



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:42 PM UTC

PDB ID : 5ECO / pdb_00005eco
Title : Crystal Structure of FIN219-FIP1 complex with JA, Leu and Mg
Authors : Chen, C.Y.; Cheng, Y.S.
Deposited on : 2015-10-20
Resolution : 1.80 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:

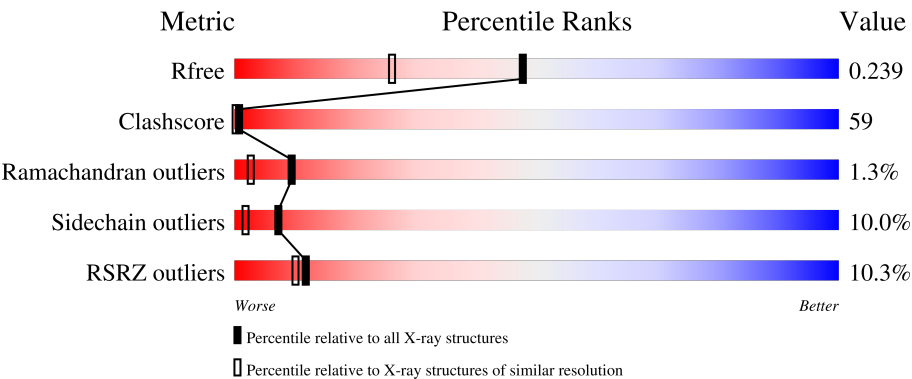
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	17% 23%58%15%..
1	D	575	11% 26%55%17%..
2	B	223	5% 33%55%8%..
2	C	223	2% 35%52%10%.
2	E	223	9% 38%48%9%.

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Mol	Chain	Length	Quality of chain
2	F	223	

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
3	JAA	A	601	-	X	-	-
4	LEU	A	602	-	-	X	-
4	LEU	D	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18387 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:

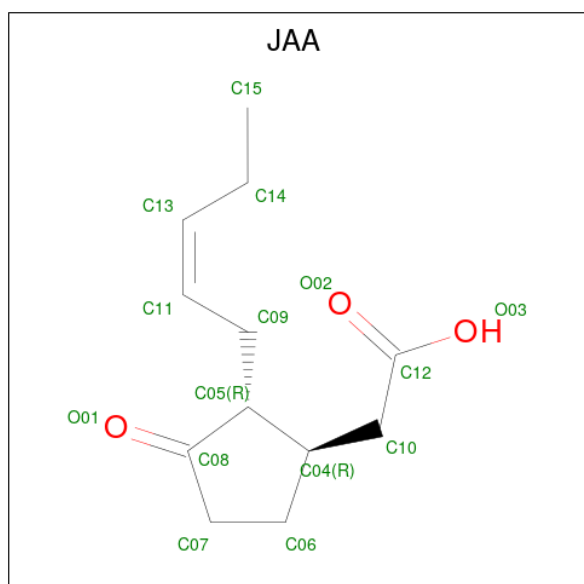
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9
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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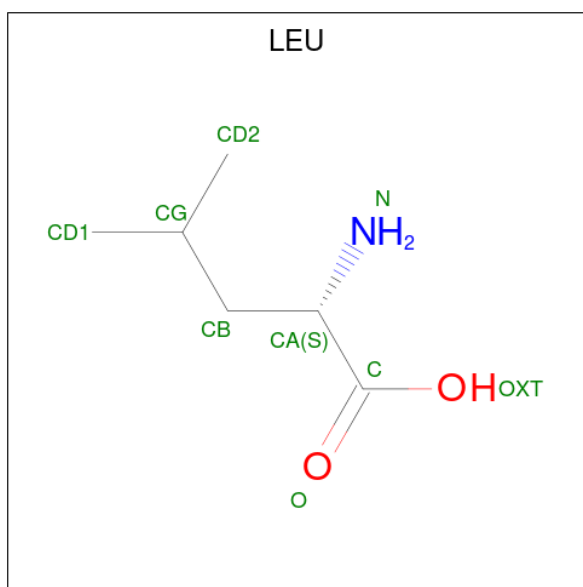
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9
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 LEUCINE (CCD ID: LEU) (formula: C₆H₁₃NO₂).

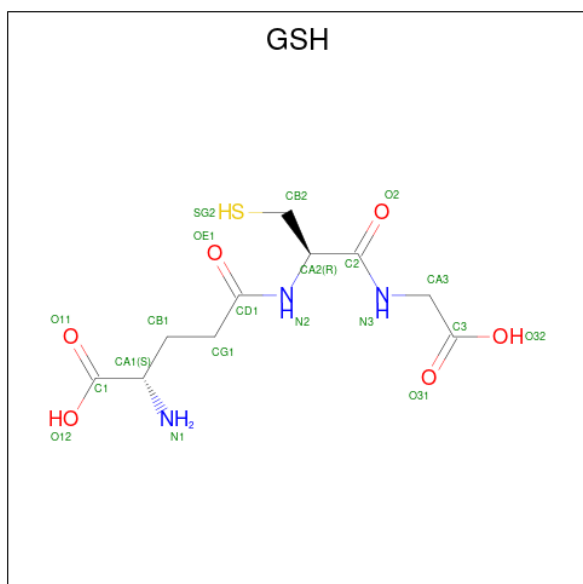


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	1	2		
4	D	1	Total	C	N	O	0	0
			9	6	1	2		

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

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

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



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

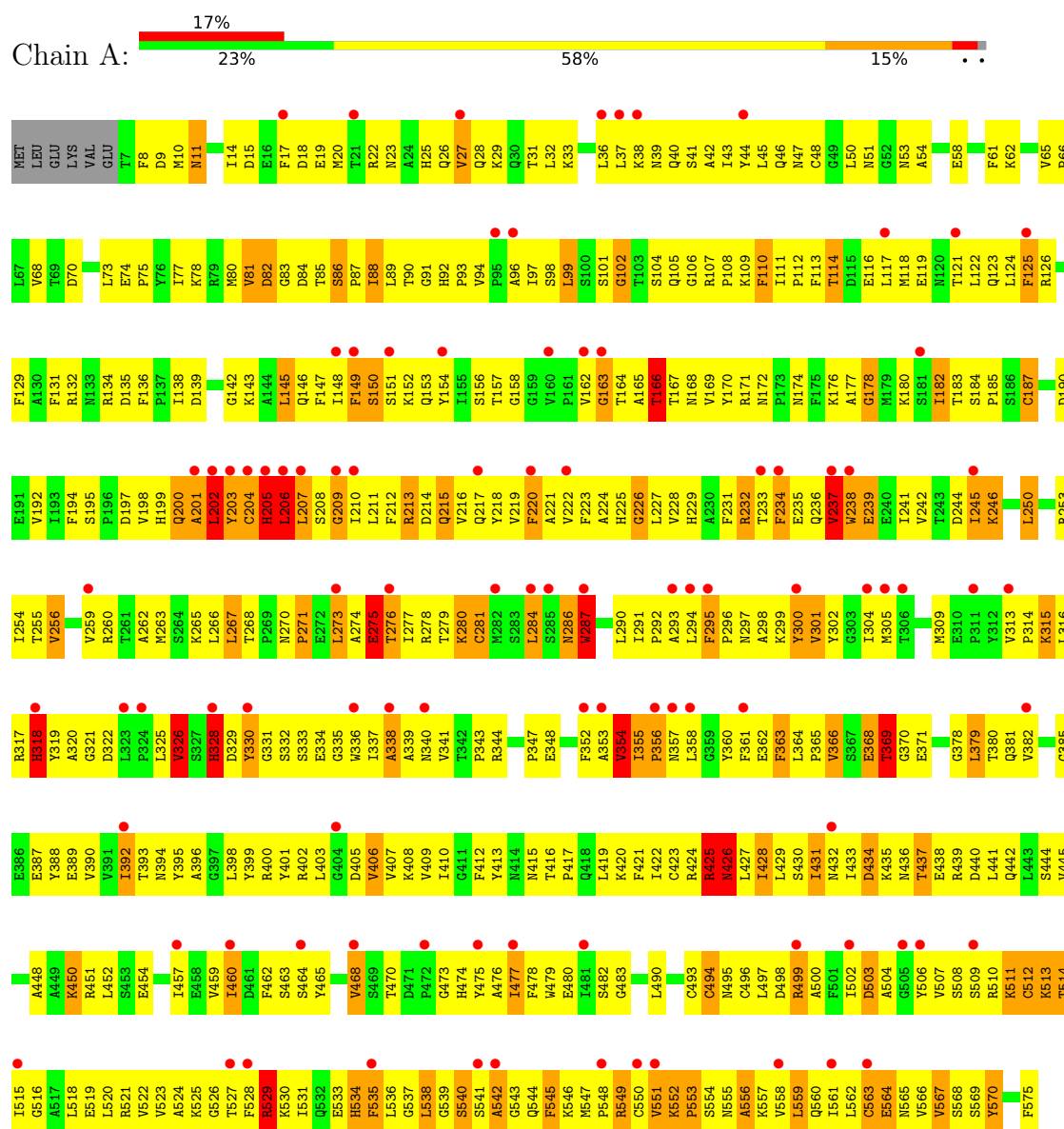
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	568	Total	O	0	0
			568	568		
7	B	270	Total	O	0	0
			270	270		
7	C	277	Total	O	0	0
			277	277		
7	D	651	Total	O	0	0
			651	651		
7	E	283	Total	O	0	0
			283	283		
7	F	259	Total	O	0	0
			259	259		

3 Residue-property plots

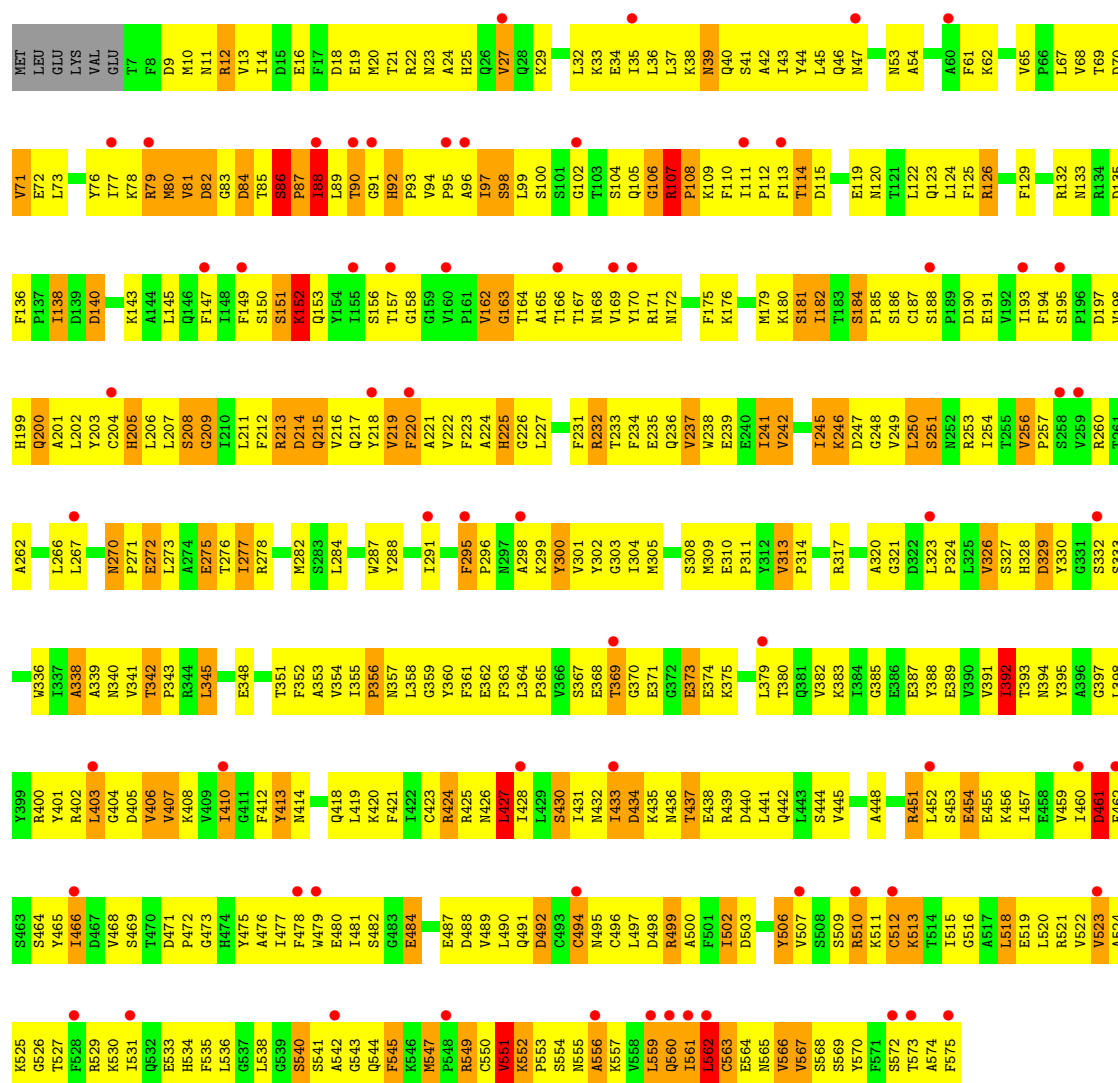
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

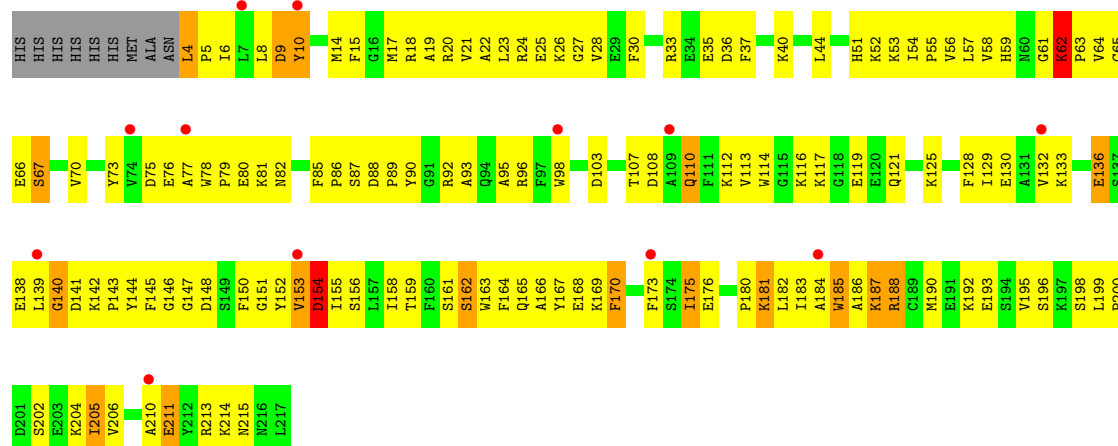


• Molecule 1: Jasmonic acid-amido synthetase JAR1





- Molecule 2: Glutathione S-transferase U20



- Molecule 2: Glutathione S-transferase U20

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.76Å 53.84Å 192.57Å 90.07° 89.96° 113.53°	Depositor
Resolution (Å)	23.48 – 1.80 23.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (23.48-1.80) 95.3 (23.48-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.222 , 0.239 0.222 , 0.239	Depositor DCC
R_{free} test set	17478 reflections (9.53%)	wwPDB-VP
Wilson B-factor (Å ²)	8.6	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 228.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.110 for -h,-k,l 0.104 for -k,-h,-l 0.088 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18387	wwPDB-VP
Average B, all atoms (Å ²)	6.0	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 50.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8822e-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: MG, GSH, JAA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	3/4581 (0.1%)	1.44	80/6219 (1.3%)
1	D	0.63	1/4581 (0.0%)	1.37	79/6219 (1.3%)
2	B	0.45	0/1799	1.08	13/2428 (0.5%)
2	C	0.49	0/1799	1.13	14/2428 (0.6%)
2	E	0.50	0/1799	1.16	10/2428 (0.4%)
2	F	0.59	1/1799 (0.1%)	1.21	17/2428 (0.7%)
All	All	0.60	5/16358 (0.0%)	1.30	213/22150 (1.0%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	HIS	N-CA	8.79	1.57	1.46
1	A	201	ALA	CA-C	-7.87	1.42	1.52
1	A	204	CYS	CA-C	6.11	1.61	1.52
2	F	175	ILE	CA-C	5.29	1.59	1.52
1	D	556	ALA	CA-CB	-5.01	1.46	1.53

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	TYR	N-CA-C	-15.33	94.67	111.07
1	A	201	ALA	CA-C-N	-14.93	94.91	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ALA	C-N-CA	-14.93	94.91	123.13
1	A	202	LEU	CB-CA-C	13.45	134.58	111.45
1	D	163	GLY	N-CA-C	12.79	130.88	111.18
1	A	563	CYS	N-CA-C	12.36	124.49	111.14
1	A	81	VAL	N-CA-C	12.26	122.05	110.53
2	F	175	ILE	N-CA-C	12.01	122.85	110.72
1	D	428	ILE	N-CA-C	-11.91	91.95	108.27
1	A	427	LEU	N-CA-C	11.61	128.06	108.20
1	A	238	TRP	N-CA-C	10.91	122.86	110.97
1	A	234	PHE	N-CA-C	-10.84	99.47	111.28
2	E	146	GLY	N-CA-C	10.83	126.64	112.77
1	D	556	ALA	N-CA-C	10.18	125.76	112.12
1	A	552	LYS	N-CA-C	-10.15	97.20	110.39
1	A	163	GLY	N-CA-C	10.08	128.04	110.80
2	E	185	TRP	N-CA-C	-9.61	100.81	111.28
1	D	427	LEU	N-CA-C	9.29	123.89	109.96
1	D	272	GLU	N-CA-C	9.24	121.43	111.36
1	A	202	LEU	N-CA-CB	-9.09	98.05	111.51
2	B	62	LYS	CA-C-N	9.08	129.76	120.14
2	B	62	LYS	C-N-CA	9.08	129.76	120.14
1	A	267	LEU	N-CA-C	8.88	123.42	110.28
1	D	206	LEU	N-CA-C	-8.69	101.77	111.07
1	A	286	ASN	N-CA-C	8.61	123.46	111.92
1	A	564	GLU	N-CA-C	8.50	120.16	111.07
1	D	563	CYS	N-CA-C	8.50	122.20	111.24
1	A	11	ASN	N-CA-C	8.47	120.29	111.14
1	D	559	LEU	N-CA-C	8.37	120.48	111.36
1	D	102	GLY	N-CA-C	-8.15	97.37	112.37
1	D	86	SER	CA-C-N	7.95	127.88	119.85
1	D	86	SER	C-N-CA	7.95	127.88	119.85
1	A	551	VAL	N-CA-C	7.92	119.56	107.99
1	D	213	ARG	N-CA-C	7.92	120.91	111.33
1	A	206	LEU	N-CA-C	-7.90	102.62	111.07
1	D	181	SER	N-CA-C	7.81	119.88	111.36
1	D	237	VAL	N-CA-C	7.79	119.87	111.77
1	A	102	GLY	N-CA-C	-7.77	98.69	112.22
1	D	560	GLN	N-CA-C	-7.76	102.90	111.36
1	A	237	VAL	N-CA-C	7.75	125.47	109.34
1	A	82	ASP	N-CA-C	7.69	121.53	107.99
2	B	188	ARG	N-CA-C	-7.42	102.34	111.40
1	A	392	ILE	N-CA-C	7.40	118.53	108.17
1	A	511	LYS	N-CA-C	-7.38	103.32	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	ALA	N-CA-C	7.37	122.72	113.43
1	D	451	ARG	N-CA-C	-7.36	103.26	111.28
1	A	232	ARG	N-CA-C	-7.33	103.30	112.90
1	D	271	PRO	N-CA-C	7.29	123.13	113.57
1	D	562	LEU	N-CA-C	7.23	118.80	111.07
1	D	551	VAL	N-CA-C	7.19	118.48	107.99
2	F	154	ASP	N-CA-C	-7.17	103.40	111.07
2	E	152	TYR	N-CA-C	7.13	125.99	110.80
1	D	10	MET	N-CA-C	7.07	118.63	111.07
1	D	392	ILE	N-CA-C	7.06	118.45	108.36
2	B	87	SER	N-CA-C	7.04	118.95	111.28
1	A	238	TRP	CA-CB-CG	7.03	126.95	113.60
1	A	220	PHE	N-CA-C	7.02	120.62	108.76
2	E	188	ARG	N-CA-C	-7.01	103.57	111.14
2	F	173	PHE	N-CA-C	-6.93	103.10	108.78
2	B	146	GLY	N-CA-C	6.93	121.64	112.77
1	D	246	LYS	N-CA-C	6.87	118.66	111.03
1	D	267	LEU	N-CA-C	6.87	121.02	109.76
1	A	213	ARG	N-CA-C	6.87	118.76	111.28
1	D	88	ILE	N-CA-C	6.86	123.61	109.34
1	A	338	ALA	N-CA-C	6.84	120.83	109.95
1	A	275	GLU	N-CA-C	-6.78	103.89	111.28
1	A	205	HIS	CA-CB-CG	6.77	120.57	113.80
1	A	503	ASP	N-CA-C	6.76	119.45	110.53
1	A	300	TYR	N-CA-C	6.74	117.47	108.38
1	D	406	VAL	N-CA-C	6.74	117.60	108.17
1	A	205	HIS	N-CA-CB	6.67	120.02	110.16
1	A	549	ARG	N-CA-C	6.66	119.54	111.82
2	C	179	SER	CA-C-N	6.64	126.08	118.85
2	C	179	SER	C-N-CA	6.64	126.08	118.85
1	D	431	ILE	N-CA-C	6.61	117.61	108.89
1	D	342	THR	CA-C-N	6.61	126.23	119.56
1	D	342	THR	C-N-CA	6.61	126.23	119.56
1	D	356	PRO	N-CA-C	6.55	123.11	114.27
1	A	482	SER	N-CA-C	6.54	119.41	111.82
1	D	107	ARG	CA-C-N	6.53	127.42	120.11
1	D	107	ARG	C-N-CA	6.53	127.42	120.11
2	F	168	GLU	N-CA-C	6.53	118.27	111.03
2	F	167	TYR	N-CA-C	-6.52	104.17	111.28
1	D	468	VAL	N-CA-C	6.50	118.34	112.17
1	D	270	ASN	CA-C-N	6.50	126.08	119.19
1	D	270	ASN	C-N-CA	6.50	126.08	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	PRO	N-CA-C	6.50	122.11	113.40
1	D	208	SER	N-CA-C	6.50	118.16	111.14
1	A	178	GLY	N-CA-C	6.47	121.05	112.77
1	A	416	THR	CA-C-N	6.43	126.40	119.78
1	A	416	THR	C-N-CA	6.43	126.40	119.78
2	B	185	TRP	N-CA-C	-6.38	104.32	111.28
1	D	552	LYS	N-CA-C	-6.33	102.85	110.13
1	D	492	ASP	N-CA-C	-6.31	104.32	111.07
2	B	154	ASP	N-CA-C	-6.27	104.36	111.07
2	F	171	GLY	N-CA-C	6.23	120.21	112.73
2	C	67	SER	N-CA-C	6.23	117.76	110.97
1	A	514	THR	N-CA-C	-6.22	104.95	112.54
1	D	81	VAL	N-CA-C	6.21	121.10	112.35
2	F	188	ARG	N-CA-C	-6.20	104.53	111.28
1	D	413	TYR	N-CA-C	-6.20	96.22	107.75
1	A	434	ASP	N-CA-C	-6.17	105.06	112.59
1	A	318	HIS	N-CA-C	-6.13	105.65	113.01
2	C	4	LEU	CA-C-N	6.12	126.32	119.90
2	C	4	LEU	C-N-CA	6.12	126.32	119.90
1	A	287	TRP	N-CA-C	6.11	123.81	110.80
1	A	281	CYS	N-CA-C	6.06	123.71	110.80
2	B	67	SER	N-CA-C	6.05	117.74	111.03
2	C	123	ALA	N-CA-C	-6.03	104.70	111.28
1	D	65	VAL	N-CA-C	6.03	113.85	107.76
1	D	574	ALA	N-CA-C	-6.02	101.02	110.36
1	D	53	ASN	CB-CA-C	-6.00	109.64	116.54
1	A	238	TRP	CB-CA-C	-5.96	101.78	110.96
1	A	280	LYS	N-CA-C	5.93	117.62	111.03
2	C	103	ASP	N-CA-C	5.92	118.69	111.82
1	D	209	GLY	N-CA-C	-5.91	105.64	112.73
1	D	106	GLY	N-CA-C	-5.89	107.63	115.40
1	D	82	ASP	N-CA-C	5.88	118.75	108.52
2	F	179	SER	CA-C-N	5.88	127.18	119.84
2	F	179	SER	C-N-CA	5.88	127.18	119.84
2	E	140	GLY	N-CA-C	-5.86	99.28	113.18
1	D	84	ASP	N-CA-C	-5.85	97.35	108.17
1	A	366	VAL	N-CA-C	-5.84	106.80	112.29
2	E	157	LEU	N-CA-C	5.83	120.67	113.50
1	A	280	LYS	CB-CA-C	-5.83	101.92	110.95
1	D	119	GLU	N-CA-C	-5.82	105.02	111.36
1	D	355	ILE	N-CA-C	-5.81	101.80	107.55
1	D	426	ASN	N-CA-C	-5.81	106.10	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	ILE	N-CA-C	5.79	116.64	108.36
2	E	30	PHE	N-CA-C	5.77	118.46	109.52
1	D	502	ILE	N-CA-C	5.76	120.18	112.98
1	D	552	LYS	CA-C-N	-5.73	112.68	119.84
1	D	552	LYS	C-N-CA	-5.73	112.68	119.84
2	B	4	LEU	CA-C-N	5.73	125.68	119.78
2	B	4	LEU	C-N-CA	5.73	125.68	119.78
1	A	86	SER	N-CA-C	5.71	116.86	109.72
1	A	149	PHE	N-CA-C	5.68	118.73	109.24
1	A	355	ILE	CA-C-N	5.67	125.03	118.85
1	A	355	ILE	C-N-CA	5.67	125.03	118.85
1	A	406	VAL	N-CA-C	5.67	116.05	108.11
1	A	354	VAL	N-CA-C	5.67	116.90	108.23
1	A	363	PHE	N-CA-C	5.66	117.61	108.34
1	A	200	GLN	N-CA-CB	5.65	119.00	110.30
1	D	434	ASP	N-CA-C	-5.65	106.25	113.02
2	F	67	SER	N-CA-C	5.63	117.10	111.07
2	B	119	GLU	N-CA-C	5.62	117.09	111.07
1	D	126	ARG	N-CA-C	-5.61	105.07	111.07
1	D	214	ASP	N-CA-C	5.58	117.45	111.36
1	D	86	SER	N-CA-C	5.58	117.77	110.08
2	C	154	ASP	N-CA-C	-5.55	105.23	111.28
1	D	300	TYR	N-CA-C	5.54	117.27	108.79
1	D	512	CYS	N-CA-C	-5.54	105.14	111.07
1	A	328	HIS	N-CA-C	5.53	119.08	110.17
2	C	16	GLY	N-CA-C	-5.51	106.12	112.73
2	C	169	LYS	N-CA-C	5.50	117.08	111.14
2	F	162	SER	N-CA-C	-5.49	106.75	113.50
2	C	48	ASN	CA-C-N	5.48	125.57	119.87
2	C	48	ASN	C-N-CA	5.48	125.57	119.87
2	C	38	SER	N-CA-C	-5.48	105.46	111.82
1	D	200	GLN	N-CA-C	-5.47	105.31	111.28
1	D	461	ASP	N-CA-C	5.47	115.59	107.88
1	D	549	ARG	N-CA-C	5.45	118.14	111.82
2	E	9	ASP	N-CA-C	5.45	118.14	109.65
1	D	506	TYR	N-CA-C	-5.42	105.37	111.28
2	F	41	SER	N-CA-C	5.42	117.38	109.84
1	A	226	GLY	N-CA-C	-5.41	106.22	112.50
1	D	170	TYR	N-CA-C	5.40	116.97	111.14
2	B	162	SER	N-CA-C	-5.39	106.70	113.28
1	A	535	PHE	N-CA-C	5.38	119.79	112.04
1	A	297	ASN	N-CA-C	5.38	119.15	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	18	ARG	N-CA-C	-5.32	105.48	111.28
1	A	246	LYS	N-CA-C	5.31	116.93	111.03
1	A	326	VAL	N-CA-C	5.30	115.59	108.17
1	D	98	SER	N-CA-C	5.30	117.92	109.81
2	F	185	TRP	N-CA-C	-5.29	105.62	111.71
1	D	152	LYS	N-CA-C	5.27	117.83	109.24
1	D	494	CYS	CA-CB-SG	5.27	126.51	114.40
1	D	466	ILE	CG1-CB-CG2	-5.25	94.94	110.70
1	A	271	PRO	N-CA-C	5.24	123.27	112.47
1	A	330	TYR	N-CA-C	5.22	117.59	108.76
1	A	428	ILE	N-CA-C	-5.22	98.48	109.34
1	D	108	PRO	N-CA-C	5.20	118.76	111.33
1	D	232	ARG	N-CA-C	-5.19	105.70	111.36
2	F	199	LEU	CA-C-N	5.19	125.19	120.21
2	F	199	LEU	C-N-CA	5.19	125.19	120.21
2	E	88	ASP	N-CA-C	5.18	116.36	109.93
1	A	256	VAL	CA-C-N	5.18	124.80	119.05
1	A	256	VAL	C-N-CA	5.18	124.80	119.05
1	A	567	VAL	N-CA-C	-5.18	104.58	111.05
1	D	454	GLU	N-CA-C	-5.18	106.80	113.01
1	A	529	ARG	N-CA-C	-5.17	105.64	111.28
1	D	487	GLU	N-CA-C	5.17	117.00	111.36
1	A	545	PHE	N-CA-C	5.15	121.34	113.61
1	A	425	ARG	CA-CB-CG	5.15	124.40	114.10
1	D	256	VAL	CA-C-N	5.15	124.76	119.05
1	D	256	VAL	C-N-CA	5.15	124.76	119.05
1	A	239	GLU	N-CA-C	-5.14	105.68	111.28
2	F	36	ASP	N-CA-C	-5.14	97.50	107.62
2	C	87	SER	N-CA-C	5.13	116.95	111.36
1	A	570	TYR	N-CA-C	5.13	117.61	109.50
1	D	338	ALA	N-CA-C	5.12	117.92	109.72
1	D	515	ILE	N-CA-C	-5.12	100.20	107.77
2	B	9	ASP	N-CA-C	5.11	116.07	108.86
1	D	180	LYS	N-CA-C	5.11	116.53	111.07
1	D	220	PHE	N-CA-C	5.10	117.73	109.06
1	A	166	THR	N-CA-C	5.08	116.50	110.97
1	A	209	GLY	N-CA-C	-5.07	106.64	112.73
1	D	87	PRO	N-CA-C	5.06	119.43	111.38
1	D	275	GLU	N-CA-C	-5.05	105.78	111.28
1	A	207	LEU	N-CA-C	5.03	116.76	111.28
1	A	410	ILE	N-CA-C	5.03	115.26	110.53
1	A	237	VAL	CB-CA-C	-5.02	103.06	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	ASN	N-CA-C	-5.01	103.72	110.68

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	LEU	Peptide
1	A	318	HIS	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4479	0	4434	662	7
1	D	4479	0	4434	587	3
2	B	1748	0	1704	168	0
2	C	1748	0	1704	193	0
2	E	1748	0	1704	170	0
2	F	1748	0	1704	169	2
3	A	15	0	0	2	0
3	D	15	0	0	2	0
4	A	9	0	10	8	0
4	D	9	0	10	6	0
5	A	1	0	0	0	0
6	B	20	0	15	1	0
6	C	20	0	15	0	0
6	E	20	0	15	2	0
6	F	20	0	15	0	0
7	A	568	0	0	103	5
7	B	270	0	0	34	1
7	C	277	0	0	27	2
7	D	651	0	0	94	2
7	E	283	0	0	36	0
7	F	259	0	0	20	2
All	All	18387	0	15764	1869	17

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 59.

All (1869) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LYS:NZ	1:D:190:ASP:OD2	1.71	1.21
1:A:202:LEU:O	1:A:205:HIS:ND1	1.81	1.10
2:C:26:LYS:HG2	2:C:81:LYS:HZ3	1.19	1.05
1:A:202:LEU:HG	1:A:205:HIS:CB	1.86	1.05
1:D:86:SER:HB3	2:E:188:ARG:HB2	1.37	1.03
1:A:278:ARG:NH2	7:A:702:HOH:O	1.91	1.02
2:F:125:LYS:NZ	7:F:402:HOH:O	1.92	1.00
1:A:202:LEU:CG	1:A:205:HIS:HB3	1.90	1.00
2:E:24:ARG:NH1	2:E:24:ARG:O	1.97	0.98
2:C:204:LYS:NZ	7:C:401:HOH:O	1.96	0.97
2:E:66:GLU:OE2	7:E:401:HOH:O	1.83	0.96
1:A:202:LEU:HG	1:A:205:HIS:HB3	0.98	0.96
1:A:202:LEU:HA	1:A:205:HIS:H	1.29	0.96
1:A:176:LYS:NZ	1:A:190:ASP:OD2	1.98	0.96
1:D:76:TYR:O	1:D:79:ARG:NH2	2.00	0.94
1:D:90:THR:HG22	1:D:397:GLY:HA2	1.49	0.94
2:E:197:LYS:NZ	7:E:402:HOH:O	1.98	0.94
2:F:26:LYS:NZ	2:F:82:ASN:O	2.02	0.93
1:A:199:HIS:HA	1:A:525:LYS:HG2	1.47	0.93
1:D:41:SER:HB3	2:E:144:TYR:HB3	1.52	0.92
2:E:125:LYS:HB3	2:E:173:PHE:HE2	1.34	0.91
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.53	0.91
1:D:88:ILE:O	7:D:701:HOH:O	1.85	0.91
1:D:100:SER:HB2	1:D:109:LYS:HD3	1.51	0.90
1:A:280:LYS:NZ	1:A:293:ALA:O	2.04	0.90
1:D:199:HIS:HB3	1:D:525:LYS:H	1.35	0.90
2:C:26:LYS:HG2	2:C:81:LYS:NZ	1.86	0.90
1:D:87:PRO:HB3	1:D:93:PRO:HD3	1.54	0.90
1:D:88:ILE:HG23	1:D:89:LEU:H	1.36	0.90
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.52	0.89
1:A:402:ARG:NH1	7:A:710:HOH:O	2.05	0.89
1:D:90:THR:OG1	1:D:91:GLY:N	1.96	0.89
1:A:99:LEU:HB3	1:A:557:LYS:H	1.36	0.89
2:F:17:MET:HE2	2:F:200:PRO:HD2	1.52	0.89
2:B:187:LYS:NZ	7:B:405:HOH:O	2.05	0.89
2:C:26:LYS:NZ	2:C:82:ASN:O	2.05	0.89
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.56	0.88
1:D:98:SER:HB2	1:D:111:ILE:HB	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:GLU:OE2	7:F:401:HOH:O	1.91	0.88
1:A:38:LYS:HZ3	1:A:395:TYR:HD1	0.94	0.87
1:D:519:GLU:OE2	1:D:569:SER:OG	1.93	0.87
2:B:162:SER:HB3	2:B:199:LEU:HD23	1.57	0.86
2:B:117:LYS:HG2	2:B:213:ARG:HH11	1.39	0.86
4:D:602:LEU:O	7:D:702:HOH:O	1.93	0.86
1:A:105:GLN:HA	1:A:430:SER:HB3	1.57	0.86
1:D:251:SER:O	7:D:703:HOH:O	1.94	0.86
1:A:87:PRO:HB3	1:A:93:PRO:HD3	1.57	0.85
2:C:33:ARG:NH1	7:C:405:HOH:O	2.09	0.85
1:D:107:ARG:HH11	1:D:107:ARG:HG3	1.42	0.85
1:D:476:ALA:O	7:D:704:HOH:O	1.95	0.85
1:A:199:HIS:HB3	1:A:525:LYS:H	1.39	0.85
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.39	0.85
1:D:424:ARG:HE	1:D:425:ARG:HD3	1.41	0.85
1:A:58:GLU:OE2	7:A:703:HOH:O	1.94	0.84
2:F:140:GLY:C	2:F:181:LYS:HZ1	1.84	0.84
1:A:526:GLY:HA2	1:A:529:ARG:HD3	1.59	0.84
1:A:152:LYS:HE2	1:A:565:ASN:HB2	1.59	0.84
1:D:95:PRO:HD3	2:E:181:LYS:HD3	1.56	0.84
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.59	0.84
2:C:135:LEU:HD22	2:C:182:LEU:HD12	1.59	0.84
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.60	0.84
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.58	0.84
2:B:88:ASP:O	7:B:401:HOH:O	1.95	0.83
1:D:90:THR:HG22	1:D:397:GLY:CA	2.07	0.83
1:A:405:ASP:HB3	1:A:541:SER:HB3	1.60	0.83
1:D:77:ILE:HG21	1:D:110:PHE:HB3	1.61	0.83
1:A:344:ARG:NH1	7:A:721:HOH:O	2.11	0.83
1:A:498:ASP:O	7:A:704:HOH:O	1.95	0.83
2:B:138:GLU:OE2	7:B:402:HOH:O	1.96	0.83
1:A:143:LYS:HZ3	1:A:187:CYS:HA	1.43	0.83
1:A:389:GLU:OE2	1:A:405:ASP:N	2.12	0.83
1:A:442:GLN:HG2	1:A:462:PHE:HZ	1.42	0.83
2:C:203:GLU:OE2	7:C:401:HOH:O	1.96	0.82
1:D:405:ASP:HB2	1:D:541:SER:HB2	1.60	0.82
2:C:184:ALA:HB1	1:D:499:ARG:NH1	1.94	0.82
2:C:66:GLU:OE2	7:C:402:HOH:O	1.97	0.82
1:D:70:ASP:OD2	7:D:705:HOH:O	1.97	0.82
1:D:77:ILE:CG2	1:D:110:PHE:HB3	2.09	0.82
1:A:424:ARG:HB2	1:A:425:ARG:NH1	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:LEU:N	7:E:410:HOH:O	2.12	0.81
2:E:125:LYS:HB3	2:E:173:PHE:CE2	2.15	0.81
1:A:154:TYR:HD1	1:A:563:CYS:HB2	1.44	0.81
2:B:116:LYS:NZ	7:B:403:HOH:O	1.99	0.81
1:A:423:CYS:SG	1:A:541:SER:OG	2.37	0.81
1:D:494:CYS:HB3	1:D:520:LEU:HB3	1.60	0.81
1:A:33:LYS:NZ	7:A:730:HOH:O	2.13	0.81
1:A:99:LEU:H	1:A:557:LYS:HG3	1.46	0.81
1:A:201:ALA:O	1:A:204:CYS:HB2	1.79	0.81
1:A:368:GLU:OE2	7:A:705:HOH:O	1.98	0.81
1:A:147:PHE:CD1	1:A:205:HIS:CD2	2.69	0.81
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.16	0.81
1:A:495:ASN:O	7:A:707:HOH:O	1.98	0.80
1:D:465:TYR:HB2	1:D:551:VAL:HG13	1.63	0.80
1:A:118:MET:SD	7:A:1034:HOH:O	2.39	0.80
1:A:317:ARG:HB2	1:A:325:LEU:HD11	1.64	0.80
2:C:117:LYS:NZ	7:C:409:HOH:O	2.13	0.80
1:A:147:PHE:HD1	1:A:205:HIS:CD2	1.99	0.80
1:A:241:ILE:O	1:A:245:ILE:HG13	1.83	0.79
1:A:238:TRP:CH2	1:A:281:CYS:HB3	2.17	0.79
1:D:46:GLN:HB2	2:E:148:ASP:HB2	1.65	0.79
2:E:180:PRO:O	7:E:403:HOH:O	2.00	0.79
2:B:18:ARG:HH12	2:B:103:ASP:CG	1.89	0.79
2:F:122:GLU:HA	2:F:125:LYS:HE2	1.64	0.79
2:C:127:GLU:OE1	7:C:403:HOH:O	2.00	0.79
1:A:87:PRO:HB2	2:B:143:PRO:HA	1.62	0.79
1:A:202:LEU:HA	1:A:205:HIS:N	1.95	0.79
1:A:229:HIS:CE1	1:A:529:ARG:HD2	2.17	0.79
2:E:64:VAL:HG13	2:E:70:VAL:HG22	1.63	0.79
1:A:202:LEU:CA	1:A:205:HIS:H	1.95	0.79
1:A:233:THR:HA	1:A:236:GLN:HB2	1.65	0.79
1:D:106:GLY:O	1:D:432:ASN:ND2	2.15	0.79
1:A:82:ASP:OD1	1:A:157:THR:OG1	2.01	0.78
1:A:39:ASN:ND2	1:A:399:TYR:OH	2.14	0.78
1:A:329:ASP:HB3	1:A:339:ALA:HA	1.64	0.78
2:B:168:GLU:OE2	7:B:404:HOH:O	2.01	0.78
1:A:202:LEU:C	1:A:205:HIS:H	1.91	0.78
1:A:199:HIS:H	1:A:524:ALA:HB1	1.48	0.78
2:C:188:ARG:NH1	1:D:499:ARG:O	2.17	0.77
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.64	0.77
1:A:231:PHE:HA	1:A:234:PHE:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:GLU:OE2	7:E:405:HOH:O	2.03	0.77
2:E:48:ASN:OD1	7:E:404:HOH:O	2.02	0.77
2:B:96:ARG:NH1	2:C:76:GLU:OE2	2.17	0.77
1:D:132:ARG:HA	1:D:343:PRO:HG3	1.66	0.77
2:E:184:ALA:HB3	7:E:403:HOH:O	1.84	0.77
1:A:143:LYS:NZ	1:A:187:CYS:HA	1.98	0.77
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.67	0.76
1:D:162:VAL:O	1:D:560:GLN:HB2	1.85	0.76
2:E:55:PRO:O	7:E:406:HOH:O	2.03	0.76
1:A:293:ALA:O	7:A:709:HOH:O	2.03	0.76
1:A:210:ILE:HG12	1:A:294:LEU:HD21	1.66	0.76
2:E:7:LEU:HD11	2:E:55:PRO:HB2	1.67	0.76
1:A:203:TYR:HD1	1:A:237:VAL:HG11	1.49	0.76
1:D:152:LYS:HG2	1:D:565:ASN:HB2	1.65	0.76
2:C:201:ASP:HB2	2:C:204:LYS:HG3	1.67	0.76
1:D:73:LEU:HD22	1:D:89:LEU:HD13	1.68	0.76
1:A:46:GLN:HB2	2:B:148:ASP:HB3	1.67	0.76
1:D:405:ASP:OD1	7:D:707:HOH:O	2.03	0.76
1:D:143:LYS:NZ	7:D:733:HOH:O	2.17	0.76
2:C:8:LEU:HD22	2:C:33:ARG:HH21	1.51	0.76
1:A:206:LEU:HG	1:A:234:PHE:HA	1.69	0.75
1:D:455:GLU:OE2	7:D:706:HOH:O	2.02	0.75
1:A:226:GLY:HA2	1:A:229:HIS:CE1	2.20	0.75
1:A:424:ARG:HB2	1:A:425:ARG:HH11	1.52	0.75
1:D:40:GLN:O	7:D:709:HOH:O	2.05	0.75
2:F:26:LYS:HG2	2:F:81:LYS:HZ3	1.52	0.75
1:A:138:ILE:HB	1:A:217:GLN:HG3	1.69	0.75
1:D:254:ILE:O	7:D:703:HOH:O	2.04	0.75
1:D:444:SER:OG	7:D:708:HOH:O	2.05	0.75
2:E:53:LYS:HG2	6:E:301:GSH:HA31	1.66	0.75
2:B:125:LYS:HB3	2:B:173:PHE:HE2	1.49	0.75
1:A:118:MET:HE3	1:A:122:LEU:HG	1.69	0.74
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.22	0.74
1:A:218:TYR:HA	1:A:298:ALA:HB1	1.70	0.74
1:D:521:ARG:HB3	1:D:566:VAL:HG12	1.70	0.74
1:A:198:VAL:HG22	1:A:524:ALA:HB3	1.69	0.74
1:A:444:SER:OG	7:A:706:HOH:O	1.98	0.74
2:E:138:GLU:OE2	2:E:142:LYS:NZ	2.13	0.74
1:A:29:LYS:HE3	1:A:58:GLU:HB2	1.69	0.74
2:E:139:LEU:C	2:E:141:ASP:H	1.95	0.74
1:D:76:TYR:HB3	1:D:88:ILE:HG12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:TYR:O	7:E:407:HOH:O	2.04	0.74
1:A:480:GLU:HB2	1:A:528:PHE:CD2	2.23	0.73
1:A:480:GLU:HB2	1:A:528:PHE:HD2	1.53	0.73
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.68	0.73
2:F:72:GLN:NE2	7:F:410:HOH:O	2.21	0.73
1:D:87:PRO:HD2	2:E:188:ARG:HB2	1.71	0.73
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.70	0.73
2:C:17:MET:HE2	2:C:200:PRO:HD2	1.69	0.73
1:A:239:GLU:OE1	7:A:711:HOH:O	2.07	0.73
1:A:507:VAL:HG13	1:A:511:LYS:HZ2	1.53	0.73
1:A:147:PHE:HD1	1:A:205:HIS:CG	2.05	0.72
2:B:18:ARG:NH1	2:B:103:ASP:OD2	2.15	0.72
1:A:17:PHE:HE1	1:A:355:ILE:HG12	1.54	0.72
1:D:199:HIS:HB2	1:D:525:LYS:HE3	1.69	0.72
1:A:81:VAL:HG11	1:A:110:PHE:HE2	1.55	0.72
1:A:253:ARG:NH2	7:A:748:HOH:O	2.21	0.72
1:D:231:PHE:O	7:D:710:HOH:O	2.06	0.72
1:A:28:GLN:HE21	1:A:361:PHE:H	1.37	0.72
1:D:143:LYS:HG3	1:D:216:VAL:HG12	1.71	0.72
1:D:534:HIS:CE1	1:D:557:LYS:HD3	2.25	0.72
1:A:362:GLU:OE2	7:A:712:HOH:O	2.07	0.72
1:A:106:GLY:C	1:A:432:ASN:HD22	1.98	0.72
1:A:305:MET:HB3	1:A:347:PRO:HB3	1.71	0.72
2:C:17:MET:SD	7:C:410:HOH:O	2.48	0.72
1:D:435:LYS:HB3	1:D:436:ASN:C	2.14	0.72
1:A:540:SER:OG	1:A:544:GLN:NE2	2.22	0.71
2:C:187:LYS:HE3	1:D:492:ASP:C	2.14	0.71
1:A:432:ASN:OD1	1:A:434:ASP:N	2.22	0.71
2:C:184:ALA:HA	2:C:187:LYS:HZ1	1.56	0.71
1:A:28:GLN:NE2	1:A:361:PHE:H	1.87	0.71
2:C:55:PRO:O	7:C:404:HOH:O	2.07	0.71
1:A:38:LYS:NZ	1:A:395:TYR:HD1	1.82	0.71
1:A:435:LYS:HZ1	1:A:438:GLU:HB3	1.55	0.71
1:A:452:LEU:HB3	1:A:457:ILE:HD11	1.72	0.71
2:E:26:LYS:HZ2	2:E:82:ASN:C	1.97	0.71
1:A:15:ASP:OD2	7:A:716:HOH:O	2.09	0.71
1:A:126:ARG:NH2	1:A:178:GLY:O	2.22	0.71
1:A:329:ASP:O	7:A:714:HOH:O	2.09	0.71
2:B:98:TRP:CE2	2:B:138:GLU:HG2	2.25	0.71
1:D:96:ALA:HB3	1:D:113:PHE:HB3	1.72	0.71
1:D:152:LYS:O	7:D:711:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.72	0.71
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.55	0.71
1:A:9:ASP:O	7:A:715:HOH:O	2.09	0.71
1:A:440:ASP:OD1	7:A:706:HOH:O	2.09	0.71
1:D:22:ARG:HH11	1:D:414:ASN:CG	1.98	0.71
2:F:10:TYR:O	2:F:20:ARG:NH2	2.20	0.71
1:A:331:GLY:HA3	1:A:336:TRP:CE3	2.24	0.71
1:A:68:VAL:HG13	1:A:401:TYR:HD1	1.56	0.71
1:A:222:VAL:HG23	1:A:223:PHE:CD1	2.26	0.71
1:A:236:GLN:NE2	7:A:751:HOH:O	2.23	0.71
1:A:507:VAL:HG13	1:A:511:LYS:NZ	2.06	0.71
1:D:212:PHE:HB3	1:D:215:GLN:HE21	1.56	0.71
1:D:435:LYS:HA	1:D:436:ASN:HB2	1.72	0.70
2:E:52:LYS:O	7:E:408:HOH:O	2.08	0.70
1:A:42:ALA:HA	2:B:143:PRO:HG3	1.73	0.70
2:E:175:ILE:HB	2:E:183:ILE:HD11	1.73	0.70
1:A:147:PHE:HB3	1:A:205:HIS:CD2	2.27	0.70
1:A:530:LYS:HE2	1:A:561:ILE:HD13	1.73	0.70
1:D:260:ARG:NH2	7:D:703:HOH:O	2.24	0.70
2:F:132:VAL:HG22	2:F:179:SER:HB2	1.73	0.70
1:A:498:ASP:OD2	1:A:510:ARG:NH1	2.25	0.70
1:A:552:LYS:O	1:A:554:SER:N	2.25	0.70
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.56	0.70
1:D:478:PHE:HE1	1:D:521:ARG:HD2	1.56	0.70
2:E:20:ARG:NH1	2:E:198:SER:O	2.24	0.70
1:A:211:LEU:O	7:A:718:HOH:O	2.10	0.70
1:A:223:PHE:CZ	1:A:536:LEU:HB3	2.27	0.70
1:A:498:ASP:HB3	1:A:510:ARG:HH22	1.56	0.70
1:D:97:ILE:O	7:D:713:HOH:O	2.10	0.70
1:A:262:ALA:HA	1:A:265:LYS:NZ	2.07	0.70
1:A:525:LYS:O	7:A:720:HOH:O	2.10	0.70
1:D:111:ILE:O	7:D:712:HOH:O	2.08	0.70
1:A:91:GLY:HA3	2:B:141:ASP:C	2.16	0.69
1:A:102:GLY:HA2	1:A:546:LYS:HB3	1.73	0.69
1:D:19:GLU:O	1:D:23:ASN:ND2	2.24	0.69
1:D:81:VAL:HG11	1:D:110:PHE:CE2	2.27	0.69
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.27	0.69
2:F:151:GLY:N	2:F:154:ASP:OD2	2.25	0.69
1:A:329:ASP:OD1	1:A:340:ASN:N	2.21	0.69
2:C:24:ARG:O	7:C:406:HOH:O	2.09	0.69
1:A:132:ARG:O	1:A:136:PHE:N	2.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASN:ND2	7:A:756:HOH:O	2.25	0.69
2:F:147:GLY:O	7:F:403:HOH:O	2.11	0.69
1:D:67:LEU:O	7:D:715:HOH:O	2.10	0.69
1:A:435:LYS:NZ	1:A:438:GLU:HB3	2.08	0.69
2:B:139:LEU:HG	2:B:142:LYS:HB2	1.75	0.69
1:A:22:ARG:O	7:A:719:HOH:O	2.10	0.69
1:D:498:ASP:CG	1:D:510:ARG:HH22	2.00	0.69
1:D:552:LYS:O	1:D:554:SER:N	2.23	0.69
1:A:150:SER:HB2	1:A:167:THR:HA	1.74	0.69
1:A:339:ALA:O	7:A:722:HOH:O	2.11	0.69
1:D:112:PRO:O	7:D:716:HOH:O	2.11	0.69
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.28	0.69
1:A:149:PHE:HD2	1:A:529:ARG:HH22	1.41	0.68
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.29	0.68
1:A:169:VAL:HG21	4:A:602:LEU:HD11	1.76	0.68
1:A:150:SER:HB3	1:A:170:TYR:CD2	2.28	0.68
1:D:39:ASN:ND2	1:D:90:THR:O	2.26	0.68
1:A:149:PHE:CE1	1:A:202:LEU:HD22	2.28	0.68
1:A:338:ALA:HA	1:A:354:VAL:HA	1.75	0.68
1:A:156:SER:HB3	1:A:162:VAL:HG13	1.76	0.68
1:D:342:THR:OG1	1:D:413:TYR:OH	2.11	0.68
1:D:562:LEU:O	7:D:717:HOH:O	2.11	0.68
2:F:135:LEU:HD22	2:F:182:LEU:HD12	1.74	0.68
1:A:166:THR:HG23	4:A:602:LEU:C	2.17	0.68
2:B:176:GLU:OE2	7:B:407:HOH:O	2.11	0.68
2:B:40:LYS:HB3	2:B:44:LEU:HD23	1.76	0.68
2:B:204:LYS:NZ	7:B:428:HOH:O	2.26	0.68
1:D:353:ALA:HB2	1:D:413:TYR:HD2	1.58	0.68
1:A:134:ARG:NH2	7:A:761:HOH:O	2.26	0.68
2:C:156:SER:O	7:C:407:HOH:O	2.11	0.68
1:D:79:ARG:NH2	1:D:88:ILE:HB	2.09	0.68
1:D:80:MET:SD	7:D:1032:HOH:O	2.51	0.68
1:D:157:THR:HB	1:D:469:SER:HB3	1.76	0.68
2:E:26:LYS:NZ	2:E:82:ASN:O	2.24	0.68
1:A:163:GLY:O	7:A:725:HOH:O	2.12	0.68
2:C:64:VAL:HB	2:C:73:TYR:CD2	2.28	0.68
1:A:287:TRP:CE3	1:A:290:LEU:HD13	2.28	0.67
2:B:202:SER:O	2:B:205:ILE:HG13	1.94	0.67
1:D:199:HIS:CE1	1:D:567:VAL:HG21	2.28	0.67
1:D:572:SER:O	7:D:714:HOH:O	2.10	0.67
1:A:219:VAL:HG11	1:A:291:ILE:HD13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:OD2	7:A:723:HOH:O	2.12	0.67
1:D:46:GLN:NE2	7:D:759:HOH:O	2.26	0.67
1:D:367:SER:O	7:D:720:HOH:O	2.13	0.67
1:A:208:SER:O	1:A:211:LEU:HB2	1.93	0.67
2:B:215:ASN:ND2	7:B:429:HOH:O	2.28	0.67
1:D:164:THR:HA	1:D:557:LYS:HG2	1.76	0.67
1:D:494:CYS:HB3	1:D:520:LEU:CB	2.24	0.67
1:D:498:ASP:OD2	7:D:719:HOH:O	2.12	0.67
2:E:139:LEU:C	2:E:141:ASP:N	2.50	0.67
1:A:166:THR:HA	4:A:602:LEU:HG	1.75	0.67
2:B:15:PHE:HB3	2:B:67:SER:HB3	1.76	0.67
2:C:31:GLU:OE2	7:C:408:HOH:O	2.12	0.67
1:A:145:LEU:O	7:A:727:HOH:O	2.13	0.67
2:B:121:GLN:NE2	7:B:422:HOH:O	2.23	0.67
1:D:20:MET:HE2	1:D:356:PRO:HD2	1.76	0.67
1:D:99:LEU:HB2	1:D:556:ALA:H	1.59	0.67
1:A:98:SER:HB2	1:A:557:LYS:HE3	1.75	0.67
1:A:145:LEU:HD23	1:A:295:PHE:HE2	1.60	0.67
1:A:238:TRP:NE1	7:A:763:HOH:O	2.27	0.67
2:B:51:HIS:HB3	2:B:53:LYS:HG3	1.76	0.67
2:E:193:GLU:HA	2:E:196:SER:HB3	1.77	0.67
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.77	0.67
2:C:184:ALA:HA	2:C:187:LYS:NZ	2.09	0.67
1:D:35:ILE:HD11	1:D:359:GLY:HA2	1.76	0.67
1:D:373:GLU:OE2	7:D:721:HOH:O	2.13	0.67
1:A:37:LEU:O	2:B:142:LYS:NZ	2.27	0.67
1:D:191:GLU:OE1	7:D:718:HOH:O	2.12	0.67
1:A:440:ASP:O	7:A:706:HOH:O	2.13	0.66
1:A:87:PRO:HD2	2:B:188:ARG:HB2	1.77	0.66
1:A:284:LEU:HD13	1:A:287:TRP:H	1.60	0.66
1:A:548:PRO:O	7:A:724:HOH:O	2.12	0.66
1:A:74:GLU:OE2	7:A:717:HOH:O	2.12	0.66
2:E:215:ASN:ND2	7:E:426:HOH:O	2.27	0.66
1:A:332:SER:OG	1:A:333:SER:N	2.26	0.66
2:C:122:GLU:HA	2:C:125:LYS:HE2	1.76	0.66
2:C:201:ASP:OD2	2:C:204:LYS:HE2	1.95	0.66
1:D:550:CYS:O	7:D:722:HOH:O	2.13	0.66
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.31	0.66
2:F:194:SER:O	2:F:198:SER:OG	2.12	0.66
1:A:17:PHE:CE1	1:A:355:ILE:HG12	2.30	0.66
1:A:348:GLU:OE2	7:A:731:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PHE:O	7:B:408:HOH:O	2.14	0.66
1:D:208:SER:O	7:D:723:HOH:O	2.14	0.66
1:D:241:ILE:O	1:D:245:ILE:HG12	1.95	0.66
1:A:206:LEU:CG	1:A:234:PHE:HA	2.25	0.66
1:D:47:ASN:O	7:D:724:HOH:O	2.14	0.66
1:A:299:LYS:O	7:A:729:HOH:O	2.13	0.66
1:A:551:VAL:HG13	1:A:555:ASN:HB2	1.78	0.66
2:E:169:LYS:NZ	2:E:206:VAL:HG13	2.10	0.66
1:D:132:ARG:O	1:D:136:PHE:N	2.29	0.66
1:D:248:GLY:O	7:D:725:HOH:O	2.14	0.66
1:D:253:ARG:HH12	1:D:484:GLU:H	1.43	0.66
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.76	0.66
1:D:440:ASP:O	7:D:708:HOH:O	2.14	0.66
2:F:188:ARG:NH2	7:F:420:HOH:O	2.29	0.66
1:A:122:LEU:HD22	1:A:126:ARG:HH21	1.60	0.66
2:B:26:LYS:HZ1	2:B:78:TRP:CG	2.14	0.66
2:C:54:ILE:HB	2:C:55:PRO:HA	1.77	0.66
1:D:99:LEU:H	1:D:557:LYS:HD2	1.59	0.66
2:F:26:LYS:HE2	2:F:75:ASP:HA	1.77	0.66
2:F:144:TYR:O	7:F:404:HOH:O	2.14	0.66
1:A:360:TYR:HB3	1:A:393:THR:HB	1.78	0.65
1:A:510:ARG:NH2	7:A:704:HOH:O	2.28	0.65
1:A:526:GLY:CA	1:A:529:ARG:HD3	2.26	0.65
1:D:98:SER:O	1:D:110:PHE:HA	1.95	0.65
1:A:90:THR:OG1	1:A:91:GLY:N	2.26	0.65
1:D:198:VAL:HG13	1:D:565:ASN:HD21	1.61	0.65
1:A:132:ARG:HA	1:A:343:PRO:HG3	1.77	0.65
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.30	0.65
2:F:216:ASN:ND2	7:F:416:HOH:O	2.27	0.65
1:A:202:LEU:C	1:A:205:HIS:HD1	1.97	0.65
1:D:81:VAL:HB	1:D:97:ILE:HD12	1.78	0.65
1:D:566:VAL:HB	1:D:569:SER:HB2	1.79	0.65
1:A:134:ARG:NH1	1:A:135:ASP:OD1	2.28	0.65
1:A:473:GLY:O	1:A:516:GLY:N	2.29	0.65
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.30	0.65
1:D:295:PHE:HD1	1:D:298:ALA:HB2	1.62	0.65
2:C:144:TYR:HB3	2:C:154:ASP:OD2	1.96	0.65
1:A:38:LYS:HB2	2:B:140:GLY:HA3	1.78	0.65
2:F:132:VAL:HG23	2:F:182:LEU:HD13	1.79	0.65
1:A:147:PHE:HB3	1:A:205:HIS:HD2	1.61	0.65
2:B:193:GLU:HA	2:B:196:SER:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LYS:HB3	1:A:436:ASN:C	2.22	0.64
1:D:223:PHE:CB	1:D:225:HIS:HD2	2.09	0.64
1:A:424:ARG:CB	1:A:425:ARG:NH1	2.59	0.64
1:A:99:LEU:HB2	1:A:556:ALA:H	1.61	0.64
2:C:132:VAL:HG23	2:C:182:LEU:HD13	1.79	0.64
2:F:109:ALA:HB1	2:F:128:PHE:HB3	1.80	0.64
1:D:552:LYS:C	1:D:554:SER:H	2.05	0.64
2:F:140:GLY:CA	2:F:181:LYS:HZ1	2.11	0.64
1:A:114:THR:H	1:A:117:LEU:HD12	1.62	0.64
1:D:284:LEU:HD13	1:D:287:TRP:HA	1.80	0.64
1:D:503:ASP:O	1:D:507:VAL:HG23	1.97	0.64
2:E:89:PRO:HB3	2:F:76:GLU:HG3	1.78	0.64
1:A:526:GLY:O	1:A:529:ARG:NH1	2.29	0.64
2:B:130:GLU:OE2	7:B:410:HOH:O	2.15	0.64
1:D:38:LYS:HB2	1:D:395:TYR:HE1	1.63	0.64
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.79	0.64
1:D:434:ASP:OD1	1:D:435:LYS:NZ	2.28	0.64
2:E:4:LEU:N	7:E:429:HOH:O	2.29	0.64
2:F:26:LYS:HG2	2:F:81:LYS:NZ	2.13	0.64
1:A:22:ARG:HE	1:A:415:ASN:HB2	1.61	0.64
1:A:154:TYR:CD1	1:A:563:CYS:HB2	2.32	0.64
1:A:344:ARG:O	7:A:735:HOH:O	2.15	0.64
1:A:381:GLN:NE2	7:A:775:HOH:O	2.29	0.64
1:A:150:SER:O	7:A:732:HOH:O	2.15	0.64
1:A:219:VAL:O	7:A:736:HOH:O	2.15	0.64
1:A:253:ARG:O	7:A:733:HOH:O	2.15	0.64
2:B:211:GLU:OE2	2:B:214:LYS:HD2	1.97	0.64
1:D:99:LEU:HB3	1:D:557:LYS:HB2	1.80	0.64
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.32	0.64
1:A:40:GLN:H	2:B:142:LYS:HE3	1.61	0.64
1:A:53:ASN:ND2	7:A:779:HOH:O	2.31	0.64
2:F:98:TRP:CD1	2:F:153:VAL:HG21	2.33	0.64
2:B:25:GLU:OE1	7:B:409:HOH:O	2.14	0.63
2:C:176:GLU:OE2	1:D:491:GLN:HG2	1.97	0.63
2:C:188:ARG:HH12	1:D:500:ALA:HA	1.63	0.63
1:D:402:ARG:NH2	7:D:768:HOH:O	2.29	0.63
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.62	0.63
2:E:11:TRP:CD1	2:E:12:PRO:HD3	2.33	0.63
1:A:403:LEU:HD23	1:A:540:SER:HB3	1.79	0.63
2:B:159:THR:HA	2:B:199:LEU:HD21	1.79	0.63
2:C:187:LYS:NZ	2:C:187:LYS:HB2	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLY:HA3	1:D:560:GLN:OE1	1.98	0.63
1:D:225:HIS:NE2	1:D:529:ARG:HG3	2.12	0.63
1:A:106:GLY:O	1:A:432:ASN:ND2	2.31	0.63
2:C:26:LYS:HE2	2:C:75:ASP:HA	1.80	0.63
2:E:11:TRP:NE1	7:E:423:HOH:O	2.27	0.63
1:A:109:LYS:NZ	1:A:111:ILE:HD11	2.12	0.63
1:A:205:HIS:CE1	1:A:206:LEU:HD13	2.34	0.63
1:A:565:ASN:ND2	7:A:783:HOH:O	2.32	0.63
1:D:437:THR:OG1	1:D:440:ASP:HB2	1.98	0.63
1:A:340:ASN:HB2	1:A:352:PHE:HD2	1.64	0.63
1:D:424:ARG:HH21	1:D:425:ARG:NE	1.95	0.63
2:E:169:LYS:HG3	2:E:170:PHE:N	2.13	0.63
2:F:72:GLN:NE2	2:F:152:TYR:OH	2.32	0.63
2:C:98:TRP:CH2	2:C:135:LEU:HG	2.34	0.63
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.33	0.63
2:B:136:GLU:HG3	2:B:181:LYS:HE3	1.78	0.63
2:C:184:ALA:HB1	1:D:499:ARG:CZ	2.27	0.63
1:D:54:ALA:O	7:D:727:HOH:O	2.16	0.63
1:D:451:ARG:O	1:D:454:GLU:HG2	1.98	0.63
1:D:498:ASP:HB3	1:D:510:ARG:HH22	1.63	0.63
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.33	0.63
1:A:536:LEU:HB2	1:A:545:PHE:CE1	2.33	0.63
1:D:114:THR:HG22	1:D:115:ASP:H	1.63	0.63
1:D:441:LEU:HD23	1:D:549:ARG:HB3	1.80	0.63
2:F:139:LEU:HB3	2:F:181:LYS:HE2	1.80	0.63
1:A:483:GLY:N	7:A:764:HOH:O	2.30	0.62
1:A:241:ILE:HG13	1:A:242:VAL:N	2.14	0.62
1:A:426:ASN:ND2	7:A:776:HOH:O	2.30	0.62
2:C:24:ARG:HB3	2:C:194:SER:HA	1.81	0.62
1:D:164:THR:OG1	1:D:557:LYS:O	2.15	0.62
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.34	0.62
2:E:121:GLN:O	2:E:125:LYS:HG3	1.99	0.62
2:E:152:TYR:OH	7:E:411:HOH:O	2.13	0.62
1:A:208:SER:HA	1:A:211:LEU:HD12	1.80	0.62
1:A:424:ARG:CB	1:A:425:ARG:HH11	2.12	0.62
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.34	0.62
1:D:79:ARG:HH22	1:D:88:ILE:HB	1.62	0.62
1:D:84:ASP:O	7:D:728:HOH:O	2.16	0.62
1:D:313:VAL:HG13	1:D:314:PRO:HD3	1.81	0.62
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.82	0.62
1:A:535:PHE:HB3	1:A:544:GLN:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD11	1:A:147:PHE:CE1	2.35	0.62
1:A:215:GLN:NE2	7:A:788:HOH:O	2.33	0.62
1:A:238:TRP:HA	1:A:241:ILE:HG12	1.81	0.62
2:B:108:ASP:OD1	7:B:411:HOH:O	2.16	0.62
1:D:147:PHE:O	1:D:529:ARG:NH2	2.30	0.62
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.35	0.62
1:D:522:VAL:HB	1:D:568:SER:OG	2.00	0.62
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.34	0.62
1:D:507:VAL:O	7:D:726:HOH:O	2.16	0.62
1:A:424:ARG:C	1:A:543:GLY:HA2	2.25	0.62
2:C:5:PRO:HG3	2:C:59:HIS:CE1	2.35	0.62
1:D:213:ARG:HG3	1:D:214:ASP:N	2.15	0.62
1:D:466:ILE:HG13	1:D:552:LYS:HA	1.81	0.62
2:F:8:LEU:HD22	2:F:33:ARG:HH21	1.64	0.62
1:A:559:LEU:HD23	1:A:562:LEU:HD13	1.82	0.61
1:D:545:PHE:O	1:D:547:MET:HE2	2.00	0.61
1:A:514:THR:O	7:A:737:HOH:O	2.16	0.61
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.82	0.61
2:F:121:GLN:O	2:F:125:LYS:HG3	2.00	0.61
1:A:199:HIS:N	1:A:524:ALA:HB1	2.14	0.61
1:A:222:VAL:HG23	1:A:223:PHE:HD1	1.64	0.61
2:C:117:LYS:HE3	2:C:213:ARG:NH1	2.16	0.61
1:D:473:GLY:O	1:D:516:GLY:N	2.33	0.61
1:A:43:ILE:HG12	1:A:88:ILE:HG23	1.81	0.61
4:A:602:LEU:N	7:A:789:HOH:O	2.33	0.61
2:E:154:ASP:O	2:E:158:ILE:HG12	2.00	0.61
1:A:143:LYS:HD2	1:A:212:PHE:HB2	1.82	0.61
2:C:164:PHE:HD2	2:C:183:ILE:HD12	1.66	0.61
1:A:212:PHE:O	1:A:216:VAL:HG23	2.00	0.61
2:B:85:PHE:HB3	2:B:92:ARG:HG2	1.82	0.61
1:D:108:PRO:HB3	1:D:555:ASN:CB	2.31	0.61
1:A:507:VAL:O	1:A:511:LYS:HB2	2.00	0.61
1:D:125:PHE:HE1	1:D:182:ILE:HD12	1.66	0.61
1:D:195:SER:OG	1:D:197:ASP:OD1	2.19	0.61
1:A:151:SER:HB3	1:A:565:ASN:ND2	2.14	0.61
1:A:528:PHE:HA	1:A:531:ILE:HG12	1.83	0.61
2:E:110:GLN:NE2	7:E:437:HOH:O	2.34	0.61
1:D:216:VAL:HG23	7:D:813:HOH:O	2.00	0.61
2:F:195:VAL:HG23	2:F:199:LEU:HD13	1.82	0.61
1:A:97:ILE:H	1:A:163:GLY:H	1.47	0.61
1:A:108:PRO:HB3	1:A:555:ASN:CG	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:HB2	1:A:538:LEU:HA	1.81	0.60
2:C:23:LEU:HD22	2:C:28:VAL:HG11	1.82	0.60
2:F:7:LEU:HD21	2:F:23:LEU:HD12	1.83	0.60
2:F:54:ILE:HB	2:F:55:PRO:HA	1.83	0.60
2:C:201:ASP:OD2	1:D:456:LYS:NZ	2.34	0.60
2:E:39:ASN:ND2	7:E:436:HOH:O	2.34	0.60
1:A:70:ASP:HA	1:A:109:LYS:HE3	1.82	0.60
1:A:92:HIS:HB3	2:B:181:LYS:HB3	1.82	0.60
1:A:212:PHE:HB3	1:A:215:GLN:HE21	1.65	0.60
1:A:504:ALA:O	1:A:507:VAL:HB	2.01	0.60
2:C:176:GLU:OE2	1:D:573:THR:OG1	2.18	0.60
1:A:451:ARG:NH1	1:A:454:GLU:OE1	2.34	0.60
2:C:98:TRP:CD1	2:C:153:VAL:HG21	2.36	0.60
1:D:410:ILE:HG13	1:D:418:GLN:HB2	1.82	0.60
1:D:478:PHE:CZ	1:D:562:LEU:HB2	2.36	0.60
1:A:222:VAL:O	1:A:304:ILE:N	2.33	0.60
1:D:87:PRO:HD2	2:E:188:ARG:CB	2.32	0.60
1:D:190:ASP:O	1:D:194:PHE:N	2.29	0.60
1:D:480:GLU:OE2	1:D:526:GLY:N	2.32	0.60
2:B:125:LYS:HB3	2:B:173:PHE:CE2	2.35	0.60
2:C:68:LEU:HB2	2:C:152:TYR:OH	2.02	0.60
1:D:105:GLN:HA	1:D:430:SER:HB3	1.83	0.60
1:D:140:ASP:OD1	1:D:140:ASP:N	2.35	0.60
1:D:200:GLN:HB3	1:D:254:ILE:HG23	1.81	0.60
1:D:332:SER:OG	1:D:333:SER:N	2.34	0.60
2:F:10:TYR:HB3	2:F:13:SER:HB2	1.84	0.60
1:A:232:ARG:NH2	7:A:781:HOH:O	2.32	0.60
1:A:305:MET:CB	1:A:347:PRO:HB3	2.31	0.60
1:D:76:TYR:C	1:D:79:ARG:HH21	2.07	0.60
2:E:63:PRO:O	7:E:412:HOH:O	2.16	0.60
2:E:114:TRP:HD1	2:E:167:TYR:HE1	1.48	0.60
1:A:442:GLN:HG2	1:A:462:PHE:CZ	2.31	0.60
2:C:18:ARG:NH2	2:C:103:ASP:OD1	2.23	0.60
1:D:107:ARG:HH21	1:D:434:ASP:HB3	1.67	0.60
1:D:329:ASP:OD1	1:D:329:ASP:N	2.35	0.59
1:A:107:ARG:HH11	1:A:433:ILE:HG13	1.67	0.59
1:A:152:LYS:HA	1:A:564:GLU:HB2	1.83	0.59
1:A:164:THR:OG1	1:A:557:LYS:O	2.21	0.59
2:C:57:LEU:HB3	2:C:64:VAL:CG2	2.32	0.59
1:D:79:ARG:HD2	2:E:188:ARG:HH22	1.67	0.59
2:E:23:LEU:HG	2:E:28:VAL:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:LYS:NZ	7:B:406:HOH:O	2.09	0.59
1:D:88:ILE:HG13	1:D:89:LEU:N	2.17	0.59
1:D:405:ASP:CB	1:D:541:SER:HB2	2.29	0.59
2:F:165:GLN:HG3	2:F:206:VAL:HG21	1.84	0.59
1:D:83:GLY:H	1:D:158:GLY:HA3	1.66	0.59
1:D:498:ASP:CB	1:D:510:ARG:HH22	2.15	0.59
2:F:33:ARG:NH2	2:F:35:GLU:OE2	2.35	0.59
1:D:288:TYR:O	7:D:730:HOH:O	2.16	0.59
2:F:40:LYS:HD2	2:F:52:LYS:HB3	1.85	0.59
1:A:213:ARG:HG3	1:A:214:ASP:N	2.18	0.59
1:A:441:LEU:HD23	1:A:549:ARG:HB3	1.84	0.59
1:D:152:LYS:NZ	1:D:561:ILE:HG23	2.17	0.59
2:F:143:PRO:O	2:F:185:TRP:HD1	1.85	0.59
1:D:181:SER:O	7:D:731:HOH:O	2.17	0.59
1:D:360:TYR:OH	1:D:362:GLU:OE2	2.11	0.59
1:D:535:PHE:O	1:D:538:LEU:HB3	2.02	0.59
1:A:74:GLU:HG2	1:A:78:LYS:HD3	1.84	0.59
1:A:424:ARG:CG	1:A:425:ARG:HH11	2.15	0.59
2:C:10:TYR:O	2:C:20:ARG:NH2	2.34	0.59
1:D:108:PRO:HB3	1:D:555:ASN:HB2	1.84	0.59
1:D:199:HIS:H	1:D:524:ALA:HB1	1.67	0.59
2:F:135:LEU:HD13	2:F:182:LEU:CD1	2.32	0.59
1:A:225:HIS:HB3	1:A:309:MET:SD	2.43	0.59
1:A:254:ILE:HG22	7:A:798:HOH:O	2.02	0.59
2:C:33:ARG:HH12	2:C:41:SER:HB2	1.67	0.59
2:F:110:GLN:HA	2:F:113:VAL:HG12	1.83	0.59
1:D:90:THR:CG2	1:D:112:PRO:HG2	2.32	0.59
1:D:507:VAL:HG12	7:D:726:HOH:O	2.02	0.59
1:D:527:THR:O	7:D:729:HOH:O	2.16	0.59
2:E:26:LYS:NZ	2:E:82:ASN:C	2.61	0.59
2:E:139:LEU:O	2:E:141:ASP:N	2.29	0.59
1:A:18:ASP:O	1:A:22:ARG:HG2	2.03	0.58
1:A:83:GLY:O	7:A:741:HOH:O	2.17	0.58
1:A:291:ILE:HD12	1:A:320:ALA:HB2	1.85	0.58
2:B:17:MET:SD	2:B:199:LEU:HG	2.43	0.58
2:B:184:ALA:HA	2:B:187:LYS:CG	2.33	0.58
1:D:526:GLY:O	1:D:530:LYS:HG3	2.03	0.58
2:F:24:ARG:HB3	2:F:194:SER:HA	1.85	0.58
2:F:57:LEU:O	2:F:64:VAL:HG22	2.03	0.58
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.38	0.58
2:F:98:TRP:CE3	2:F:101:PHE:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:CYS:HA	1:A:499:ARG:HB2	1.85	0.58
1:A:81:VAL:HG11	1:A:110:PHE:CE2	2.38	0.58
1:A:450:LYS:HE3	7:A:1031:HOH:O	2.03	0.58
1:A:477:ILE:HG13	1:A:518:LEU:HD23	1.86	0.58
2:F:86:PRO:HD3	2:F:146:GLY:O	2.04	0.58
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.38	0.58
2:C:86:PRO:HB2	7:C:434:HOH:O	2.04	0.58
2:F:114:TRP:HA	2:F:170:PHE:HD2	1.68	0.58
2:F:135:LEU:HD13	2:F:182:LEU:HD11	1.86	0.58
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.86	0.58
1:A:87:PRO:HD2	2:B:188:ARG:CB	2.33	0.58
1:A:559:LEU:O	1:A:562:LEU:HB3	2.03	0.58
2:B:169:LYS:HG3	2:B:170:PHE:N	2.18	0.58
2:E:13:SER:O	2:E:17:MET:HG3	2.03	0.58
2:E:193:GLU:HB2	2:E:197:LYS:HD3	1.85	0.58
1:A:38:LYS:O	2:B:142:LYS:HG3	2.03	0.58
2:E:24:ARG:HE	2:E:193:GLU:HG3	1.68	0.58
1:A:340:ASN:HB2	1:A:352:PHE:CD2	2.39	0.58
1:D:166:THR:HG23	4:D:602:LEU:OXT	2.03	0.58
2:F:10:TYR:HH	2:F:208:TYR:HH	1.49	0.58
1:A:171:ARG:N	7:A:708:HOH:O	2.34	0.58
1:D:97:ILE:HG22	1:D:162:VAL:CG2	2.34	0.58
2:E:56:VAL:HA	7:E:406:HOH:O	2.04	0.58
2:B:26:LYS:NZ	2:B:78:TRP:CD2	2.72	0.58
2:F:33:ARG:NH2	2:F:43:LEU:HD11	2.19	0.58
2:F:43:LEU:HD12	2:F:44:LEU:N	2.18	0.58
2:F:144:TYR:HB3	2:F:154:ASP:OD1	2.05	0.57
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.39	0.57
1:A:164:THR:HA	1:A:557:LYS:HG2	1.85	0.57
1:D:135:ASP:OD2	1:D:343:PRO:HD2	2.04	0.57
1:D:152:LYS:HG2	1:D:565:ASN:CB	2.34	0.57
1:D:163:GLY:CA	1:D:560:GLN:OE1	2.52	0.57
2:F:113:VAL:HB	2:F:128:PHE:CE2	2.39	0.57
1:A:150:SER:O	1:A:150:SER:OG	2.20	0.57
2:B:58:VAL:O	7:B:413:HOH:O	2.17	0.57
2:C:187:LYS:HZ3	1:D:496:CYS:HB2	1.69	0.57
1:D:39:ASN:HA	2:E:142:LYS:HG2	1.85	0.57
1:D:432:ASN:O	1:D:433:ILE:HG23	2.04	0.57
1:A:478:PHE:CZ	1:A:562:LEU:HG	2.40	0.57
2:C:114:TRP:HA	2:C:170:PHE:HD2	1.69	0.57
1:D:518:LEU:N	7:D:719:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:LEU:O	2:E:142:LYS:HG3	2.04	0.57
1:A:165:ALA:HB1	4:A:602:LEU:HD12	1.86	0.57
1:A:284:LEU:HD13	1:A:287:TRP:N	2.19	0.57
1:A:428:ILE:HG13	1:A:428:ILE:O	2.03	0.57
1:A:452:LEU:HD13	1:A:493:CYS:SG	2.44	0.57
2:C:7:LEU:HD21	2:C:23:LEU:HD12	1.85	0.57
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.39	0.57
1:D:97:ILE:HG22	1:D:162:VAL:HG23	1.85	0.57
1:D:369:THR:OG1	1:D:370:GLY:N	2.34	0.57
1:A:80:MET:HG3	1:A:88:ILE:HD12	1.86	0.57
1:A:206:LEU:O	1:A:210:ILE:HG13	2.04	0.57
2:B:20:ARG:NH1	2:B:198:SER:O	2.37	0.57
2:B:158:ILE:HG12	2:B:195:VAL:HG21	1.87	0.57
1:D:35:ILE:HD13	1:D:394:ASN:HA	1.86	0.57
2:E:169:LYS:HG3	2:E:170:PHE:H	1.69	0.57
2:F:72:GLN:HG2	2:F:152:TYR:HE1	1.69	0.57
1:A:465:TYR:HA	1:A:551:VAL:HB	1.87	0.57
1:D:382:VAL:HG13	1:D:388:TYR:CD2	2.40	0.57
1:A:148:ILE:HD12	1:A:170:TYR:CZ	2.39	0.57
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.39	0.57
1:D:108:PRO:HG2	1:D:552:LYS:HB3	1.85	0.57
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.35	0.57
2:E:201:ASP:HB2	2:E:204:LYS:HG3	1.87	0.57
1:A:152:LYS:HG3	1:A:565:ASN:CG	2.30	0.57
2:B:162:SER:O	2:B:205:ILE:HG12	2.05	0.57
2:C:102:VAL:O	2:C:107:THR:HG23	2.05	0.57
2:C:153:VAL:O	2:C:157:LEU:HD23	2.05	0.57
2:E:26:LYS:HE2	7:E:417:HOH:O	2.05	0.57
1:A:526:GLY:O	1:A:530:LYS:HG3	2.05	0.56
2:B:117:LYS:HG2	2:B:213:ARG:NH1	2.17	0.56
2:C:57:LEU:HB3	2:C:64:VAL:HG22	1.87	0.56
2:C:84:PHE:HB2	2:C:152:TYR:N	2.20	0.56
2:C:86:PRO:HD3	2:C:146:GLY:O	2.05	0.56
1:D:165:ALA:HB1	4:D:602:LEU:HD12	1.87	0.56
2:F:98:TRP:HE3	2:F:101:PHE:HB2	1.68	0.56
1:A:521:ARG:HB3	1:A:566:VAL:HG12	1.88	0.56
2:C:18:ARG:NH1	2:C:67:SER:OG	2.38	0.56
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.40	0.56
2:C:184:ALA:HB1	1:D:499:ARG:HH11	1.68	0.56
1:D:340:ASN:HD21	1:D:345:LEU:HD11	1.71	0.56
2:E:166:ALA:HA	2:E:169:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:HD21	2:B:90:TYR:HB3	1.70	0.56
1:A:152:LYS:HG3	1:A:565:ASN:ND2	2.21	0.56
1:A:412:PHE:CZ	1:A:417:PRO:HB3	2.41	0.56
2:C:136:GLU:HG3	2:C:181:LYS:CD	2.31	0.56
1:D:236:GLN:NE2	7:D:795:HOH:O	2.37	0.56
1:D:247:ASP:HB2	1:D:249:VAL:HG22	1.86	0.56
1:D:434:ASP:OD1	1:D:435:LYS:HG3	2.05	0.56
1:D:438:GLU:O	1:D:442:GLN:HG3	2.06	0.56
2:C:53:LYS:O	7:C:411:HOH:O	2.17	0.56
1:D:110:PHE:CE2	1:D:554:SER:HA	2.40	0.56
2:E:145:PHE:HB2	2:E:154:ASP:OD1	2.05	0.56
2:F:140:GLY:CA	2:F:181:LYS:NZ	2.69	0.56
1:A:96:ALA:HB3	1:A:113:PHE:CD2	2.40	0.56
2:C:64:VAL:HB	2:C:73:TYR:CE2	2.41	0.56
1:D:198:VAL:HG22	1:D:524:ALA:HB3	1.87	0.56
1:D:199:HIS:N	1:D:524:ALA:HB1	2.20	0.56
1:D:405:ASP:OD1	1:D:540:SER:HB2	2.05	0.56
1:A:97:ILE:N	1:A:163:GLY:H	2.04	0.56
1:A:315:LYS:O	1:A:318:HIS:HB3	2.06	0.56
1:A:506:TYR:OH	1:A:518:LEU:HD11	2.05	0.56
1:D:22:ARG:NH1	1:D:414:ASN:CG	2.64	0.56
1:D:529:ARG:NH1	1:D:533:GLU:OE2	2.38	0.56
1:A:153:GLN:HG2	1:A:167:THR:HG21	1.88	0.56
2:B:8:LEU:HB2	2:B:56:VAL:HB	1.88	0.56
2:B:139:LEU:O	2:B:141:ASP:N	2.38	0.56
1:D:18:ASP:OD1	1:D:414:ASN:ND2	2.39	0.56
1:A:182:ILE:HG13	1:A:183:THR:HG23	1.86	0.56
1:A:319:TYR:HA	7:A:753:HOH:O	2.06	0.56
2:C:98:TRP:O	2:C:101:PHE:HB2	2.05	0.56
2:C:184:ALA:O	1:D:499:ARG:NH2	2.39	0.56
1:D:92:HIS:CG	2:E:139:LEU:HD23	2.40	0.56
1:A:105:GLN:OE1	7:A:743:HOH:O	2.18	0.56
1:A:267:LEU:HG	7:A:773:HOH:O	2.06	0.56
1:A:369:THR:HG23	1:A:370:GLY:H	1.71	0.56
2:C:10:TYR:HB3	2:C:13:SER:HB2	1.88	0.56
1:D:23:ASN:O	1:D:27:VAL:HG12	2.06	0.56
1:D:76:TYR:HD2	1:D:88:ILE:HD11	1.70	0.56
1:D:143:LYS:HB2	1:D:185:PRO:O	2.06	0.56
1:D:531:ILE:HG21	1:D:547:MET:HG2	1.87	0.56
2:F:72:GLN:HG2	2:F:152:TYR:CE1	2.40	0.56
2:F:208:TYR:O	7:F:406:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HH21	1:A:296:PRO:HG3	1.72	0.55
1:A:552:LYS:HD2	1:A:553:PRO:HD2	1.89	0.55
1:D:77:ILE:HG22	1:D:110:PHE:HB3	1.86	0.55
1:D:212:PHE:O	1:D:216:VAL:HG13	2.07	0.55
2:E:53:LYS:HD3	6:E:301:GSH:HB13	1.88	0.55
1:A:152:LYS:HD3	1:A:561:ILE:O	2.06	0.55
2:B:58:VAL:HG22	2:B:63:PRO:HB3	1.88	0.55
1:A:94:VAL:HB	1:A:113:PHE:O	2.06	0.55
2:B:17:MET:HG2	2:B:20:ARG:NH1	2.21	0.55
1:D:90:THR:HG23	7:D:742:HOH:O	2.05	0.55
1:D:410:ILE:HG21	1:D:420:LYS:HB3	1.89	0.55
2:E:64:VAL:HG23	2:F:93:ALA:HB1	1.87	0.55
2:B:76:GLU:OE2	2:C:92:ARG:NE	2.39	0.55
2:B:96:ARG:HH12	2:C:76:GLU:CD	2.14	0.55
2:C:197:LYS:NZ	7:C:433:HOH:O	2.39	0.55
1:D:42:ALA:HA	2:E:143:PRO:HG3	1.87	0.55
1:D:98:SER:C	1:D:556:ALA:HB3	2.31	0.55
1:D:478:PHE:CE1	1:D:521:ARG:HD2	2.40	0.55
2:E:153:VAL:O	2:E:156:SER:OG	2.15	0.55
1:A:32:LEU:HD22	1:A:360:TYR:CZ	2.42	0.55
1:A:152:LYS:HD3	1:A:561:ILE:C	2.32	0.55
1:A:202:LEU:CD2	1:A:205:HIS:HB3	2.36	0.55
1:A:300:TYR:CD2	1:A:302:TYR:HB2	2.41	0.55
1:D:12:ARG:NH2	7:D:803:HOH:O	2.39	0.55
2:F:37:PHE:O	2:F:40:LYS:NZ	2.40	0.55
1:A:93:PRO:HG2	2:B:184:ALA:CB	2.37	0.55
1:A:164:THR:N	1:A:560:GLN:OE1	2.40	0.55
2:E:174:SER:HB3	2:E:177:SER:HB2	1.89	0.55
1:A:92:HIS:NE2	2:B:139:LEU:HB3	2.22	0.55
1:A:238:TRP:HH2	1:A:281:CYS:HB3	1.69	0.55
1:A:250:LEU:HD11	1:A:260:ARG:CZ	2.37	0.55
1:A:315:LYS:HA	1:A:318:HIS:HB3	1.89	0.55
2:C:32:TYR:CD1	2:C:34:GLU:OE2	2.60	0.55
2:F:84:PHE:HB2	2:F:152:TYR:N	2.21	0.55
2:F:214:LYS:NZ	7:F:411:HOH:O	2.22	0.55
1:A:42:ALA:HB3	1:A:45:LEU:HD22	1.88	0.55
1:A:219:VAL:HB	1:A:295:PHE:HZ	1.71	0.55
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.87	0.55
1:D:104:SER:O	1:D:107:ARG:HB2	2.07	0.55
2:E:7:LEU:HB2	2:E:57:LEU:HD13	1.89	0.55
1:A:39:ASN:ND2	1:A:90:THR:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:N	1:A:314:PRO:HD2	2.21	0.55
2:E:195:VAL:HG23	2:E:199:LEU:HD22	1.88	0.55
2:F:98:TRP:CD2	2:F:138:GLU:OE2	2.59	0.55
1:A:468:VAL:O	7:A:744:HOH:O	2.18	0.54
2:B:33:ARG:NH1	7:B:444:HOH:O	2.40	0.54
2:C:64:VAL:HG23	2:C:70:VAL:HG22	1.88	0.54
2:C:98:TRP:O	2:C:102:VAL:HG23	2.07	0.54
2:C:117:LYS:HE3	2:C:213:ARG:HH11	1.72	0.54
1:D:79:ARG:NH2	1:D:88:ILE:CB	2.70	0.54
2:F:64:VAL:HB	2:F:73:TYR:CD2	2.42	0.54
2:F:126:LYS:O	2:F:129:ILE:HG13	2.07	0.54
1:A:162:VAL:HG21	1:A:559:LEU:HD13	1.89	0.54
1:A:424:ARG:HD2	1:A:425:ARG:NH1	2.23	0.54
2:C:140:GLY:O	7:C:412:HOH:O	2.18	0.54
1:D:302:TYR:HD1	1:D:326:VAL:HG13	1.73	0.54
2:E:96:ARG:NH2	2:F:69:ASN:OD1	2.40	0.54
2:F:98:TRP:O	2:F:101:PHE:HB2	2.06	0.54
2:F:178:GLU:OE1	7:F:407:HOH:O	2.18	0.54
2:C:141:ASP:N	2:C:141:ASP:OD1	2.40	0.54
1:D:223:PHE:HB2	1:D:225:HIS:HD2	1.71	0.54
1:A:31:THR:OG1	1:A:357:ASN:HA	2.07	0.54
1:D:13:VAL:HA	1:D:16:GLU:OE2	2.07	0.54
1:D:82:ASP:N	7:D:728:HOH:O	2.39	0.54
1:D:114:THR:HG23	2:E:141:ASP:OD2	2.08	0.54
1:D:437:THR:O	1:D:440:ASP:N	2.41	0.54
1:A:85:THR:N	7:A:804:HOH:O	2.40	0.54
1:A:231:PHE:O	1:A:235:GLU:HB2	2.07	0.54
1:D:506:TYR:CE2	1:D:510:ARG:NH1	2.75	0.54
1:A:81:VAL:O	7:A:742:HOH:O	2.17	0.54
1:A:124:LEU:HD12	1:A:355:ILE:HD12	1.89	0.54
1:D:163:GLY:HA2	1:D:560:GLN:HB2	1.90	0.54
1:D:496:CYS:N	1:D:499:ARG:NH1	2.56	0.54
2:E:159:THR:HA	2:E:199:LEU:HD21	1.90	0.54
2:E:201:ASP:OD2	2:E:204:LYS:HE2	2.07	0.54
2:E:8:LEU:HD21	2:E:43:LEU:HD23	1.90	0.54
2:E:15:PHE:HB3	2:E:67:SER:CB	2.38	0.54
1:A:557:LYS:O	1:A:561:ILE:HG13	2.07	0.54
2:E:144:TYR:OH	2:E:151:GLY:N	2.28	0.54
1:A:125:PHE:HB3	1:A:182:ILE:HD12	1.88	0.54
1:A:262:ALA:HA	1:A:265:LYS:HZ2	1.73	0.54
2:C:117:LYS:HA	2:C:121:GLN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:VAL:HG23	1:D:556:ALA:HB1	1.90	0.54
2:F:9:ASP:HA	2:F:54:ILE:HD13	1.89	0.54
1:A:85:THR:O	2:B:184:ALA:HB1	2.08	0.54
1:A:266:LEU:HB2	7:A:773:HOH:O	2.08	0.54
1:D:221:ALA:HB3	1:D:227:LEU:HG	1.90	0.54
1:D:562:LEU:HD12	1:D:563:CYS:N	2.22	0.54
1:A:428:ILE:HG23	7:A:978:HOH:O	2.07	0.53
2:B:92:ARG:HG3	7:B:401:HOH:O	2.07	0.53
2:C:150:PHE:CD1	2:C:192:LYS:HG3	2.43	0.53
1:D:219:VAL:HG13	1:D:301:VAL:HG13	1.89	0.53
1:D:563:CYS:O	1:D:566:VAL:HG22	2.08	0.53
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.43	0.53
2:F:23:LEU:HD22	2:F:28:VAL:HG11	1.88	0.53
2:F:107:THR:HG22	2:F:160:PHE:CZ	2.43	0.53
1:A:363:PHE:HE1	1:A:390:VAL:HG22	1.73	0.53
1:A:40:GLN:HG2	2:B:142:LYS:HE3	1.89	0.53
1:A:99:LEU:HD23	1:A:535:PHE:HZ	1.73	0.53
1:A:154:TYR:CE2	1:A:156:SER:HA	2.43	0.53
1:A:417:PRO:HB2	7:A:800:HOH:O	2.08	0.53
2:B:57:LEU:HD22	2:B:70:VAL:HG13	1.91	0.53
1:D:47:ASN:ND2	7:D:808:HOH:O	2.41	0.53
2:E:26:LYS:HE3	2:E:81:LYS:HZ1	1.73	0.53
1:A:302:TYR:CD2	1:A:328:HIS:NE2	2.77	0.53
1:D:44:TYR:HD2	1:D:45:LEU:HD12	1.73	0.53
1:D:151:SER:O	1:D:171:ARG:NH2	2.42	0.53
1:D:494:CYS:HB2	7:D:815:HOH:O	2.07	0.53
1:A:200:GLN:HE21	1:A:259:VAL:HG11	1.74	0.53
2:B:96:ARG:HE	2:C:73:TYR:HE1	1.57	0.53
2:C:57:LEU:O	2:C:64:VAL:HG22	2.08	0.53
1:D:151:SER:HB2	1:D:194:PHE:C	2.34	0.53
1:D:169:VAL:O	1:D:175:PHE:HB2	2.09	0.53
2:E:176:GLU:HB2	2:E:183:ILE:HD12	1.90	0.53
2:F:192:LYS:NZ	7:F:436:HOH:O	2.41	0.53
1:A:99:LEU:HD12	1:A:555:ASN:CG	2.33	0.53
1:A:200:GLN:OE1	7:A:733:HOH:O	2.18	0.53
1:A:202:LEU:C	1:A:205:HIS:ND1	2.62	0.53
1:D:36:LEU:HD22	1:D:61:PHE:CE1	2.44	0.53
2:E:68:LEU:HD11	2:E:152:TYR:CE1	2.43	0.53
1:A:45:LEU:HG	1:A:50:LEU:HD22	1.90	0.53
1:A:83:GLY:H	1:A:158:GLY:HA3	1.72	0.53
1:A:314:PRO:HA	1:A:317:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:HA	1:A:398:LEU:O	2.08	0.53
2:F:120:GLU:O	7:F:405:HOH:O	2.17	0.53
1:A:151:SER:OG	1:A:195:SER:O	2.26	0.53
1:A:203:TYR:CE1	1:A:241:ILE:HG22	2.44	0.53
1:D:109:LYS:N	1:D:555:ASN:OD1	2.29	0.53
1:D:217:GLN:NE2	7:D:810:HOH:O	2.42	0.53
1:D:451:ARG:NH1	1:D:454:GLU:CD	2.67	0.53
1:A:122:LEU:O	1:A:126:ARG:HB2	2.09	0.53
1:A:158:GLY:N	7:A:742:HOH:O	2.41	0.53
1:A:512:CYS:SG	1:A:514:THR:HG23	2.48	0.53
2:B:62:LYS:HB2	2:C:90:TYR:CZ	2.43	0.53
1:D:253:ARG:NH1	1:D:484:GLU:HB3	2.24	0.53
1:D:433:ILE:HD11	1:D:552:LYS:HE3	1.90	0.53
1:A:451:ARG:NE	7:A:812:HOH:O	2.42	0.52
1:A:460:ILE:HD11	1:A:480:GLU:HG2	1.91	0.52
2:B:108:ASP:O	2:B:112:LYS:HG2	2.09	0.52
2:E:5:PRO:HB3	2:E:59:HIS:CD2	2.44	0.52
2:F:5:PRO:HG3	2:F:59:HIS:CE1	2.44	0.52
1:A:432:ASN:CG	1:A:433:ILE:N	2.67	0.52
1:D:496:CYS:HA	1:D:499:ARG:NH1	2.24	0.52
2:E:154:ASP:HB3	2:E:158:ILE:HD11	1.90	0.52
1:A:92:HIS:CE1	2:B:139:LEU:HD23	2.44	0.52
1:A:522:VAL:O	1:A:567:VAL:HG22	2.09	0.52
2:B:169:LYS:HG3	2:B:170:PHE:H	1.74	0.52
1:A:260:ARG:HB2	7:A:798:HOH:O	2.08	0.52
1:D:88:ILE:HG13	1:D:89:LEU:HG	1.90	0.52
2:F:165:GLN:HG3	2:F:206:VAL:CG2	2.39	0.52
1:A:97:ILE:O	1:A:163:GLY:N	2.42	0.52
1:A:223:PHE:CE1	1:A:304:ILE:HD12	2.45	0.52
2:C:98:TRP:CD1	2:C:153:VAL:HG11	2.44	0.52
1:A:301:VAL:HG22	7:A:889:HOH:O	2.08	0.52
1:A:540:SER:HG	1:A:544:GLN:HE21	1.55	0.52
1:D:208:SER:HA	1:D:211:LEU:HD12	1.92	0.52
1:D:451:ARG:HH11	1:D:454:GLU:CD	2.17	0.52
2:E:96:ARG:HH21	2:F:69:ASN:HA	1.75	0.52
2:F:201:ASP:HB2	2:F:204:LYS:HG3	1.92	0.52
1:A:73:LEU:HD22	1:A:89:LEU:HD13	1.91	0.52
1:A:207:LEU:HD21	1:A:263:MET:HE2	1.92	0.52
1:A:224:ALA:HB3	1:A:309:MET:HB3	1.92	0.52
1:A:302:TYR:HA	1:A:326:VAL:HG13	1.91	0.52
1:A:437:THR:O	1:A:440:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:PHE:HB3	2:C:153:VAL:HG13	1.91	0.52
2:E:74:VAL:HG12	7:E:516:HOH:O	2.09	0.52
1:A:149:PHE:CZ	1:A:202:LEU:HB2	2.44	0.52
1:A:172:ASN:ND2	7:A:817:HOH:O	2.43	0.52
1:A:432:ASN:HD21	1:A:434:ASP:CG	2.17	0.52
1:A:538:LEU:HD12	1:A:539:GLY:N	2.25	0.52
1:A:552:LYS:CD	1:A:553:PRO:HD2	2.40	0.52
2:C:183:ILE:HD11	1:D:451:ARG:HE	1.74	0.52
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.42	0.52
1:D:385:GLY:HA2	1:D:408:LYS:HE3	1.92	0.52
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.74	0.52
1:A:423:CYS:SG	1:A:543:GLY:N	2.83	0.52
1:A:498:ASP:HB2	7:A:707:HOH:O	2.10	0.52
2:C:40:LYS:HD2	2:C:52:LYS:HB3	1.92	0.52
2:E:26:LYS:HE3	2:E:81:LYS:NZ	2.25	0.52
2:E:98:TRP:CZ2	2:E:138:GLU:HB2	2.45	0.52
2:F:68:LEU:O	2:F:72:GLN:HG3	2.09	0.52
2:F:84:PHE:CG	2:F:152:TYR:HB2	2.45	0.52
1:A:405:ASP:HB3	1:A:541:SER:CB	2.35	0.52
1:A:538:LEU:HD12	1:A:539:GLY:H	1.75	0.52
2:F:108:ASP:O	2:F:112:LYS:HG2	2.10	0.52
2:F:132:VAL:HG22	2:F:179:SER:CB	2.38	0.52
2:C:8:LEU:HD21	2:C:43:LEU:HD11	1.92	0.51
2:C:187:LYS:HE3	1:D:492:ASP:O	2.10	0.51
2:F:56:VAL:HG13	7:F:465:HOH:O	2.09	0.51
1:A:153:GLN:O	1:A:564:GLU:HG2	2.10	0.51
1:A:470:THR:HG21	1:A:474:HIS:CE1	2.45	0.51
1:D:330:TYR:HE2	1:D:540:SER:H	1.53	0.51
1:D:457:ILE:HD11	1:D:481:ILE:HB	1.92	0.51
1:A:32:LEU:HB2	1:A:360:TYR:CD1	2.46	0.51
1:A:58:GLU:HG2	1:A:62:LYS:HE2	1.91	0.51
1:A:81:VAL:HG13	1:A:82:ASP:OD2	2.09	0.51
1:A:331:GLY:N	1:A:537:GLY:O	2.43	0.51
1:A:405:ASP:CB	1:A:541:SER:HB3	2.35	0.51
2:B:19:ALA:N	7:B:408:HOH:O	2.43	0.51
2:B:92:ARG:N	7:B:401:HOH:O	2.42	0.51
2:B:107:THR:HA	2:B:110:GLN:HG2	1.92	0.51
1:D:291:ILE:HB	1:D:320:ALA:HA	1.92	0.51
1:D:511:LYS:HB2	7:D:726:HOH:O	2.09	0.51
2:F:165:GLN:O	2:F:165:GLN:NE2	2.44	0.51
1:A:77:ILE:HD13	1:A:112:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ARG:CG	1:A:425:ARG:NH1	2.74	0.51
1:A:531:ILE:HA	1:A:534:HIS:NE2	2.25	0.51
2:B:96:ARG:HH11	2:C:73:TYR:HE1	1.56	0.51
1:D:90:THR:HG1	1:D:91:GLY:N	2.03	0.51
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.90	0.51
1:D:167:THR:OG1	7:D:735:HOH:O	2.19	0.51
2:F:26:LYS:HD3	2:F:78:TRP:HB2	1.91	0.51
2:F:131:ALA:O	2:F:135:LEU:HB2	2.11	0.51
2:F:145:PHE:HB3	2:F:153:VAL:HG13	1.91	0.51
2:B:188:ARG:HG2	7:B:454:HOH:O	2.10	0.51
1:D:138:ILE:O	7:D:734:HOH:O	2.19	0.51
1:D:223:PHE:HD2	1:D:225:HIS:CD2	2.28	0.51
1:D:225:HIS:HE2	1:D:529:ARG:HG3	1.73	0.51
1:D:424:ARG:NH1	1:D:424:ARG:HB3	2.25	0.51
2:E:145:PHE:N	2:E:154:ASP:OD1	2.41	0.51
2:F:110:GLN:O	2:F:113:VAL:HG12	2.10	0.51
2:F:188:ARG:HD2	2:F:191:GLU:OE2	2.09	0.51
1:A:167:THR:HB	1:A:560:GLN:CD	2.36	0.51
1:A:438:GLU:O	1:A:442:GLN:HG3	2.11	0.51
1:A:476:ALA:HA	1:A:519:GLU:O	2.11	0.51
1:D:222:VAL:HB	1:D:533:GLU:HB3	1.93	0.51
1:A:96:ALA:O	1:A:113:PHE:HB3	2.11	0.51
1:A:147:PHE:CB	1:A:205:HIS:CD2	2.94	0.51
1:A:147:PHE:CB	1:A:205:HIS:HD2	2.24	0.51
2:C:187:LYS:NZ	1:D:496:CYS:HB2	2.26	0.51
1:D:20:MET:SD	7:D:757:HOH:O	2.58	0.51
1:D:69:THR:N	1:D:72:GLU:OE1	2.43	0.51
1:D:122:LEU:HD23	1:D:125:PHE:CZ	2.46	0.51
1:D:295:PHE:CD1	1:D:298:ALA:HB2	2.43	0.51
1:D:541:SER:O	1:D:543:GLY:N	2.41	0.51
1:A:147:PHE:CD1	1:A:205:HIS:CG	2.93	0.51
2:B:166:ALA:O	2:B:170:PHE:HB2	2.10	0.51
1:D:9:ASP:N	7:D:812:HOH:O	2.42	0.51
1:D:11:ASN:O	1:D:14:ILE:HG13	2.11	0.51
1:D:62:LYS:HB3	1:D:400:ARG:HH12	1.75	0.51
1:D:218:TYR:N	7:D:813:HOH:O	2.42	0.51
1:D:383:LYS:NZ	7:D:819:HOH:O	2.44	0.51
2:E:8:LEU:HB2	7:E:438:HOH:O	2.11	0.51
2:E:57:LEU:HG	2:E:59:HIS:NE2	2.26	0.51
2:F:70:VAL:O	2:F:73:TYR:HB2	2.10	0.51
2:F:102:VAL:O	2:F:107:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CE1	1:A:328:HIS:HE1	2.29	0.51
1:D:70:ASP:OD1	1:D:71:VAL:N	2.44	0.51
1:D:153:GLN:H	1:D:564:GLU:HB2	1.76	0.51
2:F:144:TYR:HA	2:F:185:TRP:NE1	2.25	0.51
1:A:149:PHE:HZ	1:A:202:LEU:HB2	1.76	0.51
1:A:334:GLU:O	1:A:394:ASN:ND2	2.44	0.51
1:D:204:CYS:HA	1:D:207:LEU:HB3	1.93	0.51
1:D:365:PRO:HG3	1:D:388:TYR:CE2	2.46	0.51
1:D:527:THR:O	1:D:530:LYS:HB2	2.12	0.51
1:A:77:ILE:HG13	1:A:89:LEU:HD12	1.93	0.50
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.93	0.50
1:A:556:ALA:HA	1:A:559:LEU:HB2	1.93	0.50
1:D:99:LEU:CB	1:D:557:LYS:H	2.24	0.50
1:A:22:ARG:NH2	1:A:415:ASN:OD1	2.44	0.50
1:A:94:VAL:HG21	1:A:112:PRO:HA	1.94	0.50
2:B:26:LYS:NZ	2:B:78:TRP:CG	2.78	0.50
1:D:223:PHE:HZ	1:D:536:LEU:CB	2.24	0.50
1:D:235:GLU:OE1	7:D:736:HOH:O	2.20	0.50
2:E:214:LYS:NZ	7:E:409:HOH:O	2.11	0.50
1:A:112:PRO:HD2	1:A:396:ALA:O	2.11	0.50
1:A:149:PHE:CZ	1:A:202:LEU:CB	2.94	0.50
2:B:65:CYS:O	2:B:66:GLU:HB2	2.11	0.50
1:D:94:VAL:HB	1:D:113:PHE:O	2.11	0.50
1:D:299:LYS:HG3	7:D:823:HOH:O	2.12	0.50
1:D:424:ARG:HE	1:D:425:ARG:CD	2.20	0.50
1:D:510:ARG:NH1	1:D:518:LEU:HG	2.26	0.50
2:E:10:TYR:HA	2:E:34:GLU:OE2	2.12	0.50
1:A:223:PHE:CE1	1:A:533:GLU:HA	2.46	0.50
2:B:17:MET:HE2	2:B:200:PRO:HD2	1.94	0.50
1:D:200:GLN:HG2	1:D:254:ILE:HA	1.93	0.50
2:E:109:ALA:O	2:E:113:VAL:HG23	2.12	0.50
1:A:152:LYS:HE3	1:A:527:THR:HG21	1.93	0.50
1:A:237:VAL:O	1:A:241:ILE:HG23	2.11	0.50
1:A:273:LEU:HA	1:A:276:THR:HG23	1.92	0.50
1:A:276:THR:O	1:A:279:THR:OG1	2.23	0.50
1:A:526:GLY:C	1:A:529:ARG:HH11	2.19	0.50
1:D:276:THR:OG1	1:D:277:ILE:N	2.44	0.50
1:D:303:GLY:O	1:D:327:SER:HA	2.12	0.50
1:D:464:SER:HB2	1:D:550:CYS:HB2	1.93	0.50
2:F:50:ILE:HG13	2:F:51:HIS:H	1.76	0.50
2:F:97:PHE:CE1	2:F:101:PHE:HE1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:SER:O	1:D:211:LEU:HB2	2.11	0.50
1:D:296:PRO:HD2	7:D:861:HOH:O	2.11	0.50
1:D:391:VAL:HG22	1:D:402:ARG:HA	1.93	0.50
1:A:93:PRO:HG2	2:B:184:ALA:HB3	1.94	0.50
2:B:130:GLU:OE2	2:B:133:LYS:HD2	2.11	0.50
1:D:90:THR:HG23	1:D:112:PRO:HG2	1.93	0.50
1:D:114:THR:HG23	2:E:181:LYS:HZ2	1.77	0.50
1:D:522:VAL:O	1:D:567:VAL:HG12	2.12	0.50
1:D:531:ILE:HA	1:D:534:HIS:CD2	2.46	0.50
2:E:144:TYR:CZ	2:E:151:GLY:N	2.79	0.50
2:F:141:ASP:N	2:F:141:ASP:OD1	2.45	0.50
1:A:20:MET:HG2	1:A:356:PRO:CG	2.42	0.50
1:A:77:ILE:CG2	1:A:110:PHE:HB3	2.41	0.50
1:A:135:ASP:OD2	1:A:343:PRO:HD2	2.12	0.50
1:A:138:ILE:HB	1:A:217:GLN:CG	2.39	0.50
2:C:144:TYR:HB3	2:C:154:ASP:CG	2.37	0.50
1:D:122:LEU:HA	1:D:125:PHE:CE2	2.47	0.50
1:D:551:VAL:HG23	1:D:555:ASN:HB2	1.93	0.50
1:A:32:LEU:HD21	1:A:61:PHE:HD2	1.76	0.50
1:A:53:ASN:HB2	2:B:88:ASP:CG	2.37	0.50
2:B:54:ILE:HB	2:B:55:PRO:HA	1.93	0.50
2:B:90:TYR:O	2:B:93:ALA:HB3	2.12	0.50
2:C:135:LEU:HD22	2:C:182:LEU:CD1	2.34	0.50
1:D:34:GLU:O	1:D:38:LYS:HG2	2.11	0.50
1:D:85:THR:HA	7:D:866:HOH:O	2.12	0.50
1:D:231:PHE:CZ	1:D:291:ILE:HG12	2.47	0.50
1:D:491:GLN:NE2	1:D:570:TYR:HB3	2.27	0.50
2:F:17:MET:SD	2:F:199:LEU:HG	2.52	0.50
1:A:163:GLY:HA2	1:A:560:GLN:CB	2.33	0.49
2:B:161:SER:HA	2:B:164:PHE:CD2	2.47	0.49
1:D:35:ILE:HA	1:D:395:TYR:CE1	2.47	0.49
1:D:273:LEU:HA	1:D:276:THR:HG23	1.93	0.49
2:E:14:MET:O	2:E:17:MET:HB2	2.12	0.49
2:E:95:ALA:HB1	2:E:152:TYR:HD2	1.77	0.49
2:F:98:TRP:CD1	2:F:153:VAL:HG11	2.47	0.49
1:A:53:ASN:HD22	2:B:88:ASP:CG	2.19	0.49
1:A:510:ARG:NH1	1:A:575:PHE:CE2	2.80	0.49
1:D:43:ILE:HD11	1:D:88:ILE:HD11	1.94	0.49
1:A:250:LEU:HD11	1:A:260:ARG:NH1	2.28	0.49
2:C:15:PHE:O	7:C:413:HOH:O	2.19	0.49
2:C:140:GLY:N	2:C:181:LYS:HZ1	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:O	1:D:216:VAL:HA	2.12	0.49
2:F:140:GLY:O	2:F:181:LYS:NZ	2.45	0.49
1:A:22:ARG:HH21	1:A:415:ASN:CG	2.20	0.49
1:A:166:THR:HG23	4:A:602:LEU:O	2.11	0.49
1:A:421:PHE:CE1	1:A:541:SER:HA	2.47	0.49
1:D:39:ASN:O	7:D:737:HOH:O	2.20	0.49
1:D:342:THR:O	1:D:345:LEU:HG	2.12	0.49
1:A:330:TYR:HE2	1:A:352:PHE:CE1	2.31	0.49
3:A:601:JAA:C05	4:A:602:LEU:HB2	2.42	0.49
1:D:197:ASP:HB2	1:D:200:GLN:OE1	2.13	0.49
1:A:17:PHE:CE2	1:A:341:VAL:HG11	2.47	0.49
1:A:23:ASN:O	1:A:27:VAL:HG12	2.13	0.49
1:A:199:HIS:CD2	1:A:200:GLN:H	2.30	0.49
1:A:434:ASP:HB2	1:A:550:CYS:HB3	1.93	0.49
1:A:451:ARG:NH1	1:A:454:GLU:CD	2.70	0.49
1:A:506:TYR:CE2	1:A:510:ARG:NE	2.81	0.49
2:C:126:LYS:O	2:C:129:ILE:HG13	2.12	0.49
2:C:159:THR:HA	2:C:199:LEU:HD21	1.95	0.49
2:C:194:SER:O	2:C:198:SER:OG	2.25	0.49
1:D:387:GLU:HB3	1:D:406:VAL:CG1	2.42	0.49
2:F:143:PRO:O	2:F:185:TRP:CD1	2.65	0.49
1:A:244:ASP:HB3	1:A:250:LEU:HA	1.94	0.49
1:A:490:LEU:HD22	1:A:522:VAL:HG11	1.94	0.49
2:B:75:ASP:OD1	7:B:416:HOH:O	2.20	0.49
2:C:104:LYS:HG3	2:C:105:LYS:N	2.28	0.49
2:C:201:ASP:OD2	1:D:456:LYS:HG3	2.12	0.49
1:D:89:LEU:O	7:D:738:HOH:O	2.20	0.49
1:D:143:LYS:CG	1:D:216:VAL:HG12	2.42	0.49
1:D:253:ARG:NH2	7:D:756:HOH:O	2.26	0.49
1:D:303:GLY:O	1:D:328:HIS:N	2.44	0.49
1:D:510:ARG:HH21	1:D:575:PHE:HE2	1.56	0.49
1:A:378:GLY:N	1:A:381:GLN:HB2	2.28	0.49
1:A:462:PHE:O	1:A:549:ARG:NH1	2.46	0.49
1:A:528:PHE:HA	1:A:531:ILE:CG1	2.43	0.49
2:C:50:ILE:HG13	2:C:51:HIS:H	1.78	0.49
1:D:253:ARG:NH1	1:D:484:GLU:H	2.10	0.49
2:E:15:PHE:O	2:E:18:ARG:HB2	2.12	0.49
1:A:23:ASN:C	1:A:27:VAL:HG12	2.38	0.49
2:C:188:ARG:NH1	1:D:500:ALA:HA	2.27	0.49
1:D:407:VAL:HG11	1:D:419:LEU:HD13	1.94	0.49
1:D:441:LEU:HG	1:D:462:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:ARG:NE	2:E:193:GLU:HG3	2.28	0.49
2:E:92:ARG:NH1	2:F:76:GLU:OE1	2.46	0.49
2:E:184:ALA:HA	2:E:187:LYS:HB2	1.95	0.49
2:F:126:LYS:NZ	7:F:415:HOH:O	2.26	0.49
1:A:99:LEU:HB3	1:A:557:LYS:N	2.18	0.49
1:A:149:PHE:HD2	1:A:529:ARG:NH2	2.09	0.49
1:A:149:PHE:CB	1:A:530:LYS:HD3	2.43	0.49
1:A:445:VAL:HA	1:A:479:TRP:CZ2	2.48	0.49
2:C:17:MET:SD	2:C:199:LEU:HG	2.53	0.49
1:D:465:TYR:CB	1:D:551:VAL:HG13	2.37	0.49
2:E:90:TYR:O	2:E:93:ALA:HB3	2.13	0.49
1:A:87:PRO:C	1:A:88:ILE:HG13	2.38	0.48
1:D:88:ILE:HG23	1:D:89:LEU:N	2.15	0.48
1:D:538:LEU:HD23	1:D:544:GLN:HG2	1.94	0.48
2:B:151:GLY:O	2:B:154:ASP:HB2	2.13	0.48
2:C:169:LYS:HD3	2:C:206:VAL:HG13	1.95	0.48
1:D:120:ASN:CG	1:D:358:LEU:HD22	2.38	0.48
1:D:453:SER:HA	1:D:457:ILE:HG22	1.95	0.48
1:D:480:GLU:HG3	1:D:525:LYS:HA	1.94	0.48
1:D:506:TYR:OH	1:D:518:LEU:HD21	2.14	0.48
2:E:54:ILE:HG22	7:E:438:HOH:O	2.13	0.48
2:F:113:VAL:HB	2:F:128:PHE:HE2	1.77	0.48
1:A:224:ALA:O	1:A:228:VAL:HG23	2.12	0.48
2:B:30:PHE:O	7:B:417:HOH:O	2.20	0.48
1:D:151:SER:HB2	1:D:194:PHE:HA	1.96	0.48
1:D:223:PHE:CZ	1:D:536:LEU:HB3	2.48	0.48
1:D:273:LEU:O	1:D:276:THR:OG1	2.28	0.48
1:D:362:GLU:C	1:D:363:PHE:HD1	2.21	0.48
1:D:475:TYR:HB2	1:D:518:LEU:HD22	1.95	0.48
1:A:352:PHE:HD1	7:A:805:HOH:O	1.97	0.48
1:A:366:VAL:HG22	1:A:387:GLU:O	2.13	0.48
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.78	0.48
1:D:84:ASP:C	1:D:86:SER:H	2.20	0.48
1:D:465:TYR:O	1:D:475:TYR:HA	2.13	0.48
1:A:199:HIS:CD2	1:A:200:GLN:N	2.81	0.48
2:B:9:ASP:OD2	2:B:20:ARG:NE	2.43	0.48
2:C:139:LEU:O	2:C:141:ASP:N	2.46	0.48
1:D:79:ARG:HH22	1:D:88:ILE:CB	2.27	0.48
1:D:126:ARG:HA	1:D:182:ILE:HG21	1.94	0.48
1:D:314:PRO:HB3	1:D:317:ARG:HH12	1.77	0.48
2:E:154:ASP:OD2	2:E:185:TRP:NE1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HB	1:A:292:PRO:HD3	1.95	0.48
1:A:316:LEU:O	1:A:320:ALA:N	2.38	0.48
1:A:496:CYS:HA	1:A:499:ARG:CB	2.44	0.48
2:B:199:LEU:O	7:B:414:HOH:O	2.19	0.48
2:C:70:VAL:O	2:C:73:TYR:HB2	2.13	0.48
2:C:110:GLN:O	2:C:113:VAL:HG12	2.13	0.48
1:D:197:ASP:OD1	1:D:197:ASP:N	2.45	0.48
1:D:407:VAL:HG23	1:D:541:SER:OG	2.14	0.48
2:B:114:TRP:HB3	2:B:167:TYR:HE1	1.78	0.48
2:B:133:LYS:HE2	2:B:133:LYS:HB3	1.62	0.48
1:D:32:LEU:HD21	1:D:61:PHE:HD2	1.79	0.48
1:D:124:LEU:HB3	3:D:601:JAA:C15	2.44	0.48
2:F:46:GLN:O	7:F:409:HOH:O	2.20	0.48
1:A:20:MET:HG2	1:A:356:PRO:HG2	1.94	0.48
2:C:31:GLU:N	7:C:429:HOH:O	2.47	0.48
2:C:33:ARG:NH2	2:C:35:GLU:OE2	2.47	0.48
1:D:222:VAL:O	1:D:304:ILE:N	2.47	0.48
1:D:507:VAL:C	7:D:726:HOH:O	2.55	0.48
1:D:521:ARG:NH1	1:D:562:LEU:HD13	2.29	0.48
2:E:144:TYR:CE2	2:E:151:GLY:N	2.81	0.48
1:A:97:ILE:O	1:A:556:ALA:HB1	2.14	0.48
1:A:142:GLY:HA2	1:A:215:GLN:HB2	1.94	0.48
1:A:164:THR:HG21	1:A:561:ILE:HD11	1.95	0.48
1:A:464:SER:O	1:A:551:VAL:HG23	2.14	0.48
2:C:10:TYR:CD2	2:C:12:PRO:HD2	2.49	0.48
1:D:143:LYS:CD	1:D:212:PHE:HB2	2.44	0.48
1:D:405:ASP:OD1	1:D:405:ASP:N	2.45	0.48
1:A:41:SER:HA	2:B:148:ASP:HA	1.95	0.48
1:A:53:ASN:ND2	2:B:90:TYR:HB3	2.29	0.48
1:A:131:PHE:O	1:A:134:ARG:HB3	2.14	0.48
1:A:387:GLU:C	1:A:388:TYR:HD1	2.21	0.48
2:B:86:PRO:HG2	7:B:401:HOH:O	2.13	0.48
2:B:145:PHE:CD2	2:B:153:VAL:HG22	2.49	0.48
1:D:153:GLN:HG3	1:D:171:ARG:HD2	1.96	0.48
1:D:374:GLU:HB2	7:D:720:HOH:O	2.12	0.48
2:F:105:LYS:NZ	7:F:419:HOH:O	2.29	0.48
1:A:47:ASN:O	7:A:747:HOH:O	2.20	0.47
1:A:99:LEU:HD23	1:A:535:PHE:CZ	2.49	0.47
1:A:330:TYR:HD1	1:A:537:GLY:HA2	1.78	0.47
1:A:335:GLY:HA2	1:A:394:ASN:ND2	2.29	0.47
2:B:18:ARG:NH1	2:B:103:ASP:CG	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:ALA:O	2:C:135:LEU:HB2	2.14	0.47
1:D:79:ARG:HE	1:D:79:ARG:HB3	1.63	0.47
1:D:460:ILE:HD11	1:D:482:SER:HB3	1.95	0.47
1:D:29:LYS:HB2	1:D:29:LYS:HE3	1.57	0.47
1:D:168:ASN:O	1:D:172:ASN:HB2	2.14	0.47
2:F:100:ASP:OD1	7:F:408:HOH:O	2.20	0.47
1:A:406:VAL:O	1:A:541:SER:OG	2.31	0.47
2:C:32:TYR:H	2:C:32:TYR:HD2	1.62	0.47
1:D:45:LEU:HD22	7:D:737:HOH:O	2.14	0.47
1:D:87:PRO:CB	1:D:93:PRO:HD3	2.37	0.47
1:D:253:ARG:HH11	1:D:484:GLU:HB3	1.79	0.47
1:D:295:PHE:HA	7:D:861:HOH:O	2.15	0.47
1:D:336:TRP:HB2	1:D:358:LEU:HD13	1.96	0.47
1:D:552:LYS:HG3	1:D:553:PRO:HD2	1.97	0.47
2:E:30:PHE:HD1	7:E:441:HOH:O	1.96	0.47
2:E:70:VAL:HG21	7:E:406:HOH:O	2.15	0.47
1:A:152:LYS:CE	1:A:565:ASN:HB2	2.37	0.47
1:A:412:PHE:HA	1:A:417:PRO:HA	1.95	0.47
1:A:460:ILE:HG12	1:A:480:GLU:O	2.14	0.47
1:A:552:LYS:C	1:A:554:SER:H	2.23	0.47
2:B:8:LEU:HD22	2:B:35:GLU:OE2	2.14	0.47
2:B:30:PHE:HA	7:B:427:HOH:O	2.13	0.47
2:B:144:TYR:HB3	2:B:154:ASP:OD2	2.14	0.47
2:C:169:LYS:HG3	2:C:170:PHE:N	2.29	0.47
2:E:17:MET:HB2	2:E:159:THR:HB	1.95	0.47
1:A:138:ILE:HA	1:A:217:GLN:NE2	2.29	0.47
1:A:480:GLU:OE2	1:A:526:GLY:N	2.35	0.47
1:D:92:HIS:HB2	2:E:141:ASP:HA	1.95	0.47
1:D:193:ILE:HG12	1:D:205:HIS:NE2	2.30	0.47
1:D:495:ASN:C	1:D:499:ARG:NH1	2.73	0.47
2:F:98:TRP:NE1	2:F:153:VAL:HG21	2.29	0.47
2:F:211:GLU:HA	2:F:214:LYS:HE3	1.97	0.47
1:A:480:GLU:OE1	1:A:528:PHE:N	2.43	0.47
2:B:23:LEU:HD11	2:B:57:LEU:HD11	1.95	0.47
2:B:181:LYS:HB2	2:B:181:LYS:HE2	1.50	0.47
2:B:183:ILE:O	2:B:186:ALA:HB3	2.15	0.47
2:C:37:PHE:O	2:C:40:LYS:NZ	2.46	0.47
1:D:330:TYR:OH	1:D:541:SER:N	2.47	0.47
1:D:361:PHE:CD1	1:D:392:ILE:HD13	2.49	0.47
1:D:435:LYS:HB3	1:D:436:ASN:O	2.14	0.47
1:D:461:ASP:HB2	7:D:787:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:SER:N	1:D:549:ARG:O	2.48	0.47
2:E:169:LYS:HZ3	2:E:206:VAL:HG13	1.78	0.47
2:F:32:TYR:CD1	2:F:34:GLU:OE2	2.68	0.47
2:F:107:THR:HG22	2:F:160:PHE:CE2	2.49	0.47
2:F:144:TYR:HB3	2:F:154:ASP:CG	2.40	0.47
1:A:43:ILE:HG13	1:A:44:TYR:N	2.30	0.47
1:A:107:ARG:HG3	1:A:107:ARG:NH1	2.30	0.47
1:A:238:TRP:CZ2	1:A:281:CYS:SG	3.07	0.47
1:A:503:ASP:CG	1:A:504:ALA:N	2.73	0.47
2:C:90:TYR:O	2:C:94:GLN:HG3	2.15	0.47
2:C:187:LYS:HE2	1:D:496:CYS:HB2	1.96	0.47
1:D:187:CYS:O	7:D:733:HOH:O	2.21	0.47
1:D:401:TYR:HB2	7:D:817:HOH:O	2.15	0.47
1:D:432:ASN:OD1	1:D:433:ILE:N	2.38	0.47
1:D:530:LYS:HB3	7:D:797:HOH:O	2.14	0.47
2:E:21:VAL:HG12	2:E:155:ILE:HG12	1.97	0.47
2:E:187:LYS:HA	2:E:190:MET:HG3	1.96	0.47
1:A:149:PHE:HZ	1:A:202:LEU:CB	2.28	0.47
1:A:256:VAL:N	7:A:798:HOH:O	2.47	0.47
1:A:362:GLU:HG3	1:A:400:ARG:CZ	2.44	0.47
1:D:107:ARG:HG3	1:D:107:ARG:NH1	2.17	0.47
1:D:389:GLU:CD	1:D:402:ARG:HH21	2.23	0.47
1:D:552:LYS:C	1:D:554:SER:N	2.68	0.47
2:C:10:TYR:CG	2:C:12:PRO:HD2	2.50	0.47
1:D:92:HIS:CD2	1:D:93:PRO:HD2	2.49	0.47
1:D:143:LYS:C	1:D:184:SER:HB3	2.40	0.47
1:D:317:ARG:O	1:D:321:GLY:N	2.36	0.47
1:D:437:THR:HG21	1:D:439:ARG:HH21	1.79	0.47
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.44	0.47
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.50	0.47
2:C:73:TYR:HD1	2:C:76:GLU:OE2	1.98	0.47
1:D:107:ARG:HH22	1:D:552:LYS:HB2	1.80	0.47
1:D:309:MET:HE3	1:D:545:PHE:CZ	2.50	0.47
1:D:393:THR:HA	1:D:398:LEU:O	2.15	0.47
1:D:451:ARG:NH1	1:D:454:GLU:OE1	2.48	0.47
2:E:15:PHE:HB3	2:E:67:SER:HB3	1.96	0.47
2:E:17:MET:O	2:E:21:VAL:HG23	2.15	0.47
2:F:182:LEU:HD23	2:F:183:ILE:N	2.30	0.47
1:A:198:VAL:CG2	1:A:524:ALA:HB3	2.43	0.46
1:A:344:ARG:NH1	7:A:824:HOH:O	2.47	0.46
1:A:477:ILE:HD12	1:A:497:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:ALA:CB	1:D:499:ARG:NH1	2.74	0.46
1:D:82:ASP:C	1:D:84:ASP:H	2.23	0.46
1:D:179:MET:HE2	1:D:179:MET:HB3	1.69	0.46
2:E:21:VAL:CG1	2:E:155:ILE:HG12	2.45	0.46
2:F:165:GLN:O	2:F:168:GLU:HB2	2.15	0.46
1:A:255:THR:OG1	7:A:738:HOH:O	2.17	0.46
1:A:365:PRO:HG3	1:A:388:TYR:CZ	2.50	0.46
1:A:421:PHE:HB3	1:A:542:ALA:HB2	1.96	0.46
1:A:480:GLU:CD	1:A:526:GLY:H	2.21	0.46
2:B:14:MET:O	2:B:17:MET:HB2	2.15	0.46
2:C:33:ARG:CZ	2:C:35:GLU:OE2	2.62	0.46
1:D:110:PHE:CE1	1:D:555:ASN:C	2.92	0.46
1:D:202:LEU:HD23	1:D:525:LYS:HD2	1.97	0.46
2:E:144:TYR:CZ	2:E:154:ASP:HB2	2.49	0.46
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.79	0.46
2:B:107:THR:O	2:B:110:GLN:HG3	2.15	0.46
1:D:149:PHE:HZ	1:D:202:LEU:HD13	1.80	0.46
1:D:531:ILE:CG2	1:D:547:MET:HG2	2.45	0.46
1:D:552:LYS:HE2	7:D:882:HOH:O	2.14	0.46
2:E:144:TYR:CE2	2:E:154:ASP:OD1	2.68	0.46
1:A:177:ALA:O	1:A:180:LYS:HG2	2.15	0.46
2:B:176:GLU:O	2:B:180:PRO:N	2.48	0.46
2:C:68:LEU:HD23	2:C:103:ASP:OD2	2.14	0.46
1:D:99:LEU:HG	1:D:555:ASN:OD1	2.15	0.46
1:D:496:CYS:CA	1:D:499:ARG:NH1	2.78	0.46
1:D:510:ARG:HE	1:D:510:ARG:HB3	1.50	0.46
1:D:559:LEU:O	1:D:562:LEU:HG	2.15	0.46
2:E:86:PRO:HB2	2:E:88:ASP:OD1	2.16	0.46
2:F:71:VAL:O	2:F:74:VAL:HB	2.15	0.46
1:A:101:SER:HB3	1:A:535:PHE:CD2	2.51	0.46
2:B:65:CYS:HB2	2:C:97:PHE:CE1	2.50	0.46
1:D:239:GLU:O	1:D:242:VAL:HG13	2.16	0.46
1:D:262:ALA:O	1:D:266:LEU:HG	2.15	0.46
2:E:168:GLU:CD	2:E:174:SER:HA	2.40	0.46
1:A:74:GLU:N	1:A:75:PRO:HD2	2.31	0.46
1:A:139:ASP:H	1:A:217:GLN:CD	2.23	0.46
1:A:167:THR:HB	1:A:560:GLN:OE1	2.15	0.46
1:A:444:SER:HB3	1:A:497:LEU:HD23	1.97	0.46
2:B:37:PHE:CE1	6:B:301:GSH:HA32	2.50	0.46
1:D:156:SER:HB3	1:D:162:VAL:CG1	2.46	0.46
1:D:199:HIS:NE2	1:D:200:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:HB3	1:A:54:ALA:H	1.44	0.46
1:A:108:PRO:HG2	1:A:552:LYS:HB3	1.98	0.46
1:A:300:TYR:CE2	1:A:302:TYR:HB2	2.51	0.46
1:A:394:ASN:HD21	1:A:396:ALA:HB3	1.79	0.46
1:A:421:PHE:CD1	1:A:541:SER:HA	2.51	0.46
1:A:527:THR:HA	1:A:530:LYS:NZ	2.31	0.46
1:A:531:ILE:HD11	1:A:558:VAL:HG23	1.98	0.46
2:C:13:SER:O	2:C:17:MET:HG3	2.15	0.46
2:C:73:TYR:HA	2:C:76:GLU:OE2	2.16	0.46
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.51	0.46
1:D:200:GLN:O	1:D:203:TYR:HB3	2.16	0.46
1:D:314:PRO:HA	1:D:317:ARG:NH1	2.30	0.46
1:D:340:ASN:HB2	1:D:352:PHE:CD1	2.51	0.46
1:D:433:ILE:C	1:D:435:LYS:H	2.21	0.46
1:D:561:ILE:HG22	7:D:772:HOH:O	2.15	0.46
2:E:62:LYS:HA	2:E:63:PRO:HD3	1.83	0.46
1:A:147:PHE:CE1	1:A:206:LEU:HD12	2.51	0.46
1:A:450:LYS:H	1:A:450:LYS:HG2	1.44	0.46
2:B:150:PHE:O	7:B:418:HOH:O	2.21	0.46
2:C:121:GLN:O	2:C:125:LYS:HG3	2.16	0.46
1:D:78:LYS:HG3	1:D:553:PRO:O	2.14	0.46
1:D:98:SER:HA	7:D:713:HOH:O	2.16	0.46
1:D:235:GLU:HG3	7:D:710:HOH:O	2.15	0.46
2:E:20:ARG:HB2	7:E:425:HOH:O	2.15	0.46
1:A:295:PHE:CD1	1:A:298:ALA:HB2	2.50	0.46
1:A:522:VAL:HG23	1:A:567:VAL:HG23	1.98	0.46
1:A:552:LYS:CG	1:A:553:PRO:HD2	2.46	0.46
2:B:52:LYS:O	7:B:415:HOH:O	2.20	0.46
1:D:69:THR:OG1	1:D:72:GLU:OE1	2.26	0.46
1:D:80:MET:HE3	1:D:88:ILE:HG22	1.98	0.46
1:D:498:ASP:HB3	1:D:510:ARG:NH2	2.30	0.46
2:F:33:ARG:CZ	2:F:35:GLU:OE2	2.64	0.46
2:F:123:ALA:O	2:F:127:GLU:HG3	2.15	0.46
2:F:183:ILE:O	2:F:186:ALA:HB3	2.16	0.46
1:A:53:ASN:ND2	2:B:88:ASP:OD2	2.46	0.46
1:A:522:VAL:HG23	1:A:567:VAL:CG2	2.46	0.46
2:B:26:LYS:HB3	2:B:26:LYS:HE2	1.57	0.46
2:C:18:ARG:HD2	2:C:67:SER:HB2	1.96	0.46
2:C:24:ARG:HD2	2:C:198:SER:OG	2.15	0.46
2:E:70:VAL:HG13	7:E:498:HOH:O	2.16	0.46
2:E:169:LYS:HD3	2:E:206:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:HIS:CE1	1:A:380:THR:HG1	2.34	0.45
1:A:203:TYR:CD1	1:A:237:VAL:HG11	2.39	0.45
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.78	0.45
1:A:424:ARG:HG3	1:A:425:ARG:HH11	1.82	0.45
1:A:460:ILE:HD11	1:A:480:GLU:OE2	2.16	0.45
1:A:528:PHE:HB3	1:A:547:MET:HE1	1.97	0.45
2:B:14:MET:HG2	2:B:163:TRP:CD1	2.52	0.45
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.46	0.45
1:D:129:PHE:O	1:D:133:ASN:HB2	2.16	0.45
1:D:526:GLY:HA2	1:D:529:ARG:HB3	1.98	0.45
2:F:144:TYR:HA	2:F:185:TRP:HE1	1.81	0.45
1:A:48:CYS:SG	1:A:65:VAL:HG23	2.57	0.45
1:A:62:LYS:HD3	7:A:712:HOH:O	2.16	0.45
1:A:116:GLU:O	1:A:119:GLU:HB2	2.16	0.45
1:A:146:GLN:HB2	1:A:148:ILE:HG23	1.98	0.45
1:A:237:VAL:HB	1:A:241:ILE:HG23	1.98	0.45
1:A:385:GLY:N	1:A:409:VAL:O	2.33	0.45
2:B:66:GLU:O	2:B:70:VAL:HG23	2.16	0.45
2:B:181:LYS:H	2:B:181:LYS:HG3	1.48	0.45
2:C:169:LYS:HE3	2:C:169:LYS:HB2	1.78	0.45
1:D:107:ARG:NH2	1:D:552:LYS:HB2	2.32	0.45
1:D:152:LYS:HZ3	1:D:561:ILE:HG23	1.79	0.45
1:D:444:SER:HA	1:D:500:ALA:CB	2.46	0.45
1:D:531:ILE:HG12	7:D:729:HOH:O	2.16	0.45
2:E:211:GLU:O	2:E:214:LYS:HB2	2.16	0.45
2:F:138:GLU:HG3	2:F:145:PHE:HE1	1.79	0.45
2:F:140:GLY:N	2:F:181:LYS:NZ	2.65	0.45
1:A:134:ARG:NH1	1:A:135:ASP:CG	2.74	0.45
2:C:18:ARG:NH2	7:C:407:HOH:O	2.49	0.45
1:D:223:PHE:CD1	1:D:304:ILE:HB	2.50	0.45
1:D:239:GLU:HA	1:D:242:VAL:HG13	1.98	0.45
1:D:451:ARG:CZ	1:D:489:VAL:HG12	2.46	0.45
1:D:510:ARG:NH2	1:D:575:PHE:CE2	2.79	0.45
1:A:109:LYS:HZ3	1:A:111:ILE:HD11	1.80	0.45
1:A:222:VAL:HG21	7:A:789:HOH:O	2.17	0.45
1:A:437:THR:OG1	1:A:440:ASP:HB2	2.16	0.45
2:B:184:ALA:HA	2:B:187:LYS:HG2	1.98	0.45
2:C:132:VAL:HG22	7:C:414:HOH:O	2.17	0.45
2:C:170:PHE:CD2	2:C:213:ARG:HD2	2.52	0.45
1:D:91:GLY:HA3	2:E:141:ASP:O	2.16	0.45
1:D:223:PHE:HB3	1:D:225:HIS:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ASN:HB2	1:D:352:PHE:HD1	1.80	0.45
1:D:427:LEU:HD12	1:D:427:LEU:O	2.16	0.45
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.99	0.45
2:F:32:TYR:H	2:F:32:TYR:HD2	1.65	0.45
1:A:77:ILE:HA	1:A:80:MET:SD	2.56	0.45
1:A:164:THR:OG1	1:A:561:ILE:HG13	2.17	0.45
1:A:302:TYR:CG	1:A:328:HIS:NE2	2.83	0.45
2:C:24:ARG:HG3	2:C:30:PHE:CZ	2.50	0.45
1:D:68:VAL:HG11	1:D:73:LEU:HD21	1.98	0.45
1:D:498:ASP:OD2	1:D:510:ARG:NH2	2.50	0.45
2:E:86:PRO:HD3	2:E:146:GLY:O	2.17	0.45
2:E:144:TYR:C	2:E:145:PHE:HD1	2.23	0.45
2:F:163:TRP:HB3	2:F:167:TYR:CZ	2.51	0.45
1:A:61:PHE:O	1:A:65:VAL:HG12	2.17	0.45
1:A:84:ASP:C	1:A:86:SER:H	2.25	0.45
2:C:114:TRP:HA	2:C:170:PHE:CD2	2.51	0.45
2:C:138:GLU:HG3	2:C:145:PHE:HE1	1.81	0.45
2:C:173:PHE:HB3	2:C:174:SER:H	1.63	0.45
1:D:220:PHE:HD1	1:D:302:TYR:HB3	1.81	0.45
1:D:328:HIS:CG	1:D:329:ASP:N	2.84	0.45
1:D:491:GLN:HE22	1:D:570:TYR:HB3	1.81	0.45
1:D:551:VAL:HG23	1:D:555:ASN:CB	2.46	0.45
1:A:99:LEU:CD2	1:A:535:PHE:HZ	2.28	0.45
1:A:102:GLY:HA3	1:A:426:ASN:ND2	2.32	0.45
1:A:150:SER:HB2	1:A:167:THR:CA	2.45	0.45
1:A:174:ASN:O	1:A:178:GLY:N	2.40	0.45
1:A:200:GLN:OE1	1:A:254:ILE:HA	2.17	0.45
1:A:382:VAL:HG13	1:A:388:TYR:CD2	2.52	0.45
1:A:478:PHE:CE2	1:A:562:LEU:HA	2.51	0.45
1:A:498:ASP:HB3	1:A:510:ARG:NH2	2.28	0.45
2:C:109:ALA:HA	7:C:403:HOH:O	2.17	0.45
1:D:110:PHE:CD1	1:D:556:ALA:HB2	2.52	0.45
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.52	0.45
2:E:37:PHE:HZ	2:E:53:LYS:HA	1.82	0.45
2:F:68:LEU:HD12	2:F:69:ASN:N	2.32	0.45
1:A:125:PHE:O	1:A:129:PHE:HB2	2.16	0.45
1:A:168:ASN:O	1:A:172:ASN:HB2	2.17	0.45
1:A:171:ARG:HG3	1:A:194:PHE:CE1	2.52	0.45
1:A:233:THR:C	1:A:236:GLN:H	2.25	0.45
1:A:253:ARG:O	7:A:746:HOH:O	2.20	0.45
1:A:390:VAL:HG23	7:A:777:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:187:LYS:HB2	2:C:187:LYS:HZ3	1.81	0.45
1:D:12:ARG:HD2	1:D:12:ARG:HA	1.68	0.45
2:E:141:ASP:OD2	2:E:181:LYS:NZ	2.43	0.45
2:E:162:SER:HB3	2:E:199:LEU:HD23	1.98	0.45
2:F:26:LYS:HE3	2:F:78:TRP:O	2.16	0.45
1:A:149:PHE:HB2	1:A:530:LYS:HD3	1.99	0.45
1:A:315:LYS:HD2	1:A:319:TYR:CE2	2.52	0.45
1:A:444:SER:HA	1:A:500:ALA:HB3	1.98	0.45
2:C:10:TYR:HH	2:C:208:TYR:HH	1.58	0.45
2:C:71:VAL:O	2:C:74:VAL:HB	2.17	0.45
1:D:149:PHE:HB3	1:D:198:VAL:HG11	1.99	0.45
1:D:149:PHE:O	1:D:530:LYS:HE3	2.17	0.45
1:D:232:ARG:HG3	7:D:795:HOH:O	2.16	0.45
2:F:86:PRO:HB2	7:F:441:HOH:O	2.16	0.45
1:A:403:LEU:HD12	1:A:403:LEU:HA	1.84	0.45
1:A:502:ILE:HD12	1:A:503:ASP:N	2.31	0.45
2:C:145:PHE:HB3	2:C:153:VAL:CG1	2.46	0.45
1:D:125:PHE:CE1	1:D:182:ILE:HD12	2.49	0.45
1:D:223:PHE:HZ	1:D:536:LEU:HB3	1.82	0.45
2:E:7:LEU:HB3	7:E:441:HOH:O	2.17	0.45
2:E:9:ASP:OD1	2:E:10:TYR:N	2.37	0.45
1:A:11:ASN:O	1:A:14:ILE:HG13	2.16	0.44
1:D:47:ASN:O	7:D:740:HOH:O	2.21	0.44
1:D:225:HIS:HB3	1:D:309:MET:SD	2.56	0.44
1:D:226:GLY:HA3	1:D:529:ARG:HD2	1.99	0.44
1:A:97:ILE:H	1:A:163:GLY:N	2.14	0.44
1:A:124:LEU:HD13	1:A:336:TRP:CE3	2.52	0.44
1:A:192:VAL:HG12	1:A:202:LEU:CD1	2.47	0.44
1:A:242:VAL:O	1:A:246:LYS:HB2	2.17	0.44
1:A:263:MET:HE3	7:A:773:HOH:O	2.16	0.44
1:A:531:ILE:HA	1:A:534:HIS:CD2	2.53	0.44
2:B:17:MET:O	2:B:21:VAL:HG23	2.18	0.44
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.52	0.44
1:A:41:SER:HA	2:B:147:GLY:O	2.18	0.44
1:A:150:SER:OG	1:A:170:TYR:HB2	2.17	0.44
1:A:365:PRO:HG3	1:A:388:TYR:CE2	2.53	0.44
1:A:451:ARG:HA	7:A:991:HOH:O	2.17	0.44
1:A:527:THR:HB	1:A:561:ILE:CG2	2.47	0.44
1:D:407:VAL:HG12	7:D:794:HOH:O	2.17	0.44
1:D:466:ILE:HD11	1:D:552:LYS:HG3	1.98	0.44
1:D:498:ASP:OD1	1:D:518:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:LEU:HD12	2:E:139:LEU:HA	1.59	0.44
2:E:183:ILE:O	2:E:186:ALA:HB3	2.17	0.44
2:F:140:GLY:C	2:F:181:LYS:NZ	2.66	0.44
1:A:121:THR:HG23	3:A:601:JAA:C13	2.47	0.44
1:A:206:LEU:HA	7:A:1013:HOH:O	2.17	0.44
1:A:315:LYS:O	1:A:319:TYR:N	2.50	0.44
1:A:405:ASP:OD1	1:A:426:ASN:HB3	2.18	0.44
1:A:511:LYS:NZ	7:A:701:HOH:O	1.91	0.44
1:D:96:ALA:HB1	1:D:163:GLY:H	1.82	0.44
1:D:362:GLU:O	1:D:391:VAL:HB	2.16	0.44
2:E:95:ALA:HB1	2:E:152:TYR:CD2	2.52	0.44
2:F:130:GLU:O	2:F:134:ILE:HG22	2.18	0.44
1:A:39:ASN:HA	2:B:142:LYS:CG	2.48	0.44
1:A:62:LYS:HG2	1:A:400:ARG:NH1	2.32	0.44
1:A:223:PHE:HE2	1:A:545:PHE:CZ	2.36	0.44
1:A:336:TRP:HB2	1:A:358:LEU:HB3	1.99	0.44
1:A:432:ASN:CG	1:A:433:ILE:H	2.25	0.44
1:A:499:ARG:N	7:A:707:HOH:O	2.51	0.44
2:C:132:VAL:O	7:C:414:HOH:O	2.21	0.44
1:D:70:ASP:HB2	1:D:104:SER:OG	2.18	0.44
1:D:83:GLY:N	1:D:158:GLY:HA3	2.32	0.44
1:D:363:PHE:HB3	1:D:388:TYR:HB3	1.99	0.44
1:A:233:THR:HG23	1:A:525:LYS:NZ	2.32	0.44
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.98	0.44
2:B:196:SER:O	7:B:419:HOH:O	2.21	0.44
2:C:4:LEU:HA	2:C:5:PRO:HD3	1.74	0.44
2:C:113:VAL:HG21	2:C:128:PHE:CE2	2.53	0.44
1:D:107:ARG:HH11	1:D:107:ARG:CG	2.19	0.44
1:D:138:ILE:HD12	7:D:823:HOH:O	2.18	0.44
1:D:152:LYS:HG2	1:D:565:ASN:CG	2.43	0.44
1:D:190:ASP:HB2	7:D:718:HOH:O	2.18	0.44
2:E:24:ARG:HG2	2:E:194:SER:HA	1.99	0.44
2:E:65:CYS:HA	7:E:406:HOH:O	2.17	0.44
2:E:114:TRP:CD1	2:E:167:TYR:HE1	2.31	0.44
2:E:139:LEU:HG	2:E:142:LYS:H	1.83	0.44
1:D:233:THR:O	1:D:237:VAL:HG22	2.18	0.44
1:D:393:THR:OG1	1:D:400:ARG:N	2.31	0.44
1:D:523:VAL:HG12	1:D:524:ALA:H	1.83	0.44
2:E:125:LYS:O	2:E:129:ILE:HG12	2.17	0.44
2:F:109:ALA:CB	2:F:128:PHE:HB3	2.46	0.44
1:A:440:ASP:OD1	1:A:502:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LEU:HG	7:B:413:HOH:O	2.17	0.44
2:B:58:VAL:HA	2:B:63:PRO:HA	1.99	0.44
1:D:77:ILE:CG2	1:D:97:ILE:HD11	2.47	0.44
1:D:107:ARG:CZ	1:D:433:ILE:HG13	2.47	0.44
1:D:462:PHE:O	1:D:549:ARG:NH1	2.51	0.44
2:F:9:ASP:HB2	2:F:20:ARG:HH21	1.83	0.44
1:A:143:LYS:HZ2	1:A:187:CYS:HB3	1.82	0.44
1:A:305:MET:HE2	7:A:889:HOH:O	2.16	0.44
1:A:432:ASN:O	1:A:433:ILE:HG23	2.17	0.44
2:B:10:TYR:O	2:B:20:ARG:NH2	2.51	0.44
2:B:151:GLY:C	2:B:154:ASP:HB2	2.43	0.44
2:C:65:CYS:O	2:C:69:ASN:HB3	2.18	0.44
2:C:66:GLU:O	2:C:70:VAL:HG23	2.18	0.44
1:D:114:THR:HG22	1:D:115:ASP:N	2.31	0.44
1:D:253:ARG:HG2	1:D:254:ILE:HD13	2.00	0.44
2:E:9:ASP:OD1	2:E:16:GLY:HA3	2.18	0.44
2:F:8:LEU:HB2	2:F:56:VAL:HB	2.00	0.44
1:A:117:LEU:HD21	7:A:756:HOH:O	2.17	0.43
1:A:205:HIS:CE1	1:A:206:LEU:CD1	3.01	0.43
1:A:317:ARG:O	1:A:321:GLY:N	2.51	0.43
1:A:337:ILE:O	1:A:354:VAL:HG23	2.18	0.43
1:A:451:ARG:NH1	1:A:454:GLU:OE2	2.51	0.43
2:B:144:TYR:O	2:B:145:PHE:HD1	2.01	0.43
2:C:209:ALA:HB2	7:C:470:HOH:O	2.18	0.43
7:C:416:HOH:O	1:D:489:VAL:HG13	2.18	0.43
1:D:77:ILE:HD12	1:D:77:ILE:HG23	1.42	0.43
1:D:92:HIS:H	2:E:141:ASP:C	2.26	0.43
1:D:94:VAL:HG21	1:D:112:PRO:HB3	1.98	0.43
1:D:444:SER:HA	1:D:500:ALA:HB1	2.00	0.43
1:D:507:VAL:O	1:D:511:LYS:HB2	2.18	0.43
1:A:26:GLN:NE2	7:A:787:HOH:O	2.32	0.43
1:A:48:CYS:SG	1:A:66:PRO:HD2	2.58	0.43
1:A:132:ARG:HD2	1:A:326:VAL:HG21	1.99	0.43
1:A:552:LYS:HD2	1:A:552:LYS:HA	1.77	0.43
2:B:64:VAL:HG13	2:C:93:ALA:HB1	1.99	0.43
2:B:188:ARG:O	2:B:188:ARG:HD3	2.17	0.43
2:B:65:CYS:HB2	2:C:97:PHE:CZ	2.52	0.43
2:C:7:LEU:HD13	2:C:30:PHE:CD2	2.53	0.43
1:D:153:GLN:HG3	1:D:171:ARG:NH1	2.33	0.43
1:D:256:VAL:HA	1:D:257:PRO:HD3	1.79	0.43
2:E:36:ASP:OD2	2:E:38:SER:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:LYS:HE2	2:F:133:LYS:HB3	1.68	0.43
2:F:173:PHE:HB3	2:F:174:SER:H	1.72	0.43
1:A:109:LYS:CE	1:A:111:ILE:HD11	2.48	0.43
1:A:114:THR:O	1:A:117:LEU:HB2	2.18	0.43
1:A:368:GLU:HG3	1:A:369:THR:HG22	1.99	0.43
1:A:463:SER:HB2	1:A:528:PHE:HE1	1.83	0.43
2:B:128:PHE:O	2:B:132:VAL:HG13	2.17	0.43
2:C:130:GLU:O	2:C:134:ILE:HG22	2.19	0.43
1:D:238:TRP:CE2	1:D:239:GLU:HG3	2.53	0.43
1:D:401:TYR:HE2	1:D:403:LEU:HD13	1.83	0.43
1:D:441:LEU:HG	1:D:462:PHE:HE1	1.84	0.43
3:D:601:JAA:O02	4:D:602:LEU:N	2.52	0.43
2:F:114:TRP:HA	2:F:170:PHE:CD2	2.53	0.43
2:F:185:TRP:CE2	2:F:189:CYS:SG	3.11	0.43
1:A:284:LEU:H	1:A:284:LEU:HG	1.45	0.43
2:B:153:VAL:HA	2:B:156:SER:HB3	2.01	0.43
2:C:143:PRO:HB2	2:C:144:TYR:CD2	2.54	0.43
1:D:323:LEU:HD23	1:D:324:PRO:HD2	1.99	0.43
1:D:575:PHE:HB2	7:D:714:HOH:O	2.19	0.43
2:F:73:TYR:HD1	2:F:76:GLU:OE2	2.01	0.43
1:A:77:ILE:O	1:A:80:MET:HB2	2.18	0.43
1:A:195:SER:OG	7:A:726:HOH:O	2.12	0.43
1:A:227:LEU:HB2	1:A:316:LEU:HD22	2.00	0.43
1:A:568:SER:OG	7:A:749:HOH:O	2.21	0.43
2:B:18:ARG:HG2	2:B:155:ILE:O	2.19	0.43
1:D:122:LEU:HD23	1:D:125:PHE:HZ	1.83	0.43
1:D:387:GLU:HB3	1:D:406:VAL:HG12	2.00	0.43
2:E:14:MET:HB3	2:E:159:THR:OG1	2.18	0.43
2:E:145:PHE:CB	2:E:153:VAL:HB	2.49	0.43
2:F:169:LYS:HD3	2:F:206:VAL:HG13	2.00	0.43
1:A:74:GLU:HA	7:A:826:HOH:O	2.17	0.43
1:D:224:ALA:HB2	1:D:305:MET:SD	2.59	0.43
1:D:308:SER:O	1:D:311:PRO:HD2	2.18	0.43
1:D:534:HIS:HB3	4:D:602:LEU:C	2.43	0.43
2:E:122:GLU:O	2:E:125:LYS:HB2	2.19	0.43
1:A:292:PRO:O	1:A:296:PRO:HA	2.19	0.43
2:B:6:ILE:O	2:B:57:LEU:HA	2.18	0.43
2:B:77:ALA:C	2:B:79:PRO:HD3	2.43	0.43
7:C:416:HOH:O	1:D:488:ASP:HB3	2.17	0.43
1:D:223:PHE:CG	1:D:533:GLU:HG2	2.54	0.43
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:MET:SD	7:A:831:HOH:O	2.62	0.43
1:A:426:ASN:OD1	1:A:426:ASN:N	2.44	0.43
1:A:549:ARG:NE	7:A:791:HOH:O	2.47	0.43
2:C:104:LYS:CG	2:C:105:LYS:N	2.81	0.43
2:C:129:ILE:O	2:C:132:VAL:HG12	2.19	0.43
2:C:211:GLU:HA	2:C:214:LYS:HG2	2.01	0.43
1:D:38:LYS:C	2:E:142:LYS:HG2	2.44	0.43
1:D:186:SER:OG	7:D:739:HOH:O	2.20	0.43
1:A:229:HIS:HA	1:A:232:ARG:HG2	2.00	0.43
2:B:95:ALA:HB1	2:B:152:TYR:HD2	1.83	0.43
2:B:113:VAL:O	7:B:420:HOH:O	2.22	0.43
1:D:389:GLU:OE2	1:D:404:GLY:HA2	2.19	0.43
1:D:391:VAL:HG23	7:D:828:HOH:O	2.19	0.43
2:F:117:LYS:HE3	2:F:213:ARG:NH1	2.33	0.43
1:A:80:MET:HA	1:A:86:SER:O	2.19	0.42
1:A:98:SER:C	1:A:556:ALA:HB3	2.43	0.42
2:C:15:PHE:O	2:C:18:ARG:HB2	2.18	0.42
2:C:164:PHE:CD2	2:C:183:ILE:HD12	2.52	0.42
1:D:207:LEU:HD13	1:D:241:ILE:HD12	2.01	0.42
1:D:291:ILE:HG23	1:D:295:PHE:CZ	2.53	0.42
1:D:295:PHE:CD1	1:D:295:PHE:O	2.72	0.42
1:D:348:GLU:OE2	7:D:743:HOH:O	2.21	0.42
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.69	0.42
2:E:30:PHE:CD2	2:E:30:PHE:N	2.86	0.42
1:A:134:ARG:HH11	1:A:135:ASP:CG	2.22	0.42
1:A:231:PHE:CZ	1:A:291:ILE:HG12	2.54	0.42
1:A:513:LYS:NZ	1:A:575:PHE:HB3	2.33	0.42
1:D:93:PRO:HG2	7:E:403:HOH:O	2.18	0.42
1:D:99:LEU:HB3	1:D:557:LYS:H	1.83	0.42
1:D:253:ARG:NH1	7:D:840:HOH:O	2.53	0.42
2:E:18:ARG:HG3	2:E:159:THR:HG21	1.99	0.42
2:E:110:GLN:OE1	2:E:160:PHE:HD2	2.02	0.42
2:F:151:GLY:CA	2:F:154:ASP:OD2	2.67	0.42
1:A:131:PHE:CD1	1:A:341:VAL:HB	2.54	0.42
1:A:353:ALA:HB3	7:A:722:HOH:O	2.19	0.42
2:B:26:LYS:HZ3	2:B:28:VAL:HG21	1.83	0.42
2:B:170:PHE:HZ	2:B:210:ALA:HA	1.85	0.42
2:C:129:ILE:HA	2:C:132:VAL:HG12	2.01	0.42
1:D:202:LEU:HA	1:D:205:HIS:HB2	2.00	0.42
1:D:245:ILE:HG12	1:D:245:ILE:H	1.33	0.42
1:D:403:LEU:HD23	1:D:540:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:PRO:O	2:F:163:TRP:CZ2	2.73	0.42
2:F:65:CYS:O	2:F:66:GLU:HB2	2.18	0.42
1:A:212:PHE:CB	1:A:215:GLN:HE21	2.32	0.42
1:A:223:PHE:HE2	1:A:545:PHE:HZ	1.67	0.42
2:C:24:ARG:NE	7:C:440:HOH:O	2.43	0.42
2:C:113:VAL:HG23	2:C:125:LYS:HG2	2.01	0.42
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.38	0.42
1:D:182:ILE:H	1:D:182:ILE:HG13	1.62	0.42
1:D:420:LYS:NZ	7:D:783:HOH:O	2.34	0.42
1:D:563:CYS:O	1:D:566:VAL:N	2.52	0.42
2:E:31:GLU:HB3	7:E:457:HOH:O	2.19	0.42
2:F:21:VAL:HG22	2:F:195:VAL:HA	2.01	0.42
2:F:125:LYS:O	2:F:129:ILE:HG23	2.19	0.42
1:A:122:LEU:HD22	1:A:126:ARG:NH2	2.31	0.42
1:A:197:ASP:O	1:A:201:ALA:HB2	2.20	0.42
1:A:205:HIS:ND1	1:A:206:LEU:HD13	2.34	0.42
2:C:104:LYS:HG3	2:C:105:LYS:H	1.83	0.42
1:D:109:LYS:O	1:D:555:ASN:HA	2.19	0.42
1:D:150:SER:HB3	1:D:166:THR:HB	2.02	0.42
2:E:24:ARG:HE	2:E:193:GLU:CG	2.32	0.42
1:A:8:PHE:HD1	1:A:126:ARG:HG3	1.85	0.42
1:A:41:SER:HB3	2:B:144:TYR:H	1.84	0.42
1:A:91:GLY:HA2	2:B:143:PRO:HD3	2.00	0.42
1:A:102:GLY:HA3	1:A:426:ASN:HD21	1.85	0.42
1:A:104:SER:O	1:A:107:ARG:HB2	2.18	0.42
1:A:277:ILE:HG23	1:A:278:ARG:N	2.34	0.42
1:A:330:TYR:N	7:A:786:HOH:O	2.52	0.42
2:B:59:HIS:ND1	2:B:73:TYR:OH	2.42	0.42
2:C:84:PHE:HE1	2:C:85:PHE:CD2	2.38	0.42
1:D:68:VAL:HG22	1:D:69:THR:H	1.85	0.42
1:D:223:PHE:CZ	1:D:536:LEU:CB	3.03	0.42
1:D:471:ASP:HA	1:D:472:PRO:HA	1.87	0.42
1:D:495:ASN:HD22	1:D:572:SER:HB3	1.85	0.42
2:E:17:MET:SD	2:E:199:LEU:HG	2.59	0.42
2:E:102:VAL:HG23	7:E:450:HOH:O	2.20	0.42
2:F:7:LEU:HD11	2:F:23:LEU:CD1	2.48	0.42
2:F:153:VAL:HA	2:F:156:SER:HB2	2.00	0.42
1:A:97:ILE:HG21	1:A:110:PHE:CG	2.55	0.42
1:A:220:PHE:CE1	1:A:328:HIS:CE1	3.08	0.42
1:A:234:PHE:HE2	1:A:290:LEU:HD11	1.85	0.42
1:A:363:PHE:CE1	1:A:390:VAL:HG22	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ALA:HB3	1:A:479:TRP:CH2	2.54	0.42
2:B:22:ALA:HB2	2:B:155:ILE:HD13	2.01	0.42
2:C:88:ASP:O	2:C:92:ARG:HG3	2.18	0.42
1:D:76:TYR:HB2	1:D:89:LEU:HD11	2.00	0.42
1:D:153:GLN:HB2	1:D:171:ARG:NH1	2.35	0.42
1:D:299:LYS:HB2	1:D:300:TYR:HD1	1.84	0.42
1:D:555:ASN:ND2	7:D:722:HOH:O	2.50	0.42
1:A:36:LEU:HD22	1:A:61:PHE:CZ	2.54	0.42
1:A:149:PHE:CZ	1:A:202:LEU:HD22	2.54	0.42
1:A:503:ASP:O	1:A:507:VAL:HG23	2.20	0.42
2:B:98:TRP:CZ2	2:B:138:GLU:HG2	2.55	0.42
2:C:9:ASP:OD1	2:C:9:ASP:N	2.52	0.42
1:D:36:LEU:O	1:D:40:GLN:N	2.52	0.42
1:D:302:TYR:CD1	1:D:326:VAL:HG13	2.52	0.42
1:D:563:CYS:N	7:D:822:HOH:O	2.52	0.42
2:E:164:PHE:HD1	2:E:164:PHE:HA	1.62	0.42
2:F:114:TRP:CD1	2:F:167:TYR:HE1	2.38	0.42
1:A:36:LEU:HD22	1:A:61:PHE:CE2	2.55	0.42
1:A:246:LYS:HD2	1:A:274:ALA:HB2	2.01	0.42
2:B:167:TYR:N	2:B:167:TYR:CD1	2.84	0.42
2:C:97:PHE:CE1	2:C:101:PHE:HE1	2.37	0.42
2:C:187:LYS:HG2	1:D:451:ARG:HD3	2.01	0.42
1:D:83:GLY:O	1:D:85:THR:HG23	2.20	0.42
1:D:405:ASP:O	7:D:707:HOH:O	2.21	0.42
1:D:477:ILE:HG21	1:D:497:LEU:HD13	2.02	0.42
1:D:509:SER:O	1:D:513:LYS:N	2.22	0.42
2:F:110:GLN:HB3	2:F:167:TYR:CE1	2.55	0.42
2:B:165:GLN:HB2	7:B:491:HOH:O	2.20	0.42
2:C:34:GLU:N	2:C:34:GLU:CD	2.77	0.42
2:C:68:LEU:HA	2:C:71:VAL:HG12	2.02	0.42
2:C:98:TRP:CD2	2:C:138:GLU:OE2	2.73	0.42
1:D:46:GLN:NE2	7:D:845:HOH:O	2.53	0.42
1:D:232:ARG:O	1:D:235:GLU:HB2	2.20	0.42
1:D:434:ASP:CG	1:D:550:CYS:HB3	2.45	0.42
1:D:499:ARG:CZ	1:D:499:ARG:CB	2.95	0.42
2:F:18:ARG:HH21	2:F:160:PHE:HE1	1.68	0.42
2:F:98:TRP:CZ2	2:F:157:LEU:HD22	2.54	0.42
2:F:143:PRO:HB2	2:F:144:TYR:CD2	2.54	0.42
2:F:179:SER:HA	2:F:180:PRO:HD3	1.84	0.42
1:A:39:ASN:HA	2:B:142:LYS:HG2	2.01	0.41
1:A:364:LEU:HB2	1:A:389:GLU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:LYS:HG3	1:A:553:PRO:HD2	2.02	0.41
2:C:11:TRP:HZ3	2:C:205:ILE:HG13	1.84	0.41
2:C:60:ASN:O	2:C:60:ASN:ND2	2.52	0.41
1:D:149:PHE:CZ	1:D:202:LEU:HD13	2.55	0.41
1:D:187:CYS:HB2	1:D:208:SER:C	2.45	0.41
1:D:445:VAL:HG13	1:D:479:TRP:NE1	2.35	0.41
1:A:165:ALA:HB3	4:A:602:LEU:OXT	2.19	0.41
1:A:361:PHE:CE2	1:A:392:ILE:HG12	2.55	0.41
1:A:552:LYS:C	1:A:554:SER:N	2.77	0.41
1:A:568:SER:HB3	7:A:882:HOH:O	2.20	0.41
2:C:24:ARG:HG3	2:C:30:PHE:CE1	2.55	0.41
1:D:197:ASP:HB3	1:D:567:VAL:HG23	2.01	0.41
1:D:412:PHE:HB3	1:D:414:ASN:O	2.20	0.41
2:F:70:VAL:HA	2:F:73:TYR:CD2	2.55	0.41
1:A:10:MET:HG2	7:A:853:HOH:O	2.19	0.41
1:A:87:PRO:CB	1:A:93:PRO:HD3	2.40	0.41
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.84	0.41
2:B:35:GLU:HG3	2:B:44:LEU:HD22	2.01	0.41
2:B:144:TYR:OH	2:B:192:LYS:NZ	2.43	0.41
1:D:13:VAL:O	1:D:16:GLU:HG2	2.20	0.41
1:D:105:GLN:C	1:D:107:ARG:H	2.27	0.41
1:D:123:GLN:HG2	7:D:864:HOH:O	2.19	0.41
1:D:152:LYS:NZ	1:D:527:THR:OG1	2.53	0.41
1:D:169:VAL:HG21	4:D:602:LEU:HD11	2.02	0.41
1:D:250:LEU:HG	7:D:800:HOH:O	2.20	0.41
1:D:272:GLU:O	1:D:275:GLU:HB3	2.20	0.41
1:D:301:VAL:HG23	1:D:323:LEU:HD13	2.01	0.41
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.51	0.41
1:A:109:LYS:NZ	1:A:401:TYR:CZ	2.81	0.41
1:A:200:GLN:O	1:A:203:TYR:HB3	2.20	0.41
1:A:325:LEU:O	7:A:750:HOH:O	2.21	0.41
1:A:337:ILE:HG22	1:A:338:ALA:N	2.34	0.41
2:B:85:PHE:HE1	2:B:152:TYR:HB2	1.85	0.41
1:D:338:ALA:HA	1:D:354:VAL:HA	2.02	0.41
2:E:98:TRP:CE2	2:E:138:GLU:HG2	2.55	0.41
2:F:68:LEU:HG	7:F:476:HOH:O	2.19	0.41
1:A:25:HIS:HB2	7:A:866:HOH:O	2.20	0.41
1:A:101:SER:HB3	1:A:535:PHE:CG	2.55	0.41
1:A:170:TYR:CD1	1:A:170:TYR:N	2.88	0.41
1:A:362:GLU:HG3	1:A:400:ARG:NH2	2.35	0.41
1:A:363:PHE:HD2	1:A:382:VAL:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:PHE:O	1:A:531:ILE:HB	2.21	0.41
2:B:129:ILE:O	2:B:132:VAL:HG22	2.21	0.41
2:C:32:TYR:HD1	2:C:34:GLU:OE2	2.02	0.41
1:D:33:LYS:O	1:D:37:LEU:HB2	2.21	0.41
1:D:99:LEU:HB2	1:D:557:LYS:H	1.86	0.41
1:D:235:GLU:HG2	1:D:287:TRP:CG	2.56	0.41
2:E:21:VAL:HG23	7:E:425:HOH:O	2.20	0.41
2:F:15:PHE:HB3	2:F:67:SER:HB3	2.03	0.41
2:F:26:LYS:HD2	2:F:74:VAL:CG1	2.51	0.41
2:F:64:VAL:HG23	2:F:70:VAL:HG22	2.01	0.41
1:A:93:PRO:HG2	2:B:184:ALA:HB1	2.01	0.41
1:A:336:TRP:CB	1:A:358:LEU:HB3	2.50	0.41
1:A:510:ARG:HG2	1:A:515:ILE:O	2.21	0.41
1:A:527:THR:O	1:A:530:LYS:HB2	2.21	0.41
1:A:570:TYR:OH	7:A:740:HOH:O	2.17	0.41
2:B:183:ILE:O	2:B:187:LYS:HG2	2.21	0.41
1:D:104:SER:OG	1:D:109:LYS:HG3	2.20	0.41
1:D:234:PHE:HB3	7:D:710:HOH:O	2.20	0.41
1:D:351:THR:HG22	1:D:420:LYS:HB3	2.03	0.41
2:E:53:LYS:O	7:E:413:HOH:O	2.20	0.41
2:F:98:TRP:CE3	2:F:98:TRP:O	2.73	0.41
1:A:28:GLN:HE21	1:A:361:PHE:N	2.12	0.41
1:A:197:ASP:O	1:A:201:ALA:N	2.52	0.41
1:A:407:VAL:HG22	1:A:419:LEU:HD22	2.01	0.41
1:A:478:PHE:C	1:A:479:TRP:HD1	2.29	0.41
1:D:25:HIS:CE1	1:D:380:THR:HG21	2.55	0.41
1:D:153:GLN:HG2	1:D:167:THR:HG21	2.02	0.41
1:D:495:ASN:ND2	1:D:572:SER:HB3	2.36	0.41
1:A:42:ALA:HA	2:B:143:PRO:CG	2.47	0.41
1:A:134:ARG:NH2	7:A:825:HOH:O	2.48	0.41
1:A:218:TYR:CE2	1:A:220:PHE:HB2	2.55	0.41
1:A:407:VAL:HG23	1:A:420:LYS:O	2.21	0.41
1:A:555:ASN:HB3	7:A:841:HOH:O	2.19	0.41
2:B:125:LYS:O	2:B:129:ILE:HG12	2.21	0.41
2:C:5:PRO:HB3	2:C:57:LEU:HD11	2.03	0.41
2:C:23:LEU:CD2	2:C:28:VAL:HG11	2.49	0.41
2:C:62:LYS:NZ	7:C:447:HOH:O	2.50	0.41
2:C:98:TRP:HD1	2:C:153:VAL:HG11	1.85	0.41
2:E:93:ALA:HB1	2:F:73:TYR:CZ	2.56	0.41
2:F:98:TRP:CH2	2:F:135:LEU:HG	2.55	0.41
2:F:151:GLY:O	2:F:154:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:CZ	1:A:168:ASN:HB3	2.56	0.41
1:A:149:PHE:HB3	1:A:530:LYS:HD3	2.03	0.41
1:A:225:HIS:ND1	1:A:309:MET:SD	2.92	0.41
1:A:387:GLU:HA	1:A:407:VAL:O	2.21	0.41
1:A:494:CYS:SG	1:A:495:ASN:N	2.94	0.41
1:A:500:ALA:O	1:A:502:ILE:N	2.54	0.41
1:A:520:LEU:O	1:A:569:SER:HA	2.21	0.41
1:A:567:VAL:HA	7:A:834:HOH:O	2.21	0.41
2:B:81:LYS:HB2	2:B:82:ASN:H	1.73	0.41
2:B:89:PRO:HB3	2:C:76:GLU:HG3	2.02	0.41
2:C:71:VAL:HG13	2:C:152:TYR:CE1	2.56	0.41
1:D:227:LEU:O	1:D:231:PHE:HD2	2.03	0.41
1:D:238:TRP:CZ2	1:D:239:GLU:HG3	2.56	0.41
1:D:238:TRP:HZ3	1:D:278:ARG:HA	1.85	0.41
1:D:302:TYR:OH	1:D:328:HIS:ND1	2.51	0.41
1:D:364:LEU:HB2	7:D:828:HOH:O	2.21	0.41
1:D:413:TYR:O	1:D:414:ASN:HB2	2.21	0.41
1:D:437:THR:CG2	1:D:439:ARG:HH21	2.34	0.41
1:D:453:SER:C	1:D:455:GLU:N	2.79	0.41
1:D:464:SER:HA	1:D:476:ALA:O	2.21	0.41
1:D:563:CYS:HA	1:D:566:VAL:HG13	2.01	0.41
1:D:566:VAL:C	1:D:568:SER:N	2.74	0.41
2:E:36:ASP:OD1	7:E:415:HOH:O	2.21	0.41
2:E:158:ILE:O	2:E:161:SER:OG	2.30	0.41
2:F:85:PHE:HD2	2:F:92:ARG:NH1	2.19	0.41
2:F:129:ILE:O	2:F:132:VAL:HG12	2.21	0.41
2:F:151:GLY:H	2:F:154:ASP:CG	2.24	0.41
1:A:113:PHE:HA	1:A:117:LEU:HD12	2.02	0.41
1:A:202:LEU:O	1:A:205:HIS:N	2.54	0.41
1:A:202:LEU:HG	1:A:205:HIS:CA	2.48	0.41
1:A:238:TRP:CZ2	1:A:281:CYS:HB3	2.53	0.41
1:A:241:ILE:HG13	1:A:242:VAL:H	1.84	0.41
1:A:354:VAL:HG11	1:A:379:LEU:HD11	2.03	0.41
1:A:379:LEU:HD23	1:A:380:THR:HG23	2.03	0.41
1:D:21:THR:O	1:D:24:ALA:HB2	2.21	0.41
2:E:25:GLU:HG2	2:E:84:PHE:HE1	1.86	0.41
2:E:88:ASP:HA	2:E:89:PRO:HD2	1.87	0.41
2:F:14:MET:N	7:F:433:HOH:O	2.40	0.41
1:A:27:VAL:HG13	1:A:356:PRO:HB2	2.03	0.40
1:A:119:GLU:C	1:A:123:GLN:HE21	2.29	0.40
1:A:143:LYS:HB2	1:A:185:PRO:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASN:HB2	7:A:810:HOH:O	2.21	0.40
1:A:452:LEU:O	1:A:457:ILE:HG12	2.21	0.40
2:B:61:GLY:N	7:B:453:HOH:O	2.53	0.40
2:B:164:PHE:CD2	2:B:183:ILE:HG13	2.57	0.40
2:C:11:TRP:O	2:C:200:PRO:HG2	2.21	0.40
1:D:126:ARG:CZ	1:D:182:ILE:HD11	2.51	0.40
1:D:332:SER:CB	1:D:538:LEU:HA	2.50	0.40
1:D:332:SER:HB3	1:D:538:LEU:HA	2.04	0.40
1:D:341:VAL:HG23	1:D:342:THR:HG23	2.02	0.40
2:E:24:ARG:HH11	2:E:24:ARG:C	2.11	0.40
2:E:207:ALA:O	2:E:211:GLU:HB2	2.20	0.40
2:F:49:PRO:O	2:F:52:LYS:NZ	2.22	0.40
1:A:70:ASP:HB2	1:A:109:LYS:HG3	2.04	0.40
1:A:74:GLU:O	1:A:78:LYS:HB2	2.20	0.40
1:A:94:VAL:HG11	1:A:112:PRO:HB3	2.03	0.40
1:A:142:GLY:CA	1:A:215:GLN:HB2	2.52	0.40
1:D:29:LYS:O	1:D:33:LYS:HG3	2.21	0.40
1:D:92:HIS:CD2	2:E:185:TRP:HB2	2.56	0.40
1:D:92:HIS:CD2	2:E:139:LEU:HD23	2.57	0.40
1:D:143:LYS:NZ	1:D:187:CYS:HA	2.36	0.40
1:D:278:ARG:O	1:D:282:MET:HE2	2.21	0.40
1:D:284:LEU:HD13	1:D:287:TRP:CA	2.51	0.40
1:D:336:TRP:HB2	1:D:358:LEU:CD1	2.52	0.40
1:A:27:VAL:HB	7:A:862:HOH:O	2.21	0.40
1:A:275:GLU:O	1:A:279:THR:HG23	2.21	0.40
2:B:24:ARG:NH1	7:B:436:HOH:O	2.32	0.40
2:B:128:PHE:HE2	2:B:175:ILE:HG21	1.85	0.40
2:B:188:ARG:HD3	2:B:188:ARG:C	2.47	0.40
2:C:68:LEU:O	2:C:72:GLN:HG2	2.21	0.40
2:C:159:THR:O	7:C:410:HOH:O	2.22	0.40
1:D:27:VAL:HG21	1:D:356:PRO:HG2	2.02	0.40
1:D:27:VAL:HG23	1:D:357:ASN:HB3	2.03	0.40
1:D:107:ARG:NH1	1:D:433:ILE:HD11	2.37	0.40
1:D:391:VAL:HG22	1:D:402:ARG:HG2	2.04	0.40
1:D:565:ASN:O	1:D:567:VAL:N	2.53	0.40
2:E:9:ASP:HB3	2:E:32:TYR:CE1	2.56	0.40
2:E:48:ASN:ND2	2:E:65:CYS:SG	2.94	0.40
1:A:96:ALA:HB1	1:A:163:GLY:HA3	2.03	0.40
1:A:213:ARG:CG	1:A:214:ASP:N	2.85	0.40
1:A:217:GLN:O	1:A:299:LYS:N	2.51	0.40
1:A:313:VAL:N	1:A:314:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ASN:O	1:A:437:THR:C	2.65	0.40
1:A:477:ILE:O	1:A:520:LEU:HD12	2.22	0.40
1:A:490:LEU:HD13	1:A:522:VAL:HG21	2.03	0.40
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.86	0.40
2:B:26:LYS:HZ3	2:B:28:VAL:CG2	2.34	0.40
2:B:117:LYS:O	7:B:421:HOH:O	2.22	0.40
1:D:18:ASP:O	1:D:21:THR:OG1	2.33	0.40
1:D:235:GLU:HG2	1:D:287:TRP:CD2	2.56	0.40
1:D:393:THR:HG1	1:D:400:ARG:H	1.63	0.40
1:D:405:ASP:OD2	1:D:541:SER:O	2.40	0.40
1:D:423:CYS:HB2	1:D:542:ALA:C	2.47	0.40
2:E:26:LYS:HA	2:E:26:LYS:HD2	1.62	0.40
2:E:74:VAL:O	7:E:417:HOH:O	2.22	0.40
2:E:145:PHE:N	2:E:145:PHE:CD1	2.90	0.40
2:F:12:PRO:O	2:F:163:TRP:HZ2	2.04	0.40
2:F:41:SER:HA	2:F:42:PRO:HD3	2.00	0.40
1:A:110:PHE:HE1	1:A:556:ALA:HB2	1.75	0.40
1:A:260:ARG:HG2	1:A:260:ARG:HH11	1.86	0.40
1:A:475:TYR:OH	7:A:728:HOH:O	2.13	0.40
2:B:182:LEU:O	2:B:185:TRP:HB3	2.21	0.40
2:C:4:LEU:HA	2:C:4:LEU:HD23	1.82	0.40
2:C:110:GLN:HG2	2:C:167:TYR:CE2	2.57	0.40
1:D:246:LYS:HE3	1:D:246:LYS:HB3	1.84	0.40
1:D:310:GLU:N	1:D:311:PRO:CD	2.84	0.40
1:D:464:SER:O	1:D:550:CYS:HA	2.21	0.40
1:D:497:LEU:HD12	1:D:520:LEU:HD22	2.02	0.40
2:E:16:GLY:HA2	2:E:55:PRO:HG3	2.04	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:O	1:D:511:LYS:NZ[1_655]	1.97	0.23
1:A:299:LYS:NZ	1:A:431:ILE:O[1_655]	2.01	0.19
1:A:239:GLU:OE2	2:F:174:SER:N[1_554]	2.02	0.18
1:A:286:ASN:ND2	2:F:161:SER:OG[1_554]	2.03	0.17
1:A:213:ARG:NH1	1:A:436:ASN:OD1[1_655]	2.07	0.13
1:D:270:ASN:ND2	1:D:510:ARG:O[1_655]	2.08	0.12
1:A:139:ASP:OD2	7:A:717:HOH:O[1_655]	2.10	0.10
1:A:270:ASN:ND2	1:A:510:ARG:O[1_655]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:748:HOH:O	7:F:423:HOH:O[1_554]	2.15	0.05
7:A:788:HOH:O	7:A:846:HOH:O[1_655]	2.16	0.04
1:D:213:ARG:NH1	1:D:436:ASN:OD1[1_655]	2.16	0.04
1:A:207:LEU:O	1:A:508:SER:OG[1_655]	2.17	0.03
7:A:1258:HOH:O	7:A:1259:HOH:O[1_655]	2.18	0.02
7:D:1340:HOH:O	7:D:1343:HOH:O[1_445]	2.18	0.02
7:A:927:HOH:O	7:F:542:HOH:O[1_554]	2.19	0.01
7:B:483:HOH:O	7:C:472:HOH:O[1_565]	2.19	0.01
7:C:626:HOH:O	7:D:1268:HOH:O[1_455]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/575 (99%)	526 (93%)	29 (5%)	12 (2%)	5	1
1	D	567/575 (99%)	530 (94%)	30 (5%)	7 (1%)	10	3
2	B	212/223 (95%)	196 (92%)	14 (7%)	2 (1%)	14	5
2	C	212/223 (95%)	196 (92%)	15 (7%)	1 (0%)	24	14
2	E	212/223 (95%)	198 (93%)	13 (6%)	1 (0%)	24	14
2	F	212/223 (95%)	197 (93%)	12 (6%)	3 (1%)	9	2
All	All	1982/2042 (97%)	1843 (93%)	113 (6%)	26 (1%)	9	3

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	TRP
1	A	513	LYS
1	A	540	SER
1	D	369	THR
1	D	433	ILE
1	D	437	THR

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Mol	Chain	Res	Type
1	D	513	LYS
1	D	540	SER
2	E	141	ASP
1	A	368	GLU
1	A	437	THR
1	A	553	PRO
2	B	140	GLY
2	C	140	GLY
1	D	88	ILE
1	D	368	GLU
2	F	140	GLY
2	F	180	PRO
1	A	237	VAL
2	B	27	GLY
1	A	51	ASN
1	A	369	THR
1	A	542	ALA
1	A	271	PRO
1	A	88	ILE
2	F	12	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	449 (90%)	50 (10%)	7	2
1	D	499/505 (99%)	436 (87%)	63 (13%)	4	1
2	B	187/195 (96%)	171 (91%)	16 (9%)	10	3
2	C	187/195 (96%)	172 (92%)	15 (8%)	11	3
2	E	187/195 (96%)	171 (91%)	16 (9%)	10	3
2	F	187/195 (96%)	172 (92%)	15 (8%)	11	3
All	All	1746/1790 (98%)	1571 (90%)	175 (10%)	7	2

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	27	VAL
1	A	99	LEU
1	A	110	PHE
1	A	114	THR
1	A	125	PHE
1	A	145	LEU
1	A	150	SER
1	A	166	THR
1	A	182	ILE
1	A	184	SER
1	A	187	CYS
1	A	205	HIS
1	A	206	LEU
1	A	215	GLN
1	A	237	VAL
1	A	245	ILE
1	A	250	LEU
1	A	268	THR
1	A	273	LEU
1	A	275	GLU
1	A	276	THR
1	A	284	LEU
1	A	295	PHE
1	A	301	VAL
1	A	315	LYS
1	A	326	VAL
1	A	328	HIS
1	A	354	VAL
1	A	369	THR
1	A	379	LEU
1	A	422	ILE
1	A	425	ARG
1	A	426	ASN
1	A	429	LEU
1	A	431	ILE
1	A	450	LYS
1	A	459	VAL
1	A	460	ILE
1	A	468	VAL
1	A	477	ILE
1	A	494	CYS
1	A	499	ARG

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Mol	Chain	Res	Type
1	A	509	SER
1	A	512	CYS
1	A	523	VAL
1	A	529	ARG
1	A	534	HIS
1	A	538	LEU
1	A	559	LEU
2	B	10	TYR
2	B	36	ASP
2	B	62	LYS
2	B	80	GLU
2	B	110	GLN
2	B	136	GLU
2	B	153	VAL
2	B	154	ASP
2	B	170	PHE
2	B	175	ILE
2	B	181	LYS
2	B	187	LYS
2	B	190	MET
2	B	205	ILE
2	B	206	VAL
2	B	211	GLU
2	C	28	VAL
2	C	32	TYR
2	C	43	LEU
2	C	65	CYS
2	C	72	GLN
2	C	84	PHE
2	C	117	LYS
2	C	134	ILE
2	C	135	LEU
2	C	139	LEU
2	C	157	LEU
2	C	176	GLU
2	C	183	ILE
2	C	206	VAL
2	C	211	GLU
1	D	12	ARG
1	D	27	VAL
1	D	39	ASN
1	D	71	VAL

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Mol	Chain	Res	Type
1	D	79	ARG
1	D	80	MET
1	D	86	SER
1	D	90	THR
1	D	92	HIS
1	D	97	ILE
1	D	107	ARG
1	D	114	THR
1	D	138	ILE
1	D	140	ASP
1	D	151	SER
1	D	152	LYS
1	D	162	VAL
1	D	182	ILE
1	D	184	SER
1	D	188	SER
1	D	205	HIS
1	D	215	GLN
1	D	219	VAL
1	D	225	HIS
1	D	241	ILE
1	D	242	VAL
1	D	245	ILE
1	D	250	LEU
1	D	251	SER
1	D	277	ILE
1	D	295	PHE
1	D	313	VAL
1	D	326	VAL
1	D	329	ASP
1	D	345	LEU
1	D	373	GLU
1	D	375	LYS
1	D	379	LEU
1	D	392	ILE
1	D	403	LEU
1	D	407	VAL
1	D	410	ILE
1	D	421	PHE
1	D	424	ARG
1	D	427	LEU
1	D	430	SER

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Mol	Chain	Res	Type
1	D	452	LEU
1	D	459	VAL
1	D	461	ASP
1	D	484	GLU
1	D	499	ARG
1	D	502	ILE
1	D	510	ARG
1	D	512	CYS
1	D	518	LEU
1	D	523	VAL
1	D	545	PHE
1	D	547	MET
1	D	551	VAL
1	D	561	ILE
1	D	562	LEU
1	D	566	VAL
1	D	567	VAL
2	E	4	LEU
2	E	6	ILE
2	E	23	LEU
2	E	51	HIS
2	E	60	ASN
2	E	62	LYS
2	E	80	GLU
2	E	81	LYS
2	E	110	GLN
2	E	139	LEU
2	E	145	PHE
2	E	158	ILE
2	E	168	GLU
2	E	173	PHE
2	E	195	VAL
2	E	211	GLU
2	F	26	LYS
2	F	32	TYR
2	F	43	LEU
2	F	68	LEU
2	F	133	LYS
2	F	134	ILE
2	F	135	LEU
2	F	139	LEU
2	F	157	LEU

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Mol	Chain	Res	Type
2	F	175	ILE
2	F	176	GLU
2	F	182	LEU
2	F	206	VAL
2	F	211	GLU
2	F	212	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	53	ASN
1	A	123	GLN
1	A	172	ASN
1	A	215	GLN
1	A	217	GLN
1	A	236	GLN
1	A	318	HIS
2	B	51	HIS
2	C	60	ASN
2	C	72	GLN
2	C	216	ASN
1	D	47	ASN
1	D	215	GLN
1	D	225	HIS
1	D	340	ASN
2	E	48	ASN
2	F	72	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
6	GSH	F	301	-	18,19,19	1.43	3 (16%)	21,24,24	2.47	5 (23%)
6	GSH	B	301	-	18,19,19	1.55	3 (16%)	21,24,24	2.47	4 (19%)
6	GSH	C	301	-	18,19,19	1.47	3 (16%)	21,24,24	2.69	4 (19%)
6	GSH	E	301	-	18,19,19	1.56	3 (16%)	21,24,24	2.64	6 (28%)
4	LEU	D	602	-	6,8,8	0.99	1 (16%)	5,10,10	1.16	1 (20%)
3	JAA	A	601	-	15,15,15	5.26	7 (46%)	14,19,19	3.50	10 (71%)
4	LEU	A	602	5	6,8,8	0.97	1 (16%)	5,10,10	1.21	1 (20%)
3	JAA	D	601	-	15,15,15	5.39	7 (46%)	14,19,19	3.26	9 (64%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GSH	F	301	-	-	6/24/24/24	-
6	GSH	B	301	-	-	0/24/24/24	-
6	GSH	C	301	-	-	6/24/24/24	-
6	GSH	E	301	-	-	7/24/24/24	-
4	LEU	D	602	-	-	3/8/8/8	-
3	JAA	A	601	-	-	9/9/22/22	0/1/1/1
4	LEU	A	602	5	-	4/8/8/8	-
3	JAA	D	601	-	-	4/9/22/22	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	JAA	C05-C08	-13.38	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JAA	C05-C08	-12.86	1.31	1.52
3	D	601	JAA	C06-C04	-11.66	1.24	1.53
3	A	601	JAA	C06-C04	-11.55	1.24	1.53
3	D	601	JAA	C07-C08	6.50	1.61	1.51
3	A	601	JAA	C07-C08	6.42	1.61	1.51
3	A	601	JAA	C10-C04	-5.21	1.45	1.53
3	D	601	JAA	C05-C04	4.94	1.66	1.54
3	D	601	JAA	C10-C04	-4.89	1.45	1.53
3	A	601	JAA	C05-C04	4.70	1.66	1.54
3	D	601	JAA	C09-C05	-4.29	1.48	1.54
3	A	601	JAA	C09-C05	-3.71	1.49	1.54
6	E	301	GSH	C2-N3	2.89	1.40	1.33
6	C	301	GSH	CA2-N2	-2.86	1.39	1.45
6	B	301	GSH	C2-N3	2.82	1.40	1.33
6	C	301	GSH	C2-N3	2.80	1.40	1.33
6	F	301	GSH	C2-N3	2.79	1.40	1.33
6	E	301	GSH	CD1-N2	2.76	1.39	1.34
6	B	301	GSH	CD1-N2	2.73	1.39	1.34
6	B	301	GSH	CA2-N2	-2.72	1.40	1.45
6	E	301	GSH	CA2-N2	-2.70	1.40	1.45
6	F	301	GSH	CA2-N2	-2.69	1.40	1.45
6	F	301	GSH	CD1-N2	2.64	1.39	1.34
6	C	301	GSH	CD1-N2	2.42	1.39	1.34
4	D	602	LEU	OXT-C	-2.31	1.23	1.30
4	A	602	LEU	OXT-C	-2.26	1.23	1.30
3	D	601	JAA	O03-C12	-2.06	1.24	1.30
3	A	601	JAA	O03-C12	-2.00	1.24	1.30

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301	GSH	CA2-CB2-SG2	-10.54	102.28	114.16
6	B	301	GSH	CA2-CB2-SG2	-9.30	103.67	114.16
6	F	301	GSH	CA2-CB2-SG2	-8.40	104.69	114.16
6	E	301	GSH	CA2-CB2-SG2	-7.83	105.34	114.16
3	D	601	JAA	C07-C06-C04	-6.21	97.89	104.45
6	E	301	GSH	CB2-CA2-N2	-5.95	102.80	111.28
3	A	601	JAA	C07-C06-C04	-5.89	98.22	104.45
3	A	601	JAA	C09-C11-C13	-5.64	105.46	126.21
3	D	601	JAA	C09-C11-C13	-5.06	107.59	126.21
3	D	601	JAA	C06-C07-C08	-4.79	100.65	105.39
3	A	601	JAA	C06-C07-C08	-4.75	100.69	105.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	301	GSH	CB2-CA2-N2	-4.02	105.56	111.28
6	F	301	GSH	CB2-CA2-N2	-3.88	105.76	111.28
3	D	601	JAA	O03-C12-C10	3.61	125.22	114.00
3	A	601	JAA	O01-C08-C05	3.61	130.21	125.60
6	E	301	GSH	CB1-CG1-CD1	3.59	121.07	113.06
3	A	601	JAA	C14-C13-C11	-3.54	105.13	126.42
3	A	601	JAA	O03-C12-C10	3.47	124.78	114.00
3	A	601	JAA	C06-C04-C10	-3.40	107.08	113.41
3	D	601	JAA	C06-C04-C10	-3.38	107.13	113.41
6	E	301	GSH	CG1-CD1-N2	-3.31	110.03	115.86
3	A	601	JAA	O02-C12-C10	-3.30	112.70	122.84
3	D	601	JAA	C07-C08-C05	-3.28	103.66	109.06
3	A	601	JAA	C07-C08-C05	-3.25	103.72	109.06
3	D	601	JAA	O02-C12-C10	-3.20	113.02	122.84
6	C	301	GSH	CB2-CA2-N2	-3.08	106.90	111.28
3	A	601	JAA	C04-C10-C12	-3.05	107.15	113.33
6	F	301	GSH	CG1-CD1-N2	-2.96	110.65	115.86
6	F	301	GSH	CB1-CG1-CD1	2.94	119.61	113.06
3	D	601	JAA	C14-C13-C11	-2.62	110.63	126.42
4	A	602	LEU	OXT-C-O	-2.61	118.15	124.08
6	C	301	GSH	C2-CA2-N2	-2.59	104.09	111.11
4	D	602	LEU	OXT-C-O	-2.51	118.38	124.08
3	D	601	JAA	O01-C08-C05	2.48	128.77	125.60
6	E	301	GSH	OE1-CD1-CG1	2.31	126.21	122.02
6	B	301	GSH	CG1-CD1-N2	-2.29	111.83	115.86
6	F	301	GSH	OE1-CD1-CG1	2.29	126.17	122.02
6	B	301	GSH	CB1-CG1-CD1	2.16	117.87	113.06
6	E	301	GSH	CB2-CA2-C2	-2.15	104.82	109.50
6	C	301	GSH	CG1-CD1-N2	-2.14	112.09	115.86

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	JAA	C05-C04-C10-C12
3	A	601	JAA	C06-C04-C10-C12
3	A	601	JAA	C08-C05-C09-C11
6	C	301	GSH	N2-CA2-CB2-SG2
6	C	301	GSH	C2-CA2-CB2-SG2
6	E	301	GSH	N1-CA1-CB1-CG1
6	E	301	GSH	C1-CA1-CB1-CG1
6	E	301	GSH	N2-CA2-CB2-SG2

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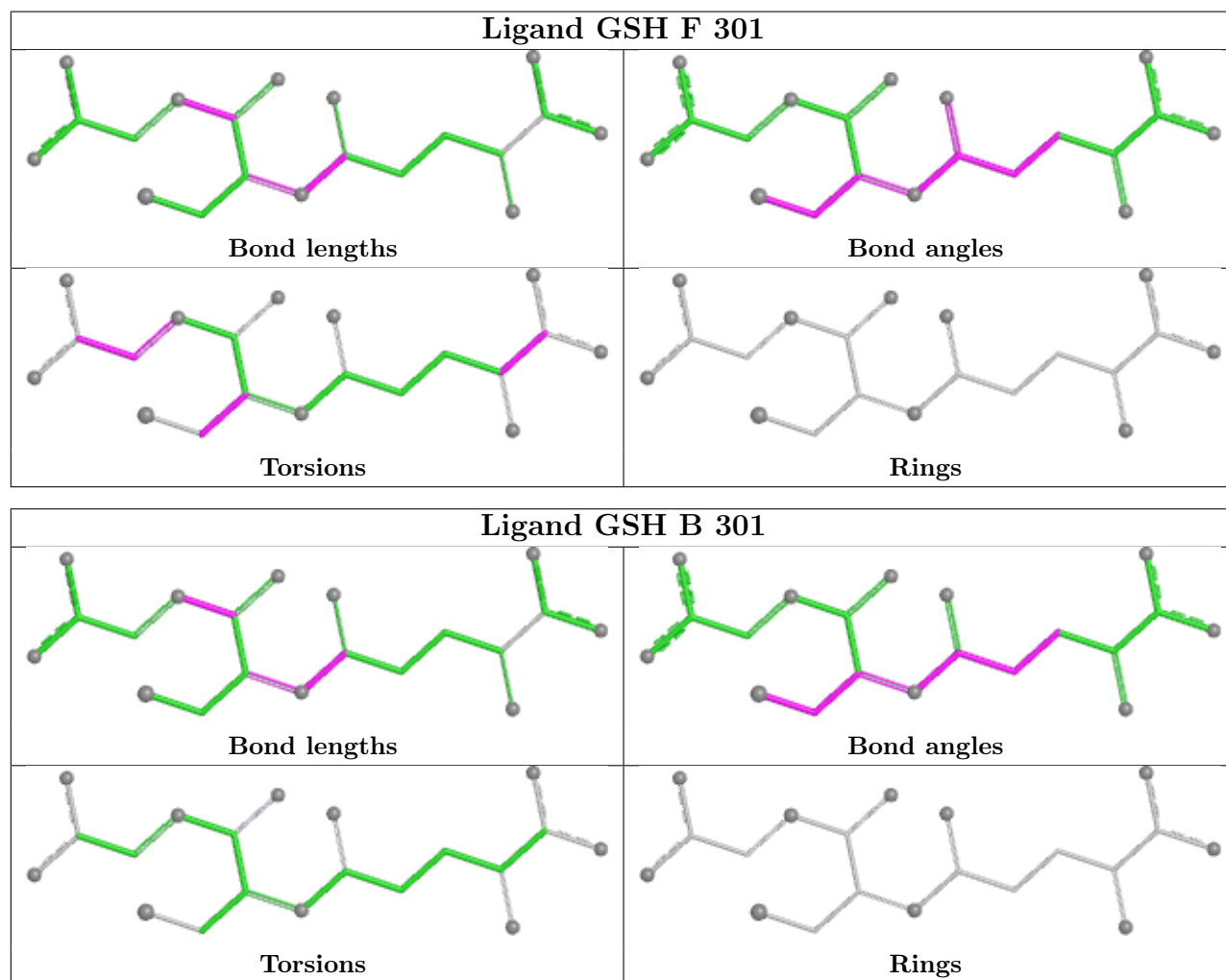
Mol	Chain	Res	Type	Atoms
6	E	301	GSH	C2-CA2-CB2-SG2
6	F	301	GSH	N2-CA2-CB2-SG2
6	F	301	GSH	C2-CA2-CB2-SG2
3	A	601	JAA	C09-C11-C13-C14
4	A	602	LEU	C-CA-CB-CG
3	D	601	JAA	C09-C11-C13-C14
6	E	301	GSH	CA1-CB1-CG1-CD1
6	C	301	GSH	O32-C3-CA3-N3
6	E	301	GSH	O32-C3-CA3-N3
6	C	301	GSH	O31-C3-CA3-N3
6	E	301	GSH	O31-C3-CA3-N3
6	F	301	GSH	O31-C3-CA3-N3
3	A	601	JAA	C11-C13-C14-C15
4	A	602	LEU	OXT-C-CA-N
3	D	601	JAA	C05-C09-C11-C13
4	A	602	LEU	O-C-CA-N
6	C	301	GSH	O12-C1-CA1-N1
3	A	601	JAA	C04-C05-C09-C11
6	F	301	GSH	O32-C3-CA3-N3
4	D	602	LEU	C-CA-CB-CG
3	A	601	JAA	C05-C09-C11-C13
3	A	601	JAA	C04-C10-C12-O03
3	A	601	JAA	C04-C10-C12-O02
3	D	601	JAA	C04-C05-C09-C11
6	F	301	GSH	O12-C1-CA1-N1
4	D	602	LEU	OXT-C-CA-N
4	A	602	LEU	N-CA-CB-CG
4	D	602	LEU	N-CA-CB-CG
6	F	301	GSH	C3-CA3-N3-C2
3	D	601	JAA	C08-C05-C09-C11
6	C	301	GSH	CA1-CB1-CG1-CD1

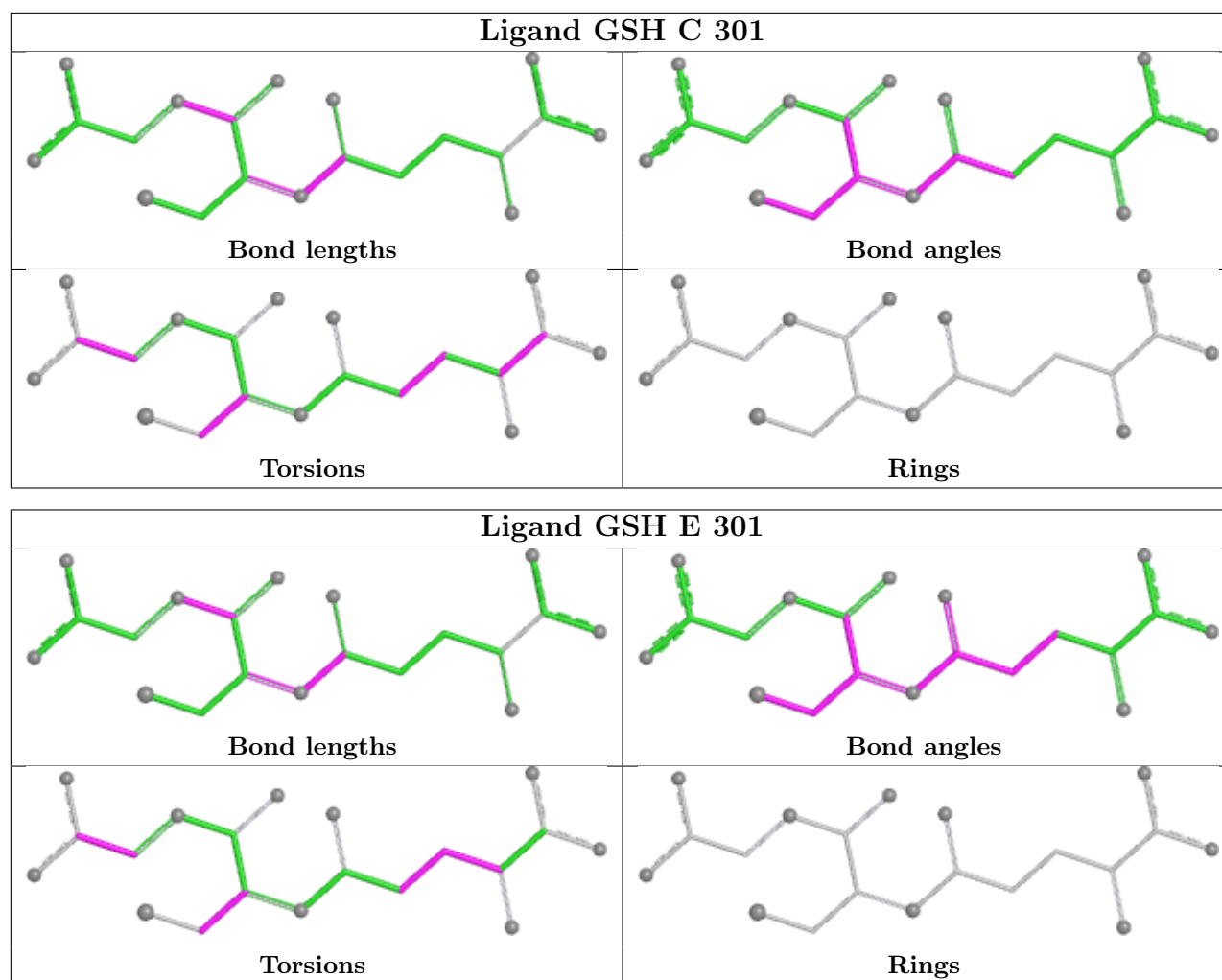
There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	301	GSH	1	0
6	E	301	GSH	2	0
4	D	602	LEU	6	0
3	A	601	JAA	2	0
4	A	602	LEU	8	0
3	D	601	JAA	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	569/575 (98%)	1.13	96 (16%) 4 3	3, 9, 15, 21	0
1	D	569/575 (98%)	0.96	65 (11%) 10 8	3, 8, 13, 20	0
2	B	214/223 (95%)	0.63	12 (5%) 30 29	3, 6, 11, 13	0
2	C	214/223 (95%)	0.47	4 (1%) 66 66	2, 3, 7, 11	0
2	E	214/223 (95%)	0.85	21 (9%) 13 11	3, 7, 11, 15	0
2	F	214/223 (95%)	0.53	7 (3%) 49 49	2, 3, 7, 11	0
All	All	1994/2042 (97%)	0.86	205 (10%) 12 10	2, 7, 13, 21	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	10.1
1	A	201	ALA	7.0
1	A	205	HIS	6.8
1	A	506	TYR	6.1
1	D	494	CYS	5.6
2	E	184	ALA	5.1
2	E	27	GLY	4.9
1	D	113	PHE	4.5
2	B	139	LEU	4.5
1	A	203	TYR	4.2
1	A	338	ALA	4.2
1	A	294	LEU	4.2
1	A	551	VAL	4.1
1	D	88	ILE	4.1
2	F	128	PHE	4.0
1	D	523	VAL	3.9
1	D	77	ILE	3.9
1	D	573	THR	3.7
1	A	328	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	295	PHE	3.7
1	A	151	SER	3.6
1	A	352	PHE	3.6
2	E	144	TYR	3.5
1	D	79	ARG	3.5
1	D	562	LEU	3.5
2	E	153	VAL	3.4
1	D	433	ILE	3.4
1	A	285	SER	3.4
1	D	90	THR	3.4
1	A	222	VAL	3.4
2	E	30	PHE	3.4
2	C	32	TYR	3.3
1	A	17	PHE	3.3
1	A	306	THR	3.3
1	D	170	TYR	3.3
2	E	95	ALA	3.3
2	E	63	PRO	3.2
1	A	284	LEU	3.2
1	A	238	TRP	3.2
1	A	210	ILE	3.2
1	D	466	ILE	3.2
1	A	535	PHE	3.1
2	E	65	CYS	3.1
2	F	176	GLU	3.0
1	A	481	ILE	3.0
1	A	300	TYR	3.0
1	A	37	LEU	2.9
1	A	206	LEU	2.9
1	D	572	SER	2.9
1	A	160	VAL	2.9
1	A	163	GLY	2.9
1	D	102	GLY	2.9
1	A	361	PHE	2.9
1	A	353	ALA	2.9
2	B	98	TRP	2.9
1	A	404	GLY	2.9
1	D	169	VAL	2.8
1	A	27	VAL	2.8
2	B	10	TYR	2.8
1	D	542	ALA	2.8
1	D	548	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	118	GLY	2.8
1	A	121	THR	2.8
1	D	559	LEU	2.8
1	A	313	VAL	2.8
1	A	558	VAL	2.8
1	A	154	TYR	2.7
2	F	85	PHE	2.7
2	E	43	LEU	2.7
1	A	509	SER	2.7
2	C	124	GLY	2.7
1	A	304	ILE	2.7
1	D	47	ASN	2.7
1	A	38	LYS	2.7
1	A	550	CYS	2.7
1	D	95	PRO	2.7
1	A	561	ILE	2.7
2	E	150	PHE	2.6
1	A	273	LEU	2.6
1	A	457	ILE	2.6
2	E	72	GLN	2.6
1	A	293	ALA	2.6
2	E	64	VAL	2.6
1	A	295	PHE	2.6
1	A	358	LEU	2.6
1	A	217	GLN	2.6
1	D	160	VAL	2.6
1	D	195	SER	2.6
1	A	95	PRO	2.5
1	A	149	PHE	2.5
1	D	149	PHE	2.5
1	D	155	ILE	2.5
2	B	153	VAL	2.5
2	E	164	PHE	2.5
1	D	323	LEU	2.5
2	E	148	ASP	2.5
1	A	323	LEU	2.5
2	E	21	VAL	2.5
1	A	204	CYS	2.4
1	D	561	ILE	2.4
1	A	162	VAL	2.4
1	A	382	VAL	2.4
1	D	27	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	510	ARG	2.4
1	A	209	GLY	2.4
1	A	357	ASN	2.4
2	F	172	ASN	2.4
1	A	330	TYR	2.4
1	A	245	ILE	2.4
1	A	21	THR	2.4
2	F	184	ALA	2.4
1	A	324	PRO	2.4
1	A	318	HIS	2.4
2	E	124	GLY	2.4
2	F	101	PHE	2.4
1	D	531	ILE	2.4
1	A	287	TRP	2.4
1	A	36	LEU	2.3
1	A	125	PHE	2.3
2	E	172	ASN	2.3
2	B	184	ALA	2.3
2	B	210	ALA	2.3
1	A	237	VAL	2.3
1	D	512	CYS	2.3
1	D	462	PHE	2.3
1	A	477	ILE	2.3
1	A	259	VAL	2.3
1	A	563	CYS	2.3
1	A	527	THR	2.3
1	A	499	ARG	2.2
1	A	548	PRO	2.2
1	A	392	ILE	2.2
1	D	410	ILE	2.2
2	C	183	ILE	2.2
2	E	74	VAL	2.2
1	A	432	ASN	2.2
1	A	356	PRO	2.2
1	A	541	SER	2.2
1	D	258	SER	2.2
2	F	79	PRO	2.2
1	A	96	ALA	2.2
1	D	60	ALA	2.2
1	A	336	TRP	2.2
1	D	147	PHE	2.2
2	E	54	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	282	MET	2.2
1	A	468	VAL	2.2
1	D	379	LEU	2.2
1	A	472	PRO	2.2
1	D	460	ILE	2.2
1	D	166	THR	2.2
1	D	91	GLY	2.2
1	A	44	TYR	2.1
1	D	218	TYR	2.1
1	A	148	ILE	2.1
1	D	35	ILE	2.1
1	D	193	ILE	2.1
1	D	479	TRP	2.1
1	D	452	LEU	2.1
1	A	542	ALA	2.1
1	D	556	ALA	2.1
2	B	77	ALA	2.1
1	D	220	PHE	2.1
1	D	111	ILE	2.1
1	D	507	VAL	2.1
1	D	204	CYS	2.1
1	A	207	LEU	2.1
1	A	311	PRO	2.1
1	D	403	LEU	2.1
2	B	7	LEU	2.1
1	D	560	GLN	2.1
2	E	166	ALA	2.1
2	B	173	PHE	2.1
1	A	515	ILE	2.1
1	D	291	ILE	2.1
1	A	181	SER	2.1
1	A	464	SER	2.1
1	D	188	SER	2.1
1	D	157	THR	2.1
1	D	369	THR	2.1
1	A	340	ASN	2.1
1	D	267	LEU	2.1
1	A	234	PHE	2.0
1	A	460	ILE	2.0
1	A	502	ILE	2.0
1	A	528	PHE	2.0
1	D	478	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	332	SER	2.0
2	E	152	TYR	2.0
1	A	276	THR	2.0
1	D	259	VAL	2.0
2	B	74	VAL	2.0
1	A	117	LEU	2.0
1	D	96	ALA	2.0
1	D	298	ALA	2.0
2	B	109	ALA	2.0
1	A	305	MET	2.0
1	A	220	PHE	2.0
1	D	428	ILE	2.0
1	D	528	PHE	2.0
1	D	575	PHE	2.0
1	A	233	THR	2.0
1	A	505	GLY	2.0
1	A	475	TYR	2.0
2	B	132	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

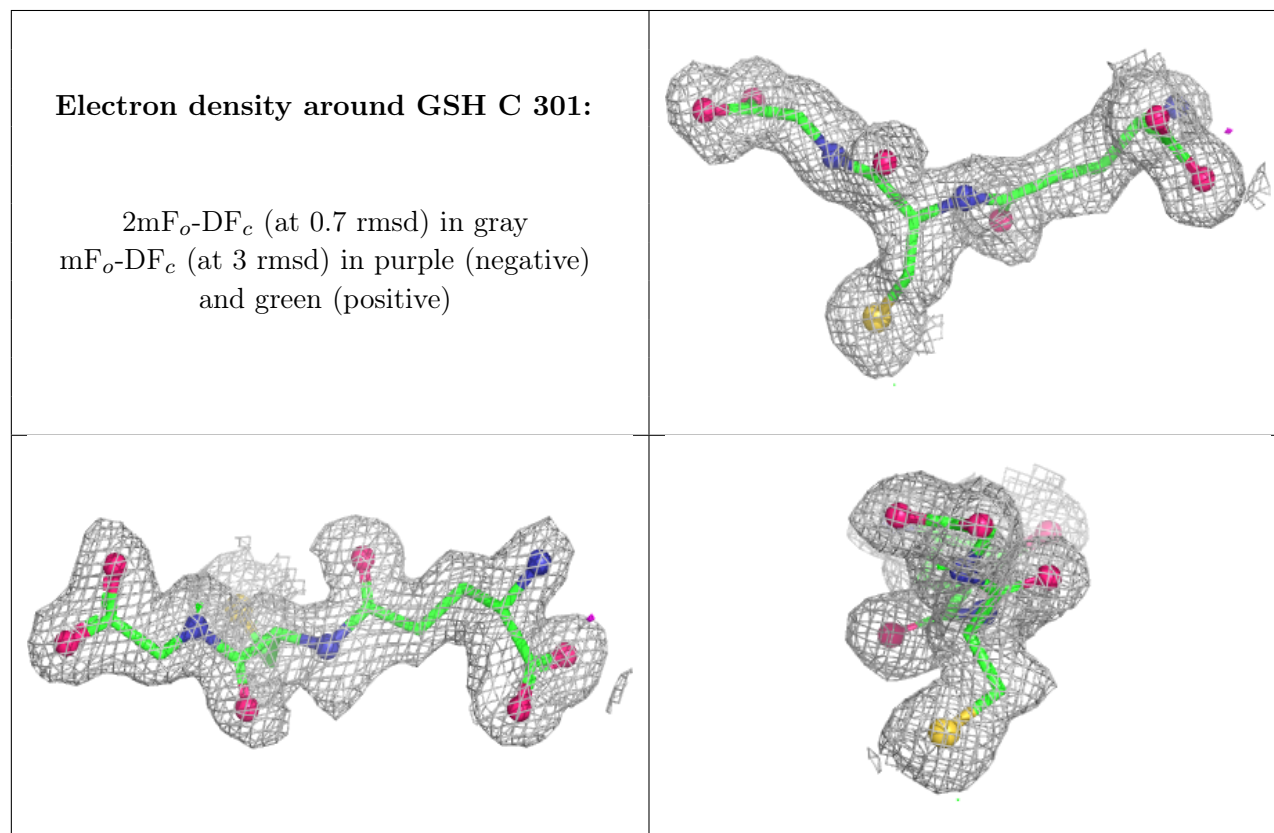
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LEU	D	602	9/9	0.82	0.12	6,8,11,22	0
4	LEU	A	602	9/9	0.84	0.11	8,10,14,15	0
3	JAA	A	601	15/15	0.85	0.16	7,11,17,18	0
3	JAA	D	601	15/15	0.85	0.12	5,9,12,15	0
6	GSH	C	301	20/20	0.92	0.07	2,4,6,7	0

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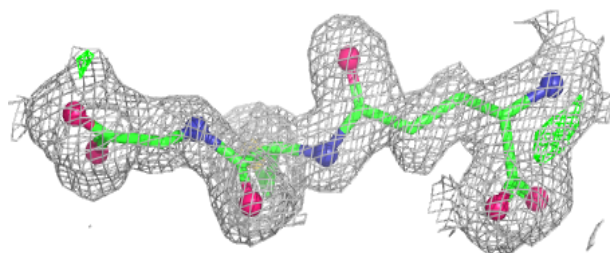
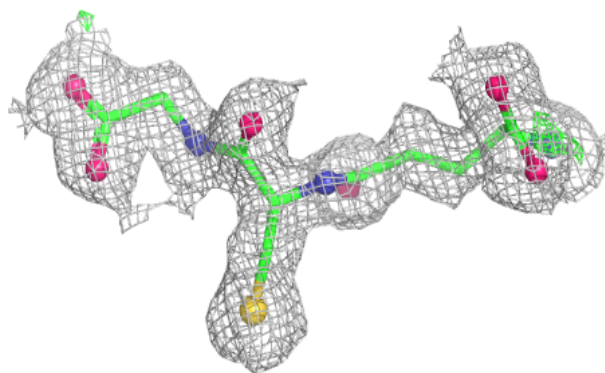
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GSH	F	301	20/20	0.92	0.08	3,5,10,10	0
6	GSH	B	301	20/20	0.94	0.08	2,5,14,15	0
6	GSH	E	301	20/20	0.96	0.07	3,9,13,17	0
5	MG	A	603	1/1	0.96	0.11	16,16,16,16	0

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.

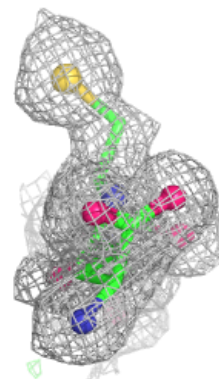
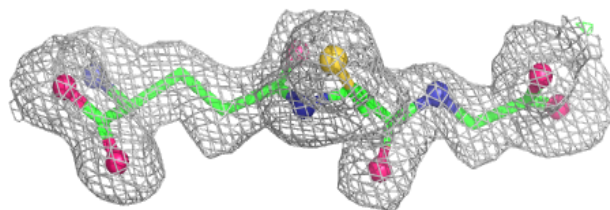
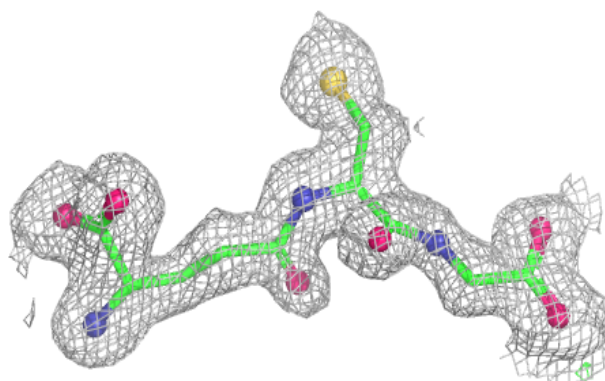


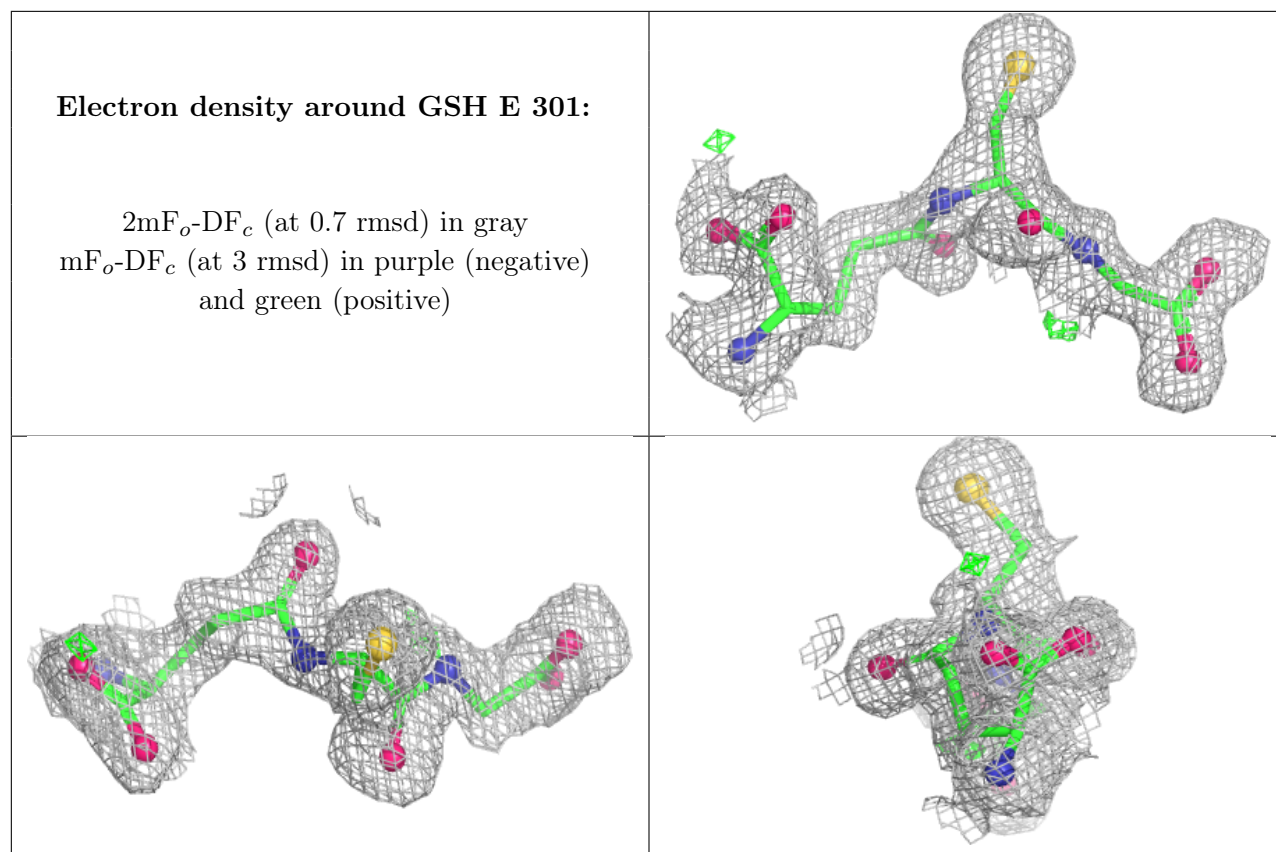
Electron density around GSH F 301:

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

**Electron density around GSH B 301:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.