	0.53
1:A:86:SER:HB2	2:B:188:ARG:HB2	1.90	0.53
1:A:465:TYR:CD1	1:A:551:VAL:HG23	2.41	0.53
2:C:84:PHE:CG	2:C:152:TYR:HB2	2.42	0.53
2:C:170:PHE:CD2	2:C:213:ARG:HD2	2.43	0.53
1:D:199:HIS:CD2	1:D:200:GLN:HG3	2.44	0.53
2:E:18:ARG:HH21	2:E:67:SER:HG	1.52	0.53
2:F:110:GLN:HB3	2:F:167:TYR:OH	2.08	0.53
2:F:188:ARG:NE	2:F:188:ARG:HA	2.24	0.53
1:A:457:ILE:HG23	1:A:482:SER:OG	2.08	0.53
2:E:130:GLU:HG3	7:E:516:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:185:TRP:CE3	2:F:186:ALA:N	2.76	0.53
1:A:106:GLY:O	1:A:432:ASN:ND2	2.41	0.53
1:A:166:THR:HG21	1:A:530:LYS:HD2	1.91	0.53
1:A:465:TYR:HB2	1:A:478:PHE:HZ	1.74	0.53
2:B:135:LEU:C	2:B:139:LEU:HD22	2.34	0.53
2:B:152:TYR:HD1	2:B:153:VAL:HG12	1.72	0.53
1:D:152:LYS:HD3	1:D:560:GLN:O	2.09	0.53
1:D:336:TRP:HB2	1:D:358:LEU:HD22	1.90	0.53
2:F:188:ARG:NH1	7:F:432:HOH:O	2.41	0.53
1:A:139:ASP:OD1	7:A:736:HOH:O	2.19	0.53
2:B:153:VAL:HA	2:B:156:SER:HG	1.74	0.53
2:C:4:LEU:HB3	2:C:31:GLU:OE1	2.08	0.53
2:C:48:ASN:O	7:C:413:HOH:O	2.19	0.53
2:C:69:ASN:HB3	2:C:73:TYR:CZ	2.44	0.53
1:D:338:ALA:HB2	1:D:354:VAL:HA	1.91	0.53
2:F:215:ASN:O	7:F:410:HOH:O	2.19	0.53
1:A:182:ILE:HD13	1:A:182:ILE:H	1.73	0.52
1:A:475:TYR:HE2	1:A:506:TYR:CE1	2.27	0.52
1:A:547:MET:HE3	1:A:548:PRO:O	2.09	0.52
1:A:557:LYS:O	1:A:561:ILE:HG13	2.10	0.52
2:C:122:GLU:OE1	7:C:414:HOH:O	2.19	0.52
1:D:309:MET:HE3	1:D:545:PHE:CZ	2.44	0.52
2:E:8:LEU:HB2	2:E:56:VAL:HG13	1.89	0.52
1:A:215:GLN:HB2	7:A:720:HOH:O	2.08	0.52
1:A:314:PRO:HA	1:A:317:ARG:NH1	2.24	0.52
1:A:329:ASP:OD1	1:A:340:ASN:N	2.27	0.52
2:B:6:ILE:CG2	2:B:33:ARG:HD2	2.39	0.52
1:D:90:THR:HG21	1:D:397:GLY:CA	2.39	0.52
2:E:45:LEU:N	7:E:401:HOH:O	2.43	0.52
2:F:26:LYS:NZ	7:F:401:HOH:O	2.17	0.52
2:F:161:SER:C	2:F:164:PHE:HB2	2.34	0.52
1:A:94:VAL:HG22	1:A:96:ALA:H	1.72	0.52
1:A:233:THR:C	7:A:769:HOH:O	2.51	0.52
1:A:363:PHE:HE2	1:A:419:LEU:HD11	1.74	0.52
1:A:442:GLN:HG2	1:A:462:PHE:CZ	2.44	0.52
1:D:336:TRP:CB	1:D:358:LEU:HD22	2.39	0.52
2:F:32:TYR:HD1	2:F:32:TYR:H	1.57	0.52
2:F:117:LYS:HA	2:F:121:GLN:HB2	1.91	0.52
2:F:181:LYS:N	7:F:411:HOH:O	2.40	0.52
1:A:41:SER:HB2	2:B:143:PRO:HD2	1.91	0.52
1:A:152:LYS:HD3	1:A:561:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ARG:HG2	1:A:425:ARG:HG3	1.91	0.52
2:B:10:TYR:CG	2:B:12:PRO:HD2	2.45	0.52
5:D:603:ATP:N3	5:D:603:ATP:C2'	2.70	0.52
1:A:94:VAL:HG11	1:A:97:ILE:HD11	1.92	0.52
1:A:165:ALA:HA	5:A:603:ATP:O5'	2.09	0.52
1:A:295:PHE:CD2	1:A:298:ALA:HB2	2.43	0.52
2:C:198:SER:O	2:C:200:PRO:HD3	2.09	0.52
1:D:332:SER:HB2	1:D:539:GLY:H	1.74	0.52
1:D:335:GLY:O	1:D:539:GLY:HA3	2.10	0.52
2:F:26:LYS:HG2	2:F:81:LYS:HZ3	1.74	0.52
1:A:122:LEU:HA	1:A:125:PHE:CZ	2.45	0.52
1:A:142:GLY:O	1:A:185:PRO:HD2	2.09	0.52
1:D:77:ILE:O	1:D:81:VAL:HG23	2.09	0.52
1:D:276:THR:OG1	1:D:277:ILE:N	2.43	0.52
1:D:461:ASP:OD2	1:D:547:MET:HE1	2.10	0.52
1:D:480:GLU:HB2	1:D:528:PHE:HZ	1.69	0.52
2:E:12:PRO:HB2	2:E:208:TYR:CE2	2.45	0.52
2:F:24:ARG:HG3	2:F:30:PHE:CZ	2.45	0.52
1:D:248:GLY:O	1:D:267:LEU:HD13	2.10	0.52
2:F:132:VAL:HG13	2:F:179:SER:CB	2.39	0.52
1:A:241:ILE:HG22	1:A:242:VAL:N	2.25	0.52
2:B:18:ARG:HG2	2:B:159:THR:HB	1.92	0.52
2:C:199:LEU:O	7:C:402:HOH:O	2.19	0.52
1:D:354:VAL:HG11	1:D:379:LEU:HD11	1.90	0.52
1:D:465:TYR:HA	1:D:551:VAL:HB	1.91	0.52
1:D:513:LYS:NZ	1:D:575:PHE:HD2	2.07	0.52
2:E:10:TYR:HB3	2:E:13:SER:CB	2.40	0.52
1:A:99:LEU:HG	1:A:555:ASN:OD1	2.09	0.52
1:A:213:ARG:HH21	1:A:296:PRO:CD	2.22	0.52
1:A:472:PRO:HD2	7:A:843:HOH:O	2.10	0.52
2:C:78:TRP:CD1	2:C:81:LYS:HZ2	2.28	0.52
1:D:241:ILE:O	1:D:245:ILE:HG23	2.10	0.52
1:D:452:LEU:HD11	1:D:490:LEU:HD23	1.91	0.52
2:E:139:LEU:O	2:E:141:ASP:N	2.43	0.52
1:A:328:HIS:CG	1:A:329:ASP:N	2.78	0.52
1:A:498:ASP:HB3	1:A:510:ARG:HH12	1.75	0.52
2:B:111:PHE:HA	2:B:114:TRP:NE1	2.25	0.52
1:D:75:PRO:O	1:D:79:ARG:HG2	2.10	0.52
1:D:262:ALA:HA	1:D:265:LYS:HE2	1.91	0.52
1:D:317:ARG:HA	1:D:320:ALA:HB3	1.92	0.52
2:E:13:SER:O	2:E:17:MET:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASN:OD1	2:B:143:PRO:HD3	2.10	0.51
1:A:250:LEU:HD21	1:A:260:ARG:HA	1.91	0.51
2:C:8:LEU:HD13	2:C:44:LEU:HB2	1.92	0.51
1:D:332:SER:C	5:D:603:ATP:N7	2.69	0.51
2:F:84:PHE:HD1	2:F:85:PHE:N	2.08	0.51
1:A:164:THR:HG23	1:A:534:HIS:CE1	2.45	0.51
1:A:366:VAL:O	7:A:739:HOH:O	2.19	0.51
2:B:168:GLU:CD	2:B:174:SER:HA	2.36	0.51
1:D:232:ARG:NH1	7:D:784:HOH:O	2.43	0.51
1:D:526:GLY:O	1:D:529:ARG:HG2	2.09	0.51
2:E:164:PHE:HE2	2:E:183:ILE:HA	1.76	0.51
1:A:109:LYS:HG2	7:A:762:HOH:O	2.10	0.51
1:A:336:TRP:HD1	5:A:603:ATP:C5	2.28	0.51
2:C:144:TYR:HB3	2:C:154:ASP:OD2	2.10	0.51
1:D:10:MET:SD	7:D:931:HOH:O	2.59	0.51
1:D:384:ILE:HG13	7:D:841:HOH:O	2.11	0.51
2:F:163:TRP:O	2:F:166:ALA:N	2.42	0.51
2:C:26:LYS:HD3	2:C:74:VAL:CG1	2.39	0.51
1:D:48:CYS:O	7:D:732:HOH:O	2.19	0.51
1:D:368:GLU:O	7:D:731:HOH:O	2.19	0.51
2:F:70:VAL:HG21	7:F:405:HOH:O	2.09	0.51
1:A:407:VAL:CG2	1:A:419:LEU:HB3	2.40	0.51
2:C:153:VAL:O	2:C:157:LEU:HD23	2.11	0.51
1:D:75:PRO:O	1:D:78:LYS:HG2	2.10	0.51
1:D:197:ASP:HB2	1:D:256:VAL:HG21	1.93	0.51
1:D:223:PHE:HB3	1:D:309:MET:SD	2.51	0.51
1:D:328:HIS:CG	1:D:329:ASP:N	2.78	0.51
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.45	0.51
2:F:203:GLU:OE2	7:F:409:HOH:O	2.18	0.51
1:A:495:ASN:HB3	1:A:499:ARG:HH11	1.76	0.51
2:C:20:ARG:HB3	2:C:198:SER:OG	2.11	0.51
1:D:99:LEU:O	1:D:557:LYS:HD3	2.09	0.51
1:D:208:SER:O	1:D:211:LEU:HB2	2.10	0.51
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.41	0.51
1:A:45:LEU:HD11	1:A:50:LEU:HD22	1.93	0.51
1:A:152:LYS:HE2	1:A:565:ASN:CB	2.31	0.51
1:A:197:ASP:OD2	1:A:200:GLN:HB2	2.10	0.51
1:A:224:ALA:O	1:A:228:VAL:HG23	2.11	0.51
2:B:86:PRO:HD3	2:B:152:TYR:HE2	1.75	0.51
2:B:135:LEU:O	2:B:139:LEU:HD22	2.11	0.51
2:C:26:LYS:HE2	2:C:75:ASP:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:PRO:HG2	2:E:184:ALA:HB3	1.92	0.51
1:D:219:VAL:HG21	1:D:231:PHE:CZ	2.44	0.51
1:D:243:THR:HA	1:D:246:LYS:HD3	1.93	0.51
1:D:256:VAL:HB	1:D:259:VAL:HG12	1.92	0.51
1:D:543:GLY:C	1:D:544:GLN:HG2	2.34	0.51
2:E:85:PHE:HB3	2:E:92:ARG:HG2	1.93	0.51
1:A:330:TYR:CG	1:A:421:PHE:HE2	2.28	0.51
1:A:455:GLU:OE1	1:A:485:THR:HB	2.11	0.51
2:B:26:LYS:HG3	2:B:28:VAL:H	1.75	0.51
1:D:203:TYR:CE2	1:D:253:ARG:HD3	2.44	0.51
1:D:213:ARG:HG3	1:D:214:ASP:H	1.76	0.51
1:D:213:ARG:HG3	1:D:214:ASP:N	2.26	0.51
1:D:238:TRP:CG	1:D:239:GLU:H	2.29	0.51
1:D:329:ASP:OD1	1:D:340:ASN:N	2.37	0.51
1:D:423:CYS:HB3	1:D:543:GLY:N	2.26	0.51
5:D:603:ATP:O2'	5:D:603:ATP:C4	2.62	0.51
2:E:192:LYS:NZ	2:E:194:SER:HB3	2.23	0.51
2:F:23:LEU:HD22	2:F:28:VAL:HG11	1.92	0.51
1:A:62:LYS:HZ1	1:A:376:PRO:HB2	1.75	0.51
1:A:277:ILE:HG23	1:A:278:ARG:N	2.25	0.51
2:B:65:CYS:O	2:B:69:ASN:HB3	2.11	0.51
2:B:145:PHE:HD2	2:B:153:VAL:HG22	1.75	0.51
2:C:31:GLU:HB3	7:C:438:HOH:O	2.11	0.51
1:D:163:GLY:HA3	1:D:168:ASN:HD21	1.75	0.51
1:D:229:HIS:ND1	1:D:529:ARG:HD3	2.25	0.51
1:D:233:THR:HG23	1:D:525:LYS:NZ	2.25	0.51
1:A:90:THR:HG21	1:A:112:PRO:HG2	1.93	0.51
1:A:407:VAL:HB	1:A:541:SER:HB2	1.94	0.50
2:B:103:ASP:O	2:B:107:THR:OG1	2.20	0.50
1:D:103:THR:HB	1:D:106:GLY:CA	2.41	0.50
1:D:478:PHE:HZ	1:D:562:LEU:HA	1.76	0.50
2:E:98:TRP:NE1	2:E:138:GLU:HG2	2.26	0.50
2:F:190:MET:HA	2:F:195:VAL:CG1	2.41	0.50
1:A:87:PRO:HD2	2:B:188:ARG:CB	2.41	0.50
1:A:201:ALA:O	1:A:205:HIS:N	2.45	0.50
1:A:330:TYR:HE1	1:A:536:LEU:O	1.95	0.50
1:A:521:ARG:HD2	1:A:562:LEU:HD11	1.94	0.50
1:D:273:LEU:O	1:D:276:THR:HG23	2.10	0.50
2:F:114:TRP:CD1	2:F:167:TYR:CE1	2.99	0.50
1:A:199:HIS:CE1	1:A:567:VAL:HG11	2.36	0.50
2:B:79:PRO:HA	7:B:423:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ARG:CA	1:D:343:PRO:HG2	2.41	0.50
1:D:149:PHE:N	7:D:788:HOH:O	2.44	0.50
1:D:334:GLU:HB3	1:D:398:LEU:HD12	1.93	0.50
1:D:509:SER:HA	1:D:512:CYS:SG	2.51	0.50
1:A:125:PHE:HD1	1:A:126:ARG:N	2.10	0.50
1:A:166:THR:HG23	4:A:602:MET:OXT	2.12	0.50
1:A:230:ALA:O	1:A:234:PHE:N	2.44	0.50
1:D:107:ARG:HB2	1:D:552:LYS:HE3	1.92	0.50
1:D:360:TYR:CE2	1:D:362:GLU:OE2	2.64	0.50
1:D:365:PRO:HA	1:D:388:TYR:CD1	2.46	0.50
2:F:68:LEU:O	2:F:72:GLN:HG2	2.11	0.50
2:F:183:ILE:O	2:F:187:LYS:HD2	2.11	0.50
1:A:87:PRO:HG2	2:B:188:ARG:HG2	1.93	0.50
1:A:93:PRO:O	2:B:181:LYS:HG2	2.12	0.50
1:A:240:GLU:HG3	1:A:251:SER:HB3	1.93	0.50
1:A:248:GLY:HA2	1:A:267:LEU:HG	1.94	0.50
1:A:479:TRP:HB3	1:A:481:ILE:HD11	1.93	0.50
2:B:127:GLU:OE1	7:B:411:HOH:O	2.19	0.50
1:D:13:VAL:HG11	1:D:130:ALA:HB3	1.93	0.50
1:D:145:LEU:HD11	1:D:210:ILE:HD13	1.93	0.50
1:D:528:PHE:CB	1:D:531:ILE:HD12	2.36	0.50
2:E:90:TYR:O	2:E:93:ALA:HB3	2.10	0.50
6:E:301:GSH:O31	7:E:413:HOH:O	2.19	0.50
2:F:8:LEU:HD22	2:F:33:ARG:HE	1.76	0.50
2:F:198:SER:N	7:F:436:HOH:O	2.45	0.50
1:A:62:LYS:HA	1:A:400:ARG:CZ	2.41	0.50
1:A:146:GLN:HB3	1:A:220:PHE:HD2	1.77	0.50
2:B:92:ARG:O	2:B:95:ALA:HB3	2.12	0.50
1:D:10:MET:HA	1:D:13:VAL:CG2	2.42	0.50
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.47	0.50
2:E:204:LYS:O	2:E:207:ALA:HB3	2.10	0.50
2:F:150:PHE:CD1	2:F:192:LYS:HG3	2.47	0.50
2:F:162:SER:HB2	2:F:205:ILE:HD13	1.92	0.50
1:A:23:ASN:O	1:A:27:VAL:HG12	2.11	0.50
1:A:272:GLU:O	1:A:275:GLU:HB3	2.11	0.50
2:B:125:LYS:O	2:B:129:ILE:HG12	2.11	0.50
2:C:98:TRP:CH2	2:C:135:LEU:HG	2.47	0.50
2:C:102:VAL:O	2:C:107:THR:HG23	2.11	0.50
1:D:339:ALA:O	1:D:353:ALA:N	2.44	0.50
1:D:396:ALA:N	7:D:775:HOH:O	2.38	0.50
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:PHE:O	1:D:532:GLN:HG3	2.12	0.50
2:E:11:TRP:CD1	2:E:12:PRO:HD3	2.47	0.50
1:A:240:GLU:O	1:A:241:ILE:C	2.54	0.50
1:A:480:GLU:HG2	1:A:525:LYS:HA	1.94	0.50
2:B:70:VAL:O	2:B:74:VAL:HB	2.11	0.50
1:D:174:ASN:OD1	1:D:174:ASN:N	2.33	0.50
1:D:440:ASP:O	1:D:444:SER:N	2.44	0.50
1:A:480:GLU:OE1	1:A:528:PHE:N	2.41	0.50
2:B:66:GLU:OE2	2:B:69:ASN:CG	2.54	0.50
1:D:70:ASP:OD2	1:D:104:SER:HA	2.12	0.50
1:D:121:THR:HG22	1:D:336:TRP:CZ2	2.45	0.50
1:D:202:LEU:HA	1:D:205:HIS:HB2	1.94	0.50
1:D:291:ILE:HG21	1:D:301:VAL:HG22	1.94	0.50
1:D:473:GLY:HA3	1:D:475:TYR:CE2	2.46	0.50
1:A:78:LYS:CE	1:A:554:SER:HA	2.41	0.49
1:A:104:SER:HB2	1:A:109:LYS:HG3	1.94	0.49
1:A:364:LEU:O	1:A:389:GLU:N	2.45	0.49
1:A:379:LEU:HG	1:A:417:PRO:HG3	1.94	0.49
1:D:223:PHE:HD2	1:D:225:HIS:HE1	1.59	0.49
1:D:301:VAL:HB	1:D:325:LEU:HD23	1.94	0.49
2:E:18:ARG:NH2	7:E:425:HOH:O	2.43	0.49
2:E:166:ALA:O	2:E:169:LYS:HG2	2.11	0.49
2:F:26:LYS:HD2	2:F:74:VAL:HG12	1.94	0.49
1:A:194:PHE:O	7:A:737:HOH:O	2.19	0.49
2:B:66:GLU:HB2	2:B:69:ASN:HB2	1.94	0.49
2:B:69:ASN:OD1	2:C:96:ARG:NE	2.45	0.49
1:D:143:LYS:CD	1:D:212:PHE:HB2	2.32	0.49
1:D:494:CYS:HB2	1:D:520:LEU:HB2	1.95	0.49
2:E:121:GLN:HG2	2:E:125:LYS:HE3	1.93	0.49
2:E:166:ALA:HA	2:E:169:LYS:HG2	1.93	0.49
1:A:389:GLU:OE2	1:A:402:ARG:NH2	2.45	0.49
2:B:207:ALA:O	2:B:211:GLU:N	2.36	0.49
2:C:84:PHE:CD1	2:C:85:PHE:N	2.79	0.49
2:C:108:ASP:O	2:C:112:LYS:HG2	2.13	0.49
1:D:39:ASN:OD1	1:D:90:THR:HA	2.12	0.49
1:D:126:ARG:HE	1:D:182:ILE:HD11	1.76	0.49
2:F:129:ILE:HG13	2:F:130:GLU:N	2.28	0.49
1:A:96:ALA:HB1	1:A:163:GLY:N	2.28	0.49
2:B:23:LEU:HD23	2:B:30:PHE:HB3	1.94	0.49
2:C:143:PRO:HG2	7:C:424:HOH:O	2.12	0.49
1:D:233:THR:O	1:D:237:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HE3	1:A:293:ALA:HB1	1.95	0.49
1:A:333:SER:O	5:A:603:ATP:H2	1.96	0.49
1:A:407:VAL:HG21	1:A:419:LEU:HB3	1.94	0.49
1:A:453:SER:C	1:A:456:LYS:H	2.20	0.49
2:B:65:CYS:HB3	7:B:437:HOH:O	2.12	0.49
2:B:195:VAL:HG11	7:B:414:HOH:O	2.13	0.49
1:D:224:ALA:HA	1:D:316:LEU:HD22	1.94	0.49
1:D:330:TYR:CE2	1:D:421:PHE:HZ	2.31	0.49
2:F:39:ASN:OD1	7:F:413:HOH:O	2.20	0.49
2:F:139:LEU:HB3	2:F:181:LYS:CD	2.32	0.49
1:A:445:VAL:HG13	1:A:479:TRP:NE1	2.27	0.49
2:C:57:LEU:O	2:C:64:VAL:HG22	2.12	0.49
2:C:60:ASN:O	2:C:60:ASN:ND2	2.44	0.49
2:C:146:GLY:HA3	2:C:151:GLY:HA3	1.95	0.49
1:A:148:ILE:HG12	1:A:170:TYR:OH	2.12	0.49
1:A:558:VAL:O	1:A:561:ILE:HB	2.13	0.49
2:B:15:PHE:HB3	2:B:67:SER:OG	2.13	0.49
2:B:26:LYS:CD	2:B:28:VAL:HB	2.43	0.49
2:B:135:LEU:HB2	2:B:182:LEU:HD11	1.95	0.49
1:D:103:THR:N	7:D:771:HOH:O	2.35	0.49
1:D:528:PHE:HA	1:D:531:ILE:CG1	2.43	0.49
2:F:70:VAL:HA	2:F:73:TYR:CD2	2.47	0.49
2:F:165:GLN:HB3	2:F:202:SER:HB3	1.95	0.49
1:A:305:MET:HB3	1:A:313:VAL:HG22	1.93	0.49
1:A:307:GLY:O	1:A:310:GLU:HB2	2.13	0.49
2:B:105:LYS:NZ	2:B:134:ILE:HD12	2.28	0.49
2:B:163:TRP:HA	2:B:205:ILE:HD11	1.95	0.49
2:C:53:LYS:NZ	7:C:444:HOH:O	2.46	0.49
2:F:108:ASP:O	2:F:112:LYS:HG2	2.13	0.49
1:A:10:MET:O	1:A:14:ILE:HG13	2.12	0.49
1:A:33:LYS:HE3	1:A:57:PRO:HG3	1.95	0.49
1:A:91:GLY:HA2	2:B:143:PRO:HG3	1.93	0.49
1:A:95:PRO:HG3	7:A:851:HOH:O	2.13	0.49
1:A:290:LEU:CD1	1:A:319:TYR:HD1	2.24	0.49
1:A:368:GLU:N	7:A:739:HOH:O	2.45	0.49
1:A:494:CYS:CB	1:A:520:LEU:HB3	2.40	0.49
1:D:388:TYR:OH	7:D:734:HOH:O	2.20	0.49
2:F:128:PHE:CE1	2:F:175:ILE:HB	2.48	0.49
1:A:43:ILE:HG13	1:A:44:TYR:N	2.27	0.48
1:A:153:GLN:HA	1:A:560:GLN:HG2	1.94	0.48
1:A:420:LYS:HG2	1:A:421:PHE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:ARG:NE	7:B:434:HOH:O	2.46	0.48
2:C:70:VAL:O	2:C:74:VAL:HG23	2.12	0.48
2:C:99:ALA:HB2	2:C:152:TYR:CE2	2.48	0.48
1:D:473:GLY:C	1:D:516:GLY:H	2.21	0.48
2:E:10:TYR:HB3	2:E:13:SER:HB3	1.95	0.48
1:A:103:THR:HG22	1:A:548:PRO:HB3	1.93	0.48
1:A:475:TYR:CE2	1:A:506:TYR:CE1	3.01	0.48
1:D:304:ILE:HG13	1:D:328:HIS:HB3	1.93	0.48
2:F:7:LEU:HD13	2:F:30:PHE:HB2	1.94	0.48
2:F:132:VAL:C	2:F:179:SER:HB3	2.39	0.48
1:A:203:TYR:HB3	1:A:237:VAL:HG21	1.95	0.48
1:D:10:MET:O	1:D:13:VAL:HG23	2.12	0.48
1:D:121:THR:HG22	3:D:601:JAA:C13	2.44	0.48
1:D:242:VAL:O	1:D:245:ILE:HG13	2.13	0.48
2:F:180:PRO:O	2:F:183:ILE:HG22	2.12	0.48
1:A:149:PHE:CZ	1:A:527:THR:HG22	2.48	0.48
1:A:421:PHE:CG	1:A:542:ALA:HB2	2.49	0.48
1:D:39:ASN:HD22	2:E:142:LYS:HA	1.78	0.48
1:D:538:LEU:HD23	1:D:540:SER:HB2	1.93	0.48
1:A:86:SER:CB	2:B:188:ARG:HE	2.26	0.48
1:A:97:ILE:H	1:A:163:GLY:H	1.61	0.48
2:C:40:LYS:HZ3	2:C:40:LYS:N	2.08	0.48
1:D:145:LEU:HG	1:D:209:GLY:HA3	1.95	0.48
1:D:198:VAL:O	1:D:202:LEU:N	2.41	0.48
1:D:490:LEU:O	1:D:520:LEU:HD23	2.13	0.48
2:F:7:LEU:HD21	2:F:23:LEU:HD12	1.94	0.48
2:F:185:TRP:O	2:F:189:CYS:N	2.42	0.48
2:B:102:VAL:HG21	2:B:157:LEU:HG	1.94	0.48
2:C:64:VAL:HB	2:C:73:TYR:CD2	2.48	0.48
2:C:113:VAL:HG23	2:C:125:LYS:HG2	1.96	0.48
1:D:62:LYS:HE3	7:D:766:HOH:O	2.14	0.48
1:D:90:THR:HG21	1:D:397:GLY:HA3	1.94	0.48
1:D:250:LEU:HD21	1:D:260:ARG:HG3	1.95	0.48
2:E:26:LYS:HG3	2:E:78:TRP:NE1	2.29	0.48
2:E:96:ARG:HD2	2:F:73:TYR:HE1	1.76	0.48
2:F:192:LYS:HA	7:F:468:HOH:O	2.13	0.48
2:B:50:ILE:HG21	2:C:134:ILE:HG13	1.95	0.48
2:C:69:ASN:HB3	2:C:73:TYR:CE2	2.49	0.48
2:F:18:ARG:NH2	2:F:102:VAL:HG12	2.28	0.48
1:A:91:GLY:HA3	2:B:141:ASP:C	2.39	0.48
1:A:351:THR:OG1	1:A:418:GLN:OE1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ASN:ND2	2:E:143:PRO:HD3	2.29	0.48
1:D:97:ILE:HD13	1:D:112:PRO:HA	1.96	0.48
1:D:168:ASN:HD22	5:D:603:ATP:PA	2.37	0.48
1:D:405:ASP:HB2	1:D:541:SER:HB2	1.96	0.48
2:F:166:ALA:HA	2:F:206:VAL:HG22	1.95	0.48
2:F:190:MET:HA	2:F:195:VAL:HG13	1.95	0.48
1:A:95:PRO:O	1:A:161:PRO:HG2	2.14	0.48
1:D:106:GLY:HA3	1:D:432:ASN:HB3	1.94	0.48
1:D:333:SER:HA	5:D:603:ATP:C8	2.48	0.48
2:E:145:PHE:CE2	2:E:157:LEU:HD13	2.48	0.48
2:F:21:VAL:HG12	2:F:155:ILE:HG12	1.96	0.48
2:F:40:LYS:H	2:F:40:LYS:HE2	1.79	0.48
2:F:163:TRP:N	2:F:163:TRP:CE3	2.81	0.48
1:A:277:ILE:O	1:A:281:CYS:SG	2.70	0.48
1:A:333:SER:HA	5:A:603:ATP:N3	2.29	0.48
1:A:421:PHE:CZ	1:A:541:SER:HA	2.48	0.48
2:B:11:TRP:CD1	2:B:12:PRO:HD3	2.49	0.48
2:B:205:ILE:HD11	7:B:403:HOH:O	2.14	0.48
1:D:98:SER:C	1:D:556:ALA:HB3	2.39	0.48
1:D:108:PRO:CG	1:D:552:LYS:H	2.24	0.48
1:D:377:VAL:HG13	1:D:378:GLY:O	2.14	0.48
1:D:538:LEU:HD21	1:D:540:SER:HB2	1.94	0.48
2:E:111:PHE:HA	2:E:114:TRP:NE1	2.28	0.48
2:F:139:LEU:HD22	2:F:181:LYS:HD3	1.96	0.48
1:D:32:LEU:HB2	1:D:360:TYR:CD1	2.49	0.47
1:D:273:LEU:HA	1:D:276:THR:HG23	1.96	0.47
1:D:477:ILE:HG21	1:D:497:LEU:HD13	1.96	0.47
2:F:161:SER:HA	2:F:164:PHE:HD2	1.78	0.47
1:A:125:PHE:CD1	1:A:126:ARG:N	2.82	0.47
1:A:150:SER:HB3	1:A:170:TYR:HD2	1.78	0.47
2:C:178:GLU:HB3	7:C:468:HOH:O	2.14	0.47
1:D:53:ASN:HB3	1:D:54:ALA:H	1.47	0.47
1:D:164:THR:HA	5:D:603:ATP:O1G	2.14	0.47
1:D:211:LEU:C	1:D:212:PHE:HD1	2.22	0.47
1:D:223:PHE:CD2	1:D:533:GLU:HA	2.49	0.47
2:E:37:PHE:CE1	6:E:301:GSH:HA32	2.49	0.47
2:E:135:LEU:HD12	2:E:182:LEU:HD11	1.97	0.47
1:A:230:ALA:C	1:A:233:THR:H	2.23	0.47
2:C:187:LYS:NZ	1:D:499:ARG:HH12	2.11	0.47
2:C:197:LYS:O	7:C:415:HOH:O	2.20	0.47
1:D:94:VAL:HG11	1:D:97:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.95	0.47
2:F:132:VAL:HG23	2:F:182:LEU:HD22	1.96	0.47
1:A:152:LYS:HG2	1:A:565:ASN:OD1	2.14	0.47
1:A:185:PRO:HA	7:A:886:HOH:O	2.13	0.47
1:A:435:LYS:HB3	1:A:437:THR:HA	1.97	0.47
1:A:478:PHE:N	1:A:478:PHE:CD1	2.82	0.47
2:B:63:PRO:O	2:C:90:TYR:HE1	1.97	0.47
1:D:303:GLY:O	1:D:327:SER:HA	2.14	0.47
2:F:91:GLY:HA2	2:F:94:GLN:OE1	2.14	0.47
1:A:70:ASP:OD1	1:A:71:VAL:HG23	2.14	0.47
1:A:310:GLU:N	1:A:311:PRO:HD2	2.29	0.47
1:A:445:VAL:HG22	1:A:479:TRP:HE1	1.79	0.47
2:C:14:MET:O	2:C:17:MET:HB2	2.14	0.47
2:C:24:ARG:HD2	7:C:427:HOH:O	2.15	0.47
2:C:176:GLU:HB2	2:C:183:ILE:HG21	1.97	0.47
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.44	0.47
1:D:389:GLU:HA	1:D:405:ASP:O	2.14	0.47
1:D:410:ILE:H	1:D:420:LYS:NZ	2.12	0.47
1:D:412:PHE:N	7:D:791:HOH:O	2.47	0.47
1:D:465:TYR:O	1:D:475:TYR:HB3	2.14	0.47
1:A:135:ASP:OD2	1:A:343:PRO:HD2	2.15	0.47
1:A:330:TYR:CE1	1:A:536:LEU:O	2.68	0.47
3:A:601:JAA:O01	4:A:602:MET:HE2	2.14	0.47
2:B:154:ASP:O	2:B:158:ILE:N	2.47	0.47
1:D:143:LYS:HA	1:D:184:SER:HB2	1.96	0.47
1:D:222:VAL:HB	1:D:533:GLU:CD	2.39	0.47
2:E:120:GLU:HB2	7:E:468:HOH:O	2.15	0.47
2:E:205:ILE:HG22	2:E:208:TYR:HE2	1.80	0.47
2:F:154:ASP:HB3	7:F:445:HOH:O	2.14	0.47
1:A:7:THR:O	1:A:7:THR:OG1	2.31	0.47
1:A:29:LYS:HE2	1:A:33:LYS:HZ1	1.79	0.47
1:A:81:VAL:CG1	1:A:97:ILE:HG13	2.43	0.47
1:A:527:THR:N	7:A:718:HOH:O	2.47	0.47
2:C:125:LYS:HD3	2:C:173:PHE:CE2	2.50	0.47
1:D:77:ILE:CG1	1:D:89:LEU:HD11	2.44	0.47
1:D:152:LYS:HD2	1:D:153:GLN:N	2.30	0.47
1:D:317:ARG:NH2	7:D:793:HOH:O	2.47	0.47
1:D:494:CYS:SG	1:D:495:ASN:ND2	2.88	0.47
2:E:10:TYR:CG	2:E:12:PRO:HD2	2.50	0.47
2:E:65:CYS:O	2:E:66:GLU:HB2	2.15	0.47
2:E:171:GLY:O	2:E:172:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.49	0.47
1:A:46:GLN:HB2	2:B:148:ASP:O	2.15	0.47
1:A:90:THR:HG21	1:A:112:PRO:CG	2.45	0.47
1:A:90:THR:HG1	1:A:91:GLY:H	1.55	0.47
1:A:103:THR:CG2	1:A:548:PRO:HB3	2.45	0.47
1:A:105:GLN:NE2	7:A:722:HOH:O	2.13	0.47
1:A:164:THR:HA	1:A:557:LYS:HG3	1.97	0.47
1:A:200:GLN:N	7:A:712:HOH:O	2.07	0.47
1:A:236:GLN:O	7:A:724:HOH:O	2.20	0.47
2:B:85:PHE:N	2:B:85:PHE:CD1	2.82	0.47
1:D:87:PRO:HD2	2:E:188:ARG:CB	2.37	0.47
1:D:164:THR:N	1:D:560:GLN:OE1	2.40	0.47
1:D:444:SER:HA	1:D:500:ALA:CB	2.43	0.47
1:D:470:THR:HG21	1:D:474:HIS:CE1	2.49	0.47
2:E:17:MET:SD	2:E:199:LEU:HG	2.55	0.47
2:F:44:LEU:HD13	2:F:56:VAL:HG21	1.96	0.47
1:A:71:VAL:HG11	1:A:105:GLN:NE2	2.30	0.47
1:A:232:ARG:HG2	1:A:232:ARG:O	2.15	0.47
1:A:552:LYS:O	1:A:554:SER:N	2.47	0.47
2:C:10:TYR:HB3	2:C:13:SER:HB2	1.97	0.47
2:E:188:ARG:O	2:E:188:ARG:HD3	2.14	0.47
1:A:363:PHE:CE2	1:A:419:LEU:HD11	2.50	0.47
1:A:475:TYR:CB	1:A:518:LEU:HD13	2.45	0.47
2:C:14:MET:HB2	2:C:14:MET:HE3	1.79	0.47
2:C:211:GLU:O	2:C:215:ASN:ND2	2.48	0.47
1:D:118:MET:HA	1:D:121:THR:OG1	2.15	0.47
1:D:301:VAL:HG11	1:D:316:LEU:HD21	1.97	0.47
1:D:361:PHE:HE1	1:D:392:ILE:HG23	1.79	0.47
1:D:467:ASP:O	1:D:475:TYR:CE2	2.68	0.47
1:D:534:HIS:HB3	4:D:602:MET:C	2.39	0.47
1:D:538:LEU:HD22	1:D:544:GLN:CD	2.40	0.47
2:E:99:ALA:O	2:E:103:ASP:HB2	2.15	0.47
2:F:155:ILE:O	2:F:158:ILE:HG22	2.15	0.47
1:A:131:PHE:HD1	1:A:134:ARG:HH22	1.62	0.46
1:A:498:ASP:OD2	1:A:510:ARG:NH2	2.48	0.46
1:A:519:GLU:HB2	1:A:571:PHE:CE1	2.50	0.46
2:B:129:ILE:HD12	7:B:453:HOH:O	2.14	0.46
1:D:76:TYR:O	1:D:80:MET:HG2	2.15	0.46
1:D:98:SER:CB	5:D:603:ATP:O2G	2.62	0.46
1:D:155:ILE:HD11	1:D:159:GLY:C	2.41	0.46
1:D:314:PRO:O	1:D:318:HIS:N	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:THR:HA	1:D:530:LYS:HD3	1.97	0.46
1:A:250:LEU:HD13	1:A:254:ILE:HB	1.97	0.46
1:A:353:ALA:HB2	1:A:413:TYR:CE2	2.49	0.46
1:D:9:ASP:O	1:D:13:VAL:HG22	2.15	0.46
1:D:362:GLU:HB2	1:D:391:VAL:HG13	1.96	0.46
2:E:16:GLY:HA2	2:E:55:PRO:HG3	1.96	0.46
2:E:17:MET:HB2	2:E:159:THR:HG22	1.96	0.46
2:F:24:ARG:HG3	2:F:30:PHE:CE1	2.50	0.46
2:F:151:GLY:O	2:F:154:ASP:HB2	2.14	0.46
1:A:99:LEU:HG	1:A:555:ASN:CG	2.40	0.46
1:A:169:VAL:CB	5:A:603:ATP:O3'	2.51	0.46
2:B:96:ARG:HB2	2:C:69:ASN:OD1	2.15	0.46
1:D:85:THR:CB	2:E:184:ALA:HB1	2.44	0.46
1:D:377:VAL:HB	7:D:782:HOH:O	2.14	0.46
1:D:496:CYS:HA	1:D:499:ARG:NH1	2.30	0.46
1:A:35:ILE:HG12	1:A:395:TYR:CZ	2.49	0.46
1:A:114:THR:HG21	2:B:141:ASP:HB3	1.97	0.46
1:A:154:TYR:CB	1:A:560:GLN:HA	2.45	0.46
1:A:225:HIS:HB2	1:A:529:ARG:HH21	1.80	0.46
1:A:527:THR:O	1:A:530:LYS:HB3	2.15	0.46
2:C:65:CYS:O	2:C:66:GLU:HB2	2.16	0.46
2:C:110:GLN:HE21	2:C:167:TYR:HE2	1.63	0.46
2:C:164:PHE:CZ	2:C:182:LEU:HD21	2.50	0.46
1:D:106:GLY:C	1:D:432:ASN:HB3	2.40	0.46
1:D:152:LYS:CD	1:D:561:ILE:HA	2.45	0.46
1:D:441:LEU:O	1:D:445:VAL:HG23	2.15	0.46
1:D:529:ARG:O	1:D:533:GLU:HG3	2.16	0.46
1:D:557:LYS:HD2	5:D:603:ATP:PG	2.56	0.46
2:F:124:GLY:HA2	2:F:127:GLU:CD	2.41	0.46
2:F:167:TYR:N	2:F:167:TYR:HD1	2.13	0.46
1:A:72:GLU:O	1:A:76:TYR:CD2	2.69	0.46
2:B:66:GLU:O	2:B:70:VAL:HG23	2.15	0.46
1:D:402:ARG:NH2	7:D:729:HOH:O	2.43	0.46
1:D:461:ASP:OD2	1:D:547:MET:CE	2.63	0.46
2:E:48:ASN:HB2	7:E:446:HOH:O	2.15	0.46
1:A:104:SER:N	1:A:107:ARG:O	2.43	0.46
1:A:313:VAL:HA	7:A:940:HOH:O	2.15	0.46
1:A:465:TYR:O	1:A:476:ALA:N	2.46	0.46
1:D:97:ILE:HG22	1:D:98:SER:N	2.31	0.46
2:F:26:LYS:HE3	2:F:78:TRP:O	2.15	0.46
2:B:132:VAL:HG22	2:B:182:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:191:GLU:HA	1:D:450:LYS:HD2	1.98	0.46
1:D:477:ILE:O	1:D:477:ILE:HG12	2.15	0.46
2:F:185:TRP:O	2:F:188:ARG:N	2.49	0.46
1:A:303:GLY:O	1:A:328:HIS:N	2.49	0.46
1:A:544:GLN:NE2	7:A:730:HOH:O	2.17	0.46
2:C:10:TYR:HB3	2:C:13:SER:CB	2.46	0.46
1:D:165:ALA:HB1	5:D:603:ATP:C2	2.51	0.46
1:D:222:VAL:HG21	4:D:602:MET:N	2.30	0.46
1:D:467:ASP:OD2	1:D:475:TYR:HE1	1.99	0.46
2:E:51:HIS:O	2:E:53:LYS:HD2	2.16	0.46
2:E:135:LEU:HD13	2:E:157:LEU:HD11	1.96	0.46
2:F:22:ALA:O	2:F:74:VAL:HG11	2.16	0.46
1:A:97:ILE:N	1:A:163:GLY:H	2.14	0.46
1:A:157:THR:HG22	1:A:469:SER:HB3	1.98	0.46
2:C:187:LYS:HG2	1:D:451:ARG:HD3	1.98	0.46
1:D:87:PRO:HB2	2:E:143:PRO:HB3	1.96	0.46
1:D:124:LEU:HA	1:D:127:THR:HG22	1.97	0.46
1:D:152:LYS:HD3	1:D:561:ILE:CA	2.43	0.46
1:D:222:VAL:HB	1:D:533:GLU:HB3	1.97	0.46
1:D:398:LEU:HA	1:D:398:LEU:HD23	1.70	0.46
2:F:214:LYS:HE2	2:F:214:LYS:HB3	1.72	0.46
1:A:507:VAL:O	1:A:511:LYS:HB2	2.16	0.46
2:B:90:TYR:CZ	2:C:62:LYS:HB3	2.51	0.46
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.79	0.46
2:C:164:PHE:CD2	2:C:183:ILE:HD13	2.48	0.46
2:C:182:LEU:O	2:C:185:TRP:HE3	1.99	0.46
1:D:254:ILE:HD12	1:D:263:MET:SD	2.56	0.46
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.63	0.46
2:E:50:ILE:HD12	2:E:51:HIS:N	2.24	0.46
2:E:102:VAL:HG21	2:E:157:LEU:HG	1.97	0.46
2:E:158:ILE:N	7:E:403:HOH:O	2.48	0.46
2:F:167:TYR:N	2:F:167:TYR:CD1	2.84	0.46
1:A:154:TYR:HD1	1:A:155:ILE:N	2.14	0.45
1:A:207:LEU:O	1:A:210:ILE:HG12	2.16	0.45
1:A:396:ALA:HA	7:A:768:HOH:O	2.16	0.45
1:A:547:MET:O	1:A:547:MET:HG3	2.13	0.45
2:B:9:ASP:OD1	2:B:16:GLY:HA3	2.15	0.45
2:B:40:LYS:HZ1	2:B:52:LYS:HB2	1.81	0.45
2:C:146:GLY:O	7:C:417:HOH:O	2.21	0.45
1:D:98:SER:HB2	1:D:557:LYS:CD	2.46	0.45
2:E:66:GLU:CD	2:F:100:ASP:OD2	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:HB3	2:B:144:TYR:HB2	1.99	0.45
1:A:76:TYR:HB3	1:A:88:ILE:HG21	1.98	0.45
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.46	0.45
2:B:96:ARG:C	2:C:69:ASN:HD21	2.24	0.45
2:C:10:TYR:OH	2:C:208:TYR:OH	2.27	0.45
2:C:72:GLN:NE2	7:C:425:HOH:O	2.35	0.45
1:D:437:THR:O	1:D:440:ASP:N	2.48	0.45
2:E:10:TYR:CD2	2:E:12:PRO:HD2	2.51	0.45
2:E:110:GLN:O	2:E:113:VAL:HG12	2.15	0.45
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.51	0.45
2:F:42:PRO:HA	2:F:45:LEU:HG	1.98	0.45
2:F:84:PHE:CD1	2:F:85:PHE:N	2.83	0.45
2:F:106:PHE:O	2:F:110:GLN:HG3	2.16	0.45
2:C:187:LYS:HE3	1:D:493:CYS:HA	1.98	0.45
1:D:24:ALA:HA	1:D:27:VAL:HG12	1.98	0.45
1:D:99:LEU:HA	1:D:109:LYS:O	2.16	0.45
1:D:108:PRO:HG3	1:D:555:ASN:ND2	2.30	0.45
1:D:113:PHE:CE1	1:D:333:SER:HB3	2.52	0.45
1:D:330:TYR:CZ	1:D:421:PHE:HZ	2.34	0.45
1:D:393:THR:HG23	1:D:399:TYR:HA	1.97	0.45
2:E:17:MET:HA	2:E:20:ARG:CD	2.47	0.45
2:F:21:VAL:O	2:F:194:SER:HB2	2.15	0.45
1:A:132:ARG:O	1:A:136:PHE:N	2.48	0.45
1:A:310:GLU:HA	1:A:313:VAL:HG23	1.97	0.45
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.86	0.45
2:B:62:LYS:HB3	2:C:90:TYR:CE2	2.52	0.45
2:C:41:SER:O	7:C:416:HOH:O	2.21	0.45
2:E:11:TRP:O	2:E:200:PRO:HG3	2.15	0.45
2:F:10:TYR:CD2	2:F:12:PRO:HD2	2.52	0.45
2:F:135:LEU:HD22	2:F:182:LEU:HD11	1.97	0.45
1:A:150:SER:CB	1:A:167:THR:HA	2.46	0.45
1:A:179:MET:HE2	1:A:179:MET:HB3	1.90	0.45
1:A:398:LEU:HD13	1:A:401:TYR:CD1	2.52	0.45
1:A:426:ASN:ND2	7:A:730:HOH:O	2.50	0.45
2:B:176:GLU:HB2	2:B:183:ILE:HG21	1.98	0.45
2:C:23:LEU:HD23	2:C:78:TRP:HH2	1.81	0.45
1:D:42:ALA:HB3	1:D:45:LEU:HG	1.99	0.45
1:D:253:ARG:NH2	7:D:796:HOH:O	2.49	0.45
1:D:521:ARG:HB3	1:D:566:VAL:CG1	2.46	0.45
2:E:14:MET:HE3	2:E:15:PHE:HE1	1.82	0.45
2:F:84:PHE:HE1	2:F:85:PHE:CD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:107:THR:O	2:F:110:GLN:HB2	2.16	0.45
2:F:114:TRP:HA	2:F:170:PHE:CD2	2.50	0.45
1:A:107:ARG:HG3	1:A:433:ILE:HD11	1.99	0.45
1:A:229:HIS:CE1	1:A:525:LYS:HD2	2.51	0.45
1:A:315:LYS:HD2	1:A:315:LYS:HA	1.58	0.45
2:B:9:ASP:HB3	2:B:32:TYR:CE2	2.52	0.45
2:C:62:LYS:HA	2:C:63:PRO:HD3	1.81	0.45
1:D:10:MET:HB3	1:D:10:MET:HE2	1.64	0.45
1:D:17:PHE:CD1	1:D:18:ASP:N	2.85	0.45
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.99	0.45
1:D:295:PHE:HA	1:D:296:PRO:HD2	1.73	0.45
1:D:428:ILE:O	7:D:735:HOH:O	2.21	0.45
2:F:24:ARG:HB3	2:F:194:SER:HA	1.99	0.45
2:F:160:PHE:O	2:F:164:PHE:CG	2.70	0.45
1:A:121:THR:HG22	1:A:175:PHE:HE1	1.66	0.45
1:A:490:LEU:HD11	7:A:745:HOH:O	2.17	0.45
1:A:549:ARG:N	7:A:786:HOH:O	2.49	0.45
1:A:552:LYS:C	1:A:554:SER:N	2.74	0.45
2:C:11:TRP:CZ2	2:C:208:TYR:HB2	2.52	0.45
1:D:461:ASP:OD1	1:D:462:PHE:N	2.43	0.45
2:E:102:VAL:HG22	2:E:160:PHE:HE2	1.82	0.45
2:E:158:ILE:O	2:E:161:SER:OG	2.31	0.45
2:F:207:ALA:O	2:F:211:GLU:N	2.37	0.45
1:A:73:LEU:HA	1:A:76:TYR:HD2	1.82	0.45
1:A:94:VAL:HG23	1:A:113:PHE:O	2.17	0.45
1:A:125:PHE:O	1:A:129:PHE:HB2	2.17	0.45
1:A:162:VAL:HG23	7:A:702:HOH:O	2.16	0.45
1:A:501:PHE:HD2	1:A:506:TYR:CZ	2.35	0.45
1:D:41:SER:OG	2:E:144:TYR:O	2.35	0.45
1:D:95:PRO:HD3	2:E:181:LYS:NZ	2.32	0.45
1:D:477:ILE:HB	1:D:479:TRP:HZ3	1.82	0.45
1:D:525:LYS:HG2	7:D:701:HOH:O	2.16	0.45
2:E:70:VAL:O	2:E:74:VAL:N	2.43	0.45
2:F:142:LYS:HE2	7:F:515:HOH:O	2.15	0.45
2:F:163:TRP:HB3	2:F:167:TYR:CE1	2.51	0.45
1:A:199:HIS:HB2	1:A:525:LYS:HE2	1.99	0.45
1:A:361:PHE:HD1	1:A:392:ILE:HG12	1.82	0.45
1:A:394:ASN:OD1	7:A:741:HOH:O	2.21	0.45
1:A:435:LYS:HD3	1:A:438:GLU:H	1.82	0.45
1:A:466:ILE:CG1	1:A:552:LYS:HA	2.47	0.45
1:D:103:THR:HB	1:D:106:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PRO:HB3	1:D:555:ASN:N	2.32	0.45
1:D:160:VAL:O	1:D:162:VAL:HG22	2.17	0.45
1:D:510:ARG:HH11	1:D:575:PHE:HZ	1.64	0.45
2:E:17:MET:HB3	2:E:199:LEU:HD12	1.98	0.45
2:E:128:PHE:HE2	2:E:175:ILE:HG12	1.81	0.45
2:E:194:SER:OG	2:E:195:VAL:N	2.50	0.45
2:F:157:LEU:HG	2:F:185:TRP:HH2	1.82	0.45
1:A:102:GLY:O	1:A:548:PRO:HD3	2.17	0.45
1:A:536:LEU:HD21	7:A:765:HOH:O	2.16	0.45
2:C:136:GLU:HG2	7:C:471:HOH:O	2.16	0.45
1:D:97:ILE:HG21	1:D:110:PHE:CD1	2.52	0.45
1:D:124:LEU:HD11	1:D:339:ALA:HB2	1.98	0.45
1:D:272:GLU:O	1:D:275:GLU:HB3	2.17	0.45
1:D:351:THR:HG22	1:D:420:LYS:HD2	1.98	0.45
1:D:361:PHE:CE1	1:D:392:ILE:HG23	2.51	0.45
1:D:503:ASP:O	1:D:507:VAL:HG23	2.17	0.45
1:D:509:SER:O	1:D:513:LYS:N	2.49	0.45
2:E:24:ARG:HD2	2:E:198:SER:OG	2.16	0.45
2:F:69:ASN:OD1	2:F:70:VAL:N	2.50	0.45
1:A:238:TRP:CH2	1:A:281:CYS:SG	3.10	0.44
1:A:437:THR:HG21	1:A:439:ARG:NH2	2.10	0.44
2:B:68:LEU:HD12	2:B:69:ASN:N	2.32	0.44
2:C:89:PRO:O	2:C:92:ARG:HB2	2.17	0.44
1:D:96:ALA:HB1	1:D:163:GLY:N	2.31	0.44
1:D:152:LYS:HG2	1:D:565:ASN:HB2	1.99	0.44
1:D:330:TYR:CE2	1:D:338:ALA:HB3	2.51	0.44
1:D:409:VAL:HA	1:D:420:LYS:HZ1	1.81	0.44
1:D:455:GLU:O	1:D:456:LYS:HB2	2.17	0.44
2:E:18:ARG:HD2	2:E:156:SER:HA	1.99	0.44
2:F:142:LYS:HE3	2:F:142:LYS:HB2	1.84	0.44
1:A:219:VAL:CG1	1:A:291:ILE:HG21	2.47	0.44
1:A:464:SER:HB3	1:A:550:CYS:CB	2.46	0.44
1:A:480:GLU:HB2	1:A:528:PHE:CE2	2.51	0.44
1:D:97:ILE:CG2	1:D:111:ILE:H	2.31	0.44
1:D:113:PHE:HD1	1:D:117:LEU:CD1	2.30	0.44
1:D:132:ARG:O	1:D:136:PHE:N	2.47	0.44
1:D:193:ILE:H	1:D:193:ILE:HG12	1.54	0.44
2:F:172:ASN:O	2:F:172:ASN:ND2	2.50	0.44
1:A:53:ASN:HB3	1:A:54:ALA:H	1.41	0.44
1:A:86:SER:CB	2:B:188:ARG:HB2	2.47	0.44
1:A:494:CYS:SG	1:A:495:ASN:N	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:TYR:CD2	2:C:12:PRO:HD2	2.52	0.44
1:D:145:LEU:HD13	1:D:295:PHE:CD1	2.52	0.44
1:D:291:ILE:HG13	7:D:844:HOH:O	2.17	0.44
1:D:464:SER:HA	1:D:477:ILE:N	2.20	0.44
2:E:155:ILE:O	2:E:158:ILE:HG22	2.16	0.44
1:A:320:ALA:O	1:A:323:LEU:HB2	2.17	0.44
1:A:501:PHE:CD2	1:A:506:TYR:CZ	3.06	0.44
2:B:40:LYS:NZ	2:B:52:LYS:HB2	2.33	0.44
2:C:172:ASN:O	2:C:172:ASN:ND2	2.50	0.44
1:D:12:ARG:C	1:D:14:ILE:N	2.72	0.44
1:D:225:HIS:ND1	1:D:309:MET:SD	2.74	0.44
1:D:447:SER:HB2	1:D:496:CYS:SG	2.57	0.44
2:E:17:MET:HB2	2:E:159:THR:CG2	2.47	0.44
2:E:54:ILE:HB	2:E:55:PRO:HA	2.00	0.44
1:A:153:GLN:HG2	7:A:726:HOH:O	2.17	0.44
1:A:154:TYR:CD1	1:A:155:ILE:N	2.86	0.44
1:A:167:THR:O	1:A:171:ARG:HG2	2.17	0.44
1:A:195:SER:HA	1:A:196:PRO:HD3	1.90	0.44
1:A:204:CYS:SG	7:A:970:HOH:O	2.51	0.44
1:A:238:TRP:HH2	1:A:287:TRP:HZ2	1.63	0.44
1:A:242:VAL:CG2	1:A:277:ILE:HD13	2.47	0.44
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.81	0.44
2:B:4:LEU:HB3	2:B:31:GLU:OE1	2.17	0.44
2:B:171:GLY:O	2:B:172:ASN:HB2	2.17	0.44
2:C:128:PHE:HE1	2:C:175:ILE:HG22	1.83	0.44
2:C:150:PHE:HE2	2:C:155:ILE:HG12	1.82	0.44
1:D:138:ILE:HD12	1:D:139:ASP:O	2.17	0.44
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.53	0.44
1:D:528:PHE:HA	1:D:531:ILE:HG13	1.97	0.44
2:E:40:LYS:HB2	2:E:40:LYS:HE3	1.60	0.44
2:E:99:ALA:HB2	2:E:152:TYR:HE1	1.82	0.44
1:A:232:ARG:HA	1:A:235:GLU:CG	2.32	0.44
1:A:363:PHE:HB3	1:A:388:TYR:CB	2.48	0.44
1:A:434:ASP:OD1	1:A:435:LYS:HG3	2.18	0.44
1:A:439:ARG:O	1:A:443:LEU:HB2	2.16	0.44
1:A:463:SER:HB2	1:A:528:PHE:CE1	2.52	0.44
2:B:155:ILE:HG21	7:B:516:HOH:O	2.17	0.44
2:C:187:LYS:NZ	1:D:496:CYS:HB2	2.32	0.44
1:D:14:ILE:C	1:D:16:GLU:N	2.72	0.44
1:D:80:MET:CE	1:D:88:ILE:HG13	2.46	0.44
1:D:163:GLY:HA2	1:D:560:GLN:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:20:ARG:HB2	2:E:198:SER:HB3	2.00	0.44
2:E:116:LYS:HA	2:E:116:LYS:HD3	1.65	0.44
1:A:73:LEU:HD13	1:A:89:LEU:HD13	1.99	0.44
1:A:351:THR:HB	1:A:410:ILE:HG12	1.98	0.44
2:C:169:LYS:HB2	2:C:169:LYS:HE3	1.77	0.44
2:F:8:LEU:HD22	2:F:33:ARG:HH21	1.83	0.44
1:A:95:PRO:HD3	2:B:181:LYS:NZ	2.33	0.44
1:A:143:LYS:NZ	1:A:187:CYS:HA	2.33	0.44
1:D:433:ILE:CD1	1:D:552:LYS:HD2	2.48	0.44
1:D:477:ILE:CD1	1:D:520:LEU:HA	2.37	0.44
2:E:98:TRP:O	2:E:102:VAL:HG12	2.18	0.44
1:A:79:ARG:O	1:A:84:ASP:O	2.36	0.44
1:A:265:LYS:HG2	1:A:266:LEU:HG	2.00	0.44
1:A:330:TYR:CD1	1:A:421:PHE:HE2	2.36	0.44
1:A:337:ILE:HG13	1:A:338:ALA:H	1.83	0.44
1:A:358:LEU:N	1:A:358:LEU:HD23	2.33	0.44
2:C:16:GLY:HA3	2:C:20:ARG:NH2	2.33	0.44
2:C:129:ILE:HA	2:C:132:VAL:HG12	2.00	0.44
1:D:81:VAL:HG12	1:D:156:SER:OG	2.18	0.44
1:D:104:SER:O	1:D:107:ARG:HG2	2.18	0.44
1:D:332:SER:OG	1:D:333:SER:N	2.51	0.44
2:E:125:LYS:HB3	2:E:173:PHE:CE2	2.52	0.44
2:F:72:GLN:O	2:F:76:GLU:HG2	2.17	0.44
2:F:177:SER:O	2:F:180:PRO:HG3	2.18	0.44
1:A:99:LEU:CD1	1:A:558:VAL:H	2.26	0.43
1:A:108:PRO:HD2	1:A:433:ILE:HD11	2.00	0.43
1:A:244:ASP:HB2	1:A:250:LEU:HA	2.00	0.43
1:A:387:GLU:C	1:A:388:TYR:HD1	2.26	0.43
1:D:35:ILE:HG23	7:E:454:HOH:O	2.18	0.43
2:E:65:CYS:O	2:E:69:ASN:ND2	2.42	0.43
2:E:202:SER:O	2:E:206:VAL:HG22	2.18	0.43
2:F:163:TRP:HE3	2:F:163:TRP:H	1.64	0.43
1:A:198:VAL:HG23	1:A:524:ALA:HB3	1.99	0.43
2:C:163:TRP:HB3	2:C:167:TYR:CE1	2.53	0.43
1:D:98:SER:CA	1:D:556:ALA:HB3	2.48	0.43
1:D:227:LEU:HG	7:D:838:HOH:O	2.18	0.43
1:D:465:TYR:N	1:D:476:ALA:HA	2.15	0.43
1:D:531:ILE:HA	1:D:534:HIS:CE1	2.53	0.43
2:E:166:ALA:HA	2:E:169:LYS:CD	2.48	0.43
1:A:540:SER:HG	1:A:541:SER:N	2.16	0.43
2:B:181:LYS:H	2:B:181:LYS:HG3	1.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:PHE:CD1	1:D:17:PHE:C	2.96	0.43
1:D:528:PHE:HA	1:D:531:ILE:HD12	2.00	0.43
2:F:98:TRP:CE3	2:F:138:GLU:OE2	2.72	0.43
2:F:203:GLU:HB2	7:F:454:HOH:O	2.18	0.43
1:A:66:PRO:HA	7:A:787:HOH:O	2.18	0.43
1:A:197:ASP:CG	1:A:256:VAL:HG21	2.44	0.43
1:A:481:ILE:N	1:A:481:ILE:HD12	2.33	0.43
2:B:77:ALA:HB3	2:B:78:TRP:CZ3	2.54	0.43
1:D:13:VAL:HG21	1:D:130:ALA:CB	2.49	0.43
1:D:212:PHE:N	1:D:212:PHE:CD1	2.87	0.43
1:D:238:TRP:C	1:D:240:GLU:H	2.26	0.43
1:D:441:LEU:HB3	7:D:808:HOH:O	2.17	0.43
1:D:482:SER:CA	1:D:525:LYS:HD2	2.42	0.43
2:E:65:CYS:HB3	2:F:97:PHE:CE1	2.53	0.43
2:E:165:GLN:O	2:E:169:LYS:HE3	2.19	0.43
2:F:65:CYS:N	7:F:402:HOH:O	2.52	0.43
2:F:132:VAL:CG2	2:F:182:LEU:HD13	2.48	0.43
1:A:95:PRO:HD3	2:B:181:LYS:HZ3	1.83	0.43
2:C:135:LEU:HD23	2:C:145:PHE:CZ	2.54	0.43
2:C:188:ARG:HH12	1:D:500:ALA:HA	1.84	0.43
1:D:117:LEU:O	1:D:120:ASN:HB2	2.18	0.43
1:D:126:ARG:HE	1:D:182:ILE:CD1	2.31	0.43
1:D:176:LYS:HB2	1:D:176:LYS:HE3	1.84	0.43
1:D:461:ASP:OD2	1:D:547:MET:SD	2.77	0.43
2:E:96:ARG:NH2	2:F:76:GLU:OE2	2.52	0.43
1:A:17:PHE:CE1	1:A:127:THR:HG21	2.54	0.43
1:A:74:GLU:CD	1:A:107:ARG:HE	2.27	0.43
1:A:147:PHE:HE1	1:A:206:LEU:HG	1.83	0.43
1:A:421:PHE:CB	1:A:542:ALA:HB2	2.48	0.43
1:A:426:ASN:ND2	1:A:544:GLN:NE2	2.65	0.43
1:A:429:LEU:HD12	1:A:429:LEU:HA	1.71	0.43
1:A:504:ALA:O	1:A:507:VAL:HB	2.18	0.43
1:A:509:SER:HB3	1:A:515:ILE:CD1	2.47	0.43
2:C:14:MET:HA	2:C:17:MET:SD	2.58	0.43
2:C:117:LYS:CA	2:C:121:GLN:HB2	2.45	0.43
1:D:81:VAL:HG13	1:D:162:VAL:HG11	2.01	0.43
1:D:364:LEU:HA	1:D:365:PRO:HD3	1.92	0.43
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.54	0.43
2:F:163:TRP:O	2:F:164:PHE:C	2.60	0.43
1:A:125:PHE:CD1	1:A:182:ILE:HG13	2.54	0.43
1:A:182:ILE:HG12	1:A:183:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:TRP:CH2	1:A:287:TRP:CZ2	3.03	0.43
1:A:360:TYR:CZ	1:A:362:GLU:OE2	2.71	0.43
2:C:84:PHE:HE1	2:C:85:PHE:CD2	2.36	0.43
1:D:124:LEU:HB3	3:D:601:JAA:C15	2.49	0.43
1:D:208:SER:HA	1:D:211:LEU:HG	2.01	0.43
1:D:460:ILE:HD12	7:D:701:HOH:O	2.17	0.43
1:D:560:GLN:C	1:D:562:LEU:H	2.26	0.43
1:A:94:VAL:HG22	1:A:96:ALA:N	2.34	0.43
1:A:242:VAL:HG22	1:A:277:ILE:HD13	2.00	0.43
1:A:510:ARG:HH21	1:A:518:LEU:H	1.67	0.43
2:C:18:ARG:HH21	2:C:160:PHE:HE1	1.62	0.43
1:D:13:VAL:HG21	1:D:130:ALA:HB1	2.01	0.43
1:D:94:VAL:HG11	1:D:97:ILE:CG1	2.49	0.43
1:D:548:PRO:HG3	7:D:824:HOH:O	2.18	0.43
2:E:169:LYS:HZ1	2:E:206:VAL:HG11	1.84	0.43
1:A:117:LEU:HB2	5:A:603:ATP:C4	2.54	0.43
1:A:155:ILE:HA	1:A:161:PRO:HA	1.99	0.43
2:B:127:GLU:OE1	7:B:412:HOH:O	2.22	0.43
2:C:11:TRP:HZ2	2:C:208:TYR:HB2	1.83	0.43
1:D:198:VAL:HG22	1:D:524:ALA:HB3	2.01	0.43
1:D:217:GLN:O	7:D:738:HOH:O	2.21	0.43
1:D:336:TRP:CZ2	5:D:603:ATP:N7	2.87	0.43
2:E:18:ARG:CD	2:E:156:SER:HA	2.49	0.43
2:F:135:LEU:HD12	7:F:426:HOH:O	2.17	0.43
1:A:187:CYS:HB2	1:A:208:SER:HB3	2.00	0.43
1:A:273:LEU:O	1:A:277:ILE:HG22	2.18	0.43
2:C:23:LEU:O	2:C:28:VAL:HG12	2.19	0.43
2:C:95:ALA:HB1	7:C:461:HOH:O	2.18	0.43
1:D:69:THR:OG1	1:D:72:GLU:OE1	2.31	0.43
1:D:89:LEU:H	1:D:89:LEU:HG	1.54	0.43
1:D:231:PHE:HA	1:D:234:PHE:CD2	2.45	0.43
2:E:18:ARG:N	2:E:159:THR:HG21	2.33	0.43
1:A:125:PHE:O	1:A:129:PHE:HD1	2.01	0.42
1:A:191:GLU:HA	1:A:194:PHE:HB2	2.01	0.42
1:A:336:TRP:HB2	5:A:603:ATP:N6	2.34	0.42
1:A:445:VAL:HG11	1:A:462:PHE:CD2	2.54	0.42
1:A:531:ILE:CD1	1:A:558:VAL:HG22	2.45	0.42
2:B:33:ARG:N	7:B:405:HOH:O	2.33	0.42
2:C:6:ILE:HB	2:C:58:VAL:HB	2.00	0.42
2:C:66:GLU:HB2	2:C:69:ASN:HB2	2.01	0.42
1:D:87:PRO:HB2	2:E:143:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ASP:CB	1:D:256:VAL:HG21	2.48	0.42
1:D:270:ASN:N	7:D:706:HOH:O	2.43	0.42
1:D:433:ILE:HD12	1:D:552:LYS:HD2	2.01	0.42
2:E:146:GLY:HA3	2:E:151:GLY:HA3	2.00	0.42
1:A:93:PRO:HG2	2:B:184:ALA:C	2.43	0.42
1:A:295:PHE:HA	1:A:296:PRO:HD2	1.71	0.42
1:A:336:TRP:CD1	5:A:603:ATP:N7	2.87	0.42
1:D:96:ALA:HB1	1:D:163:GLY:H	1.84	0.42
1:D:143:LYS:HZ2	1:D:212:PHE:H	1.66	0.42
1:D:152:LYS:HD2	1:D:152:LYS:C	2.43	0.42
1:D:203:TYR:OH	1:D:482:SER:O	2.35	0.42
1:D:246:LYS:HG2	1:D:247:ASP:N	2.33	0.42
1:D:531:ILE:HD13	1:D:558:VAL:HG22	2.01	0.42
2:F:6:ILE:C	2:F:7:LEU:HD12	2.44	0.42
2:F:110:GLN:CB	2:F:167:TYR:HE2	2.32	0.42
1:A:213:ARG:HD3	7:A:704:HOH:O	2.18	0.42
1:A:286:ASN:O	1:A:318:HIS:NE2	2.51	0.42
1:A:539:GLY:O	1:A:540:SER:HB3	2.18	0.42
2:B:11:TRP:CG	2:B:12:PRO:HD3	2.54	0.42
2:B:51:HIS:O	2:B:53:LYS:HG3	2.18	0.42
2:C:102:VAL:HG21	2:C:157:LEU:HB3	2.02	0.42
2:C:152:TYR:OH	7:C:404:HOH:O	2.06	0.42
2:C:162:SER:HB2	2:C:205:ILE:HD13	2.00	0.42
1:D:143:LYS:O	7:D:740:HOH:O	2.22	0.42
1:D:168:ASN:ND2	5:D:603:ATP:O3A	2.40	0.42
1:A:91:GLY:HA3	2:B:142:LYS:N	2.34	0.42
1:A:133:ASN:HA	1:A:136:PHE:O	2.18	0.42
1:A:223:PHE:HB2	1:A:225:HIS:CE1	2.54	0.42
1:A:234:PHE:CE1	1:A:294:LEU:HD11	2.54	0.42
1:A:239:GLU:O	1:A:240:GLU:C	2.62	0.42
1:A:465:TYR:OH	7:A:734:HOH:O	2.18	0.42
2:C:97:PHE:CE2	2:C:101:PHE:CZ	3.07	0.42
1:D:65:VAL:HA	1:D:66:PRO:HD2	1.82	0.42
1:D:86:SER:HB2	2:E:188:ARG:NE	2.34	0.42
1:D:314:PRO:HA	1:D:317:ARG:NH1	2.35	0.42
1:D:520:LEU:HD11	1:D:522:VAL:HG13	2.02	0.42
1:D:531:ILE:HD11	1:D:558:VAL:HG13	2.02	0.42
2:F:118:GLY:HA2	7:F:513:HOH:O	2.18	0.42
2:F:166:ALA:HB1	2:F:209:ALA:CB	2.49	0.42
2:F:213:ARG:HG3	7:F:493:HOH:O	2.19	0.42
1:A:114:THR:O	1:A:117:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:CD2	1:A:220:PHE:HB2	2.54	0.42
1:A:256:VAL:HB	1:A:259:VAL:HG12	2.00	0.42
1:A:273:LEU:HA	1:A:273:LEU:HD23	1.77	0.42
1:A:431:ILE:H	1:A:431:ILE:HG12	1.66	0.42
2:B:13:SER:O	2:B:17:MET:HG3	2.20	0.42
1:D:14:ILE:HG22	1:D:16:GLU:CB	2.49	0.42
1:D:80:MET:HA	1:D:80:MET:HE2	2.02	0.42
1:D:113:PHE:CD2	5:D:603:ATP:O1B	2.72	0.42
1:D:169:VAL:HG13	1:D:170:TYR:N	2.35	0.42
1:D:182:ILE:O	1:D:182:ILE:HG22	2.19	0.42
2:E:169:LYS:HB3	2:E:169:LYS:HE2	1.50	0.42
2:F:42:PRO:O	2:F:45:LEU:HG	2.19	0.42
1:A:98:SER:HB2	5:A:603:ATP:O3B	2.20	0.42
1:A:208:SER:HA	1:A:211:LEU:CD1	2.49	0.42
1:A:286:ASN:ND2	1:A:288:TYR:CE2	2.85	0.42
2:B:105:LYS:HE2	2:B:131:ALA:HB2	2.01	0.42
2:C:116:LYS:HD3	2:C:116:LYS:HA	1.86	0.42
1:D:333:SER:N	5:D:603:ATP:N7	2.68	0.42
2:F:131:ALA:O	2:F:135:LEU:HB2	2.20	0.42
1:A:38:LYS:HD3	1:A:395:TYR:CE1	2.55	0.42
1:A:169:VAL:HG23	1:A:175:PHE:CE1	2.55	0.42
2:B:21:VAL:HG13	2:B:194:SER:HB2	2.01	0.42
2:B:142:LYS:HA	2:B:143:PRO:HD3	1.97	0.42
2:C:32:TYR:HD1	2:C:32:TYR:H	1.66	0.42
2:C:51:HIS:O	2:C:53:LYS:HG3	2.19	0.42
1:D:435:LYS:HA	1:D:436:ASN:HB2	2.00	0.42
2:E:4:LEU:HA	2:E:5:PRO:HD3	1.91	0.42
2:E:130:GLU:O	2:E:134:ILE:HG13	2.20	0.42
2:F:136:GLU:HB2	2:F:179:SER:HA	2.02	0.42
1:A:18:ASP:O	1:A:22:ARG:HG3	2.20	0.42
1:A:80:MET:SD	1:A:94:VAL:HG12	2.60	0.42
1:A:143:LYS:O	1:A:216:VAL:HA	2.20	0.42
1:A:200:GLN:HG3	7:A:712:HOH:O	2.19	0.42
1:A:369:THR:HG23	1:A:370:GLY:H	1.84	0.42
2:C:125:LYS:CE	2:C:171:GLY:HA2	2.47	0.42
2:C:202:SER:OG	1:D:454:GLU:OE2	2.36	0.42
1:D:74:GLU:N	1:D:75:PRO:HD2	2.34	0.42
2:E:45:LEU:HB2	7:E:401:HOH:O	2.20	0.42
2:F:47:SER:HB2	2:F:63:PRO:HB2	2.02	0.42
2:F:54:ILE:HB	2:F:55:PRO:HA	2.00	0.42
2:F:176:GLU:OE1	2:F:176:GLU:N	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG11	1:A:291:ILE:HG21	2.01	0.42
1:A:221:ALA:CB	1:A:227:LEU:HG	2.43	0.42
1:A:251:SER:OG	7:A:725:HOH:O	2.15	0.42
1:A:360:TYR:N	1:A:393:THR:O	2.43	0.42
1:A:403:LEU:HD12	7:A:730:HOH:O	2.20	0.42
1:A:459:VAL:HA	1:A:481:ILE:HA	2.02	0.42
1:A:475:TYR:HB2	1:A:518:LEU:HD13	2.02	0.42
1:A:480:GLU:HB2	1:A:528:PHE:HD2	1.81	0.42
2:C:125:LYS:HD3	2:C:173:PHE:CD2	2.55	0.42
1:D:65:VAL:HG21	1:D:399:TYR:CE2	2.52	0.42
1:D:150:SER:OG	1:D:170:TYR:HB2	2.20	0.42
1:D:519:GLU:HG3	1:D:570:TYR:O	2.18	0.42
2:E:205:ILE:H	2:E:205:ILE:HG12	1.72	0.42
1:A:190:ASP:HA	1:A:193:ILE:HD12	2.02	0.42
1:A:357:ASN:ND2	7:A:746:HOH:O	2.25	0.42
2:B:146:GLY:N	2:B:151:GLY:HA3	2.33	0.42
1:D:113:PHE:HE1	1:D:333:SER:C	2.28	0.42
1:D:144:ALA:HB1	1:D:218:TYR:CE1	2.55	0.42
1:D:212:PHE:HD1	1:D:212:PHE:N	2.17	0.42
2:E:68:LEU:HD21	2:E:99:ALA:HB1	2.02	0.42
2:E:211:GLU:HA	2:E:214:LYS:HD2	2.02	0.42
2:F:92:ARG:O	2:F:96:ARG:HG3	2.19	0.42
2:F:154:ASP:O	2:F:158:ILE:HB	2.19	0.42
1:A:98:SER:HB3	1:A:111:ILE:CB	2.40	0.41
1:A:111:ILE:HD13	1:A:334:GLU:OE2	2.19	0.41
1:A:336:TRP:HB3	1:A:358:LEU:CD1	2.50	0.41
1:A:455:GLU:CD	1:A:457:ILE:HD12	2.45	0.41
1:A:474:HIS:NE2	1:A:521:ARG:NH2	2.68	0.41
1:A:490:LEU:HA	1:A:490:LEU:HD23	1.86	0.41
1:D:530:LYS:HG3	7:D:769:HOH:O	2.19	0.41
1:D:561:ILE:H	1:D:561:ILE:HG12	1.48	0.41
1:A:118:MET:HE2	1:A:172:ASN:ND2	2.35	0.41
1:A:152:LYS:HD3	1:A:561:ILE:CA	2.50	0.41
1:A:197:ASP:C	7:A:712:HOH:O	2.63	0.41
1:A:547:MET:HE3	1:A:549:ARG:HA	2.03	0.41
1:D:104:SER:HB3	1:D:107:ARG:O	2.20	0.41
1:D:106:GLY:CA	1:D:432:ASN:HB3	2.49	0.41
1:D:279:THR:HG23	1:D:282:MET:HE2	2.02	0.41
2:E:151:GLY:H	2:E:154:ASP:CB	2.31	0.41
2:F:185:TRP:CE2	2:F:189:CYS:SG	3.13	0.41
1:A:306:THR:HA	1:A:310:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:LEU:HB2	2:C:31:GLU:O	2.20	0.41
2:C:12:PRO:O	2:C:163:TRP:CZ2	2.73	0.41
2:C:181:LYS:HE3	2:C:181:LYS:HB2	1.91	0.41
1:D:67:LEU:HA	1:D:400:ARG:O	2.20	0.41
1:D:70:ASP:OD1	1:D:71:VAL:N	2.54	0.41
1:D:82:ASP:OD1	7:D:742:HOH:O	2.22	0.41
1:D:99:LEU:HD22	1:D:555:ASN:CG	2.45	0.41
1:D:143:LYS:HG3	1:D:216:VAL:HG13	2.02	0.41
1:D:154:TYR:HA	1:D:563:CYS:HB3	2.01	0.41
1:D:470:THR:HG23	1:D:473:GLY:HA2	2.01	0.41
2:E:5:PRO:HB2	2:E:57:LEU:HD11	2.02	0.41
2:E:142:LYS:HB3	2:E:144:TYR:O	2.20	0.41
1:A:241:ILE:C	1:A:245:ILE:HG12	2.43	0.41
1:A:318:HIS:CD2	1:A:318:HIS:C	2.98	0.41
1:A:421:PHE:HB3	1:A:542:ALA:CB	2.49	0.41
1:A:487:GLU:OE1	1:A:568:SER:HB3	2.20	0.41
1:D:117:LEU:HD11	1:D:396:ALA:HB2	2.01	0.41
1:D:287:TRP:CE3	1:D:290:LEU:CD1	2.96	0.41
1:D:308:SER:O	1:D:311:PRO:HD2	2.20	0.41
1:D:328:HIS:CE1	1:D:329:ASP:OD2	2.74	0.41
1:D:340:ASN:HA	1:D:352:PHE:HA	2.02	0.41
1:D:382:VAL:HG22	1:D:388:TYR:HD2	1.86	0.41
2:E:96:ARG:NH2	2:F:73:TYR:CE1	2.86	0.41
2:E:151:GLY:O	2:E:154:ASP:HB2	2.20	0.41
2:F:161:SER:O	2:F:164:PHE:HB2	2.19	0.41
1:A:205:HIS:NE2	7:A:755:HOH:O	2.37	0.41
1:A:312:TYR:HD1	7:A:914:HOH:O	2.01	0.41
1:A:313:VAL:HG13	1:A:325:LEU:HD13	2.03	0.41
2:B:18:ARG:CD	2:B:156:SER:HA	2.37	0.41
2:B:66:GLU:HG3	2:C:97:PHE:CD1	2.56	0.41
2:C:5:PRO:HB3	2:C:59:HIS:NE2	2.35	0.41
1:D:58:GLU:O	1:D:62:LYS:HD3	2.21	0.41
1:D:125:PHE:O	1:D:129:PHE:HB2	2.20	0.41
1:D:238:TRP:C	1:D:240:GLU:N	2.79	0.41
1:D:240:GLU:OE2	1:D:253:ARG:NH1	2.52	0.41
1:A:118:MET:SD	5:A:603:ATP:H4'	2.60	0.41
1:A:315:LYS:HB2	7:A:914:HOH:O	2.21	0.41
1:A:462:PHE:CE1	1:A:549:ARG:HD2	2.56	0.41
1:A:519:GLU:HB2	1:A:571:PHE:CD1	2.55	0.41
1:A:551:VAL:HG12	1:A:555:ASN:HD22	1.86	0.41
2:C:9:ASP:OD2	2:C:32:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:LEU:HD23	2:C:183:ILE:N	2.35	0.41
1:D:41:SER:O	1:D:42:ALA:C	2.63	0.41
1:D:247:ASP:O	1:D:249:VAL:HG23	2.20	0.41
1:A:144:ALA:HB2	1:A:184:SER:OG	2.21	0.41
1:A:150:SER:HB3	1:A:170:TYR:CD2	2.55	0.41
1:A:331:GLY:N	1:A:537:GLY:O	2.53	0.41
1:A:521:ARG:NH1	7:A:797:HOH:O	2.53	0.41
2:B:157:LEU:HD23	2:B:157:LEU:HA	1.89	0.41
2:C:17:MET:HA	2:C:20:ARG:HD2	2.03	0.41
2:C:49:PRO:O	2:C:52:LYS:HG3	2.20	0.41
1:D:31:THR:HG21	1:D:359:GLY:CA	2.50	0.41
1:D:40:GLN:OE1	7:D:737:HOH:O	2.21	0.41
1:D:130:ALA:O	1:D:134:ARG:N	2.48	0.41
1:D:474:HIS:O	1:D:474:HIS:CG	2.73	0.41
2:E:98:TRP:HH2	2:E:134:ILE:HG22	1.85	0.41
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.90	0.41
2:F:102:VAL:CG1	2:F:160:PHE:HE2	2.33	0.41
2:F:145:PHE:HB3	2:F:153:VAL:CG1	2.51	0.41
1:A:145:LEU:HB2	1:A:209:GLY:HA3	2.03	0.41
2:C:197:LYS:HB2	7:C:427:HOH:O	2.20	0.41
1:D:43:ILE:CG2	1:D:88:ILE:HG23	2.51	0.41
1:D:222:VAL:O	1:D:223:PHE:HD1	2.04	0.41
1:D:299:LYS:O	1:D:324:PRO:HD2	2.21	0.41
1:D:437:THR:O	1:D:438:GLU:C	2.63	0.41
1:D:531:ILE:CD1	1:D:558:VAL:HG22	2.51	0.41
2:E:25:GLU:HG2	2:E:84:PHE:CE1	2.55	0.41
2:F:73:TYR:HE2	7:F:402:HOH:O	2.03	0.41
1:A:43:ILE:HA	1:A:46:GLN:HB3	2.02	0.41
1:A:72:GLU:C	1:A:75:PRO:HD2	2.46	0.41
1:A:277:ILE:O	1:A:278:ARG:C	2.64	0.41
1:A:448:ALA:HB2	1:A:496:CYS:HB3	2.03	0.41
1:A:548:PRO:O	7:A:742:HOH:O	2.22	0.41
2:B:158:ILE:HD11	7:B:414:HOH:O	2.20	0.41
2:B:163:TRP:CG	2:B:205:ILE:HD13	2.55	0.41
2:B:201:ASP:OD1	2:B:202:SER:N	2.53	0.41
7:B:538:HOH:O	2:C:104:LYS:HG2	2.20	0.41
2:C:168:GLU:CD	1:D:488:ASP:OD2	2.63	0.41
1:D:45:LEU:HD13	1:D:50:LEU:HD13	2.02	0.41
1:D:120:ASN:CG	1:D:358:LEU:HD23	2.46	0.41
1:D:169:VAL:HG11	7:D:803:HOH:O	2.20	0.41
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:154:ASP:O	2:E:158:ILE:HB	2.20	0.41
2:F:203:GLU:O	2:F:206:VAL:HB	2.20	0.41
1:A:11:ASN:HA	1:A:14:ILE:HD12	2.02	0.41
1:A:93:PRO:HG2	2:B:184:ALA:HB3	2.03	0.41
1:A:110:PHE:O	1:A:111:ILE:HG13	2.21	0.41
1:A:464:SER:O	1:A:551:VAL:N	2.40	0.41
2:B:58:VAL:HA	2:B:63:PRO:HA	2.04	0.41
2:B:117:LYS:HA	2:B:121:GLN:NE2	2.36	0.41
2:B:163:TRP:HZ3	2:B:209:ALA:HB2	1.86	0.41
1:D:19:GLU:O	1:D:23:ASN:ND2	2.41	0.41
1:D:362:GLU:OE1	7:D:739:HOH:O	2.22	0.41
1:A:228:VAL:O	1:A:229:HIS:C	2.65	0.40
1:A:337:ILE:O	1:A:355:ILE:N	2.32	0.40
1:A:362:GLU:O	1:A:363:PHE:HD1	2.04	0.40
2:B:48:ASN:HA	2:B:49:PRO:HD2	1.81	0.40
2:B:86:PRO:HG2	2:B:92:ARG:HG3	2.03	0.40
2:C:57:LEU:HB3	2:C:64:VAL:CG2	2.51	0.40
1:D:87:PRO:HB2	2:E:143:PRO:CB	2.51	0.40
1:D:441:LEU:O	1:D:441:LEU:HD12	2.22	0.40
1:D:445:VAL:HG13	1:D:479:TRP:CZ2	2.56	0.40
1:D:481:ILE:HD12	1:D:483:GLY:O	2.21	0.40
1:D:500:ALA:O	7:D:743:HOH:O	2.22	0.40
2:E:98:TRP:CE2	2:E:138:GLU:HG2	2.56	0.40
1:A:122:LEU:HD23	1:A:125:PHE:CZ	2.56	0.40
1:A:204:CYS:O	1:A:207:LEU:HB3	2.21	0.40
1:A:274:ALA:HB3	7:A:716:HOH:O	2.20	0.40
1:A:308:SER:HB2	1:A:545:PHE:CE2	2.55	0.40
1:A:559:LEU:O	1:A:562:LEU:N	2.43	0.40
2:B:153:VAL:O	2:B:157:LEU:HB2	2.21	0.40
1:D:113:PHE:CE1	1:D:333:SER:C	2.99	0.40
1:D:113:PHE:CD2	5:D:603:ATP:PB	3.14	0.40
1:D:139:ASP:OD1	1:D:141:ASN:N	2.53	0.40
1:D:155:ILE:HG22	7:D:831:HOH:O	2.21	0.40
1:D:295:PHE:CD1	1:D:295:PHE:N	2.89	0.40
1:D:366:VAL:HA	1:D:371:GLU:O	2.21	0.40
2:E:8:LEU:O	2:E:55:PRO:HA	2.22	0.40
2:E:156:SER:HB2	7:E:415:HOH:O	2.21	0.40
2:F:24:ARG:NH1	2:F:198:SER:OG	2.55	0.40
1:A:189:PRO:O	1:A:192:VAL:HG12	2.22	0.40
1:A:225:HIS:HD1	1:A:309:MET:CE	2.33	0.40
1:A:330:TYR:CZ	1:A:538:LEU:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.85	0.40
1:A:436:ASN:O	1:A:437:THR:C	2.64	0.40
1:D:35:ILE:HD13	1:D:394:ASN:HA	2.04	0.40
1:D:76:TYR:CD2	1:D:88:ILE:HD13	2.49	0.40
1:D:116:GLU:HB2	1:D:395:TYR:CE1	2.56	0.40
1:D:144:ALA:HB2	1:D:184:SER:OG	2.21	0.40
1:D:167:THR:HB	1:D:560:GLN:OE1	2.22	0.40
1:D:210:ILE:O	1:D:213:ARG:N	2.53	0.40
1:D:246:LYS:HA	1:D:270:ASN:O	2.22	0.40
1:D:308:SER:OG	1:D:536:LEU:HD12	2.21	0.40
2:E:66:GLU:O	2:E:70:VAL:HG13	2.22	0.40
2:E:128:PHE:CE2	2:E:175:ILE:HG12	2.56	0.40
2:F:138:GLU:CD	2:F:145:PHE:CE1	3.00	0.40
1:A:121:THR:HG22	1:A:122:LEU:N	2.35	0.40
2:C:128:PHE:CE1	2:C:175:ILE:HG22	2.55	0.40
1:D:39:ASN:ND2	2:E:142:LYS:HA	2.36	0.40
1:D:94:VAL:HG11	1:D:97:ILE:HD11	2.02	0.40
1:D:187:CYS:SG	1:D:209:GLY:HA2	2.62	0.40
1:D:256:VAL:O	1:D:260:ARG:HB3	2.21	0.40
1:D:393:THR:HA	1:D:398:LEU:O	2.21	0.40
1:D:424:ARG:HG3	1:D:425:ARG:HD2	2.04	0.40
2:F:176:GLU:O	2:F:177:SER:OG	2.32	0.40
1:A:35:ILE:HA	1:A:395:TYR:CE1	2.56	0.40
1:A:118:MET:HE3	1:A:175:PHE:HE2	1.86	0.40
1:A:256:VAL:HA	1:A:257:PRO:HD3	1.91	0.40
1:A:337:ILE:HG13	1:A:338:ALA:N	2.36	0.40
1:D:245:ILE:HD11	1:D:274:ALA:HB2	2.03	0.40
1:D:434:ASP:HB2	1:D:550:CYS:SG	2.61	0.40
2:E:10:TYR:HB3	2:E:13:SER:HB2	2.03	0.40
2:E:205:ILE:HA	2:E:208:TYR:CD2	2.57	0.40
2:F:11:TRP:CZ3	2:F:205:ILE:HG13	2.57	0.40
2:F:47:SER:HB2	2:F:63:PRO:CB	2.52	0.40
2:F:123:ALA:O	2:F:127:GLU:HG3	2.21	0.40

All (22) 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:D:297:ASN:ND2	1:D:435:LYS:O[1_655]	1.96	0.24
7:F:552:HOH:O	7:F:577:HOH:O[1_665]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLU:OE1	2:F:178:GLU:N[1_554]	2.01	0.19
7:D:936:HOH:O	7:D:988:HOH:O[1_655]	2.04	0.16
7:D:989:HOH:O	7:D:1008:HOH:O[1_665]	2.04	0.16
7:A:953:HOH:O	7:F:463:HOH:O[1_454]	2.05	0.15
1:A:268:THR:OG1	7:A:708:HOH:O[1_655]	2.08	0.12
1:D:207:LEU:O	7:D:713:HOH:O[1_655]	2.08	0.12
1:A:503:ASP:O	7:A:706:HOH:O[1_455]	2.09	0.11
2:B:33:ARG:NH2	2:C:215:ASN:O[1_455]	2.09	0.11
7:A:1006:HOH:O	7:A:1015:HOH:O[1_665]	2.11	0.09
7:B:457:HOH:O	7:C:517:HOH:O[1_565]	2.11	0.09
7:A:719:HOH:O	7:F:432:HOH:O[1_554]	2.13	0.07
1:A:297:ASN:ND2	1:A:435:LYS:O[1_655]	2.14	0.06
7:D:773:HOH:O	7:E:507:HOH:O[1_545]	2.14	0.06
7:B:590:HOH:O	7:B:591:HOH:O[1_655]	2.17	0.03
1:D:26:GLN:NE2	2:E:211:GLU:OE1[1_545]	2.17	0.03
1:A:270:ASN:ND2	1:A:510:ARG:O[1_655]	2.18	0.02
7:A:1049:HOH:O	7:A:1056:HOH:O[1_665]	2.18	0.02
1:D:139:ASP:OD2	1:D:552:LYS:NZ[1_655]	2.18	0.02
1:D:213:ARG:NE	1:D:503:ASP:OD2[1_655]	2.18	0.02
1:A:436:ASN:ND2	7:A:704: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%)	514 (91%)	38 (7%)	15 (3%)	42
1	D	567/575 (99%)	516 (91%)	36 (6%)	15 (3%)	42
2	B	212/223 (95%)	200 (94%)	10 (5%)	2 (1%)	1412
2	C	212/223 (95%)	198 (93%)	12 (6%)	2 (1%)	1412
2	E	212/223 (95%)	199 (94%)	12 (6%)	1 (0%)	2424
2	F	212/223 (95%)	196 (92%)	11 (5%)	5 (2%)	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1982/2042 (97%)	1823 (92%)	119 (6%)	40 (2%)	6 3

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	TRP
1	A	241	ILE
1	A	368	GLU
1	A	540	SER
1	A	542	ALA
2	B	66	GLU
1	D	286	ASN
1	D	368	GLU
1	D	476	ALA
1	D	540	SER
2	F	12	PRO
1	A	76	TYR
1	A	88	ILE
1	A	165	ALA
1	A	235	GLU
1	A	437	THR
2	C	104	LYS
1	D	83	GLY
1	D	239	GLU
1	D	477	ILE
1	D	561	ILE
2	F	177	SER
1	A	544	GLN
1	D	211	LEU
1	D	271	PRO
2	E	140	GLY
1	A	90	THR
1	A	307	GLY
1	D	14	ILE
1	D	369	THR
1	D	437	THR
2	F	141	ASP
1	A	236	GLN
1	D	13	VAL
1	A	240	GLU
2	F	66	GLU
2	B	140	GLY

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Mol	Chain	Res	Type
2	C	12	PRO
2	F	83	PRO
1	D	88	ILE

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%)	411 (82%)	88 (18%)	2	0
1	D	499/505 (99%)	396 (79%)	103 (21%)	1	0
2	B	187/195 (96%)	172 (92%)	15 (8%)	11	9
2	C	187/195 (96%)	160 (86%)	27 (14%)	3	1
2	E	187/195 (96%)	156 (83%)	31 (17%)	2	0
2	F	187/195 (96%)	145 (78%)	42 (22%)	1	0
All	All	1746/1790 (98%)	1440 (82%)	306 (18%)	2	0

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	20	MET
1	A	46	GLN
1	A	67	LEU
1	A	77	ILE
1	A	78	LYS
1	A	80	MET
1	A	90	THR
1	A	99	LEU
1	A	101	SER
1	A	103	THR
1	A	108	PRO
1	A	109	LYS
1	A	110	PHE
1	A	116	GLU

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Mol	Chain	Res	Type
1	A	117	LEU
1	A	121	THR
1	A	125	PHE
1	A	140	ASP
1	A	146	GLN
1	A	149	PHE
1	A	150	SER
1	A	152	LYS
1	A	155	ILE
1	A	182	ILE
1	A	183	THR
1	A	184	SER
1	A	187	CYS
1	A	188	SER
1	A	198	VAL
1	A	202	LEU
1	A	206	LEU
1	A	213	ARG
1	A	216	VAL
1	A	235	GLU
1	A	237	VAL
1	A	238	TRP
1	A	239	GLU
1	A	240	GLU
1	A	244	ASP
1	A	265	LYS
1	A	266	LEU
1	A	267	LEU
1	A	276	THR
1	A	277	ILE
1	A	278	ARG
1	A	279	THR
1	A	285	SER
1	A	287	TRP
1	A	291	ILE
1	A	315	LYS
1	A	333	SER
1	A	340	ASN
1	A	342	THR
1	A	369	THR
1	A	371	GLU
1	A	375	LYS

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Mol	Chain	Res	Type
1	A	377	VAL
1	A	403	LEU
1	A	406	VAL
1	A	416	THR
1	A	422	ILE
1	A	427	LEU
1	A	431	ILE
1	A	437	THR
1	A	440	ASP
1	A	459	VAL
1	A	461	ASP
1	A	463	SER
1	A	468	VAL
1	A	478	PHE
1	A	479	TRP
1	A	480	GLU
1	A	494	CYS
1	A	498	ASP
1	A	502	ILE
1	A	512	CYS
1	A	515	ILE
1	A	525	LYS
1	A	533	GLU
1	A	535	PHE
1	A	536	LEU
1	A	545	PHE
1	A	547	MET
1	A	562	LEU
1	A	563	CYS
1	A	569	SER
1	A	573	THR
2	B	4	LEU
2	B	6	ILE
2	B	40	LYS
2	B	48	ASN
2	B	50	ILE
2	B	66	GLU
2	B	74	VAL
2	B	81	LYS
2	B	132	VAL
2	B	138	GLU
2	B	139	LEU

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Mol	Chain	Res	Type
2	B	153	VAL
2	B	157	LEU
2	B	168	GLU
2	B	182	LEU
2	C	4	LEU
2	C	9	ASP
2	C	14	MET
2	C	32	TYR
2	C	38	SER
2	C	40	LYS
2	C	43	LEU
2	C	50	ILE
2	C	64	VAL
2	C	65	CYS
2	C	68	LEU
2	C	71	VAL
2	C	80	GLU
2	C	81	LYS
2	C	84	PHE
2	C	85	PHE
2	C	104	LYS
2	C	133	LYS
2	C	135	LEU
2	C	136	GLU
2	C	157	LEU
2	C	158	ILE
2	C	162	SER
2	C	176	GLU
2	C	182	LEU
2	C	183	ILE
2	C	206	VAL
1	D	13	VAL
1	D	14	ILE
1	D	33	LYS
1	D	44	TYR
1	D	47	ASN
1	D	55	THR
1	D	62	LYS
1	D	63	SER
1	D	65	VAL
1	D	69	THR
1	D	80	MET

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Mol	Chain	Res	Type
1	D	85	THR
1	D	89	LEU
1	D	90	THR
1	D	94	VAL
1	D	107	ARG
1	D	109	LYS
1	D	110	PHE
1	D	111	ILE
1	D	114	THR
1	D	121	THR
1	D	124	LEU
1	D	129	PHE
1	D	145	LEU
1	D	151	SER
1	D	152	LYS
1	D	162	VAL
1	D	174	ASN
1	D	186	SER
1	D	187	CYS
1	D	188	SER
1	D	190	ASP
1	D	193	ILE
1	D	212	PHE
1	D	216	VAL
1	D	227	LEU
1	D	236	GLN
1	D	240	GLU
1	D	246	LYS
1	D	250	LEU
1	D	251	SER
1	D	254	ILE
1	D	259	VAL
1	D	264	SER
1	D	276	THR
1	D	284	LEU
1	D	290	LEU
1	D	295	PHE
1	D	299	LYS
1	D	306	THR
1	D	329	ASP
1	D	333	SER
1	D	337	ILE

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Mol	Chain	Res	Type
1	D	342	THR
1	D	345	LEU
1	D	349	GLU
1	D	369	THR
1	D	377	VAL
1	D	379	LEU
1	D	380	THR
1	D	386	GLU
1	D	391	VAL
1	D	400	ARG
1	D	403	LEU
1	D	420	LYS
1	D	421	PHE
1	D	422	ILE
1	D	423	CYS
1	D	424	ARG
1	D	425	ARG
1	D	427	LEU
1	D	428	ILE
1	D	433	ILE
1	D	437	THR
1	D	443	LEU
1	D	447	SER
1	D	450	LYS
1	D	452	LEU
1	D	458	GLU
1	D	467	ASP
1	D	477	ILE
1	D	480	GLU
1	D	481	ILE
1	D	484	GLU
1	D	494	CYS
1	D	499	ARG
1	D	502	ILE
1	D	513	LYS
1	D	522	VAL
1	D	523	VAL
1	D	527	THR
1	D	528	PHE
1	D	536	LEU
1	D	538	LEU
1	D	545	PHE

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Mol	Chain	Res	Type
1	D	547	MET
1	D	552	LYS
1	D	554	SER
1	D	561	ILE
1	D	562	LEU
1	D	563	CYS
1	D	565	ASN
1	D	573	THR
2	E	7	LEU
2	E	43	LEU
2	E	45	LEU
2	E	48	ASN
2	E	50	ILE
2	E	51	HIS
2	E	53	LYS
2	E	56	VAL
2	E	58	VAL
2	E	66	GLU
2	E	68	LEU
2	E	74	VAL
2	E	101	PHE
2	E	103	ASP
2	E	116	LYS
2	E	119	GLU
2	E	120	GLU
2	E	133	LYS
2	E	142	LYS
2	E	153	VAL
2	E	157	LEU
2	E	158	ILE
2	E	173	PHE
2	E	177	SER
2	E	178	GLU
2	E	179	SER
2	E	183	ILE
2	E	190	MET
2	E	204	LYS
2	E	205	ILE
2	E	211	GLU
2	F	26	LYS
2	F	32	TYR
2	F	33	ARG

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Mol	Chain	Res	Type
2	F	35	GLU
2	F	36	ASP
2	F	40	LYS
2	F	41	SER
2	F	43	LEU
2	F	45	LEU
2	F	51	HIS
2	F	71	VAL
2	F	72	GLN
2	F	75	ASP
2	F	84	PHE
2	F	105	LYS
2	F	117	LYS
2	F	129	ILE
2	F	133	LYS
2	F	134	ILE
2	F	135	LEU
2	F	136	GLU
2	F	138	GLU
2	F	139	LEU
2	F	157	LEU
2	F	158	ILE
2	F	161	SER
2	F	162	SER
2	F	164	PHE
2	F	169	LYS
2	F	173	PHE
2	F	175	ILE
2	F	176	GLU
2	F	178	GLU
2	F	181	LYS
2	F	182	LEU
2	F	185	TRP
2	F	190	MET
2	F	191	GLU
2	F	195	VAL
2	F	197	LYS
2	F	204	LYS
2	F	211	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	46	GLN
1	A	51	ASN
1	A	120	ASN
1	A	123	GLN
1	A	146	GLN
1	A	426	ASN
1	A	544	GLN
2	C	46	GLN
2	C	69	ASN
2	C	110	GLN
2	C	121	GLN
2	C	172	ASN
2	C	215	ASN
1	D	39	ASN
1	D	146	GLN
1	D	432	ASN
1	D	495	ASN
1	D	534	HIS
1	D	544	GLN
2	E	60	ASN
2	E	72	GLN
2	E	121	GLN
2	E	172	ASN
2	F	110	GLN
2	F	172	ASN
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

10 ligands are modelled in this entry.

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	2.67	5 (23%)
3	JAA	A	601	-	15,15,15	5.38	6 (40%)	14,19,19	2.78	8 (57%)
5	ATP	D	603	-	32,33,33	4.73	20 (62%)	48,52,52	2.90	21 (43%)
3	JAA	D	601	-	15,15,15	5.34	7 (46%)	14,19,19	2.61	7 (50%)
6	GSH	F	301	-	18,19,19	1.58	4 (22%)	21,24,24	3.50	7 (33%)
4	MET	A	602	-	7,8,8	1.12	1 (14%)	5,9,9	0.94	0
6	GSH	E	301	-	18,19,19	1.50	4 (22%)	21,24,24	2.72	6 (28%)
5	ATP	A	603	-	32,33,33	4.34	21 (65%)	48,52,52	3.34	25 (52%)
4	MET	D	602	-	7,8,8	0.96	1 (14%)	5,9,9	0.93	1 (20%)
6	GSH	B	301	-	18,19,19	1.73	4 (22%)	21,24,24	2.74	6 (28%)

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	-	-	3/24/24/24	-
3	JAA	A	601	-	-	4/9/22/22	0/1/1/1
5	ATP	D	603	-	-	5/22/38/38	0/3/3/3
3	JAA	D	601	-	-	4/9/22/22	0/1/1/1
6	GSH	F	301	-	-	5/24/24/24	-
4	MET	A	602	-	-	3/8/8/8	-
6	GSH	E	301	-	-	4/24/24/24	-
5	ATP	A	603	-	-	8/22/38/38	0/3/3/3
4	MET	D	602	-	-	4/8/8/8	-
6	GSH	B	301	-	-	3/24/24/24	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JAA	C05-C08	-13.88	1.29	1.52
3	D	601	JAA	C05-C08	-13.62	1.30	1.52
3	D	601	JAA	C06-C04	-11.40	1.25	1.53
5	D	603	ATP	C1'-N9	-11.02	1.15	1.46
3	A	601	JAA	C06-C04	-11.01	1.26	1.53
5	A	603	ATP	C6-N6	-9.76	1.09	1.34
5	A	603	ATP	O4'-C4'	-9.49	1.23	1.45
5	D	603	ATP	O4'-C4'	-8.95	1.25	1.45
5	A	603	ATP	O4'-C1'	8.04	1.60	1.42
5	D	603	ATP	O4'-C1'	8.02	1.60	1.42
5	D	603	ATP	C6-N6	-7.91	1.14	1.34
5	A	603	ATP	C1'-N9	-7.07	1.26	1.46
5	D	603	ATP	PA-O3A	-6.93	1.52	1.59
3	A	601	JAA	C07-C08	6.76	1.61	1.51
5	A	603	ATP	PA-O3A	-6.38	1.52	1.59
5	D	603	ATP	C4-N3	6.25	1.46	1.34
5	D	603	ATP	O3'-C3'	-6.06	1.27	1.43
5	A	603	ATP	PB-O3B	-5.75	1.53	1.59
3	D	601	JAA	C07-C08	5.72	1.60	1.51
5	A	603	ATP	C8-N9	-5.64	1.27	1.37
5	D	603	ATP	C2-N1	5.60	1.43	1.33
5	A	603	ATP	C2-N1	5.51	1.43	1.33
5	D	603	ATP	C2'-C1'	-5.29	1.36	1.53
3	D	601	JAA	C10-C04	-5.28	1.44	1.53
5	A	603	ATP	C2'-C1'	-5.07	1.37	1.53
5	D	603	ATP	C8-N9	-5.06	1.28	1.37
5	D	603	ATP	C5-N7	-4.86	1.30	1.39
3	A	601	JAA	C05-C04	4.73	1.66	1.54
3	A	601	JAA	C10-C04	-4.72	1.45	1.53
5	D	603	ATP	PB-O3A	-4.67	1.54	1.59
5	A	603	ATP	O3'-C3'	-4.55	1.31	1.43
5	D	603	ATP	C2-N3	-4.44	1.26	1.33
3	D	601	JAA	C05-C04	4.41	1.65	1.54
3	A	601	JAA	C09-C05	-4.39	1.48	1.54
5	D	603	ATP	PB-O3B	-4.39	1.54	1.59
5	A	603	ATP	C5-C4	4.36	1.46	1.39
5	D	603	ATP	C3'-C4'	4.35	1.64	1.53
5	D	603	ATP	C2'-C3'	-4.25	1.41	1.53
5	D	603	ATP	C5'-C4'	-4.14	1.39	1.51
5	A	603	ATP	C2'-C3'	-4.11	1.42	1.53
3	D	601	JAA	C09-C05	-3.94	1.48	1.54
5	A	603	ATP	C3'-C4'	3.92	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	GSH	CD1-N2	3.87	1.42	1.34
5	D	603	ATP	C5-C4	-3.57	1.32	1.39
6	F	301	GSH	CA2-N2	-3.53	1.38	1.45
5	A	603	ATP	PB-O3A	-3.44	1.55	1.59
6	E	301	GSH	C2-N3	3.41	1.41	1.33
5	A	603	ATP	C5-C6	-3.34	1.31	1.41
6	B	301	GSH	C2-N3	3.08	1.40	1.33
5	A	603	ATP	PG-O1G	-2.99	1.41	1.50
6	C	301	GSH	CB2-CA2	-2.98	1.49	1.53
6	B	301	GSH	CB2-CA2	-2.84	1.50	1.53
6	F	301	GSH	C2-N3	2.78	1.40	1.33
6	C	301	GSH	CA2-N2	-2.75	1.40	1.45
3	D	601	JAA	O03-C12	-2.72	1.21	1.30
5	A	603	ATP	C2-N3	-2.71	1.29	1.33
6	C	301	GSH	C2-N3	2.59	1.39	1.33
4	A	602	MET	OXT-C	-2.55	1.22	1.30
5	A	603	ATP	C5'-C4'	-2.49	1.44	1.51
5	A	603	ATP	O5'-C5'	-2.39	1.35	1.44
6	E	301	GSH	CD1-N2	2.36	1.39	1.34
4	D	602	MET	OXT-C	-2.36	1.23	1.30
6	E	301	GSH	CA2-N2	-2.36	1.41	1.45
5	D	603	ATP	PG-O1G	-2.30	1.43	1.50
5	D	603	ATP	C5-C6	2.27	1.47	1.41
6	F	301	GSH	CB2-CA2	-2.22	1.50	1.53
5	A	603	ATP	C6-N1	-2.20	1.29	1.35
6	F	301	GSH	CB2-SG2	-2.18	1.77	1.81
6	B	301	GSH	CB2-SG2	-2.09	1.77	1.81
6	E	301	GSH	CB2-CA2	-2.03	1.50	1.53
6	C	301	GSH	CD1-N2	2.02	1.38	1.34
5	A	603	ATP	PG-O2G	2.02	1.62	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	301	GSH	CA2-CB2-SG2	-13.78	98.63	114.16
5	A	603	ATP	C4-C5-N7	-12.20	96.64	110.58
6	B	301	GSH	CA2-CB2-SG2	-10.33	102.51	114.16
6	E	301	GSH	CA2-CB2-SG2	-10.15	102.72	114.16
6	C	301	GSH	CA2-CB2-SG2	-9.68	103.25	114.16
5	A	603	ATP	C5-N7-C8	7.63	115.44	103.45
5	D	603	ATP	N9-C8-N7	-7.43	103.39	113.94
5	D	603	ATP	C5-N7-C8	6.72	114.02	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	ATP	O3A-PA-O1A	-6.31	91.72	110.70
5	A	603	ATP	O4'-C1'-N9	5.40	118.46	108.09
5	A	603	ATP	C6-C5-N7	5.39	142.49	132.09
5	D	603	ATP	O2A-PA-O3A	-5.32	92.90	107.27
5	D	603	ATP	C4-C5-N7	-5.16	104.68	110.58
5	D	603	ATP	O3B-PB-O1B	-5.08	95.43	110.70
3	A	601	JAA	C09-C11-C13	-4.89	108.23	126.21
5	D	603	ATP	N3-C2-N1	-4.78	121.35	128.58
3	D	601	JAA	C09-C11-C13	-4.70	108.93	126.21
5	D	603	ATP	C4'-O4'-C1'	-4.54	99.43	109.47
5	A	603	ATP	O3G-PG-O3B	4.46	119.60	104.64
5	D	603	ATP	C4-N9-C8	4.33	110.29	105.74
5	A	603	ATP	O2A-PA-O3A	4.21	118.66	107.27
3	D	601	JAA	C06-C07-C08	-4.13	101.30	105.39
3	D	601	JAA	C07-C06-C04	-4.12	100.09	104.45
3	A	601	JAA	O03-C12-C10	4.09	126.72	114.00
5	D	603	ATP	O4'-C1'-N9	4.04	115.86	108.09
5	D	603	ATP	C2'-C1'-N9	4.03	123.31	113.30
5	A	603	ATP	C4'-O4'-C1'	-3.97	100.69	109.47
5	D	603	ATP	C2-N1-C6	3.96	125.24	118.73
6	F	301	GSH	CB2-CA2-N2	-3.96	105.64	111.28
5	A	603	ATP	O2B-PB-O3B	-3.95	96.58	107.27
5	A	603	ATP	C5-C4-N9	3.90	110.06	105.81
6	C	301	GSH	C2-CA2-N2	-3.82	100.79	111.11
3	A	601	JAA	C06-C04-C10	-3.79	106.36	113.41
5	A	603	ATP	O4'-C1'-C2'	-3.74	98.60	106.62
3	D	601	JAA	C06-C04-C10	-3.68	106.56	113.41
5	D	603	ATP	O4'-C1'-C2'	-3.64	98.82	106.62
6	B	301	GSH	CB2-CA2-C2	-3.58	101.72	109.50
6	E	301	GSH	CG1-CD1-N2	-3.53	109.65	115.86
3	A	601	JAA	C14-C13-C11	-3.52	105.26	126.42
5	A	603	ATP	C5-C4-N3	-3.38	122.07	126.72
5	A	603	ATP	N9-C8-N7	-3.33	109.22	113.94
5	D	603	ATP	O2B-PB-O3A	3.23	115.99	107.27
3	A	601	JAA	C06-C04-C05	3.20	107.85	103.36
5	A	603	ATP	O2B-PB-O3A	3.17	115.83	107.27
6	E	301	GSH	CB1-CG1-CD1	3.15	120.09	113.06
3	D	601	JAA	C04-C10-C12	-3.15	106.95	113.33
3	A	601	JAA	O02-C12-C10	-3.10	113.32	122.84
5	D	603	ATP	O3G-PG-O3B	3.06	114.88	104.64
6	F	301	GSH	CG1-CD1-N2	-3.04	110.50	115.86
6	F	301	GSH	OE1-CD1-CG1	3.00	127.46	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	301	GSH	C2-CA2-N2	-2.92	103.20	111.11
5	D	603	ATP	C5-C4-N3	-2.90	122.72	126.72
6	C	301	GSH	CG1-CD1-N2	-2.79	110.95	115.86
6	F	301	GSH	CB1-CG1-CD1	2.78	119.26	113.06
5	A	603	ATP	C5'-C4'-C3'	-2.76	105.28	115.21
5	A	603	ATP	O3A-PB-O1B	2.76	119.01	110.70
5	D	603	ATP	N6-C6-N1	2.76	124.52	118.38
5	A	603	ATP	C4-N9-C8	2.73	108.60	105.74
5	A	603	ATP	O3'-C3'-C2'	2.72	120.55	111.82
5	D	603	ATP	C6-C5-C4	2.72	120.89	117.18
3	A	601	JAA	C04-C10-C12	-2.71	107.83	113.33
6	C	301	GSH	CB1-CG1-CD1	2.70	119.08	113.06
5	A	603	ATP	PA-O5'-C5'	-2.67	106.05	121.35
5	A	603	ATP	C6-C5-C4	2.60	120.73	117.18
3	D	601	JAA	C14-C13-C11	-2.56	111.01	126.42
5	D	603	ATP	O2G-PG-O3B	2.52	113.09	104.64
5	D	603	ATP	O4'-C4'-C5'	2.46	117.23	109.33
6	F	301	GSH	CG1-CB1-CA1	-2.43	108.28	113.86
3	A	601	JAA	O01-C08-C05	2.41	128.67	125.60
6	C	301	GSH	OE1-CD1-CG1	2.36	126.29	122.02
6	E	301	GSH	C2-CA2-N2	-2.36	104.73	111.11
6	B	301	GSH	C2-CA2-N2	-2.34	104.77	111.11
6	E	301	GSH	CG1-CB1-CA1	-2.34	108.49	113.86
5	A	603	ATP	C2'-C1'-N9	2.33	119.09	113.30
5	A	603	ATP	N6-C6-N1	2.23	123.34	118.38
5	A	603	ATP	O5'-C5'-C4'	2.21	116.53	108.99
5	D	603	ATP	O2'-C2'-C1'	-2.20	102.52	110.10
5	D	603	ATP	C2-N3-C4	2.17	117.14	111.83
5	A	603	ATP	O3B-PB-O1B	-2.17	104.19	110.70
5	A	603	ATP	C1'-N9-C8	-2.16	122.30	127.09
6	B	301	GSH	CB2-CA2-N2	-2.07	108.34	111.28
6	B	301	GSH	CG1-CD1-N2	-2.06	112.23	115.86
6	B	301	GSH	CG1-CB1-CA1	-2.06	109.13	113.86
4	D	602	MET	OXT-C-O	-2.02	119.49	124.08
3	D	601	JAA	O01-C08-C05	2.02	128.18	125.60
6	E	301	GSH	CB2-CA2-N2	-2.01	108.42	111.28

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	JAA	C08-C05-C09-C11

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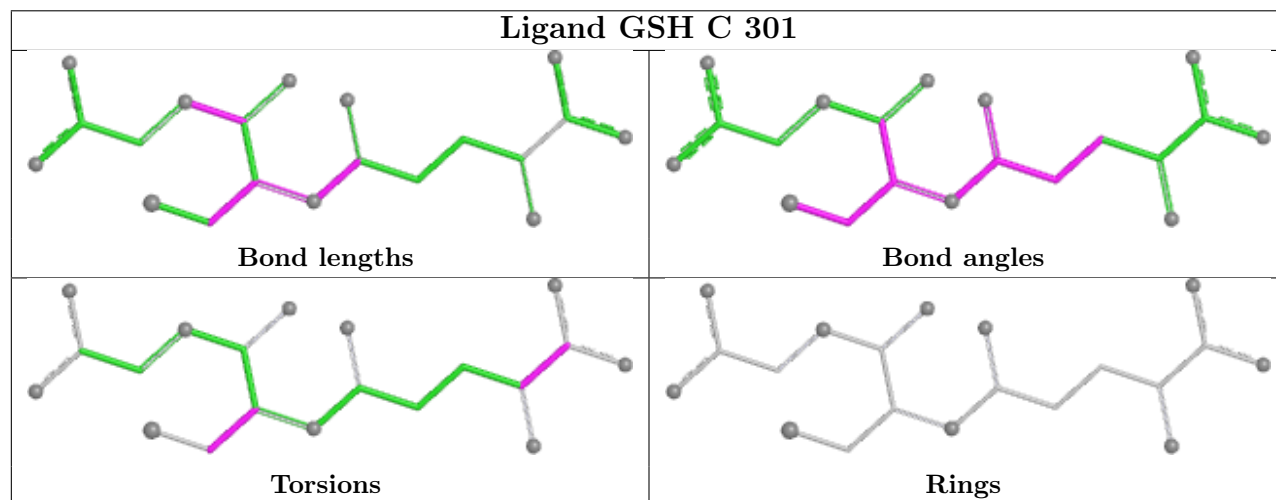
Mol	Chain	Res	Type	Atoms
4	A	602	MET	N-CA-CB-CG
4	A	602	MET	C-CA-CB-CG
4	D	602	MET	N-CA-CB-CG
4	D	602	MET	C-CA-CB-CG
5	A	603	ATP	C5'-O5'-PA-O2A
5	A	603	ATP	C5'-O5'-PA-O3A
5	A	603	ATP	O4'-C1'-N9-C8
5	A	603	ATP	O4'-C1'-N9-C4
5	D	603	ATP	PB-O3B-PG-O3G
5	D	603	ATP	C2'-C1'-N9-C8
5	D	603	ATP	C2'-C1'-N9-C4
6	B	301	GSH	N2-CA2-CB2-SG2
6	B	301	GSH	C2-CA2-CB2-SG2
6	C	301	GSH	N2-CA2-CB2-SG2
6	C	301	GSH	C2-CA2-CB2-SG2
6	F	301	GSH	N2-CA2-CB2-SG2
6	F	301	GSH	C2-CA2-CB2-SG2
3	A	601	JAA	C09-C11-C13-C14
6	F	301	GSH	CA1-CB1-CG1-CD1
4	A	602	MET	CB-CG-SD-CE
6	F	301	GSH	O31-C3-CA3-N3
6	F	301	GSH	O32-C3-CA3-N3
3	D	601	JAA	C09-C11-C13-C14
4	D	602	MET	CA-CB-CG-SD
3	A	601	JAA	C04-C05-C09-C11
3	D	601	JAA	C11-C13-C14-C15
6	B	301	GSH	C1-CA1-CB1-CG1
3	D	601	JAA	C08-C05-C09-C11
5	D	603	ATP	C4'-C5'-O5'-PA
3	D	601	JAA	C05-C09-C11-C13
5	A	603	ATP	PA-O3A-PB-O2B
5	A	603	ATP	PB-O3A-PA-O2A
5	D	603	ATP	PB-O3B-PG-O1G
3	A	601	JAA	C05-C09-C11-C13
6	E	301	GSH	O32-C3-CA3-N3
6	E	301	GSH	CA1-CB1-CG1-CD1
6	E	301	GSH	O11-C1-CA1-N1
5	A	603	ATP	PB-O3A-PA-O1A
6	C	301	GSH	O11-C1-CA1-N1
4	D	602	MET	OXT-C-CA-N
6	E	301	GSH	O31-C3-CA3-N3
5	A	603	ATP	PA-O3A-PB-O1B

There are no ring outliers.

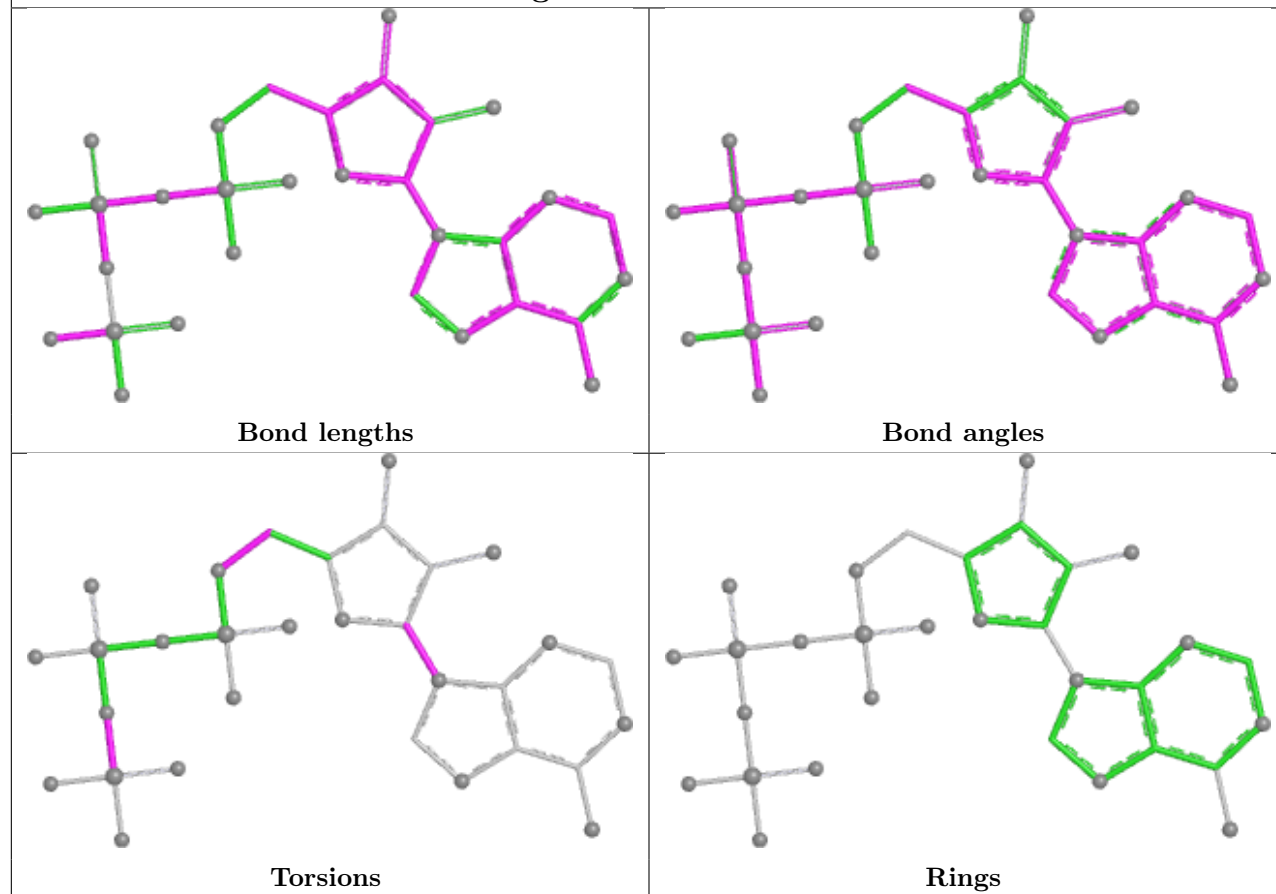
8 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	JAA	2	0
5	D	603	ATP	26	0
3	D	601	JAA	2	0
4	A	602	MET	4	0
6	E	301	GSH	3	0
5	A	603	ATP	17	0
4	D	602	MET	5	0
6	B	301	GSH	1	0

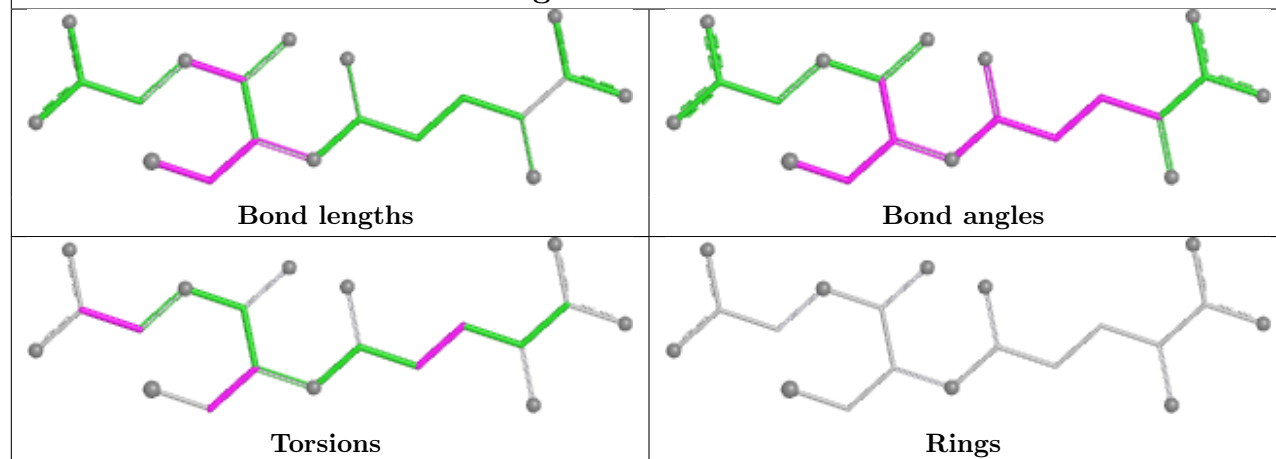
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



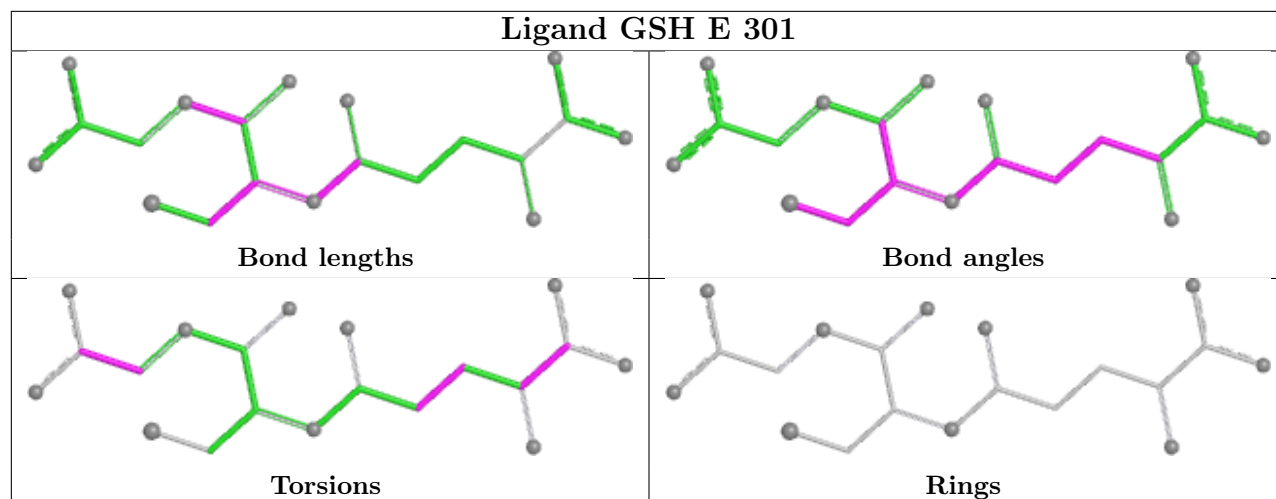
Ligand ATP D 603



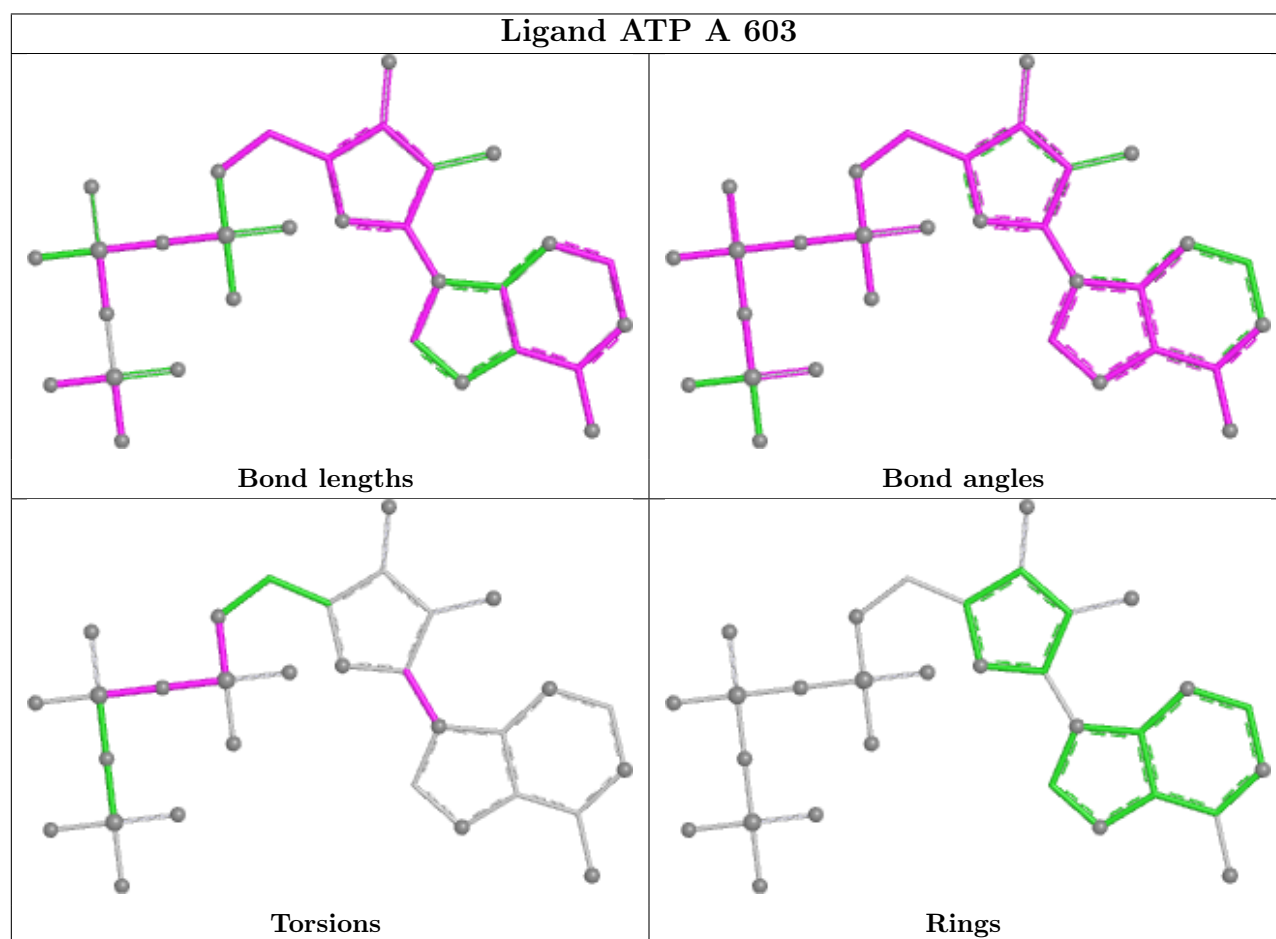
Ligand GSH F 301

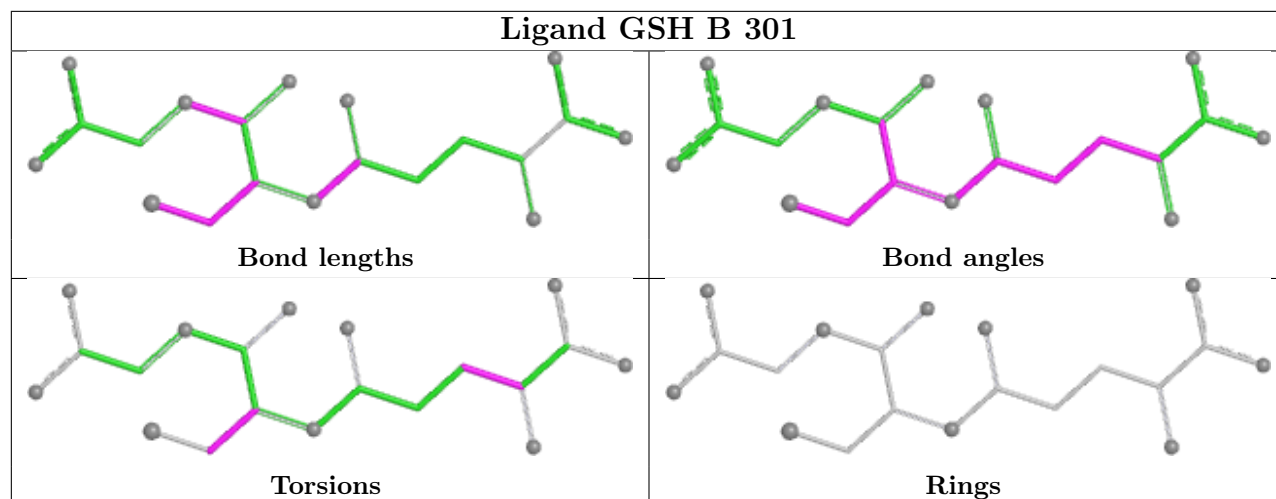


Ligand GSH E 301



Ligand ATP A 603





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%)	0.60	32 (5%) 30 28	3, 14, 22, 28	0
1	D	569/575 (98%)	0.70	31 (5%) 31 29	3, 15, 24, 31	0
2	B	214/223 (95%)	0.40	10 (4%) 36 35	4, 11, 20, 28	0
2	C	214/223 (95%)	0.07	2 (0%) 81 82	2, 3, 7, 11	0
2	E	214/223 (95%)	0.37	9 (4%) 40 40	4, 9, 16, 27	0
2	F	214/223 (95%)	0.04	0 100 100	2, 3, 7, 11	0
All	All	1994/2042 (97%)	0.46	84 (4%) 40 40	2, 12, 22, 31	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	153	VAL	3.8
1	D	276	THR	3.6
1	A	554	SER	3.6
1	D	30	GLN	3.5
1	D	554	SER	3.4
1	A	338	ALA	3.3
2	C	123	ALA	3.3
1	A	524	ALA	3.2
1	D	77	ILE	3.1
1	A	224	ALA	3.1
1	A	433	ILE	3.1
1	D	241	ILE	3.0
1	D	71	VAL	3.0
1	A	507	VAL	3.0
1	D	226	GLY	2.9
2	B	61	GLY	2.9
1	D	380	THR	2.9
1	A	514	THR	2.9
1	D	36	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	407	VAL	2.9
2	B	205	ILE	2.9
2	B	86	PRO	2.8
2	E	11	TRP	2.8
1	A	512	CYS	2.8
1	D	335	GLY	2.8
2	B	210	ALA	2.8
1	A	169	VAL	2.8
1	D	507	VAL	2.8
1	D	102	GLY	2.7
1	A	276	THR	2.7
2	E	194	SER	2.7
1	D	111	ILE	2.6
1	A	518	LEU	2.5
1	D	37	LEU	2.5
1	A	204	CYS	2.5
2	B	89	PRO	2.5
1	A	155	ILE	2.5
1	A	245	ILE	2.5
2	E	184	ALA	2.5
1	D	196	PRO	2.5
1	A	113	PHE	2.5
2	B	216	ASN	2.5
1	A	142	GLY	2.5
1	A	464	SER	2.4
1	A	501	PHE	2.4
1	A	475	TYR	2.4
1	A	229	HIS	2.4
1	D	75	PRO	2.4
1	A	303	GLY	2.4
2	E	95	ALA	2.4
2	E	140	GLY	2.4
1	A	138	ILE	2.4
1	D	211	LEU	2.4
1	D	539	GLY	2.3
1	A	237	VAL	2.3
2	B	95	ALA	2.3
1	A	148	ILE	2.3
1	A	277	ILE	2.3
1	D	80	MET	2.3
1	D	201	ALA	2.2
1	D	500	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	124	LEU	2.2
1	D	110	PHE	2.2
2	E	101	PHE	2.2
1	A	118	MET	2.2
2	C	118	GLY	2.2
1	D	31	THR	2.2
1	A	358	LEU	2.2
1	D	73	LEU	2.2
1	A	242	VAL	2.2
2	E	63	PRO	2.2
1	D	279	THR	2.2
1	A	147	PHE	2.1
1	D	479	TRP	2.1
1	D	74	GLU	2.1
1	A	429	LEU	2.1
2	E	79	PRO	2.1
1	D	522	VAL	2.1
2	E	64	VAL	2.1
1	D	336	TRP	2.1
2	B	215	ASN	2.0
1	A	106	GLY	2.0
1	A	478	PHE	2.0
2	B	139	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

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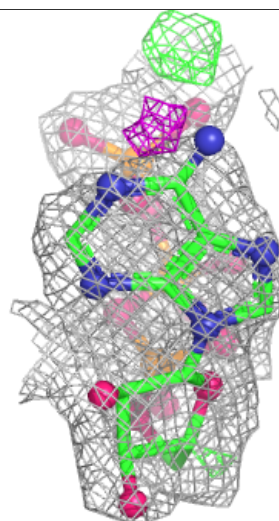
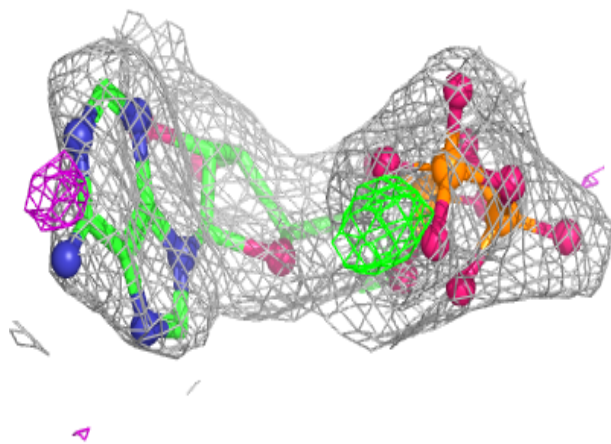
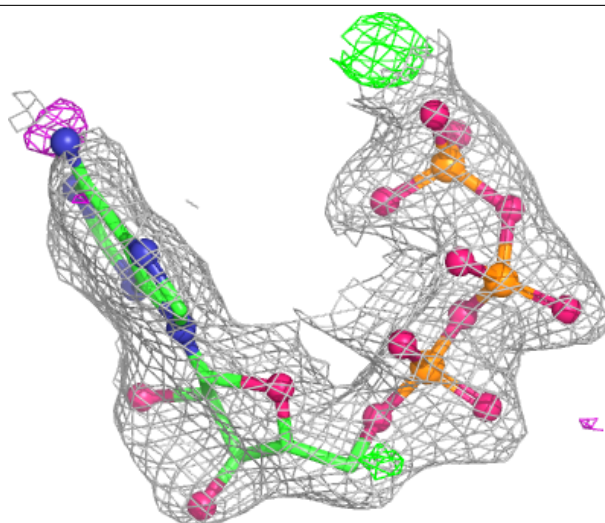
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JAA	D	601	15/15	0.79	0.18	12,19,30,35	0
3	JAA	A	601	15/15	0.82	0.13	12,19,24,28	0
4	MET	D	602	9/9	0.87	0.14	14,20,29,39	0
4	MET	A	602	9/9	0.91	0.14	14,20,24,26	0
5	ATP	D	603	31/31	0.91	0.10	13,20,30,32	0
6	GSH	F	301	20/20	0.92	0.09	9,16,23,25	0
6	GSH	E	301	20/20	0.94	0.09	6,13,21,22	0
5	ATP	A	603	31/31	0.95	0.10	8,19,26,28	0
6	GSH	B	301	20/20	0.96	0.07	3,5,8,8	0
6	GSH	C	301	20/20	0.96	0.07	5,9,17,20	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.

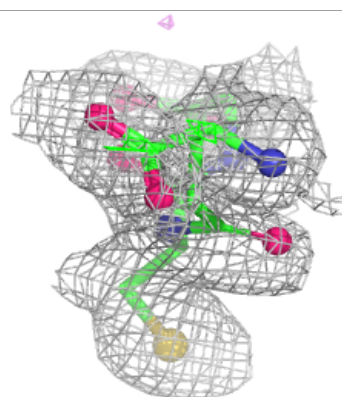
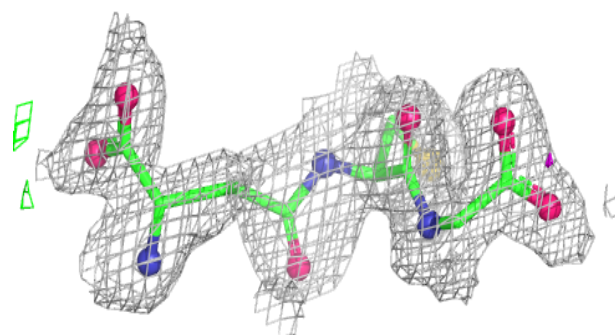
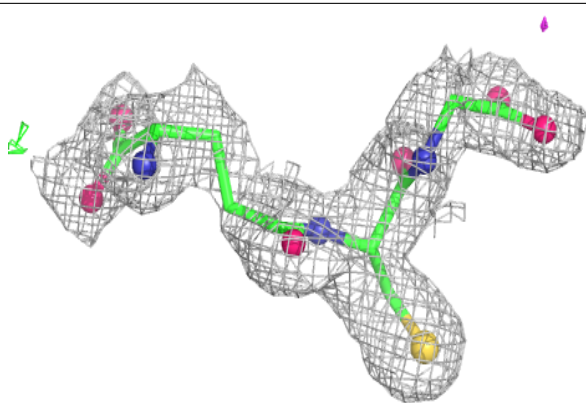
Electron density around ATP D 603:

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

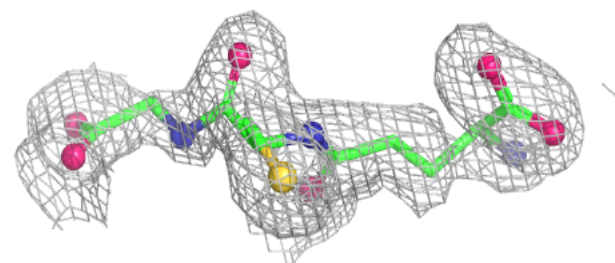
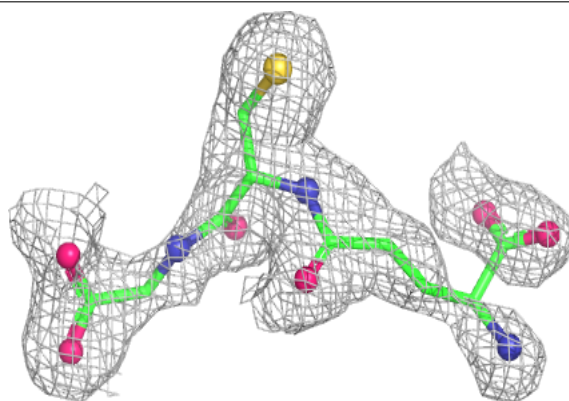


Electron density around GSH F 301:

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

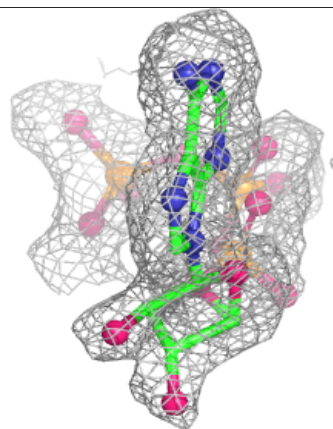
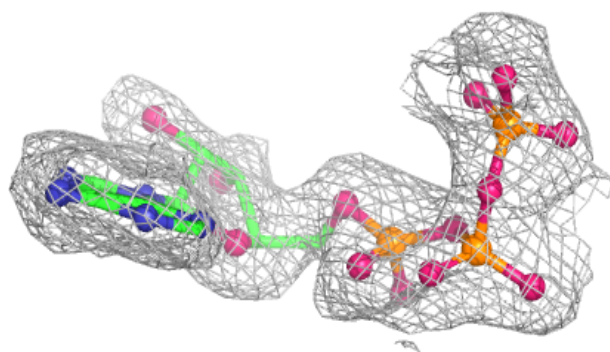
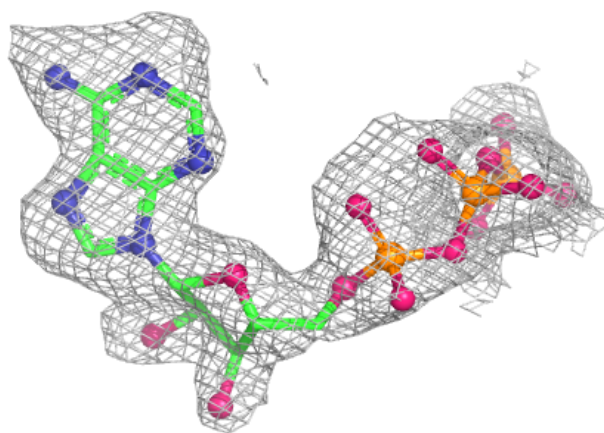
**Electron density around GSH E 301:**

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

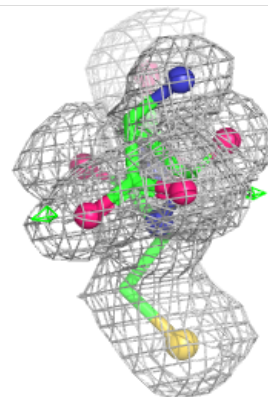
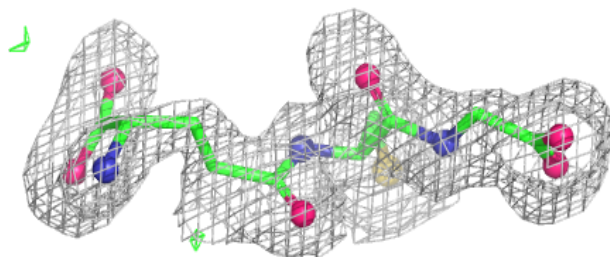
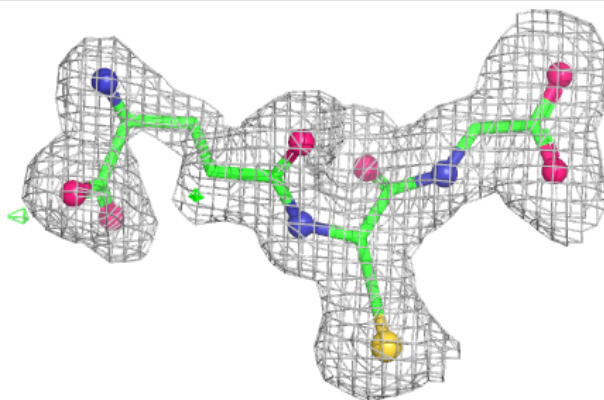


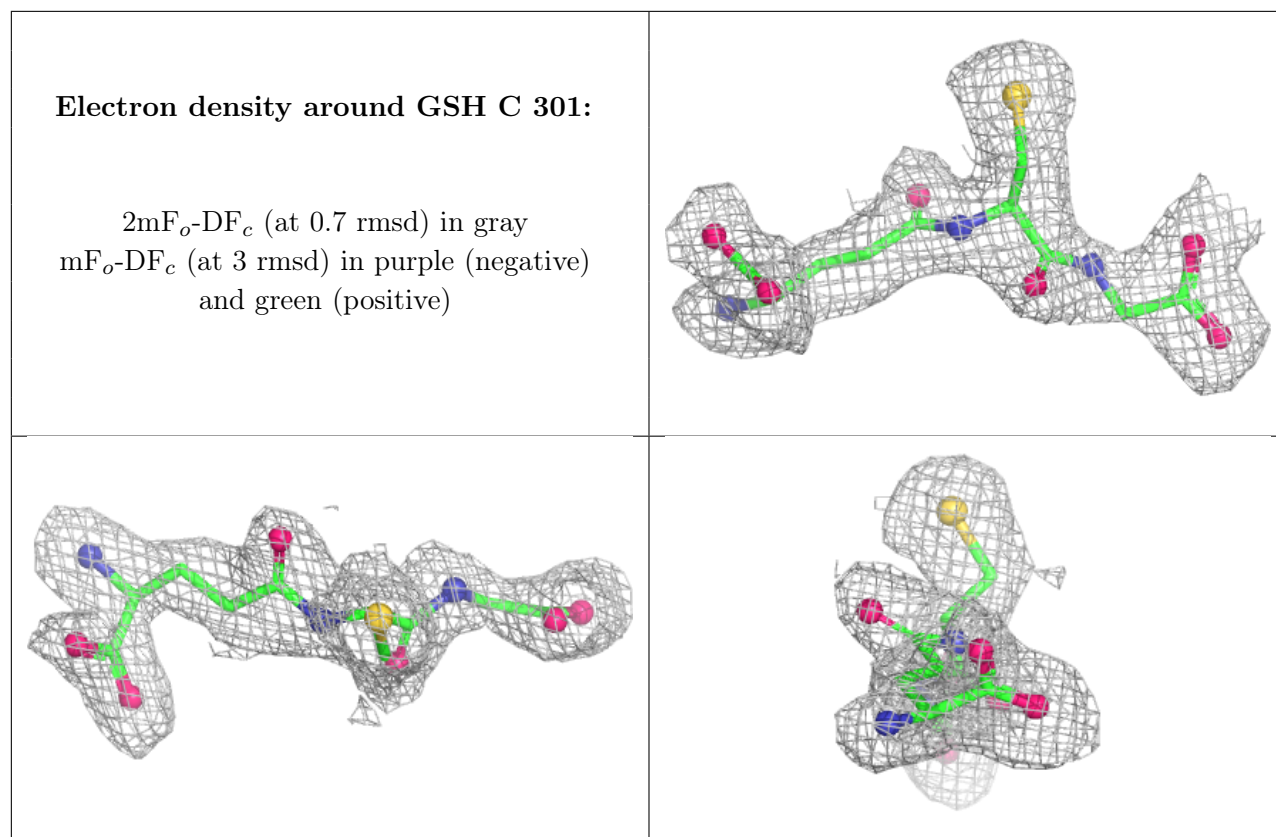
Electron density around ATP A 603:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.