



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:31 AM UTC

PDB ID : 5ECR / pdb_00005ecr
Title : Crystal Structure of FIN219-FIP1 complex with JA, VAL and Mg
Authors : Chen, C.Y.; Cheng, Y.S.
Deposited on : 2015-10-20
Resolution : 1.72 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

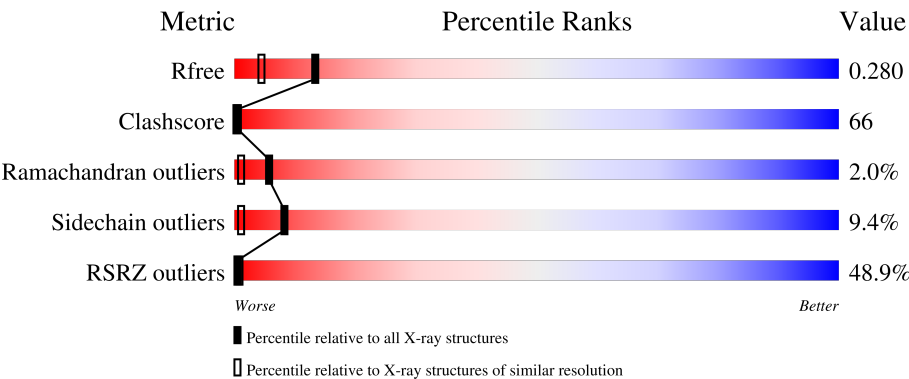
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	67% 21% 64% 13% ..
1	D	575	50% 22% 64% 13% ..
2	B	223	38% 36% 52% 8% .
2	C	223	23% 29% 56% 11% .
2	E	223	51% 32% 57% 8% .

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Mol	Chain	Length	Quality of chain
2	F	223	24% 30% 54% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	VAL	A	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17885 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:

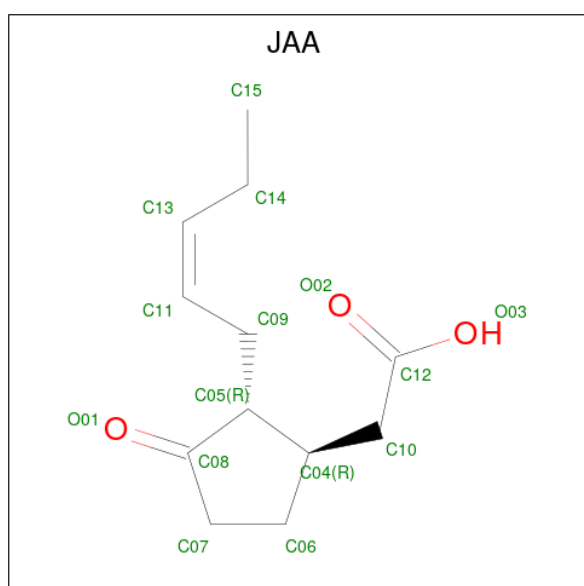
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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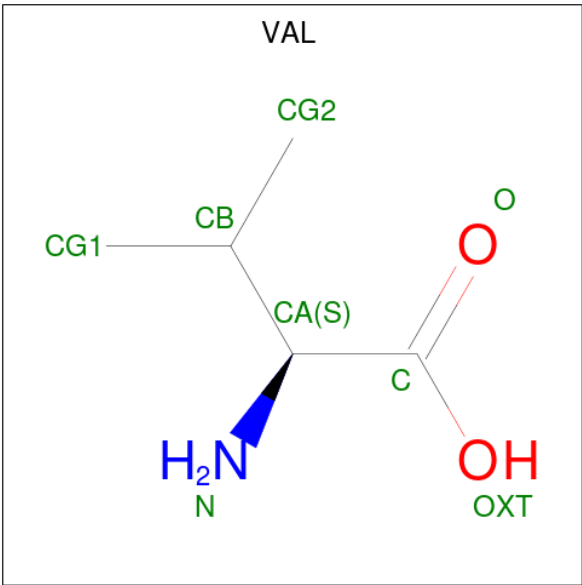
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9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



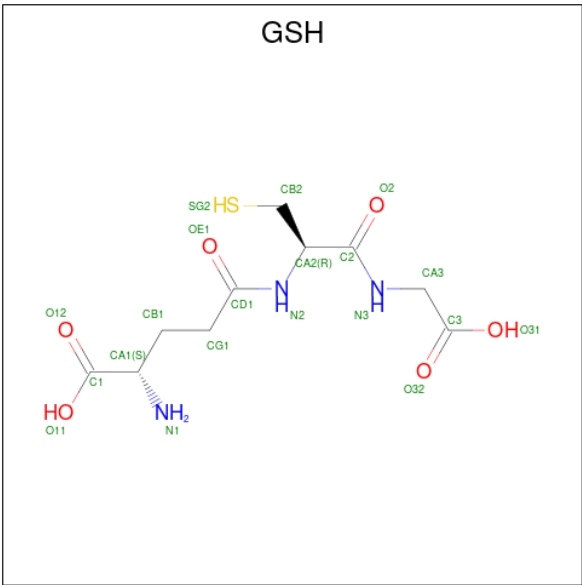
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	5	1	2		
4	D	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 5 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



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

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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

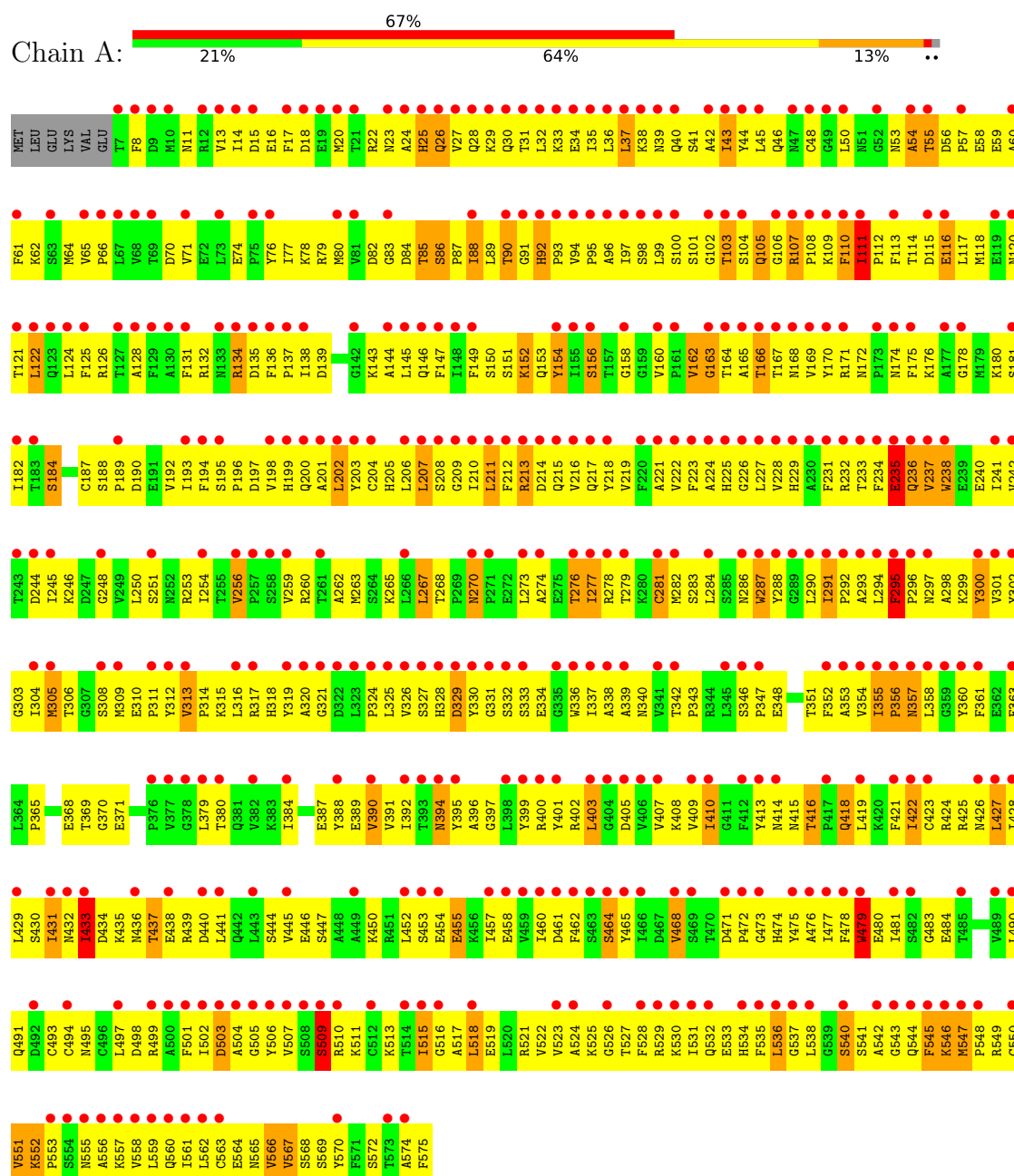
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	512	Total	O	0	0
			512	512		
7	B	203	Total	O	0	0
			203	203		
7	C	198	Total	O	0	0
			198	198		
7	D	510	Total	O	0	0
			510	510		
7	E	186	Total	O	0	0
			186	186		
7	F	199	Total	O	0	0
			199	199		

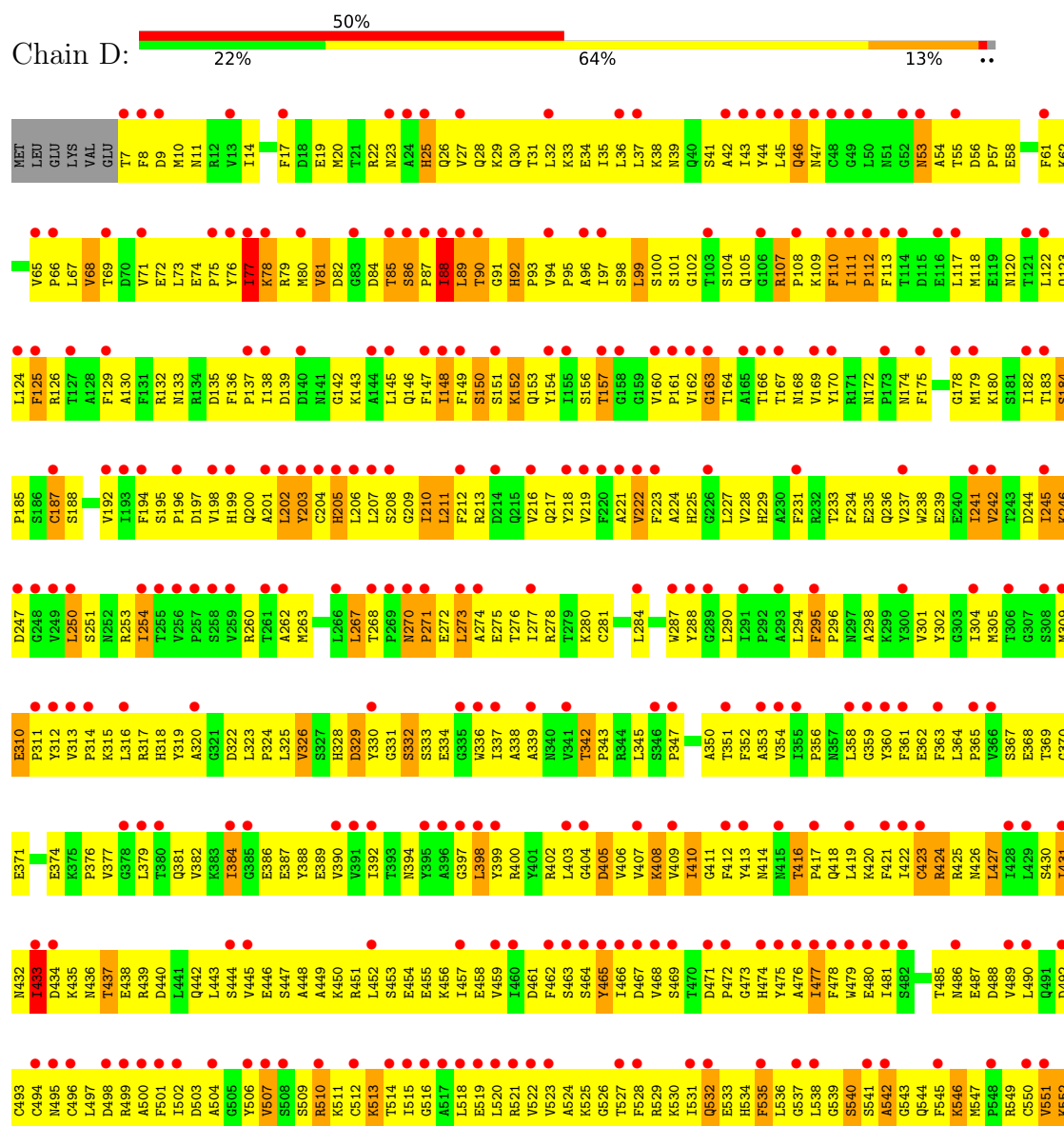
3 Residue-property plots

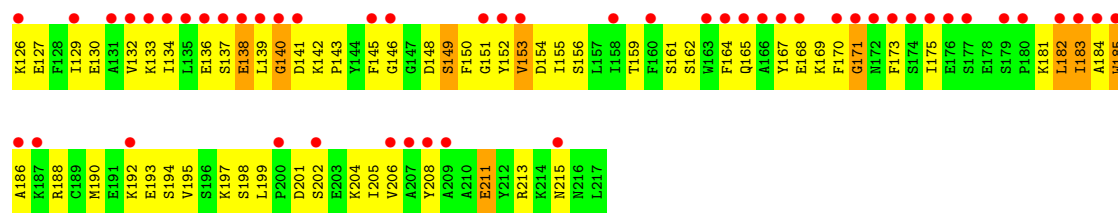
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

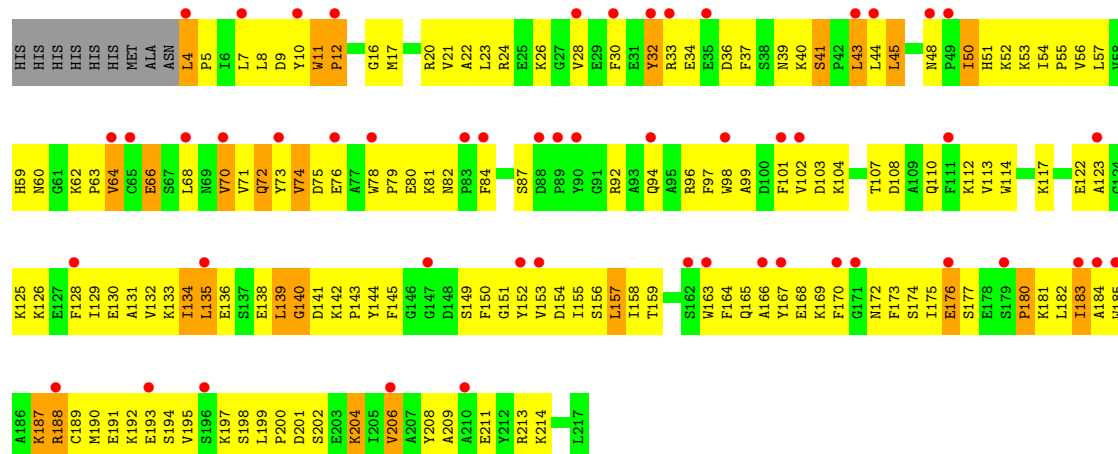


• Molecule 1: Jasmonic acid-amido synthetase JAR1

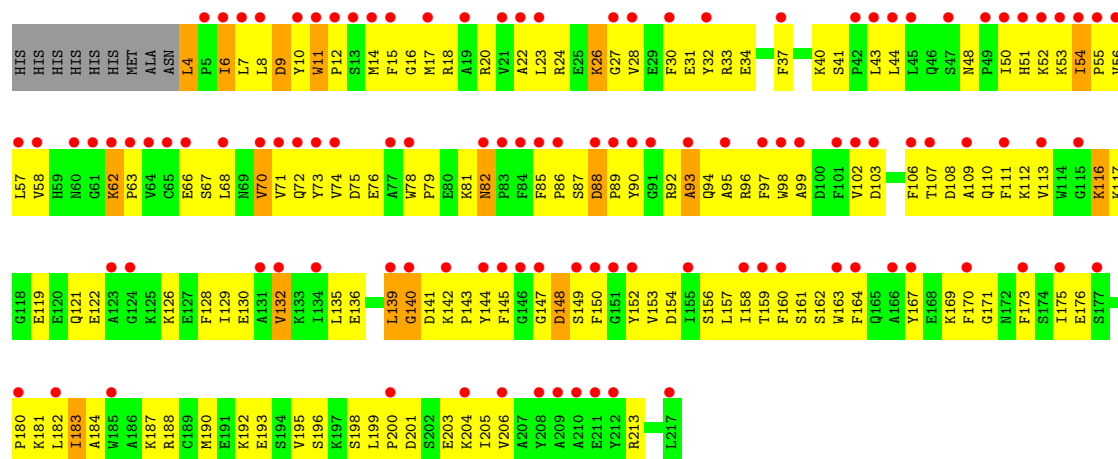




• Molecule 2: Glutathione S-transferase U20

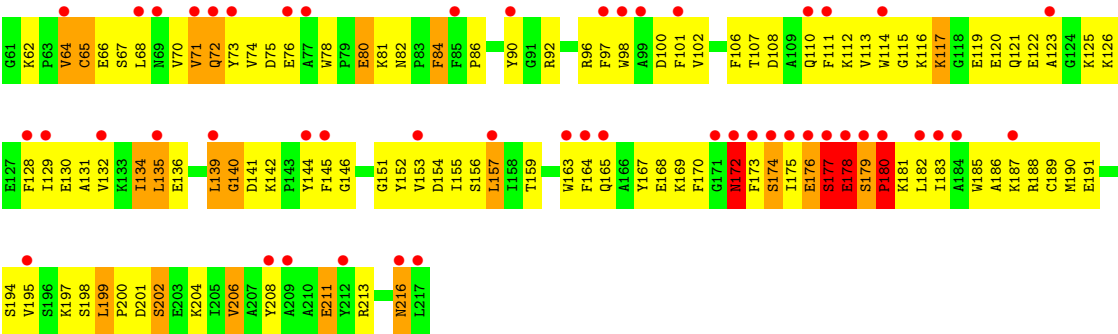


• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.84Å 53.85Å 193.64Å 90.03° 90.04° 113.41°	Depositor
Resolution (Å)	24.20 – 1.72 24.20 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.20-1.72) 99.5 (24.20-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.262 , 0.281 0.262 , 0.280	Depositor DCC
R_{free} test set	21132 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.56 , 181.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.099 for -h,-k,l 0.088 for k,h,-l 0.097 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	17885	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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 52.28 % 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 4.9763e-05. 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: JAA, GSH, MG

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	0.63	2/4581 (0.0%)	1.23	45/6219 (0.7%)
1	D	0.61	0/4581	1.21	35/6219 (0.6%)
2	B	0.46	0/1799	0.97	9/2428 (0.4%)
2	C	0.54	0/1799	1.07	9/2428 (0.4%)
2	E	0.51	1/1799 (0.1%)	1.01	9/2428 (0.4%)
2	F	0.59	2/1799 (0.1%)	1.14	10/2428 (0.4%)
All	All	0.58	5/16358 (0.0%)	1.15	117/22150 (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	2
1	D	0	2
2	E	0	1
2	F	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	93	ALA	CA-CB	-7.91	1.42	1.54
2	F	180	PRO	CA-CB	-5.92	1.45	1.53
1	A	235	GLU	C-O	-5.91	1.17	1.24
1	A	237	VAL	CA-C	5.24	1.59	1.52
2	F	176	GLU	CA-C	-5.01	1.44	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	178	GLU	N-CA-C	-12.33	98.33	113.50
1	A	355	ILE	CA-C-N	12.13	131.58	118.97
1	A	355	ILE	C-N-CA	12.13	131.58	118.97
1	A	86	SER	CA-C-N	11.89	131.65	119.76
1	A	86	SER	C-N-CA	11.89	131.65	119.76
1	D	86	SER	CA-C-N	11.43	132.34	119.99
1	D	86	SER	C-N-CA	11.43	132.34	119.99
1	A	552	LYS	CA-C-N	-11.08	107.82	120.12
1	A	552	LYS	C-N-CA	-11.08	107.82	120.12
1	D	270	ASN	CA-C-N	10.52	129.91	118.97
1	D	270	ASN	C-N-CA	10.52	129.91	118.97
2	F	179	SER	CA-C-N	-9.58	107.87	119.84
2	F	179	SER	C-N-CA	-9.58	107.87	119.84
1	D	295	PHE	CA-C-N	9.19	129.43	119.87
1	D	295	PHE	C-N-CA	9.19	129.43	119.87
1	A	213	ARG	N-CA-C	8.66	120.72	111.28
2	B	185	TRP	N-CA-C	-8.28	102.21	111.07
1	D	163	GLY	N-CA-C	7.93	125.72	110.66
2	C	11	TRP	CA-C-N	-7.82	110.06	119.84
2	C	11	TRP	C-N-CA	-7.82	110.06	119.84
1	A	238	TRP	CA-CB-CG	7.78	128.38	113.60
1	D	107	ARG	CA-C-N	7.65	128.11	119.93
1	D	107	ARG	C-N-CA	7.65	128.11	119.93
1	D	310	GLU	CA-C-N	-7.50	112.07	119.87
1	D	310	GLU	C-N-CA	-7.50	112.07	119.87
1	A	237	VAL	N-CA-C	7.46	124.85	109.34
1	D	567	VAL	N-CA-C	-7.29	101.66	111.44
1	A	107	ARG	CA-C-N	7.20	127.19	119.78
1	A	107	ARG	C-N-CA	7.20	127.19	119.78
1	A	226	GLY	N-CA-C	-7.20	103.56	112.77
1	A	256	VAL	CA-C-N	7.19	126.81	119.19
1	A	256	VAL	C-N-CA	7.19	126.81	119.19
2	E	11	TRP	CA-C-N	-7.17	110.87	119.84
2	E	11	TRP	C-N-CA	-7.17	110.87	119.84
2	E	82	ASN	CA-C-N	-7.17	112.59	119.76
2	E	82	ASN	C-N-CA	-7.17	112.59	119.76
1	A	346	SER	CA-C-N	6.90	127.19	119.32
1	A	346	SER	C-N-CA	6.90	127.19	119.32
2	B	4	LEU	CA-C-N	6.80	126.77	119.76
2	B	4	LEU	C-N-CA	6.80	126.77	119.76
1	D	86	SER	N-CA-C	6.79	118.35	109.93
2	C	4	LEU	CA-C-N	6.78	127.84	119.98
2	C	4	LEU	C-N-CA	6.78	127.84	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	62	LYS	CA-C-N	6.73	126.97	119.90
2	E	62	LYS	C-N-CA	6.73	126.97	119.90
2	F	199	LEU	CA-C-N	6.68	127.59	120.11
2	F	199	LEU	C-N-CA	6.68	127.59	120.11
1	A	531	ILE	N-CA-C	-6.62	104.03	110.72
1	A	211	LEU	N-CA-C	6.61	118.49	111.28
1	A	235	GLU	N-CA-C	-6.52	104.17	111.28
1	A	295	PHE	CA-C-N	6.47	127.92	119.84
1	A	295	PHE	C-N-CA	6.47	127.92	119.84
1	A	342	THR	CA-C-N	6.47	126.16	119.56
1	A	342	THR	C-N-CA	6.47	126.16	119.56
2	C	41	SER	CA-C-N	6.44	126.66	119.32
2	C	41	SER	C-N-CA	6.44	126.66	119.32
1	A	163	GLY	N-CA-C	6.30	123.07	110.97
2	B	11	TRP	CA-C-N	-6.28	113.44	121.04
2	B	11	TRP	C-N-CA	-6.28	113.44	121.04
2	F	11	TRP	CA-C-N	-6.27	112.00	119.84
2	F	11	TRP	C-N-CA	-6.27	112.00	119.84
1	A	551	VAL	N-CA-C	6.22	117.08	107.99
1	D	271	PRO	N-CA-C	6.21	122.35	113.47
1	A	356	PRO	N-CA-C	6.08	122.17	113.47
2	B	171	GLY	N-CA-C	-6.05	107.16	114.66
1	A	300	TYR	N-CA-C	6.05	117.43	108.60
1	D	504	ALA	N-CA-C	6.01	118.62	111.71
1	A	422	ILE	N-CA-C	-5.98	106.67	112.29
1	D	203	TYR	N-CA-C	-5.95	104.87	111.71
1	A	267	LEU	N-CA-C	5.93	119.49	109.76
1	A	563	CYS	N-CA-C	5.92	117.53	111.14
2	E	9	ASP	N-CA-C	5.88	117.15	108.86
1	A	236	GLN	N-CA-C	5.88	120.31	113.20
1	D	465	TYR	N-CA-C	5.86	118.05	108.55
1	A	394	ASN	N-CA-C	5.85	115.96	108.24
1	A	567	VAL	N-CA-C	-5.75	103.90	111.09
1	D	88	ILE	N-CA-C	5.70	121.19	109.34
1	D	184	SER	CA-C-N	5.62	125.94	119.93
1	D	184	SER	C-N-CA	5.62	125.94	119.93
1	A	479	TRP	N-CA-C	5.62	118.59	108.48
2	B	116	LYS	N-CA-C	5.60	117.48	109.14
1	D	77	ILE	N-CA-C	-5.58	104.84	113.16
2	B	88	ASP	CA-C-N	5.53	124.99	119.24
2	B	88	ASP	C-N-CA	5.53	124.99	119.24
1	D	342	THR	CA-C-N	5.48	125.15	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	342	THR	C-N-CA	5.48	125.15	119.56
1	A	238	TRP	N-CA-C	5.46	119.94	113.16
1	D	246	LYS	N-CA-C	5.46	117.68	111.02
1	D	563	CYS	N-CA-C	5.44	117.02	111.14
1	D	211	LEU	N-CA-C	5.38	117.14	111.28
1	D	267	LEU	N-CA-C	5.36	117.83	108.76
2	E	88	ASP	CA-C-N	5.36	126.54	119.84
2	E	88	ASP	C-N-CA	5.36	126.54	119.84
1	D	111	ILE	CA-C-N	5.34	125.28	119.78
1	D	111	ILE	C-N-CA	5.34	125.28	119.78
1	D	102	GLY	N-CA-C	-5.31	101.30	112.45
1	A	427	LEU	N-CA-C	5.30	117.38	107.99
2	F	176	GLU	N-CA-C	-5.30	107.35	112.97
1	D	464	SER	N-CA-C	5.29	115.11	108.45
1	A	503	ASP	N-CA-C	5.28	118.09	110.28
2	C	70	VAL	N-CA-C	5.27	115.99	110.62
1	A	111	ILE	CA-C-N	5.25	125.17	119.76
1	A	111	ILE	C-N-CA	5.25	125.17	119.76
1	A	88	ILE	N-CA-C	5.24	120.25	109.34
1	D	205	HIS	N-CA-CB	5.21	117.96	110.20
2	F	41	SER	CA-C-N	5.20	125.25	119.32
2	F	41	SER	C-N-CA	5.20	125.25	119.32
1	D	112	PRO	N-CA-C	5.20	119.47	111.21
1	D	332	SER	N-CA-C	5.18	114.67	107.73
1	A	287	TRP	CA-CB-CG	-5.16	103.79	113.60
1	A	270	ASN	N-CA-C	5.12	117.27	108.82
1	D	535	PHE	N-CA-C	5.10	117.97	111.69
1	A	235	GLU	O-C-N	-5.05	116.77	122.12
2	C	188	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	A	291	ILE	CA-C-N	-5.05	114.59	120.04
1	A	291	ILE	C-N-CA	-5.05	114.59	120.04
2	C	188	ARG	NE-CZ-NH2	5.03	123.72	119.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	LEU	Peptide
1	A	431	ILE	Peptide
1	D	427	LEU	Peptide
1	D	565	ASN	Peptide
2	E	140	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	F	177	SER	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	721	6
1	D	4479	0	4434	643	5
2	B	1748	0	1704	198	1
2	C	1748	0	1704	247	2
2	E	1748	0	1704	185	0
2	F	1748	0	1704	218	1
3	A	15	0	0	4	0
3	D	15	0	0	2	0
4	A	8	0	8	4	0
4	D	8	0	8	2	0
5	B	20	0	15	4	0
5	C	20	0	15	1	0
5	E	20	0	15	1	0
5	F	20	0	15	3	0
6	D	1	0	0	0	0
7	A	512	0	0	130	4
7	B	203	0	0	28	4
7	C	198	0	0	64	3
7	D	510	0	0	106	4
7	E	186	0	0	27	1
7	F	199	0	0	47	1
All	All	17885	0	15760	2089	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 66.

All (2089) 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:152:LYS:HZ1	1:A:530:LYS:NZ	1.21	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:NZ	1:A:530:LYS:HZ1	1.30	1.26
1:D:488:ASP:OD1	7:D:701:HOH:O	1.53	1.24
2:C:188:ARG:NH1	1:D:499:ARG:O	1.70	1.22
2:E:92:ARG:NH1	2:F:76:GLU:OE1	1.79	1.15
1:A:446:GLU:OE2	7:A:701:HOH:O	1.67	1.12
1:D:152:LYS:NZ	1:D:527:THR:OG1	1.81	1.12
2:C:188:ARG:HH12	1:D:500:ALA:HA	1.11	1.11
1:A:176:LYS:NZ	1:A:190:ASP:OD2	1.83	1.10
2:C:9:ASP:OD2	7:C:402:HOH:O	1.71	1.09
1:A:134:ARG:NH1	7:A:702:HOH:O	1.86	1.04
2:C:176:GLU:OE2	1:D:573:THR:OG1	1.76	1.04
2:E:139:LEU:HG	2:E:142:LYS:HB2	1.35	1.01
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.44	1.00
1:A:106:GLY:HA3	1:A:432:ASN:HD21	1.27	0.99
1:A:166:THR:HG22	4:A:602:VAL:HG13	1.44	0.98
1:A:510:ARG:NH1	1:A:516:GLY:O	1.94	0.98
2:E:26:LYS:HZ3	2:E:74:VAL:HG22	1.29	0.98
2:E:40:LYS:NZ	2:E:52:LYS:O	1.96	0.98
1:A:519:GLU:OE2	1:A:569:SER:OG	1.84	0.96
2:F:60:ASN:ND2	7:F:409:HOH:O	1.99	0.95
1:A:284:LEU:HD13	1:A:287:TRP:H	1.30	0.95
2:F:120:GLU:OE1	7:F:401:HOH:O	1.85	0.94
1:A:152:LYS:HA	1:A:564:GLU:HB2	1.49	0.94
2:B:26:LYS:NZ	2:B:82:ASN:H	1.64	0.94
2:C:184:ALA:HB1	1:D:499:ARG:CZ	1.98	0.93
1:A:491:GLN:OE1	7:A:703:HOH:O	1.87	0.93
1:D:254:ILE:O	1:D:260:ARG:NH1	2.01	0.93
1:A:510:ARG:NH1	1:A:515:ILE:HD12	1.84	0.93
2:C:66:GLU:OE2	7:C:405:HOH:O	1.87	0.92
2:C:92:ARG:NH1	7:C:414:HOH:O	2.03	0.92
2:F:190:MET:SD	7:F:436:HOH:O	2.26	0.92
1:A:39:ASN:ND2	2:B:141:ASP:O	2.01	0.92
1:A:199:HIS:HB3	1:A:525:LYS:H	1.32	0.92
1:D:452:LEU:HB3	1:D:457:ILE:HD11	1.49	0.92
1:A:93:PRO:HG3	2:B:184:ALA:HB3	1.52	0.91
2:C:188:ARG:NH1	1:D:500:ALA:HA	1.84	0.91
2:B:116:LYS:O	2:B:213:ARG:NH1	2.02	0.91
1:D:466:ILE:HB	1:D:552:LYS:HA	1.53	0.91
1:A:498:ASP:O	7:A:704:HOH:O	1.88	0.91
1:D:99:LEU:HB3	1:D:557:LYS:H	1.32	0.91
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:156:SER:OG	7:F:402:HOH:O	1.85	0.91
1:A:208:SER:HA	1:A:211:LEU:HD12	1.52	0.90
1:A:225:HIS:HA	1:A:228:VAL:HG22	1.54	0.90
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.54	0.90
1:A:475:TYR:H	1:A:510:ARG:HH22	1.15	0.89
1:A:165:ALA:H	1:A:557:LYS:NZ	1.70	0.89
2:F:122:GLU:OE2	7:F:403:HOH:O	1.89	0.89
2:F:26:LYS:NZ	2:F:82:ASN:O	2.06	0.89
2:C:181:LYS:NZ	7:C:416:HOH:O	2.04	0.89
1:A:165:ALA:N	1:A:557:LYS:HZ3	1.68	0.88
2:F:20:ARG:NH1	7:F:404:HOH:O	1.90	0.88
1:A:152:LYS:NZ	1:A:530:LYS:NZ	2.03	0.88
2:C:117:LYS:NZ	7:C:403:HOH:O	1.77	0.88
2:F:136:GLU:OE2	2:F:180:PRO:HD3	1.73	0.88
1:D:172:ASN:ND2	1:D:174:ASN:OD1	2.07	0.88
2:C:26:LYS:NZ	2:C:82:ASN:O	2.07	0.87
2:C:98:TRP:O	7:C:406:HOH:O	1.91	0.87
2:C:41:SER:N	7:C:415:HOH:O	2.03	0.87
1:A:402:ARG:NH1	7:A:726:HOH:O	2.08	0.87
1:A:100:SER:OG	1:A:334:GLU:OE2	1.92	0.86
2:C:176:GLU:OE1	7:D:701:HOH:O	1.93	0.86
1:D:123:GLN:NE2	7:D:713:HOH:O	2.06	0.86
1:A:134:ARG:NH1	7:A:731:HOH:O	2.09	0.86
1:A:164:THR:HG22	1:A:557:LYS:HD3	1.57	0.86
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.56	0.86
2:C:184:ALA:O	1:D:499:ARG:NH2	2.09	0.86
1:D:552:LYS:O	1:D:554:SER:N	2.09	0.86
1:D:309:MET:O	7:D:702:HOH:O	1.92	0.85
1:A:143:LYS:NZ	1:A:187:CYS:HB3	1.91	0.85
1:A:38:LYS:NZ	1:A:395:TYR:OH	2.10	0.85
1:A:277:ILE:HG23	1:A:278:ARG:HG3	1.58	0.85
2:C:168:GLU:OE1	7:C:407:HOH:O	1.93	0.85
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.59	0.85
1:D:93:PRO:HG2	2:E:181:LYS:HA	1.58	0.85
2:F:26:LYS:HG2	2:F:81:LYS:NZ	1.92	0.84
2:F:197:LYS:O	7:F:405:HOH:O	1.94	0.84
1:D:337:ILE:HD13	1:D:539:GLY:HA3	1.59	0.84
2:F:132:VAL:HG23	2:F:182:LEU:HD13	1.57	0.84
1:A:143:LYS:HD3	1:A:212:PHE:HB2	1.59	0.84
1:A:551:VAL:HG11	1:A:559:LEU:HD11	1.60	0.84
1:D:408:LYS:HG2	1:D:420:LYS:HG2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:187:LYS:O	7:E:401:HOH:O	1.96	0.84
2:E:93:ALA:HB1	2:F:73:TYR:HE1	1.43	0.83
2:C:172:ASN:OD1	7:C:408:HOH:O	1.96	0.83
1:A:74:GLU:OE2	7:A:706:HOH:O	1.97	0.83
2:C:193:GLU:HG3	7:C:442:HOH:O	1.79	0.83
2:E:143:PRO:HB2	2:E:188:ARG:HH12	1.44	0.83
2:F:18:ARG:NH2	7:F:414:HOH:O	2.10	0.83
1:D:480:GLU:OE1	7:D:703:HOH:O	1.94	0.83
1:D:509:SER:O	1:D:513:LYS:N	2.10	0.83
1:A:103:THR:HB	1:A:106:GLY:HA2	1.61	0.83
2:E:143:PRO:HB2	2:E:188:ARG:NH1	1.93	0.83
2:C:26:LYS:HG2	2:C:81:LYS:NZ	1.93	0.83
2:F:120:GLU:O	7:F:406:HOH:O	1.97	0.82
1:A:20:MET:HG2	1:A:356:PRO:HG2	1.61	0.82
1:A:87:PRO:HB2	2:B:143:PRO:HA	1.60	0.82
1:D:199:HIS:HB3	1:D:525:LYS:H	1.43	0.82
1:D:405:ASP:HB2	1:D:541:SER:HB3	1.58	0.82
1:D:495:ASN:C	1:D:499:ARG:HH12	1.87	0.82
1:A:106:GLY:HA3	1:A:432:ASN:ND2	1.94	0.82
2:E:40:LYS:HZ3	2:E:52:LYS:HB2	1.45	0.82
2:E:50:ILE:HG13	2:E:51:HIS:H	1.43	0.82
1:A:225:HIS:HB3	1:A:312:TYR:CE2	2.15	0.82
2:C:79:PRO:O	7:C:410:HOH:O	1.97	0.81
2:C:184:ALA:HB1	1:D:499:ARG:NH1	1.95	0.81
1:D:495:ASN:C	1:D:499:ARG:NH1	2.37	0.81
2:E:26:LYS:NZ	2:E:74:VAL:HG22	1.93	0.81
1:A:478:PHE:CZ	1:A:562:LEU:HA	2.15	0.81
2:C:17:MET:HE2	2:C:200:PRO:HD2	1.63	0.81
1:D:305:MET:SD	7:D:1023:HOH:O	2.38	0.81
1:D:213:ARG:NE	1:D:294:LEU:O	2.12	0.81
2:C:28:VAL:O	7:C:409:HOH:O	1.97	0.81
1:A:45:LEU:HD22	1:A:50:LEU:HD12	1.62	0.81
1:A:138:ILE:HD12	1:A:217:GLN:HB2	1.61	0.81
1:D:42:ALA:HA	2:E:143:PRO:HG3	1.62	0.81
1:D:199:HIS:H	1:D:524:ALA:HB1	1.44	0.81
1:D:239:GLU:OE2	7:D:704:HOH:O	1.98	0.81
1:D:499:ARG:CZ	1:D:499:ARG:HB2	2.08	0.80
1:D:531:ILE:HA	1:D:534:HIS:CE1	2.15	0.80
2:F:72:GLN:OE1	7:F:407:HOH:O	1.99	0.80
2:E:92:ARG:HH12	2:F:76:GLU:CD	1.90	0.80
1:A:143:LYS:HZ2	1:A:209:GLY:HA2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:VAL:HG13	1:A:555:ASN:HB3	1.63	0.80
1:A:424:ARG:NH1	7:A:747:HOH:O	2.15	0.80
1:A:18:ASP:OD1	1:A:414:ASN:ND2	2.14	0.80
1:A:143:LYS:HZ2	1:A:187:CYS:HB3	1.44	0.80
2:F:178:GLU:O	7:F:410:HOH:O	2.00	0.80
1:A:413:TYR:OH	7:A:707:HOH:O	1.97	0.80
1:D:87:PRO:HG2	2:E:188:ARG:HD2	1.64	0.80
1:D:150:SER:HB2	1:D:167:THR:HA	1.61	0.80
2:B:24:ARG:HH12	2:B:197:LYS:HE3	1.47	0.79
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.63	0.79
1:A:458:GLU:O	7:A:708:HOH:O	2.01	0.79
2:B:136:GLU:OE2	7:B:401:HOH:O	1.99	0.79
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.62	0.79
1:D:432:ASN:ND2	7:D:735:HOH:O	2.15	0.79
2:C:132:VAL:HG23	2:C:182:LEU:HD13	1.63	0.79
2:C:9:ASP:OD1	7:C:412:HOH:O	2.00	0.79
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.65	0.79
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.47	0.79
2:B:145:PHE:HB2	2:B:154:ASP:HB3	1.64	0.79
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.65	0.79
1:A:62:LYS:HG2	1:A:400:ARG:NH1	1.99	0.78
1:A:306:THR:OG1	1:A:330:TYR:OH	2.01	0.78
1:A:117:LEU:HD11	1:A:333:SER:HA	1.65	0.78
1:D:138:ILE:HB	1:D:217:GLN:HG3	1.64	0.78
1:A:304:ILE:HG13	1:A:328:HIS:HB3	1.65	0.78
1:A:305:MET:HE3	1:A:347:PRO:HG3	1.64	0.78
1:A:236:GLN:OE1	7:A:710:HOH:O	2.02	0.78
2:B:215:ASN:ND2	7:B:405:HOH:O	2.08	0.78
1:D:44:TYR:HB2	1:D:89:LEU:HG	1.66	0.78
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.64	0.78
2:B:76:GLU:OE1	7:C:404:HOH:O	2.01	0.78
1:D:268:THR:O	7:D:705:HOH:O	2.02	0.78
1:D:322:ASP:O	7:D:706:HOH:O	2.02	0.78
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.48	0.78
1:A:150:SER:OG	7:A:709:HOH:O	2.02	0.78
1:A:452:LEU:HD23	1:A:481:ILE:HG12	1.64	0.78
1:A:425:ARG:NH2	7:A:734:HOH:O	2.09	0.78
1:A:332:SER:HG	1:A:534:HIS:HE2	1.32	0.78
1:A:465:TYR:HA	1:A:551:VAL:HB	1.66	0.78
1:A:152:LYS:CE	1:A:530:LYS:HZ1	1.97	0.77
1:A:224:ALA:HA	1:A:227:LEU:HD12	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PHE:HB2	1:A:506:TYR:CZ	2.19	0.77
1:D:418:GLN:OE1	7:D:707:HOH:O	2.02	0.77
2:E:40:LYS:NZ	2:E:52:LYS:HB2	1.98	0.77
1:A:464:SER:HG	1:A:550:CYS:HG	1.07	0.77
1:A:165:ALA:H	1:A:557:LYS:HZ3	0.84	0.77
1:D:99:LEU:HD23	1:D:558:VAL:H	1.49	0.77
2:B:18:ARG:HD3	2:B:156:SER:HA	1.65	0.77
1:A:527:THR:HG23	1:A:561:ILE:HG21	1.65	0.77
2:F:119:GLU:O	7:F:411:HOH:O	2.03	0.77
1:A:152:LYS:HD2	1:A:561:ILE:HG23	1.65	0.76
2:B:201:ASP:O	7:B:402:HOH:O	2.02	0.76
1:D:439:ARG:NH1	7:D:741:HOH:O	2.17	0.76
2:F:164:PHE:HD2	2:F:183:ILE:HD13	1.49	0.76
1:A:92:HIS:HE1	2:B:185:TRP:HZ2	1.34	0.76
1:D:198:VAL:HG22	1:D:565:ASN:HD22	1.48	0.76
2:E:70:VAL:HA	2:E:73:TYR:CE2	2.21	0.76
1:A:454:GLU:OE1	7:A:711:HOH:O	2.03	0.76
2:F:8:LEU:HD22	2:F:33:ARG:HH21	1.50	0.76
1:A:340:ASN:OD1	7:A:714:HOH:O	2.04	0.76
2:E:93:ALA:HB1	2:F:73:TYR:CE1	2.21	0.75
1:A:555:ASN:N	7:A:718:HOH:O	2.20	0.75
1:D:389:GLU:OE2	1:D:404:GLY:HA2	1.87	0.75
1:A:238:TRP:HA	1:A:241:ILE:HB	1.69	0.75
1:A:340:ASN:ND2	7:A:755:HOH:O	2.18	0.75
2:C:164:PHE:HD2	2:C:183:ILE:HD12	1.52	0.75
2:C:201:ASP:OD2	1:D:456:LYS:NZ	2.18	0.75
1:A:146:GLN:NE2	7:A:758:HOH:O	2.19	0.75
2:F:56:VAL:HG13	7:F:426:HOH:O	1.85	0.75
2:E:122:GLU:OE2	7:E:402:HOH:O	2.05	0.75
2:B:96:ARG:HH11	2:C:73:TYR:HE1	1.32	0.74
2:F:8:LEU:HD21	2:F:43:LEU:HD11	1.68	0.74
1:A:152:LYS:HG3	1:A:561:ILE:HA	1.69	0.74
2:F:62:LYS:NZ	7:F:408:HOH:O	1.99	0.74
1:D:310:GLU:HG2	1:D:311:PRO:HD3	1.69	0.74
2:B:96:ARG:NH1	2:C:73:TYR:CE1	2.54	0.74
1:D:211:LEU:O	7:D:712:HOH:O	2.06	0.74
2:C:64:VAL:HG23	2:C:70:VAL:HG22	1.69	0.74
1:D:246:LYS:HE2	1:D:271:PRO:HA	1.69	0.74
1:A:108:PRO:HB3	1:A:555:ASN:HB2	1.69	0.74
1:A:558:VAL:O	7:A:713:HOH:O	2.04	0.74
2:C:80:GLU:OE2	7:C:417:HOH:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLN:NE2	7:D:743:HOH:O	2.17	0.74
1:A:361:PHE:O	7:A:712:HOH:O	2.04	0.74
1:A:552:LYS:O	7:A:718:HOH:O	2.06	0.74
2:C:33:ARG:NE	7:C:422:HOH:O	2.12	0.74
1:A:331:GLY:HA2	7:A:764:HOH:O	1.87	0.74
1:A:143:LYS:NZ	1:A:209:GLY:HA2	2.02	0.74
1:D:87:PRO:HB2	2:E:143:PRO:HA	1.69	0.73
1:A:79:ARG:HH22	2:B:188:ARG:NH1	1.85	0.73
1:A:301:VAL:HG11	1:A:316:LEU:HD21	1.69	0.73
1:A:401:TYR:HE2	1:A:403:LEU:HD13	1.52	0.73
2:F:180:PRO:HD2	2:F:181:LYS:HG2	1.68	0.73
1:A:397:GLY:O	7:A:721:HOH:O	2.06	0.73
1:A:548:PRO:O	7:A:716:HOH:O	2.05	0.73
2:C:64:VAL:HB	2:C:73:TYR:CD2	2.22	0.73
1:D:9:ASP:O	7:D:710:HOH:O	2.05	0.73
1:D:143:LYS:HD3	1:D:187:CYS:HB3	1.71	0.73
1:A:479:TRP:NE1	7:A:762:HOH:O	2.20	0.73
1:A:132:ARG:NH1	7:A:754:HOH:O	2.22	0.73
1:A:337:ILE:N	7:A:764:HOH:O	2.21	0.73
2:C:142:LYS:NZ	7:C:401:HOH:O	1.60	0.73
1:D:164:THR:OG1	1:D:557:LYS:O	2.07	0.73
1:D:477:ILE:HG13	1:D:520:LEU:HA	1.71	0.73
1:A:304:ILE:O	7:A:715:HOH:O	2.05	0.73
1:A:304:ILE:O	7:A:722:HOH:O	2.06	0.73
1:A:494:CYS:HA	1:A:497:LEU:HD12	1.69	0.73
2:C:26:LYS:HD2	2:C:74:VAL:HG13	1.70	0.73
2:C:33:ARG:HH22	2:C:43:LEU:HD11	1.53	0.73
2:C:191:GLU:OE1	1:D:447:SER:OG	2.07	0.73
2:B:24:ARG:NE	2:B:198:SER:OG	2.20	0.73
2:C:211:GLU:OE1	7:C:418:HOH:O	2.06	0.73
1:A:138:ILE:HG13	1:A:217:GLN:OE1	1.88	0.73
1:A:351:THR:HG21	1:A:410:ILE:HG12	1.71	0.73
2:E:89:PRO:HB3	2:F:76:GLU:HG3	1.71	0.73
2:F:136:GLU:HG3	2:F:181:LYS:HD3	1.71	0.73
1:A:284:LEU:HD22	1:A:287:TRP:HA	1.71	0.72
1:A:529:ARG:NH1	7:A:767:HOH:O	2.22	0.72
1:D:236:GLN:NE2	7:D:748:HOH:O	2.18	0.72
1:D:423:CYS:SG	1:D:541:SER:OG	2.46	0.72
2:B:50:ILE:HG13	2:C:134:ILE:HD12	1.72	0.72
2:F:98:TRP:HE3	2:F:101:PHE:HB2	1.54	0.72
2:F:122:GLU:HA	2:F:125:LYS:HE2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASP:OD1	7:A:717:HOH:O	2.06	0.72
1:A:64:MET:O	7:A:723:HOH:O	2.06	0.72
1:D:22:ARG:HH11	1:D:414:ASN:CG	1.96	0.72
1:D:426:ASN:ND2	7:D:758:HOH:O	2.21	0.72
2:F:168:GLU:OE2	2:F:176:GLU:OE2	2.06	0.72
2:F:26:LYS:HG2	2:F:81:LYS:HZ3	1.52	0.72
1:A:223:PHE:CZ	1:A:536:LEU:HB2	2.24	0.72
1:A:150:SER:O	1:A:171:ARG:NH1	2.23	0.72
1:A:337:ILE:HG12	1:A:361:PHE:CZ	2.24	0.72
2:B:92:ARG:NH2	2:C:76:GLU:OE1	2.22	0.72
1:D:524:ALA:HB2	1:D:567:VAL:HG11	1.71	0.72
2:E:20:ARG:HB3	2:E:24:ARG:NH1	2.04	0.72
1:A:446:GLU:OE2	7:A:728:HOH:O	2.08	0.72
1:D:518:LEU:O	7:D:715:HOH:O	2.08	0.71
1:D:534:HIS:O	7:D:714:HOH:O	2.07	0.71
1:A:331:GLY:HA3	1:A:336:TRP:CE3	2.25	0.71
2:C:189:CYS:HB3	7:C:432:HOH:O	1.89	0.71
1:A:295:PHE:O	7:A:725:HOH:O	2.07	0.71
1:D:152:LYS:HE3	1:D:565:ASN:HB2	1.71	0.71
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.72	0.71
2:E:14:MET:HA	2:E:17:MET:HE3	1.72	0.71
2:B:119:GLU:OE2	7:B:404:HOH:O	2.08	0.71
5:B:301:GSH:O31	7:B:407:HOH:O	2.09	0.71
1:A:139:ASP:O	7:A:727:HOH:O	2.08	0.71
1:A:244:ASP:OD2	7:A:724:HOH:O	2.07	0.71
2:F:117:LYS:HE3	2:F:213:ARG:NH1	2.06	0.71
1:A:199:HIS:N	1:A:524:ALA:HB1	2.05	0.71
1:D:208:SER:O	7:D:716:HOH:O	2.08	0.71
1:A:199:HIS:H	1:A:524:ALA:HB1	1.56	0.70
1:D:301:VAL:HG11	1:D:316:LEU:HD21	1.71	0.70
2:F:176:GLU:O	2:F:180:PRO:HB3	1.91	0.70
2:C:4:LEU:N	7:C:427:HOH:O	2.23	0.70
2:C:187:LYS:NZ	1:D:496:CYS:HB2	2.06	0.70
1:D:10:MET:SD	7:D:754:HOH:O	2.48	0.70
1:D:37:LEU:O	7:D:717:HOH:O	2.08	0.70
2:B:103:ASP:O	7:B:406:HOH:O	2.09	0.70
2:C:139:LEU:HD23	7:C:430:HOH:O	1.90	0.70
1:A:331:GLY:N	1:A:537:GLY:O	2.25	0.70
2:B:24:ARG:NH2	2:B:193:GLU:O	2.25	0.70
1:D:496:CYS:HA	1:D:499:ARG:NH2	2.06	0.70
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:OG	1:A:333:SER:N	2.23	0.70
1:D:108:PRO:HG2	1:D:552:LYS:H	1.57	0.70
1:A:97:ILE:O	7:A:732:HOH:O	2.09	0.70
2:C:7:LEU:HD21	2:C:23:LEU:HD12	1.74	0.70
1:D:199:HIS:O	7:D:718:HOH:O	2.09	0.70
2:E:201:ASP:O	7:E:404:HOH:O	2.09	0.70
1:D:32:LEU:HA	1:D:35:ILE:HD12	1.72	0.70
1:D:406:VAL:O	1:D:541:SER:OG	2.10	0.70
2:E:92:ARG:NH1	2:F:76:GLU:CD	2.49	0.70
2:F:98:TRP:CE3	2:F:101:PHE:HB2	2.26	0.70
1:A:246:LYS:NZ	1:A:278:ARG:HH22	1.89	0.70
1:A:181:SER:O	7:A:730:HOH:O	2.08	0.70
2:C:26:LYS:HG2	2:C:81:LYS:HZ1	1.53	0.70
1:D:53:ASN:N	2:E:90:TYR:OH	2.24	0.70
1:D:549:ARG:NH1	7:D:726:HOH:O	2.24	0.70
1:A:354:VAL:HG21	1:A:379:LEU:HD21	1.73	0.70
1:A:494:CYS:SG	7:A:703:HOH:O	2.50	0.70
1:D:513:LYS:HZ2	1:D:575:PHE:HB3	1.57	0.70
1:A:16:GLU:OE2	7:A:733:HOH:O	2.09	0.69
2:C:33:ARG:NH2	2:C:43:LEU:HD21	2.07	0.69
2:C:139:LEU:HG	2:C:145:PHE:CZ	2.27	0.69
1:D:389:GLU:OE2	1:D:402:ARG:NE	2.25	0.69
2:B:20:ARG:HD3	2:B:198:SER:HB3	1.73	0.69
1:D:109:LYS:O	7:D:719:HOH:O	2.09	0.69
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.25	0.69
1:A:118:MET:SD	7:A:810:HOH:O	2.50	0.69
2:B:18:ARG:NH2	2:B:67:SER:OG	2.25	0.69
2:E:116:LYS:O	2:E:213:ARG:NH1	2.25	0.69
1:A:39:ASN:HA	2:B:142:LYS:HG3	1.73	0.69
2:C:188:ARG:HD2	2:C:191:GLU:OE2	1.92	0.69
2:E:176:GLU:OE2	7:E:405:HOH:O	2.10	0.69
2:B:182:LEU:HD13	2:B:185:TRP:CZ3	2.27	0.69
1:A:53:ASN:OD1	1:A:54:ALA:N	2.24	0.69
1:A:464:SER:HB2	1:A:477:ILE:HD13	1.74	0.69
2:B:18:ARG:HD2	2:B:155:ILE:HD12	1.74	0.69
1:D:549:ARG:NH2	7:D:769:HOH:O	2.26	0.69
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.28	0.69
2:F:139:LEU:HG	2:F:145:PHE:CZ	2.27	0.69
1:A:22:ARG:NH1	7:A:779:HOH:O	2.25	0.69
1:A:407:VAL:HG22	1:A:541:SER:HB2	1.75	0.69
2:C:101:PHE:O	7:C:419:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:HE2	1:A:111:ILE:HD11	1.73	0.69
1:A:166:THR:OG1	1:A:167:THR:N	2.24	0.69
1:D:332:SER:OG	1:D:333:SER:N	2.26	0.69
2:E:180:PRO:HD2	2:E:181:LYS:HG3	1.74	0.69
1:A:483:GLY:O	7:A:736:HOH:O	2.11	0.69
2:C:144:TYR:HB3	2:C:154:ASP:OD2	1.93	0.69
1:D:38:LYS:HB3	2:E:140:GLY:HA3	1.74	0.69
1:D:107:ARG:NH2	1:D:552:LYS:HB3	2.08	0.69
1:D:514:THR:O	7:D:724:HOH:O	2.11	0.69
2:E:119:GLU:OE2	7:E:406:HOH:O	2.11	0.69
1:A:99:LEU:HB3	1:A:557:LYS:HB2	1.75	0.68
1:A:224:ALA:HB1	1:A:316:LEU:HD22	1.75	0.68
3:A:601:JAA:O02	7:A:737:HOH:O	2.11	0.68
1:D:54:ALA:O	7:D:721:HOH:O	2.10	0.68
1:D:487:GLU:HG2	1:D:570:TYR:CZ	2.29	0.68
1:D:495:ASN:HB3	1:D:499:ARG:NH1	2.07	0.68
2:E:159:THR:HA	2:E:199:LEU:HD21	1.74	0.68
2:F:30:PHE:O	7:F:413:HOH:O	2.10	0.68
2:F:64:VAL:N	7:F:426:HOH:O	2.27	0.68
1:A:184:SER:HB2	1:A:217:GLN:NE2	2.09	0.68
1:A:202:LEU:HD21	1:A:529:ARG:HH22	1.57	0.68
2:B:142:LYS:NZ	2:B:145:PHE:O	2.19	0.68
1:D:77:ILE:CG1	1:D:110:PHE:HB3	2.24	0.68
1:D:461:ASP:OD1	7:D:723:HOH:O	2.11	0.68
2:E:66:GLU:OE2	7:E:408:HOH:O	2.12	0.68
1:A:552:LYS:HG3	1:A:553:PRO:HD2	1.75	0.68
1:A:560:GLN:OE1	7:A:735:HOH:O	2.10	0.68
1:D:147:PHE:CE1	1:D:202:LEU:HD13	2.28	0.68
1:D:245:ILE:O	7:D:705:HOH:O	2.10	0.68
2:F:119:GLU:OE2	7:F:416:HOH:O	2.12	0.68
1:A:560:GLN:HB3	7:A:784:HOH:O	1.94	0.68
2:C:59:HIS:O	7:C:421:HOH:O	2.12	0.68
1:D:81:VAL:O	7:D:709:HOH:O	2.11	0.68
1:D:81:VAL:HG11	1:D:110:PHE:CE2	2.29	0.68
1:A:30:GLN:HA	1:A:33:LYS:HG2	1.75	0.68
1:A:168:ASN:O	1:A:172:ASN:HB2	1.94	0.68
1:D:104:SER:HB2	1:D:109:LYS:HB2	1.75	0.68
1:A:171:ARG:O	7:A:738:HOH:O	2.12	0.68
2:B:113:VAL:O	7:B:408:HOH:O	2.11	0.68
1:D:125:PHE:HE2	1:D:328:HIS:CE1	2.12	0.68
1:D:125:PHE:HE2	1:D:328:HIS:HE1	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:HIS:N	1:D:524:ALA:HB1	2.08	0.68
2:C:104:LYS:NZ	7:C:413:HOH:O	2.02	0.67
1:D:56:ASP:OD2	7:D:722:HOH:O	2.11	0.67
2:F:106:PHE:O	7:F:417:HOH:O	2.12	0.67
1:A:231:PHE:O	1:A:235:GLU:HB3	1.93	0.67
1:A:399:TYR:O	7:A:740:HOH:O	2.12	0.67
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.29	0.67
1:D:143:LYS:HG2	1:D:216:VAL:HG22	1.76	0.67
1:D:183:THR:O	7:D:729:HOH:O	2.12	0.67
1:A:339:ALA:HB2	1:A:355:ILE:HD11	1.77	0.67
1:D:66:PRO:O	7:D:728:HOH:O	2.12	0.67
1:A:435:LYS:HE3	1:A:438:GLU:HB3	1.76	0.67
1:A:440:ASP:O	7:A:705:HOH:O	2.12	0.67
1:A:445:VAL:HG13	1:A:479:TRP:HE1	1.59	0.67
1:A:96:ALA:HA	1:A:162:VAL:HA	1.77	0.67
1:D:210:ILE:HA	1:D:213:ARG:HG3	1.76	0.67
2:F:26:LYS:O	7:F:415:HOH:O	2.11	0.67
2:F:81:LYS:N	7:F:423:HOH:O	2.22	0.67
1:A:86:SER:HB2	2:B:188:ARG:HE	1.60	0.67
2:B:82:ASN:OD1	7:B:409:HOH:O	2.12	0.67
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.30	0.67
1:D:336:TRP:HB2	1:D:358:LEU:HD13	1.77	0.67
1:D:519:GLU:OE2	1:D:569:SER:OG	2.06	0.67
1:D:542:ALA:O	7:D:725:HOH:O	2.11	0.67
1:A:300:TYR:HA	7:A:741:HOH:O	1.93	0.67
1:A:340:ASN:HB2	1:A:352:PHE:CD2	2.30	0.67
1:A:423:CYS:HB3	1:A:542:ALA:HB3	1.75	0.67
2:C:68:LEU:HA	2:C:71:VAL:HG12	1.76	0.67
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.77	0.67
2:B:154:ASP:OD1	2:B:155:ILE:N	2.27	0.67
2:E:31:GLU:OE2	7:E:407:HOH:O	2.12	0.67
2:F:136:GLU:OE2	2:F:180:PRO:CD	2.43	0.67
2:C:22:ALA:HA	2:C:155:ILE:HD13	1.76	0.66
2:C:57:LEU:O	7:C:420:HOH:O	2.11	0.66
1:D:87:PRO:HD2	2:E:188:ARG:HB2	1.77	0.66
1:D:154:TYR:HD2	1:D:559:LEU:HD13	1.60	0.66
2:F:211:GLU:HG3	7:F:456:HOH:O	1.93	0.66
2:B:51:HIS:CD2	2:B:53:LYS:HE2	2.30	0.66
2:F:98:TRP:CD1	2:F:153:VAL:HG11	2.30	0.66
1:A:109:LYS:NZ	1:A:401:TYR:CZ	2.64	0.66
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:HIS:HA	1:A:510:ARG:HH12	1.59	0.66
2:C:187:LYS:HG2	1:D:451:ARG:HD3	1.76	0.66
2:F:114:TRP:CD1	2:F:167:TYR:HE1	2.13	0.66
2:F:165:GLN:HG2	2:F:206:VAL:HG21	1.77	0.66
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.30	0.66
1:A:92:HIS:CE1	2:B:185:TRP:HZ2	2.13	0.66
1:A:103:THR:HB	1:A:106:GLY:CA	2.24	0.66
1:A:329:ASP:OD1	1:A:330:TYR:N	2.28	0.66
2:C:23:LEU:HD22	2:C:28:VAL:HG11	1.78	0.66
1:A:128:ALA:HA	1:A:131:PHE:CE2	2.30	0.66
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.30	0.66
2:C:151:GLY:O	7:C:424:HOH:O	2.13	0.66
1:D:386:GLU:OE1	1:D:387:GLU:N	2.28	0.66
2:E:169:LYS:HZ2	2:E:206:VAL:HG21	1.60	0.66
2:F:7:LEU:HD21	2:F:23:LEU:HD12	1.78	0.66
2:F:24:ARG:HB3	2:F:194:SER:HA	1.78	0.66
2:F:163:TRP:HB3	2:F:167:TYR:CZ	2.31	0.66
1:A:324:PRO:O	7:A:741:HOH:O	2.12	0.66
1:A:424:ARG:HD2	1:A:425:ARG:NH1	2.11	0.66
2:C:187:LYS:HD3	1:D:492:ASP:HB3	1.78	0.66
1:D:105:GLN:HA	1:D:430:SER:HB3	1.76	0.66
1:D:147:PHE:CD2	1:D:529:ARG:NH1	2.63	0.65
1:D:205:HIS:O	7:D:727:HOH:O	2.12	0.65
2:E:57:LEU:HB3	2:E:73:TYR:OH	1.97	0.65
1:A:402:ARG:NH2	7:A:798:HOH:O	2.30	0.65
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.30	0.65
1:D:195:SER:OG	1:D:197:ASP:OD1	2.14	0.65
1:A:458:GLU:OE2	7:A:744:HOH:O	2.13	0.65
1:D:168:ASN:O	1:D:172:ASN:HB3	1.96	0.65
1:D:313:VAL:HG23	1:D:325:LEU:HD12	1.79	0.65
2:F:23:LEU:HD22	2:F:28:VAL:HG11	1.78	0.65
1:D:241:ILE:O	1:D:245:ILE:HG12	1.97	0.65
2:E:159:THR:HG22	2:E:199:LEU:HD11	1.78	0.65
5:F:301:GSH:N1	7:F:430:HOH:O	2.30	0.65
1:A:421:PHE:CD1	1:A:541:SER:HA	2.32	0.65
2:C:40:LYS:HB3	2:C:44:LEU:HD23	1.78	0.65
2:C:166:ALA:HB3	7:C:484:HOH:O	1.95	0.65
1:D:23:ASN:OD1	1:D:26:GLN:HB3	1.96	0.65
2:F:153:VAL:O	2:F:157:LEU:HD23	1.96	0.65
1:A:41:SER:HA	2:B:148:ASP:HA	1.78	0.65
1:A:94:VAL:HG21	1:A:112:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:VAL:O	2:B:136:GLU:HG2	1.97	0.65
1:D:314:PRO:HB3	1:D:317:ARG:HH12	1.61	0.65
2:F:122:GLU:HG3	7:F:470:HOH:O	1.96	0.65
1:A:432:ASN:O	7:A:746:HOH:O	2.14	0.65
1:A:455:GLU:OE1	7:A:739:HOH:O	2.12	0.65
1:D:77:ILE:HG13	1:D:110:PHE:HB3	1.77	0.65
1:D:533:GLU:O	7:D:731:HOH:O	2.14	0.65
2:E:4:LEU:HD13	2:E:31:GLU:HB2	1.79	0.65
1:A:286:ASN:HA	1:A:287:TRP:CE3	2.32	0.65
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.62	0.65
2:C:214:LYS:NZ	7:C:411:HOH:O	1.99	0.65
1:A:126:ARG:NH1	7:A:795:HOH:O	2.29	0.64
1:A:445:VAL:HG13	1:A:479:TRP:NE1	2.12	0.64
1:A:484:GLU:O	7:A:742:HOH:O	2.13	0.64
1:D:359:GLY:O	7:D:734:HOH:O	2.15	0.64
1:A:547:MET:O	7:A:743:HOH:O	2.13	0.64
1:D:152:LYS:HG2	1:D:565:ASN:H	1.61	0.64
1:D:312:TYR:N	7:D:773:HOH:O	2.27	0.64
2:E:8:LEU:HD21	7:E:403:HOH:O	1.97	0.64
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.32	0.64
1:D:480:GLU:OE2	1:D:526:GLY:N	2.30	0.64
2:B:96:ARG:NH1	2:C:73:TYR:HE1	1.91	0.64
2:E:107:THR:HA	2:E:110:GLN:HG2	1.78	0.64
1:A:169:VAL:O	1:A:175:PHE:HB2	1.97	0.64
1:A:290:LEU:HD12	1:A:293:ALA:HB3	1.78	0.64
2:C:183:ILE:HG12	1:D:492:ASP:CG	2.22	0.64
1:D:273:LEU:HA	1:D:276:THR:HG23	1.79	0.64
1:D:328:HIS:NE2	3:D:601:JAA:O03	2.29	0.64
1:D:382:VAL:O	7:D:736:HOH:O	2.15	0.64
2:F:132:VAL:HG22	2:F:179:SER:HB2	1.80	0.64
1:A:464:SER:OG	1:A:550:CYS:SG	2.32	0.64
1:D:151:SER:OG	1:D:565:ASN:ND2	2.29	0.64
1:D:367:SER:HB2	1:D:386:GLU:OE2	1.98	0.64
1:A:97:ILE:HB	1:A:162:VAL:HB	1.80	0.64
1:D:200:GLN:HA	1:D:203:TYR:CE2	2.33	0.64
1:D:463:SER:OG	7:D:726:HOH:O	2.12	0.64
1:D:477:ILE:HD12	1:D:497:LEU:HD13	1.79	0.64
1:D:98:SER:HB3	1:D:557:LYS:HE3	1.79	0.64
1:D:139:ASP:O	7:D:733:HOH:O	2.15	0.64
1:D:180:LYS:O	7:D:737:HOH:O	2.15	0.64
1:A:143:LYS:CD	1:A:212:PHE:HB2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.62	0.64
1:D:162:VAL:O	1:D:560:GLN:HB2	1.98	0.64
1:A:332:SER:HB2	1:A:538:LEU:HA	1.79	0.64
1:A:424:ARG:HD2	1:A:425:ARG:HH11	1.61	0.64
2:C:139:LEU:O	2:C:141:ASP:N	2.30	0.64
1:A:22:ARG:HG2	1:A:414:ASN:HB3	1.81	0.63
2:C:45:LEU:HD12	7:C:444:HOH:O	1.98	0.63
1:A:432:ASN:O	1:A:433:ILE:HG23	1.99	0.63
2:B:90:TYR:O	2:B:93:ALA:HB3	1.99	0.63
1:D:386:GLU:O	7:D:738:HOH:O	2.15	0.63
1:A:313:VAL:HG22	1:A:314:PRO:HD3	1.81	0.63
2:F:176:GLU:OE1	2:F:176:GLU:N	2.29	0.63
1:A:91:GLY:O	7:A:748:HOH:O	2.15	0.63
2:C:98:TRP:CZ2	2:C:157:LEU:HD22	2.34	0.63
1:D:270:ASN:HB3	1:D:273:LEU:HD11	1.79	0.63
1:D:288:TYR:HA	1:D:318:HIS:CD2	2.33	0.63
1:A:105:GLN:HB2	1:A:430:SER:HB2	1.81	0.63
1:A:217:GLN:O	1:A:299:LYS:N	2.29	0.63
1:A:361:PHE:CE1	1:A:392:ILE:HG22	2.34	0.62
1:A:532:GLN:HG3	1:A:547:MET:HE2	1.81	0.62
1:D:46:GLN:NE2	7:D:749:HOH:O	2.29	0.62
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.81	0.62
2:E:24:ARG:NE	7:E:419:HOH:O	2.30	0.62
2:E:121:GLN:NE2	2:E:170:PHE:O	2.32	0.62
2:F:10:TYR:HH	2:F:208:TYR:HH	1.47	0.62
1:A:92:HIS:NE2	2:B:136:GLU:O	2.31	0.62
2:E:90:TYR:O	2:E:94:GLN:HG2	1.99	0.62
2:F:33:ARG:NH1	2:F:41:SER:OG	2.31	0.62
1:A:113:PHE:HD1	1:A:117:LEU:HD13	1.64	0.62
1:D:132:ARG:HA	1:D:343:PRO:HG3	1.82	0.62
1:A:236:GLN:NE2	7:A:797:HOH:O	2.29	0.62
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.34	0.62
1:A:240:GLU:HB3	7:A:757:HOH:O	1.98	0.62
2:C:102:VAL:HG23	7:C:406:HOH:O	2.00	0.62
2:E:23:LEU:HD22	2:E:28:VAL:HB	1.81	0.62
1:A:76:TYR:O	1:A:88:ILE:HD12	1.99	0.62
1:A:79:ARG:NH1	2:B:188:ARG:HH22	1.98	0.62
2:B:110:GLN:HB2	2:B:167:TYR:CE2	2.34	0.62
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.18	0.62
2:E:48:ASN:ND2	7:E:409:HOH:O	2.32	0.62
2:F:19:ALA:N	7:F:429:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:SER:HA	1:D:211:LEU:HG	1.82	0.62
1:D:305:MET:HE3	1:D:325:LEU:HB3	1.82	0.62
2:B:195:VAL:HG13	2:B:199:LEU:HD13	1.82	0.62
1:A:93:PRO:HG2	2:B:181:LYS:HA	1.81	0.61
2:B:114:TRP:O	7:B:412:HOH:O	2.16	0.61
2:B:121:GLN:NE2	2:B:170:PHE:O	2.34	0.61
1:D:166:THR:OG1	1:D:561:ILE:HD11	2.00	0.61
2:B:125:LYS:NZ	7:B:403:HOH:O	2.05	0.61
1:D:126:ARG:HD3	1:D:182:ILE:HD13	1.81	0.61
1:D:475:TYR:CZ	1:D:506:TYR:HE1	2.18	0.61
2:E:93:ALA:CB	2:F:73:TYR:HE1	2.12	0.61
2:C:53:LYS:HG2	5:C:301:GSH:HA31	1.81	0.61
2:C:64:VAL:N	7:C:420:HOH:O	2.11	0.61
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.33	0.61
1:D:25:HIS:O	1:D:29:LYS:HG2	2.00	0.61
1:D:507:VAL:HG12	1:D:510:ARG:NH2	2.16	0.61
2:E:8:LEU:HD13	2:E:44:LEU:HB2	1.81	0.61
1:A:461:ASP:HB3	1:A:528:PHE:CD2	2.34	0.61
2:B:9:ASP:OD1	2:B:10:TYR:N	2.29	0.61
2:E:53:LYS:O	7:E:409:HOH:O	2.16	0.61
2:F:111:PHE:O	7:F:419:HOH:O	2.16	0.61
1:A:244:ASP:HB2	1:A:250:LEU:HA	1.83	0.61
2:B:24:ARG:HH22	2:B:197:LYS:HB2	1.64	0.61
2:B:139:LEU:CD2	2:B:142:LYS:H	2.14	0.61
1:D:364:LEU:HD12	1:D:402:ARG:HH22	1.66	0.61
1:D:451:ARG:NH1	1:D:454:GLU:CD	2.59	0.61
2:C:114:TRP:HA	2:C:170:PHE:HD2	1.66	0.61
2:E:51:HIS:HB3	2:E:53:LYS:HG3	1.82	0.61
1:A:149:PHE:CB	1:A:530:LYS:HZ3	2.14	0.61
1:A:224:ALA:HB3	1:A:312:TYR:CE1	2.36	0.61
1:A:286:ASN:HA	1:A:287:TRP:HE3	1.64	0.61
1:D:94:VAL:HG11	1:D:112:PRO:HB3	1.83	0.61
1:D:150:SER:HB3	1:D:170:TYR:CD2	2.35	0.61
2:C:32:TYR:H	2:C:32:TYR:HD2	1.49	0.61
1:D:337:ILE:HD13	1:D:539:GLY:CA	2.30	0.61
1:D:420:LYS:NZ	7:D:774:HOH:O	2.27	0.61
1:A:109:LYS:NZ	1:A:401:TYR:OH	2.28	0.60
1:A:242:VAL:HG21	1:A:278:ARG:HD3	1.82	0.60
1:A:309:MET:HB3	1:A:312:TYR:CE2	2.36	0.60
1:A:547:MET:SD	1:A:549:ARG:NH2	2.71	0.60
2:B:139:LEU:HD21	2:B:142:LYS:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:THR:HA	1:D:236:GLN:HE21	1.66	0.60
1:D:360:TYR:C	1:D:361:PHE:HD1	2.10	0.60
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.35	0.60
2:B:73:TYR:OH	7:B:411:HOH:O	2.16	0.60
1:D:76:TYR:O	1:D:79:ARG:HB2	2.01	0.60
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.36	0.60
1:D:122:LEU:HD23	7:D:828:HOH:O	2.01	0.60
1:D:362:GLU:HG3	1:D:400:ARG:NH2	2.15	0.60
1:A:232:ARG:O	1:A:235:GLU:HG2	2.01	0.60
1:A:295:PHE:HD1	1:A:298:ALA:HB2	1.65	0.60
2:B:59:HIS:CE1	2:B:60:ASN:HD22	2.19	0.60
2:C:122:GLU:HA	2:C:125:LYS:HE2	1.83	0.60
1:D:150:SER:CB	1:D:167:THR:HA	2.32	0.60
1:D:153:GLN:HA	1:D:560:GLN:HG2	1.83	0.60
1:D:462:PHE:O	1:D:549:ARG:NH1	2.35	0.60
2:F:17:MET:HE2	2:F:200:PRO:HD2	1.83	0.60
2:F:183:ILE:HD12	2:F:186:ALA:HB3	1.83	0.60
1:A:92:HIS:ND1	2:B:181:LYS:HB3	2.16	0.60
1:A:246:LYS:HZ3	1:A:278:ARG:HH22	1.49	0.60
2:C:201:ASP:HB2	2:C:204:LYS:HG3	1.84	0.60
1:D:339:ALA:O	7:D:740:HOH:O	2.16	0.60
1:D:559:LEU:HA	1:D:562:LEU:HB2	1.83	0.60
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.37	0.60
2:B:139:LEU:HG	2:B:142:LYS:HB2	1.84	0.60
2:C:202:SER:OG	1:D:454:GLU:OE2	2.17	0.60
1:A:465:TYR:HB3	1:A:476:ALA:HB3	1.83	0.60
1:D:535:PHE:HB3	1:D:544:GLN:O	2.02	0.60
2:F:176:GLU:O	2:F:177:SER:HB2	2.00	0.60
2:B:150:PHE:HB2	2:B:192:LYS:HZ2	1.66	0.60
2:C:73:TYR:HA	2:C:76:GLU:OE2	2.02	0.60
2:F:8:LEU:HB2	2:F:56:VAL:HB	1.84	0.60
2:F:64:VAL:HB	2:F:73:TYR:CD2	2.37	0.60
2:F:144:TYR:HB3	2:F:154:ASP:OD2	2.01	0.60
1:A:363:PHE:O	7:A:750:HOH:O	2.17	0.60
1:D:467:ASP:OD1	1:D:474:HIS:N	2.32	0.60
2:E:41:SER:OG	7:E:403:HOH:O	2.06	0.60
1:A:524:ALA:O	7:A:749:HOH:O	2.17	0.60
2:B:120:GLU:O	7:B:414:HOH:O	2.17	0.60
1:D:425:ARG:NH2	7:D:791:HOH:O	2.33	0.60
1:A:41:SER:H	2:B:142:LYS:HG2	1.65	0.60
1:A:223:PHE:HD2	1:A:225:HIS:CD2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:LEU:O	1:D:126:ARG:HG2	2.02	0.60
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.84	0.60
1:D:454:GLU:HG2	7:D:798:HOH:O	2.01	0.60
2:E:92:ARG:CZ	2:E:96:ARG:HH12	2.13	0.60
1:A:28:GLN:OE1	1:A:379:LEU:HD22	2.02	0.59
1:A:437:THR:O	1:A:440:ASP:N	2.35	0.59
2:C:64:VAL:HB	2:C:73:TYR:CE2	2.37	0.59
1:D:148:ILE:O	1:D:205:HIS:HE1	1.84	0.59
1:D:506:TYR:HB3	1:D:510:ARG:HH21	1.67	0.59
1:D:513:LYS:NZ	1:D:575:PHE:HB3	2.16	0.59
2:E:58:VAL:HG22	2:E:63:PRO:HB3	1.82	0.59
2:F:67:SER:OG	5:F:301:GSH:O12	2.13	0.59
2:F:70:VAL:O	2:F:73:TYR:HB2	2.02	0.59
2:F:170:PHE:C	2:F:172:ASN:H	2.08	0.59
1:A:42:ALA:HB1	1:A:44:TYR:CE1	2.38	0.59
1:A:149:PHE:HB2	1:A:530:LYS:HZ3	1.66	0.59
2:B:66:GLU:N	7:B:420:HOH:O	2.21	0.59
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.36	0.59
1:A:113:PHE:CD1	1:A:117:LEU:HD13	2.37	0.59
1:A:143:LYS:HZ2	1:A:187:CYS:CB	2.15	0.59
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.36	0.59
2:E:92:ARG:NH1	2:E:96:ARG:HH12	1.99	0.59
2:F:82:ASN:O	7:F:420:HOH:O	2.17	0.59
2:F:195:VAL:HG23	2:F:199:LEU:HD13	1.84	0.59
1:A:260:ARG:NE	7:A:796:HOH:O	2.29	0.59
1:A:287:TRP:CD1	1:A:290:LEU:HD13	2.37	0.59
1:D:473:GLY:O	1:D:516:GLY:N	2.32	0.59
2:E:50:ILE:HD12	2:F:101:PHE:CZ	2.37	0.59
2:F:114:TRP:HA	2:F:170:PHE:HD2	1.66	0.59
1:A:93:PRO:HG3	2:B:184:ALA:CB	2.27	0.59
1:A:154:TYR:OH	1:A:156:SER:OG	2.19	0.59
1:A:248:GLY:HA2	1:A:267:LEU:HD22	1.83	0.59
2:B:96:ARG:NH1	2:C:73:TYR:CD1	2.69	0.59
1:D:61:PHE:O	1:D:65:VAL:HG12	2.02	0.59
1:A:407:VAL:HG11	1:A:419:LEU:HD13	1.84	0.59
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.37	0.59
2:E:8:LEU:O	2:E:55:PRO:HA	2.02	0.59
1:A:473:GLY:O	1:A:516:GLY:N	2.34	0.59
2:C:180:PRO:HG2	1:D:574:ALA:HA	1.85	0.59
2:B:107:THR:HA	2:B:110:GLN:HG2	1.85	0.59
1:A:84:ASP:C	1:A:86:SER:H	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:VAL:N	7:D:738:HOH:O	2.31	0.59
2:E:136:GLU:OE2	2:E:181:LYS:HD3	2.02	0.59
1:A:24:ALA:O	7:A:752:HOH:O	2.17	0.59
1:A:184:SER:HB2	1:A:217:GLN:HE21	1.68	0.59
1:D:495:ASN:O	1:D:499:ARG:NH1	2.35	0.59
1:A:40:GLN:HG2	2:B:142:LYS:HD2	1.85	0.58
1:A:79:ARG:NH2	2:B:188:ARG:NH1	2.51	0.58
1:A:314:PRO:HB3	1:A:317:ARG:HH12	1.66	0.58
1:A:424:ARG:C	1:A:543:GLY:HA2	2.27	0.58
1:D:73:LEU:HD22	1:D:89:LEU:HD13	1.84	0.58
1:D:209:GLY:N	7:D:727:HOH:O	2.36	0.58
2:F:164:PHE:CD2	2:F:183:ILE:HD13	2.34	0.58
2:C:26:LYS:HG2	2:C:81:LYS:HZ3	1.68	0.58
2:C:26:LYS:HE2	2:C:75:ASP:HA	1.85	0.58
1:D:22:ARG:NH1	1:D:414:ASN:CG	2.62	0.58
1:A:99:LEU:HB2	1:A:557:LYS:H	1.68	0.58
1:A:291:ILE:HB	1:A:320:ALA:HA	1.84	0.58
1:A:401:TYR:CE2	1:A:403:LEU:HD13	2.37	0.58
1:A:434:ASP:OD2	7:A:751:HOH:O	2.17	0.58
2:B:165:GLN:HB3	7:B:486:HOH:O	2.02	0.58
2:E:62:LYS:HD3	2:F:90:TYR:CD2	2.39	0.58
2:F:165:GLN:OE1	2:F:202:SER:HB2	2.02	0.58
1:A:48:CYS:HB3	1:A:65:VAL:HG22	1.85	0.58
1:D:521:ARG:NH2	1:D:563:CYS:SG	2.77	0.58
2:F:188:ARG:HD2	2:F:191:GLU:OE2	2.03	0.58
1:D:417:PRO:O	7:D:742:HOH:O	2.17	0.58
2:E:116:LYS:O	7:E:410:HOH:O	2.17	0.58
2:F:142:LYS:HB3	7:F:424:HOH:O	2.03	0.58
1:A:90:THR:HG23	1:A:397:GLY:CA	2.33	0.58
1:A:107:ARG:HH21	1:A:433:ILE:HG12	1.68	0.58
1:A:424:ARG:HG3	1:A:425:ARG:H	1.68	0.58
2:B:152:TYR:O	2:B:155:ILE:HG13	2.04	0.58
2:C:98:TRP:CZ2	2:C:135:LEU:HD21	2.38	0.58
1:D:62:LYS:HE2	1:D:376:PRO:HG2	1.85	0.58
1:D:80:MET:SD	1:D:87:PRO:HA	2.44	0.58
2:F:9:ASP:HB3	7:F:482:HOH:O	2.04	0.58
2:F:33:ARG:HH12	2:F:41:SER:CB	2.16	0.58
1:A:48:CYS:SG	1:A:65:VAL:HG13	2.44	0.58
1:A:79:ARG:HH22	2:B:188:ARG:HH12	1.51	0.58
1:A:152:LYS:CG	1:A:561:ILE:HA	2.33	0.58
1:D:88:ILE:HD12	1:D:89:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:GLN:H	1:D:564:GLU:HB2	1.68	0.58
1:D:480:GLU:OE2	1:D:527:THR:N	2.36	0.58
2:E:66:GLU:CD	2:F:97:PHE:HD1	2.11	0.58
1:A:36:LEU:HD22	1:A:61:PHE:HZ	1.68	0.58
1:A:149:PHE:HB2	1:A:530:LYS:NZ	2.19	0.58
2:E:8:LEU:HD12	2:E:56:VAL:HB	1.85	0.58
1:D:143:LYS:N	7:D:765:HOH:O	2.29	0.58
1:D:231:PHE:HB3	1:D:290:LEU:HD13	1.85	0.58
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.38	0.58
2:B:125:LYS:HB3	2:B:173:PHE:HE2	1.68	0.57
2:C:51:HIS:ND1	7:C:423:HOH:O	2.33	0.57
1:D:38:LYS:O	2:E:142:LYS:HG3	2.02	0.57
1:A:445:VAL:HG22	7:A:762:HOH:O	2.04	0.57
1:A:450:LYS:HA	1:A:453:SER:HB3	1.86	0.57
2:B:125:LYS:O	2:B:129:ILE:HG12	2.04	0.57
1:D:44:TYR:CB	1:D:89:LEU:HG	2.34	0.57
1:D:363:PHE:HB3	1:D:388:TYR:HB3	1.85	0.57
2:F:135:LEU:HD13	2:F:182:LEU:HD11	1.86	0.57
1:A:274:ALA:HB1	1:A:278:ARG:CZ	2.34	0.57
1:A:287:TRP:HD1	1:A:290:LEU:HD13	1.68	0.57
1:D:11:ASN:O	1:D:14:ILE:HG13	2.04	0.57
1:D:99:LEU:HD12	1:D:100:SER:N	2.19	0.57
1:D:107:ARG:HH22	1:D:552:LYS:HB3	1.69	0.57
1:D:407:VAL:HG22	1:D:541:SER:HB2	1.85	0.57
2:E:195:VAL:HG13	2:E:199:LEU:HD13	1.85	0.57
2:F:98:TRP:CZ2	2:F:157:LEU:HD22	2.39	0.57
1:A:23:ASN:OD1	1:A:26:GLN:HG2	2.04	0.57
1:A:348:GLU:OE1	7:A:753:HOH:O	2.18	0.57
1:D:394:ASN:OD1	1:D:398:LEU:HD11	2.04	0.57
1:A:559:LEU:O	1:A:562:LEU:HG	2.04	0.57
1:D:77:ILE:HG12	1:D:110:PHE:C	2.29	0.57
1:D:330:TYR:OH	1:D:541:SER:N	2.36	0.57
1:D:528:PHE:HA	1:D:531:ILE:HG12	1.87	0.57
1:A:32:LEU:HB2	1:A:360:TYR:CD1	2.39	0.57
1:D:154:TYR:HB3	1:D:560:GLN:HA	1.86	0.57
1:D:342:THR:OG1	1:D:413:TYR:OH	2.12	0.57
1:D:377:VAL:O	7:D:745:HOH:O	2.18	0.57
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.39	0.57
1:A:122:LEU:HD21	1:A:178:GLY:HA3	1.86	0.57
1:A:338:ALA:HA	1:A:354:VAL:HA	1.85	0.57
1:A:441:LEU:HG	1:A:462:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:VAL:O	2:C:73:TYR:HB2	2.04	0.57
1:D:168:ASN:ND2	7:D:732:HOH:O	2.15	0.57
1:D:207:LEU:O	1:D:210:ILE:HG22	2.05	0.57
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.87	0.57
2:C:184:ALA:HB1	1:D:499:ARG:NE	2.19	0.57
1:D:108:PRO:HB2	1:D:554:SER:OG	2.05	0.57
1:D:389:GLU:OE1	7:D:744:HOH:O	2.17	0.57
1:A:26:GLN:HA	1:A:29:LYS:HG2	1.86	0.57
1:A:32:LEU:HD21	1:A:61:PHE:HD2	1.70	0.57
1:A:237:VAL:HG11	7:A:1029:HOH:O	2.05	0.57
2:C:17:MET:SD	2:C:199:LEU:HG	2.44	0.57
1:D:8:PHE:CD1	1:D:182:ILE:HG22	2.39	0.57
1:D:382:VAL:HG13	1:D:388:TYR:CE2	2.40	0.57
2:E:113:VAL:O	7:E:410:HOH:O	2.17	0.57
2:B:14:MET:HE1	2:B:110:GLN:HE22	1.70	0.57
1:A:231:PHE:HA	1:A:234:PHE:HB3	1.86	0.56
2:B:152:TYR:OH	7:B:413:HOH:O	2.16	0.56
2:B:162:SER:HB3	2:B:199:LEU:HD23	1.86	0.56
1:D:284:LEU:HD13	1:D:287:TRP:H	1.69	0.56
1:A:37:LEU:HD11	2:B:90:TYR:HE2	1.69	0.56
1:D:405:ASP:OD1	1:D:405:ASP:N	2.36	0.56
2:F:98:TRP:CZ2	2:F:135:LEU:HD21	2.40	0.56
1:A:132:ARG:O	1:A:136:PHE:N	2.38	0.56
1:A:206:LEU:HD12	1:A:207:LEU:N	2.20	0.56
2:C:123:ALA:HB2	7:C:476:HOH:O	2.05	0.56
1:D:196:PRO:HA	1:D:565:ASN:OD1	2.06	0.56
2:F:29:GLU:N	7:F:433:HOH:O	2.38	0.56
1:A:207:LEU:HD13	1:A:245:ILE:HD11	1.87	0.56
1:A:506:TYR:HA	1:A:509:SER:HB2	1.87	0.56
1:D:451:ARG:NH1	1:D:454:GLU:OE1	2.38	0.56
2:F:68:LEU:HA	2:F:71:VAL:HG12	1.88	0.56
1:A:174:ASN:ND2	7:A:818:HOH:O	2.39	0.56
2:B:150:PHE:HB2	2:B:192:LYS:NZ	2.20	0.56
1:D:99:LEU:HD22	1:D:555:ASN:HB3	1.88	0.56
2:E:85:PHE:CE1	2:E:152:TYR:HB2	2.40	0.56
1:A:233:THR:O	1:A:236:GLN:N	2.39	0.56
1:D:330:TYR:HE1	1:D:536:LEU:O	1.89	0.56
1:A:120:ASN:O	1:A:124:LEU:HG	2.06	0.56
1:A:228:VAL:O	1:A:232:ARG:N	2.38	0.56
2:C:10:TYR:HH	2:C:208:TYR:HH	1.53	0.56
1:D:221:ALA:HB3	1:D:227:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:SER:HB3	1:A:535:PHE:CD2	2.41	0.56
1:A:165:ALA:HB3	4:A:602:VAL:HA	1.87	0.56
1:A:523:VAL:HG22	1:A:524:ALA:H	1.71	0.56
1:D:242:VAL:O	1:D:246:LYS:HB2	2.05	0.56
1:D:566:VAL:HG23	1:D:568:SER:C	2.31	0.56
2:E:144:TYR:HB3	2:E:154:ASP:OD2	2.06	0.56
2:F:183:ILE:O	2:F:186:ALA:N	2.37	0.56
1:A:86:SER:HB2	2:B:188:ARG:NE	2.21	0.56
1:D:110:PHE:CD2	1:D:554:SER:HA	2.41	0.56
1:D:146:GLN:NE2	7:D:760:HOH:O	2.22	0.56
1:D:166:THR:HG22	4:D:602:VAL:HB	1.87	0.56
1:D:233:THR:O	1:D:237:VAL:HG22	2.06	0.56
2:E:50:ILE:HG13	2:E:51:HIS:N	2.18	0.56
1:A:171:ARG:HB2	7:A:709:HOH:O	2.05	0.56
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.87	0.56
2:B:37:PHE:CE1	5:B:301:GSH:HA32	2.41	0.56
1:A:523:VAL:HG11	1:A:527:THR:HG21	1.88	0.55
1:D:96:ALA:HA	1:D:161:PRO:O	2.05	0.55
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.70	0.55
2:F:64:VAL:HG23	2:F:70:VAL:HG22	1.88	0.55
2:F:185:TRP:NE1	2:F:189:CYS:SG	2.79	0.55
1:A:503:ASP:CG	1:A:505:GLY:H	2.13	0.55
1:D:47:ASN:OD1	7:D:749:HOH:O	2.18	0.55
1:D:113:PHE:CD1	1:D:117:LEU:HD12	2.40	0.55
1:D:169:VAL:HG23	7:D:770:HOH:O	2.06	0.55
1:D:188:SER:OG	1:D:205:HIS:CD2	2.59	0.55
1:D:434:ASP:HB2	1:D:550:CYS:HB3	1.88	0.55
1:D:495:ASN:CB	1:D:499:ARG:NH1	2.68	0.55
2:F:17:MET:SD	2:F:199:LEU:HG	2.46	0.55
1:A:38:LYS:HZ2	1:A:395:TYR:HE1	1.52	0.55
1:A:79:ARG:HH12	2:B:188:ARG:HH12	1.53	0.55
1:A:92:HIS:CE1	2:B:139:LEU:HD22	2.42	0.55
1:A:97:ILE:HD13	1:A:112:PRO:HA	1.87	0.55
1:A:493:CYS:HB3	7:A:940:HOH:O	2.06	0.55
2:C:135:LEU:HD13	2:C:182:LEU:HD11	1.87	0.55
1:D:101:SER:HB3	1:D:535:PHE:CD2	2.41	0.55
1:D:110:PHE:O	7:D:746:HOH:O	2.18	0.55
1:D:332:SER:HB2	1:D:538:LEU:HA	1.88	0.55
1:D:541:SER:O	1:D:543:GLY:N	2.39	0.55
2:E:173:PHE:HE1	2:E:175:ILE:HG13	1.72	0.55
2:E:193:GLU:OE1	2:E:196:SER:OG	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LYS:NZ	1:A:208:SER:O	2.39	0.55
1:A:152:LYS:HZ1	1:A:530:LYS:HZ3	1.39	0.55
1:D:80:MET:HE3	1:D:94:VAL:HG22	1.87	0.55
1:D:149:PHE:HB2	1:D:530:LYS:HE2	1.89	0.55
1:D:223:PHE:HD2	1:D:225:HIS:CE1	2.25	0.55
2:E:20:ARG:HB3	2:E:24:ARG:HH12	1.69	0.55
2:F:123:ALA:HB2	7:F:411:HOH:O	2.05	0.55
1:A:150:SER:OG	1:A:150:SER:O	2.22	0.55
1:A:437:THR:OG1	1:A:440:ASP:HB2	2.07	0.55
2:C:185:TRP:NE1	2:C:189:CYS:SG	2.80	0.55
1:D:39:ASN:ND2	1:D:399:TYR:OH	2.39	0.55
1:D:68:VAL:HG12	1:D:72:GLU:HB2	1.88	0.55
1:D:328:HIS:CG	1:D:329:ASP:N	2.74	0.55
1:A:121:THR:HG22	1:A:336:TRP:CZ2	2.41	0.55
2:C:54:ILE:HB	2:C:55:PRO:HA	1.88	0.55
1:D:164:THR:HA	1:D:557:LYS:HG3	1.87	0.55
1:D:228:VAL:HG13	1:D:319:TYR:HE2	1.72	0.55
1:D:551:VAL:HB	1:D:555:ASN:HB2	1.87	0.55
2:F:73:TYR:HA	2:F:76:GLU:OE2	2.07	0.55
1:A:238:TRP:CA	1:A:241:ILE:HB	2.36	0.55
1:A:340:ASN:ND2	1:A:343:PRO:HA	2.20	0.55
2:C:165:GLN:HA	2:C:168:GLU:OE1	2.07	0.55
1:D:150:SER:O	1:D:150:SER:OG	2.20	0.55
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.41	0.55
2:E:141:ASP:OD2	2:E:181:LYS:NZ	2.36	0.55
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.42	0.55
1:A:28:GLN:HG3	1:A:356:PRO:O	2.07	0.55
1:A:169:VAL:HG13	1:A:170:TYR:CD1	2.42	0.55
1:A:503:ASP:OD2	1:A:505:GLY:N	2.38	0.55
2:B:139:LEU:O	2:B:141:ASP:N	2.40	0.55
2:C:96:ARG:N	7:C:440:HOH:O	2.40	0.55
1:D:75:PRO:O	1:D:79:ARG:HG3	2.07	0.55
1:D:437:THR:O	1:D:440:ASP:N	2.40	0.55
1:D:495:ASN:O	1:D:498:ASP:HB2	2.06	0.55
1:D:524:ALA:HB2	1:D:567:VAL:CG1	2.36	0.55
2:E:93:ALA:CB	2:F:73:TYR:CE1	2.90	0.55
2:F:200:PRO:HG3	7:F:494:HOH:O	2.06	0.55
2:C:87:SER:HB3	7:C:502:HOH:O	2.06	0.55
1:D:43:ILE:O	1:D:46:GLN:HG2	2.07	0.55
1:A:201:ALA:O	1:A:205:HIS:N	2.40	0.55
1:A:228:VAL:O	1:A:232:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:GLU:OE2	2:C:92:ARG:NH2	2.40	0.55
2:E:205:ILE:HG12	7:E:404:HOH:O	2.06	0.55
1:A:78:LYS:NZ	7:A:720:HOH:O	2.06	0.54
1:A:315:LYS:O	1:A:318:HIS:HB3	2.07	0.54
2:B:93:ALA:HB1	2:C:73:TYR:CZ	2.43	0.54
1:D:467:ASP:CG	1:D:474:HIS:H	2.15	0.54
2:E:201:ASP:OD2	2:E:204:LYS:HE3	2.07	0.54
1:A:15:ASP:OD1	1:A:16:GLU:N	2.40	0.54
1:A:80:MET:HE1	1:A:94:VAL:HG22	1.89	0.54
1:A:92:HIS:HD2	2:B:140:GLY:O	1.89	0.54
1:A:151:SER:HB2	1:A:194:PHE:HA	1.88	0.54
1:A:212:PHE:HB3	1:A:215:GLN:NE2	2.23	0.54
2:C:8:LEU:HD22	2:C:33:ARG:NH2	2.22	0.54
2:C:209:ALA:HB2	7:C:434:HOH:O	2.06	0.54
1:D:107:ARG:CZ	1:D:433:ILE:HG13	2.38	0.54
1:D:363:PHE:HE1	1:D:390:VAL:HG23	1.71	0.54
2:E:70:VAL:HA	2:E:73:TYR:HE2	1.71	0.54
2:F:86:PRO:HD3	2:F:146:GLY:O	2.08	0.54
1:A:77:ILE:CG2	1:A:110:PHE:HB3	2.37	0.54
1:A:314:PRO:HA	1:A:317:ARG:NH1	2.22	0.54
2:C:44:LEU:HB3	7:C:415:HOH:O	2.07	0.54
2:C:102:VAL:O	2:C:107:THR:HG23	2.07	0.54
2:C:168:GLU:OE2	1:D:488:ASP:OD2	2.26	0.54
1:D:337:ILE:CD1	1:D:361:PHE:HE2	2.20	0.54
1:D:202:LEU:HD23	1:D:525:LYS:HD2	1.89	0.54
2:F:121:GLN:O	2:F:125:LYS:HG3	2.08	0.54
1:A:104:SER:C	1:A:106:GLY:N	2.65	0.54
1:A:340:ASN:HB2	1:A:352:PHE:CE2	2.42	0.54
2:C:50:ILE:HD12	7:C:489:HOH:O	2.07	0.54
2:C:164:PHE:O	2:C:168:GLU:HG3	2.08	0.54
1:A:118:MET:O	1:A:121:THR:OG1	2.24	0.54
2:B:124:GLY:HA2	2:B:127:GLU:CD	2.33	0.54
1:D:42:ALA:HB3	1:D:45:LEU:HD13	1.89	0.54
1:D:425:ARG:NH1	1:D:546:LYS:HE3	2.23	0.54
1:A:92:HIS:CE1	2:B:185:TRP:CZ2	2.96	0.54
1:A:193:ILE:HA	1:A:205:HIS:CE1	2.43	0.54
1:A:32:LEU:HD22	1:A:360:TYR:CE2	2.43	0.54
1:A:334:GLU:OE1	1:A:403:LEU:HD21	2.07	0.54
1:A:369:THR:OG1	1:A:370:GLY:N	2.40	0.54
1:D:10:MET:HA	7:D:710:HOH:O	2.08	0.54
1:D:99:LEU:H	1:D:557:LYS:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ALA:HB2	1:D:413:TYR:HD2	1.72	0.54
1:D:382:VAL:HG13	1:D:388:TYR:CD2	2.43	0.54
2:E:92:ARG:NH2	7:E:424:HOH:O	2.40	0.54
2:E:107:THR:HG22	2:E:160:PHE:CZ	2.43	0.54
1:A:203:TYR:HD2	1:A:254:ILE:HD11	1.73	0.54
2:B:108:ASP:O	2:B:112:LYS:HG2	2.08	0.54
2:C:24:ARG:HB3	2:C:194:SER:HA	1.90	0.54
2:C:187:LYS:HZ3	1:D:496:CYS:HB2	1.73	0.54
1:D:452:LEU:HD23	1:D:481:ILE:HG21	1.89	0.54
1:D:551:VAL:HG21	1:D:559:LEU:HD23	1.90	0.54
2:E:17:MET:SD	2:E:200:PRO:HD2	2.48	0.54
1:A:83:GLY:H	1:A:158:GLY:HA3	1.72	0.53
1:A:128:ALA:HA	1:A:131:PHE:CD2	2.43	0.53
1:A:152:LYS:CE	1:A:530:LYS:NZ	2.65	0.53
1:A:339:ALA:N	1:A:353:ALA:O	2.29	0.53
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.88	0.53
1:A:562:LEU:HB3	7:A:713:HOH:O	2.08	0.53
1:D:76:TYR:HB3	1:D:88:ILE:HD13	1.90	0.53
1:D:195:SER:HB3	1:D:201:ALA:HB2	1.90	0.53
1:D:246:LYS:CE	1:D:271:PRO:HA	2.37	0.53
2:E:193:GLU:HA	2:E:196:SER:OG	2.09	0.53
1:A:94:VAL:HB	1:A:113:PHE:O	2.07	0.53
1:A:154:TYR:CE2	1:A:559:LEU:HB3	2.42	0.53
1:A:216:VAL:HG21	7:A:778:HOH:O	2.07	0.53
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.44	0.53
2:C:98:TRP:CD1	2:C:153:VAL:HG11	2.44	0.53
1:A:233:THR:HG23	1:A:525:LYS:NZ	2.22	0.53
1:A:310:GLU:HG3	1:A:311:PRO:HD3	1.90	0.53
1:A:435:LYS:HE3	1:A:438:GLU:CB	2.38	0.53
2:C:40:LYS:HD2	2:C:52:LYS:HB3	1.91	0.53
1:D:79:ARG:NH1	7:D:800:HOH:O	2.40	0.53
1:D:445:VAL:HG21	1:D:462:PHE:CD1	2.43	0.53
2:F:57:LEU:O	2:F:64:VAL:HG22	2.08	0.53
1:A:36:LEU:HD22	1:A:61:PHE:CZ	2.44	0.53
1:A:144:ALA:HA	7:A:745:HOH:O	2.08	0.53
1:A:287:TRP:HB3	7:A:1021:HOH:O	2.08	0.53
1:A:291:ILE:HG21	1:A:301:VAL:HG22	1.91	0.53
1:D:85:THR:HB	2:E:184:ALA:HB1	1.90	0.53
1:D:302:TYR:HD1	1:D:326:VAL:HG13	1.72	0.53
1:D:475:TYR:HB2	1:D:518:LEU:HG	1.90	0.53
2:F:51:HIS:O	7:F:421:HOH:O	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASN:O	1:A:14:ILE:HG13	2.08	0.53
1:A:311:PRO:C	1:A:314:PRO:HD2	2.34	0.53
1:A:334:GLU:O	1:A:394:ASN:ND2	2.40	0.53
2:B:134:ILE:HG22	2:B:138:GLU:OE2	2.08	0.53
2:C:108:ASP:O	2:C:112:LYS:HG2	2.08	0.53
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.44	0.53
1:D:126:ARG:HD2	1:D:182:ILE:HG21	1.91	0.53
1:D:199:HIS:HA	1:D:525:LYS:HB2	1.91	0.53
2:B:151:GLY:H	2:B:154:ASP:CG	2.17	0.53
2:C:102:VAL:HG21	2:C:157:LEU:HB3	1.91	0.53
1:D:295:PHE:HD1	1:D:298:ALA:HB2	1.74	0.53
2:F:108:ASP:O	2:F:112:LYS:HG2	2.07	0.53
1:A:164:THR:OG1	1:A:166:THR:OG1	2.16	0.53
1:A:510:ARG:CZ	1:A:515:ILE:HD12	2.38	0.53
2:B:24:ARG:HG3	2:B:30:PHE:HE1	1.74	0.53
2:C:187:LYS:NZ	2:C:187:LYS:HB2	2.23	0.53
1:D:244:ASP:OD1	1:D:251:SER:HB2	2.09	0.53
1:D:381:GLN:O	7:D:750:HOH:O	2.19	0.53
1:D:495:ASN:CB	1:D:499:ARG:HH12	2.20	0.53
1:D:559:LEU:O	1:D:562:LEU:HB3	2.09	0.53
2:E:53:LYS:HG2	5:E:301:GSH:HA31	1.90	0.53
1:A:218:TYR:HA	1:A:298:ALA:HB1	1.91	0.53
2:B:168:GLU:OE1	7:B:415:HOH:O	2.18	0.53
2:C:188:ARG:HH12	1:D:500:ALA:CA	2.02	0.53
1:D:139:ASP:OD2	1:D:142:GLY:N	2.42	0.53
1:D:400:ARG:HB2	7:D:728:HOH:O	2.09	0.53
1:D:522:VAL:O	1:D:567:VAL:HG22	2.09	0.53
2:E:26:LYS:HG3	2:E:82:ASN:HD21	1.72	0.53
1:A:295:PHE:C	1:A:297:ASN:H	2.17	0.53
2:B:201:ASP:HB2	2:B:204:LYS:HG3	1.91	0.53
1:D:534:HIS:CD2	1:D:557:LYS:HD3	2.44	0.53
1:A:538:LEU:HD22	1:A:544:GLN:HE21	1.74	0.53
1:D:206:LEU:O	1:D:210:ILE:HB	2.09	0.53
1:D:251:SER:O	1:D:254:ILE:HG12	2.07	0.53
1:D:465:TYR:HB3	1:D:476:ALA:HB3	1.89	0.53
1:D:507:VAL:O	1:D:511:LYS:HB2	2.09	0.53
2:B:165:GLN:O	2:B:168:GLU:HG2	2.09	0.52
2:C:158:ILE:HG12	7:C:432:HOH:O	2.08	0.52
1:D:10:MET:HB2	7:D:881:HOH:O	2.08	0.52
1:D:112:PRO:HD2	1:D:397:GLY:HA3	1.90	0.52
1:D:152:LYS:CE	1:D:565:ASN:HB2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:TYR:HB2	1:D:352:PHE:CD2	2.43	0.52
2:E:162:SER:HB3	2:E:199:LEU:HD23	1.91	0.52
1:A:137:PRO:O	7:A:756:HOH:O	2.18	0.52
1:A:202:LEU:HD21	1:A:529:ARG:NH2	2.23	0.52
1:A:305:MET:CE	1:A:325:LEU:HG	2.38	0.52
1:A:461:ASP:HB3	1:A:528:PHE:HD2	1.74	0.52
2:B:18:ARG:CD	2:B:156:SER:HA	2.38	0.52
2:B:24:ARG:NH2	2:B:197:LYS:HB2	2.23	0.52
1:D:154:TYR:CD2	1:D:559:LEU:HD13	2.44	0.52
1:D:387:GLU:O	7:D:747:HOH:O	2.18	0.52
1:D:412:PHE:N	7:D:707:HOH:O	2.41	0.52
1:D:432:ASN:O	7:D:751:HOH:O	2.19	0.52
2:E:135:LEU:HD23	2:E:157:LEU:HD21	1.91	0.52
2:F:70:VAL:HA	2:F:73:TYR:CD2	2.44	0.52
1:A:236:GLN:NE2	7:A:729:HOH:O	2.08	0.52
1:D:425:ARG:HG2	1:D:545:PHE:CE1	2.45	0.52
1:A:290:LEU:N	1:A:319:TYR:O	2.42	0.52
2:C:5:PRO:HG3	2:C:59:HIS:CE1	2.43	0.52
1:D:235:GLU:HG2	1:D:287:TRP:CG	2.44	0.52
1:A:90:THR:HG23	1:A:397:GLY:HA2	1.91	0.52
1:A:551:VAL:CG1	1:A:555:ASN:HB3	2.36	0.52
2:E:62:LYS:NZ	7:E:426:HOH:O	2.41	0.52
2:E:97:PHE:CE1	2:F:65:CYS:HB2	2.45	0.52
7:C:407:HOH:O	1:D:451:ARG:NH2	2.42	0.52
1:D:412:PHE:HB3	1:D:414:ASN:O	2.10	0.52
1:D:437:THR:OG1	1:D:440:ASP:HB2	2.09	0.52
1:A:91:GLY:O	1:A:92:HIS:C	2.53	0.52
1:A:151:SER:HA	1:A:194:PHE:HA	1.91	0.52
1:A:292:PRO:HA	7:A:725:HOH:O	2.10	0.52
1:A:478:PHE:CZ	1:A:523:VAL:HB	2.44	0.52
1:D:151:SER:HA	1:D:194:PHE:HA	1.92	0.52
2:F:121:GLN:HB3	7:F:457:HOH:O	2.10	0.52
2:C:20:ARG:HB3	2:C:198:SER:HB3	1.92	0.52
2:C:142:LYS:HB3	7:C:430:HOH:O	2.09	0.52
1:D:451:ARG:HH11	1:D:454:GLU:CD	2.18	0.52
2:E:40:LYS:HD3	2:E:52:LYS:HE3	1.91	0.52
2:F:139:LEU:O	2:F:141:ASP:N	2.38	0.52
2:F:176:GLU:N	2:F:176:GLU:CD	2.68	0.52
1:A:96:ALA:HB1	1:A:163:GLY:H	1.75	0.52
1:D:172:ASN:HD21	1:D:174:ASN:CG	2.17	0.52
2:F:131:ALA:O	2:F:135:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:CYS:HA	1:A:207:LEU:HD23	1.91	0.52
1:D:337:ILE:HD11	1:D:361:PHE:HE2	1.75	0.52
1:D:364:LEU:HD12	1:D:402:ARG:NH2	2.25	0.52
2:E:145:PHE:HB2	2:E:154:ASP:CG	2.36	0.52
2:E:150:PHE:CZ	2:E:158:ILE:HD12	2.45	0.52
1:A:365:PRO:HA	1:A:388:TYR:CD1	2.44	0.51
1:A:391:VAL:HG12	1:A:402:ARG:HA	1.93	0.51
2:B:161:SER:HB2	2:B:186:ALA:HB1	1.92	0.51
1:D:33:LYS:O	1:D:37:LEU:HB2	2.10	0.51
1:D:403:LEU:HD22	7:D:803:HOH:O	2.09	0.51
1:D:535:PHE:O	1:D:538:LEU:HB3	2.09	0.51
1:A:32:LEU:HB2	1:A:360:TYR:CG	2.45	0.51
1:A:187:CYS:HB2	1:A:208:SER:HB3	1.92	0.51
1:A:215:GLN:NE2	7:A:824:HOH:O	2.43	0.51
1:A:224:ALA:HB3	1:A:312:TYR:HE1	1.74	0.51
2:B:129:ILE:HD12	2:B:175:ILE:HD11	1.92	0.51
2:C:112:LYS:HG3	7:C:450:HOH:O	2.11	0.51
1:D:202:LEU:O	1:D:205:HIS:N	2.43	0.51
2:E:7:LEU:HD11	2:E:32:TYR:CD1	2.45	0.51
2:B:62:LYS:HZ1	2:C:94:GLN:HG3	1.74	0.51
2:B:125:LYS:HE2	2:B:171:GLY:HA2	1.93	0.51
1:D:87:PRO:HD2	2:E:188:ARG:CB	2.40	0.51
1:A:300:TYR:CE1	1:A:302:TYR:HB2	2.46	0.51
1:A:574:ALA:O	1:A:575:PHE:HB2	2.10	0.51
2:B:132:VAL:HG13	2:B:182:LEU:HD23	1.92	0.51
2:C:104:LYS:N	7:C:419:HOH:O	2.43	0.51
2:C:169:LYS:HD3	2:C:206:VAL:HG13	1.93	0.51
1:D:126:ARG:CD	1:D:182:ILE:HG21	2.40	0.51
1:D:351:THR:HG22	1:D:420:LYS:HB3	1.92	0.51
2:E:193:GLU:HB2	7:E:516:HOH:O	2.11	0.51
1:A:87:PRO:HB2	2:B:143:PRO:CA	2.37	0.51
1:A:405:ASP:HB3	1:A:541:SER:HB3	1.93	0.51
1:A:534:HIS:HA	4:A:602:VAL:N	2.26	0.51
2:B:17:MET:HA	2:B:20:ARG:HD2	1.93	0.51
1:D:97:ILE:HG12	1:D:162:VAL:HG22	1.93	0.51
1:D:310:GLU:O	1:D:313:VAL:HG12	2.10	0.51
2:F:73:TYR:HD1	2:F:76:GLU:OE2	1.94	0.51
1:A:151:SER:OG	1:A:195:SER:O	2.29	0.51
1:D:223:PHE:CZ	1:D:536:LEU:HB2	2.46	0.51
1:D:281:CYS:O	1:D:284:LEU:HG	2.10	0.51
1:D:361:PHE:CZ	1:D:392:ILE:HG23	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:GLU:HB3	7:D:703:HOH:O	2.10	0.51
2:E:76:GLU:OE2	2:F:92:ARG:NH2	2.44	0.51
2:F:165:GLN:HG2	2:F:206:VAL:CG2	2.41	0.51
1:A:219:VAL:HB	1:A:295:PHE:CE1	2.45	0.51
1:A:410:ILE:HD11	1:A:418:GLN:OE1	2.10	0.51
2:C:12:PRO:O	2:C:163:TRP:CZ2	2.64	0.51
2:C:194:SER:N	7:C:442:HOH:O	2.43	0.51
1:D:198:VAL:HG13	1:D:565:ASN:HD21	1.74	0.51
1:D:475:TYR:CE1	1:D:506:TYR:HE1	2.28	0.51
1:D:552:LYS:HE3	1:D:554:SER:OG	2.10	0.51
1:A:46:GLN:HB2	2:B:148:ASP:HB2	1.93	0.51
1:A:113:PHE:HE1	1:A:117:LEU:HD22	1.75	0.51
1:A:337:ILE:HG22	1:A:338:ALA:HB2	1.92	0.51
1:A:423:CYS:SG	1:A:543:GLY:N	2.84	0.51
2:C:164:PHE:CD2	2:C:183:ILE:HD12	2.40	0.51
1:D:437:THR:HG21	1:D:439:ARG:HH21	1.75	0.51
2:E:68:LEU:HA	2:E:71:VAL:HG22	1.92	0.51
1:A:37:LEU:HD11	2:B:90:TYR:CE2	2.45	0.51
1:A:131:PHE:HD1	1:A:343:PRO:HG3	1.75	0.51
2:C:141:ASP:N	2:C:141:ASP:OD1	2.44	0.51
2:C:153:VAL:O	2:C:157:LEU:HD23	2.11	0.51
2:E:144:TYR:CZ	2:E:188:ARG:NH1	2.79	0.51
2:F:115:GLY:HA3	7:F:419:HOH:O	2.10	0.51
2:F:117:LYS:HE3	2:F:213:ARG:HH11	1.74	0.51
1:A:45:LEU:HA	1:A:48:CYS:HB2	1.92	0.51
1:A:95:PRO:HD3	2:B:181:LYS:HZ2	1.76	0.51
1:A:156:SER:HB2	1:A:160:VAL:O	2.11	0.51
1:A:495:ASN:ND2	7:A:703:HOH:O	2.44	0.51
2:C:125:LYS:HD2	2:C:173:PHE:CE1	2.46	0.51
1:A:34:GLU:C	1:A:38:LYS:HE3	2.35	0.50
1:A:154:TYR:HD2	1:A:560:GLN:HA	1.76	0.50
1:A:167:THR:HG21	1:A:560:GLN:HG3	1.92	0.50
2:B:161:SER:HA	2:B:164:PHE:CD2	2.46	0.50
2:C:195:VAL:HG23	2:C:199:LEU:HD13	1.93	0.50
1:D:99:LEU:HB2	1:D:556:ALA:H	1.76	0.50
1:D:118:MET:HG3	7:D:828:HOH:O	2.10	0.50
1:D:332:SER:CB	1:D:538:LEU:HA	2.41	0.50
2:F:32:TYR:H	2:F:32:TYR:HD2	1.57	0.50
1:A:56:ASP:O	1:A:60:ALA:N	2.35	0.50
2:B:205:ILE:HG12	7:B:402:HOH:O	2.10	0.50
1:D:20:MET:SD	7:D:713:HOH:O	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HA	1:A:216:VAL:CG2	2.41	0.50
1:A:535:PHE:HB3	1:A:544:GLN:O	2.11	0.50
1:D:46:GLN:HG3	1:D:47:ASN:N	2.25	0.50
2:E:171:GLY:HA3	2:E:173:PHE:CE2	2.47	0.50
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.46	0.50
1:D:197:ASP:HA	1:D:567:VAL:HG12	1.94	0.50
1:D:223:PHE:HE2	1:D:532:GLN:HB2	1.77	0.50
2:B:183:ILE:O	2:B:186:ALA:HB3	2.12	0.50
1:D:10:MET:HE1	1:D:133:ASN:HB3	1.92	0.50
1:D:76:TYR:O	1:D:88:ILE:HG21	2.12	0.50
1:D:329:ASP:HB3	1:D:338:ALA:O	2.11	0.50
1:D:337:ILE:O	1:D:354:VAL:HA	2.11	0.50
1:D:337:ILE:HG22	1:D:338:ALA:HB2	1.94	0.50
1:D:529:ARG:NH2	1:D:533:GLU:OE1	2.45	0.50
1:A:195:SER:HB3	1:A:201:ALA:HB2	1.92	0.50
2:B:37:PHE:O	7:B:416:HOH:O	2.19	0.50
1:D:32:LEU:O	1:D:36:LEU:HD12	2.11	0.50
1:D:33:LYS:NZ	1:D:58:GLU:HB2	2.27	0.50
1:D:506:TYR:C	1:D:510:ARG:HE	2.19	0.50
1:D:529:ARG:HH21	1:D:530:LYS:HD3	1.76	0.50
1:A:91:GLY:HA3	2:B:142:LYS:N	2.26	0.50
1:A:279:THR:HA	1:A:282:MET:SD	2.52	0.50
1:D:435:LYS:HB3	1:D:436:ASN:C	2.36	0.50
1:A:43:ILE:HD11	1:A:88:ILE:HG23	1.93	0.50
1:A:153:GLN:H	1:A:564:GLU:HB2	1.77	0.50
1:A:237:VAL:O	7:A:757:HOH:O	2.19	0.50
1:A:305:MET:HA	7:A:715:HOH:O	2.12	0.50
1:A:521:ARG:HB3	1:A:566:VAL:HG22	1.94	0.50
2:C:60:ASN:HB3	7:C:421:HOH:O	2.12	0.50
1:D:17:PHE:HA	1:D:20:MET:HB3	1.93	0.50
1:D:476:ALA:HA	1:D:519:GLU:O	2.12	0.50
2:F:114:TRP:HA	2:F:170:PHE:CD2	2.47	0.50
1:A:91:GLY:HA3	2:B:141:ASP:C	2.36	0.50
1:A:291:ILE:HD12	1:A:320:ALA:HB2	1.93	0.50
1:D:270:ASN:HB3	1:D:273:LEU:CD1	2.42	0.50
2:E:110:GLN:HG3	2:E:111:PHE:N	2.25	0.50
2:F:40:LYS:HD2	2:F:52:LYS:HB3	1.93	0.50
1:A:87:PRO:HD2	2:B:188:ARG:HB2	1.93	0.49
1:A:440:ASP:OD1	1:A:501:PHE:HA	2.12	0.49
1:A:505:GLY:C	1:A:507:VAL:H	2.19	0.49
2:C:5:PRO:HB3	2:C:57:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:TYR:HB3	2:C:154:ASP:CG	2.37	0.49
1:D:330:TYR:HE2	1:D:540:SER:H	1.56	0.49
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.46	0.49
1:A:33:LYS:HA	1:A:36:LEU:CD2	2.42	0.49
1:A:103:THR:OG1	1:A:429:LEU:HD11	2.12	0.49
1:A:197:ASP:HA	1:A:567:VAL:HG12	1.94	0.49
1:A:421:PHE:CE1	1:A:541:SER:HA	2.47	0.49
1:A:428:ILE:O	7:A:759:HOH:O	2.20	0.49
2:B:94:GLN:O	2:B:98:TRP:HD1	1.95	0.49
2:B:110:GLN:NE2	7:B:444:HOH:O	2.45	0.49
2:C:187:LYS:HE3	1:D:492:ASP:C	2.36	0.49
1:D:410:ILE:HG13	1:D:418:GLN:HB2	1.94	0.49
2:F:33:ARG:HG3	7:F:518:HOH:O	2.12	0.49
2:F:145:PHE:HA	7:F:424:HOH:O	2.11	0.49
1:A:224:ALA:CB	1:A:316:LEU:HD22	2.43	0.49
1:A:295:PHE:CD1	1:A:298:ALA:HB2	2.45	0.49
2:B:9:ASP:OD1	2:B:16:GLY:HA3	2.12	0.49
2:B:15:PHE:HA	2:B:18:ARG:HG3	1.94	0.49
2:C:98:TRP:CD1	2:C:153:VAL:HG21	2.47	0.49
2:F:71:VAL:O	2:F:74:VAL:HB	2.13	0.49
2:F:172:ASN:O	2:F:173:PHE:HD1	1.94	0.49
1:A:302:TYR:OH	7:A:719:HOH:O	2.06	0.49
1:A:311:PRO:O	1:A:314:PRO:HD2	2.13	0.49
2:C:57:LEU:O	2:C:64:VAL:HG22	2.13	0.49
1:D:151:SER:HB2	1:D:195:SER:O	2.13	0.49
2:E:132:VAL:HG13	2:E:182:LEU:HD23	1.93	0.49
2:F:110:GLN:HG2	2:F:167:TYR:CE2	2.47	0.49
1:A:104:SER:HB3	1:A:107:ARG:O	2.12	0.49
1:A:149:PHE:CB	1:A:530:LYS:NZ	2.75	0.49
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.93	0.49
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.47	0.49
1:A:316:LEU:O	1:A:320:ALA:N	2.41	0.49
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.95	0.49
1:D:55:THR:C	1:D:57:PRO:HD3	2.36	0.49
2:E:102:VAL:O	2:E:106:PHE:HB3	2.12	0.49
2:E:129:ILE:HD11	2:E:173:PHE:CD1	2.47	0.49
2:F:140:GLY:N	2:F:181:LYS:NZ	2.60	0.49
1:A:103:THR:CB	1:A:106:GLY:HA2	2.40	0.49
1:A:549:ARG:HG3	7:A:865:HOH:O	2.11	0.49
2:B:113:VAL:HG23	7:B:436:HOH:O	2.12	0.49
2:C:129:ILE:HA	2:C:132:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LYS:HE2	7:C:481:HOH:O	2.13	0.49
1:D:110:PHE:CE2	1:D:554:SER:HA	2.48	0.49
1:D:145:LEU:HD23	1:D:295:PHE:CZ	2.47	0.49
1:D:342:THR:O	1:D:345:LEU:HG	2.13	0.49
1:D:435:LYS:HD3	1:D:438:GLU:N	2.28	0.49
2:F:92:ARG:HE	2:F:96:ARG:HH22	1.59	0.49
2:F:98:TRP:HD1	2:F:153:VAL:HG11	1.77	0.49
1:A:200:GLN:HA	7:A:963:HOH:O	2.11	0.49
2:C:32:TYR:HA	7:C:412:HOH:O	2.12	0.49
2:C:130:GLU:OE2	7:C:425:HOH:O	2.20	0.49
1:D:498:ASP:OD1	1:D:518:LEU:HD13	2.12	0.49
2:E:15:PHE:HB3	2:E:67:SER:HB3	1.95	0.49
1:A:8:PHE:CD1	1:A:182:ILE:HG22	2.47	0.49
1:A:308:SER:HB3	1:A:424:ARG:HA	1.94	0.49
1:A:551:VAL:HG11	1:A:559:LEU:CD1	2.38	0.49
2:C:24:ARG:HG3	2:C:30:PHE:CE1	2.47	0.49
1:D:223:PHE:CG	1:D:533:GLU:HG2	2.48	0.49
1:D:475:TYR:HE1	1:D:515:ILE:HG21	1.76	0.49
1:D:543:GLY:O	1:D:544:GLN:HG3	2.13	0.49
2:E:139:LEU:O	2:E:141:ASP:N	2.45	0.49
1:A:55:THR:C	1:A:57:PRO:HD3	2.37	0.49
1:A:524:ALA:HB2	1:A:567:VAL:HG11	1.95	0.49
2:C:44:LEU:HB2	7:C:460:HOH:O	2.13	0.49
2:C:84:PHE:HB2	2:C:152:TYR:N	2.28	0.49
1:D:94:VAL:HG21	1:D:97:ILE:HG22	1.95	0.49
1:D:386:GLU:HB3	7:D:771:HOH:O	2.13	0.49
1:D:452:LEU:HD11	1:D:490:LEU:HD23	1.95	0.49
2:F:125:LYS:O	2:F:129:ILE:HG23	2.13	0.49
2:C:174:SER:OG	7:D:701:HOH:O	2.15	0.49
1:D:398:LEU:HD12	1:D:398:LEU:O	2.13	0.49
2:F:37:PHE:HZ	2:F:54:ILE:HG12	1.77	0.49
2:F:145:PHE:CD2	2:F:157:LEU:HD21	2.47	0.49
1:A:41:SER:HB2	2:B:142:LYS:HG2	1.94	0.48
1:A:238:TRP:CE3	1:A:277:ILE:HD11	2.48	0.48
1:A:387:GLU:O	1:A:388:TYR:HD1	1.96	0.48
1:A:468:VAL:HG23	7:A:856:HOH:O	2.13	0.48
2:B:125:LYS:HB3	2:B:173:PHE:CE2	2.48	0.48
2:C:188:ARG:NH1	1:D:499:ARG:C	2.61	0.48
1:D:84:ASP:C	1:D:86:SER:H	2.21	0.48
1:D:223:PHE:HZ	1:D:536:LEU:HB2	1.78	0.48
1:D:476:ALA:HB1	1:D:478:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:ARG:HH12	2:F:41:SER:HB2	1.77	0.48
2:F:201:ASP:HB2	2:F:204:LYS:HE2	1.94	0.48
1:A:104:SER:O	1:A:107:ARG:HG2	2.13	0.48
1:A:225:HIS:HA	1:A:228:VAL:CG2	2.36	0.48
1:A:309:MET:CE	1:A:536:LEU:HD12	2.43	0.48
2:C:32:TYR:CD1	2:C:34:GLU:OE2	2.66	0.48
1:D:263:MET:HE2	1:D:267:LEU:HD11	1.94	0.48
1:D:509:SER:HA	1:D:512:CYS:SG	2.53	0.48
2:E:24:ARG:CZ	2:E:30:PHE:HZ	2.25	0.48
2:E:98:TRP:HB3	2:E:153:VAL:HG21	1.94	0.48
2:F:14:MET:HG3	2:F:163:TRP:CH2	2.48	0.48
1:A:238:TRP:HA	1:A:241:ILE:CB	2.38	0.48
1:A:284:LEU:HB2	7:A:812:HOH:O	2.12	0.48
1:A:402:ARG:HD3	7:A:913:HOH:O	2.12	0.48
1:A:452:LEU:HD11	1:A:490:LEU:HD23	1.96	0.48
2:C:44:LEU:HD22	7:C:517:HOH:O	2.14	0.48
2:C:96:ARG:NH1	7:C:404:HOH:O	1.84	0.48
1:D:20:MET:HE2	1:D:356:PRO:HG2	1.95	0.48
1:D:311:PRO:O	1:D:314:PRO:HD2	2.13	0.48
1:D:496:CYS:HA	1:D:499:ARG:HH22	1.77	0.48
2:E:71:VAL:HG23	2:E:152:TYR:HE1	1.78	0.48
2:F:153:VAL:HA	7:F:402:HOH:O	2.13	0.48
1:A:317:ARG:O	1:A:321:GLY:N	2.45	0.48
2:C:150:PHE:CD1	2:C:192:LYS:HG3	2.48	0.48
1:D:41:SER:HB3	2:E:144:TYR:HB2	1.94	0.48
1:D:73:LEU:HD12	7:D:808:HOH:O	2.13	0.48
1:D:407:VAL:HG13	1:D:421:PHE:CE1	2.48	0.48
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.42	0.48
2:E:129:ILE:HD11	2:E:173:PHE:CE1	2.49	0.48
2:F:151:GLY:N	2:F:154:ASP:OD2	2.47	0.48
1:A:50:LEU:HD13	1:A:61:PHE:CE1	2.49	0.48
1:A:120:ASN:ND2	7:A:828:HOH:O	2.45	0.48
1:A:202:LEU:O	1:A:205:HIS:N	2.46	0.48
1:A:309:MET:C	1:A:311:PRO:HD2	2.38	0.48
1:A:405:ASP:HB2	1:A:540:SER:HB3	1.94	0.48
2:B:15:PHE:HB3	2:B:67:SER:HB3	1.94	0.48
2:C:33:ARG:NH2	2:C:43:LEU:HD11	2.27	0.48
1:D:179:MET:HE1	7:D:743:HOH:O	2.12	0.48
1:D:192:VAL:HG21	1:D:204:CYS:HB3	1.95	0.48
1:D:242:VAL:HA	1:D:245:ILE:HD11	1.95	0.48
2:F:125:LYS:HA	2:F:128:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:LEU:HB3	2:F:181:LYS:HE2	1.96	0.48
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.95	0.48
1:A:198:VAL:CG2	1:A:524:ALA:HB3	2.43	0.48
1:A:336:TRP:HB2	1:A:358:LEU:HD13	1.95	0.48
1:A:460:ILE:HG13	7:A:708:HOH:O	2.13	0.48
1:A:464:SER:OG	1:A:465:TYR:N	2.45	0.48
1:A:522:VAL:O	1:A:567:VAL:HG22	2.13	0.48
2:C:68:LEU:HB2	2:C:152:TYR:OH	2.14	0.48
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.78	0.48
1:D:236:GLN:NE2	7:D:809:HOH:O	2.47	0.48
1:D:334:GLU:O	1:D:398:LEU:HD21	2.14	0.48
1:D:410:ILE:HG21	1:D:420:LYS:HB3	1.96	0.48
1:D:492:ASP:O	1:D:495:ASN:HB2	2.13	0.48
2:F:170:PHE:C	2:F:172:ASN:N	2.63	0.48
1:A:85:THR:O	1:A:93:PRO:HB3	2.13	0.48
1:A:97:ILE:CB	1:A:162:VAL:HB	2.43	0.48
1:A:284:LEU:HD12	1:A:284:LEU:O	2.14	0.48
1:A:302:TYR:OH	7:A:754:HOH:O	2.18	0.48
2:B:182:LEU:HD13	2:B:185:TRP:CE3	2.49	0.48
2:B:182:LEU:HA	2:B:185:TRP:CD2	2.49	0.48
2:C:10:TYR:CD2	2:C:12:PRO:HD2	2.49	0.48
2:C:37:PHE:HD1	2:C:40:LYS:HG2	1.78	0.48
1:D:53:ASN:O	1:D:57:PRO:HB3	2.13	0.48
1:D:423:CYS:HG	1:D:541:SER:HG	1.50	0.48
2:F:199:LEU:HA	2:F:200:PRO:HD2	1.72	0.48
1:A:82:ASP:OD2	7:A:760:HOH:O	2.20	0.48
1:A:309:MET:HE2	1:A:536:LEU:HD12	1.95	0.48
1:A:433:ILE:CD1	1:A:552:LYS:NZ	2.77	0.48
1:A:452:LEU:CD2	1:A:481:ILE:HG12	2.39	0.48
2:C:98:TRP:HZ2	2:C:157:LEU:HD22	1.78	0.48
2:C:131:ALA:O	2:C:135:LEU:HB2	2.14	0.48
1:D:92:HIS:H	2:E:141:ASP:C	2.22	0.48
1:D:198:VAL:CG2	1:D:524:ALA:HB3	2.43	0.48
2:E:68:LEU:O	2:E:72:GLN:HG3	2.14	0.48
1:A:231:PHE:CZ	1:A:291:ILE:HG12	2.49	0.48
1:A:356:PRO:HG3	7:A:917:HOH:O	2.14	0.48
1:A:474:HIS:HB2	1:A:517:ALA:O	2.13	0.48
2:E:75:ASP:HA	7:E:455:HOH:O	2.14	0.48
1:A:27:VAL:CG1	1:A:356:PRO:HB3	2.43	0.47
1:A:91:GLY:HA3	2:B:142:LYS:C	2.39	0.47
1:A:217:GLN:N	7:A:745:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:TRP:HH2	2:C:135:LEU:HD11	1.79	0.47
1:D:405:ASP:OD2	1:D:540:SER:HB3	2.13	0.47
1:D:459:VAL:HG22	1:D:481:ILE:HG22	1.95	0.47
1:A:25:HIS:ND1	1:A:380:THR:HG21	2.29	0.47
1:A:26:GLN:O	1:A:30:GLN:HB2	2.13	0.47
1:A:41:SER:O	2:B:143:PRO:HG2	2.13	0.47
1:A:111:ILE:HG23	1:A:396:ALA:O	2.14	0.47
1:A:268:THR:HA	7:A:861:HOH:O	2.14	0.47
2:B:102:VAL:O	2:B:107:THR:OG1	2.28	0.47
1:D:374:GLU:OE1	7:D:753:HOH:O	2.20	0.47
1:D:495:ASN:HB3	1:D:499:ARG:HH11	1.77	0.47
2:E:181:LYS:HG3	2:E:181:LYS:H	1.43	0.47
2:F:179:SER:HA	2:F:180:PRO:HD3	1.62	0.47
1:A:92:HIS:CE1	2:B:136:GLU:HA	2.50	0.47
2:B:24:ARG:NH1	2:B:197:LYS:HE3	2.23	0.47
2:C:185:TRP:O	2:C:188:ARG:HB3	2.15	0.47
1:D:126:ARG:NH2	1:D:178:GLY:O	2.47	0.47
1:D:313:VAL:HG13	1:D:314:PRO:HD3	1.96	0.47
1:D:450:LYS:HA	1:D:453:SER:HB3	1.96	0.47
1:D:494:CYS:SG	1:D:495:ASN:N	2.88	0.47
1:A:225:HIS:NE2	1:A:532:GLN:OE1	2.46	0.47
2:B:99:ALA:O	2:B:103:ASP:HB2	2.14	0.47
2:B:116:LYS:HD3	2:B:120:GLU:HG2	1.97	0.47
2:C:187:LYS:HE3	1:D:493:CYS:HA	1.96	0.47
1:D:97:ILE:HG13	1:D:556:ALA:CB	2.44	0.47
1:D:157:THR:OG1	1:D:469:SER:HB3	2.14	0.47
2:F:201:ASP:HB2	2:F:204:LYS:HG3	1.95	0.47
1:A:154:TYR:CE1	1:A:156:SER:HA	2.50	0.47
2:C:12:PRO:O	2:C:163:TRP:HZ2	1.97	0.47
2:C:57:LEU:HB3	2:C:64:VAL:HG22	1.96	0.47
2:C:153:VAL:HG23	2:C:156:SER:HB2	1.95	0.47
2:C:181:LYS:HA	2:C:184:ALA:HB3	1.97	0.47
2:C:185:TRP:NE1	2:C:189:CYS:HG	2.11	0.47
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.48	0.47
1:D:450:LYS:HE2	1:D:450:LYS:HB3	1.65	0.47
1:A:309:MET:SD	1:A:545:PHE:CZ	3.08	0.47
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.79	0.47
2:C:33:ARG:CZ	2:C:43:LEU:HD21	2.44	0.47
2:C:159:THR:HA	2:C:199:LEU:HD21	1.96	0.47
2:F:129:ILE:HA	2:F:132:VAL:HG12	1.97	0.47
2:F:159:THR:HA	2:F:199:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:N	7:A:789:HOH:O	2.28	0.47
1:A:99:LEU:H	1:A:557:LYS:HG2	1.79	0.47
2:B:122:GLU:OE2	2:B:125:LYS:NZ	2.42	0.47
1:D:143:LYS:O	1:D:216:VAL:HA	2.15	0.47
1:D:207:LEU:O	1:D:211:LEU:HG	2.14	0.47
2:F:80:GLU:N	7:F:423:HOH:O	2.48	0.47
2:F:114:TRP:HD1	2:F:167:TYR:CE1	2.33	0.47
2:F:141:ASP:HA	7:F:464:HOH:O	2.15	0.47
1:A:225:HIS:HB3	1:A:312:TYR:CD2	2.50	0.47
1:A:311:PRO:HB2	7:A:1024:HOH:O	2.14	0.47
5:B:301:GSH:OE1	7:B:418:HOH:O	2.21	0.47
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.96	0.47
2:C:24:ARG:HG3	2:C:30:PHE:CZ	2.49	0.47
2:C:138:GLU:HG3	2:C:145:PHE:HE1	1.80	0.47
1:D:78:LYS:HE2	1:D:554:SER:HB3	1.97	0.47
1:D:147:PHE:HD2	1:D:529:ARG:NH1	2.10	0.47
2:F:8:LEU:HD13	2:F:44:LEU:HB2	1.97	0.47
2:F:130:GLU:O	2:F:134:ILE:HG22	2.15	0.47
2:F:145:PHE:HB3	2:F:153:VAL:CG1	2.44	0.47
1:A:92:HIS:HB2	2:B:141:ASP:OD1	2.15	0.47
1:A:199:HIS:O	7:A:761:HOH:O	2.20	0.47
2:C:23:LEU:CD2	2:C:28:VAL:HG11	2.43	0.47
1:D:98:SER:C	1:D:556:ALA:HB3	2.40	0.47
2:E:17:MET:SD	2:E:199:LEU:HG	2.55	0.47
2:F:57:LEU:HB3	2:F:64:VAL:HG22	1.97	0.47
2:F:90:TYR:OH	7:F:412:HOH:O	2.09	0.47
1:A:294:LEU:HB3	1:A:295:PHE:CD2	2.50	0.47
1:A:481:ILE:HG22	1:A:483:GLY:H	1.80	0.47
2:C:97:PHE:CE2	2:C:101:PHE:CZ	3.03	0.47
2:C:197:LYS:HB3	2:C:197:LYS:HE3	1.77	0.47
1:D:431:ILE:HD13	1:D:431:ILE:HA	1.68	0.47
1:D:448:ALA:CB	1:D:496:CYS:HB3	2.45	0.47
1:D:526:GLY:O	1:D:530:LYS:HG2	2.15	0.47
1:D:547:MET:HG3	7:D:726:HOH:O	2.15	0.47
2:E:20:ARG:NH1	7:E:429:HOH:O	2.44	0.47
2:E:163:TRP:HB3	2:E:167:TYR:CZ	2.49	0.47
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.49	0.47
2:F:140:GLY:N	2:F:181:LYS:HZ1	2.13	0.47
1:A:98:SER:C	1:A:556:ALA:HB3	2.40	0.46
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.96	0.46
1:A:566:VAL:HG13	1:A:568:SER:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:CYS:O	2:B:66:GLU:HB2	2.14	0.46
2:B:202:SER:HB3	7:B:517:HOH:O	2.15	0.46
2:C:5:PRO:HG2	2:C:28:VAL:CG2	2.45	0.46
1:D:75:PRO:HG2	1:D:76:TYR:HD1	1.80	0.46
1:D:108:PRO:HA	7:D:842:HOH:O	2.15	0.46
2:F:26:LYS:HE2	2:F:75:ASP:HA	1.96	0.46
2:F:26:LYS:CG	2:F:81:LYS:HZ3	2.26	0.46
1:A:223:PHE:HE1	1:A:304:ILE:HD12	1.81	0.46
1:A:441:LEU:HG	1:A:462:PHE:HE2	1.80	0.46
2:C:9:ASP:CG	7:C:412:HOH:O	2.53	0.46
1:D:316:LEU:HD23	1:D:320:ALA:HB2	1.98	0.46
1:D:537:GLY:N	7:D:767:HOH:O	2.37	0.46
2:F:33:ARG:HH22	2:F:41:SER:HB2	1.81	0.46
2:F:174:SER:O	2:F:174:SER:OG	2.25	0.46
1:A:26:GLN:HG3	1:A:27:VAL:N	2.25	0.46
1:A:92:HIS:HB3	2:B:181:LYS:HZ1	1.80	0.46
1:A:246:LYS:HZ1	1:A:278:ARG:HH22	1.63	0.46
1:A:501:PHE:O	1:A:506:TYR:OH	2.20	0.46
2:C:21:VAL:HG12	2:C:155:ILE:HG12	1.97	0.46
2:C:170:PHE:CD2	2:C:213:ARG:HD2	2.50	0.46
1:D:29:LYS:O	1:D:33:LYS:HG2	2.15	0.46
1:D:82:ASP:HA	7:D:709:HOH:O	2.16	0.46
1:D:274:ALA:O	1:D:277:ILE:HG13	2.15	0.46
1:A:97:ILE:H	1:A:162:VAL:HA	1.79	0.46
1:D:152:LYS:HD3	1:D:561:ILE:CG2	2.39	0.46
1:D:219:VAL:HG21	1:D:231:PHE:HZ	1.80	0.46
1:D:238:TRP:O	1:D:242:VAL:HG12	2.16	0.46
1:A:242:VAL:HG11	1:A:278:ARG:HH21	1.80	0.46
2:C:177:SER:HB3	7:C:498:HOH:O	2.16	0.46
1:D:8:PHE:CG	1:D:182:ILE:HG22	2.50	0.46
1:D:489:VAL:O	1:D:492:ASP:HB2	2.15	0.46
1:D:521:ARG:HG3	1:D:569:SER:HB2	1.97	0.46
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.95	0.46
1:A:70:ASP:HB3	1:A:109:LYS:HD2	1.98	0.46
1:A:79:ARG:NH1	2:B:188:ARG:HH12	2.13	0.46
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.51	0.46
1:A:145:LEU:HB2	7:A:778:HOH:O	2.15	0.46
1:A:262:ALA:O	1:A:265:LYS:HG2	2.16	0.46
1:A:390:VAL:CG2	1:A:540:SER:HA	2.45	0.46
1:A:405:ASP:HB3	1:A:541:SER:CB	2.46	0.46
1:A:476:ALA:HA	1:A:519:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PHE:HZ	2:B:182:LEU:HD11	1.81	0.46
1:D:284:LEU:HD13	1:D:287:TRP:N	2.30	0.46
1:D:313:VAL:CG1	1:D:314:PRO:HD3	2.45	0.46
1:D:390:VAL:HG11	1:D:540:SER:CB	2.45	0.46
2:E:22:ALA:HB1	2:E:74:VAL:HG11	1.96	0.46
2:E:26:LYS:HG3	2:E:82:ASN:ND2	2.30	0.46
1:A:222:VAL:HG11	1:A:533:GLU:O	2.16	0.46
1:A:284:LEU:HD12	1:A:284:LEU:C	2.41	0.46
1:A:497:LEU:HD11	7:A:940:HOH:O	2.15	0.46
1:D:74:GLU:O	1:D:78:LYS:HB2	2.16	0.46
1:D:97:ILE:CG1	1:D:162:VAL:HG13	2.45	0.46
1:D:480:GLU:HB2	1:D:528:PHE:CD1	2.50	0.46
2:E:154:ASP:O	2:E:158:ILE:HG13	2.16	0.46
2:F:135:LEU:HD13	2:F:182:LEU:CD1	2.46	0.46
1:A:87:PRO:CB	2:B:143:PRO:HA	2.40	0.46
1:A:208:SER:O	1:A:211:LEU:HB2	2.16	0.46
1:A:240:GLU:OE2	1:A:253:ARG:NE	2.43	0.46
2:B:169:LYS:HD3	2:B:206:VAL:HG13	1.96	0.46
2:C:51:HIS:CD2	7:C:489:HOH:O	2.68	0.46
2:C:57:LEU:HB3	2:C:64:VAL:CG2	2.46	0.46
2:E:149:SER:HB3	2:E:150:PHE:H	1.60	0.46
2:F:100:ASP:HA	7:F:431:HOH:O	2.16	0.46
1:A:143:LYS:HG3	1:A:144:ALA:N	2.28	0.46
1:A:143:LYS:O	1:A:216:VAL:HA	2.16	0.46
1:A:166:THR:HG23	4:A:602:VAL:OXT	2.15	0.46
1:A:210:ILE:HG12	1:A:294:LEU:HD11	1.98	0.46
1:A:326:VAL:HA	7:A:844:HOH:O	2.16	0.46
2:B:134:ILE:O	2:B:137:SER:OG	2.16	0.46
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.46	0.46
2:E:18:ARG:NE	2:E:156:SER:O	2.41	0.46
2:F:201:ASP:OD2	2:F:204:LYS:HE2	2.16	0.46
1:A:17:PHE:HA	1:A:20:MET:HB3	1.97	0.46
1:A:143:LYS:HZ1	1:A:212:PHE:H	1.64	0.46
1:A:210:ILE:HG12	1:A:294:LEU:HD21	1.98	0.46
1:A:309:MET:SD	1:A:312:TYR:HE2	2.39	0.46
1:D:68:VAL:HG11	1:D:73:LEU:HD23	1.97	0.46
1:D:135:ASP:HB2	7:D:827:HOH:O	2.16	0.46
1:D:439:ARG:O	1:D:443:LEU:HB2	2.16	0.46
2:E:10:TYR:HA	2:E:34:GLU:OE2	2.16	0.46
2:F:185:TRP:O	2:F:188:ARG:HB3	2.16	0.46
2:F:195:VAL:HG22	7:F:436:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:HG23	1:A:80:MET:SD	2.55	0.45
1:A:154:TYR:H	1:A:560:GLN:HA	1.81	0.45
2:C:97:PHE:CE2	2:C:101:PHE:HZ	2.34	0.45
1:D:97:ILE:H	1:D:162:VAL:HA	1.80	0.45
1:D:187:CYS:HB2	1:D:208:SER:C	2.41	0.45
2:E:128:PHE:HE2	2:E:175:ILE:HG12	1.81	0.45
2:F:5:PRO:HB3	2:F:59:HIS:NE2	2.30	0.45
2:F:126:LYS:O	2:F:129:ILE:HG13	2.15	0.45
1:A:98:SER:HA	7:A:732:HOH:O	2.16	0.45
2:B:6:ILE:O	2:B:57:LEU:HA	2.17	0.45
2:B:26:LYS:HZ3	2:B:82:ASN:H	1.56	0.45
1:D:410:ILE:HG13	1:D:411:GLY:N	2.30	0.45
2:E:9:ASP:OD1	2:E:16:GLY:HA3	2.16	0.45
2:E:16:GLY:O	2:E:20:ARG:HG3	2.15	0.45
1:A:20:MET:HE2	1:A:356:PRO:HB2	1.97	0.45
1:A:101:SER:HB3	1:A:535:PHE:CG	2.52	0.45
1:A:203:TYR:HE1	1:A:241:ILE:HG13	1.81	0.45
1:A:281:CYS:HB3	1:A:287:TRP:HE1	1.80	0.45
1:D:231:PHE:CD1	1:D:290:LEU:HD22	2.50	0.45
1:D:315:LYS:HD2	1:D:315:LYS:HA	1.80	0.45
1:D:552:LYS:C	1:D:554:SER:H	2.15	0.45
2:E:23:LEU:HD23	2:E:23:LEU:HA	1.80	0.45
2:E:37:PHE:HA	2:E:40:LYS:HG2	1.97	0.45
2:F:11:TRP:O	7:F:404:HOH:O	2.21	0.45
2:F:32:TYR:CD1	2:F:34:GLU:OE2	2.69	0.45
1:A:128:ALA:HB1	7:A:754:HOH:O	2.16	0.45
1:A:151:SER:CB	1:A:194:PHE:HA	2.47	0.45
1:A:330:TYR:HE2	1:A:352:PHE:CD1	2.34	0.45
2:B:26:LYS:HZ1	2:B:82:ASN:H	1.57	0.45
1:D:152:LYS:HG3	1:D:565:ASN:CG	2.41	0.45
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.77	0.45
2:F:23:LEU:CD2	2:F:28:VAL:HG11	2.43	0.45
1:A:121:THR:HG22	1:A:336:TRP:HZ2	1.80	0.45
1:A:152:LYS:H	1:A:152:LYS:HG2	1.58	0.45
2:C:8:LEU:HD13	2:C:44:LEU:HB2	1.98	0.45
2:C:150:PHE:CE1	2:C:192:LYS:HG3	2.52	0.45
1:D:129:PHE:HZ	1:D:218:TYR:HH	1.64	0.45
2:E:24:ARG:HD2	2:E:198:SER:OG	2.16	0.45
2:E:205:ILE:HG22	7:E:441:HOH:O	2.15	0.45
2:F:117:LYS:HA	2:F:121:GLN:HB2	1.98	0.45
1:A:79:ARG:NH2	2:B:188:ARG:HH12	2.12	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:HA	1:A:87:PRO:HD2	1.54	0.45
1:A:87:PRO:HB3	1:A:91:GLY:O	2.17	0.45
1:A:97:ILE:HG23	1:A:111:ILE:H	1.82	0.45
1:A:276:THR:CG2	1:A:277:ILE:N	2.79	0.45
2:C:180:PRO:HB2	1:D:574:ALA:HB2	1.98	0.45
1:D:295:PHE:HA	1:D:296:PRO:HD2	1.86	0.45
2:E:107:THR:HG22	2:E:160:PHE:CE2	2.52	0.45
2:F:5:PRO:HB3	2:F:57:LEU:HD11	1.99	0.45
1:A:76:TYR:CD2	1:A:89:LEU:HD21	2.52	0.45
1:A:309:MET:CB	1:A:312:TYR:CE2	3.00	0.45
2:B:17:MET:HA	2:B:20:ARG:CG	2.47	0.45
2:C:188:ARG:HA	2:C:188:ARG:HD3	1.84	0.45
1:D:34:GLU:O	1:D:38:LYS:HG2	2.17	0.45
1:D:331:GLY:HA3	1:D:336:TRP:HA	1.97	0.45
1:D:451:ARG:CZ	1:D:489:VAL:HG12	2.46	0.45
2:E:26:LYS:NZ	2:E:78:TRP:CE3	2.79	0.45
2:F:102:VAL:O	2:F:107:THR:HG23	2.16	0.45
1:A:39:ASN:OD1	1:A:399:TYR:OH	2.35	0.45
1:A:222:VAL:HG23	7:A:819:HOH:O	2.16	0.45
1:A:363:PHE:HD1	1:A:390:VAL:HA	1.82	0.45
1:A:498:ASP:OD2	7:A:763:HOH:O	2.21	0.45
1:D:69:THR:OG1	1:D:71:VAL:HG12	2.16	0.45
1:D:273:LEU:H	1:D:273:LEU:HG	1.42	0.45
1:D:332:SER:HB3	1:D:538:LEU:HD12	1.98	0.45
2:E:92:ARG:HG3	2:E:96:ARG:HH12	1.82	0.45
2:F:12:PRO:O	2:F:163:TRP:CZ2	2.70	0.45
2:F:26:LYS:HD2	2:F:74:VAL:CG1	2.47	0.45
2:F:176:GLU:C	2:F:180:PRO:HB3	2.41	0.45
1:A:108:PRO:CB	1:A:555:ASN:HB2	2.43	0.45
1:A:143:LYS:CE	1:A:187:CYS:HB3	2.47	0.45
1:A:206:LEU:HD11	1:A:241:ILE:HD11	1.98	0.45
1:A:358:LEU:HA	7:A:828:HOH:O	2.16	0.45
1:A:525:LYS:HD3	7:A:833:HOH:O	2.15	0.45
2:B:165:GLN:HA	2:B:168:GLU:OE2	2.17	0.45
2:C:24:ARG:NH1	2:C:30:PHE:HZ	2.15	0.45
1:D:26:GLN:O	1:D:30:GLN:HB2	2.17	0.45
1:D:288:TYR:HA	1:D:318:HIS:HD2	1.79	0.45
1:D:430:SER:OG	1:D:431:ILE:N	2.49	0.45
1:D:534:HIS:NE2	1:D:557:LYS:HD3	2.32	0.45
2:E:48:ASN:OD1	2:E:50:ILE:HD11	2.16	0.45
1:A:188:SER:HB3	1:A:192:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HA	1:A:244:ASP:OD1	2.16	0.45
1:A:310:GLU:HG3	1:A:311:PRO:CD	2.47	0.45
2:B:48:ASN:HD22	2:B:53:LYS:H	1.65	0.45
2:C:163:TRP:HD1	7:C:484:HOH:O	2.00	0.45
2:C:184:ALA:CB	1:D:499:ARG:NH1	2.75	0.45
2:E:108:ASP:O	2:E:112:LYS:HG2	2.17	0.45
1:A:23:ASN:CG	1:A:26:GLN:HG2	2.42	0.44
1:A:58:GLU:OE2	1:A:360:TYR:OH	2.34	0.44
1:A:384:ILE:HA	1:A:409:VAL:HG12	1.98	0.44
2:C:8:LEU:CD2	2:C:33:ARG:NH2	2.80	0.44
1:D:143:LYS:NZ	1:D:187:CYS:HA	2.33	0.44
1:D:150:SER:OG	1:D:170:TYR:HB2	2.17	0.44
1:D:288:TYR:CE1	1:D:318:HIS:HA	2.52	0.44
2:F:145:PHE:HB3	2:F:153:VAL:HG13	1.98	0.44
1:A:25:HIS:CD2	1:A:25:HIS:H	2.33	0.44
1:A:224:ALA:HA	1:A:227:LEU:CD1	2.43	0.44
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.52	0.44
2:C:153:VAL:HG21	7:C:406:HOH:O	2.17	0.44
1:D:133:ASN:OD1	1:D:138:ILE:HG12	2.16	0.44
1:D:150:SER:HB2	1:D:167:THR:CA	2.40	0.44
1:D:188:SER:HB3	1:D:192:VAL:CG1	2.47	0.44
1:D:206:LEU:HD13	1:D:234:PHE:HD1	1.82	0.44
2:F:125:LYS:HB2	7:F:470:HOH:O	2.16	0.44
2:F:173:PHE:HB3	2:F:174:SER:H	1.47	0.44
1:A:176:LYS:O	1:A:180:LYS:HB2	2.18	0.44
2:B:17:MET:HG3	2:B:20:ARG:NH1	2.33	0.44
2:C:128:PHE:O	2:C:132:VAL:HG12	2.17	0.44
1:D:219:VAL:HB	1:D:295:PHE:CE1	2.52	0.44
1:D:338:ALA:HA	1:D:354:VAL:HA	1.99	0.44
1:D:423:CYS:HB2	1:D:542:ALA:C	2.42	0.44
1:D:485:THR:OG1	1:D:486:ASN:N	2.50	0.44
1:A:147:PHE:HE1	1:A:206:LEU:HB3	1.83	0.44
1:A:217:GLN:CG	1:A:218:TYR:CD2	3.00	0.44
1:A:232:ARG:HA	1:A:235:GLU:CG	2.48	0.44
1:A:351:THR:N	7:A:787:HOH:O	2.50	0.44
1:A:413:TYR:N	1:A:416:THR:O	2.47	0.44
1:A:498:ASP:OD1	1:A:518:LEU:HD12	2.17	0.44
2:B:23:LEU:HD22	2:B:28:VAL:HG11	1.99	0.44
2:C:48:ASN:ND2	7:C:423:HOH:O	2.12	0.44
2:C:68:LEU:HD23	2:C:103:ASP:OD2	2.17	0.44
2:C:187:LYS:HE3	1:D:492:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:LYS:HE2	1:D:456:LYS:HZ3	1.81	0.44
1:D:31:THR:O	1:D:35:ILE:HG13	2.18	0.44
1:D:92:HIS:ND1	2:E:181:LYS:O	2.51	0.44
1:D:329:ASP:N	1:D:329:ASP:OD1	2.50	0.44
1:D:449:ALA:HB1	1:D:459:VAL:HG23	1.98	0.44
1:D:549:ARG:HD3	1:D:549:ARG:HA	1.75	0.44
2:E:48:ASN:C	2:E:50:ILE:H	2.26	0.44
2:E:92:ARG:CZ	2:E:96:ARG:NH1	2.80	0.44
2:E:121:GLN:HG3	7:E:410:HOH:O	2.17	0.44
2:F:10:TYR:CD2	2:F:12:PRO:HD2	2.52	0.44
2:F:141:ASP:N	2:F:141:ASP:OD1	2.50	0.44
1:A:97:ILE:O	1:A:556:ALA:HB1	2.18	0.44
1:A:97:ILE:CG2	1:A:111:ILE:H	2.29	0.44
1:A:552:LYS:HA	1:A:552:LYS:HD2	1.53	0.44
2:B:7:LEU:HD23	2:B:32:TYR:HD1	1.82	0.44
1:D:38:LYS:HA	1:D:38:LYS:HD2	1.84	0.44
1:D:95:PRO:HD3	2:E:181:LYS:HE3	1.99	0.44
1:D:99:LEU:HD13	1:D:555:ASN:OD1	2.18	0.44
1:D:122:LEU:HD12	1:D:123:GLN:N	2.33	0.44
1:D:328:HIS:CG	1:D:329:ASP:H	2.36	0.44
2:E:98:TRP:CZ2	2:E:135:LEU:HA	2.52	0.44
2:E:175:ILE:HB	2:E:183:ILE:HD11	1.99	0.44
1:A:305:MET:CE	1:A:347:PRO:HG3	2.43	0.44
1:A:479:TRP:O	1:A:523:VAL:HG12	2.17	0.44
2:B:62:LYS:NZ	2:C:94:GLN:HG3	2.32	0.44
1:D:97:ILE:HG12	1:D:162:VAL:HG13	1.99	0.44
1:D:194:PHE:O	7:D:757:HOH:O	2.21	0.44
2:E:92:ARG:NH1	2:E:96:ARG:NH1	2.66	0.44
2:E:128:PHE:HD1	7:E:411:HOH:O	2.00	0.44
1:A:70:ASP:OD2	1:A:104:SER:HA	2.18	0.44
1:A:233:THR:CG2	1:A:525:LYS:NZ	2.81	0.44
1:A:527:THR:HB	7:A:749:HOH:O	2.16	0.44
2:B:101:PHE:HA	7:B:474:HOH:O	2.17	0.44
2:B:186:ALA:O	2:B:190:MET:HG2	2.17	0.44
1:D:434:ASP:O	1:D:435:LYS:HG3	2.18	0.44
2:F:10:TYR:HB3	2:F:13:SER:HB2	1.99	0.44
2:F:170:PHE:C	2:F:170:PHE:CD1	2.94	0.44
1:A:13:VAL:HG11	7:A:771:HOH:O	2.17	0.44
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.78	0.44
1:A:112:PRO:HD2	1:A:396:ALA:O	2.17	0.44
1:A:305:MET:SD	1:A:325:LEU:HG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASP:HB2	1:A:550:CYS:HB3	2.00	0.44
2:B:139:LEU:HD23	2:B:142:LYS:H	1.81	0.44
2:B:151:GLY:O	2:B:155:ILE:HG23	2.18	0.44
2:C:9:ASP:HB2	2:C:20:ARG:NH2	2.33	0.44
1:D:23:ASN:O	1:D:27:VAL:HG23	2.18	0.44
1:D:81:VAL:HA	1:D:160:VAL:HG11	1.98	0.44
1:D:125:PHE:CE1	1:D:129:PHE:HE1	2.36	0.44
1:D:130:ALA:O	7:D:754:HOH:O	2.20	0.44
1:D:203:TYR:OH	1:D:254:ILE:HG23	2.17	0.44
1:D:270:ASN:HA	1:D:271:PRO:HD2	1.75	0.44
1:D:359:GLY:HA3	1:D:361:PHE:HE1	1.83	0.44
1:D:455:GLU:OE1	1:D:485:THR:HB	2.17	0.44
2:E:88:ASP:HB2	2:E:90:TYR:CE1	2.53	0.44
2:E:95:ALA:O	2:E:99:ALA:N	2.47	0.44
2:E:148:ASP:OD1	2:E:148:ASP:N	2.51	0.44
1:A:23:ASN:O	1:A:27:VAL:HG12	2.17	0.44
1:A:92:HIS:CG	2:B:181:LYS:HE3	2.53	0.44
1:A:189:PRO:O	1:A:192:VAL:HG12	2.18	0.44
1:A:190:ASP:HA	1:A:193:ILE:HD12	2.00	0.44
1:A:212:PHE:O	1:A:216:VAL:HG23	2.17	0.44
1:A:281:CYS:O	1:A:287:TRP:CZ2	2.71	0.44
1:A:409:VAL:HG13	7:A:794:HOH:O	2.17	0.44
2:B:26:LYS:NZ	2:B:82:ASN:N	2.49	0.44
2:C:142:LYS:HG2	2:C:144:TYR:H	1.83	0.44
1:D:108:PRO:HB3	1:D:555:ASN:N	2.32	0.44
1:D:142:GLY:O	1:D:185:PRO:HD2	2.18	0.44
2:F:26:LYS:HD2	2:F:74:VAL:HG13	2.00	0.44
2:F:54:ILE:HB	2:F:55:PRO:HA	2.00	0.44
2:F:188:ARG:HD3	2:F:188:ARG:HA	1.56	0.44
1:A:99:LEU:HD22	1:A:555:ASN:OD1	2.18	0.43
1:A:114:THR:OG1	2:B:141:ASP:OD2	2.31	0.43
1:A:138:ILE:HA	1:A:138:ILE:HD13	1.76	0.43
1:A:202:LEU:HA	1:A:205:HIS:HB2	2.00	0.43
1:A:222:VAL:HG22	3:A:601:JAA:C07	2.48	0.43
1:A:231:PHE:HB2	1:A:319:TYR:CE2	2.53	0.43
1:A:309:MET:SD	1:A:312:TYR:CE2	3.11	0.43
2:B:51:HIS:HD2	2:B:53:LYS:HE2	1.76	0.43
1:D:7:THR:HG21	7:D:990:HOH:O	2.18	0.43
1:D:534:HIS:CE1	1:D:557:LYS:HD3	2.53	0.43
1:A:109:LYS:HE3	1:A:109:LYS:HB2	1.67	0.43
1:A:229:HIS:O	1:A:233:THR:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:SER:HA	7:A:703:HOH:O	2.18	0.43
2:C:71:VAL:O	2:C:74:VAL:HB	2.18	0.43
2:C:190:MET:HE3	7:C:470:HOH:O	2.17	0.43
2:C:195:VAL:HG11	7:C:432:HOH:O	2.18	0.43
1:D:164:THR:HG22	1:D:166:THR:H	1.83	0.43
1:D:446:GLU:HG2	7:D:1050:HOH:O	2.19	0.43
2:E:68:LEU:HD13	2:E:99:ALA:HB1	2.00	0.43
2:E:82:ASN:OD1	2:E:82:ASN:N	2.51	0.43
2:E:106:PHE:O	7:E:411:HOH:O	2.21	0.43
2:F:12:PRO:O	2:F:163:TRP:HZ2	2.02	0.43
1:A:99:LEU:HB3	1:A:557:LYS:CB	2.47	0.43
1:A:143:LYS:HE2	1:A:216:VAL:CG2	2.49	0.43
2:B:11:TRP:HZ2	2:B:208:TYR:CE1	2.36	0.43
2:C:99:ALA:HA	7:C:406:HOH:O	2.18	0.43
1:D:27:VAL:HG11	1:D:356:PRO:HG2	2.00	0.43
1:D:132:ARG:O	1:D:136:PHE:N	2.38	0.43
1:D:363:PHE:CE1	1:D:390:VAL:HG23	2.52	0.43
1:D:387:GLU:HG3	1:D:408:LYS:HB2	2.01	0.43
2:E:15:PHE:HB3	2:E:67:SER:CB	2.48	0.43
2:E:135:LEU:HD22	2:E:182:LEU:HD21	1.99	0.43
1:A:41:SER:OG	2:B:142:LYS:HE3	2.18	0.43
1:A:102:GLY:N	1:A:546:LYS:O	2.48	0.43
1:A:219:VAL:HG13	1:A:301:VAL:HG13	2.00	0.43
1:A:288:TYR:CZ	1:A:321:GLY:HA2	2.53	0.43
1:A:475:TYR:HB2	1:A:518:LEU:HD23	2.00	0.43
1:A:494:CYS:SG	1:A:495:ASN:N	2.91	0.43
2:B:121:GLN:O	2:B:125:LYS:HG3	2.19	0.43
1:D:67:LEU:HB3	7:D:856:HOH:O	2.18	0.43
1:D:91:GLY:HA3	2:E:142:LYS:HA	1.99	0.43
2:E:126:LYS:O	2:E:130:GLU:HG3	2.18	0.43
2:E:201:ASP:HB3	2:E:203:GLU:HG2	2.00	0.43
2:F:98:TRP:CD1	2:F:153:VAL:HG21	2.53	0.43
2:F:181:LYS:O	2:F:185:TRP:N	2.40	0.43
2:F:185:TRP:NE1	2:F:189:CYS:HG	2.14	0.43
1:A:195:SER:OG	1:A:259:VAL:HG21	2.17	0.43
1:A:312:TYR:CD1	1:A:312:TYR:C	2.97	0.43
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.62	0.43
1:A:423:CYS:HA	7:A:747:HOH:O	2.18	0.43
1:A:434:ASP:O	1:A:435:LYS:HG3	2.18	0.43
1:A:537:GLY:HA3	3:A:601:JAA:O02	2.19	0.43
2:B:65:CYS:SG	2:C:97:PHE:CZ	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:PHE:CD1	1:D:556:ALA:HB2	2.53	0.43
1:D:198:VAL:HG22	1:D:565:ASN:ND2	2.24	0.43
1:D:435:LYS:HA	1:D:436:ASN:HB2	1.99	0.43
1:D:552:LYS:C	1:D:554:SER:N	2.75	0.43
2:E:88:ASP:HA	2:E:89:PRO:HD3	1.86	0.43
2:F:10:TYR:CG	2:F:12:PRO:HD2	2.53	0.43
1:A:151:SER:CA	1:A:194:PHE:HA	2.49	0.43
1:A:250:LEU:HD21	1:A:260:ARG:HG2	2.00	0.43
1:A:274:ALA:O	1:A:278:ARG:NE	2.52	0.43
1:A:478:PHE:HZ	1:A:562:LEU:HA	1.79	0.43
2:B:93:ALA:HB1	2:C:73:TYR:CE1	2.54	0.43
2:B:112:LYS:HB2	7:B:414:HOH:O	2.18	0.43
1:D:413:TYR:O	1:D:416:THR:HG22	2.18	0.43
2:E:169:LYS:NZ	2:E:206:VAL:HG11	2.33	0.43
2:E:206:VAL:HA	7:E:441:HOH:O	2.18	0.43
1:A:274:ALA:C	1:A:278:ARG:NE	2.77	0.43
1:A:337:ILE:HG13	7:A:764:HOH:O	2.18	0.43
1:A:475:TYR:HB2	1:A:518:LEU:CD2	2.48	0.43
1:A:527:THR:HG22	1:A:528:PHE:CD1	2.53	0.43
2:C:149:SER:HB3	2:C:150:PHE:H	1.71	0.43
1:D:77:ILE:HG12	1:D:110:PHE:O	2.19	0.43
1:D:444:SER:HA	1:D:500:ALA:CB	2.48	0.43
1:D:521:ARG:HG3	1:D:521:ARG:HH11	1.83	0.43
2:E:16:GLY:O	2:E:20:ARG:NE	2.50	0.43
2:E:85:PHE:N	2:E:85:PHE:CD1	2.87	0.43
2:F:194:SER:O	2:F:198:SER:OG	2.20	0.43
1:A:116:GLU:OE2	1:A:395:TYR:CE1	2.72	0.43
2:C:54:ILE:N	7:C:428:HOH:O	2.50	0.43
2:C:62:LYS:HA	2:C:63:PRO:HD2	1.87	0.43
2:C:190:MET:HB3	1:D:450:LYS:HG3	2.00	0.43
1:D:39:ASN:HA	2:E:142:LYS:CG	2.49	0.43
1:D:87:PRO:CB	2:E:143:PRO:HA	2.45	0.43
1:D:453:SER:C	1:D:455:GLU:H	2.26	0.43
2:E:109:ALA:HB3	7:E:411:HOH:O	2.18	0.43
2:E:164:PHE:CD2	2:E:183:ILE:HG12	2.53	0.43
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.69	0.43
2:F:8:LEU:HD22	2:F:33:ARG:NH2	2.26	0.43
2:F:98:TRP:CE3	2:F:98:TRP:O	2.72	0.43
1:A:25:HIS:HD2	7:A:889:HOH:O	2.02	0.43
1:A:96:ALA:HB3	1:A:113:PHE:CD2	2.53	0.43
1:A:135:ASP:HB2	7:A:929:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG13	3:A:601:JAA:C06	2.48	0.43
1:A:429:LEU:HD12	1:A:429:LEU:HA	1.79	0.43
1:A:505:GLY:C	1:A:507:VAL:N	2.76	0.43
1:A:555:ASN:O	1:A:559:LEU:HD22	2.19	0.43
1:D:36:LEU:HD13	1:D:61:PHE:CE2	2.54	0.43
1:D:96:ALA:O	1:D:113:PHE:HB3	2.19	0.43
1:D:316:LEU:O	1:D:320:ALA:N	2.50	0.43
1:D:424:ARG:O	1:D:543:GLY:HA2	2.18	0.43
2:E:24:ARG:NH1	2:E:198:SER:OG	2.51	0.43
2:E:48:ASN:HB3	2:E:52:LYS:HA	2.01	0.43
2:E:62:LYS:HA	2:E:63:PRO:HD2	1.79	0.43
1:A:56:ASP:HB2	1:A:59:GLU:HB2	2.01	0.43
1:A:213:ARG:HG3	1:A:214:ASP:N	2.34	0.43
1:A:305:MET:HE2	1:A:327:SER:OG	2.19	0.43
2:C:168:GLU:CD	1:D:488:ASP:OD2	2.62	0.43
1:D:124:LEU:HB3	3:D:601:JAA:C15	2.49	0.43
1:D:362:GLU:HG3	1:D:400:ARG:HH22	1.82	0.43
1:D:575:PHE:O	7:D:756:HOH:O	2.21	0.43
2:E:26:LYS:HE2	2:E:26:LYS:HB2	1.91	0.43
2:E:161:SER:HA	2:E:164:PHE:CG	2.54	0.43
2:F:33:ARG:HH22	2:F:41:SER:CB	2.31	0.43
1:A:33:LYS:HA	1:A:36:LEU:HD23	2.00	0.42
1:A:66:PRO:HD3	7:A:723:HOH:O	2.19	0.42
1:A:70:ASP:OD1	1:A:71:VAL:N	2.52	0.42
1:A:97:ILE:HA	1:A:111:ILE:O	2.19	0.42
1:A:291:ILE:HD11	1:A:316:LEU:HD11	2.01	0.42
1:A:303:GLY:O	1:A:327:SER:HA	2.19	0.42
1:A:433:ILE:CD1	1:A:552:LYS:HZ2	2.32	0.42
1:A:446:GLU:CD	7:A:884:HOH:O	2.62	0.42
2:C:104:LYS:NZ	7:C:439:HOH:O	2.39	0.42
2:C:114:TRP:HA	2:C:170:PHE:CD2	2.49	0.42
1:D:402:ARG:NH2	7:D:759:HOH:O	2.21	0.42
1:D:407:VAL:HG21	7:D:920:HOH:O	2.19	0.42
2:F:185:TRP:CE2	2:F:189:CYS:SG	3.11	0.42
1:A:53:ASN:CG	1:A:54:ALA:N	2.77	0.42
1:A:238:TRP:CZ2	1:A:281:CYS:HB2	2.54	0.42
1:A:240:GLU:CD	1:A:253:ARG:HE	2.25	0.42
1:A:274:ALA:CB	1:A:278:ARG:CZ	2.96	0.42
1:A:355:ILE:HA	1:A:356:PRO:HD3	1.49	0.42
1:A:389:GLU:OE2	1:A:402:ARG:HG2	2.19	0.42
2:B:18:ARG:HG2	2:B:159:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:PRO:HD3	2:B:146:GLY:O	2.20	0.42
2:C:4:LEU:HA	2:C:5:PRO:HD3	1.65	0.42
1:D:32:LEU:O	1:D:35:ILE:HB	2.20	0.42
1:D:32:LEU:HD13	1:D:360:TYR:CD2	2.54	0.42
1:D:163:GLY:HA2	1:D:560:GLN:HB2	2.02	0.42
1:D:224:ALA:HA	1:D:316:LEU:HD12	2.00	0.42
1:D:229:HIS:O	1:D:233:THR:HG23	2.20	0.42
1:D:365:PRO:HD2	1:D:374:GLU:HG2	2.01	0.42
2:F:145:PHE:CE2	2:F:157:LEU:HD21	2.53	0.42
2:F:169:LYS:HD3	2:F:206:VAL:HG13	2.01	0.42
1:A:86:SER:HB2	2:B:188:ARG:HB2	2.02	0.42
1:A:145:LEU:HD13	1:A:209:GLY:CA	2.43	0.42
1:A:154:TYR:CZ	1:A:559:LEU:HD23	2.54	0.42
2:B:15:PHE:O	2:B:18:ARG:HB2	2.19	0.42
2:B:194:SER:O	2:B:198:SER:HB2	2.19	0.42
1:D:28:GLN:HA	7:D:734:HOH:O	2.19	0.42
1:D:168:ASN:HB2	7:D:770:HOH:O	2.19	0.42
1:D:452:LEU:HD13	1:D:493:CYS:SG	2.59	0.42
2:F:187:LYS:O	2:F:187:LYS:HG2	2.18	0.42
1:A:248:GLY:O	1:A:267:LEU:HB3	2.20	0.42
1:A:510:ARG:C	1:A:513:LYS:H	2.27	0.42
2:B:27:GLY:HA2	7:B:503:HOH:O	2.19	0.42
2:C:104:LYS:HD2	2:C:104:LYS:C	2.44	0.42
1:D:196:PRO:O	1:D:565:ASN:HA	2.19	0.42
1:D:494:CYS:HB2	1:D:520:LEU:HB3	2.01	0.42
1:D:541:SER:C	1:D:543:GLY:H	2.27	0.42
2:F:144:TYR:HB3	2:F:154:ASP:CG	2.45	0.42
2:F:180:PRO:C	2:F:182:LEU:N	2.76	0.42
1:A:167:THR:HG21	1:A:560:GLN:CG	2.50	0.42
1:A:244:ASP:HB2	1:A:251:SER:H	1.85	0.42
1:A:504:ALA:O	1:A:507:VAL:HB	2.19	0.42
1:A:524:ALA:HB2	1:A:567:VAL:CG1	2.50	0.42
1:A:532:GLN:NE2	7:A:777:HOH:O	2.25	0.42
2:B:51:HIS:HB2	2:B:53:LYS:HG2	2.01	0.42
1:D:44:TYR:OH	1:D:68:VAL:HG22	2.18	0.42
1:D:111:ILE:HA	1:D:112:PRO:HD3	1.90	0.42
1:D:184:SER:HB3	7:D:733:HOH:O	2.18	0.42
1:D:253:ARG:NH2	7:D:819:HOH:O	2.52	0.42
1:D:336:TRP:C	1:D:337:ILE:HD12	2.44	0.42
1:D:501:PHE:CE2	1:D:518:LEU:HD21	2.54	0.42
2:E:6:ILE:HG23	2:E:31:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:150:PHE:CD2	2:E:192:LYS:HD2	2.54	0.42
1:A:32:LEU:HD22	1:A:360:TYR:CD2	2.54	0.42
1:A:198:VAL:HG22	1:A:524:ALA:HB3	2.00	0.42
1:A:207:LEU:HD21	1:A:263:MET:HE2	2.00	0.42
1:A:213:ARG:HA	1:A:216:VAL:HG23	2.01	0.42
2:B:139:LEU:HD21	2:B:142:LYS:H	1.84	0.42
2:B:197:LYS:HE3	2:B:197:LYS:HB2	1.73	0.42
1:D:305:MET:HB3	1:D:347:PRO:HB3	2.02	0.42
2:E:14:MET:HE1	7:E:550:HOH:O	2.19	0.42
2:F:57:LEU:HB3	2:F:64:VAL:CG2	2.50	0.42
2:F:216:ASN:HA	7:F:459:HOH:O	2.19	0.42
1:A:27:VAL:HG11	1:A:356:PRO:HB3	2.01	0.42
1:A:92:HIS:HE1	2:B:136:GLU:HA	1.84	0.42
1:A:152:LYS:HD3	1:A:565:ASN:ND2	2.34	0.42
1:A:233:THR:CG2	1:A:525:LYS:HZ1	2.32	0.42
1:A:351:THR:HG21	1:A:410:ILE:CG1	2.46	0.42
2:B:65:CYS:O	2:B:69:ASN:HB3	2.19	0.42
2:B:149:SER:HB2	2:B:150:PHE:H	1.67	0.42
1:D:41:SER:HA	2:E:147:GLY:O	2.20	0.42
1:D:97:ILE:HG13	1:D:556:ALA:HB1	2.01	0.42
1:D:534:HIS:CD2	1:D:535:PHE:CD1	3.08	0.42
1:D:534:HIS:HD2	1:D:535:PHE:CD1	2.38	0.42
2:F:26:LYS:HE3	2:F:78:TRP:O	2.19	0.42
1:A:222:VAL:HG12	1:A:223:PHE:CD1	2.55	0.42
1:A:223:PHE:CD2	1:A:309:MET:HE1	2.54	0.42
1:A:238:TRP:CZ3	1:A:277:ILE:HG12	2.55	0.42
1:A:509:SER:HB3	1:A:515:ILE:HG12	2.02	0.42
1:D:384:ILE:H	1:D:384:ILE:HG13	1.60	0.42
1:D:551:VAL:HG23	1:D:555:ASN:H	1.84	0.42
2:E:102:VAL:HA	2:E:106:PHE:HB2	2.01	0.42
2:F:102:VAL:O	2:F:106:PHE:HB3	2.20	0.42
1:A:79:ARG:HH11	1:A:88:ILE:CD1	2.32	0.42
1:A:117:LEU:O	1:A:121:THR:HG23	2.19	0.42
1:A:237:VAL:HB	7:A:757:HOH:O	2.20	0.42
1:A:246:LYS:NZ	1:A:278:ARG:NH2	2.63	0.42
1:A:390:VAL:HG21	1:A:540:SER:HA	2.02	0.42
2:B:8:LEU:HD21	2:B:43:LEU:HD13	2.01	0.42
2:B:21:VAL:O	2:B:25:GLU:HB2	2.19	0.42
2:B:50:ILE:HG13	2:C:134:ILE:CD1	2.47	0.42
2:C:126:LYS:O	2:C:129:ILE:HG13	2.20	0.42
1:D:101:SER:N	1:D:535:PHE:CZ	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LEU:HD21	1:D:329:ASP:HB2	2.02	0.42
1:D:233:THR:HG22	7:D:748:HOH:O	2.19	0.42
1:D:408:LYS:O	1:D:419:LEU:HA	2.20	0.42
1:D:477:ILE:O	1:D:520:LEU:HD12	2.20	0.42
2:E:7:LEU:CD1	2:E:9:ASP:HB2	2.49	0.42
5:F:301:GSH:N1	7:F:425:HOH:O	2.25	0.42
1:A:92:HIS:O	1:A:93:PRO:C	2.62	0.42
1:A:94:VAL:HG11	1:A:112:PRO:HB3	2.01	0.42
1:A:98:SER:OG	1:A:111:ILE:HB	2.20	0.42
1:A:198:VAL:O	1:A:202:LEU:HD12	2.20	0.42
1:A:217:GLN:HG3	1:A:218:TYR:HD2	1.84	0.42
1:A:242:VAL:HG11	1:A:278:ARG:NH2	2.34	0.42
1:A:305:MET:HG3	7:A:715:HOH:O	2.20	0.42
1:A:310:GLU:N	1:A:311:PRO:HD2	2.34	0.42
1:A:491:GLN:NE2	1:A:570:TYR:CD2	2.88	0.42
2:C:185:TRP:CE2	2:C:189:CYS:SG	3.12	0.42
1:D:108:PRO:HB3	1:D:555:ASN:CB	2.50	0.42
1:D:277:ILE:HD12	1:D:278:ARG:N	2.35	0.42
1:D:364:LEU:HB2	1:D:402:ARG:HH22	1.84	0.42
1:D:523:VAL:HG23	7:D:785:HOH:O	2.20	0.42
2:E:26:LYS:HZ3	2:E:74:VAL:CG2	2.15	0.42
2:E:33:ARG:NH2	2:E:43:LEU:HD13	2.35	0.42
2:F:21:VAL:HG12	2:F:155:ILE:HG12	2.01	0.42
1:A:95:PRO:HD3	2:B:181:LYS:NZ	2.34	0.41
1:A:392:ILE:HG13	1:A:401:TYR:HB3	2.02	0.41
1:A:532:GLN:O	1:A:535:PHE:N	2.49	0.41
2:B:110:GLN:O	2:B:113:VAL:HB	2.20	0.41
2:C:8:LEU:HG	2:C:56:VAL:HB	2.02	0.41
2:C:26:LYS:HE3	2:C:78:TRP:O	2.19	0.41
1:D:95:PRO:O	1:D:161:PRO:HB2	2.20	0.41
1:D:118:MET:HG2	1:D:172:ASN:ND2	2.35	0.41
1:D:254:ILE:HD13	1:D:254:ILE:N	2.35	0.41
1:D:403:LEU:HD23	1:D:403:LEU:HA	1.51	0.41
1:D:465:TYR:HD1	1:D:551:VAL:HG13	1.84	0.41
1:D:485:THR:OG1	7:D:755:HOH:O	2.21	0.41
1:A:31:THR:OG1	1:A:357:ASN:HA	2.20	0.41
1:A:224:ALA:HB3	1:A:312:TYR:CD1	2.54	0.41
1:A:510:ARG:HB3	1:A:575:PHE:CE2	2.55	0.41
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.83	0.41
2:B:34:GLU:HA	7:B:465:HOH:O	2.20	0.41
2:B:193:GLU:HB3	2:B:197:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:ASP:O	2:C:39:ASN:N	2.47	0.41
2:C:72:GLN:OE1	7:C:426:HOH:O	2.22	0.41
2:C:81:LYS:HG3	2:C:82:ASN:H	1.85	0.41
1:D:156:SER:OG	7:D:709:HOH:O	2.04	0.41
1:D:169:VAL:O	1:D:175:PHE:HB2	2.20	0.41
2:F:168:GLU:CD	2:F:176:GLU:OE2	2.63	0.41
1:A:45:LEU:C	1:A:48:CYS:H	2.28	0.41
1:A:105:GLN:N	7:A:829:HOH:O	2.46	0.41
1:A:107:ARG:NH2	7:A:746:HOH:O	2.53	0.41
1:A:188:SER:HB3	1:A:192:VAL:CG1	2.51	0.41
1:A:238:TRP:HA	1:A:241:ILE:CG1	2.50	0.41
1:A:314:PRO:CB	1:A:317:ARG:HH12	2.33	0.41
1:A:471:ASP:HA	1:A:472:PRO:HA	1.80	0.41
2:B:126:LYS:O	2:B:130:GLU:HG2	2.21	0.41
2:C:8:LEU:N	2:C:8:LEU:HD23	2.35	0.41
2:C:184:ALA:CB	1:D:499:ARG:CZ	2.85	0.41
1:D:90:THR:OG1	1:D:397:GLY:HA2	2.20	0.41
1:D:250:LEU:HB2	1:D:254:ILE:HG13	2.02	0.41
1:D:446:GLU:HG3	7:D:824:HOH:O	2.20	0.41
1:D:453:SER:HB2	7:D:786:HOH:O	2.20	0.41
2:E:190:MET:HE3	2:E:190:MET:HB3	1.87	0.41
2:F:110:GLN:O	2:F:113:VAL:HG12	2.20	0.41
1:A:145:LEU:HD21	1:A:147:PHE:CZ	2.55	0.41
1:A:196:PRO:HG2	1:A:256:VAL:HG11	2.01	0.41
1:A:282:MET:HG3	1:A:283:SER:N	2.36	0.41
1:A:305:MET:HE2	1:A:305:MET:HB2	1.82	0.41
1:A:310:GLU:O	1:A:314:PRO:HD3	2.21	0.41
1:A:384:ILE:HA	1:A:409:VAL:CG1	2.49	0.41
2:C:110:GLN:O	2:C:113:VAL:HG12	2.20	0.41
1:D:133:ASN:CG	1:D:137:PRO:HA	2.45	0.41
1:D:425:ARG:HH12	1:D:546:LYS:HE3	1.84	0.41
2:B:8:LEU:HD22	2:B:35:GLU:OE2	2.19	0.41
2:B:53:LYS:HD3	5:B:301:GSH:HB13	2.02	0.41
2:C:9:ASP:HB2	2:C:20:ARG:HH21	1.85	0.41
1:D:94:VAL:HG21	1:D:97:ILE:CG2	2.51	0.41
1:D:192:VAL:HA	1:D:195:SER:HB2	2.01	0.41
1:D:445:VAL:HG13	1:D:479:TRP:NE1	2.34	0.41
1:D:480:GLU:HB2	1:D:528:PHE:HD1	1.85	0.41
1:D:521:ARG:HG3	1:D:521:ARG:NH1	2.35	0.41
2:E:86:PRO:HD2	2:E:92:ARG:HA	2.02	0.41
1:A:35:ILE:O	1:A:39:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:HE2	1:A:162:VAL:HG22	1.85	0.41
1:A:225:HIS:HB3	1:A:312:TYR:CZ	2.53	0.41
2:B:70:VAL:O	2:B:74:VAL:HG23	2.20	0.41
2:C:57:LEU:O	2:C:64:VAL:HG13	2.21	0.41
1:D:99:LEU:CB	1:D:556:ALA:H	2.34	0.41
1:D:345:LEU:HD13	1:D:350:ALA:HA	2.02	0.41
1:D:471:ASP:HA	1:D:472:PRO:HA	1.88	0.41
1:A:203:TYR:CD2	1:A:254:ILE:HD11	2.53	0.41
1:A:357:ASN:ND2	7:A:843:HOH:O	2.54	0.41
1:A:452:LEU:O	1:A:457:ILE:HB	2.21	0.41
1:A:527:THR:HG23	1:A:561:ILE:CG2	2.44	0.41
2:C:187:LYS:HZ3	2:C:187:LYS:HB2	1.84	0.41
1:D:19:GLU:O	1:D:23:ASN:HB2	2.21	0.41
1:D:68:VAL:HG11	1:D:73:LEU:CD2	2.51	0.41
1:D:247:ASP:HA	7:D:992:HOH:O	2.19	0.41
1:D:323:LEU:HA	1:D:324:PRO:HD3	1.95	0.41
1:D:425:ARG:HB2	1:D:427:LEU:HB2	2.03	0.41
1:A:87:PRO:HD3	1:A:93:PRO:HD3	2.03	0.41
1:A:117:LEU:O	1:A:120:ASN:HB2	2.21	0.41
2:B:96:ARG:NH1	2:C:76:GLU:OE2	2.54	0.41
2:C:64:VAL:HG12	7:C:447:HOH:O	2.21	0.41
1:D:91:GLY:HA3	2:E:142:LYS:CA	2.51	0.41
1:D:91:GLY:O	1:D:92:HIS:C	2.64	0.41
1:D:262:ALA:HB3	7:D:783:HOH:O	2.20	0.41
1:D:295:PHE:CD2	1:D:295:PHE:N	2.88	0.41
1:D:440:ASP:OD1	1:D:501:PHE:HA	2.20	0.41
2:F:115:GLY:O	2:F:116:LYS:HD2	2.21	0.41
1:A:46:GLN:OE1	2:B:149:SER:HB3	2.20	0.41
1:A:57:PRO:HG3	7:A:809:HOH:O	2.21	0.41
1:A:77:ILE:HG22	1:A:110:PHE:HB3	2.02	0.41
1:A:92:HIS:NE2	2:B:139:LEU:HB3	2.35	0.41
1:A:223:PHE:HB3	1:A:312:TYR:OH	2.21	0.41
1:A:447:SER:O	1:A:450:LYS:HG2	2.21	0.41
1:A:507:VAL:HG13	1:A:511:LYS:HD2	2.03	0.41
2:B:5:PRO:HB3	2:B:57:LEU:HD21	2.01	0.41
2:C:7:LEU:HD21	2:C:23:LEU:CD1	2.48	0.41
2:C:26:LYS:HD2	2:C:74:VAL:CG1	2.47	0.41
2:C:64:VAL:HB	2:C:73:TYR:HD2	1.82	0.41
2:C:142:LYS:HA	2:C:143:PRO:HD3	1.97	0.41
2:C:151:GLY:N	2:C:154:ASP:OD2	2.54	0.41
2:C:174:SER:C	2:C:176:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LYS:HB2	1:D:33:LYS:HE2	2.03	0.41
1:D:79:ARG:HD2	7:D:1040:HOH:O	2.21	0.41
1:D:82:ASP:O	7:D:761:HOH:O	2.22	0.41
1:D:222:VAL:O	1:D:304:ILE:N	2.35	0.41
1:D:222:VAL:HG11	4:D:602:VAL:N	2.36	0.41
1:D:563:CYS:O	1:D:566:VAL:HG12	2.20	0.41
2:E:54:ILE:H	2:E:54:ILE:HG13	1.72	0.41
2:E:66:GLU:CD	2:F:97:PHE:CD1	2.97	0.41
1:A:113:PHE:CE1	1:A:117:LEU:HD22	2.56	0.41
1:A:117:LEU:HD11	1:A:333:SER:CA	2.42	0.41
1:A:288:TYR:HA	1:A:318:HIS:O	2.21	0.41
1:A:465:TYR:HD1	1:A:551:VAL:CG1	2.34	0.41
1:D:92:HIS:HB2	2:E:141:ASP:CB	2.51	0.41
1:D:109:LYS:HE3	1:D:111:ILE:HG13	2.02	0.41
1:D:133:ASN:OD1	1:D:138:ILE:N	2.50	0.41
2:E:199:LEU:HA	2:E:200:PRO:HD2	1.97	0.41
2:F:9:ASP:HB2	2:F:20:ARG:NH2	2.36	0.41
2:F:14:MET:HE3	2:F:14:MET:HB2	1.94	0.41
2:F:182:LEU:O	2:F:185:TRP:HE3	2.04	0.41
1:A:114:THR:HG22	1:A:115:ASP:H	1.86	0.40
1:A:143:LYS:CE	1:A:212:PHE:HB2	2.50	0.40
2:B:211:GLU:OE1	7:B:421:HOH:O	2.22	0.40
2:C:143:PRO:HB2	2:C:144:TYR:CD2	2.56	0.40
1:D:77:ILE:O	1:D:81:VAL:HG12	2.21	0.40
1:D:108:PRO:HG2	1:D:552:LYS:N	2.30	0.40
1:D:330:TYR:HB2	1:D:352:PHE:HD2	1.85	0.40
1:D:363:PHE:HB2	1:D:388:TYR:HD2	1.87	0.40
1:D:449:ALA:O	1:D:452:LEU:HB2	2.21	0.40
2:F:117:LYS:HE3	2:F:213:ARG:HH12	1.84	0.40
2:F:169:LYS:HE3	2:F:169:LYS:HB2	1.68	0.40
1:A:117:LEU:HA	1:A:120:ASN:ND2	2.37	0.40
1:A:337:ILE:O	1:A:354:VAL:HA	2.22	0.40
1:A:444:SER:OG	7:A:705:HOH:O	1.96	0.40
2:B:62:LYS:NZ	2:C:94:GLN:CG	2.84	0.40
2:B:77:ALA:C	2:B:79:PRO:HD3	2.46	0.40
2:C:20:ARG:CB	2:C:198:SER:HB3	2.51	0.40
1:D:125:PHE:CE2	1:D:328:HIS:CE1	3.02	0.40
1:D:302:TYR:CD1	1:D:326:VAL:HG13	2.53	0.40
1:D:433:ILE:C	1:D:435:LYS:H	2.29	0.40
2:E:99:ALA:O	2:E:103:ASP:HB2	2.21	0.40
1:A:33:LYS:O	1:A:37:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:CG2	1:A:97:ILE:HD12	2.51	0.40
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.43	0.40
1:A:256:VAL:O	1:A:260:ARG:HB2	2.21	0.40
1:A:273:LEU:O	1:A:276:THR:HG22	2.20	0.40
2:C:153:VAL:HG22	2:C:157:LEU:HD23	2.03	0.40
2:C:211:GLU:O	2:C:214:LYS:HG2	2.21	0.40
1:D:36:LEU:HD22	1:D:61:PHE:CE1	2.57	0.40
1:D:65:VAL:HA	1:D:66:PRO:HD3	1.92	0.40
1:D:68:VAL:CG1	1:D:72:GLU:HB2	2.49	0.40
1:D:101:SER:HB3	1:D:535:PHE:CE2	2.56	0.40
1:D:147:PHE:CE1	1:D:149:PHE:HE2	2.40	0.40
1:D:329:ASP:CB	1:D:339:ALA:HA	2.44	0.40
2:F:110:GLN:HG3	7:F:417:HOH:O	2.22	0.40
1:A:78:LYS:HE2	1:A:553:PRO:HG2	2.04	0.40
1:A:90:THR:O	2:B:143:PRO:HD3	2.21	0.40
1:A:201:ALA:O	1:A:205:HIS:ND1	2.50	0.40
1:A:290:LEU:O	1:A:293:ALA:N	2.54	0.40
1:A:428:ILE:HD13	7:A:1133:HOH:O	2.21	0.40
2:B:24:ARG:HE	2:B:198:SER:HG	1.62	0.40
2:B:133:LYS:HA	2:B:136:GLU:OE2	2.22	0.40
2:B:134:ILE:HG22	2:B:138:GLU:CD	2.47	0.40
1:D:105:GLN:C	1:D:107:ARG:H	2.30	0.40
1:D:120:ASN:CG	1:D:358:LEU:HD22	2.46	0.40
1:D:272:GLU:O	1:D:275:GLU:HB3	2.21	0.40
1:D:365:PRO:HG3	1:D:388:TYR:CZ	2.56	0.40
1:D:390:VAL:HG11	1:D:540:SER:OG	2.22	0.40
2:E:117:LYS:HB2	2:E:117:LYS:HE3	1.94	0.40
2:F:10:TYR:O	2:F:20:ARG:NH2	2.42	0.40
1:A:96:ALA:HB3	1:A:113:PHE:HB3	2.04	0.40
1:A:480:GLU:C	1:A:481:ILE:HD12	2.47	0.40
1:A:566:VAL:O	1:A:566:VAL:HG12	2.20	0.40
2:B:65:CYS:HB2	7:B:420:HOH:O	2.21	0.40
1:D:198:VAL:HG22	1:D:524:ALA:HB3	2.04	0.40
1:D:204:CYS:O	1:D:208:SER:OG	2.27	0.40
1:D:354:VAL:HG11	1:D:379:LEU:HD21	2.02	0.40
1:D:506:TYR:O	1:D:510:ARG:HB3	2.21	0.40
2:E:93:ALA:HB2	2:E:96:ARG:NH1	2.36	0.40
2:F:23:LEU:HB3	2:F:28:VAL:CG1	2.51	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:A:211:LEU:O	1:A:509:SER:OG[1_655]	1.76	0.44
1:A:270:ASN:O	1:A:511:LYS:NZ[1_655]	1.80	0.40
1:A:238:TRP:N	2:F:177:SER:OG[1_554]	1.91	0.29
7:B:427:HOH:O	7:C:482:HOH:O[1_455]	1.98	0.22
7:D:1210:HOH:O	7:E:581:HOH:O[1_655]	2.00	0.20
7:A:1075:HOH:O	7:B:533:HOH:O[1_545]	2.07	0.13
1:A:270:ASN:ND2	1:A:510:ARG:O[1_655]	2.10	0.10
1:D:270:ASN:ND2	1:D:510:ARG:O[1_655]	2.10	0.10
7:D:1071:HOH:O	7:D:1097:HOH:O[1_665]	2.11	0.09
7:B:476:HOH:O	7:C:503:HOH:O[1_455]	2.12	0.08
1:D:280:LYS:NZ	1:D:503:ASP:OD1[1_655]	2.12	0.08
1:A:22:ARG:NH2	2:B:173:PHE:O[1_545]	2.13	0.07
1:A:276:THR:OG1	1:A:501:PHE:O[1_655]	2.13	0.07
7:A:1066:HOH:O	7:F:489:HOH:O[1_554]	2.13	0.07
7:A:1159:HOH:O	7:A:1172:HOH:O[1_565]	2.13	0.07
7:B:502:HOH:O	7:C:527:HOH:O[1_455]	2.13	0.07
7:A:1161:HOH:O	7:A:1200:HOH:O[1_565]	2.15	0.05
7:D:953:HOH:O	7:D:1024:HOH:O[1_655]	2.15	0.05
2:C:140:GLY:O	1:D:246:LYS:NZ[1_455]	2.17	0.03
7:D:1019:HOH:O	7:D:1095:HOH:O[1_565]	2.17	0.03
2:C:141:ASP:OD2	1:D:278:ARG:NH2[1_455]	2.18	0.02
1:D:270:ASN:O	1:D:511:LYS:NZ[1_655]	2.18	0.02

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%)	513 (90%)	41 (7%)	13 (2%)	5 1
1	D	567/575 (99%)	504 (89%)	53 (9%)	10 (2%)	6 1
2	B	212/223 (95%)	197 (93%)	12 (6%)	3 (1%)	9 2
2	C	212/223 (95%)	193 (91%)	15 (7%)	4 (2%)	6 1
2	E	212/223 (95%)	192 (91%)	18 (8%)	2 (1%)	14 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	212/223 (95%)	191 (90%)	14 (7%)	7 (3%)	3 0
All	All	1982/2042 (97%)	1790 (90%)	153 (8%)	39 (2%)	6 1

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	ILE
1	A	540	SER
1	D	433	ILE
1	D	540	SER
1	D	542	ALA
2	F	177	SER
2	F	180	PRO
1	A	166	THR
1	A	437	THR
1	A	566	VAL
2	C	140	GLY
1	D	53	ASN
1	D	437	THR
1	D	566	VAL
2	F	140	GLY
2	F	174	SER
1	A	54	ALA
1	A	92	HIS
1	A	368	GLU
2	B	26	LYS
2	B	140	GLY
1	D	368	GLU
1	D	574	ALA
2	F	66	GLU
1	A	105	GLN
1	A	329	ASP
2	B	79	PRO
1	D	369	THR
2	F	172	ASN
1	A	85	THR
2	C	66	GLU
2	C	180	PRO
1	D	553	PRO
1	A	509	SER
2	F	27	GLY
1	A	296	PRO

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Mol	Chain	Res	Type
2	E	27	GLY
2	E	79	PRO
2	C	12	PRO

5.3.2 Protein sidechains [i](#)

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%)	449 (90%)	50 (10%)	7	1
1	D	499/505 (99%)	446 (89%)	53 (11%)	6	1
2	B	187/195 (96%)	178 (95%)	9 (5%)	23	4
2	C	187/195 (96%)	169 (90%)	18 (10%)	8	1
2	E	187/195 (96%)	175 (94%)	12 (6%)	16	2
2	F	187/195 (96%)	166 (89%)	21 (11%)	6	1
All	All	1746/1790 (98%)	1583 (91%)	163 (9%)	8	1

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	26	GLN
1	A	37	LEU
1	A	43	ILE
1	A	55	THR
1	A	90	THR
1	A	103	THR
1	A	110	PHE
1	A	111	ILE
1	A	116	GLU
1	A	122	LEU
1	A	125	PHE
1	A	134	ARG
1	A	152	LYS
1	A	154	TYR

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Mol	Chain	Res	Type
1	A	156	SER
1	A	162	VAL
1	A	184	SER
1	A	202	LEU
1	A	207	LEU
1	A	235	GLU
1	A	276	THR
1	A	277	ILE
1	A	281	CYS
1	A	295	PHE
1	A	305	MET
1	A	313	VAL
1	A	357	ASN
1	A	390	VAL
1	A	403	LEU
1	A	410	ILE
1	A	416	THR
1	A	418	GLN
1	A	422	ILE
1	A	426	ASN
1	A	431	ILE
1	A	433	ILE
1	A	455	GLU
1	A	464	SER
1	A	468	VAL
1	A	479	TRP
1	A	499	ARG
1	A	502	ILE
1	A	509	SER
1	A	515	ILE
1	A	518	LEU
1	A	536	LEU
1	A	545	PHE
1	A	546	LYS
1	A	547	MET
2	B	65	CYS
2	B	110	GLN
2	B	113	VAL
2	B	138	GLU
2	B	149	SER
2	B	153	VAL
2	B	182	LEU

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Mol	Chain	Res	Type
2	B	183	ILE
2	B	211	GLU
2	C	32	TYR
2	C	43	LEU
2	C	45	LEU
2	C	50	ILE
2	C	64	VAL
2	C	72	GLN
2	C	74	VAL
2	C	133	LYS
2	C	134	ILE
2	C	135	LEU
2	C	139	LEU
2	C	157	LEU
2	C	175	ILE
2	C	176	GLU
2	C	183	ILE
2	C	187	LYS
2	C	204	LYS
2	C	206	VAL
1	D	25	HIS
1	D	46	GLN
1	D	68	VAL
1	D	77	ILE
1	D	78	LYS
1	D	81	VAL
1	D	85	THR
1	D	88	ILE
1	D	89	LEU
1	D	90	THR
1	D	92	HIS
1	D	99	LEU
1	D	110	PHE
1	D	125	PHE
1	D	148	ILE
1	D	150	SER
1	D	152	LYS
1	D	157	THR
1	D	187	CYS
1	D	202	LEU
1	D	210	ILE
1	D	222	VAL

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Mol	Chain	Res	Type
1	D	241	ILE
1	D	242	VAL
1	D	245	ILE
1	D	250	LEU
1	D	254	ILE
1	D	273	LEU
1	D	326	VAL
1	D	329	ASP
1	D	384	ILE
1	D	398	LEU
1	D	405	ASP
1	D	408	LYS
1	D	410	ILE
1	D	416	THR
1	D	422	ILE
1	D	423	CYS
1	D	424	ARG
1	D	431	ILE
1	D	433	ILE
1	D	458	GLU
1	D	468	VAL
1	D	477	ILE
1	D	502	ILE
1	D	507	VAL
1	D	510	ARG
1	D	513	LYS
1	D	532	GLN
1	D	546	LYS
1	D	551	VAL
1	D	552	LYS
1	D	566	VAL
2	E	4	LEU
2	E	6	ILE
2	E	26	LYS
2	E	54	ILE
2	E	70	VAL
2	E	81	LYS
2	E	87	SER
2	E	116	LYS
2	E	132	VAL
2	E	139	LEU
2	E	148	ASP

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Mol	Chain	Res	Type
2	E	183	ILE
2	F	32	TYR
2	F	43	LEU
2	F	50	ILE
2	F	64	VAL
2	F	65	CYS
2	F	71	VAL
2	F	72	GLN
2	F	80	GLU
2	F	84	PHE
2	F	117	LYS
2	F	134	ILE
2	F	135	LEU
2	F	139	LEU
2	F	157	LEU
2	F	172	ASN
2	F	175	ILE
2	F	178	GLU
2	F	202	SER
2	F	206	VAL
2	F	211	GLU
2	F	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	217	GLN
1	A	357	ASN
1	A	394	ASN
1	A	491	GLN
2	B	48	ASN
2	B	60	ASN
2	B	165	GLN
2	C	60	ASN
2	C	216	ASN
1	D	172	ASN
1	D	205	HIS
1	D	236	GLN
1	D	318	HIS
1	D	565	ASN
2	F	110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GSH	F	301	-	18,19,19	1.56	3 (16%)	21,24,24	2.58	5 (23%)
3	JAA	A	601	-	15,15,15	5.29	7 (46%)	14,19,19	2.96	8 (57%)
5	GSH	B	301	-	18,19,19	1.49	3 (16%)	21,24,24	1.93	5 (23%)
5	GSH	E	301	-	18,19,19	1.47	4 (22%)	21,24,24	2.49	5 (23%)
3	JAA	D	601	6	15,15,15	5.29	6 (40%)	14,19,19	3.28	10 (71%)
4	VAL	A	602	-	6,7,7	0.97	1 (16%)	8,9,9	1.53	1 (12%)
5	GSH	C	301	-	18,19,19	1.59	4 (22%)	21,24,24	3.03	8 (38%)
4	VAL	D	602	-	6,7,7	1.09	1 (16%)	8,9,9	0.99	1 (12%)

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
5	GSH	F	301	-	-	2/24/24/24	-
3	JAA	A	601	-	-	3/9/22/22	0/1/1/1
5	GSH	B	301	-	-	6/24/24/24	-
5	GSH	E	301	-	-	10/24/24/24	-
3	JAA	D	601	6	-	4/9/22/22	0/1/1/1
4	VAL	A	602	-	-	5/8/8/8	-
5	GSH	C	301	-	-	7/24/24/24	-
4	VAL	D	602	-	-	1/8/8/8	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JAA	C05-C08	-13.04	1.31	1.52
3	D	601	JAA	C05-C08	-12.78	1.31	1.52
3	A	601	JAA	C06-C04	-11.89	1.23	1.53
3	D	601	JAA	C06-C04	-11.75	1.24	1.53
3	D	601	JAA	C07-C08	6.34	1.61	1.51
3	A	601	JAA	C07-C08	5.94	1.60	1.51
3	D	601	JAA	C05-C04	4.93	1.66	1.54
3	D	601	JAA	C10-C04	-4.83	1.45	1.53
3	A	601	JAA	C05-C04	4.82	1.66	1.54
3	A	601	JAA	C10-C04	-4.60	1.45	1.53
3	D	601	JAA	C09-C05	-4.46	1.48	1.54
3	A	601	JAA	C09-C05	-4.00	1.48	1.54
5	F	301	GSH	CA2-N2	-3.38	1.38	1.45
5	C	301	GSH	CA2-N2	-3.21	1.39	1.45
5	B	301	GSH	C2-N3	3.12	1.41	1.33
5	E	301	GSH	CA2-N2	-3.07	1.39	1.45
5	E	301	GSH	C2-N3	3.04	1.40	1.33
5	B	301	GSH	CD1-N2	2.86	1.40	1.34
5	B	301	GSH	CA2-N2	-2.63	1.40	1.45
5	F	301	GSH	C2-N3	2.61	1.39	1.33
5	C	301	GSH	C2-N3	2.53	1.39	1.33
4	D	602	VAL	OXT-C	-2.38	1.23	1.30
5	C	301	GSH	CD1-N2	2.37	1.39	1.34
5	E	301	GSH	CD1-N2	2.32	1.38	1.34
4	A	602	VAL	OXT-C	-2.12	1.23	1.30
5	F	301	GSH	CD1-N2	2.11	1.38	1.34
3	A	601	JAA	O03-C12	-2.07	1.24	1.30
5	C	301	GSH	O11-C1	-2.01	1.24	1.30
5	E	301	GSH	CB2-CA2	-2.01	1.50	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	GSH	CA2-CB2-SG2	-9.93	102.97	114.16
5	F	301	GSH	CA2-CB2-SG2	-9.21	103.78	114.16
5	E	301	GSH	CA2-CB2-SG2	-6.62	106.70	114.16
3	D	601	JAA	C07-C06-C04	-6.25	97.85	104.45
5	B	301	GSH	CA2-CB2-SG2	-6.11	107.28	114.16
5	E	301	GSH	CB2-CA2-N2	-6.02	102.70	111.28
3	D	601	JAA	C09-C11-C13	-5.70	105.26	126.21
3	A	601	JAA	O01-C08-C05	5.04	132.05	125.60
3	A	601	JAA	C09-C11-C13	-4.67	109.04	126.21
5	F	301	GSH	CB2-CA2-N2	-4.65	104.65	111.28
5	C	301	GSH	CB2-CA2-N2	-4.59	104.74	111.28
3	A	601	JAA	C07-C08-C05	-4.29	102.01	109.06
5	C	301	GSH	CG1-CD1-N2	-4.02	108.79	115.86
3	A	601	JAA	O03-C12-C10	3.93	126.20	114.00
3	A	601	JAA	C06-C04-C10	-3.85	106.24	113.41
5	C	301	GSH	CB1-CG1-CD1	3.61	121.12	113.06
3	D	601	JAA	O01-C08-C05	3.56	130.15	125.60
5	E	301	GSH	CB1-CG1-CD1	3.55	120.97	113.06
3	D	601	JAA	O03-C12-C10	3.52	124.95	114.00
4	A	602	VAL	OXT-C-O	-3.46	116.23	124.08
5	C	301	GSH	CG1-CB1-CA1	-3.45	105.94	113.86
5	E	301	GSH	CG1-CD1-N2	-3.45	109.79	115.86
3	D	601	JAA	C07-C08-C05	-3.18	103.84	109.06
5	C	301	GSH	C2-CA2-N2	-3.16	102.57	111.11
3	D	601	JAA	C06-C07-C08	-3.10	102.32	105.39
3	D	601	JAA	C06-C04-C10	-3.07	107.69	113.41
3	A	601	JAA	O02-C12-C10	-3.02	113.56	122.84
3	D	601	JAA	C04-C10-C12	-2.91	107.43	113.33
3	A	601	JAA	C14-C13-C11	-2.89	109.03	126.42
5	F	301	GSH	C3-CA3-N3	-2.78	104.42	113.06
5	C	301	GSH	OE1-CD1-CG1	2.78	127.05	122.02
5	B	301	GSH	C2-CA2-N2	-2.69	103.83	111.11
3	D	601	JAA	O02-C12-C10	-2.67	114.65	122.84
5	F	301	GSH	CG1-CD1-N2	-2.57	111.34	115.86
5	E	301	GSH	OE1-CD1-CG1	2.52	126.58	122.02
3	D	601	JAA	C14-C13-C11	-2.48	111.49	126.42
5	B	301	GSH	CB2-CA2-N2	-2.41	107.84	111.28
4	D	602	VAL	OXT-C-O	-2.34	118.78	124.08
5	B	301	GSH	CB1-CG1-CD1	2.24	118.06	113.06
5	C	301	GSH	CA3-N3-C2	-2.15	115.95	121.38
3	A	601	JAA	C07-C06-C04	-2.08	102.26	104.45
5	B	301	GSH	CG1-CD1-N2	-2.05	112.25	115.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	301	GSH	C2-CA2-N2	-2.03	105.62	111.11

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	VAL	OXT-C-CA-N
4	A	602	VAL	N-CA-CB-CG1
4	A	602	VAL	N-CA-CB-CG2
4	A	602	VAL	C-CA-CB-CG1
4	A	602	VAL	C-CA-CB-CG2
5	B	301	GSH	N1-CA1-CB1-CG1
5	B	301	GSH	C1-CA1-CB1-CG1
5	B	301	GSH	C2-CA2-CB2-SG2
5	C	301	GSH	N2-CA2-CB2-SG2
5	C	301	GSH	C2-CA2-CB2-SG2
5	E	301	GSH	N2-CA2-CB2-SG2
5	E	301	GSH	C2-CA2-CB2-SG2
5	F	301	GSH	N2-CA2-CB2-SG2
5	F	301	GSH	C2-CA2-CB2-SG2
3	D	601	JAA	C09-C11-C13-C14
3	A	601	JAA	C09-C11-C13-C14
5	C	301	GSH	CA1-CB1-CG1-CD1
5	E	301	GSH	O31-C3-CA3-N3
5	C	301	GSH	O11-C1-CA1-N1
5	E	301	GSH	CA1-CB1-CG1-CD1
5	E	301	GSH	O32-C3-CA3-N3
3	D	601	JAA	C11-C13-C14-C15
5	B	301	GSH	O32-C3-CA3-N3
5	C	301	GSH	O12-C1-CA1-N1
3	D	601	JAA	C04-C05-C09-C11
5	B	301	GSH	O31-C3-CA3-N3
3	A	601	JAA	C05-C09-C11-C13
5	E	301	GSH	C1-CA1-CB1-CG1
3	D	601	JAA	C08-C05-C09-C11
5	B	301	GSH	N2-CA2-CB2-SG2
5	C	301	GSH	O31-C3-CA3-N3
5	E	301	GSH	OE1-CD1-CG1-CB1
5	E	301	GSH	C3-CA3-N3-C2
5	E	301	GSH	N2-CD1-CG1-CB1
5	C	301	GSH	O32-C3-CA3-N3
4	D	602	VAL	C-CA-CB-CG2

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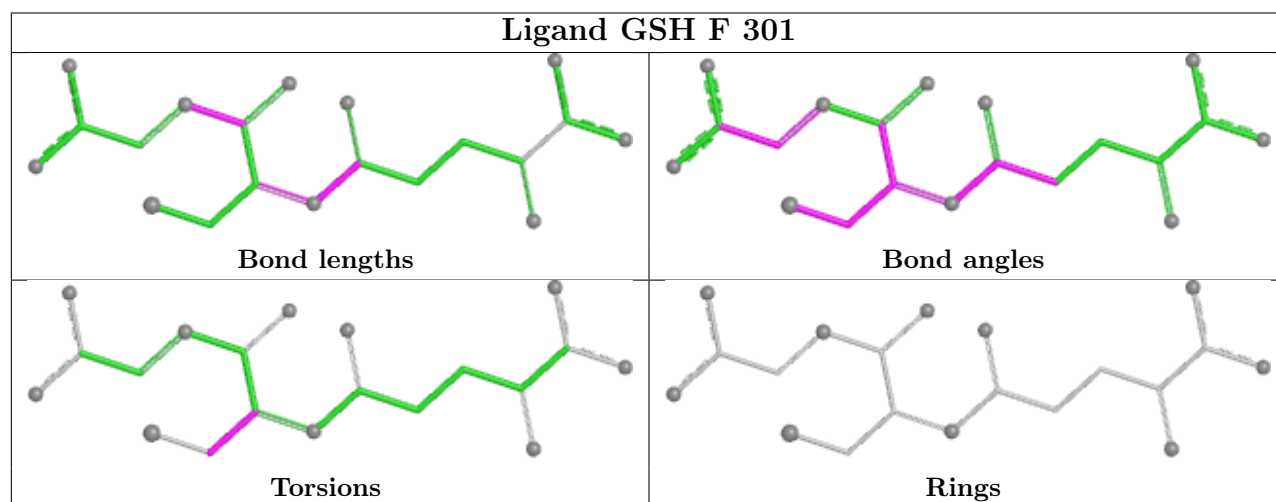
Mol	Chain	Res	Type	Atoms
5	E	301	GSH	O2-C2-CA2-N2
3	A	601	JAA	C04-C10-C12-O03

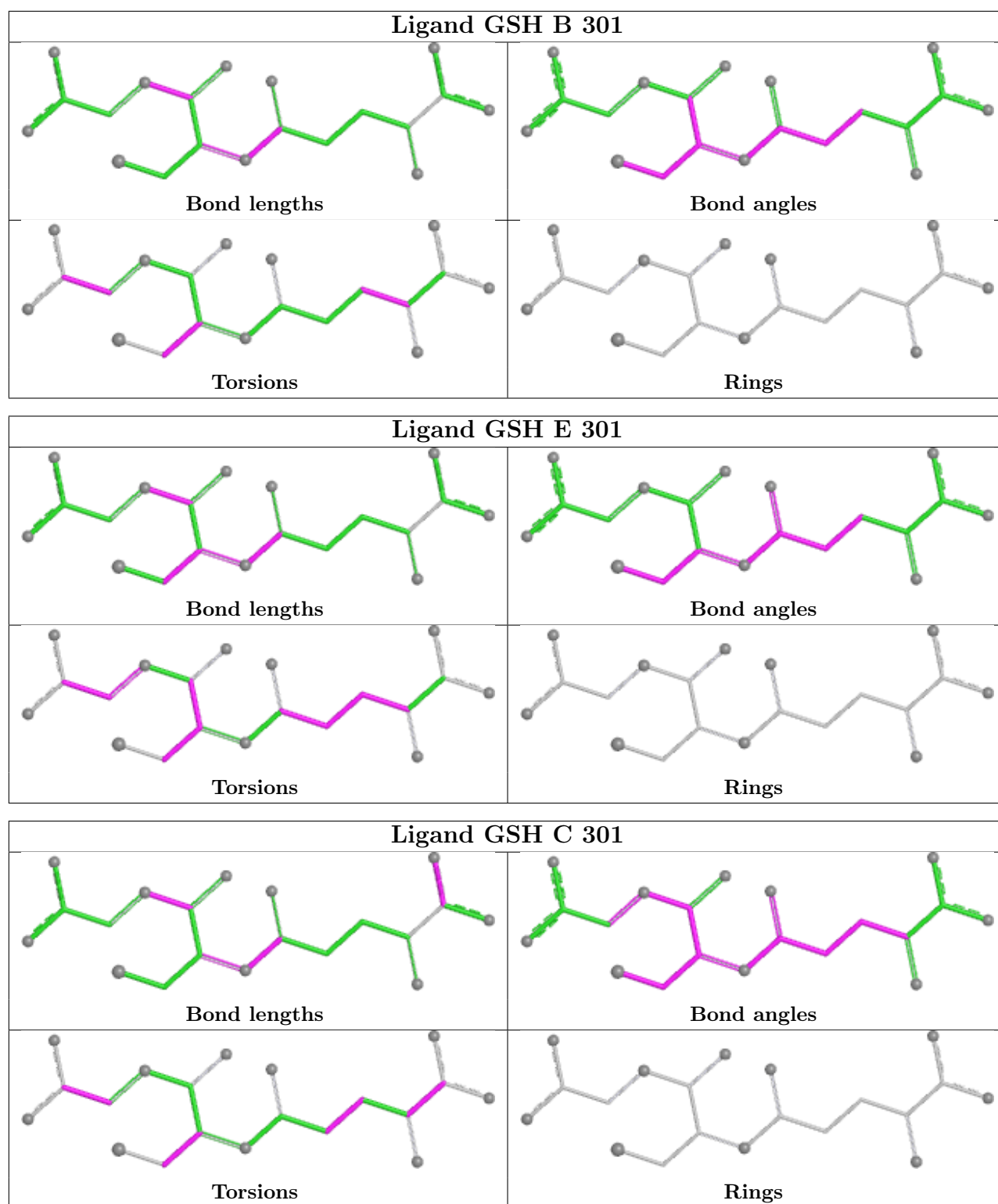
There are no ring outliers.

8 monomers are involved in 21 short contacts:

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

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	569/575 (98%)	2.85	388 (68%) 0 0	5, 17, 25, 32	0
1	D	569/575 (98%)	2.10	286 (50%) 0 0	4, 12, 19, 26	0
2	B	214/223 (95%)	1.94	84 (39%) 1 1	6, 13, 21, 28	0
2	C	214/223 (95%)	1.37	52 (24%) 2 3	3, 7, 11, 18	0
2	E	214/223 (95%)	2.12	113 (52%) 0 0	7, 12, 20, 26	0
2	F	214/223 (95%)	1.56	53 (24%) 2 3	4, 9, 14, 22	0
All	All	1994/2042 (97%)	2.16	976 (48%) 0 1	3, 12, 22, 32	0

All (976) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	174	SER	9.2
2	E	97	PHE	9.1
1	A	27	VAL	9.0
1	A	515	ILE	9.0
1	D	161	PRO	8.6
1	A	432	ASN	8.3
1	A	294	LEU	8.2
2	B	139	LEU	8.1
2	E	95	ALA	8.0
1	A	202	LEU	7.7
1	A	429	LEU	7.5
2	F	176	GLU	7.4
1	A	66	PRO	7.4
1	A	36	LEU	7.2
1	D	566	VAL	7.2
1	A	274	ALA	7.2
1	A	35	ILE	6.9
1	A	210	ILE	6.9
1	A	17	PHE	6.9

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Mol	Chain	Res	Type	RSRZ
2	C	90	TYR	6.8
1	A	279	THR	6.7
1	A	38	LYS	6.7
1	A	287	TRP	6.6
2	B	140	GLY	6.6
1	A	238	TRP	6.6
2	B	123	ALA	6.6
1	A	538	LEU	6.4
1	A	523	VAL	6.3
1	A	65	VAL	6.3
1	A	284	LEU	6.2
1	A	104	SER	6.2
2	F	172	ASN	6.2
2	F	180	PRO	6.1
2	B	175	ILE	6.1
1	A	305	MET	6.0
1	D	409	VAL	6.0
1	A	556	ALA	5.9
2	E	124	GLY	5.9
1	A	145	LEU	5.9
1	A	346	SER	5.9
1	D	398	LEU	5.9
1	A	459	VAL	5.9
1	D	397	GLY	5.9
1	A	37	LEU	5.8
1	A	237	VAL	5.8
1	A	531	ILE	5.8
1	D	361	PHE	5.8
1	A	354	VAL	5.7
1	A	106	GLY	5.7
1	A	506	TYR	5.7
2	E	63	PRO	5.7
1	A	14	ILE	5.6
2	F	177	SER	5.5
1	A	113	PHE	5.5
1	A	309	MET	5.5
1	A	468	VAL	5.4
1	A	181	SER	5.4
1	A	313	VAL	5.4
1	D	160	VAL	5.4
2	E	71	VAL	5.4
2	B	183	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	507	VAL	5.3
1	A	125	PHE	5.3
1	A	13	VAL	5.2
1	A	406	VAL	5.2
2	F	165	GLN	5.2
1	A	497	LEU	5.2
1	A	500	ALA	5.2
2	E	74	VAL	5.2
1	D	203	TYR	5.2
2	F	179	SER	5.2
1	A	536	LEU	5.1
1	A	110	PHE	5.1
1	D	506	TYR	5.1
1	A	563	CYS	5.1
1	D	274	ALA	5.1
1	A	423	CYS	5.0
2	B	185	TRP	5.0
1	A	67	LEU	5.0
1	D	466	ILE	5.0
1	A	220	PHE	5.0
1	A	19	GLU	5.0
1	A	546	LYS	4.9
1	A	464	SER	4.9
1	D	517	ALA	4.9
1	A	295	PHE	4.9
1	A	535	PHE	4.9
2	F	173	PHE	4.9
1	A	169	VAL	4.9
2	B	132	VAL	4.9
1	D	163	GLY	4.9
1	D	288	TYR	4.9
1	D	475	TYR	4.9
1	A	323	LEU	4.9
1	D	457	ILE	4.9
1	D	114	THR	4.8
1	D	167	THR	4.8
1	D	162	VAL	4.8
1	A	170	TYR	4.8
1	A	392	ILE	4.8
1	A	28	GLN	4.8
1	A	469	SER	4.8
1	A	460	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	330	TYR	4.7
2	B	166	ALA	4.7
1	A	108	PRO	4.7
2	B	153	VAL	4.7
1	A	475	TYR	4.7
1	A	241	ILE	4.7
1	D	46	GLN	4.7
1	A	545	PHE	4.7
1	A	154	TYR	4.6
1	A	301	VAL	4.6
1	A	561	ILE	4.6
2	F	68	LEU	4.6
1	D	271	PRO	4.6
1	A	75	PRO	4.6
1	A	136	PHE	4.5
1	A	116	GLU	4.5
1	D	202	LEU	4.5
2	E	44	LEU	4.5
1	A	355	ILE	4.5
2	C	10	TYR	4.5
1	A	311	PRO	4.5
1	A	21	THR	4.5
1	A	214	ASP	4.5
1	A	312	TYR	4.5
1	D	523	VAL	4.5
2	C	193	GLU	4.5
1	A	325	LEU	4.5
2	B	86	PRO	4.4
1	A	290	LEU	4.4
1	D	89	LEU	4.4
1	A	42	ALA	4.4
2	E	109	ALA	4.4
1	A	233	THR	4.4
1	A	433	ILE	4.4
1	D	516	GLY	4.4
1	A	234	PHE	4.4
1	D	507	VAL	4.4
1	D	512	CYS	4.4
1	D	76	TYR	4.4
2	E	10	TYR	4.4
1	A	129	PHE	4.4
1	A	231	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
2	E	64	VAL	4.4
1	A	379	LEU	4.4
1	A	321	GLY	4.4
2	E	91	GLY	4.4
1	A	428	ILE	4.4
1	D	77	ILE	4.4
1	D	515	ILE	4.4
1	A	548	PRO	4.3
1	A	149	PHE	4.3
1	A	103	THR	4.3
1	A	242	VAL	4.3
1	A	326	VAL	4.3
1	A	395	TYR	4.3
2	B	60	ASN	4.3
1	A	217	GLN	4.3
1	A	277	ILE	4.3
1	A	98	SER	4.3
1	A	122	LEU	4.3
2	E	206	VAL	4.3
1	A	512	CYS	4.3
1	A	166	THR	4.2
2	F	208	TYR	4.2
1	A	211	LEU	4.2
1	D	548	PRO	4.2
1	D	335	GLY	4.2
2	E	98	TRP	4.2
1	A	457	ILE	4.2
1	A	198	VAL	4.2
1	D	178	GLY	4.2
2	E	61	GLY	4.2
2	F	171	GLY	4.2
1	D	155	ILE	4.2
1	D	481	ILE	4.2
1	A	276	THR	4.2
1	A	339	ALA	4.1
1	A	322	ASP	4.1
1	A	553	PRO	4.1
2	E	70	VAL	4.1
1	D	182	ILE	4.1
1	D	262	ALA	4.1
1	A	91	GLY	4.1
1	D	113	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	550	CYS	4.1
1	D	428	ILE	4.1
1	D	165	ALA	4.1
1	A	341	VAL	4.1
1	D	192	VAL	4.1
1	D	249	VAL	4.1
1	A	502	ILE	4.1
2	E	50	ILE	4.1
1	A	93	PRO	4.0
2	B	174	SER	4.0
1	D	522	VAL	4.0
1	A	148	ILE	4.0
1	A	431	ILE	4.0
1	D	337	ILE	4.0
1	A	407	VAL	4.0
2	B	186	ALA	4.0
2	E	175	ILE	4.0
1	A	33	LYS	4.0
1	D	495	ASN	4.0
2	C	68	LEU	4.0
1	D	287	TRP	4.0
1	A	352	PHE	4.0
2	E	173	PHE	4.0
1	D	65	VAL	4.0
1	A	83	GLY	4.0
2	C	147	GLY	4.0
2	F	175	ILE	3.9
2	B	78	TRP	3.9
1	A	257	PRO	3.9
1	D	111	ILE	3.9
2	B	135	LEU	3.9
2	E	54	ILE	3.9
1	A	124	LEU	3.9
1	A	282	MET	3.9
1	A	60	ALA	3.9
1	A	382	VAL	3.8
1	A	558	VAL	3.8
1	A	123	GLN	3.8
1	A	505	GLY	3.8
1	A	54	ALA	3.8
1	A	96	ALA	3.8
1	A	203	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	353	ALA	3.8
2	E	22	ALA	3.8
1	A	189	PRO	3.8
2	E	101	PHE	3.8
1	A	560	GLN	3.8
1	A	216	VAL	3.8
1	D	479	TRP	3.8
2	B	206	VAL	3.8
1	A	526	GLY	3.8
2	E	27	GLY	3.8
1	A	273	LEU	3.8
1	A	57	PRO	3.8
2	E	90	TYR	3.8
1	A	426	ASN	3.8
2	F	183	ILE	3.8
1	A	377	VAL	3.7
1	A	403	LEU	3.7
1	A	230	ALA	3.7
1	A	477	ILE	3.7
1	D	149	PHE	3.7
1	D	571	PHE	3.7
1	D	259	VAL	3.7
1	D	459	VAL	3.7
2	E	49	PRO	3.7
1	A	130	ALA	3.7
2	F	114	TRP	3.7
1	D	55	THR	3.7
1	A	92	HIS	3.7
1	A	390	VAL	3.7
2	B	70	VAL	3.7
1	A	293	ALA	3.7
1	A	559	LEU	3.7
1	D	476	ALA	3.7
1	D	538	LEU	3.7
2	F	99	ALA	3.7
2	B	136	GLU	3.7
2	E	32	TYR	3.7
1	D	208	SER	3.7
2	E	158	ILE	3.6
2	F	97	PHE	3.6
1	D	567	VAL	3.6
1	A	345	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	20	MET	3.6
1	A	324	PRO	3.6
1	D	347	PRO	3.6
2	E	93	ALA	3.6
2	F	72	GLN	3.6
2	F	98	TRP	3.6
2	B	120	GLU	3.6
1	A	342	THR	3.6
1	A	501	PHE	3.6
2	E	30	PHE	3.6
1	A	465	TYR	3.6
1	A	90	THR	3.5
1	A	357	ASN	3.5
1	A	393	THR	3.5
2	B	137	SER	3.5
1	A	304	ILE	3.5
1	A	209	GLY	3.5
1	A	223	PHE	3.5
1	D	545	PHE	3.5
2	B	173	PHE	3.5
2	B	209	ALA	3.5
1	D	562	LEU	3.5
1	A	503	ASP	3.5
1	D	304	ILE	3.5
1	D	462	PHE	3.5
2	E	150	PHE	3.5
1	D	71	VAL	3.5
1	D	445	VAL	3.5
1	D	518	LEU	3.5
1	A	281	CYS	3.5
1	D	563	CYS	3.5
2	B	172	ASN	3.5
1	A	327	SER	3.5
1	A	508	SER	3.5
1	A	360	TYR	3.5
1	D	261	THR	3.5
2	C	32	TYR	3.5
1	A	128	ALA	3.5
1	D	502	ILE	3.5
1	D	250	LEU	3.5
1	A	222	VAL	3.5
2	F	216	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	550	CYS	3.5
1	A	292	PRO	3.5
2	F	90	TYR	3.5
1	A	109	LYS	3.4
1	A	361	PHE	3.4
1	A	358	LEU	3.4
1	D	122	LEU	3.4
1	D	173	PRO	3.4
2	E	73	TYR	3.4
2	B	134	ILE	3.4
2	B	202	SER	3.4
2	E	134	ILE	3.4
2	B	101	PHE	3.4
1	A	259	VAL	3.4
1	A	445	VAL	3.4
1	D	27	VAL	3.4
1	A	404	GLY	3.4
1	D	465	TYR	3.4
2	B	184	ALA	3.4
1	D	561	ILE	3.4
2	B	133	LYS	3.4
1	A	528	PHE	3.4
1	D	32	LEU	3.4
1	D	124	LEU	3.4
2	B	170	PHE	3.4
2	E	43	LEU	3.4
1	D	69	THR	3.4
1	D	222	VAL	3.4
2	B	64	VAL	3.4
1	D	196	PRO	3.4
2	B	180	PRO	3.4
1	A	201	ALA	3.3
1	D	353	ALA	3.3
2	C	123	ALA	3.3
2	E	123	ALA	3.3
1	D	413	TYR	3.3
1	A	335	GLY	3.3
1	D	103	THR	3.3
1	D	48	CYS	3.3
1	D	198	VAL	3.3
1	D	313	VAL	3.3
1	A	63	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	29	LYS	3.3
1	D	320	ALA	3.3
1	D	205	HIS	3.3
1	A	388	TYR	3.3
1	A	232	ARG	3.3
1	A	245	ILE	3.3
1	A	316	LEU	3.3
1	A	412	PHE	3.3
2	C	153	VAL	3.3
1	A	144	ALA	3.3
2	E	99	ALA	3.3
1	D	521	ARG	3.3
1	A	454	GLU	3.3
1	D	148	ILE	3.3
1	D	431	ILE	3.3
1	A	32	LEU	3.3
1	A	419	LEU	3.3
2	E	57	LEU	3.3
1	A	147	PHE	3.3
1	D	42	ALA	3.3
1	D	47	ASN	3.3
1	A	516	GLY	3.2
1	A	288	TYR	3.2
2	B	32	TYR	3.2
2	F	73	TYR	3.2
1	A	183	THR	3.2
1	D	510	ARG	3.2
2	C	44	LEU	3.2
2	F	157	LEU	3.2
1	D	110	PHE	3.2
1	D	575	PHE	3.2
1	D	94	VAL	3.2
1	A	537	GLY	3.2
1	A	236	GLN	3.2
2	B	167	TYR	3.2
1	A	161	PRO	3.2
1	D	421	PHE	3.2
2	B	37	PHE	3.2
1	A	24	ALA	3.2
1	A	163	GLY	3.2
2	E	151	GLY	3.2
2	F	184	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	195	SER	3.2
1	D	169	VAL	3.2
1	A	380	THR	3.2
1	D	380	THR	3.2
1	D	154	TYR	3.2
1	D	399	TYR	3.2
2	B	129	ILE	3.2
2	E	11	TRP	3.2
1	A	61	PHE	3.2
1	A	131	PHE	3.2
1	D	147	PHE	3.2
2	B	145	PHE	3.2
1	A	71	VAL	3.2
1	D	366	VAL	3.2
2	F	132	VAL	3.2
2	F	153	VAL	3.2
1	A	34	GLU	3.2
2	E	14	MET	3.1
1	A	413	TYR	3.1
2	C	83	PRO	3.1
1	A	45	LEU	3.1
1	A	73	LEU	3.1
1	D	37	LEU	3.1
1	D	403	LEU	3.1
1	A	204	CYS	3.1
2	B	93	ALA	3.1
1	D	528	PHE	3.1
1	A	127	THR	3.1
1	D	166	THR	3.1
1	A	394	ASN	3.1
2	E	102	VAL	3.1
1	A	44	TYR	3.1
1	A	218	TYR	3.1
1	A	482	SER	3.1
2	B	141	ASP	3.1
1	A	328	HIS	3.1
1	A	466	ILE	3.1
2	E	51	HIS	3.1
1	A	518	LEU	3.1
1	A	562	LEU	3.1
2	E	65	CYS	3.1
1	A	212	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	421	PHE	3.1
2	E	60	ASN	3.1
1	A	68	VAL	3.1
1	D	472	PRO	3.1
1	A	453	SER	3.1
2	B	177	SER	3.1
1	D	247	ASP	3.1
2	F	10	TYR	3.1
1	D	385	GLY	3.1
2	B	16	GLY	3.1
1	A	43	ILE	3.1
1	A	111	ILE	3.1
1	A	48	CYS	3.1
1	A	167	THR	3.1
1	D	220	PHE	3.1
1	D	478	PHE	3.1
2	B	164	PHE	3.1
2	F	111	PHE	3.1
1	D	492	ASP	3.1
2	B	98	TRP	3.0
2	B	114	TRP	3.0
2	E	21	VAL	3.0
1	D	170	TYR	3.0
1	D	88	ILE	3.0
1	A	338	ALA	3.0
1	D	201	ALA	3.0
1	D	221	ALA	3.0
1	D	501	PHE	3.0
1	D	112	PRO	3.0
2	E	132	VAL	3.0
1	D	53	ASN	3.0
1	A	99	LEU	3.0
1	A	254	ILE	3.0
1	A	337	ILE	3.0
1	A	476	ALA	3.0
1	A	485	THR	3.0
1	D	24	ALA	3.0
1	D	207	LEU	3.0
1	D	351	THR	3.0
1	D	464	SER	3.0
1	A	175	PHE	3.0
1	D	378	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	171	GLY	3.0
1	A	489	VAL	3.0
2	C	73	TYR	3.0
1	A	18	ASP	3.0
1	A	333	SER	3.0
1	D	573	THR	3.0
2	E	107	THR	3.0
1	A	441	LEU	3.0
1	D	392	ILE	3.0
1	D	520	LEU	3.0
2	B	182	LEU	3.0
2	F	182	LEU	3.0
2	E	42	PRO	3.0
1	D	468	VAL	2.9
1	A	544	GLN	2.9
1	A	499	ARG	2.9
1	A	514	THR	2.9
1	A	504	ALA	2.9
1	D	556	ALA	2.9
2	E	210	ALA	2.9
1	D	336	TRP	2.9
2	C	76	GLU	2.9
1	D	117	LEU	2.9
2	F	135	LEU	2.9
1	A	182	ILE	2.9
1	D	254	ILE	2.9
1	D	277	ILE	2.9
2	E	6	ILE	2.9
1	D	23	ASN	2.9
2	B	63	PRO	2.9
2	B	200	PRO	2.9
1	D	498	ASP	2.9
2	C	179	SER	2.9
2	F	64	VAL	2.9
1	A	177	ALA	2.9
1	A	120	ASN	2.9
1	D	44	TYR	2.9
1	D	218	TYR	2.9
1	A	227	LEU	2.9
1	D	66	PRO	2.9
1	D	499	ARG	2.9
1	D	127	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	300	TYR	2.9
1	A	302	TYR	2.9
2	E	144	TYR	2.9
2	C	33	ARG	2.9
1	A	207	LEU	2.9
1	A	443	LEU	2.9
1	A	481	ILE	2.9
2	E	66	GLU	2.9
2	E	180	PRO	2.9
2	E	13	SER	2.9
2	B	163	TRP	2.9
1	A	8	PHE	2.8
1	D	85	THR	2.8
1	D	242	VAL	2.8
1	D	489	VAL	2.8
2	C	64	VAL	2.8
1	A	80	MET	2.8
1	A	554	SER	2.8
1	D	45	LEU	2.8
1	D	269	PRO	2.8
1	D	311	PRO	2.8
1	D	241	ILE	2.8
1	A	479	TRP	2.8
1	D	116	GLU	2.8
2	C	176	GLU	2.8
1	A	226	GLY	2.8
1	D	144	ALA	2.8
1	D	293	ALA	2.8
2	F	77	ALA	2.8
1	D	216	VAL	2.8
2	B	13	SER	2.8
1	A	95	PRO	2.8
1	D	108	PRO	2.8
1	D	429	LEU	2.8
1	D	494	CYS	2.8
1	A	88	ILE	2.8
1	A	168	ASN	2.8
1	A	213	ARG	2.8
1	A	278	ARG	2.8
2	B	158	ILE	2.8
1	A	142	GLY	2.8
1	A	289	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	359	GLY	2.8
1	A	100	SER	2.8
1	D	17	PHE	2.8
1	D	129	PHE	2.8
1	D	194	PHE	2.8
1	D	308	SER	2.8
2	F	101	PHE	2.8
1	A	81	VAL	2.8
1	D	206	LEU	2.8
1	D	97	ILE	2.8
1	A	440	ASP	2.8
2	B	88	ASP	2.8
1	A	243	THR	2.8
1	D	157	THR	2.8
1	D	8	PHE	2.7
1	D	61	PHE	2.7
1	A	409	VAL	2.7
1	A	530	LYS	2.7
1	D	557	LYS	2.7
2	E	113	VAL	2.7
1	D	360	TYR	2.7
1	D	531	ILE	2.7
2	E	177	SER	2.7
1	D	49	GLY	2.7
1	A	286	ASN	2.7
2	E	77	ALA	2.7
1	D	535	PHE	2.7
2	E	84	PHE	2.7
2	C	28	VAL	2.7
1	A	494	CYS	2.7
1	D	183	THR	2.7
1	A	97	ILE	2.7
2	E	211	GLU	2.7
1	A	178	GLY	2.7
1	D	270	ASN	2.7
1	A	524	ALA	2.7
1	D	396	ALA	2.7
1	A	329	ASP	2.7
1	A	347	PRO	2.7
1	A	363	PHE	2.7
2	E	106	PHE	2.7
1	A	206	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	121	THR	2.7
1	D	204	CYS	2.7
1	D	514	THR	2.7
2	C	102	VAL	2.7
1	A	401	TYR	2.7
1	D	570	TYR	2.7
2	B	90	TYR	2.7
1	A	270	ASN	2.7
1	A	331	GLY	2.7
2	C	48	ASN	2.7
1	A	410	ILE	2.7
1	A	542	ALA	2.7
1	D	96	ALA	2.7
2	E	19	ALA	2.7
1	A	356	PRO	2.6
1	D	199	HIS	2.6
1	A	509	SER	2.6
1	A	478	PHE	2.6
1	D	363	PHE	2.6
2	E	85	PHE	2.6
1	A	39	ASN	2.6
1	A	414	ASN	2.6
1	D	306	THR	2.6
1	A	473	GLY	2.6
1	D	106	GLY	2.6
1	D	187	CYS	2.6
2	C	171	GLY	2.6
1	D	419	LEU	2.6
2	E	139	LEU	2.6
1	A	570	TYR	2.6
2	C	152	TYR	2.6
2	F	32	TYR	2.6
2	C	78	TRP	2.6
1	A	134	ARG	2.6
2	E	166	ALA	2.6
1	A	271	PRO	2.6
1	D	125	PHE	2.6
1	D	268	THR	2.6
1	D	295	PHE	2.6
2	B	151	GLY	2.6
2	B	160	PHE	2.6
1	A	427	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	36	LEU	2.6
1	D	219	VAL	2.6
1	D	460	ILE	2.6
1	A	208	SER	2.6
1	A	251	SER	2.6
1	D	500	ALA	2.6
1	D	508	SER	2.6
2	C	184	ALA	2.6
1	A	417	PRO	2.6
2	F	187	LYS	2.6
1	A	164	THR	2.6
1	A	510	ARG	2.6
1	A	235	GLU	2.6
1	D	90	THR	2.6
1	D	289	GLY	2.6
2	B	138	GLU	2.6
1	A	398	LEU	2.6
1	D	559	LEU	2.6
1	D	354	VAL	2.6
1	D	390	VAL	2.6
2	E	56	VAL	2.6
1	D	258	SER	2.6
1	D	309	MET	2.6
1	A	133	ASN	2.6
2	B	131	ALA	2.6
1	D	75	PRO	2.6
1	D	137	PRO	2.6
2	E	12	PRO	2.6
2	E	55	PRO	2.6
2	E	163	TRP	2.6
2	B	92	ARG	2.6
2	F	178	GLU	2.6
1	D	255	THR	2.5
2	E	159	THR	2.5
1	A	26	GLN	2.5
1	A	50	LEU	2.5
1	A	490	LEU	2.5
1	A	171	ARG	2.5
1	D	551	VAL	2.5
1	D	558	VAL	2.5
2	E	58	VAL	2.5
1	D	291	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	183	ILE	2.5
2	B	207	ALA	2.5
2	C	49	PRO	2.5
1	A	461	ASP	2.5
1	A	31	THR	2.5
1	D	527	THR	2.5
2	C	185	TRP	2.5
1	A	332	SER	2.5
1	A	458	GLU	2.5
1	A	194	PHE	2.5
2	C	101	PHE	2.5
2	C	135	LEU	2.5
2	E	45	LEU	2.5
2	F	144	TYR	2.5
1	A	165	ALA	2.5
1	A	173	PRO	2.5
1	A	224	ALA	2.5
2	B	89	PRO	2.5
2	B	95	ALA	2.5
2	E	28	VAL	2.5
1	A	52	GLY	2.5
1	D	78	LYS	2.5
2	F	76	GLU	2.5
2	E	185	TRP	2.5
1	D	412	PHE	2.5
2	E	8	LEU	2.5
2	E	160	PHE	2.5
1	A	449	ALA	2.5
1	D	87	PRO	2.5
2	E	89	PRO	2.5
2	E	212	TYR	2.5
1	A	94	VAL	2.5
1	D	404	GLY	2.5
1	D	407	VAL	2.5
2	B	118	GLY	2.5
2	E	155	ILE	2.5
1	A	308	SER	2.5
2	E	72	GLN	2.4
1	A	405	ASP	2.4
1	A	557	LYS	2.4
1	D	231	PHE	2.4
2	C	43	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	23	LEU	2.4
2	E	204	LYS	2.4
2	F	139	LEU	2.4
1	A	225	HIS	2.4
1	A	229	HIS	2.4
1	A	102	GLY	2.4
1	A	359	GLY	2.4
1	D	158	GLY	2.4
2	B	115	GLY	2.4
2	C	188	ARG	2.4
1	D	330	TYR	2.4
1	D	395	TYR	2.4
1	A	193	ILE	2.4
1	A	291	ILE	2.4
1	A	422	ILE	2.4
1	D	477	ILE	2.4
2	B	187	LYS	2.4
1	A	534	HIS	2.4
1	D	179	MET	2.4
1	D	537	GLY	2.4
2	E	78	TRP	2.4
2	C	89	PRO	2.4
2	E	164	PHE	2.4
1	A	156	SER	2.4
1	D	415	ASN	2.4
1	D	568	SER	2.4
2	F	123	ALA	2.4
1	A	399	TYR	2.4
1	D	384	ILE	2.4
1	D	422	ILE	2.4
1	A	15	ASP	2.4
1	A	529	ARG	2.4
1	A	25	HIS	2.4
1	D	226	GLY	2.4
2	E	140	GLY	2.4
2	E	146	GLY	2.4
1	A	23	ASN	2.4
1	A	258	SER	2.4
1	D	314	PRO	2.4
2	E	200	PRO	2.4
1	A	266	LEU	2.4
1	D	273	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	574	ALA	2.4
2	E	37	PHE	2.4
1	A	76	TYR	2.4
2	B	208	TYR	2.4
2	E	167	TYR	2.4
1	D	433	ILE	2.4
2	F	129	ILE	2.4
1	A	160	VAL	2.4
1	A	463	SER	2.3
1	D	482	SER	2.3
2	E	115	GLY	2.3
2	C	35	GLU	2.3
1	A	69	THR	2.3
1	A	135	ASP	2.3
1	A	261	THR	2.3
1	D	145	LEU	2.3
1	D	316	LEU	2.3
1	D	504	ALA	2.3
2	E	7	LEU	2.3
2	E	88	ASP	2.3
2	B	126	LYS	2.3
1	A	462	PHE	2.3
2	B	84	PHE	2.3
2	C	128	PHE	2.3
2	E	145	PHE	2.3
2	F	85	PHE	2.3
2	C	98	TRP	2.3
2	F	212	TYR	2.3
1	D	256	VAL	2.3
2	B	215	ASN	2.3
1	D	572	SER	2.3
2	B	179	SER	2.3
1	A	438	GLU	2.3
1	D	140	ASP	2.3
1	D	471	ASP	2.3
1	A	296	PRO	2.3
2	C	12	PRO	2.3
2	E	53	LYS	2.3
1	D	542	ALA	2.3
1	D	490	LEU	2.3
1	D	175	PHE	2.3
1	D	212	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	84	PHE	2.3
2	C	170	PHE	2.3
1	D	312	TYR	2.3
2	F	69	ASN	2.3
1	D	444	SER	2.3
2	C	162	SER	2.3
1	A	378	GLY	2.3
1	A	10	MET	2.3
1	D	80	MET	2.3
1	A	121	THR	2.3
1	A	215	GLN	2.3
1	D	532	GLN	2.3
1	D	358	LEU	2.3
1	D	379	LEU	2.3
2	C	7	LEU	2.3
1	A	12	ARG	2.3
1	A	540	SER	2.3
1	D	463	SER	2.3
2	F	164	PHE	2.3
2	E	142	LYS	2.3
1	D	138	ILE	2.3
1	D	214	ASP	2.3
1	D	248	GLY	2.3
1	D	467	ASP	2.3
1	A	228	VAL	2.3
1	D	341	VAL	2.3
2	C	70	VAL	2.3
1	A	376	PRO	2.2
1	D	339	ALA	2.2
2	C	65	CYS	2.2
2	C	166	ALA	2.2
1	D	52	GLY	2.2
2	B	15	PHE	2.2
2	E	15	PHE	2.2
2	E	170	PHE	2.2
2	F	128	PHE	2.2
2	E	152	TYR	2.2
1	A	40	GLN	2.2
1	D	391	VAL	2.2
2	B	12	PRO	2.2
1	A	317	ARG	2.2
2	E	82	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	209	ALA	2.2
1	D	151	SER	2.2
2	E	62	LYS	2.2
1	A	492	ASP	2.2
2	E	182	LEU	2.2
1	D	519	GLU	2.2
2	C	111	PHE	2.2
2	F	15	PHE	2.2
1	A	384	ILE	2.2
1	D	43	ILE	2.2
1	A	297	ASN	2.2
1	A	555	ASN	2.2
1	D	417	PRO	2.2
2	E	5	PRO	2.2
1	D	346	SER	2.2
2	E	47	SER	2.2
1	A	320	ALA	2.2
1	A	471	ASP	2.2
2	C	88	ASP	2.2
1	A	336	TRP	2.2
1	D	423	CYS	2.2
1	D	496	CYS	2.2
2	C	163	TRP	2.2
1	A	30	GLN	2.2
1	A	158	GLY	2.2
1	A	248	GLY	2.2
1	A	452	LEU	2.2
1	D	266	LEU	2.2
2	E	217	LEU	2.2
2	B	85	PHE	2.2
2	C	30	PHE	2.2
2	E	208	TYR	2.2
1	A	7	THR	2.2
1	D	257	PRO	2.2
1	A	9	ASP	2.1
1	A	115	ASP	2.1
1	A	244	ASP	2.1
1	D	9	ASP	2.1
1	A	256	VAL	2.1
2	B	176	GLU	2.1
1	A	107	ARG	2.1
1	A	199	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	68	LEU	2.1
1	A	47	ASN	2.1
1	A	436	ASN	2.1
1	D	486	ASN	2.1
1	D	541	SER	2.1
2	E	149	SER	2.1
2	E	86	PRO	2.1
2	F	145	PHE	2.1
1	A	146	GLN	2.1
1	A	319	TYR	2.1
2	B	152	TYR	2.1
2	B	165	GLN	2.1
2	C	94	GLN	2.1
1	D	193	ILE	2.1
2	C	167	TYR	2.1
1	A	221	ALA	2.1
1	D	13	VAL	2.1
2	B	56	VAL	2.1
2	C	206	VAL	2.1
1	D	25	HIS	2.1
1	A	49	GLY	2.1
2	B	65	CYS	2.1
2	B	68	LEU	2.1
2	C	4	LEU	2.1
1	D	434	ASP	2.1
1	D	480	GLU	2.1
2	B	168	GLU	2.1
1	A	532	GLN	2.1
1	A	400	ARG	2.1
1	D	7	THR	2.1
1	A	472	PRO	2.1
1	D	365	PRO	2.1
1	D	223	PHE	2.1
2	E	111	PHE	2.1
1	A	138	ILE	2.1
1	D	300	TYR	2.1
1	D	83	GLY	2.1
2	E	131	ALA	2.1
2	F	195	VAL	2.1
1	A	547	MET	2.1
2	B	108	ASP	2.1
2	E	103	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	110	GLN	2.1
1	D	284	LEU	2.1
1	A	55	THR	2.1
1	A	573	THR	2.1
1	A	137	PRO	2.1
2	E	83	PRO	2.1
2	F	163	TRP	2.1
2	B	192	LYS	2.1
2	B	97	PHE	2.1
1	A	155	ILE	2.1
1	A	543	GLY	2.0
2	B	146	GLY	2.0
2	E	147	GLY	2.0
1	A	174	ASN	2.0
2	C	210	ALA	2.0
2	E	209	ALA	2.0
2	E	17	MET	2.0
1	D	237	VAL	2.0
1	D	469	SER	2.0
2	F	71	VAL	2.0
1	D	50	LEU	2.0
1	D	452	LEU	2.0
2	F	217	LEU	2.0
1	D	474	HIS	2.0
2	E	52	LYS	2.0
1	A	119	GLU	2.0
1	A	200	GLN	2.0
1	D	245	ILE	2.0
1	D	355	ILE	2.0
2	B	54	ILE	2.0
2	B	73	TYR	2.0
1	D	86	SER	2.0
2	C	196	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

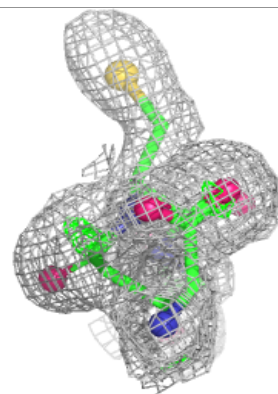
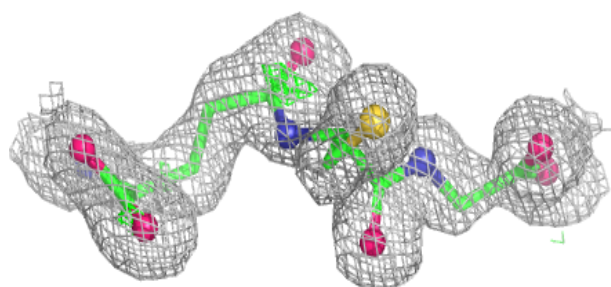
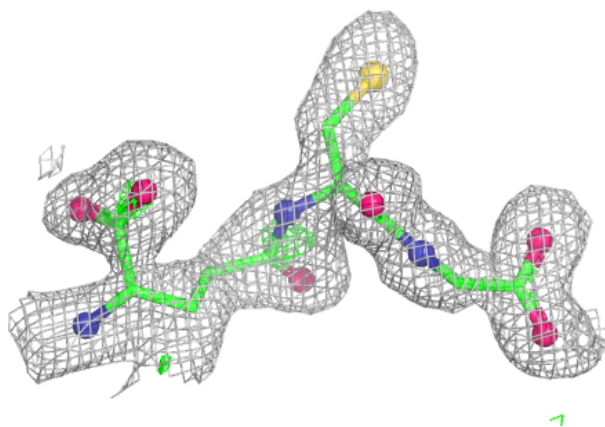
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	VAL	A	602	8/8	0.72	0.19	15,20,22,28	0
4	VAL	D	602	8/8	0.77	0.18	12,17,23,28	0
3	JAA	D	601	15/15	0.82	0.14	7,13,19,20	0
3	JAA	A	601	15/15	0.83	0.17	12,15,20,24	0
5	GSH	E	301	20/20	0.88	0.14	5,13,20,35	0
5	GSH	F	301	20/20	0.89	0.12	6,10,14,19	0
5	GSH	C	301	20/20	0.92	0.10	4,11,20,27	0
5	GSH	B	301	20/20	0.94	0.14	5,21,23,28	0
6	MG	D	603	1/1	0.95	0.17	19,19,19,19	0

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

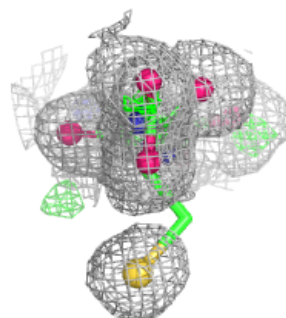
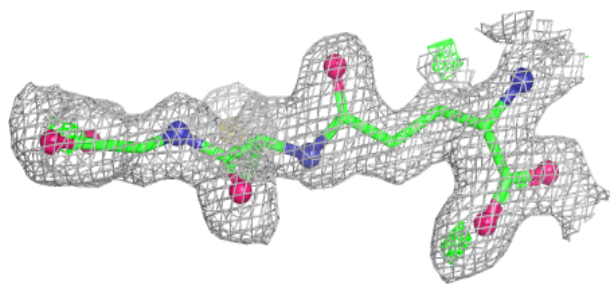
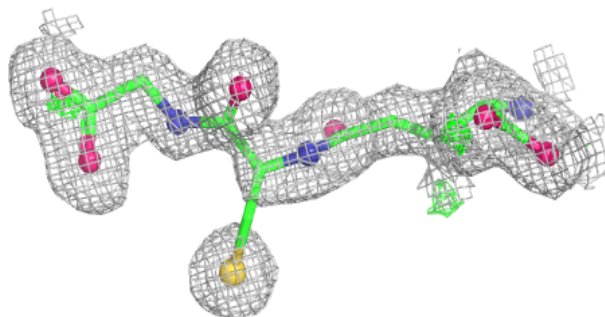
Electron density around GSH E 301:

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

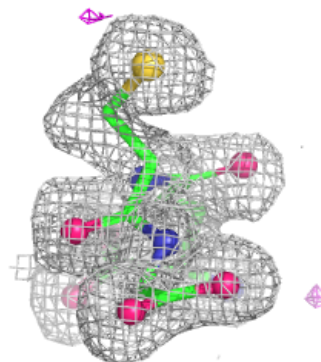
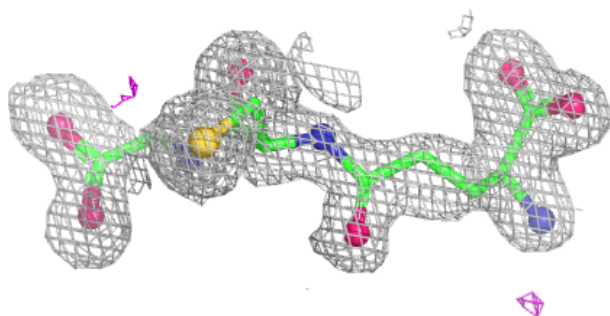
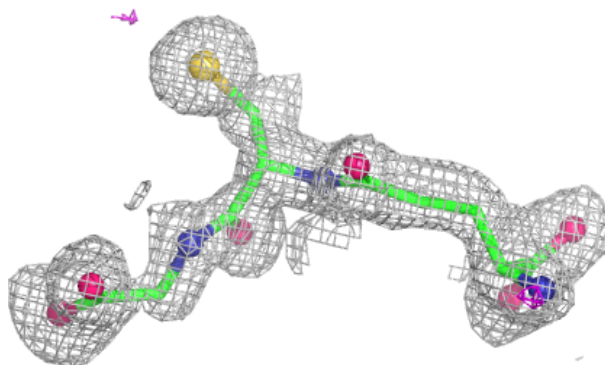


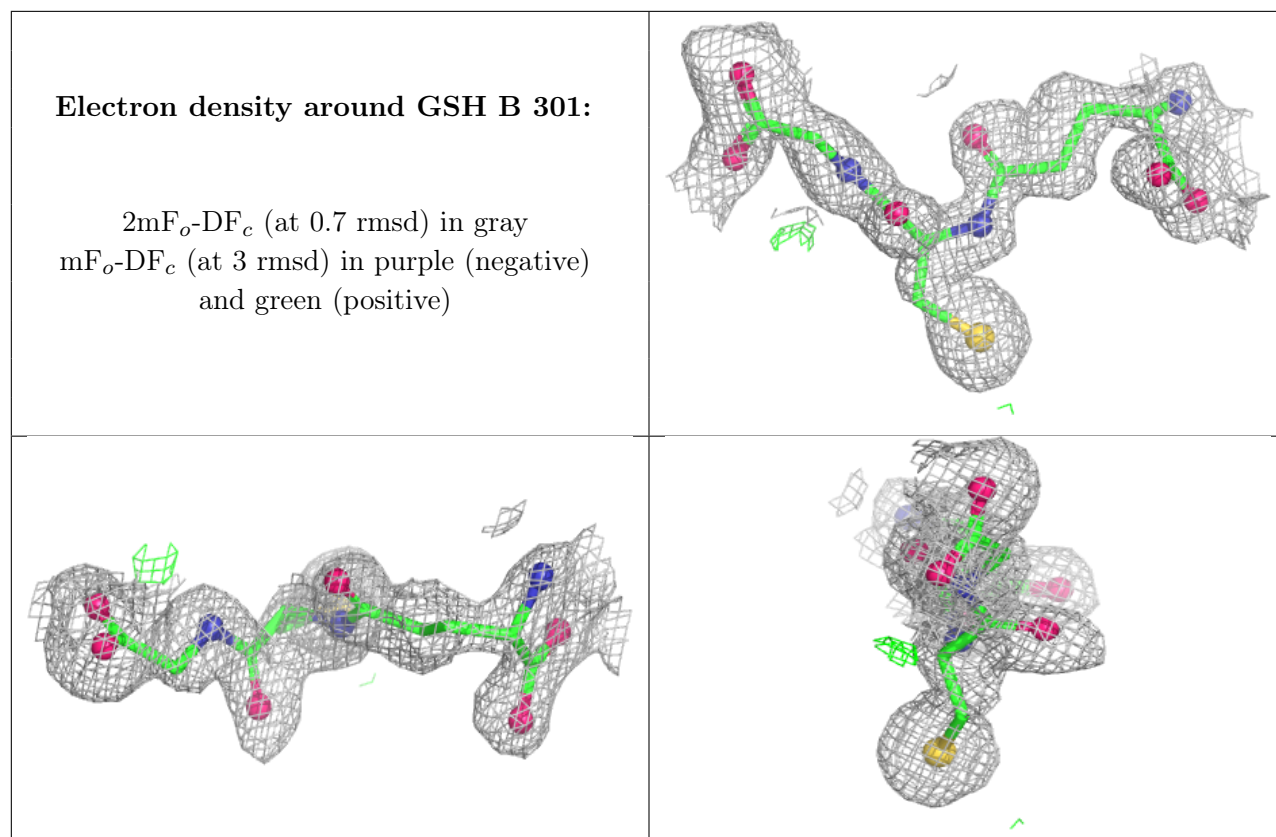
Electron density around GSH F 301:

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

**Electron density around GSH C 301:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.