



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2016 – 05:35 PM EDT

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

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

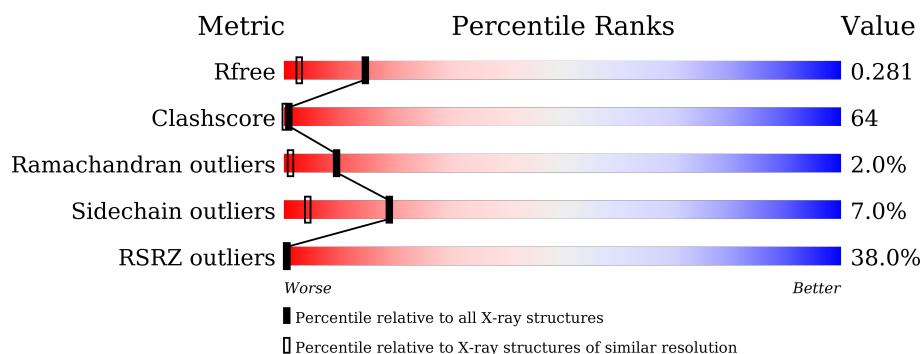
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	575	<div> <div>51%</div> <div>23% 67% 8% ..</div> </div>
1	D	575	<div> <div>41%</div> <div>23% 66% 9% ..</div> </div>
2	B	223	<div> <div>26%</div> <div>38% 55% . .</div> </div>
2	C	223	<div> <div>21%</div> <div>29% 58% 9% .</div> </div>
2	E	223	<div> <div>33%</div> <div>33% 61% . .</div> </div>
2	F	223	<div> <div>22%</div> <div>30% 57% 9% . .</div> </div>

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

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17885 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Jasmonic acid-amido synthetase JAR1.

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

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

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

There are 24 discrepancies between the modelled and reference sequences:

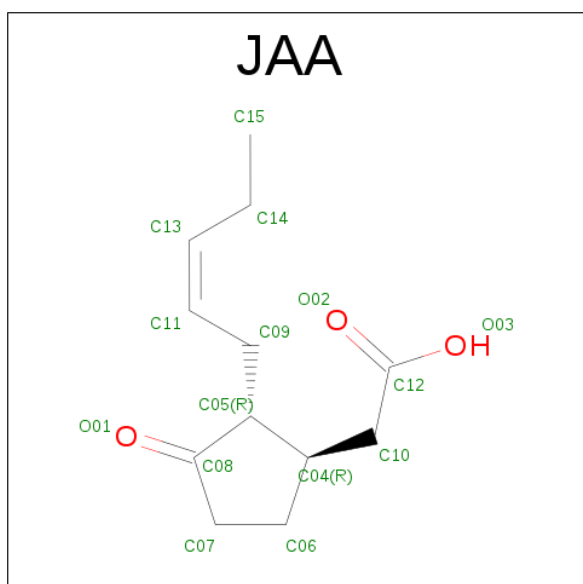
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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

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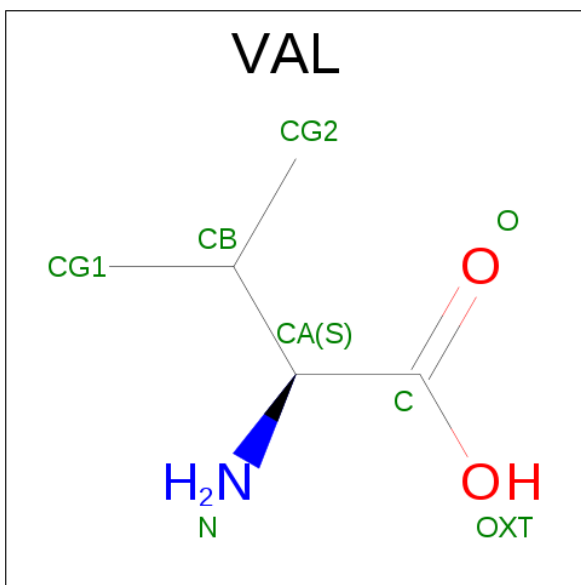
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9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

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



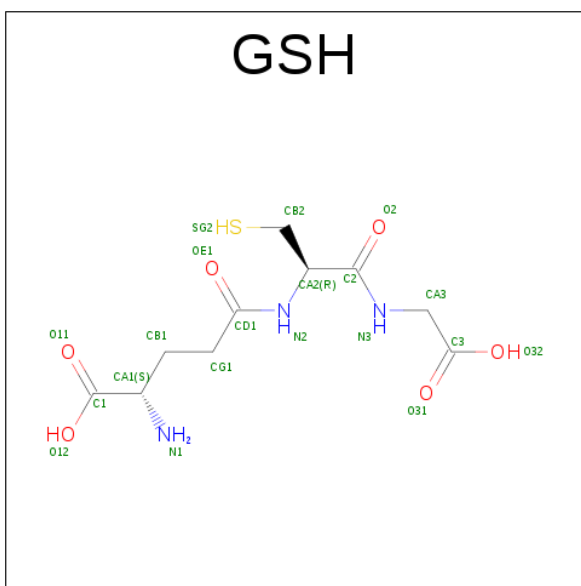
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



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

- Molecule 5 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



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

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

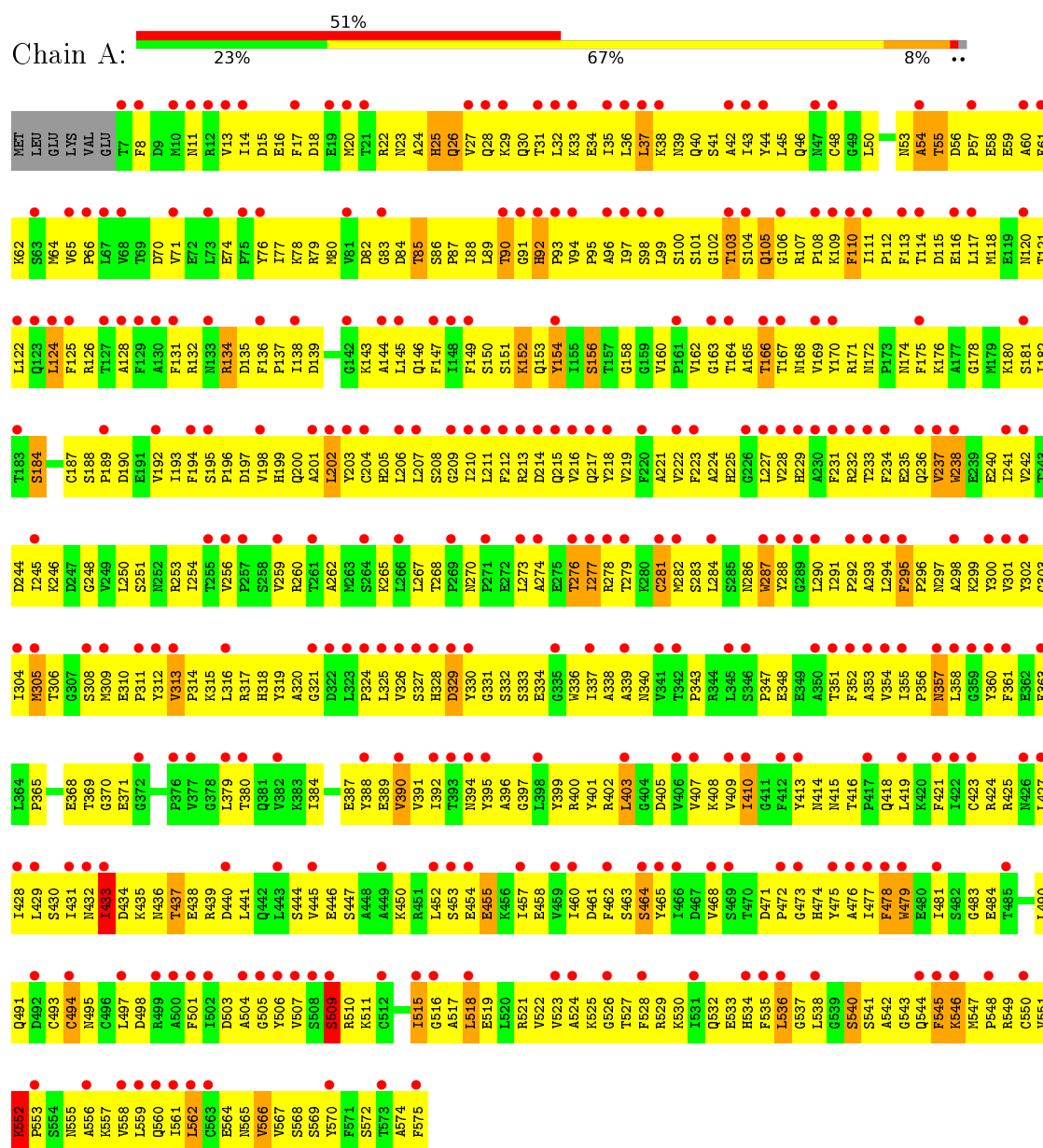
- Molecule 7 is water.

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

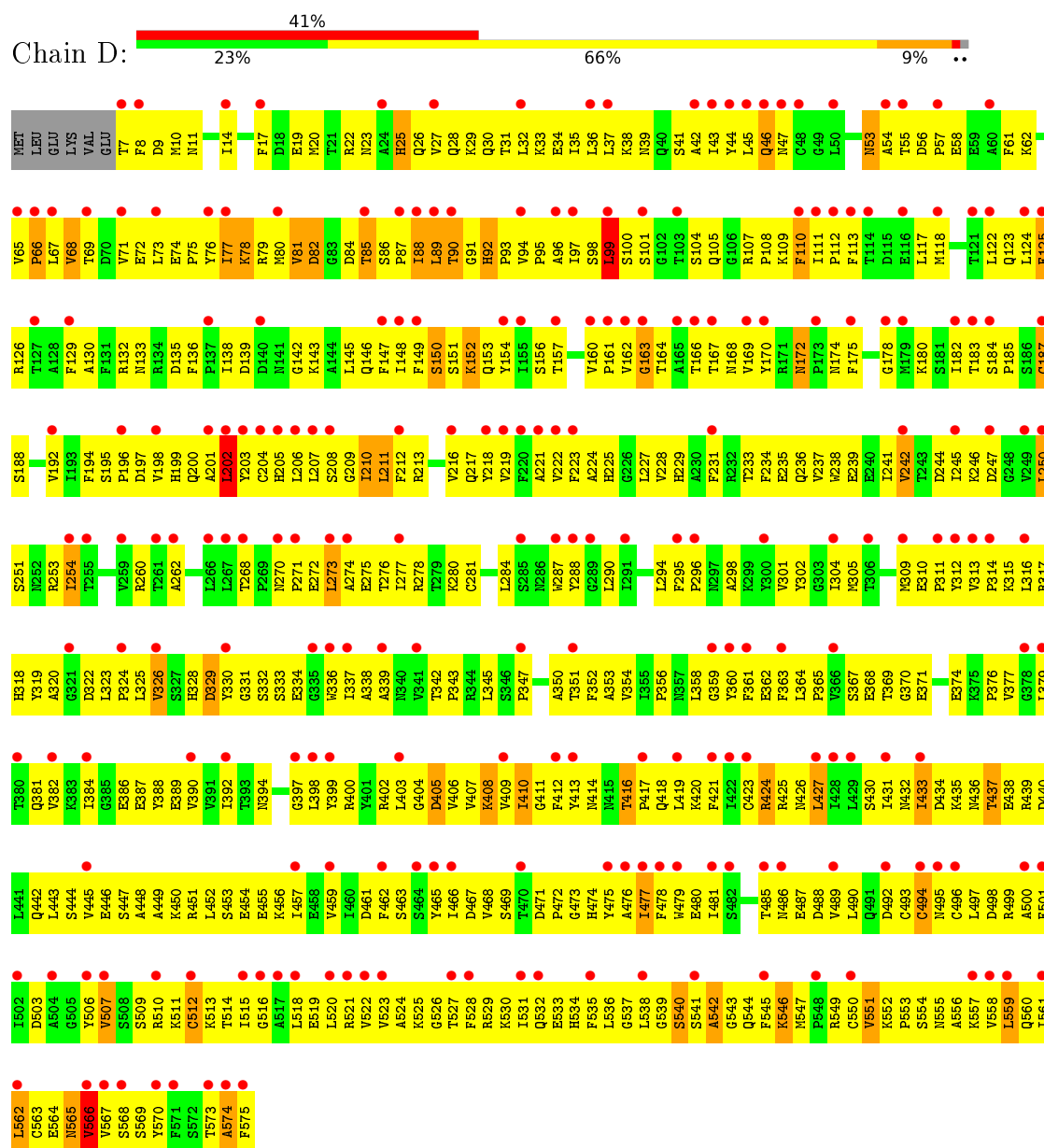
3 Residue-property plots

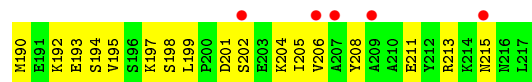
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Jasmonic acid-amido synthetase JAR1

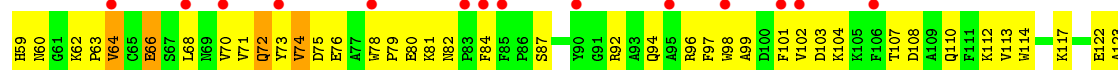


- Molecule 1: Jasmonic acid-amido synthetase JAR1

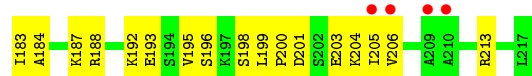
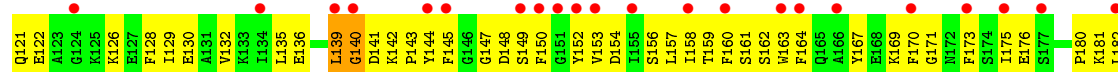
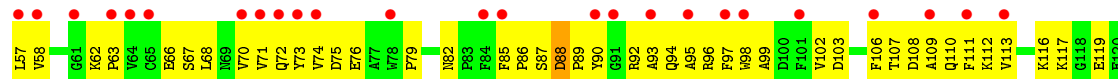
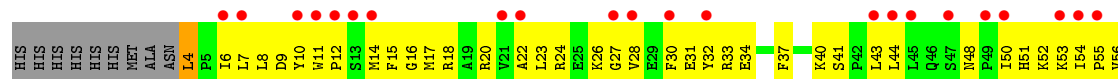




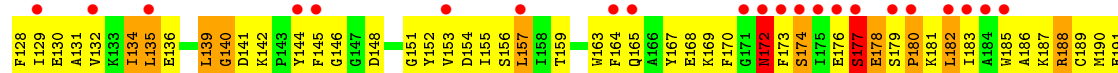
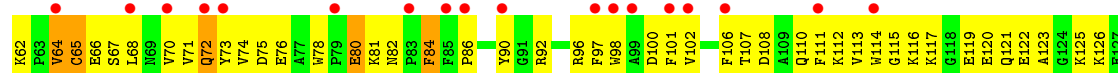
• Molecule 2: Glutathione S-transferase U20

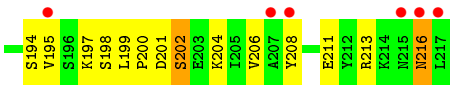


• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.84Å 53.85Å 193.64Å 90.03° 90.04° 113.41°	Depositor
Resolution (Å)	24.20 – 1.72 24.21 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.20-1.72) 99.5 (24.21-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.262 , 0.281 0.262 , 0.281	Depositor DCC
R_{free} test set	21133 reflections (10.01%)	DCC
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 218.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.099 for -h,-k,l 0.088 for k,h,-l 0.097 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17885	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.9763e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/4581	0.79	6/6219 (0.1%)
1	D	0.48	0/4581	0.79	6/6219 (0.1%)
2	B	0.38	0/1799	0.58	1/2428 (0.0%)
2	C	0.47	0/1799	0.72	4/2428 (0.2%)
2	E	0.41	0/1799	0.63	0/2428
2	F	0.51	0/1799	0.73	1/2428 (0.0%)
All	All	0.46	0/16358	0.74	18/22150 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
2	E	0	1
2	F	0	1
All	All	0	6

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	TRP	CA-CB-CG	7.72	128.38	113.70
2	C	188	ARG	NE-CZ-NH1	-7.70	116.45	120.30
2	C	188	ARG	NE-CZ-NH2	6.85	123.72	120.30
2	F	188	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	A	562	LEU	CA-CB-CG	6.47	130.18	115.30
1	D	559	LEU	CA-CB-CG	6.08	129.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	LEU	CA-CB-CG	6.01	129.12	115.30
1	D	562	LEU	CA-CB-CG	5.80	128.65	115.30
2	B	182	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	552	LYS	C-N-CD	5.29	139.51	128.40
1	A	287	TRP	CA-CB-CG	-5.22	103.79	113.70
1	D	99	LEU	CA-CB-CG	5.19	127.24	115.30
1	D	202	LEU	CB-CG-CD1	5.17	119.79	111.00
2	C	45	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	237	VAL	N-CA-C	5.13	124.85	111.00
1	A	124	LEU	CA-CB-CG	5.10	127.04	115.30
2	C	11	TRP	C-N-CD	5.08	139.06	128.40
1	D	163	GLY	N-CA-C	5.05	125.72	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	LEU	Peptide
1	A	431	ILE	Peptide
1	D	427	LEU	Peptide
1	D	565	ASN	Peptide
2	E	140	GLY	Peptide
2	F	177	SER	Peptide

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	704	6
1	D	4479	0	4434	630	5
2	B	1748	0	1704	195	1
2	C	1748	0	1704	243	2
2	E	1748	0	1704	181	0
2	F	1748	0	1704	209	1
3	A	15	0	0	4	0
3	D	15	0	0	2	0
4	A	8	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	8	2	0
5	B	20	0	15	4	0
5	C	20	0	15	1	0
5	E	20	0	15	1	0
5	F	20	0	15	3	0
6	D	1	0	0	0	0
7	A	512	0	0	129	4
7	B	203	0	0	28	4
7	C	198	0	0	61	3
7	D	510	0	0	105	4
7	E	186	0	0	26	1
7	F	199	0	0	47	1
All	All	17885	0	15760	2041	22

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (2041) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:HZ1	1:A:530:LYS:NZ	1.21	1.34
1:A:152:LYS:NZ	1:A:530:LYS:HZ1	1.30	1.26
1:D:488:ASP:OD1	7:D:701:HOH:O	1.53	1.24
2:C:188:ARG:NH1	1:D:499:ARG:O	1.70	1.22
2:E:92:ARG:NH1	2:F:76:GLU:OE1	1.79	1.15
1:A:446:GLU:OE2	7:A:701:HOH:O	1.67	1.12
1:D:152:LYS:NZ	1:D:527:THR:OG1	1.81	1.12
2:C:188:ARG:HH12	1:D:500:ALA:HA	1.11	1.11
1:A:176:LYS:NZ	1:A:190:ASP:OD2	1.83	1.10
2:C:9:ASP:OD2	7:C:402:HOH:O	1.71	1.09
1:A:134:ARG:NH1	7:A:702:HOH:O	1.86	1.04
2:C:176:GLU:OE2	1:D:573:THR:OG1	1.76	1.04
2:E:139:LEU:HG	2:E:142:LYS:HB2	1.35	1.01
2:E:26:LYS:HZ3	2:E:74:VAL:HG22	1.24	1.00
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.44	1.00
1:A:106:GLY:HA3	1:A:432:ASN:HD21	1.27	0.99
1:A:166:THR:HG22	4:A:602:VAL:HG13	1.44	0.98
1:A:510:ARG:NH1	1:A:516:GLY:O	1.94	0.98
2:E:40:LYS:NZ	2:E:52:LYS:O	1.96	0.98
1:A:519:GLU:OE2	1:A:569:SER:OG	1.84	0.96
2:F:60:ASN:ND2	7:F:409:HOH:O	1.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HD13	1:A:287:TRP:H	1.30	0.95
2:F:120:GLU:OE1	7:F:401:HOH:O	1.85	0.94
1:A:152:LYS:HA	1:A:564:GLU:HB2	1.49	0.94
2:B:26:LYS:NZ	2:B:82:ASN:H	1.64	0.94
2:C:184:ALA:HB1	1:D:499:ARG:CZ	1.98	0.93
1:A:491:GLN:OE1	7:A:703:HOH:O	1.87	0.93
1:D:254:ILE:O	1:D:260:ARG:NH1	2.01	0.93
1:A:510:ARG:NH1	1:A:515:ILE:HD12	1.84	0.93
2:C:66:GLU:OE2	7:C:405:HOH:O	1.87	0.92
2:C:92:ARG:NH1	7:C:414:HOH:O	2.03	0.92
2:F:190:MET:SD	7:F:436:HOH:O	2.26	0.92
1:A:39:ASN:ND2	2:B:141:ASP:O	2.01	0.92
1:A:199:HIS:HB3	1:A:525:LYS:H	1.32	0.92
1:D:452:LEU:HB3	1:D:457:ILE:HD11	1.49	0.92
1:A:93:PRO:HG3	2:B:184:ALA:HB3	1.52	0.91
2:C:188:ARG:NH1	1:D:500:ALA:HA	1.84	0.91
2:B:116:LYS:O	2:B:213:ARG:NH1	2.02	0.91
1:D:466:ILE:HB	1:D:552:LYS:HA	1.53	0.91
1:A:498:ASP:O	7:A:704:HOH:O	1.88	0.91
1:D:99:LEU:HB3	1:D:557:LYS:H	1.32	0.91
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.52	0.91
1:A:208:SER:HA	1:A:211:LEU:HD12	1.52	0.90
1:A:225:HIS:HA	1:A:228:VAL:HG22	1.54	0.90
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.54	0.90
1:A:475:TYR:H	1:A:510:ARG:HH22	1.15	0.89
1:A:165:ALA:H	1:A:557:LYS:NZ	1.70	0.89
2:F:122:GLU:OE2	7:F:403:HOH:O	1.89	0.89
1:A:165:ALA:H	1:A:557:LYS:HZ3	0.91	0.89
2:F:26:LYS:NZ	2:F:82:ASN:O	2.06	0.89
2:F:20:ARG:NH1	7:F:404:HOH:O	1.90	0.88
1:A:152:LYS:NZ	1:A:530:LYS:NZ	2.03	0.88
2:C:117:LYS:NZ	7:C:403:HOH:O	1.77	0.88
2:F:136:GLU:OE2	2:F:180:PRO:HD3	1.73	0.88
1:D:172:ASN:ND2	1:D:174:ASN:OD1	2.07	0.88
2:C:26:LYS:NZ	2:C:82:ASN:O	2.07	0.87
2:C:98:TRP:O	7:C:406:HOH:O	1.91	0.87
2:C:41:SER:N	7:C:415:HOH:O	2.03	0.87
1:A:402:ARG:NH1	7:A:726:HOH:O	2.08	0.87
1:A:100:SER:OG	1:A:334:GLU:OE2	1.92	0.86
2:C:176:GLU:OE1	7:D:701:HOH:O	1.93	0.86
1:D:123:GLN:NE2	7:D:713:HOH:O	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NH1	7:A:731:HOH:O	2.09	0.86
1:A:164:THR:HG22	1:A:557:LYS:HD3	1.57	0.86
1:A:165:ALA:N	1:A:557:LYS:HZ3	1.73	0.86
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.56	0.86
2:C:184:ALA:O	1:D:499:ARG:NH2	2.09	0.86
1:D:552:LYS:O	1:D:554:SER:N	2.09	0.86
1:D:309:MET:O	7:D:702:HOH:O	1.92	0.85
1:A:143:LYS:NZ	1:A:187:CYS:HB3	1.91	0.85
1:A:277:ILE:HG23	1:A:278:ARG:HG3	1.58	0.85
1:A:38:LYS:NZ	1:A:395:TYR:OH	2.10	0.85
2:C:168:GLU:OE1	7:C:407:HOH:O	1.93	0.85
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.59	0.85
1:D:93:PRO:HG2	2:E:181:LYS:HA	1.58	0.85
2:F:26:LYS:HG2	2:F:81:LYS:NZ	1.92	0.84
2:F:197:LYS:O	7:F:405:HOH:O	1.94	0.84
1:D:337:ILE:HD13	1:D:539:GLY:HA3	1.59	0.84
2:F:132:VAL:HG23	2:F:182:LEU:HD13	1.57	0.84
1:A:143:LYS:HD3	1:A:212:PHE:HB2	1.59	0.84
1:A:551:VAL:HG11	1:A:559:LEU:HD11	1.60	0.84
1:A:143:LYS:HZ2	1:A:187:CYS:HB3	1.40	0.84
1:D:408:LYS:HG2	1:D:420:LYS:HG2	1.60	0.84
2:E:187:LYS:O	7:E:401:HOH:O	1.96	0.84
2:E:93:ALA:HB1	2:F:73:TYR:HE1	1.43	0.83
2:C:172:ASN:OD1	7:C:408:HOH:O	1.96	0.83
1:A:74:GLU:OE2	7:A:706:HOH:O	1.97	0.83
2:C:193:GLU:HG3	7:C:442:HOH:O	1.79	0.83
2:E:143:PRO:HB2	2:E:188:ARG:HH12	1.44	0.83
2:F:18:ARG:NH2	7:F:414:HOH:O	2.10	0.83
1:D:480:GLU:OE1	7:D:703:HOH:O	1.94	0.83
1:D:509:SER:O	1:D:513:LYS:N	2.10	0.83
1:A:103:THR:HB	1:A:106:GLY:HA2	1.61	0.83
2:E:143:PRO:HB2	2:E:188:ARG:NH1	1.93	0.83
2:C:26:LYS:HG2	2:C:81:LYS:NZ	1.93	0.83
2:F:120:GLU:O	7:F:406:HOH:O	1.97	0.82
1:A:20:MET:HG2	1:A:356:PRO:HG2	1.61	0.82
1:A:87:PRO:HB2	2:B:143:PRO:HA	1.60	0.82
1:D:405:ASP:HB2	1:D:541:SER:HB3	1.58	0.82
1:D:199:HIS:HB3	1:D:525:LYS:H	1.43	0.82
1:A:106:GLY:HA3	1:A:432:ASN:ND2	1.94	0.82
2:E:50:ILE:HG13	2:E:51:HIS:H	1.43	0.82
1:A:225:HIS:HB3	1:A:312:TYR:CE2	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:PRO:O	7:C:410:HOH:O	1.97	0.81
2:C:184:ALA:HB1	1:D:499:ARG:NH1	1.95	0.81
2:E:26:LYS:NZ	2:E:74:VAL:HG22	1.93	0.81
1:A:478:PHE:CZ	1:A:562:LEU:HA	2.15	0.81
1:D:305:MET:SD	7:D:1023:HOH:O	2.38	0.81
1:D:213:ARG:NE	1:D:294:LEU:O	2.12	0.81
2:C:28:VAL:O	7:C:409:HOH:O	1.97	0.81
1:A:138:ILE:HD12	1:A:217:GLN:HB2	1.61	0.81
1:A:45:LEU:HD22	1:A:50:LEU:HD12	1.62	0.81
2:F:156:SER:OG	7:F:402:HOH:O	1.85	0.81
1:D:199:HIS:H	1:D:524:ALA:HB1	1.44	0.81
1:D:42:ALA:HA	2:E:143:PRO:HG3	1.62	0.81
1:D:239:GLU:OE2	7:D:704:HOH:O	1.98	0.81
1:D:499:ARG:HB2	1:D:499:ARG:CZ	2.08	0.80
1:D:531:ILE:HA	1:D:534:HIS:CE1	2.15	0.80
2:F:72:GLN:OE1	7:F:407:HOH:O	1.99	0.80
1:A:551:VAL:HG13	1:A:555:ASN:HB3	1.63	0.80
1:A:424:ARG:NH1	7:A:747:HOH:O	2.15	0.80
1:A:18:ASP:OD1	1:A:414:ASN:ND2	2.14	0.80
2:F:178:GLU:O	7:F:410:HOH:O	2.00	0.80
1:D:150:SER:HB2	1:D:167:THR:HA	1.61	0.80
1:D:87:PRO:HG2	2:E:188:ARG:HD2	1.64	0.80
2:B:24:ARG:HH12	2:B:197:LYS:HE3	1.47	0.79
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.63	0.79
1:A:458:GLU:O	7:A:708:HOH:O	2.01	0.79
2:B:136:GLU:OE2	7:B:401:HOH:O	1.99	0.79
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.62	0.79
1:D:432:ASN:ND2	7:D:735:HOH:O	2.15	0.79
2:C:132:VAL:HG23	2:C:182:LEU:HD13	1.63	0.79
2:C:9:ASP:OD1	7:C:412:HOH:O	2.00	0.79
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.65	0.79
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.47	0.79
2:B:145:PHE:HB2	2:B:154:ASP:HB3	1.64	0.79
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.65	0.79
1:A:306:THR:OG1	1:A:330:TYR:OH	2.01	0.78
1:A:62:LYS:HG2	1:A:400:ARG:NH1	1.99	0.78
1:A:117:LEU:HD11	1:A:333:SER:HA	1.65	0.78
1:D:138:ILE:HB	1:D:217:GLN:HG3	1.64	0.78
1:A:304:ILE:HG13	1:A:328:HIS:HB3	1.65	0.78
1:A:236:GLN:OE1	7:A:710:HOH:O	2.02	0.78
2:B:215:ASN:ND2	7:B:405:HOH:O	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.64	0.78
1:D:44:TYR:HB2	1:D:89:LEU:HG	1.66	0.78
2:B:76:GLU:OE1	7:C:404:HOH:O	2.01	0.78
1:D:268:THR:O	7:D:705:HOH:O	2.02	0.78
1:D:322:ASP:O	7:D:706:HOH:O	2.02	0.78
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.48	0.78
1:A:150:SER:OG	7:A:709:HOH:O	2.02	0.78
1:A:452:LEU:HD23	1:A:481:ILE:HG12	1.64	0.78
1:A:425:ARG:NH2	7:A:734:HOH:O	2.09	0.78
1:A:332:SER:HG	1:A:534:HIS:HE2	1.32	0.78
1:A:465:TYR:HA	1:A:551:VAL:HB	1.66	0.78
1:D:495:ASN:C	1:D:499:ARG:HH12	1.87	0.77
1:A:224:ALA:HA	1:A:227:LEU:HD12	1.64	0.77
1:A:501:PHE:HB2	1:A:506:TYR:CZ	2.19	0.77
1:A:152:LYS:CE	1:A:530:LYS:HZ1	1.97	0.77
1:D:418:GLN:OE1	7:D:707:HOH:O	2.02	0.77
2:E:40:LYS:NZ	2:E:52:LYS:HB2	1.98	0.77
1:A:464:SER:HG	1:A:550:CYS:HG	1.07	0.77
1:D:99:LEU:HD23	1:D:558:VAL:H	1.49	0.77
1:D:495:ASN:C	1:D:499:ARG:NH1	2.37	0.77
2:B:18:ARG:HD3	2:B:156:SER:HA	1.65	0.77
1:A:413:TYR:OH	7:A:707:HOH:O	1.97	0.77
1:A:527:THR:HG23	1:A:561:ILE:HG21	1.65	0.77
2:F:119:GLU:O	7:F:411:HOH:O	2.03	0.77
1:A:152:LYS:HD2	1:A:561:ILE:HG23	1.65	0.76
2:B:201:ASP:O	7:B:402:HOH:O	2.02	0.76
1:D:439:ARG:NH1	7:D:741:HOH:O	2.17	0.76
2:F:164:PHE:HD2	2:F:183:ILE:HD13	1.49	0.76
1:A:143:LYS:HZ2	1:A:209:GLY:HA2	1.50	0.76
1:A:92:HIS:HE1	2:B:185:TRP:HZ2	1.34	0.76
1:D:198:VAL:HG22	1:D:565:ASN:HD22	1.48	0.76
2:E:70:VAL:HA	2:E:73:TYR:CE2	2.21	0.76
1:A:454:GLU:OE1	7:A:711:HOH:O	2.03	0.76
2:F:8:LEU:HD22	2:F:33:ARG:HH21	1.50	0.76
1:A:340:ASN:OD1	7:A:714:HOH:O	2.04	0.76
2:E:93:ALA:HB1	2:F:73:TYR:CE1	2.21	0.75
1:A:555:ASN:N	7:A:718:HOH:O	2.20	0.75
1:D:389:GLU:OE2	1:D:404:GLY:HA2	1.87	0.75
1:A:238:TRP:HA	1:A:241:ILE:HB	1.69	0.75
1:A:340:ASN:ND2	7:A:755:HOH:O	2.18	0.75
2:C:164:PHE:HD2	2:C:183:ILE:HD12	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:ASP:OD2	1:D:456:LYS:NZ	2.18	0.75
1:A:146:GLN:NE2	7:A:758:HOH:O	2.19	0.75
2:F:56:VAL:HG13	7:F:426:HOH:O	1.85	0.75
2:E:122:GLU:OE2	7:E:402:HOH:O	2.05	0.75
2:B:96:ARG:HH11	2:C:73:TYR:HE1	1.32	0.74
2:F:8:LEU:HD21	2:F:43:LEU:HD11	1.68	0.74
1:A:152:LYS:HG3	1:A:561:ILE:HA	1.69	0.74
2:F:62:LYS:NZ	7:F:408:HOH:O	1.99	0.74
1:D:310:GLU:HG2	1:D:311:PRO:HD3	1.69	0.74
1:A:305:MET:HE3	1:A:347:PRO:HG3	1.69	0.74
2:B:96:ARG:NH1	2:C:73:TYR:CE1	2.54	0.74
1:D:211:LEU:O	7:D:712:HOH:O	2.06	0.74
2:C:64:VAL:HG23	2:C:70:VAL:HG22	1.69	0.74
1:D:246:LYS:HE2	1:D:271:PRO:HA	1.69	0.74
1:A:108:PRO:HB3	1:A:555:ASN:HB2	1.69	0.74
1:A:558:VAL:O	7:A:713:HOH:O	2.04	0.74
2:C:80:GLU:OE2	7:C:417:HOH:O	2.06	0.74
1:D:146:GLN:NE2	7:D:743:HOH:O	2.17	0.74
1:A:361:PHE:O	7:A:712:HOH:O	2.04	0.74
1:A:552:LYS:O	7:A:718:HOH:O	2.06	0.74
2:C:33:ARG:NE	7:C:422:HOH:O	2.12	0.74
1:A:331:GLY:HA2	7:A:764:HOH:O	1.87	0.74
1:A:143:LYS:NZ	1:A:209:GLY:HA2	2.02	0.74
1:D:87:PRO:HB2	2:E:143:PRO:HA	1.69	0.73
1:A:301:VAL:HG11	1:A:316:LEU:HD21	1.69	0.73
1:A:401:TYR:HE2	1:A:403:LEU:HD13	1.52	0.73
1:A:79:ARG:HH22	2:B:188:ARG:NH1	1.85	0.73
2:F:180:PRO:HD2	2:F:181:LYS:HG2	1.68	0.73
1:A:397:GLY:O	7:A:721:HOH:O	2.06	0.73
1:A:548:PRO:O	7:A:716:HOH:O	2.05	0.73
2:C:64:VAL:HB	2:C:73:TYR:CD2	2.22	0.73
1:D:143:LYS:HD3	1:D:187:CYS:HB3	1.71	0.73
1:D:9:ASP:O	7:D:710:HOH:O	2.05	0.73
1:A:479:TRP:NE1	7:A:762:HOH:O	2.20	0.73
1:A:132:ARG:NH1	7:A:754:HOH:O	2.22	0.73
1:A:337:ILE:N	7:A:764:HOH:O	2.21	0.73
2:C:142:LYS:NZ	7:C:401:HOH:O	1.60	0.73
1:D:164:THR:OG1	1:D:557:LYS:O	2.07	0.73
1:D:477:ILE:HG13	1:D:520:LEU:HA	1.71	0.73
1:A:304:ILE:O	7:A:715:HOH:O	2.05	0.73
1:A:304:ILE:O	7:A:722:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:CYS:HA	1:A:497:LEU:HD12	1.69	0.73
2:C:33:ARG:HH22	2:C:43:LEU:HD11	1.53	0.73
2:C:26:LYS:HD2	2:C:74:VAL:HG13	1.70	0.73
2:E:92:ARG:HH12	2:F:76:GLU:CD	1.90	0.73
2:C:191:GLU:OE1	1:D:447:SER:OG	2.07	0.73
2:B:24:ARG:NE	2:B:198:SER:OG	2.20	0.73
2:C:211:GLU:OE1	7:C:418:HOH:O	2.06	0.73
1:A:138:ILE:HG13	1:A:217:GLN:OE1	1.88	0.73
1:A:351:THR:HG21	1:A:410:ILE:HG12	1.71	0.73
2:F:136:GLU:HG3	2:F:181:LYS:HD3	1.71	0.73
2:E:89:PRO:HB3	2:F:76:GLU:HG3	1.71	0.73
1:A:284:LEU:HD22	1:A:287:TRP:HA	1.71	0.72
1:A:529:ARG:NH1	7:A:767:HOH:O	2.22	0.72
1:D:236:GLN:NE2	7:D:748:HOH:O	2.18	0.72
1:D:423:CYS:SG	1:D:541:SER:OG	2.46	0.72
2:B:50:ILE:HG13	2:C:134:ILE:HD12	1.72	0.72
2:F:122:GLU:HA	2:F:125:LYS:HE2	1.69	0.72
2:F:98:TRP:HE3	2:F:101:PHE:HB2	1.54	0.72
1:A:329:ASP:OD1	7:A:717:HOH:O	2.06	0.72
1:A:64:MET:O	7:A:723:HOH:O	2.06	0.72
1:D:426:ASN:ND2	7:D:758:HOH:O	2.21	0.72
2:F:168:GLU:OE2	2:F:176:GLU:OE2	2.06	0.72
1:A:223:PHE:CZ	1:A:536:LEU:HB2	2.24	0.72
1:A:150:SER:O	1:A:171:ARG:NH1	2.23	0.72
1:A:337:ILE:HG12	1:A:361:PHE:CZ	2.24	0.72
2:B:92:ARG:NH2	2:C:76:GLU:OE1	2.22	0.72
1:D:524:ALA:HB2	1:D:567:VAL:HG11	1.71	0.72
2:E:20:ARG:HB3	2:E:24:ARG:NH1	2.04	0.72
1:A:446:GLU:OE2	7:A:728:HOH:O	2.08	0.72
1:D:518:LEU:O	7:D:715:HOH:O	2.08	0.71
1:D:534:HIS:O	7:D:714:HOH:O	2.07	0.71
1:A:331:GLY:HA3	1:A:336:TRP:CE3	2.25	0.71
2:C:189:CYS:HB3	7:C:432:HOH:O	1.89	0.71
1:A:295:PHE:O	7:A:725:HOH:O	2.07	0.71
1:D:152:LYS:HE3	1:D:565:ASN:HB2	1.71	0.71
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.72	0.71
2:B:119:GLU:OE2	7:B:404:HOH:O	2.08	0.71
5:B:301:GSH:O31	7:B:407:HOH:O	2.09	0.71
1:A:139:ASP:O	7:A:727:HOH:O	2.08	0.71
1:A:244:ASP:OD2	7:A:724:HOH:O	2.07	0.71
2:F:117:LYS:HE3	2:F:213:ARG:NH1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:N	1:A:524:ALA:HB1	2.05	0.71
2:C:26:LYS:HG2	2:C:81:LYS:HZ1	1.52	0.71
1:D:208:SER:O	7:D:716:HOH:O	2.08	0.71
1:A:199:HIS:H	1:A:524:ALA:HB1	1.56	0.70
1:D:301:VAL:HG11	1:D:316:LEU:HD21	1.71	0.70
2:F:176:GLU:O	2:F:180:PRO:HB3	1.91	0.70
2:C:187:LYS:NZ	1:D:496:CYS:HB2	2.06	0.70
2:C:4:LEU:N	7:C:427:HOH:O	2.23	0.70
1:D:10:MET:SD	7:D:754:HOH:O	2.48	0.70
1:D:37:LEU:O	7:D:717:HOH:O	2.08	0.70
2:B:103:ASP:O	7:B:406:HOH:O	2.09	0.70
2:C:139:LEU:HD23	7:C:430:HOH:O	1.90	0.70
1:A:331:GLY:N	1:A:537:GLY:O	2.25	0.70
2:B:24:ARG:NH2	2:B:193:GLU:O	2.25	0.70
1:D:496:CYS:HA	1:D:499:ARG:NH2	2.06	0.70
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.25	0.70
1:A:332:SER:OG	1:A:333:SER:N	2.23	0.70
1:D:108:PRO:HG2	1:D:552:LYS:H	1.57	0.70
1:A:97:ILE:O	7:A:732:HOH:O	2.09	0.70
2:C:7:LEU:HD21	2:C:23:LEU:HD12	1.74	0.70
1:D:199:HIS:O	7:D:718:HOH:O	2.09	0.70
2:E:201:ASP:O	7:E:404:HOH:O	2.09	0.70
1:D:32:LEU:HA	1:D:35:ILE:HD12	1.72	0.70
1:D:406:VAL:O	1:D:541:SER:OG	2.10	0.70
2:F:98:TRP:CE3	2:F:101:PHE:HB2	2.26	0.70
1:A:246:LYS:NZ	1:A:278:ARG:HH22	1.89	0.70
1:A:181:SER:O	7:A:730:HOH:O	2.08	0.70
1:D:549:ARG:NH1	7:D:726:HOH:O	2.24	0.70
1:D:53:ASN:N	2:E:90:TYR:OH	2.24	0.70
1:A:354:VAL:HG21	1:A:379:LEU:HD21	1.73	0.70
1:A:494:CYS:SG	7:A:703:HOH:O	2.50	0.70
1:A:16:GLU:OE2	7:A:733:HOH:O	2.09	0.69
2:C:139:LEU:HG	2:C:145:PHE:CZ	2.27	0.69
2:C:33:ARG:NH2	2:C:43:LEU:HD21	2.07	0.69
1:D:389:GLU:OE2	1:D:402:ARG:NE	2.25	0.69
1:A:166:THR:OG1	1:A:167:THR:N	2.24	0.69
2:B:20:ARG:HD3	2:B:198:SER:HB3	1.73	0.69
1:D:109:LYS:O	7:D:719:HOH:O	2.09	0.69
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.25	0.69
1:A:118:MET:SD	7:A:810:HOH:O	2.50	0.69
2:B:18:ARG:NH2	2:B:67:SER:OG	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:LYS:O	2:E:213:ARG:NH1	2.25	0.69
1:A:39:ASN:HA	2:B:142:LYS:HG3	1.73	0.69
2:C:188:ARG:HD2	2:C:191:GLU:OE2	1.92	0.69
2:E:176:GLU:OE2	7:E:405:HOH:O	2.10	0.69
2:B:182:LEU:HD13	2:B:185:TRP:CZ3	2.27	0.69
1:A:464:SER:HB2	1:A:477:ILE:HD13	1.74	0.69
1:A:53:ASN:OD1	1:A:54:ALA:N	2.24	0.69
2:B:18:ARG:HD2	2:B:155:ILE:HD12	1.74	0.69
1:D:549:ARG:NH2	7:D:769:HOH:O	2.26	0.69
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.28	0.69
2:F:139:LEU:HG	2:F:145:PHE:CZ	2.27	0.69
1:A:407:VAL:HG22	1:A:541:SER:HB2	1.75	0.69
1:A:22:ARG:NH1	7:A:779:HOH:O	2.25	0.69
2:C:101:PHE:O	7:C:419:HOH:O	2.09	0.69
1:A:109:LYS:HE2	1:A:111:ILE:HD11	1.73	0.69
1:D:332:SER:OG	1:D:333:SER:N	2.26	0.69
2:E:180:PRO:HD2	2:E:181:LYS:HG3	1.74	0.69
1:A:483:GLY:O	7:A:736:HOH:O	2.11	0.69
2:C:144:TYR:HB3	2:C:154:ASP:OD2	1.93	0.69
1:D:107:ARG:NH2	1:D:552:LYS:HB3	2.08	0.69
1:D:514:THR:O	7:D:724:HOH:O	2.11	0.69
2:E:119:GLU:OE2	7:E:406:HOH:O	2.11	0.69
1:D:38:LYS:HB3	2:E:140:GLY:HA3	1.74	0.69
1:A:224:ALA:HB1	1:A:316:LEU:HD22	1.75	0.68
3:A:601:JAA:O02	7:A:737:HOH:O	2.11	0.68
1:A:99:LEU:HB3	1:A:557:LYS:HB2	1.75	0.68
1:D:54:ALA:O	7:D:721:HOH:O	2.10	0.68
1:D:487:GLU:HG2	1:D:570:TYR:CZ	2.29	0.68
1:D:495:ASN:HB3	1:D:499:ARG:NH1	2.07	0.68
2:E:159:THR:HA	2:E:199:LEU:HD21	1.74	0.68
2:F:30:PHE:O	7:F:413:HOH:O	2.10	0.68
1:A:38:LYS:HZ2	1:A:395:TYR:HE1	1.40	0.68
2:F:64:VAL:N	7:F:426:HOH:O	2.27	0.68
1:A:184:SER:HB2	1:A:217:GLN:NE2	2.09	0.68
1:A:202:LEU:HD21	1:A:529:ARG:HH22	1.57	0.68
2:B:142:LYS:NZ	2:B:145:PHE:O	2.19	0.68
1:D:77:ILE:CG1	1:D:110:PHE:HB3	2.24	0.68
1:D:461:ASP:OD1	7:D:723:HOH:O	2.11	0.68
2:E:40:LYS:HZ1	2:E:52:LYS:HB2	1.55	0.68
2:E:66:GLU:OE2	7:E:408:HOH:O	2.12	0.68
1:A:552:LYS:HG3	1:A:553:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLN:OE1	7:A:735:HOH:O	2.10	0.68
1:D:147:PHE:CE1	1:D:202:LEU:HD13	2.28	0.68
1:D:245:ILE:O	7:D:705:HOH:O	2.10	0.68
2:F:119:GLU:OE2	7:F:416:HOH:O	2.12	0.68
1:A:560:GLN:HB3	7:A:784:HOH:O	1.94	0.68
2:C:59:HIS:O	7:C:421:HOH:O	2.12	0.68
1:D:81:VAL:HG11	1:D:110:PHE:CE2	2.29	0.68
1:D:81:VAL:O	7:D:709:HOH:O	2.11	0.68
1:A:168:ASN:O	1:A:172:ASN:HB2	1.94	0.68
1:A:30:GLN:HA	1:A:33:LYS:HG2	1.75	0.68
1:D:104:SER:HB2	1:D:109:LYS:HB2	1.75	0.68
1:A:171:ARG:O	7:A:738:HOH:O	2.12	0.68
2:B:113:VAL:O	7:B:408:HOH:O	2.11	0.68
1:D:125:PHE:HE2	1:D:328:HIS:CE1	2.12	0.68
1:D:125:PHE:HE2	1:D:328:HIS:HE1	1.41	0.68
1:D:22:ARG:HH11	1:D:414:ASN:CG	1.96	0.68
1:D:199:HIS:N	1:D:524:ALA:HB1	2.08	0.68
2:C:104:LYS:NZ	7:C:413:HOH:O	2.02	0.67
1:D:56:ASP:OD2	7:D:722:HOH:O	2.11	0.67
2:F:106:PHE:O	7:F:417:HOH:O	2.12	0.67
1:A:231:PHE:O	1:A:235:GLU:HB3	1.93	0.67
1:A:399:TYR:O	7:A:740:HOH:O	2.12	0.67
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.29	0.67
1:D:143:LYS:HG2	1:D:216:VAL:HG22	1.76	0.67
1:D:183:THR:O	7:D:729:HOH:O	2.12	0.67
1:A:339:ALA:HB2	1:A:355:ILE:HD11	1.77	0.67
1:D:66:PRO:O	7:D:728:HOH:O	2.12	0.67
1:A:435:LYS:HE3	1:A:438:GLU:HB3	1.76	0.67
1:A:440:ASP:O	7:A:705:HOH:O	2.12	0.67
1:A:445:VAL:HG13	1:A:479:TRP:HE1	1.59	0.67
1:A:96:ALA:HA	1:A:162:VAL:HA	1.77	0.67
1:D:210:ILE:HA	1:D:213:ARG:HG3	1.76	0.67
2:F:26:LYS:O	7:F:415:HOH:O	2.11	0.67
2:F:81:LYS:N	7:F:423:HOH:O	2.22	0.67
1:A:86:SER:HB2	2:B:188:ARG:HE	1.60	0.67
2:B:82:ASN:OD1	7:B:409:HOH:O	2.12	0.67
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.30	0.67
1:D:336:TRP:HB2	1:D:358:LEU:HD13	1.77	0.67
1:D:519:GLU:OE2	1:D:569:SER:OG	2.06	0.67
1:D:542:ALA:O	7:D:725:HOH:O	2.11	0.67
1:A:300:TYR:HA	7:A:741:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HB2	1:A:352:PHE:CD2	2.30	0.67
1:A:423:CYS:HB3	1:A:542:ALA:HB3	1.75	0.67
2:C:68:LEU:HA	2:C:71:VAL:HG12	1.76	0.67
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.77	0.67
2:B:154:ASP:OD1	2:B:155:ILE:N	2.27	0.67
2:E:31:GLU:OE2	7:E:407:HOH:O	2.12	0.67
2:F:136:GLU:OE2	2:F:180:PRO:CD	2.43	0.67
2:C:22:ALA:HA	2:C:155:ILE:HD13	1.76	0.66
2:C:57:LEU:O	7:C:420:HOH:O	2.11	0.66
1:D:154:TYR:HD2	1:D:559:LEU:HD13	1.60	0.66
1:D:87:PRO:HD2	2:E:188:ARG:HB2	1.77	0.66
2:F:211:GLU:HG3	7:F:456:HOH:O	1.93	0.66
2:B:51:HIS:CD2	2:B:53:LYS:HE2	2.30	0.66
2:F:98:TRP:CD1	2:F:153:VAL:HG11	2.30	0.66
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.59	0.66
1:A:109:LYS:NZ	1:A:401:TYR:CZ	2.64	0.66
1:A:474:HIS:HA	1:A:510:ARG:HH12	1.59	0.66
2:C:187:LYS:HG2	1:D:451:ARG:HD3	1.76	0.66
2:F:114:TRP:CD1	2:F:167:TYR:HE1	2.13	0.66
2:F:165:GLN:HG2	2:F:206:VAL:HG21	1.77	0.66
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.30	0.66
1:A:103:THR:HB	1:A:106:GLY:CA	2.24	0.66
1:A:329:ASP:OD1	1:A:330:TYR:N	2.28	0.66
1:A:92:HIS:CE1	2:B:185:TRP:HZ2	2.13	0.66
2:C:23:LEU:HD22	2:C:28:VAL:HG11	1.78	0.66
1:A:128:ALA:HA	1:A:131:PHE:CE2	2.30	0.66
2:C:151:GLY:O	7:C:424:HOH:O	2.13	0.66
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.30	0.66
1:D:386:GLU:OE1	1:D:387:GLU:N	2.28	0.66
2:E:169:LYS:HZ2	2:E:206:VAL:HG21	1.60	0.66
2:F:163:TRP:HB3	2:F:167:TYR:CZ	2.31	0.66
2:F:24:ARG:HB3	2:F:194:SER:HA	1.78	0.66
2:F:7:LEU:HD21	2:F:23:LEU:HD12	1.78	0.66
1:A:324:PRO:O	7:A:741:HOH:O	2.12	0.66
1:A:424:ARG:HD2	1:A:425:ARG:NH1	2.11	0.66
1:D:105:GLN:HA	1:D:430:SER:HB3	1.76	0.66
2:C:187:LYS:HD3	1:D:492:ASP:HB3	1.78	0.66
1:D:147:PHE:CD2	1:D:529:ARG:NH1	2.63	0.65
1:D:205:HIS:O	7:D:727:HOH:O	2.12	0.65
2:E:57:LEU:HB3	2:E:73:TYR:OH	1.97	0.65
1:A:402:ARG:NH2	7:A:798:HOH:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.30	0.65
1:D:195:SER:OG	1:D:197:ASP:OD1	2.14	0.65
2:F:26:LYS:HG2	2:F:81:LYS:HZ3	1.61	0.65
1:A:458:GLU:OE2	7:A:744:HOH:O	2.13	0.65
1:D:168:ASN:O	1:D:172:ASN:HB3	1.96	0.65
1:D:313:VAL:HG23	1:D:325:LEU:HD12	1.79	0.65
2:E:92:ARG:NH1	2:F:76:GLU:CD	2.49	0.65
2:F:23:LEU:HD22	2:F:28:VAL:HG11	1.78	0.65
1:D:241:ILE:O	1:D:245:ILE:HG12	1.97	0.65
2:E:159:THR:HG22	2:E:199:LEU:HD11	1.78	0.65
5:F:301:GSH:N1	7:F:430:HOH:O	2.30	0.65
1:A:421:PHE:CD1	1:A:541:SER:HA	2.32	0.65
2:C:166:ALA:HB3	7:C:484:HOH:O	1.95	0.65
2:C:40:LYS:HB3	2:C:44:LEU:HD23	1.78	0.65
1:D:23:ASN:OD1	1:D:26:GLN:HB3	1.96	0.65
2:F:153:VAL:O	2:F:157:LEU:HD23	1.96	0.65
1:A:94:VAL:HG21	1:A:112:PRO:HA	1.79	0.65
1:A:41:SER:HA	2:B:148:ASP:HA	1.78	0.65
2:B:132:VAL:O	2:B:136:GLU:HG2	1.97	0.65
1:D:314:PRO:HB3	1:D:317:ARG:HH12	1.61	0.65
2:F:122:GLU:HG3	7:F:470:HOH:O	1.96	0.65
1:A:432:ASN:O	7:A:746:HOH:O	2.14	0.65
1:A:455:GLU:OE1	7:A:739:HOH:O	2.12	0.65
1:D:533:GLU:O	7:D:731:HOH:O	2.14	0.65
1:D:77:ILE:HG13	1:D:110:PHE:HB3	1.77	0.65
2:E:4:LEU:HD13	2:E:31:GLU:HB2	1.79	0.65
1:A:286:ASN:HA	1:A:287:TRP:CE3	2.32	0.65
2:C:214:LYS:NZ	7:C:411:HOH:O	1.99	0.65
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.62	0.65
1:A:126:ARG:NH1	7:A:795:HOH:O	2.29	0.64
1:A:445:VAL:HG13	1:A:479:TRP:NE1	2.12	0.64
1:A:484:GLU:O	7:A:742:HOH:O	2.13	0.64
1:D:359:GLY:O	7:D:734:HOH:O	2.15	0.64
1:A:547:MET:O	7:A:743:HOH:O	2.13	0.64
1:D:152:LYS:HG2	1:D:565:ASN:H	1.61	0.64
1:D:312:TYR:N	7:D:773:HOH:O	2.27	0.64
2:E:8:LEU:HD21	7:E:403:HOH:O	1.97	0.64
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.32	0.64
1:D:480:GLU:OE2	1:D:526:GLY:N	2.30	0.64
2:B:96:ARG:NH1	2:C:73:TYR:HE1	1.91	0.64
2:E:107:THR:HA	2:E:110:GLN:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:VAL:O	1:A:175:PHE:HB2	1.97	0.64
1:A:290:LEU:HD12	1:A:293:ALA:HB3	1.78	0.64
1:D:273:LEU:HA	1:D:276:THR:HG23	1.79	0.64
1:D:382:VAL:O	7:D:736:HOH:O	2.15	0.64
1:D:328:HIS:NE2	3:D:601:JAA:O03	2.29	0.64
2:F:132:VAL:HG22	2:F:179:SER:HB2	1.80	0.64
1:A:464:SER:OG	1:A:550:CYS:SG	2.32	0.64
1:D:151:SER:OG	1:D:565:ASN:ND2	2.29	0.64
1:D:367:SER:HB2	1:D:386:GLU:OE2	1.98	0.64
1:A:97:ILE:HB	1:A:162:VAL:HB	1.80	0.64
1:D:200:GLN:HA	1:D:203:TYR:CE2	2.33	0.64
1:D:463:SER:OG	7:D:726:HOH:O	2.12	0.64
1:D:477:ILE:HD12	1:D:497:LEU:HD13	1.79	0.64
1:D:139:ASP:O	7:D:733:HOH:O	2.15	0.64
1:D:180:LYS:O	7:D:737:HOH:O	2.15	0.64
1:D:98:SER:HB3	1:D:557:LYS:HE3	1.79	0.64
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.62	0.64
1:A:143:LYS:CD	1:A:212:PHE:HB2	2.26	0.64
1:D:162:VAL:O	1:D:560:GLN:HB2	1.98	0.64
1:A:332:SER:HB2	1:A:538:LEU:HA	1.79	0.64
1:A:424:ARG:HD2	1:A:425:ARG:HH11	1.61	0.64
2:C:139:LEU:O	2:C:141:ASP:N	2.30	0.64
1:A:22:ARG:HG2	1:A:414:ASN:HB3	1.81	0.63
2:C:45:LEU:HD12	7:C:444:HOH:O	1.98	0.63
1:A:432:ASN:O	1:A:433:ILE:HG23	1.99	0.63
2:B:90:TYR:O	2:B:93:ALA:HB3	1.99	0.63
1:D:386:GLU:O	7:D:738:HOH:O	2.15	0.63
1:A:313:VAL:HG22	1:A:314:PRO:HD3	1.81	0.63
2:F:176:GLU:N	2:F:176:GLU:OE1	2.29	0.63
1:A:143:LYS:HZ2	1:A:187:CYS:CB	2.11	0.63
1:A:91:GLY:O	7:A:748:HOH:O	2.15	0.63
2:C:98:TRP:CZ2	2:C:157:LEU:HD22	2.34	0.63
1:D:270:ASN:HB3	1:D:273:LEU:HD11	1.79	0.63
1:D:288:TYR:HA	1:D:318:HIS:CD2	2.33	0.63
1:A:217:GLN:O	1:A:299:LYS:N	2.29	0.63
1:A:105:GLN:HB2	1:A:430:SER:HB2	1.81	0.63
1:A:361:PHE:CE1	1:A:392:ILE:HG22	2.34	0.62
1:D:46:GLN:NE2	7:D:749:HOH:O	2.29	0.62
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.81	0.62
2:E:121:GLN:NE2	2:E:170:PHE:O	2.32	0.62
2:E:24:ARG:NE	7:E:419:HOH:O	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:TYR:HH	2:F:208:TYR:HH	1.47	0.62
1:A:92:HIS:NE2	2:B:136:GLU:O	2.31	0.62
2:E:90:TYR:O	2:E:94:GLN:HG2	1.99	0.62
2:F:33:ARG:NH1	2:F:41:SER:OG	2.31	0.62
1:A:113:PHE:HD1	1:A:117:LEU:HD13	1.64	0.62
1:D:132:ARG:HA	1:D:343:PRO:HG3	1.82	0.62
1:A:236:GLN:NE2	7:A:797:HOH:O	2.29	0.62
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.34	0.62
1:A:240:GLU:HB3	7:A:757:HOH:O	1.98	0.62
2:C:102:VAL:HG23	7:C:406:HOH:O	2.00	0.62
2:E:23:LEU:HD22	2:E:28:VAL:HB	1.81	0.62
1:A:76:TYR:O	1:A:88:ILE:HD12	1.99	0.62
2:B:110:GLN:HB2	2:B:167:TYR:CE2	2.34	0.62
1:A:79:ARG:NH1	2:B:188:ARG:HH22	1.98	0.62
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.18	0.62
2:E:48:ASN:ND2	7:E:409:HOH:O	2.32	0.62
2:F:19:ALA:N	7:F:429:HOH:O	2.32	0.62
1:D:208:SER:HA	1:D:211:LEU:HG	1.82	0.62
2:B:195:VAL:HG13	2:B:199:LEU:HD13	1.82	0.62
2:B:114:TRP:O	7:B:412:HOH:O	2.16	0.61
2:B:121:GLN:NE2	2:B:170:PHE:O	2.34	0.61
1:A:93:PRO:HG2	2:B:181:LYS:HA	1.81	0.61
1:D:166:THR:OG1	1:D:561:ILE:HD11	2.00	0.61
2:B:125:LYS:NZ	7:B:403:HOH:O	2.05	0.61
1:D:126:ARG:HD3	1:D:182:ILE:HD13	1.81	0.61
1:D:475:TYR:CZ	1:D:506:TYR:HE1	2.18	0.61
2:E:93:ALA:CB	2:F:73:TYR:HE1	2.12	0.61
2:C:53:LYS:HG2	5:C:301:GSH:HA31	1.81	0.61
2:C:64:VAL:N	7:C:420:HOH:O	2.11	0.61
1:D:25:HIS:O	1:D:29:LYS:HG2	2.00	0.61
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.33	0.61
1:D:507:VAL:HG12	1:D:510:ARG:NH2	2.16	0.61
2:E:8:LEU:HD13	2:E:44:LEU:HB2	1.81	0.61
1:A:461:ASP:HB3	1:A:528:PHE:CD2	2.34	0.61
2:B:9:ASP:OD1	2:B:10:TYR:N	2.29	0.61
2:E:53:LYS:O	7:E:409:HOH:O	2.16	0.61
2:F:111:PHE:O	7:F:419:HOH:O	2.16	0.61
1:A:244:ASP:HB2	1:A:250:LEU:HA	1.83	0.61
2:B:139:LEU:CD2	2:B:142:LYS:H	2.14	0.61
2:B:24:ARG:HH22	2:B:197:LYS:HB2	1.64	0.61
1:D:364:LEU:HD12	1:D:402:ARG:HH22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:TRP:HA	2:C:170:PHE:HD2	1.66	0.61
2:E:51:HIS:HB3	2:E:53:LYS:HG3	1.82	0.61
1:A:224:ALA:HB3	1:A:312:TYR:CE1	2.36	0.61
1:A:286:ASN:HA	1:A:287:TRP:HE3	1.64	0.61
1:A:149:PHE:CB	1:A:530:LYS:HZ3	2.14	0.61
1:D:150:SER:HB3	1:D:170:TYR:CD2	2.35	0.61
1:D:94:VAL:HG11	1:D:112:PRO:HB3	1.83	0.61
2:C:32:TYR:HD2	2:C:32:TYR:H	1.49	0.61
1:D:337:ILE:HD13	1:D:539:GLY:CA	2.30	0.61
1:D:420:LYS:NZ	7:D:774:HOH:O	2.27	0.61
1:A:242:VAL:HG21	1:A:278:ARG:HD3	1.82	0.60
1:A:309:MET:HB3	1:A:312:TYR:CE2	2.36	0.60
1:A:109:LYS:NZ	1:A:401:TYR:OH	2.28	0.60
1:A:547:MET:SD	1:A:549:ARG:NH2	2.71	0.60
2:B:139:LEU:HD21	2:B:142:LYS:O	2.00	0.60
1:D:233:THR:HA	1:D:236:GLN:HE21	1.66	0.60
1:D:20:MET:HE2	1:D:356:PRO:HG2	1.83	0.60
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.35	0.60
2:B:73:TYR:OH	7:B:411:HOH:O	2.16	0.60
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.36	0.60
1:D:122:LEU:HD23	7:D:828:HOH:O	2.01	0.60
1:D:362:GLU:HG3	1:D:400:ARG:NH2	2.15	0.60
1:D:76:TYR:O	1:D:79:ARG:HB2	2.01	0.60
1:A:232:ARG:O	1:A:235:GLU:HG2	2.01	0.60
1:A:295:PHE:HD1	1:A:298:ALA:HB2	1.65	0.60
2:B:59:HIS:CE1	2:B:60:ASN:HD22	2.19	0.60
2:C:122:GLU:HA	2:C:125:LYS:HE2	1.83	0.60
1:D:150:SER:CB	1:D:167:THR:HA	2.32	0.60
1:D:153:GLN:HA	1:D:560:GLN:HG2	1.83	0.60
1:D:462:PHE:O	1:D:549:ARG:NH1	2.35	0.60
2:F:183:ILE:HD12	2:F:186:ALA:HB3	1.83	0.60
1:A:246:LYS:HZ3	1:A:278:ARG:HH22	1.49	0.60
1:A:92:HIS:ND1	2:B:181:LYS:HB3	2.16	0.60
2:C:201:ASP:HB2	2:C:204:LYS:HG3	1.84	0.60
1:D:339:ALA:O	7:D:740:HOH:O	2.16	0.60
1:D:559:LEU:HA	1:D:562:LEU:HB2	1.83	0.60
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.37	0.60
2:B:139:LEU:HG	2:B:142:LYS:HB2	1.84	0.60
2:C:202:SER:OG	1:D:454:GLU:OE2	2.17	0.60
1:A:465:TYR:HB3	1:A:476:ALA:HB3	1.83	0.60
1:D:535:PHE:HB3	1:D:544:GLN:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:176:GLU:O	2:F:177:SER:HB2	2.00	0.60
2:C:73:TYR:HA	2:C:76:GLU:OE2	2.02	0.60
1:D:495:ASN:O	1:D:499:ARG:NH1	2.35	0.60
2:F:144:TYR:HB3	2:F:154:ASP:OD2	2.01	0.60
2:F:64:VAL:HB	2:F:73:TYR:CD2	2.37	0.60
2:F:8:LEU:HB2	2:F:56:VAL:HB	1.84	0.60
1:A:363:PHE:O	7:A:750:HOH:O	2.17	0.60
1:D:467:ASP:OD1	1:D:474:HIS:N	2.32	0.60
2:E:41:SER:OG	7:E:403:HOH:O	2.06	0.60
1:A:524:ALA:O	7:A:749:HOH:O	2.17	0.60
2:B:120:GLU:O	7:B:414:HOH:O	2.17	0.60
1:D:425:ARG:NH2	7:D:791:HOH:O	2.33	0.60
1:A:223:PHE:HD2	1:A:225:HIS:CD2	2.19	0.60
1:A:41:SER:H	2:B:142:LYS:HG2	1.65	0.60
1:D:122:LEU:O	1:D:126:ARG:HG2	2.02	0.60
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.84	0.60
1:D:454:GLU:HG2	7:D:798:HOH:O	2.01	0.60
2:E:92:ARG:CZ	2:E:96:ARG:HH12	2.13	0.60
1:A:28:GLN:OE1	1:A:379:LEU:HD22	2.02	0.59
1:A:437:THR:O	1:A:440:ASP:N	2.35	0.59
2:C:64:VAL:HB	2:C:73:TYR:CE2	2.37	0.59
1:D:148:ILE:O	1:D:205:HIS:HE1	1.84	0.59
1:D:506:TYR:HB3	1:D:510:ARG:HH21	1.67	0.59
1:D:513:LYS:NZ	1:D:575:PHE:HB3	2.16	0.59
2:E:58:VAL:HG22	2:E:63:PRO:HB3	1.82	0.59
2:F:67:SER:OG	5:F:301:GSH:O12	2.13	0.59
2:F:70:VAL:O	2:F:73:TYR:HB2	2.02	0.59
1:A:149:PHE:HB2	1:A:530:LYS:HZ3	1.66	0.59
1:A:42:ALA:HB1	1:A:44:TYR:CE1	2.38	0.59
2:B:66:GLU:N	7:B:420:HOH:O	2.21	0.59
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.36	0.59
1:A:113:PHE:CD1	1:A:117:LEU:HD13	2.37	0.59
2:B:150:PHE:HB2	2:B:192:LYS:HZ2	1.67	0.59
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.36	0.59
2:C:183:ILE:HG12	1:D:492:ASP:CG	2.22	0.59
2:E:92:ARG:NH1	2:E:96:ARG:HH12	1.99	0.59
2:F:195:VAL:HG23	2:F:199:LEU:HD13	1.84	0.59
2:F:82:ASN:O	7:F:420:HOH:O	2.17	0.59
1:A:260:ARG:NE	7:A:796:HOH:O	2.29	0.59
1:A:287:TRP:CD1	1:A:290:LEU:HD13	2.37	0.59
1:D:473:GLY:O	1:D:516:GLY:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:ILE:HD12	2:F:101:PHE:CZ	2.37	0.59
2:F:114:TRP:HA	2:F:170:PHE:HD2	1.66	0.59
1:A:154:TYR:OH	1:A:156:SER:OG	2.19	0.59
1:A:248:GLY:HA2	1:A:267:LEU:HD22	1.83	0.59
1:A:93:PRO:HG3	2:B:184:ALA:CB	2.27	0.59
2:B:96:ARG:NH1	2:C:73:TYR:CD1	2.69	0.59
1:D:61:PHE:O	1:D:65:VAL:HG12	2.02	0.59
1:A:407:VAL:HG11	1:A:419:LEU:HD13	1.84	0.59
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.37	0.59
2:E:8:LEU:O	2:E:55:PRO:HA	2.02	0.59
1:A:473:GLY:O	1:A:516:GLY:N	2.34	0.59
2:C:180:PRO:HG2	1:D:574:ALA:HA	1.85	0.59
2:B:107:THR:HA	2:B:110:GLN:HG2	1.85	0.59
1:D:409:VAL:N	7:D:738:HOH:O	2.31	0.59
2:E:136:GLU:OE2	2:E:181:LYS:HD3	2.02	0.59
1:A:184:SER:HB2	1:A:217:GLN:HE21	1.68	0.59
1:A:24:ALA:O	7:A:752:HOH:O	2.17	0.59
1:A:314:PRO:HB3	1:A:317:ARG:HH12	1.66	0.58
1:A:40:GLN:HG2	2:B:142:LYS:HD2	1.85	0.58
1:A:79:ARG:NH2	2:B:188:ARG:NH1	2.51	0.58
1:D:209:GLY:N	7:D:727:HOH:O	2.36	0.58
1:D:73:LEU:HD22	1:D:89:LEU:HD13	1.84	0.58
2:F:164:PHE:CD2	2:F:183:ILE:HD13	2.34	0.58
2:C:26:LYS:HE2	2:C:75:ASP:HA	1.85	0.58
1:A:291:ILE:HB	1:A:320:ALA:HA	1.84	0.58
1:A:401:TYR:CE2	1:A:403:LEU:HD13	2.37	0.58
1:A:434:ASP:OD2	7:A:751:HOH:O	2.17	0.58
1:A:99:LEU:HB2	1:A:557:LYS:H	1.68	0.58
2:B:165:GLN:HB3	7:B:486:HOH:O	2.02	0.58
2:F:165:GLN:OE1	2:F:202:SER:HB2	2.02	0.58
2:E:62:LYS:HD3	2:F:90:TYR:CD2	2.39	0.58
1:A:48:CYS:HB3	1:A:65:VAL:HG22	1.85	0.58
1:D:521:ARG:NH2	1:D:563:CYS:SG	2.77	0.58
2:F:188:ARG:HD2	2:F:191:GLU:OE2	2.03	0.58
1:D:417:PRO:O	7:D:742:HOH:O	2.17	0.58
2:E:116:LYS:O	7:E:410:HOH:O	2.17	0.58
2:F:142:LYS:HB3	7:F:424:HOH:O	2.03	0.58
1:A:107:ARG:HH21	1:A:433:ILE:HG12	1.68	0.58
1:A:424:ARG:HG3	1:A:425:ARG:H	1.68	0.58
1:A:90:THR:HG23	1:A:397:GLY:CA	2.33	0.58
2:B:152:TYR:O	2:B:155:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:TRP:CZ2	2:C:135:LEU:HD21	2.38	0.58
1:D:62:LYS:HE2	1:D:376:PRO:HG2	1.85	0.58
1:D:80:MET:SD	1:D:87:PRO:HA	2.44	0.58
2:F:33:ARG:HH12	2:F:41:SER:CB	2.16	0.58
2:F:9:ASP:HB3	7:F:482:HOH:O	2.04	0.58
1:A:48:CYS:SG	1:A:65:VAL:HG13	2.44	0.58
1:A:152:LYS:CG	1:A:561:ILE:HA	2.33	0.58
1:A:79:ARG:HH22	2:B:188:ARG:HH12	1.51	0.58
1:D:480:GLU:OE2	1:D:527:THR:N	2.36	0.58
1:D:153:GLN:H	1:D:564:GLU:HB2	1.68	0.58
1:D:88:ILE:HD12	1:D:89:LEU:HB2	1.85	0.58
1:A:149:PHE:HB2	1:A:530:LYS:NZ	2.19	0.58
1:A:36:LEU:HD22	1:A:61:PHE:HZ	1.68	0.58
2:E:8:LEU:HD12	2:E:56:VAL:HB	1.85	0.58
1:D:143:LYS:N	7:D:765:HOH:O	2.29	0.58
1:D:231:PHE:HB3	1:D:290:LEU:HD13	1.85	0.58
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.38	0.58
2:B:125:LYS:HB3	2:B:173:PHE:HE2	1.68	0.57
2:C:140:GLY:N	2:C:181:LYS:HZ3	2.02	0.57
2:C:51:HIS:ND1	7:C:423:HOH:O	2.33	0.57
1:D:38:LYS:O	2:E:142:LYS:HG3	2.02	0.57
1:A:445:VAL:HG22	7:A:762:HOH:O	2.04	0.57
1:A:450:LYS:HA	1:A:453:SER:HB3	1.86	0.57
2:B:125:LYS:O	2:B:129:ILE:HG12	2.04	0.57
1:D:363:PHE:HB3	1:D:388:TYR:HB3	1.85	0.57
1:D:44:TYR:CB	1:D:89:LEU:HG	2.34	0.57
2:F:135:LEU:HD13	2:F:182:LEU:HD11	1.86	0.57
1:A:274:ALA:HB1	1:A:278:ARG:CZ	2.34	0.57
1:A:287:TRP:HD1	1:A:290:LEU:HD13	1.68	0.57
1:D:11:ASN:O	1:D:14:ILE:HG13	2.04	0.57
1:D:407:VAL:HG22	1:D:541:SER:HB2	1.85	0.57
1:D:107:ARG:HH22	1:D:552:LYS:HB3	1.69	0.57
1:D:99:LEU:HD12	1:D:100:SER:N	2.19	0.57
2:E:195:VAL:HG13	2:E:199:LEU:HD13	1.85	0.57
2:F:98:TRP:CZ2	2:F:157:LEU:HD22	2.39	0.57
1:A:23:ASN:OD1	1:A:26:GLN:HG2	2.04	0.57
1:A:348:GLU:OE1	7:A:753:HOH:O	2.18	0.57
2:C:26:LYS:HG2	2:C:81:LYS:HZ3	1.69	0.57
1:D:394:ASN:OD1	1:D:398:LEU:HD11	2.04	0.57
1:A:559:LEU:O	1:A:562:LEU:HG	2.04	0.57
1:D:528:PHE:HA	1:D:531:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:TYR:OH	1:D:541:SER:N	2.36	0.57
1:A:32:LEU:HB2	1:A:360:TYR:CD1	2.39	0.57
1:D:342:THR:OG1	1:D:413:TYR:OH	2.12	0.57
1:D:377:VAL:O	7:D:745:HOH:O	2.18	0.57
1:D:154:TYR:HB3	1:D:560:GLN:HA	1.86	0.57
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.39	0.57
1:A:122:LEU:HD21	1:A:178:GLY:HA3	1.86	0.57
1:A:338:ALA:HA	1:A:354:VAL:HA	1.85	0.57
1:A:441:LEU:HG	1:A:462:PHE:CE2	2.39	0.57
2:C:70:VAL:O	2:C:73:TYR:HB2	2.04	0.57
1:D:168:ASN:ND2	7:D:732:HOH:O	2.15	0.57
1:D:207:LEU:O	1:D:210:ILE:HG22	2.05	0.57
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.87	0.57
1:D:108:PRO:HB2	1:D:554:SER:OG	2.05	0.57
1:D:389:GLU:OE1	7:D:744:HOH:O	2.17	0.57
2:C:184:ALA:HB1	1:D:499:ARG:NE	2.19	0.57
1:A:237:VAL:HG11	7:A:1029:HOH:O	2.05	0.57
1:A:26:GLN:HA	1:A:29:LYS:HG2	1.86	0.57
1:A:32:LEU:HD21	1:A:61:PHE:HD2	1.70	0.57
2:C:17:MET:SD	2:C:199:LEU:HG	2.44	0.57
1:D:8:PHE:CD1	1:D:182:ILE:HG22	2.39	0.57
1:D:382:VAL:HG13	1:D:388:TYR:CE2	2.40	0.57
2:E:113:VAL:O	7:E:410:HOH:O	2.17	0.57
1:A:231:PHE:HA	1:A:234:PHE:HB3	1.86	0.56
2:B:152:TYR:OH	7:B:413:HOH:O	2.16	0.56
2:B:162:SER:HB3	2:B:199:LEU:HD23	1.86	0.56
1:D:284:LEU:HD13	1:D:287:TRP:H	1.69	0.56
1:A:37:LEU:HD11	2:B:90:TYR:HE2	1.69	0.56
1:D:405:ASP:OD1	1:D:405:ASP:N	2.36	0.56
2:F:98:TRP:CZ2	2:F:135:LEU:HD21	2.40	0.56
1:A:206:LEU:HD12	1:A:207:LEU:N	2.20	0.56
1:D:196:PRO:HA	1:D:565:ASN:OD1	2.06	0.56
2:F:29:GLU:N	7:F:433:HOH:O	2.38	0.56
1:A:132:ARG:O	1:A:136:PHE:N	2.38	0.56
2:C:123:ALA:HB2	7:C:476:HOH:O	2.05	0.56
1:A:207:LEU:HD13	1:A:245:ILE:HD11	1.87	0.56
1:A:506:TYR:HA	1:A:509:SER:HB2	1.87	0.56
1:D:451:ARG:NH1	1:D:454:GLU:OE1	2.38	0.56
2:F:68:LEU:HA	2:F:71:VAL:HG12	1.88	0.56
1:A:174:ASN:ND2	7:A:818:HOH:O	2.39	0.56
2:B:150:PHE:HB2	2:B:192:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HD22	1:D:555:ASN:HB3	1.88	0.56
2:E:85:PHE:CE1	2:E:152:TYR:HB2	2.40	0.56
1:A:233:THR:O	1:A:236:GLN:N	2.39	0.56
1:D:330:TYR:HE1	1:D:536:LEU:O	1.89	0.56
1:A:120:ASN:O	1:A:124:LEU:HG	2.06	0.56
1:A:228:VAL:O	1:A:232:ARG:N	2.38	0.56
2:C:10:TYR:HH	2:C:208:TYR:HH	1.53	0.56
1:D:221:ALA:HB3	1:D:227:LEU:HG	1.87	0.56
1:D:360:TYR:C	1:D:361:PHE:HD1	2.10	0.56
1:A:101:SER:HB3	1:A:535:PHE:CD2	2.41	0.56
1:A:165:ALA:HB3	4:A:602:VAL:HA	1.87	0.56
1:A:523:VAL:HG22	1:A:524:ALA:H	1.71	0.56
1:D:242:VAL:O	1:D:246:LYS:HB2	2.05	0.56
1:D:451:ARG:NH1	1:D:454:GLU:CD	2.59	0.56
2:E:144:TYR:HB3	2:E:154:ASP:OD2	2.06	0.56
2:F:183:ILE:O	2:F:186:ALA:N	2.37	0.56
1:A:86:SER:HB2	2:B:188:ARG:NE	2.21	0.56
1:D:110:PHE:CD2	1:D:554:SER:HA	2.41	0.56
1:D:146:GLN:NE2	7:D:760:HOH:O	2.22	0.56
1:D:233:THR:O	1:D:237:VAL:HG22	2.06	0.56
1:D:166:THR:HG22	4:D:602:VAL:HB	1.87	0.56
2:E:50:ILE:HG13	2:E:51:HIS:N	2.18	0.56
1:A:171:ARG:HB2	7:A:709:HOH:O	2.05	0.56
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.87	0.56
2:B:37:PHE:CE1	5:B:301:GSH:HA32	2.41	0.56
1:A:523:VAL:HG11	1:A:527:THR:HG21	1.88	0.55
1:D:96:ALA:HA	1:D:161:PRO:O	2.05	0.55
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.70	0.55
2:F:185:TRP:NE1	2:F:189:CYS:SG	2.79	0.55
2:F:64:VAL:HG23	2:F:70:VAL:HG22	1.88	0.55
1:D:113:PHE:CD1	1:D:117:LEU:HD12	2.40	0.55
1:D:169:VAL:HG23	7:D:770:HOH:O	2.06	0.55
1:D:188:SER:OG	1:D:205:HIS:CD2	2.59	0.55
1:D:434:ASP:HB2	1:D:550:CYS:HB3	1.88	0.55
1:D:47:ASN:OD1	7:D:749:HOH:O	2.18	0.55
1:D:495:ASN:CB	1:D:499:ARG:NH1	2.68	0.55
2:F:17:MET:SD	2:F:199:LEU:HG	2.46	0.55
1:A:97:ILE:HD13	1:A:112:PRO:HA	1.87	0.55
1:A:493:CYS:HB3	7:A:940:HOH:O	2.06	0.55
1:A:92:HIS:CE1	2:B:139:LEU:HD22	2.42	0.55
1:A:79:ARG:HH12	2:B:188:ARG:HH12	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:LEU:HD13	2:C:182:LEU:HD11	1.87	0.55
1:D:101:SER:HB3	1:D:535:PHE:CD2	2.41	0.55
1:D:110:PHE:O	7:D:746:HOH:O	2.18	0.55
1:D:332:SER:HB2	1:D:538:LEU:HA	1.88	0.55
1:D:541:SER:O	1:D:543:GLY:N	2.39	0.55
2:E:173:PHE:HE1	2:E:175:ILE:HG13	1.72	0.55
2:E:193:GLU:OE1	2:E:196:SER:OG	2.23	0.55
1:A:143:LYS:NZ	1:A:208:SER:O	2.39	0.55
1:A:152:LYS:HZ1	1:A:530:LYS:HZ3	1.39	0.55
1:D:149:PHE:HB2	1:D:530:LYS:HE2	1.89	0.55
1:D:223:PHE:HD2	1:D:225:HIS:CE1	2.25	0.55
2:E:20:ARG:HB3	2:E:24:ARG:HH12	1.69	0.55
2:F:123:ALA:HB2	7:F:411:HOH:O	2.05	0.55
1:A:150:SER:OG	1:A:150:SER:O	2.22	0.55
1:A:437:THR:OG1	1:A:440:ASP:HB2	2.07	0.55
1:D:328:HIS:CG	1:D:329:ASP:N	2.74	0.55
1:D:39:ASN:ND2	1:D:399:TYR:OH	2.39	0.55
1:D:68:VAL:HG12	1:D:72:GLU:HB2	1.88	0.55
2:F:170:PHE:C	2:F:172:ASN:H	2.08	0.55
1:A:121:THR:HG22	1:A:336:TRP:CZ2	2.41	0.55
2:C:54:ILE:HB	2:C:55:PRO:HA	1.88	0.55
1:D:164:THR:HA	1:D:557:LYS:HG3	1.87	0.55
1:D:228:VAL:HG13	1:D:319:TYR:HE2	1.72	0.55
1:D:551:VAL:HB	1:D:555:ASN:HB2	1.87	0.55
2:F:73:TYR:HA	2:F:76:GLU:OE2	2.07	0.55
1:A:238:TRP:CA	1:A:241:ILE:HB	2.36	0.55
1:A:340:ASN:ND2	1:A:343:PRO:HA	2.20	0.55
2:C:165:GLN:HA	2:C:168:GLU:OE1	2.07	0.55
1:D:150:SER:O	1:D:150:SER:OG	2.20	0.55
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.41	0.55
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.42	0.55
1:A:169:VAL:HG13	1:A:170:TYR:CD1	2.42	0.55
1:A:28:GLN:HG3	1:A:356:PRO:O	2.07	0.55
1:A:503:ASP:OD2	1:A:505:GLY:N	2.38	0.55
2:B:139:LEU:O	2:B:141:ASP:N	2.40	0.55
2:C:96:ARG:N	7:C:440:HOH:O	2.40	0.55
1:D:437:THR:O	1:D:440:ASP:N	2.40	0.55
1:D:495:ASN:O	1:D:498:ASP:HB2	2.06	0.55
1:D:524:ALA:HB2	1:D:567:VAL:CG1	2.36	0.55
1:D:75:PRO:O	1:D:79:ARG:HG3	2.07	0.55
2:E:93:ALA:CB	2:F:73:TYR:CE1	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:200:PRO:HG3	7:F:494:HOH:O	2.06	0.55
2:C:87:SER:HB3	7:C:502:HOH:O	2.06	0.55
1:D:43:ILE:O	1:D:46:GLN:HG2	2.07	0.55
1:A:201:ALA:O	1:A:205:HIS:N	2.40	0.55
1:A:228:VAL:O	1:A:232:ARG:HG3	2.06	0.55
2:B:76:GLU:OE2	2:C:92:ARG:NH2	2.40	0.55
2:E:205:ILE:HG12	7:E:404:HOH:O	2.06	0.55
1:A:315:LYS:O	1:A:318:HIS:HB3	2.07	0.54
1:A:78:LYS:NZ	7:A:720:HOH:O	2.06	0.54
2:B:93:ALA:HB1	2:C:73:TYR:CZ	2.43	0.54
2:C:185:TRP:NE1	2:C:189:CYS:SG	2.80	0.54
2:E:201:ASP:OD2	2:E:204:LYS:HE3	2.07	0.54
1:A:15:ASP:OD1	1:A:16:GLU:N	2.40	0.54
1:A:151:SER:HB2	1:A:194:PHE:HA	1.88	0.54
1:A:212:PHE:HB3	1:A:215:GLN:NE2	2.23	0.54
1:A:92:HIS:HD2	2:B:140:GLY:O	1.89	0.54
2:C:209:ALA:HB2	7:C:434:HOH:O	2.06	0.54
2:C:8:LEU:HD22	2:C:33:ARG:NH2	2.22	0.54
1:D:363:PHE:HE1	1:D:390:VAL:HG23	1.71	0.54
1:D:107:ARG:CZ	1:D:433:ILE:HG13	2.38	0.54
1:D:513:LYS:HZ2	1:D:575:PHE:HB3	1.71	0.54
2:E:70:VAL:HA	2:E:73:TYR:HE2	1.71	0.54
2:F:86:PRO:HD3	2:F:146:GLY:O	2.08	0.54
1:A:77:ILE:CG2	1:A:110:PHE:HB3	2.37	0.54
1:A:314:PRO:HA	1:A:317:ARG:NH1	2.22	0.54
2:C:102:VAL:O	2:C:107:THR:HG23	2.07	0.54
2:C:44:LEU:HB3	7:C:415:HOH:O	2.07	0.54
1:D:337:ILE:CD1	1:D:361:PHE:HE2	2.20	0.54
2:C:168:GLU:OE2	1:D:488:ASP:OD2	2.26	0.54
2:E:14:MET:HA	2:E:17:MET:HE3	1.88	0.54
1:A:84:ASP:C	1:A:86:SER:H	2.11	0.54
1:D:202:LEU:HD23	1:D:525:LYS:HD2	1.89	0.54
2:F:121:GLN:O	2:F:125:LYS:HG3	2.08	0.54
1:A:340:ASN:HB2	1:A:352:PHE:CE2	2.42	0.54
2:C:164:PHE:O	2:C:168:GLU:HG3	2.08	0.54
2:C:50:ILE:HD12	7:C:489:HOH:O	2.07	0.54
1:A:118:MET:O	1:A:121:THR:OG1	2.24	0.54
1:A:424:ARG:C	1:A:543:GLY:HA2	2.27	0.54
1:D:42:ALA:HB3	1:D:45:LEU:HD13	1.89	0.54
1:D:425:ARG:NH1	1:D:546:LYS:HE3	2.23	0.54
1:A:193:ILE:HA	1:A:205:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:CE1	2:B:185:TRP:CZ2	2.96	0.54
1:A:32:LEU:HD22	1:A:360:TYR:CE2	2.43	0.54
1:A:334:GLU:OE1	1:A:403:LEU:HD21	2.07	0.54
1:A:369:THR:OG1	1:A:370:GLY:N	2.40	0.54
1:D:10:MET:HA	7:D:710:HOH:O	2.08	0.54
1:D:77:ILE:HG12	1:D:110:PHE:C	2.29	0.54
1:D:22:ARG:NH1	1:D:414:ASN:CG	2.62	0.54
1:D:353:ALA:HB2	1:D:413:TYR:HD2	1.72	0.54
1:D:382:VAL:HG13	1:D:388:TYR:CD2	2.43	0.54
1:D:99:LEU:H	1:D:557:LYS:HB2	1.73	0.54
2:E:107:THR:HG22	2:E:160:PHE:CZ	2.43	0.54
2:E:92:ARG:NH2	7:E:424:HOH:O	2.40	0.54
1:A:203:TYR:HD2	1:A:254:ILE:HD11	1.73	0.54
2:B:108:ASP:O	2:B:112:LYS:HG2	2.08	0.54
2:C:187:LYS:HZ3	1:D:496:CYS:HB2	1.73	0.54
2:C:24:ARG:HB3	2:C:194:SER:HA	1.90	0.54
1:D:452:LEU:HD23	1:D:481:ILE:HG21	1.89	0.54
1:D:551:VAL:HG21	1:D:559:LEU:HD23	1.90	0.54
2:E:17:MET:SD	2:E:200:PRO:HD2	2.48	0.54
1:A:128:ALA:HA	1:A:131:PHE:CD2	2.43	0.53
1:A:152:LYS:CE	1:A:530:LYS:NZ	2.65	0.53
1:A:339:ALA:N	1:A:353:ALA:O	2.29	0.53
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.88	0.53
1:A:562:LEU:HB3	7:A:713:HOH:O	2.08	0.53
1:A:83:GLY:H	1:A:158:GLY:HA3	1.72	0.53
1:D:195:SER:HB3	1:D:201:ALA:HB2	1.90	0.53
1:D:246:LYS:CE	1:D:271:PRO:HA	2.37	0.53
1:D:76:TYR:HB3	1:D:88:ILE:HD13	1.90	0.53
2:E:193:GLU:HA	2:E:196:SER:OG	2.09	0.53
1:A:94:VAL:HB	1:A:113:PHE:O	2.07	0.53
1:A:216:VAL:HG21	7:A:778:HOH:O	2.07	0.53
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.44	0.53
1:A:154:TYR:CE2	1:A:559:LEU:HB3	2.42	0.53
2:C:98:TRP:CD1	2:C:153:VAL:HG11	2.44	0.53
1:A:233:THR:HG23	1:A:525:LYS:NZ	2.22	0.53
1:A:310:GLU:HG3	1:A:311:PRO:HD3	1.90	0.53
1:A:435:LYS:HE3	1:A:438:GLU:CB	2.38	0.53
2:C:40:LYS:HD2	2:C:52:LYS:HB3	1.91	0.53
1:D:445:VAL:HG21	1:D:462:PHE:CD1	2.43	0.53
1:D:79:ARG:NH1	7:D:800:HOH:O	2.40	0.53
2:F:57:LEU:O	2:F:64:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:HA	7:A:745:HOH:O	2.08	0.53
1:A:287:TRP:HB3	7:A:1021:HOH:O	2.08	0.53
1:A:291:ILE:HG21	1:A:301:VAL:HG22	1.91	0.53
1:A:36:LEU:HD22	1:A:61:PHE:CZ	2.44	0.53
1:D:302:TYR:HD1	1:D:326:VAL:HG13	1.72	0.53
1:D:475:TYR:HB2	1:D:518:LEU:HG	1.90	0.53
1:D:85:THR:HB	2:E:184:ALA:HB1	1.90	0.53
2:E:66:GLU:CD	2:F:97:PHE:HD1	2.11	0.53
2:F:51:HIS:O	7:F:421:HOH:O	2.17	0.53
1:A:11:ASN:O	1:A:14:ILE:HG13	2.08	0.53
1:A:334:GLU:O	1:A:394:ASN:ND2	2.40	0.53
2:B:134:ILE:HG22	2:B:138:GLU:OE2	2.08	0.53
2:C:108:ASP:O	2:C:112:LYS:HG2	2.08	0.53
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.44	0.53
1:D:126:ARG:HD2	1:D:182:ILE:HG21	1.91	0.53
1:D:199:HIS:HA	1:D:525:LYS:HB2	1.91	0.53
2:C:102:VAL:HG21	2:C:157:LEU:HB3	1.91	0.53
1:D:295:PHE:HD1	1:D:298:ALA:HB2	1.74	0.53
2:F:108:ASP:O	2:F:112:LYS:HG2	2.07	0.53
1:A:510:ARG:CZ	1:A:515:ILE:HD12	2.38	0.53
2:B:24:ARG:HG3	2:B:30:PHE:HE1	1.74	0.53
2:C:187:LYS:NZ	2:C:187:LYS:HB2	2.23	0.53
1:D:244:ASP:OD1	1:D:251:SER:HB2	2.09	0.53
1:D:381:GLN:O	7:D:750:HOH:O	2.19	0.53
1:D:495:ASN:CB	1:D:499:ARG:HH12	2.20	0.53
1:D:559:LEU:O	1:D:562:LEU:HB3	2.09	0.53
2:E:53:LYS:HG2	5:E:301:GSH:HA31	1.90	0.53
2:F:26:LYS:HG2	2:F:81:LYS:HZ1	1.71	0.53
1:A:218:TYR:HA	1:A:298:ALA:HB1	1.91	0.53
2:B:168:GLU:OE1	7:B:415:HOH:O	2.18	0.53
2:C:188:ARG:HH12	1:D:500:ALA:CA	2.02	0.53
1:D:139:ASP:OD2	1:D:142:GLY:N	2.42	0.53
1:D:400:ARG:HB2	7:D:728:HOH:O	2.09	0.53
1:D:522:VAL:O	1:D:567:VAL:HG22	2.09	0.53
2:E:26:LYS:HG3	2:E:82:ASN:HD21	1.72	0.53
2:B:201:ASP:HB2	2:B:204:LYS:HG3	1.91	0.53
1:D:534:HIS:CD2	1:D:557:LYS:HD3	2.44	0.53
1:A:538:LEU:HD22	1:A:544:GLN:HE21	1.74	0.53
1:D:206:LEU:O	1:D:210:ILE:HB	2.09	0.53
1:D:251:SER:O	1:D:254:ILE:HG12	2.07	0.53
1:D:465:TYR:HB3	1:D:476:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:VAL:O	1:D:511:LYS:HB2	2.09	0.53
2:B:165:GLN:O	2:B:168:GLU:HG2	2.09	0.52
2:C:158:ILE:HG12	7:C:432:HOH:O	2.08	0.52
1:D:10:MET:HB2	7:D:881:HOH:O	2.08	0.52
1:D:330:TYR:HB2	1:D:352:PHE:CD2	2.43	0.52
1:D:112:PRO:HD2	1:D:397:GLY:HA3	1.90	0.52
1:D:152:LYS:CE	1:D:565:ASN:HB2	2.37	0.52
2:E:162:SER:HB3	2:E:199:LEU:HD23	1.91	0.52
1:A:137:PRO:O	7:A:756:HOH:O	2.18	0.52
1:A:305:MET:CE	1:A:325:LEU:HG	2.38	0.52
1:A:461:ASP:HB3	1:A:528:PHE:HD2	1.74	0.52
1:A:202:LEU:HD21	1:A:529:ARG:NH2	2.23	0.52
2:B:18:ARG:CD	2:B:156:SER:HA	2.38	0.52
2:B:24:ARG:NH2	2:B:197:LYS:HB2	2.23	0.52
1:D:154:TYR:CD2	1:D:559:LEU:HD13	2.44	0.52
1:D:387:GLU:O	7:D:747:HOH:O	2.18	0.52
1:D:412:PHE:N	7:D:707:HOH:O	2.41	0.52
1:D:432:ASN:O	7:D:751:HOH:O	2.19	0.52
2:E:135:LEU:HD23	2:E:157:LEU:HD21	1.91	0.52
2:F:70:VAL:HA	2:F:73:TYR:CD2	2.44	0.52
1:A:236:GLN:NE2	7:A:729:HOH:O	2.08	0.52
1:D:425:ARG:HG2	1:D:545:PHE:CE1	2.45	0.52
1:A:164:THR:OG1	1:A:166:THR:OG1	2.16	0.52
1:A:26:GLN:HG3	1:A:27:VAL:N	2.25	0.52
1:A:290:LEU:N	1:A:319:TYR:O	2.42	0.52
2:C:5:PRO:HG3	2:C:59:HIS:CE1	2.43	0.52
1:D:235:GLU:HG2	1:D:287:TRP:CG	2.44	0.52
1:A:90:THR:HG23	1:A:397:GLY:HA2	1.91	0.52
1:A:551:VAL:CG1	1:A:555:ASN:HB3	2.36	0.52
2:E:62:LYS:NZ	7:E:426:HOH:O	2.41	0.52
2:E:97:PHE:CE1	2:F:65:CYS:HB2	2.45	0.52
1:D:412:PHE:HB3	1:D:414:ASN:O	2.10	0.52
1:D:437:THR:OG1	1:D:440:ASP:HB2	2.09	0.52
7:C:407:HOH:O	1:D:451:ARG:NH2	2.42	0.52
1:A:151:SER:HA	1:A:194:PHE:HA	1.91	0.52
1:A:292:PRO:HA	7:A:725:HOH:O	2.10	0.52
1:A:478:PHE:CZ	1:A:523:VAL:HB	2.44	0.52
1:D:151:SER:HA	1:D:194:PHE:HA	1.92	0.52
2:F:121:GLN:HB3	7:F:457:HOH:O	2.10	0.52
2:C:142:LYS:HB3	7:C:430:HOH:O	2.09	0.52
2:C:20:ARG:HB3	2:C:198:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:LYS:HD3	2:E:52:LYS:HE3	1.91	0.52
2:F:139:LEU:O	2:F:141:ASP:N	2.38	0.52
2:F:170:PHE:C	2:F:172:ASN:N	2.63	0.52
1:A:96:ALA:HB1	1:A:163:GLY:H	1.75	0.52
2:F:131:ALA:O	2:F:135:LEU:HB2	2.09	0.52
1:A:204:CYS:HA	1:A:207:LEU:HD23	1.91	0.52
1:D:337:ILE:HD11	1:D:361:PHE:HE2	1.75	0.52
1:D:364:LEU:HD12	1:D:402:ARG:NH2	2.25	0.52
2:E:150:PHE:CZ	2:E:158:ILE:HD12	2.45	0.52
1:A:365:PRO:HA	1:A:388:TYR:CD1	2.44	0.51
1:A:391:VAL:HG12	1:A:402:ARG:HA	1.93	0.51
2:B:161:SER:HB2	2:B:186:ALA:HB1	1.92	0.51
1:D:33:LYS:O	1:D:37:LEU:HB2	2.10	0.51
1:D:403:LEU:HD22	7:D:803:HOH:O	2.09	0.51
1:D:535:PHE:O	1:D:538:LEU:HB3	2.09	0.51
1:A:187:CYS:HB2	1:A:208:SER:HB3	1.92	0.51
1:A:215:GLN:NE2	7:A:824:HOH:O	2.43	0.51
1:A:224:ALA:HB3	1:A:312:TYR:HE1	1.74	0.51
1:A:32:LEU:HB2	1:A:360:TYR:CG	2.45	0.51
2:B:129:ILE:HD12	2:B:175:ILE:HD11	1.92	0.51
2:C:112:LYS:HG3	7:C:450:HOH:O	2.11	0.51
1:D:202:LEU:O	1:D:205:HIS:N	2.43	0.51
2:E:7:LEU:HD11	2:E:32:TYR:CD1	2.45	0.51
2:B:125:LYS:HE2	2:B:171:GLY:HA2	1.93	0.51
2:B:62:LYS:HZ1	2:C:94:GLN:HG3	1.74	0.51
1:D:87:PRO:HD2	2:E:188:ARG:CB	2.40	0.51
1:A:300:TYR:CE1	1:A:302:TYR:HB2	2.46	0.51
1:A:574:ALA:O	1:A:575:PHE:HB2	2.10	0.51
2:B:132:VAL:HG13	2:B:182:LEU:HD23	1.92	0.51
2:C:104:LYS:N	7:C:419:HOH:O	2.43	0.51
2:C:169:LYS:HD3	2:C:206:VAL:HG13	1.93	0.51
1:D:126:ARG:CD	1:D:182:ILE:HG21	2.40	0.51
1:D:351:THR:HG22	1:D:420:LYS:HB3	1.92	0.51
2:E:193:GLU:HB2	7:E:516:HOH:O	2.11	0.51
1:A:405:ASP:HB3	1:A:541:SER:HB3	1.93	0.51
1:A:534:HIS:HA	4:A:602:VAL:N	2.26	0.51
1:A:87:PRO:HB2	2:B:143:PRO:CA	2.37	0.51
2:B:17:MET:HA	2:B:20:ARG:HD2	1.93	0.51
1:D:97:ILE:HG12	1:D:162:VAL:HG22	1.93	0.51
1:D:310:GLU:O	1:D:313:VAL:HG12	2.10	0.51
1:D:566:VAL:HG23	1:D:568:SER:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:TYR:HD1	2:F:76:GLU:OE2	1.94	0.51
1:A:151:SER:OG	1:A:195:SER:O	2.29	0.51
1:D:143:LYS:HZ3	1:D:187:CYS:HA	1.74	0.51
1:D:281:CYS:O	1:D:284:LEU:HG	2.10	0.51
1:D:361:PHE:CZ	1:D:392:ILE:HG23	2.46	0.51
1:D:480:GLU:HB3	7:D:703:HOH:O	2.10	0.51
1:D:223:PHE:CZ	1:D:536:LEU:HB2	2.46	0.51
2:E:76:GLU:OE2	2:F:92:ARG:NH2	2.44	0.51
2:F:165:GLN:HG2	2:F:206:VAL:CG2	2.41	0.51
1:A:219:VAL:HB	1:A:295:PHE:CE1	2.45	0.51
1:A:410:ILE:HD11	1:A:418:GLN:OE1	2.10	0.51
2:C:12:PRO:O	2:C:163:TRP:CZ2	2.64	0.51
2:C:194:SER:N	7:C:442:HOH:O	2.43	0.51
1:D:475:TYR:CE1	1:D:506:TYR:HE1	2.28	0.51
1:D:552:LYS:HE3	1:D:554:SER:OG	2.10	0.51
1:D:198:VAL:HG13	1:D:565:ASN:HD21	1.74	0.51
1:A:113:PHE:HE1	1:A:117:LEU:HD22	1.75	0.51
1:A:337:ILE:HG22	1:A:338:ALA:HB2	1.92	0.51
1:A:423:CYS:SG	1:A:543:GLY:N	2.84	0.51
1:A:46:GLN:HB2	2:B:148:ASP:HB2	1.93	0.51
2:C:164:PHE:CD2	2:C:183:ILE:HD12	2.40	0.51
1:D:437:THR:HG21	1:D:439:ARG:HH21	1.75	0.51
2:E:68:LEU:HA	2:E:71:VAL:HG22	1.92	0.51
1:A:131:PHE:HD1	1:A:343:PRO:HG3	1.75	0.51
1:A:503:ASP:CG	1:A:505:GLY:H	2.13	0.51
1:A:37:LEU:HD11	2:B:90:TYR:CE2	2.45	0.51
2:C:141:ASP:N	2:C:141:ASP:OD1	2.44	0.51
2:C:153:VAL:O	2:C:157:LEU:HD23	2.11	0.51
2:E:141:ASP:OD2	2:E:181:LYS:NZ	2.36	0.51
2:E:144:TYR:CZ	2:E:188:ARG:NH1	2.79	0.51
2:F:115:GLY:HA3	7:F:419:HOH:O	2.10	0.51
2:F:117:LYS:HE3	2:F:213:ARG:HH11	1.74	0.51
1:A:156:SER:HB2	1:A:160:VAL:O	2.11	0.51
1:A:45:LEU:HA	1:A:48:CYS:HB2	1.92	0.51
1:A:495:ASN:ND2	7:A:703:HOH:O	2.44	0.51
2:C:125:LYS:HD2	2:C:173:PHE:CE1	2.46	0.51
1:A:167:THR:HG21	1:A:560:GLN:HG3	1.92	0.50
1:A:154:TYR:HD2	1:A:560:GLN:HA	1.76	0.50
2:B:161:SER:HA	2:B:164:PHE:CD2	2.46	0.50
2:C:195:VAL:HG23	2:C:199:LEU:HD13	1.93	0.50
1:D:118:MET:HG3	7:D:828:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:SER:CB	1:D:538:LEU:HA	2.41	0.50
1:D:99:LEU:HB2	1:D:556:ALA:H	1.76	0.50
2:F:32:TYR:HD2	2:F:32:TYR:H	1.57	0.50
1:A:56:ASP:O	1:A:60:ALA:N	2.35	0.50
2:B:205:ILE:HG12	7:B:402:HOH:O	2.10	0.50
1:D:20:MET:SD	7:D:713:HOH:O	2.60	0.50
1:A:213:ARG:HA	1:A:216:VAL:CG2	2.41	0.50
1:A:535:PHE:HB3	1:A:544:GLN:O	2.11	0.50
1:D:46:GLN:HG3	1:D:47:ASN:N	2.25	0.50
2:E:171:GLY:HA3	2:E:173:PHE:CE2	2.47	0.50
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.46	0.50
1:D:223:PHE:HE2	1:D:532:GLN:HB2	1.77	0.50
1:D:197:ASP:HA	1:D:567:VAL:HG12	1.94	0.50
2:B:183:ILE:O	2:B:186:ALA:HB3	2.12	0.50
1:D:329:ASP:HB3	1:D:338:ALA:O	2.11	0.50
1:D:337:ILE:HG22	1:D:338:ALA:HB2	1.94	0.50
1:D:337:ILE:O	1:D:354:VAL:HA	2.11	0.50
1:D:529:ARG:NH2	1:D:533:GLU:OE1	2.45	0.50
1:D:76:TYR:O	1:D:88:ILE:HG21	2.12	0.50
1:A:195:SER:HB3	1:A:201:ALA:HB2	1.92	0.50
2:B:37:PHE:O	7:B:416:HOH:O	2.19	0.50
1:D:33:LYS:NZ	1:D:58:GLU:HB2	2.27	0.50
1:D:32:LEU:O	1:D:36:LEU:HD12	2.11	0.50
1:D:529:ARG:HH21	1:D:530:LYS:HD3	1.76	0.50
1:A:279:THR:HA	1:A:282:MET:SD	2.52	0.50
1:A:91:GLY:HA3	2:B:142:LYS:N	2.26	0.50
1:A:237:VAL:O	7:A:757:HOH:O	2.19	0.50
1:A:305:MET:HA	7:A:715:HOH:O	2.12	0.50
1:A:153:GLN:H	1:A:564:GLU:HB2	1.77	0.50
1:A:521:ARG:HB3	1:A:566:VAL:HG22	1.94	0.50
1:A:43:ILE:HD11	1:A:88:ILE:HG23	1.93	0.50
2:C:60:ASN:HB3	7:C:421:HOH:O	2.12	0.50
1:D:17:PHE:HA	1:D:20:MET:HB3	1.93	0.50
1:D:476:ALA:HA	1:D:519:GLU:O	2.12	0.50
2:F:114:TRP:HA	2:F:170:PHE:CD2	2.47	0.50
1:A:291:ILE:HD12	1:A:320:ALA:HB2	1.93	0.50
1:D:270:ASN:HB3	1:D:273:LEU:CD1	2.42	0.50
1:D:467:ASP:CG	1:D:474:HIS:H	2.15	0.50
2:E:110:GLN:HG3	2:E:111:PHE:N	2.25	0.50
2:F:40:LYS:HD2	2:F:52:LYS:HB3	1.93	0.50
1:A:440:ASP:OD1	1:A:501:PHE:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:HD2	2:B:188:ARG:HB2	1.93	0.49
2:B:153:VAL:O	2:B:156:SER:OG	2.21	0.49
2:C:5:PRO:HB3	2:C:57:LEU:HD11	1.93	0.49
1:D:330:TYR:HE2	1:D:540:SER:H	1.56	0.49
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.46	0.49
1:A:103:THR:OG1	1:A:429:LEU:HD11	2.12	0.49
1:A:197:ASP:HA	1:A:567:VAL:HG12	1.94	0.49
1:A:33:LYS:HA	1:A:36:LEU:CD2	2.42	0.49
1:A:421:PHE:CE1	1:A:541:SER:HA	2.47	0.49
1:A:428:ILE:O	7:A:759:HOH:O	2.20	0.49
2:B:110:GLN:NE2	7:B:444:HOH:O	2.45	0.49
2:B:94:GLN:O	2:B:98:TRP:HD1	1.95	0.49
1:D:410:ILE:HG13	1:D:418:GLN:HB2	1.94	0.49
2:F:145:PHE:HA	7:F:424:HOH:O	2.11	0.49
2:F:33:ARG:HG3	7:F:518:HOH:O	2.12	0.49
1:A:295:PHE:CD1	1:A:298:ALA:HB2	2.45	0.49
1:A:224:ALA:CB	1:A:316:LEU:HD22	2.43	0.49
2:B:9:ASP:OD1	2:B:16:GLY:HA3	2.12	0.49
2:B:15:PHE:HA	2:B:18:ARG:HG3	1.94	0.49
2:C:98:TRP:CD1	2:C:153:VAL:HG21	2.47	0.49
2:F:172:ASN:O	2:F:173:PHE:HD1	1.94	0.49
2:F:71:VAL:O	2:F:74:VAL:HB	2.13	0.49
1:A:104:SER:C	1:A:106:GLY:N	2.65	0.49
1:A:302:TYR:OH	7:A:719:HOH:O	2.06	0.49
1:A:311:PRO:O	1:A:314:PRO:HD2	2.13	0.49
2:C:57:LEU:O	2:C:64:VAL:HG22	2.13	0.49
1:D:151:SER:HB2	1:D:195:SER:O	2.13	0.49
2:E:132:VAL:HG13	2:E:182:LEU:HD23	1.93	0.49
2:F:110:GLN:HG2	2:F:167:TYR:CE2	2.47	0.49
1:A:104:SER:HB3	1:A:107:ARG:O	2.12	0.49
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.93	0.49
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.47	0.49
1:A:316:LEU:O	1:A:320:ALA:N	2.41	0.49
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.95	0.49
1:A:149:PHE:CB	1:A:530:LYS:NZ	2.75	0.49
2:B:124:GLY:HA2	2:B:127:GLU:CD	2.33	0.49
2:E:102:VAL:O	2:E:106:PHE:HB3	2.12	0.49
2:E:129:ILE:HD11	2:E:173:PHE:CD1	2.47	0.49
2:F:140:GLY:N	2:F:181:LYS:NZ	2.60	0.49
1:A:103:THR:CB	1:A:106:GLY:HA2	2.40	0.49
1:A:549:ARG:HG3	7:A:865:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:VAL:HG23	7:B:436:HOH:O	2.12	0.49
2:C:129:ILE:HA	2:C:132:VAL:HG12	1.94	0.49
2:C:197:LYS:HE2	7:C:481:HOH:O	2.13	0.49
1:D:145:LEU:HD23	1:D:295:PHE:CZ	2.47	0.49
1:D:342:THR:O	1:D:345:LEU:HG	2.13	0.49
1:D:435:LYS:HD3	1:D:438:GLU:N	2.28	0.49
1:D:110:PHE:CE2	1:D:554:SER:HA	2.48	0.49
2:F:98:TRP:HD1	2:F:153:VAL:HG11	1.77	0.49
2:F:92:ARG:HE	2:F:96:ARG:HH22	1.59	0.49
1:A:200:GLN:HA	7:A:963:HOH:O	2.11	0.49
2:C:130:GLU:OE2	7:C:425:HOH:O	2.20	0.49
2:C:32:TYR:HA	7:C:412:HOH:O	2.12	0.49
1:D:498:ASP:OD1	1:D:518:LEU:HD13	2.12	0.49
2:E:15:PHE:HB3	2:E:67:SER:HB3	1.95	0.49
1:A:38:LYS:NZ	1:A:395:TYR:CZ	2.78	0.49
1:A:308:SER:HB3	1:A:424:ARG:HA	1.94	0.49
1:A:551:VAL:HG11	1:A:559:LEU:CD1	2.38	0.49
1:A:8:PHE:CD1	1:A:182:ILE:HG22	2.47	0.49
2:C:24:ARG:HG3	2:C:30:PHE:CE1	2.47	0.49
1:D:223:PHE:CG	1:D:533:GLU:HG2	2.48	0.49
1:D:475:TYR:HE1	1:D:515:ILE:HG21	1.76	0.49
1:D:543:GLY:O	1:D:544:GLN:HG3	2.13	0.49
2:E:139:LEU:O	2:E:141:ASP:N	2.45	0.49
1:A:524:ALA:HB2	1:A:567:VAL:HG11	1.95	0.49
2:C:84:PHE:HB2	2:C:152:TYR:N	2.28	0.49
2:C:44:LEU:HB2	7:C:460:HOH:O	2.13	0.49
1:D:386:GLU:HB3	7:D:771:HOH:O	2.13	0.49
1:D:452:LEU:HD11	1:D:490:LEU:HD23	1.95	0.49
1:D:94:VAL:HG21	1:D:97:ILE:HG22	1.95	0.49
2:F:125:LYS:O	2:F:129:ILE:HG23	2.13	0.49
2:C:174:SER:OG	7:D:701:HOH:O	2.15	0.49
1:D:398:LEU:O	1:D:398:LEU:HD12	2.13	0.49
2:F:145:PHE:CD2	2:F:157:LEU:HD21	2.47	0.49
2:F:37:PHE:HZ	2:F:54:ILE:HG12	1.77	0.49
1:A:238:TRP:CE3	1:A:277:ILE:HD11	2.48	0.48
1:A:387:GLU:O	1:A:388:TYR:HD1	1.96	0.48
1:A:41:SER:HB2	2:B:142:LYS:HG2	1.94	0.48
1:A:468:VAL:HG23	7:A:856:HOH:O	2.13	0.48
2:B:125:LYS:HB3	2:B:173:PHE:CE2	2.48	0.48
1:D:223:PHE:HZ	1:D:536:LEU:HB2	1.78	0.48
1:D:476:ALA:HB1	1:D:478:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:ASP:HB2	2:F:204:LYS:HE2	1.94	0.48
2:F:33:ARG:HH12	2:F:41:SER:HB2	1.77	0.48
1:A:104:SER:O	1:A:107:ARG:HG2	2.13	0.48
1:A:225:HIS:HA	1:A:228:VAL:CG2	2.36	0.48
1:A:309:MET:CE	1:A:536:LEU:HD12	2.43	0.48
2:C:32:TYR:CD1	2:C:34:GLU:OE2	2.66	0.48
1:D:509:SER:HA	1:D:512:CYS:SG	2.53	0.48
2:E:98:TRP:HB3	2:E:153:VAL:HG21	1.94	0.48
2:E:24:ARG:CZ	2:E:30:PHE:HZ	2.25	0.48
2:F:14:MET:HG3	2:F:163:TRP:CH2	2.48	0.48
1:A:238:TRP:HA	1:A:241:ILE:CB	2.38	0.48
1:A:284:LEU:HB2	7:A:812:HOH:O	2.12	0.48
1:A:311:PRO:C	1:A:314:PRO:HD2	2.34	0.48
1:A:402:ARG:HD3	7:A:913:HOH:O	2.12	0.48
1:A:452:LEU:HD11	1:A:490:LEU:HD23	1.96	0.48
2:C:44:LEU:HD22	7:C:517:HOH:O	2.14	0.48
2:C:96:ARG:NH1	7:C:404:HOH:O	1.84	0.48
1:D:311:PRO:O	1:D:314:PRO:HD2	2.13	0.48
1:D:496:CYS:HA	1:D:499:ARG:HH22	1.77	0.48
2:E:71:VAL:HG23	2:E:152:TYR:HE1	1.78	0.48
2:F:153:VAL:HA	7:F:402:HOH:O	2.13	0.48
1:A:317:ARG:O	1:A:321:GLY:N	2.45	0.48
2:C:150:PHE:CD1	2:C:192:LYS:HG3	2.48	0.48
1:D:407:VAL:HG13	1:D:421:PHE:CE1	2.48	0.48
1:D:41:SER:HB3	2:E:144:TYR:HB2	1.94	0.48
1:D:73:LEU:HD12	7:D:808:HOH:O	2.13	0.48
2:B:151:GLY:H	2:B:154:ASP:CG	2.17	0.48
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.42	0.48
2:E:129:ILE:HD11	2:E:173:PHE:CE1	2.49	0.48
2:F:151:GLY:N	2:F:154:ASP:OD2	2.47	0.48
1:A:120:ASN:ND2	7:A:828:HOH:O	2.45	0.48
1:A:202:LEU:O	1:A:205:HIS:N	2.46	0.48
1:A:405:ASP:HB2	1:A:540:SER:HB3	1.94	0.48
1:A:50:LEU:HD13	1:A:61:PHE:CE1	2.49	0.48
2:B:15:PHE:HB3	2:B:67:SER:HB3	1.94	0.48
2:C:33:ARG:NH2	2:C:43:LEU:HD11	2.27	0.48
1:D:192:VAL:HG21	1:D:204:CYS:HB3	1.95	0.48
1:D:242:VAL:HA	1:D:245:ILE:HD11	1.95	0.48
2:F:125:LYS:HA	2:F:128:PHE:CD2	2.48	0.48
2:F:139:LEU:HB3	2:F:181:LYS:HE2	1.96	0.48
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PHE:C	1:A:297:ASN:H	2.17	0.48
1:A:336:TRP:HB2	1:A:358:LEU:HD13	1.95	0.48
1:A:460:ILE:HG13	7:A:708:HOH:O	2.13	0.48
1:A:464:SER:OG	1:A:465:TYR:N	2.45	0.48
1:A:198:VAL:CG2	1:A:524:ALA:HB3	2.43	0.48
1:A:522:VAL:O	1:A:567:VAL:HG22	2.13	0.48
2:C:68:LEU:HB2	2:C:152:TYR:OH	2.14	0.48
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.78	0.48
1:D:236:GLN:NE2	7:D:809:HOH:O	2.47	0.48
1:D:334:GLU:O	1:D:398:LEU:HD21	2.14	0.48
1:D:410:ILE:HG21	1:D:420:LYS:HB3	1.96	0.48
1:D:492:ASP:O	1:D:495:ASN:HB2	2.13	0.48
1:A:97:ILE:CB	1:A:162:VAL:HB	2.43	0.48
1:A:284:LEU:O	1:A:284:LEU:HD12	2.14	0.48
1:A:302:TYR:OH	7:A:754:HOH:O	2.18	0.48
1:A:85:THR:O	1:A:93:PRO:HB3	2.13	0.48
2:B:182:LEU:HA	2:B:185:TRP:CD2	2.49	0.48
2:B:182:LEU:HD13	2:B:185:TRP:CE3	2.49	0.48
2:C:10:TYR:CD2	2:C:12:PRO:HD2	2.49	0.48
2:C:37:PHE:HD1	2:C:40:LYS:HG2	1.78	0.48
1:D:53:ASN:O	1:D:57:PRO:HB3	2.13	0.48
2:F:199:LEU:HA	2:F:200:PRO:HD2	1.72	0.48
1:A:433:ILE:CD1	1:A:552:LYS:NZ	2.77	0.48
1:A:452:LEU:CD2	1:A:481:ILE:HG12	2.39	0.48
1:A:82:ASP:OD2	7:A:760:HOH:O	2.20	0.48
2:C:131:ALA:O	2:C:135:LEU:HB2	2.14	0.48
2:C:98:TRP:HZ2	2:C:157:LEU:HD22	1.78	0.48
1:D:198:VAL:CG2	1:D:524:ALA:HB3	2.43	0.48
2:E:68:LEU:O	2:E:72:GLN:HG3	2.14	0.48
1:A:231:PHE:CZ	1:A:291:ILE:HG12	2.49	0.48
1:A:356:PRO:HG3	7:A:917:HOH:O	2.14	0.48
1:A:474:HIS:HB2	1:A:517:ALA:O	2.13	0.48
2:C:17:MET:HE3	2:C:163:TRP:CH2	2.49	0.48
2:E:75:ASP:HA	7:E:455:HOH:O	2.14	0.48
1:A:217:GLN:N	7:A:745:HOH:O	2.47	0.47
1:A:27:VAL:CG1	1:A:356:PRO:HB3	2.43	0.47
2:C:98:TRP:HH2	2:C:135:LEU:HD11	1.79	0.47
1:D:459:VAL:HG22	1:D:481:ILE:HG22	1.95	0.47
1:D:405:ASP:OD2	1:D:540:SER:HB3	2.13	0.47
1:A:111:ILE:HG23	1:A:396:ALA:O	2.14	0.47
1:A:268:THR:HA	7:A:861:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:O	1:A:30:GLN:HB2	2.13	0.47
1:A:25:HIS:ND1	1:A:380:THR:HG21	2.29	0.47
1:A:41:SER:O	2:B:143:PRO:HG2	2.13	0.47
2:B:102:VAL:O	2:B:107:THR:OG1	2.28	0.47
1:D:374:GLU:OE1	7:D:753:HOH:O	2.20	0.47
1:D:495:ASN:HB3	1:D:499:ARG:HH11	1.77	0.47
2:E:181:LYS:HG3	2:E:181:LYS:H	1.43	0.47
2:F:179:SER:HA	2:F:180:PRO:HD3	1.62	0.47
1:A:92:HIS:CE1	2:B:136:GLU:HA	2.50	0.47
2:B:24:ARG:NH1	2:B:197:LYS:HE3	2.23	0.47
2:C:185:TRP:O	2:C:188:ARG:HB3	2.15	0.47
1:D:126:ARG:NH2	1:D:178:GLY:O	2.47	0.47
1:D:313:VAL:HG13	1:D:314:PRO:HD3	1.96	0.47
1:D:450:LYS:HA	1:D:453:SER:HB3	1.96	0.47
1:D:494:CYS:SG	1:D:495:ASN:N	2.88	0.47
1:A:225:HIS:NE2	1:A:532:GLN:OE1	2.46	0.47
2:B:116:LYS:HD3	2:B:120:GLU:HG2	1.97	0.47
2:B:99:ALA:O	2:B:103:ASP:HB2	2.14	0.47
1:D:157:THR:OG1	1:D:469:SER:HB3	2.14	0.47
2:C:187:LYS:HE3	1:D:493:CYS:HA	1.96	0.47
1:D:97:ILE:HG13	1:D:556:ALA:CB	2.44	0.47
2:F:201:ASP:HB2	2:F:204:LYS:HG3	1.95	0.47
1:A:154:TYR:CE1	1:A:156:SER:HA	2.50	0.47
1:A:305:MET:HE1	1:A:325:LEU:HG	1.96	0.47
2:C:12:PRO:O	2:C:163:TRP:HZ2	1.97	0.47
2:C:153:VAL:HG23	2:C:156:SER:HB2	1.95	0.47
2:C:181:LYS:HA	2:C:184:ALA:HB3	1.97	0.47
2:C:57:LEU:HB3	2:C:64:VAL:HG22	1.96	0.47
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.48	0.47
1:D:450:LYS:HE2	1:D:450:LYS:HB3	1.65	0.47
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.79	0.47
1:A:309:MET:SD	1:A:545:PHE:CZ	3.08	0.47
1:A:91:GLY:O	1:A:92:HIS:C	2.53	0.47
2:C:159:THR:HA	2:C:199:LEU:HD21	1.96	0.47
2:C:17:MET:HE3	2:C:163:TRP:HH2	1.80	0.47
2:C:33:ARG:CZ	2:C:43:LEU:HD21	2.44	0.47
2:F:129:ILE:HA	2:F:132:VAL:HG12	1.97	0.47
2:F:159:THR:HA	2:F:199:LEU:HD21	1.96	0.47
1:A:99:LEU:H	1:A:557:LYS:HG2	1.79	0.47
1:A:95:PRO:HD3	2:B:181:LYS:HZ2	1.79	0.47
1:D:207:LEU:O	1:D:211:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:O	1:D:216:VAL:HA	2.15	0.47
2:F:141:ASP:HA	7:F:464:HOH:O	2.15	0.47
1:A:90:THR:N	7:A:789:HOH:O	2.28	0.47
1:D:172:ASN:HD21	1:D:174:ASN:CG	2.17	0.47
2:F:114:TRP:HD1	2:F:167:TYR:CE1	2.33	0.47
2:F:80:GLU:N	7:F:423:HOH:O	2.48	0.47
1:A:225:HIS:HB3	1:A:312:TYR:CD2	2.50	0.47
1:A:311:PRO:HB2	7:A:1024:HOH:O	2.14	0.47
5:B:301:GSH:OE1	7:B:418:HOH:O	2.21	0.47
2:C:138:GLU:HG3	2:C:145:PHE:HE1	1.80	0.47
2:C:24:ARG:HG3	2:C:30:PHE:CZ	2.49	0.47
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.96	0.47
1:D:147:PHE:HD2	1:D:529:ARG:NH1	2.10	0.47
1:D:78:LYS:HE2	1:D:554:SER:HB3	1.97	0.47
2:E:145:PHE:HB2	2:E:154:ASP:CG	2.36	0.47
2:F:130:GLU:O	2:F:134:ILE:HG22	2.15	0.47
2:F:145:PHE:HB3	2:F:153:VAL:CG1	2.44	0.47
2:F:176:GLU:N	2:F:176:GLU:CD	2.68	0.47
2:F:8:LEU:HD13	2:F:44:LEU:HB2	1.97	0.47
1:A:199:HIS:O	7:A:761:HOH:O	2.20	0.47
1:A:92:HIS:HB2	2:B:141:ASP:OD1	2.15	0.47
2:C:23:LEU:CD2	2:C:28:VAL:HG11	2.43	0.47
2:E:17:MET:SD	2:E:199:LEU:HG	2.55	0.47
2:F:57:LEU:HB3	2:F:64:VAL:HG22	1.97	0.47
2:F:90:TYR:OH	7:F:412:HOH:O	2.09	0.47
1:A:294:LEU:HB3	1:A:295:PHE:CD2	2.50	0.47
1:A:481:ILE:HG22	1:A:483:GLY:H	1.80	0.47
2:C:197:LYS:HE3	2:C:197:LYS:HB3	1.77	0.47
2:C:97:PHE:CE2	2:C:101:PHE:CZ	3.03	0.47
1:D:431:ILE:HD13	1:D:431:ILE:HA	1.68	0.47
1:D:448:ALA:CB	1:D:496:CYS:HB3	2.45	0.47
1:D:526:GLY:O	1:D:530:LYS:HG2	2.15	0.47
1:D:547:MET:HG3	7:D:726:HOH:O	2.15	0.47
2:E:163:TRP:HB3	2:E:167:TYR:CZ	2.49	0.47
2:E:20:ARG:NH1	7:E:429:HOH:O	2.44	0.47
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.49	0.47
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.96	0.46
2:B:202:SER:HB3	7:B:517:HOH:O	2.15	0.46
2:B:65:CYS:O	2:B:66:GLU:HB2	2.14	0.46
2:C:5:PRO:HG2	2:C:28:VAL:CG2	2.45	0.46
1:D:108:PRO:HA	7:D:842:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:PRO:HG2	1:D:76:TYR:HD1	1.80	0.46
2:F:26:LYS:HE2	2:F:75:ASP:HA	1.96	0.46
1:A:223:PHE:HE1	1:A:304:ILE:HD12	1.81	0.46
1:A:441:LEU:HG	1:A:462:PHE:HE2	1.80	0.46
1:D:316:LEU:HD23	1:D:320:ALA:HB2	1.98	0.46
1:D:537:GLY:N	7:D:767:HOH:O	2.37	0.46
2:F:174:SER:O	2:F:174:SER:OG	2.25	0.46
2:F:33:ARG:HH22	2:F:41:SER:HB2	1.81	0.46
1:A:246:LYS:HZ1	1:A:278:ARG:HH22	1.63	0.46
2:C:21:VAL:HG12	2:C:155:ILE:HG12	1.97	0.46
2:C:170:PHE:CD2	2:C:213:ARG:HD2	2.50	0.46
1:D:129:PHE:HZ	1:D:218:TYR:HH	1.63	0.46
1:D:274:ALA:O	1:D:277:ILE:HG13	2.15	0.46
1:D:29:LYS:O	1:D:33:LYS:HG2	2.15	0.46
1:D:82:ASP:HA	7:D:709:HOH:O	2.16	0.46
1:A:97:ILE:H	1:A:162:VAL:HA	1.79	0.46
1:D:152:LYS:HD3	1:D:561:ILE:CG2	2.39	0.46
1:D:219:VAL:HG21	1:D:231:PHE:HZ	1.80	0.46
1:D:238:TRP:O	1:D:242:VAL:HG12	2.16	0.46
1:A:242:VAL:HG11	1:A:278:ARG:HH21	1.80	0.46
2:C:177:SER:HB3	7:C:498:HOH:O	2.16	0.46
1:D:489:VAL:O	1:D:492:ASP:HB2	2.15	0.46
1:D:521:ARG:HG3	1:D:569:SER:HB2	1.97	0.46
1:D:8:PHE:CG	1:D:182:ILE:HG22	2.50	0.46
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.95	0.46
1:A:145:LEU:HB2	7:A:778:HOH:O	2.15	0.46
1:A:262:ALA:O	1:A:265:LYS:HG2	2.16	0.46
1:A:390:VAL:CG2	1:A:540:SER:HA	2.45	0.46
1:A:476:ALA:HA	1:A:519:GLU:O	2.16	0.46
1:A:405:ASP:HB3	1:A:541:SER:CB	2.46	0.46
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.51	0.46
1:A:70:ASP:HB3	1:A:109:LYS:HD2	1.98	0.46
2:B:164:PHE:HZ	2:B:182:LEU:HD11	1.81	0.46
1:A:79:ARG:NH1	2:B:188:ARG:HH12	2.13	0.46
1:D:284:LEU:HD13	1:D:287:TRP:N	2.30	0.46
1:D:313:VAL:CG1	1:D:314:PRO:HD3	2.45	0.46
1:D:390:VAL:HG11	1:D:540:SER:CB	2.45	0.46
2:E:22:ALA:HB1	2:E:74:VAL:HG11	1.96	0.46
2:E:26:LYS:HG3	2:E:82:ASN:ND2	2.30	0.46
1:A:497:LEU:HD11	7:A:940:HOH:O	2.15	0.46
1:A:222:VAL:HG11	1:A:533:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:GLU:HB2	1:D:528:PHE:CD1	2.50	0.46
1:D:74:GLU:O	1:D:78:LYS:HB2	2.16	0.46
1:D:97:ILE:CG1	1:D:162:VAL:HG13	2.45	0.46
2:E:154:ASP:O	2:E:158:ILE:HG13	2.16	0.46
2:F:135:LEU:HD13	2:F:182:LEU:CD1	2.46	0.46
1:A:208:SER:O	1:A:211:LEU:HB2	2.16	0.46
1:A:240:GLU:OE2	1:A:253:ARG:NE	2.43	0.46
1:A:34:GLU:C	1:A:38:LYS:HE3	2.35	0.46
1:A:87:PRO:CB	2:B:143:PRO:HA	2.40	0.46
2:B:169:LYS:HD3	2:B:206:VAL:HG13	1.96	0.46
2:C:51:HIS:CD2	7:C:489:HOH:O	2.68	0.46
2:C:57:LEU:HB3	2:C:64:VAL:CG2	2.46	0.46
2:C:187:LYS:HE3	1:D:492:ASP:C	2.36	0.46
2:E:149:SER:HB3	2:E:150:PHE:H	1.60	0.46
2:F:100:ASP:HA	7:F:431:HOH:O	2.16	0.46
1:A:143:LYS:HG3	1:A:144:ALA:N	2.28	0.46
1:A:210:ILE:HG12	1:A:294:LEU:HD11	1.98	0.46
1:A:143:LYS:O	1:A:216:VAL:HA	2.16	0.46
1:A:326:VAL:HA	7:A:844:HOH:O	2.16	0.46
1:A:305:MET:CE	1:A:347:PRO:HG3	2.43	0.46
1:A:166:THR:HG23	4:A:602:VAL:OXT	2.15	0.46
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.46	0.46
2:E:18:ARG:NE	2:E:156:SER:O	2.41	0.46
2:F:201:ASP:OD2	2:F:204:LYS:HE2	2.16	0.46
1:A:17:PHE:HA	1:A:20:MET:HB3	1.97	0.46
1:A:210:ILE:HG12	1:A:294:LEU:HD21	1.98	0.46
1:A:309:MET:SD	1:A:312:TYR:HE2	2.39	0.46
1:D:135:ASP:HB2	7:D:827:HOH:O	2.16	0.46
1:D:439:ARG:O	1:D:443:LEU:HB2	2.16	0.46
1:D:68:VAL:HG11	1:D:73:LEU:HD23	1.97	0.46
2:E:10:TYR:HA	2:E:34:GLU:OE2	2.16	0.46
2:F:185:TRP:O	2:F:188:ARG:HB3	2.16	0.46
2:F:195:VAL:HG22	7:F:436:HOH:O	2.15	0.46
1:A:154:TYR:H	1:A:560:GLN:HA	1.81	0.45
1:A:77:ILE:HG23	1:A:80:MET:SD	2.55	0.45
2:C:97:PHE:CE2	2:C:101:PHE:HZ	2.34	0.45
1:D:97:ILE:H	1:D:162:VAL:HA	1.80	0.45
1:D:451:ARG:HH11	1:D:454:GLU:CD	2.18	0.45
2:E:128:PHE:HE2	2:E:175:ILE:HG12	1.81	0.45
2:F:126:LYS:O	2:F:129:ILE:HG13	2.15	0.45
2:F:5:PRO:HB3	2:F:59:HIS:NE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:SER:HA	7:A:732:HOH:O	2.16	0.45
2:B:6:ILE:O	2:B:57:LEU:HA	2.17	0.45
2:B:26:LYS:HZ3	2:B:82:ASN:H	1.56	0.45
1:D:410:ILE:HG13	1:D:411:GLY:N	2.30	0.45
2:E:9:ASP:OD1	2:E:16:GLY:HA3	2.16	0.45
2:E:16:GLY:O	2:E:20:ARG:HG3	2.15	0.45
1:A:203:TYR:HE1	1:A:241:ILE:HG13	1.81	0.45
1:A:281:CYS:HB3	1:A:287:TRP:HE1	1.80	0.45
1:A:101:SER:HB3	1:A:535:PHE:CG	2.52	0.45
1:D:231:PHE:CD1	1:D:290:LEU:HD22	2.50	0.45
1:D:315:LYS:HD2	1:D:315:LYS:HA	1.80	0.45
1:D:506:TYR:C	1:D:510:ARG:HE	2.19	0.45
2:E:23:LEU:HD23	2:E:23:LEU:HA	1.80	0.45
2:E:37:PHE:HA	2:E:40:LYS:HG2	1.97	0.45
2:F:11:TRP:O	7:F:404:HOH:O	2.21	0.45
2:F:32:TYR:CD1	2:F:34:GLU:OE2	2.69	0.45
1:A:128:ALA:HB1	7:A:754:HOH:O	2.16	0.45
1:A:151:SER:CB	1:A:194:PHE:HA	2.47	0.45
1:A:330:TYR:HE2	1:A:352:PHE:CD1	2.34	0.45
2:B:26:LYS:HZ1	2:B:82:ASN:H	1.57	0.45
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.77	0.45
1:D:435:LYS:HB3	1:D:436:ASN:C	2.36	0.45
2:F:23:LEU:CD2	2:F:28:VAL:HG11	2.43	0.45
1:A:152:LYS:HG2	1:A:152:LYS:H	1.58	0.45
1:A:121:THR:HG22	1:A:336:TRP:HZ2	1.80	0.45
1:A:505:GLY:C	1:A:507:VAL:H	2.19	0.45
2:C:150:PHE:CE1	2:C:192:LYS:HG3	2.52	0.45
2:C:8:LEU:HD13	2:C:44:LEU:HB2	1.98	0.45
2:E:24:ARG:HD2	2:E:198:SER:OG	2.16	0.45
2:E:205:ILE:HG22	7:E:441:HOH:O	2.15	0.45
2:F:117:LYS:HA	2:F:121:GLN:HB2	1.98	0.45
1:A:276:THR:CG2	1:A:277:ILE:N	2.79	0.45
1:A:79:ARG:NH2	2:B:188:ARG:HH12	2.12	0.45
1:A:87:PRO:HB3	1:A:91:GLY:O	2.17	0.45
1:A:86:SER:HA	1:A:87:PRO:HD2	1.54	0.45
1:A:97:ILE:HG23	1:A:111:ILE:H	1.82	0.45
1:A:91:GLY:HA3	2:B:141:ASP:C	2.36	0.45
1:D:295:PHE:HA	1:D:296:PRO:HD2	1.86	0.45
2:C:180:PRO:HB2	1:D:574:ALA:HB2	1.98	0.45
2:E:107:THR:HG22	2:E:160:PHE:CE2	2.52	0.45
2:F:5:PRO:HB3	2:F:57:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:MET:CB	1:A:312:TYR:CE2	3.00	0.45
1:A:76:TYR:CD2	1:A:89:LEU:HD21	2.52	0.45
2:B:17:MET:HA	2:B:20:ARG:CG	2.47	0.45
2:C:144:TYR:HB3	2:C:154:ASP:CG	2.37	0.45
2:C:188:ARG:HA	2:C:188:ARG:HD3	1.84	0.45
1:D:331:GLY:HA3	1:D:336:TRP:HA	1.97	0.45
1:D:34:GLU:O	1:D:38:LYS:HG2	2.17	0.45
1:D:451:ARG:CZ	1:D:489:VAL:HG12	2.46	0.45
2:F:102:VAL:O	2:F:107:THR:HG23	2.16	0.45
1:A:222:VAL:HG23	7:A:819:HOH:O	2.16	0.45
1:A:363:PHE:HD1	1:A:390:VAL:HA	1.82	0.45
1:A:39:ASN:OD1	1:A:399:TYR:OH	2.35	0.45
1:A:498:ASP:OD2	7:A:763:HOH:O	2.21	0.45
1:D:273:LEU:HG	1:D:273:LEU:H	1.42	0.45
1:D:332:SER:HB3	1:D:538:LEU:HD12	1.98	0.45
1:D:69:THR:OG1	1:D:71:VAL:HG12	2.16	0.45
2:E:92:ARG:HG3	2:E:96:ARG:HH12	1.82	0.45
2:F:12:PRO:O	2:F:163:TRP:CZ2	2.70	0.45
2:F:26:LYS:HD2	2:F:74:VAL:CG1	2.47	0.45
1:A:143:LYS:CE	1:A:187:CYS:HB3	2.47	0.45
1:A:206:LEU:HD11	1:A:241:ILE:HD11	1.98	0.45
1:A:358:LEU:HA	7:A:828:HOH:O	2.16	0.45
1:A:525:LYS:HD3	7:A:833:HOH:O	2.15	0.45
1:A:108:PRO:CB	1:A:555:ASN:HB2	2.43	0.45
2:B:122:GLU:OE2	2:B:125:LYS:NZ	2.42	0.45
2:B:165:GLN:HA	2:B:168:GLU:OE2	2.17	0.45
2:C:24:ARG:NH1	2:C:30:PHE:HZ	2.15	0.45
1:D:26:GLN:O	1:D:30:GLN:HB2	2.17	0.45
1:D:288:TYR:HA	1:D:318:HIS:HD2	1.79	0.45
1:D:430:SER:OG	1:D:431:ILE:N	2.49	0.45
1:D:534:HIS:NE2	1:D:557:LYS:HD3	2.32	0.45
2:E:48:ASN:OD1	2:E:50:ILE:HD11	2.16	0.45
1:A:188:SER:HB3	1:A:192:VAL:HG13	1.98	0.45
1:A:241:ILE:HA	1:A:244:ASP:OD1	2.16	0.45
1:A:310:GLU:HG3	1:A:311:PRO:CD	2.47	0.45
2:B:48:ASN:HD22	2:B:53:LYS:H	1.65	0.45
2:C:163:TRP:HD1	7:C:484:HOH:O	2.00	0.45
2:C:184:ALA:CB	1:D:499:ARG:NH1	2.75	0.45
1:D:55:THR:C	1:D:57:PRO:HD3	2.36	0.45
2:E:108:ASP:O	2:E:112:LYS:HG2	2.17	0.45
1:A:58:GLU:OE2	1:A:360:TYR:OH	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:HA	1:A:409:VAL:HG12	1.98	0.44
2:C:8:LEU:CD2	2:C:33:ARG:NH2	2.80	0.44
1:D:150:SER:OG	1:D:170:TYR:HB2	2.17	0.44
1:D:288:TYR:CE1	1:D:318:HIS:HA	2.52	0.44
2:F:145:PHE:HB3	2:F:153:VAL:HG13	1.98	0.44
1:A:224:ALA:HA	1:A:227:LEU:CD1	2.43	0.44
1:A:25:HIS:CD2	1:A:25:HIS:H	2.33	0.44
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.52	0.44
2:C:153:VAL:HG21	7:C:406:HOH:O	2.17	0.44
1:D:133:ASN:OD1	1:D:138:ILE:HG12	2.16	0.44
1:D:150:SER:HB2	1:D:167:THR:CA	2.40	0.44
1:D:188:SER:HB3	1:D:192:VAL:CG1	2.47	0.44
1:D:206:LEU:HD13	1:D:234:PHE:HD1	1.82	0.44
2:F:125:LYS:HB2	7:F:470:HOH:O	2.16	0.44
2:F:173:PHE:HB3	2:F:174:SER:H	1.47	0.44
1:A:176:LYS:O	1:A:180:LYS:HB2	2.18	0.44
2:B:17:MET:HG3	2:B:20:ARG:NH1	2.33	0.44
2:C:128:PHE:O	2:C:132:VAL:HG12	2.17	0.44
1:D:219:VAL:HB	1:D:295:PHE:CE1	2.52	0.44
1:D:338:ALA:HA	1:D:354:VAL:HA	1.99	0.44
1:D:485:THR:OG1	1:D:486:ASN:N	2.50	0.44
1:A:147:PHE:HE1	1:A:206:LEU:HB3	1.83	0.44
1:A:217:GLN:CG	1:A:218:TYR:CD2	3.00	0.44
1:A:232:ARG:HA	1:A:235:GLU:CG	2.48	0.44
1:A:351:THR:N	7:A:787:HOH:O	2.50	0.44
1:A:413:TYR:N	1:A:416:THR:O	2.47	0.44
1:A:498:ASP:OD1	1:A:518:LEU:HD12	2.17	0.44
2:B:23:LEU:HD22	2:B:28:VAL:HG11	1.99	0.44
2:C:187:LYS:HE3	1:D:492:ASP:O	2.18	0.44
2:C:48:ASN:ND2	7:C:423:HOH:O	2.12	0.44
2:C:68:LEU:HD23	2:C:103:ASP:OD2	2.17	0.44
1:D:31:THR:O	1:D:35:ILE:HG13	2.18	0.44
1:D:329:ASP:OD1	1:D:329:ASP:N	2.50	0.44
1:D:449:ALA:HB1	1:D:459:VAL:HG23	1.98	0.44
2:C:204:LYS:HE2	1:D:456:LYS:HZ3	1.81	0.44
1:D:549:ARG:HD3	1:D:549:ARG:HA	1.75	0.44
1:D:92:HIS:ND1	2:E:181:LYS:O	2.51	0.44
2:E:121:GLN:HG3	7:E:410:HOH:O	2.17	0.44
2:E:40:LYS:HZ3	2:E:52:LYS:HB2	1.76	0.44
2:E:92:ARG:CZ	2:E:96:ARG:NH1	2.80	0.44
2:F:10:TYR:CD2	2:F:12:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:141:ASP:N	2:F:141:ASP:OD1	2.50	0.44
1:A:97:ILE:CG2	1:A:111:ILE:H	2.29	0.44
1:A:552:LYS:HA	1:A:552:LYS:HD2	1.53	0.44
1:A:97:ILE:O	1:A:556:ALA:HB1	2.18	0.44
1:A:55:THR:C	1:A:57:PRO:HD3	2.37	0.44
2:B:7:LEU:HD23	2:B:32:TYR:HD1	1.82	0.44
1:D:122:LEU:HD12	1:D:123:GLN:N	2.33	0.44
1:D:143:LYS:NZ	1:D:187:CYS:HA	2.33	0.44
1:D:328:HIS:CG	1:D:329:ASP:H	2.36	0.44
1:D:38:LYS:HD2	1:D:38:LYS:HA	1.84	0.44
1:D:95:PRO:HD3	2:E:181:LYS:HE3	1.99	0.44
1:D:99:LEU:HD13	1:D:555:ASN:OD1	2.18	0.44
2:E:98:TRP:CZ2	2:E:135:LEU:HA	2.52	0.44
2:E:175:ILE:HB	2:E:183:ILE:HD11	1.99	0.44
1:A:479:TRP:O	1:A:523:VAL:HG12	2.17	0.44
1:A:92:HIS:HB3	2:B:181:LYS:HZ1	1.83	0.44
2:B:62:LYS:NZ	2:C:94:GLN:HG3	2.32	0.44
1:D:97:ILE:HG12	1:D:162:VAL:HG13	1.99	0.44
1:D:194:PHE:O	7:D:757:HOH:O	2.21	0.44
2:E:128:PHE:HD1	7:E:411:HOH:O	2.00	0.44
2:E:92:ARG:NH1	2:E:96:ARG:NH1	2.66	0.44
1:A:233:THR:CG2	1:A:525:LYS:NZ	2.81	0.44
1:A:527:THR:HB	7:A:749:HOH:O	2.16	0.44
1:A:70:ASP:OD2	1:A:104:SER:HA	2.18	0.44
2:B:101:PHE:HA	7:B:474:HOH:O	2.17	0.44
2:B:186:ALA:O	2:B:190:MET:HG2	2.17	0.44
2:C:188:ARG:NH1	1:D:499:ARG:C	2.61	0.44
1:D:434:ASP:O	1:D:435:LYS:HG3	2.18	0.44
1:D:84:ASP:C	1:D:86:SER:H	2.21	0.44
2:F:10:TYR:HB3	2:F:13:SER:HB2	1.99	0.44
1:A:112:PRO:HD2	1:A:396:ALA:O	2.17	0.44
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.78	0.44
1:A:13:VAL:HG11	7:A:771:HOH:O	2.17	0.44
1:A:305:MET:SD	1:A:325:LEU:HG	2.58	0.44
1:A:38:LYS:NZ	1:A:395:TYR:CE1	2.78	0.44
1:A:434:ASP:HB2	1:A:550:CYS:HB3	2.00	0.44
2:B:139:LEU:HD23	2:B:142:LYS:H	1.81	0.44
2:B:151:GLY:O	2:B:155:ILE:HG23	2.18	0.44
2:C:9:ASP:HB2	2:C:20:ARG:NH2	2.33	0.44
1:D:125:PHE:CE1	1:D:129:PHE:HE1	2.36	0.44
1:D:130:ALA:O	7:D:754:HOH:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:HA	1:D:160:VAL:HG11	1.98	0.44
1:D:203:TYR:OH	1:D:254:ILE:HG23	2.17	0.44
1:D:23:ASN:O	1:D:27:VAL:HG23	2.18	0.44
1:D:270:ASN:HA	1:D:271:PRO:HD2	1.75	0.44
1:D:359:GLY:HA3	1:D:361:PHE:HE1	1.83	0.44
1:D:455:GLU:OE1	1:D:485:THR:HB	2.17	0.44
2:E:148:ASP:N	2:E:148:ASP:OD1	2.51	0.44
2:E:88:ASP:HB2	2:E:90:TYR:CE1	2.53	0.44
2:E:95:ALA:O	2:E:99:ALA:N	2.47	0.44
1:A:190:ASP:HA	1:A:193:ILE:HD12	2.00	0.44
1:A:189:PRO:O	1:A:192:VAL:HG12	2.18	0.44
1:A:212:PHE:O	1:A:216:VAL:HG23	2.17	0.44
1:A:23:ASN:O	1:A:27:VAL:HG12	2.17	0.44
1:A:281:CYS:O	1:A:287:TRP:CZ2	2.71	0.44
1:A:409:VAL:HG13	7:A:794:HOH:O	2.17	0.44
1:A:92:HIS:CG	2:B:181:LYS:HE3	2.53	0.44
2:B:26:LYS:NZ	2:B:82:ASN:N	2.49	0.44
2:C:142:LYS:HG2	2:C:144:TYR:H	1.83	0.44
1:D:10:MET:HE3	1:D:133:ASN:HD22	1.83	0.44
1:D:142:GLY:O	1:D:185:PRO:HD2	2.18	0.44
1:D:496:CYS:N	1:D:499:ARG:HH12	2.16	0.44
1:D:108:PRO:HB3	1:D:555:ASN:N	2.32	0.44
1:D:80:MET:HE3	1:D:94:VAL:HG22	2.00	0.44
2:F:188:ARG:HD3	2:F:188:ARG:HA	1.56	0.44
2:F:26:LYS:HD2	2:F:74:VAL:HG13	2.00	0.44
2:F:54:ILE:HB	2:F:55:PRO:HA	2.00	0.44
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.76	0.43
1:A:202:LEU:HA	1:A:205:HIS:HB2	2.00	0.43
1:A:222:VAL:HG22	3:A:601:JAA:C07	2.48	0.43
1:A:231:PHE:HB2	1:A:319:TYR:CE2	2.53	0.43
1:A:309:MET:SD	1:A:312:TYR:CE2	3.11	0.43
1:A:99:LEU:HD22	1:A:555:ASN:OD1	2.18	0.43
1:A:114:THR:OG1	2:B:141:ASP:OD2	2.31	0.43
2:B:51:HIS:HD2	2:B:53:LYS:HE2	1.76	0.43
1:D:534:HIS:CE1	1:D:557:LYS:HD3	2.53	0.43
1:D:7:THR:HG21	7:D:990:HOH:O	2.18	0.43
1:A:109:LYS:HE3	1:A:109:LYS:HB2	1.67	0.43
1:A:229:HIS:O	1:A:233:THR:N	2.47	0.43
1:A:572:SER:HA	7:A:703:HOH:O	2.18	0.43
2:C:195:VAL:HG11	7:C:432:HOH:O	2.18	0.43
2:C:71:VAL:O	2:C:74:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:THR:HG22	1:D:166:THR:H	1.83	0.43
1:D:446:GLU:HG2	7:D:1050:HOH:O	2.19	0.43
2:E:106:PHE:O	7:E:411:HOH:O	2.21	0.43
2:E:68:LEU:HD13	2:E:99:ALA:HB1	2.00	0.43
2:E:82:ASN:N	2:E:82:ASN:OD1	2.51	0.43
2:F:12:PRO:O	2:F:163:TRP:HZ2	2.02	0.43
1:A:143:LYS:HE2	1:A:216:VAL:CG2	2.49	0.43
1:A:309:MET:C	1:A:311:PRO:HD2	2.38	0.43
1:A:99:LEU:HB3	1:A:557:LYS:CB	2.47	0.43
2:B:11:TRP:HZ2	2:B:208:TYR:CE1	2.36	0.43
2:C:99:ALA:HA	7:C:406:HOH:O	2.18	0.43
1:D:132:ARG:O	1:D:136:PHE:N	2.38	0.43
1:D:27:VAL:HG11	1:D:356:PRO:HG2	2.00	0.43
1:D:363:PHE:CE1	1:D:390:VAL:HG23	2.52	0.43
1:D:387:GLU:HG3	1:D:408:LYS:HB2	2.01	0.43
1:D:408:LYS:HG3	1:D:409:VAL:N	2.32	0.43
2:E:135:LEU:HD22	2:E:182:LEU:HD21	1.99	0.43
2:E:15:PHE:HB3	2:E:67:SER:CB	2.48	0.43
1:A:219:VAL:HG13	1:A:301:VAL:HG13	2.00	0.43
1:A:288:TYR:CZ	1:A:321:GLY:HA2	2.53	0.43
1:A:41:SER:OG	2:B:142:LYS:HE3	2.18	0.43
1:A:475:TYR:HB2	1:A:518:LEU:HD23	2.00	0.43
1:A:494:CYS:SG	1:A:495:ASN:N	2.91	0.43
1:A:102:GLY:N	1:A:546:LYS:O	2.48	0.43
2:B:121:GLN:O	2:B:125:LYS:HG3	2.19	0.43
1:D:67:LEU:HB3	7:D:856:HOH:O	2.18	0.43
2:E:126:LYS:O	2:E:130:GLU:HG3	2.18	0.43
1:D:91:GLY:HA3	2:E:142:LYS:HA	1.99	0.43
2:E:201:ASP:HB3	2:E:203:GLU:HG2	2.00	0.43
2:E:37:PHE:HE1	2:E:40:LYS:HZ2	1.67	0.43
2:F:98:TRP:CD1	2:F:153:VAL:HG21	2.53	0.43
2:F:181:LYS:O	2:F:185:TRP:N	2.40	0.43
1:A:195:SER:OG	1:A:259:VAL:HG21	2.17	0.43
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.62	0.43
1:A:423:CYS:HA	7:A:747:HOH:O	2.18	0.43
1:A:434:ASP:O	1:A:435:LYS:HG3	2.18	0.43
1:A:537:GLY:HA3	3:A:601:JAA:O02	2.19	0.43
2:B:65:CYS:SG	2:C:97:PHE:CZ	3.06	0.43
1:D:110:PHE:CD1	1:D:556:ALA:HB2	2.53	0.43
1:D:198:VAL:HG22	1:D:565:ASN:ND2	2.24	0.43
1:D:435:LYS:HA	1:D:436:ASN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:ASP:HA	2:E:89:PRO:HD3	1.86	0.43
2:F:10:TYR:CG	2:F:12:PRO:HD2	2.53	0.43
1:A:151:SER:CA	1:A:194:PHE:HA	2.49	0.43
1:A:250:LEU:HD21	1:A:260:ARG:HG2	2.00	0.43
1:A:274:ALA:O	1:A:278:ARG:NE	2.52	0.43
1:A:478:PHE:HZ	1:A:562:LEU:HA	1.79	0.43
2:B:112:LYS:HB2	7:B:414:HOH:O	2.18	0.43
2:B:93:ALA:HB1	2:C:73:TYR:CE1	2.54	0.43
1:D:413:TYR:O	1:D:416:THR:HG22	2.18	0.43
1:D:92:HIS:H	2:E:141:ASP:C	2.22	0.43
2:E:206:VAL:HA	7:E:441:HOH:O	2.18	0.43
2:E:169:LYS:NZ	2:E:206:VAL:HG11	2.33	0.43
1:A:337:ILE:HG13	7:A:764:HOH:O	2.18	0.43
1:A:475:TYR:HB2	1:A:518:LEU:CD2	2.48	0.43
1:A:527:THR:HG22	1:A:528:PHE:CD1	2.53	0.43
2:C:149:SER:HB3	2:C:150:PHE:H	1.71	0.43
1:D:444:SER:HA	1:D:500:ALA:CB	2.48	0.43
1:D:521:ARG:HH11	1:D:521:ARG:HG3	1.83	0.43
1:D:77:ILE:HG12	1:D:110:PHE:O	2.19	0.43
2:E:16:GLY:O	2:E:20:ARG:NE	2.50	0.43
2:E:85:PHE:CD1	2:E:85:PHE:N	2.87	0.43
2:F:194:SER:O	2:F:198:SER:OG	2.20	0.43
1:A:116:GLU:OE2	1:A:395:TYR:CE1	2.72	0.43
1:A:91:GLY:HA3	2:B:142:LYS:C	2.39	0.43
2:C:190:MET:HB3	1:D:450:LYS:HG3	2.00	0.43
2:C:54:ILE:N	7:C:428:HOH:O	2.50	0.43
2:C:62:LYS:HA	2:C:63:PRO:HD2	1.87	0.43
1:D:39:ASN:HA	2:E:142:LYS:CG	2.49	0.43
2:E:109:ALA:HB3	7:E:411:HOH:O	2.18	0.43
1:D:87:PRO:CB	2:E:143:PRO:HA	2.45	0.43
2:E:164:PHE:CD2	2:E:183:ILE:HG12	2.53	0.43
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.69	0.43
2:F:8:LEU:HD22	2:F:33:ARG:NH2	2.26	0.43
2:F:98:TRP:O	2:F:98:TRP:CE3	2.72	0.43
1:A:96:ALA:HB3	1:A:113:PHE:CD2	2.53	0.43
1:A:135:ASP:HB2	7:A:929:HOH:O	2.17	0.43
1:A:222:VAL:HG13	3:A:601:JAA:C06	2.48	0.43
1:A:25:HIS:HD2	7:A:889:HOH:O	2.02	0.43
1:A:429:LEU:HD12	1:A:429:LEU:HA	1.79	0.43
1:A:555:ASN:O	1:A:559:LEU:HD22	2.19	0.43
1:D:96:ALA:O	1:D:113:PHE:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:LEU:O	1:D:320:ALA:N	2.50	0.43
1:D:36:LEU:HD13	1:D:61:PHE:CE2	2.54	0.43
1:D:424:ARG:O	1:D:543:GLY:HA2	2.18	0.43
2:E:24:ARG:NH1	2:E:198:SER:OG	2.51	0.43
2:E:48:ASN:HB3	2:E:52:LYS:HA	2.01	0.43
2:E:62:LYS:HA	2:E:63:PRO:HD2	1.79	0.43
1:A:213:ARG:HG3	1:A:214:ASP:N	2.34	0.43
1:A:56:ASP:HB2	1:A:59:GLU:HB2	2.01	0.43
1:D:362:GLU:HG3	1:D:400:ARG:HH22	1.82	0.43
1:D:575:PHE:O	7:D:756:HOH:O	2.21	0.43
1:D:124:LEU:HB3	3:D:601:JAA:C15	2.49	0.43
2:E:161:SER:HA	2:E:164:PHE:CG	2.54	0.43
2:E:26:LYS:HB2	2:E:26:LYS:HE2	1.91	0.43
2:F:33:ARG:HH22	2:F:41:SER:CB	2.31	0.43
1:A:291:ILE:HD11	1:A:316:LEU:HD11	2.01	0.42
1:A:303:GLY:O	1:A:327:SER:HA	2.19	0.42
1:A:33:LYS:HA	1:A:36:LEU:HD23	2.00	0.42
1:A:66:PRO:HD3	7:A:723:HOH:O	2.19	0.42
1:A:70:ASP:OD1	1:A:71:VAL:N	2.52	0.42
1:A:97:ILE:HA	1:A:111:ILE:O	2.19	0.42
2:C:104:LYS:NZ	7:C:439:HOH:O	2.39	0.42
2:C:114:TRP:HA	2:C:170:PHE:CD2	2.49	0.42
1:D:402:ARG:NH2	7:D:759:HOH:O	2.21	0.42
1:D:407:VAL:HG21	7:D:920:HOH:O	2.19	0.42
1:A:274:ALA:CB	1:A:278:ARG:CZ	2.96	0.42
1:A:238:TRP:CZ2	1:A:281:CYS:HB2	2.54	0.42
1:A:355:ILE:HA	1:A:356:PRO:HD3	1.49	0.42
1:A:389:GLU:OE2	1:A:402:ARG:HG2	2.19	0.42
2:B:18:ARG:HG2	2:B:159:THR:HG21	2.00	0.42
2:B:86:PRO:HD3	2:B:146:GLY:O	2.20	0.42
2:C:4:LEU:HA	2:C:5:PRO:HD3	1.65	0.42
1:D:229:HIS:O	1:D:233:THR:HG23	2.20	0.42
1:D:224:ALA:HA	1:D:316:LEU:HD12	2.00	0.42
1:D:32:LEU:O	1:D:35:ILE:HB	2.20	0.42
1:D:32:LEU:HD13	1:D:360:TYR:CD2	2.54	0.42
1:D:365:PRO:HD2	1:D:374:GLU:HG2	2.01	0.42
1:D:163:GLY:HA2	1:D:560:GLN:HB2	2.02	0.42
2:F:145:PHE:CE2	2:F:157:LEU:HD21	2.53	0.42
2:F:169:LYS:HD3	2:F:206:VAL:HG13	2.01	0.42
1:A:145:LEU:HD13	1:A:209:GLY:CA	2.43	0.42
1:A:154:TYR:CZ	1:A:559:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:HB2	2:B:188:ARG:HB2	2.02	0.42
2:B:15:PHE:O	2:B:18:ARG:HB2	2.19	0.42
2:B:194:SER:O	2:B:198:SER:HB2	2.19	0.42
2:C:17:MET:HE2	2:C:200:PRO:HD2	2.01	0.42
1:D:168:ASN:HB2	7:D:770:HOH:O	2.19	0.42
1:D:28:GLN:HA	7:D:734:HOH:O	2.19	0.42
1:D:452:LEU:HD13	1:D:493:CYS:SG	2.59	0.42
2:F:187:LYS:HG2	2:F:187:LYS:O	2.18	0.42
1:A:248:GLY:O	1:A:267:LEU:HB3	2.20	0.42
2:B:27:GLY:HA2	7:B:503:HOH:O	2.19	0.42
1:D:196:PRO:O	1:D:565:ASN:HA	2.19	0.42
1:D:494:CYS:HB2	1:D:520:LEU:HB3	2.01	0.42
2:F:26:LYS:CG	2:F:81:LYS:HZ3	2.30	0.42
1:A:167:THR:HG21	1:A:560:GLN:CG	2.50	0.42
1:A:244:ASP:HB2	1:A:251:SER:H	1.85	0.42
1:A:504:ALA:O	1:A:507:VAL:HB	2.19	0.42
1:A:524:ALA:HB2	1:A:567:VAL:CG1	2.50	0.42
1:A:532:GLN:NE2	7:A:777:HOH:O	2.25	0.42
2:B:51:HIS:HB2	2:B:53:LYS:HG2	2.01	0.42
1:D:111:ILE:HA	1:D:112:PRO:HD3	1.90	0.42
1:D:184:SER:HB3	7:D:733:HOH:O	2.18	0.42
1:D:253:ARG:NH2	7:D:819:HOH:O	2.52	0.42
1:D:44:TYR:OH	1:D:68:VAL:HG22	2.18	0.42
1:D:501:PHE:CE2	1:D:518:LEU:HD21	2.54	0.42
2:E:150:PHE:CD2	2:E:192:LYS:HD2	2.54	0.42
2:E:6:ILE:HG23	2:E:31:GLU:HB3	2.02	0.42
1:A:213:ARG:HA	1:A:216:VAL:HG23	2.01	0.42
1:A:32:LEU:HD22	1:A:360:TYR:CD2	2.54	0.42
1:A:198:VAL:HG22	1:A:524:ALA:HB3	2.00	0.42
1:A:95:PRO:HD3	2:B:181:LYS:NZ	2.34	0.42
2:B:139:LEU:HD21	2:B:142:LYS:H	1.84	0.42
2:B:197:LYS:HE3	2:B:197:LYS:HB2	1.73	0.42
1:D:305:MET:HB3	1:D:347:PRO:HB3	2.02	0.42
2:F:216:ASN:HA	7:F:459:HOH:O	2.19	0.42
2:F:57:LEU:HB3	2:F:64:VAL:CG2	2.50	0.42
1:A:152:LYS:HD3	1:A:565:ASN:ND2	2.34	0.42
1:A:143:LYS:HZ1	1:A:212:PHE:H	1.67	0.42
1:A:351:THR:HG21	1:A:410:ILE:CG1	2.46	0.42
1:A:27:VAL:HG11	1:A:356:PRO:HB3	2.01	0.42
1:A:92:HIS:HE1	2:B:136:GLU:HA	1.84	0.42
2:B:149:SER:HB2	2:B:150:PHE:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:CYS:O	2:B:69:ASN:HB3	2.19	0.42
1:D:534:HIS:HD2	1:D:535:PHE:CD1	2.38	0.42
1:D:534:HIS:CD2	1:D:535:PHE:CD1	3.08	0.42
1:D:97:ILE:HG13	1:D:556:ALA:HB1	2.01	0.42
1:D:98:SER:C	1:D:556:ALA:HB3	2.40	0.42
1:D:41:SER:HA	2:E:147:GLY:O	2.20	0.42
2:F:140:GLY:N	2:F:181:LYS:HZ1	2.18	0.42
2:F:26:LYS:HE3	2:F:78:TRP:O	2.19	0.42
1:A:222:VAL:HG12	1:A:223:PHE:CD1	2.55	0.42
1:A:238:TRP:CZ3	1:A:277:ILE:HG12	2.55	0.42
1:A:509:SER:HB3	1:A:515:ILE:HG12	2.02	0.42
1:D:384:ILE:H	1:D:384:ILE:HG13	1.60	0.42
1:D:551:VAL:HG23	1:D:555:ASN:H	1.84	0.42
2:E:102:VAL:HA	2:E:106:PHE:HB2	2.01	0.42
2:F:102:VAL:O	2:F:106:PHE:HB3	2.20	0.42
1:A:117:LEU:O	1:A:121:THR:HG23	2.19	0.42
1:A:237:VAL:HB	7:A:757:HOH:O	2.20	0.42
1:A:246:LYS:NZ	1:A:278:ARG:NH2	2.63	0.42
1:A:390:VAL:HG21	1:A:540:SER:HA	2.02	0.42
1:A:566:VAL:HG13	1:A:568:SER:C	2.41	0.42
1:A:79:ARG:HH11	1:A:88:ILE:CD1	2.32	0.42
1:A:98:SER:C	1:A:556:ALA:HB3	2.40	0.42
2:B:21:VAL:O	2:B:25:GLU:HB2	2.19	0.42
2:B:50:ILE:HG13	2:C:134:ILE:CD1	2.47	0.42
2:B:8:LEU:HD21	2:B:43:LEU:HD13	2.01	0.42
2:C:126:LYS:O	2:C:129:ILE:HG13	2.20	0.42
1:D:233:THR:HG22	7:D:748:HOH:O	2.19	0.42
1:D:124:LEU:HD21	1:D:329:ASP:HB2	2.02	0.42
1:D:408:LYS:O	1:D:419:LEU:HA	2.20	0.42
1:D:477:ILE:O	1:D:520:LEU:HD12	2.20	0.42
1:D:101:SER:N	1:D:535:PHE:CZ	2.87	0.42
2:E:7:LEU:CD1	2:E:9:ASP:HB2	2.49	0.42
5:F:301:GSH:N1	7:F:425:HOH:O	2.25	0.42
1:A:98:SER:OG	1:A:111:ILE:HB	2.20	0.42
1:A:198:VAL:O	1:A:202:LEU:HD12	2.20	0.42
1:A:217:GLN:HG3	1:A:218:TYR:HD2	1.84	0.42
1:A:242:VAL:HG11	1:A:278:ARG:NH2	2.34	0.42
1:A:305:MET:HG3	7:A:715:HOH:O	2.20	0.42
1:A:310:GLU:N	1:A:311:PRO:HD2	2.34	0.42
1:A:491:GLN:NE2	1:A:570:TYR:CD2	2.88	0.42
1:A:94:VAL:HG11	1:A:112:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PRO:HB3	1:D:555:ASN:CB	2.50	0.42
1:D:10:MET:HE1	1:D:133:ASN:HB3	2.00	0.42
1:D:277:ILE:HD12	1:D:278:ARG:N	2.35	0.42
1:D:364:LEU:HB2	1:D:402:ARG:HH22	1.84	0.42
1:D:523:VAL:HG23	7:D:785:HOH:O	2.20	0.42
2:E:33:ARG:NH2	2:E:43:LEU:HD13	2.35	0.42
2:F:21:VAL:HG12	2:F:155:ILE:HG12	2.01	0.42
1:A:284:LEU:C	1:A:284:LEU:HD12	2.41	0.41
1:A:392:ILE:HG13	1:A:401:TYR:HB3	2.02	0.41
1:A:532:GLN:O	1:A:535:PHE:N	2.49	0.41
2:B:110:GLN:O	2:B:113:VAL:HB	2.20	0.41
2:C:26:LYS:HE3	2:C:78:TRP:O	2.19	0.41
2:C:8:LEU:HG	2:C:56:VAL:HB	2.02	0.41
1:D:118:MET:HG2	1:D:172:ASN:ND2	2.35	0.41
1:D:254:ILE:N	1:D:254:ILE:HD13	2.35	0.41
1:D:403:LEU:HD23	1:D:403:LEU:HA	1.51	0.41
1:D:465:TYR:HD1	1:D:551:VAL:HG13	1.84	0.41
1:D:485:THR:OG1	7:D:755:HOH:O	2.21	0.41
1:D:95:PRO:O	1:D:161:PRO:HB2	2.20	0.41
1:A:224:ALA:HB3	1:A:312:TYR:CD1	2.54	0.41
1:A:31:THR:OG1	1:A:357:ASN:HA	2.20	0.41
1:A:510:ARG:HB3	1:A:575:PHE:CE2	2.55	0.41
2:B:193:GLU:HB3	2:B:197:LYS:HE2	2.01	0.41
2:B:34:GLU:HA	7:B:465:HOH:O	2.20	0.41
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.83	0.41
2:C:36:ASP:O	2:C:39:ASN:N	2.47	0.41
2:C:72:GLN:OE1	7:C:426:HOH:O	2.22	0.41
2:C:81:LYS:HG3	2:C:82:ASN:H	1.85	0.41
1:D:156:SER:OG	7:D:709:HOH:O	2.04	0.41
1:D:169:VAL:O	1:D:175:PHE:HB2	2.20	0.41
1:A:105:GLN:N	7:A:829:HOH:O	2.46	0.41
1:A:107:ARG:NH2	7:A:746:HOH:O	2.53	0.41
1:A:188:SER:HB3	1:A:192:VAL:CG1	2.51	0.41
1:A:238:TRP:HA	1:A:241:ILE:CG1	2.50	0.41
1:A:314:PRO:CB	1:A:317:ARG:HH12	2.33	0.41
1:A:471:ASP:HA	1:A:472:PRO:HA	1.80	0.41
2:B:126:LYS:O	2:B:130:GLU:HG2	2.21	0.41
2:C:8:LEU:HD23	2:C:8:LEU:N	2.35	0.41
1:D:250:LEU:HB2	1:D:254:ILE:HG13	2.02	0.41
1:D:90:THR:OG1	1:D:397:GLY:HA2	2.20	0.41
1:D:446:GLU:HG3	7:D:824:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:SER:HB2	7:D:786:HOH:O	2.20	0.41
2:C:184:ALA:CB	1:D:499:ARG:CZ	2.85	0.41
2:F:110:GLN:O	2:F:113:VAL:HG12	2.20	0.41
1:A:145:LEU:HD21	1:A:147:PHE:CZ	2.55	0.41
1:A:196:PRO:HG2	1:A:256:VAL:HG11	2.01	0.41
1:A:282:MET:HG3	1:A:283:SER:N	2.36	0.41
1:A:310:GLU:O	1:A:314:PRO:HD3	2.21	0.41
1:A:384:ILE:HA	1:A:409:VAL:CG1	2.49	0.41
1:A:80:MET:HE1	1:A:94:VAL:HG22	2.02	0.41
2:C:110:GLN:O	2:C:113:VAL:HG12	2.20	0.41
1:D:425:ARG:HH12	1:D:546:LYS:HE3	1.84	0.41
2:B:53:LYS:HD3	5:B:301:GSH:HB13	2.02	0.41
2:B:8:LEU:HD22	2:B:35:GLU:OE2	2.19	0.41
2:C:9:ASP:HB2	2:C:20:ARG:HH21	1.85	0.41
1:D:192:VAL:HA	1:D:195:SER:HB2	2.01	0.41
1:D:445:VAL:HG13	1:D:479:TRP:NE1	2.34	0.41
1:D:521:ARG:HG3	1:D:521:ARG:NH1	2.35	0.41
1:D:480:GLU:HB2	1:D:528:PHE:HD1	1.85	0.41
1:D:94:VAL:HG21	1:D:97:ILE:CG2	2.51	0.41
2:E:86:PRO:HD2	2:E:92:ARG:HA	2.02	0.41
1:A:154:TYR:HE2	1:A:162:VAL:HG22	1.85	0.41
1:A:225:HIS:HB3	1:A:312:TYR:CZ	2.53	0.41
1:A:35:ILE:O	1:A:39:ASN:HB2	2.20	0.41
2:B:70:VAL:O	2:B:74:VAL:HG23	2.20	0.41
2:C:57:LEU:O	2:C:64:VAL:HG13	2.21	0.41
1:D:345:LEU:HD13	1:D:350:ALA:HA	2.02	0.41
1:D:471:ASP:HA	1:D:472:PRO:HA	1.88	0.41
1:D:99:LEU:CB	1:D:556:ALA:H	2.34	0.41
1:A:203:TYR:CD2	1:A:254:ILE:HD11	2.53	0.41
1:A:357:ASN:ND2	7:A:843:HOH:O	2.54	0.41
1:A:452:LEU:O	1:A:457:ILE:HB	2.21	0.41
1:A:527:THR:HG23	1:A:561:ILE:CG2	2.44	0.41
2:C:187:LYS:HB2	2:C:187:LYS:HZ3	1.84	0.41
1:D:19:GLU:O	1:D:23:ASN:HB2	2.21	0.41
1:D:247:ASP:HA	7:D:992:HOH:O	2.19	0.41
1:D:323:LEU:HA	1:D:324:PRO:HD3	1.95	0.41
1:D:425:ARG:HB2	1:D:427:LEU:HB2	2.03	0.41
1:D:68:VAL:HG11	1:D:73:LEU:CD2	2.51	0.41
1:A:117:LEU:O	1:A:120:ASN:HB2	2.21	0.41
1:A:87:PRO:HD3	1:A:93:PRO:HD3	2.03	0.41
2:C:64:VAL:HG12	7:C:447:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ARG:NH1	2:C:76:GLU:OE2	2.54	0.41
1:D:262:ALA:HB3	7:D:783:HOH:O	2.20	0.41
1:D:295:PHE:N	1:D:295:PHE:CD2	2.88	0.41
1:D:440:ASP:OD1	1:D:501:PHE:HA	2.20	0.41
1:D:91:GLY:HA3	2:E:142:LYS:CA	2.51	0.41
2:F:115:GLY:O	2:F:116:LYS:HD2	2.21	0.41
1:A:77:ILE:HG22	1:A:110:PHE:HB3	2.02	0.41
1:A:223:PHE:HB3	1:A:312:TYR:OH	2.21	0.41
1:A:447:SER:O	1:A:450:LYS:HG2	2.21	0.41
1:A:507:VAL:HG13	1:A:511:LYS:HD2	2.03	0.41
1:A:92:HIS:NE2	2:B:139:LEU:HB3	2.35	0.41
1:A:46:GLN:OE1	2:B:149:SER:HB3	2.20	0.41
2:C:142:LYS:HA	2:C:143:PRO:HD3	1.97	0.41
2:C:151:GLY:N	2:C:154:ASP:OD2	2.54	0.41
2:C:26:LYS:HD2	2:C:74:VAL:CG1	2.47	0.41
2:C:64:VAL:HB	2:C:73:TYR:HD2	1.82	0.41
1:D:187:CYS:HB2	1:D:208:SER:C	2.41	0.41
1:D:222:VAL:O	1:D:304:ILE:N	2.35	0.41
1:D:563:CYS:O	1:D:566:VAL:HG12	2.20	0.41
1:D:79:ARG:HD2	7:D:1040:HOH:O	2.21	0.41
1:A:57:PRO:HG3	7:A:809:HOH:O	2.21	0.41
2:B:5:PRO:HB3	2:B:57:LEU:HD21	2.01	0.41
2:C:7:LEU:HD21	2:C:23:LEU:CD1	2.48	0.41
1:D:222:VAL:HG11	4:D:602:VAL:N	2.36	0.41
1:D:29:LYS:HB2	1:D:33:LYS:HE2	2.03	0.41
1:D:82:ASP:O	7:D:761:HOH:O	2.22	0.41
2:E:54:ILE:H	2:E:54:ILE:HG13	1.72	0.41
1:A:117:LEU:HD11	1:A:333:SER:CA	2.42	0.41
1:A:113:PHE:CE1	1:A:117:LEU:HD22	2.56	0.41
1:A:288:TYR:HA	1:A:318:HIS:O	2.21	0.41
1:A:465:TYR:HD1	1:A:551:VAL:CG1	2.34	0.41
1:D:109:LYS:HE3	1:D:111:ILE:HG13	2.02	0.41
1:D:133:ASN:OD1	1:D:138:ILE:N	2.50	0.41
1:D:92:HIS:HB2	2:E:141:ASP:CB	2.51	0.41
2:E:199:LEU:HA	2:E:200:PRO:HD2	1.97	0.41
2:F:182:LEU:O	2:F:185:TRP:HE3	2.04	0.41
2:F:9:ASP:HB2	2:F:20:ARG:NH2	2.36	0.41
1:A:114:THR:HG22	1:A:115:ASP:H	1.86	0.40
1:A:143:LYS:CE	1:A:212:PHE:HB2	2.50	0.40
1:A:309:MET:HE3	1:A:536:LEU:HD12	2.03	0.40
2:B:211:GLU:OE1	7:B:421:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:PRO:HB2	2:C:144:TYR:CD2	2.56	0.40
1:D:108:PRO:HG2	1:D:552:LYS:N	2.30	0.40
1:D:330:TYR:HB2	1:D:352:PHE:HD2	1.85	0.40
1:D:363:PHE:HB2	1:D:388:TYR:HD2	1.87	0.40
1:D:449:ALA:O	1:D:452:LEU:HB2	2.21	0.40
1:D:152:LYS:HG3	1:D:565:ASN:CG	2.41	0.40
1:D:77:ILE:O	1:D:81:VAL:HG12	2.21	0.40
2:F:117:LYS:HE3	2:F:213:ARG:HH12	1.84	0.40
2:F:169:LYS:HB2	2:F:169:LYS:HE3	1.68	0.40
1:A:117:LEU:HA	1:A:120:ASN:ND2	2.37	0.40
1:A:337:ILE:O	1:A:354:VAL:HA	2.22	0.40
1:A:444:SER:OG	7:A:705:HOH:O	1.96	0.40
2:C:17:MET:CE	2:C:200:PRO:HD2	2.52	0.40
2:C:20:ARG:CB	2:C:198:SER:HB3	2.51	0.40
2:B:62:LYS:NZ	2:C:94:GLN:CG	2.84	0.40
1:D:302:TYR:CD1	1:D:326:VAL:HG13	2.53	0.40
1:D:125:PHE:CE2	1:D:328:HIS:CE1	3.02	0.40
2:E:99:ALA:O	2:E:103:ASP:HB2	2.21	0.40
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.43	0.40
1:A:256:VAL:O	1:A:260:ARG:HB2	2.21	0.40
1:A:273:LEU:O	1:A:276:THR:HG22	2.20	0.40
1:A:33:LYS:O	1:A:37:LEU:HB2	2.21	0.40
1:A:77:ILE:CG2	1:A:97:ILE:HD12	2.51	0.40
2:C:153:VAL:HG22	2:C:157:LEU:HD23	2.03	0.40
2:C:211:GLU:O	2:C:214:LYS:HG2	2.21	0.40
1:D:101:SER:HB3	1:D:535:PHE:CE2	2.56	0.40
1:D:147:PHE:CE1	1:D:149:PHE:HE2	2.40	0.40
1:D:329:ASP:CB	1:D:339:ALA:HA	2.44	0.40
1:D:36:LEU:HD22	1:D:61:PHE:CE1	2.57	0.40
1:D:65:VAL:HA	1:D:66:PRO:HD3	1.92	0.40
1:D:68:VAL:CG1	1:D:72:GLU:HB2	2.49	0.40
2:F:110:GLN:HG3	7:F:417:HOH:O	2.22	0.40
1:A:201:ALA:O	1:A:205:HIS:ND1	2.50	0.40
1:A:290:LEU:O	1:A:293:ALA:N	2.54	0.40
1:A:428:ILE:HD13	7:A:1133:HOH:O	2.21	0.40
1:A:78:LYS:HE2	1:A:553:PRO:HG2	2.04	0.40
2:B:133:LYS:HA	2:B:136:GLU:OE2	2.22	0.40
1:A:90:THR:O	2:B:143:PRO:HD3	2.21	0.40
2:B:24:ARG:HE	2:B:198:SER:HG	1.62	0.40
1:D:272:GLU:O	1:D:275:GLU:HB3	2.21	0.40
1:D:365:PRO:HG3	1:D:388:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:VAL:HG11	1:D:540:SER:OG	2.22	0.40
2:E:117:LYS:HE3	2:E:117:LYS:HB2	1.94	0.40
2:F:10:TYR:O	2:F:20:ARG:NH2	2.42	0.40
1:A:566:VAL:HG12	1:A:566:VAL:O	2.20	0.40
1:A:96:ALA:HB3	1:A:113:PHE:HB3	2.04	0.40
2:B:65:CYS:HB2	7:B:420:HOH:O	2.21	0.40
1:D:198:VAL:HG22	1:D:524:ALA:HB3	2.04	0.40
1:D:354:VAL:HG11	1:D:379:LEU:HD21	2.02	0.40
1:D:506:TYR:O	1:D:510:ARG:HB3	2.21	0.40
2:E:93:ALA:HB2	2:E:96:ARG:NH1	2.36	0.40
2:F:23:LEU:HB3	2:F:28:VAL:CG1	2.51	0.40

All (22) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:O	1:A:509:SER:OG[1_655]	1.76	0.44
1:A:270:ASN:O	1:A:511:LYS:NZ[1_655]	1.80	0.40
1:A:238:TRP:N	2:F:177:SER:OG[1_554]	1.91	0.29
7:B:427:HOH:O	7:C:482:HOH:O[1_455]	1.98	0.22
7:D:1210:HOH:O	7:E:581:HOH:O[1_655]	2.00	0.20
7:A:1075:HOH:O	7:B:533:HOH:O[1_545]	2.07	0.13
1:D:270:ASN:ND2	1:D:510:ARG:O[1_655]	2.10	0.10
1:A:270:ASN:ND2	1:A:510:ARG:O[1_655]	2.10	0.10
7:D:1071:HOH:O	7:D:1097:HOH:O[1_665]	2.11	0.09
7:B:476:HOH:O	7:C:503:HOH:O[1_455]	2.12	0.08
1:D:280:LYS:NZ	1:D:503:ASP:OD1[1_655]	2.12	0.08
1:A:22:ARG:NH2	2:B:173:PHE:O[1_545]	2.13	0.07
7:A:1159:HOH:O	7:A:1172:HOH:O[1_565]	2.13	0.07
7:A:1066:HOH:O	7:F:489:HOH:O[1_554]	2.13	0.07
7:B:502:HOH:O	7:C:527:HOH:O[1_455]	2.13	0.07
1:A:276:THR:OG1	1:A:501:PHE:O[1_655]	2.13	0.07
7:D:953:HOH:O	7:D:1024:HOH:O[1_655]	2.15	0.05
7:A:1161:HOH:O	7:A:1200:HOH:O[1_565]	2.15	0.05
2:C:140:GLY:O	1:D:246:LYS:NZ[1_455]	2.17	0.03
7:D:1019:HOH:O	7:D:1095:HOH:O[1_565]	2.17	0.03
1:D:270:ASN:O	1:D:511:LYS:NZ[1_655]	2.18	0.02
2:C:141:ASP:OD2	1:D:278:ARG:NH2[1_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/575 (99%)	513 (90%)	41 (7%)	13 (2%)	8	1
1	D	567/575 (99%)	504 (89%)	53 (9%)	10 (2%)	11	1
2	B	212/223 (95%)	197 (93%)	12 (6%)	3 (1%)	14	2
2	C	212/223 (95%)	193 (91%)	15 (7%)	4 (2%)	10	1
2	E	212/223 (95%)	192 (91%)	18 (8%)	2 (1%)	21	5
2	F	212/223 (95%)	191 (90%)	14 (7%)	7 (3%)	5	0
All	All	1982/2042 (97%)	1790 (90%)	153 (8%)	39 (2%)	9	1

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	ILE
1	A	540	SER
1	D	433	ILE
1	D	540	SER
1	D	542	ALA
2	F	177	SER
2	F	180	PRO
1	A	166	THR
1	A	437	THR
1	A	566	VAL
2	C	140	GLY
1	D	53	ASN
1	D	437	THR
1	D	566	VAL
2	F	140	GLY
2	F	174	SER
1	A	54	ALA
1	A	92	HIS
1	A	368	GLU
2	B	26	LYS

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Mol	Chain	Res	Type
2	B	140	GLY
1	D	368	GLU
1	D	574	ALA
2	F	66	GLU
1	A	105	GLN
1	A	329	ASP
2	B	79	PRO
1	D	369	THR
2	F	172	ASN
1	A	85	THR
2	C	66	GLU
2	C	180	PRO
1	D	553	PRO
1	A	509	SER
2	F	27	GLY
1	A	296	PRO
2	E	27	GLY
2	E	79	PRO
2	C	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%)	461 (92%)	38 (8%)	16	3
1	D	499/505 (99%)	458 (92%)	41 (8%)	14	3
2	B	187/195 (96%)	180 (96%)	7 (4%)	41	17
2	C	187/195 (96%)	172 (92%)	15 (8%)	15	3
2	E	187/195 (96%)	183 (98%)	4 (2%)	61	40
2	F	187/195 (96%)	170 (91%)	17 (9%)	12	2
All	All	1746/1790 (98%)	1624 (93%)	122 (7%)	19	4

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	26	GLN
1	A	37	LEU
1	A	55	THR
1	A	90	THR
1	A	103	THR
1	A	110	PHE
1	A	125	PHE
1	A	134	ARG
1	A	152	LYS
1	A	154	TYR
1	A	156	SER
1	A	184	SER
1	A	202	LEU
1	A	276	THR
1	A	277	ILE
1	A	281	CYS
1	A	295	PHE
1	A	305	MET
1	A	313	VAL
1	A	357	ASN
1	A	390	VAL
1	A	403	LEU
1	A	410	ILE
1	A	433	ILE
1	A	455	GLU
1	A	463	SER
1	A	464	SER
1	A	478	PHE
1	A	479	TRP
1	A	494	CYS
1	A	509	SER
1	A	515	ILE
1	A	518	LEU
1	A	536	LEU
1	A	545	PHE
1	A	546	LYS
1	A	552	LYS
2	B	39	ASN
2	B	43	LEU
2	B	65	CYS
2	B	103	ASP
2	B	149	SER

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Mol	Chain	Res	Type
2	B	182	LEU
2	B	188	ARG
2	C	32	TYR
2	C	45	LEU
2	C	50	ILE
2	C	64	VAL
2	C	72	GLN
2	C	74	VAL
2	C	133	LYS
2	C	134	ILE
2	C	135	LEU
2	C	139	LEU
2	C	157	LEU
2	C	176	GLU
2	C	183	ILE
2	C	185	TRP
2	C	204	LYS
1	D	25	HIS
1	D	46	GLN
1	D	66	PRO
1	D	68	VAL
1	D	77	ILE
1	D	78	LYS
1	D	81	VAL
1	D	82	ASP
1	D	85	THR
1	D	88	ILE
1	D	89	LEU
1	D	90	THR
1	D	92	HIS
1	D	99	LEU
1	D	110	PHE
1	D	125	PHE
1	D	150	SER
1	D	152	LYS
1	D	172	ASN
1	D	187	CYS
1	D	202	LEU
1	D	210	ILE
1	D	242	VAL
1	D	250	LEU
1	D	254	ILE

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Mol	Chain	Res	Type
1	D	273	LEU
1	D	326	VAL
1	D	329	ASP
1	D	405	ASP
1	D	408	LYS
1	D	410	ILE
1	D	416	THR
1	D	424	ARG
1	D	468	VAL
1	D	477	ILE
1	D	494	CYS
1	D	507	VAL
1	D	512	CYS
1	D	546	LYS
1	D	551	VAL
1	D	566	VAL
2	E	4	LEU
2	E	87	SER
2	E	88	ASP
2	E	139	LEU
2	F	32	TYR
2	F	43	LEU
2	F	64	VAL
2	F	65	CYS
2	F	72	GLN
2	F	80	GLU
2	F	84	PHE
2	F	134	ILE
2	F	135	LEU
2	F	139	LEU
2	F	148	ASP
2	F	157	LEU
2	F	172	ASN
2	F	178	GLU
2	F	182	LEU
2	F	202	SER
2	F	216	ASN

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

Mol	Chain	Res	Type
1	A	26	GLN

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Mol	Chain	Res	Type
1	A	146	GLN
1	A	217	GLN
1	A	394	ASN
1	A	491	GLN
1	A	565	ASN
2	B	60	ASN
2	C	72	GLN
1	D	39	ASN
1	D	123	GLN
1	D	172	ASN
1	D	205	HIS
1	D	236	GLN
1	D	318	HIS
1	D	565	ASN
2	F	110	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
3	JAA	A	601	-	12,15,15	5.68	6 (50%)	12,19,19	3.47	5 (41%)
4	VAL	A	602	-	4,7,7	0.66	0	3,9,9	0.74	0
5	GSH	B	301	-	13,19,19	1.69	3 (23%)	15,24,24	2.27	6 (40%)
5	GSH	C	301	-	13,19,19	1.64	3 (23%)	15,24,24	3.76	8 (53%)
3	JAA	D	601	6	12,15,15	5.68	6 (50%)	12,19,19	3.62	7 (58%)
4	VAL	D	602	-	4,7,7	0.71	0	3,9,9	0.03	0
5	GSH	E	301	-	13,19,19	1.66	3 (23%)	15,24,24	2.92	6 (40%)
5	GSH	F	301	-	13,19,19	1.63	3 (23%)	15,24,24	2.98	3 (20%)

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
3	JAA	A	601	-	-	0/7/22/22	0/1/1/1
4	VAL	A	602	-	-	0/4/8/8	0/0/0/0
5	GSH	B	301	-	-	0/18/24/24	0/0/0/0
5	GSH	C	301	-	-	0/18/24/24	0/0/0/0
3	JAA	D	601	6	-	0/7/22/22	0/1/1/1
4	VAL	D	602	-	-	0/4/8/8	0/0/0/0
5	GSH	E	301	-	-	0/18/24/24	0/0/0/0
5	GSH	F	301	-	-	0/18/24/24	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JAA	C05-C08	-12.87	1.31	1.52
3	D	601	JAA	C05-C08	-12.62	1.31	1.52
3	A	601	JAA	C06-C04	-11.13	1.23	1.53
3	D	601	JAA	C06-C04	-11.00	1.24	1.53
3	D	601	JAA	C10-C04	-5.24	1.45	1.53
3	A	601	JAA	C10-C04	-5.02	1.45	1.53
3	D	601	JAA	C09-C05	-4.44	1.48	1.54
3	A	601	JAA	C09-C05	-3.97	1.48	1.54
5	F	301	GSH	CA2-N2	-3.14	1.38	1.45
5	C	301	GSH	CA2-N2	-2.98	1.39	1.45
5	E	301	GSH	CA2-N2	-2.85	1.39	1.45
5	B	301	GSH	CA2-N2	-2.44	1.40	1.45
5	F	301	GSH	CD1-N2	2.18	1.38	1.34
5	E	301	GSH	CD1-N2	2.40	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	GSH	CD1-N2	2.45	1.39	1.34
5	C	301	GSH	C2-N3	2.87	1.39	1.33
5	F	301	GSH	C2-N3	2.96	1.39	1.33
5	B	301	GSH	CD1-N2	2.97	1.40	1.34
5	E	301	GSH	C2-N3	3.44	1.40	1.33
5	B	301	GSH	C2-N3	3.54	1.41	1.33
3	A	601	JAA	C05-C04	4.55	1.66	1.55
3	D	601	JAA	C05-C04	4.65	1.66	1.55
3	A	601	JAA	C07-C08	5.38	1.60	1.50
3	D	601	JAA	C07-C08	5.75	1.61	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	GSH	CA2-CB2-SG2	-10.03	102.97	113.99
5	F	301	GSH	CA2-CB2-SG2	-9.30	103.78	113.99
3	A	601	JAA	C07-C08-C05	-8.13	102.01	109.04
3	D	601	JAA	C07-C06-C04	-6.65	97.85	104.57
5	E	301	GSH	CA2-CB2-SG2	-6.63	106.70	113.99
5	E	301	GSH	CB2-CA2-N2	-6.48	102.70	111.43
5	B	301	GSH	CA2-CB2-SG2	-6.11	107.28	113.99
3	D	601	JAA	C07-C08-C05	-6.01	103.84	109.04
3	D	601	JAA	C09-C11-C13	-5.99	105.26	126.48
5	F	301	GSH	CB2-CA2-N2	-5.04	104.65	111.43
5	C	301	GSH	CB2-CA2-N2	-4.97	104.74	111.43
3	A	601	JAA	C09-C11-C13	-4.93	109.04	126.48
5	C	301	GSH	CA3-N3-C2	-4.53	115.95	122.36
5	C	301	GSH	CG1-CD1-N2	-4.20	108.79	115.85
3	A	601	JAA	C14-C13-C11	-3.89	109.03	127.15
5	E	301	GSH	CG1-CD1-N2	-3.60	109.79	115.85
5	C	301	GSH	CG1-CB1-CA1	-3.50	105.94	114.18
3	D	601	JAA	C14-C13-C11	-3.36	111.49	127.15
5	C	301	GSH	C2-CA2-N2	-3.08	102.57	111.28
3	D	601	JAA	C06-C07-C08	-3.02	102.32	105.47
5	F	301	GSH	CG1-CD1-N2	-2.68	111.34	115.85
5	B	301	GSH	CB2-CA2-N2	-2.67	107.84	111.43
5	B	301	GSH	C2-CA2-N2	-2.63	103.83	111.28
5	B	301	GSH	CA3-N3-C2	-2.42	118.94	122.36
3	A	601	JAA	C07-C06-C04	-2.29	102.26	104.57
5	B	301	GSH	CG1-CD1-N2	-2.14	112.25	115.85
5	B	301	GSH	CB1-CG1-CD1	2.10	118.06	113.26
5	E	301	GSH	CA2-N2-CD1	2.17	126.44	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	JAA	C10-C04-C05	2.27	120.11	114.80
5	E	301	GSH	OE1-CD1-CG1	2.66	126.58	121.97
5	C	301	GSH	OE1-CD1-CG1	2.93	127.05	121.97
5	E	301	GSH	CB1-CG1-CD1	3.37	120.97	113.26
5	C	301	GSH	CB1-CG1-CD1	3.44	121.12	113.26
3	D	601	JAA	O01-C08-C05	3.67	130.15	125.41
3	A	601	JAA	O01-C08-C05	5.14	132.05	125.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

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

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%)	2.34	296 (52%) 0 0	5, 17, 25, 32	0
1	D	569/575 (98%)	1.84	234 (41%) 0 0	4, 12, 19, 26	0
2	B	214/223 (95%)	1.50	58 (27%) 1 1	6, 13, 21, 28	0
2	C	214/223 (95%)	1.24	47 (21%) 1 1	3, 7, 11, 18	0
2	E	214/223 (95%)	1.64	73 (34%) 0 0	7, 12, 20, 26	0
2	F	214/223 (95%)	1.45	50 (23%) 1 1	4, 9, 14, 22	0
All	All	1994/2042 (97%)	1.82	758 (38%) 0 0	3, 12, 22, 32	0

All (758) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	VAL	9.7
2	E	97	PHE	9.1
1	A	515	ILE	9.0
2	F	174	SER	8.6
1	A	429	LEU	8.5
1	A	36	LEU	8.1
1	D	161	PRO	8.1
1	A	294	LEU	7.8
1	A	432	ASN	7.5
1	A	17	PHE	7.5
2	C	90	TYR	7.3
1	A	210	ILE	7.1
1	A	346	SER	7.1
2	E	95	ALA	7.0
1	A	287	TRP	6.7
1	A	13	VAL	6.6
2	B	123	ALA	6.6
2	F	176	GLU	6.5
1	A	202	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	523	VAL	6.4
1	A	284	LEU	6.3
1	A	305	MET	6.2
2	F	172	ASN	6.2
1	D	361	PHE	6.1
1	A	506	TYR	6.0
1	A	309	MET	6.0
1	D	173	PRO	5.8
1	A	423	CYS	5.8
1	A	354	VAL	5.7
1	A	459	VAL	5.7
1	D	566	VAL	5.7
1	A	125	PHE	5.7
1	A	457	ILE	5.6
1	A	377	VAL	5.6
1	A	274	ALA	5.5
1	A	531	ILE	5.5
1	A	233	THR	5.4
1	A	500	ALA	5.4
1	A	237	VAL	5.3
2	B	132	VAL	5.3
1	A	468	VAL	5.2
1	D	517	ALA	5.2
1	A	35	ILE	5.2
1	A	295	PHE	5.1
1	D	203	TYR	5.1
2	B	140	GLY	5.1
1	A	48	CYS	5.0
1	A	556	ALA	5.0
1	A	60	ALA	5.0
1	A	301	VAL	5.0
1	A	66	PRO	5.0
1	A	145	LEU	4.9
1	D	114	THR	4.9
1	A	65	VAL	4.9
2	E	70	VAL	4.9
1	A	279	THR	4.9
1	D	506	TYR	4.9
1	D	507	VAL	4.9
1	A	406	VAL	4.9
1	A	238	TRP	4.9
1	A	169	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	104	SER	4.8
1	A	234	PHE	4.8
2	B	139	LEU	4.8
1	D	398	LEU	4.8
1	D	155	ILE	4.8
1	A	257	PRO	4.8
1	A	37	LEU	4.8
1	A	475	TYR	4.8
1	D	475	TYR	4.8
1	A	538	LEU	4.8
1	A	220	PHE	4.7
2	F	180	PRO	4.7
1	A	392	ILE	4.6
1	D	466	ILE	4.6
1	D	271	PRO	4.6
1	A	8	PHE	4.6
1	A	497	LEU	4.5
1	D	262	ALA	4.5
1	D	77	ILE	4.5
1	A	563	CYS	4.5
1	A	507	VAL	4.5
1	D	523	VAL	4.5
1	D	202	LEU	4.5
1	D	162	VAL	4.5
1	A	154	TYR	4.4
1	D	111	ILE	4.4
1	A	170	TYR	4.4
2	C	10	TYR	4.4
1	D	46	GLN	4.4
2	B	135	LEU	4.4
1	A	110	PHE	4.4
1	A	113	PHE	4.4
2	B	153	VAL	4.4
1	A	460	ILE	4.3
1	D	89	LEU	4.3
1	D	160	VAL	4.3
1	D	515	ILE	4.3
1	A	433	ILE	4.3
1	A	469	SER	4.3
1	D	409	VAL	4.3
1	A	546	LYS	4.3
2	F	165	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	241	ILE	4.2
2	B	183	ILE	4.2
2	F	173	PHE	4.2
1	A	67	LEU	4.2
1	D	288	TYR	4.2
1	A	129	PHE	4.2
1	A	545	PHE	4.2
2	B	64	VAL	4.1
2	E	173	PHE	4.1
1	D	457	ILE	4.1
2	B	70	VAL	4.1
1	A	131	PHE	4.1
1	D	76	TYR	4.0
2	E	61	GLY	4.0
1	A	326	VAL	4.0
1	D	313	VAL	4.0
1	D	397	GLY	4.0
1	A	477	ILE	4.0
1	D	428	ILE	4.0
1	A	136	PHE	4.0
2	E	49	PRO	4.0
2	B	175	ILE	4.0
1	A	211	LEU	3.9
1	A	149	PHE	3.9
1	A	428	ILE	3.9
1	D	481	ILE	3.9
1	A	345	LEU	3.9
2	F	114	TRP	3.9
2	E	71	VAL	3.9
1	D	42	ALA	3.9
2	F	73	TYR	3.9
1	A	535	PHE	3.9
1	A	431	ILE	3.9
1	D	65	VAL	3.9
2	F	179	SER	3.9
2	B	185	TRP	3.9
1	A	312	TYR	3.9
1	D	113	PHE	3.9
1	A	324	PRO	3.9
1	A	230	ALA	3.8
1	D	266	LEU	3.8
1	A	38	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	153	VAL	3.8
1	A	311	PRO	3.8
1	A	466	ILE	3.8
1	A	558	VAL	3.8
1	D	71	VAL	3.8
1	A	175	PHE	3.8
2	C	193	GLU	3.8
2	F	175	ILE	3.8
2	E	57	LEU	3.8
1	A	14	ILE	3.7
2	E	158	ILE	3.7
2	F	68	LEU	3.7
2	E	74	VAL	3.7
1	D	204	CYS	3.7
1	A	526	GLY	3.7
1	D	32	LEU	3.7
1	A	353	ALA	3.7
1	A	407	VAL	3.7
2	F	90	TYR	3.7
1	A	19	GLU	3.7
1	D	149	PHE	3.7
1	D	304	ILE	3.7
1	A	166	THR	3.7
1	D	85	THR	3.7
1	D	380	THR	3.7
2	F	144	TYR	3.7
1	A	116	GLU	3.7
1	D	274	ALA	3.7
1	D	462	PHE	3.7
1	A	443	LEU	3.7
1	D	219	VAL	3.7
2	E	206	VAL	3.7
1	A	327	SER	3.6
1	A	42	ALA	3.6
1	A	352	PHE	3.6
1	D	528	PHE	3.6
1	A	379	LEU	3.6
2	F	177	SER	3.6
1	A	43	ILE	3.6
1	D	531	ILE	3.6
1	A	313	VAL	3.6
1	D	287	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	330	TYR	3.6
1	A	388	TYR	3.6
1	A	33	LYS	3.6
1	A	122	LEU	3.6
1	A	325	LEU	3.6
1	A	403	LEU	3.6
1	A	198	VAL	3.6
2	F	99	ALA	3.6
2	B	78	TRP	3.6
1	A	454	GLU	3.5
1	D	154	TYR	3.5
1	A	290	LEU	3.5
1	D	167	THR	3.5
2	E	139	LEU	3.5
2	F	64	VAL	3.5
1	A	282	MET	3.5
2	F	183	ILE	3.5
1	A	147	PHE	3.5
1	A	281	CYS	3.5
1	A	393	THR	3.5
1	A	524	ALA	3.5
1	D	476	ALA	3.5
2	E	109	ALA	3.5
1	D	250	LEU	3.5
1	D	285	SER	3.5
2	B	202	SER	3.5
1	A	323	LEU	3.4
1	D	242	VAL	3.4
1	D	384	ILE	3.4
2	F	98	TRP	3.4
1	D	571	PHE	3.4
1	D	179	MET	3.4
1	D	550	CYS	3.4
1	A	57	PRO	3.4
1	A	28	GLN	3.4
1	A	536	LEU	3.4
1	D	429	LEU	3.4
2	E	175	ILE	3.4
2	B	60	ASN	3.4
2	E	98	TRP	3.4
1	A	217	GLN	3.4
1	D	206	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	522	VAL	3.4
2	C	28	VAL	3.4
1	A	203	TYR	3.4
1	D	561	ILE	3.4
1	D	7	THR	3.4
1	D	147	PHE	3.4
1	A	339	ALA	3.3
1	A	161	PRO	3.3
1	D	316	LEU	3.3
1	D	182	ILE	3.3
1	D	479	TRP	3.3
1	A	419	LEU	3.3
1	D	419	LEU	3.3
1	A	473	GLY	3.3
1	A	548	PRO	3.3
2	E	21	VAL	3.3
2	E	134	ILE	3.3
1	A	71	VAL	3.3
1	D	192	VAL	3.3
2	E	63	PRO	3.3
1	A	218	TYR	3.3
2	F	208	TYR	3.3
1	D	512	CYS	3.3
1	A	231	PHE	3.2
1	D	520	LEU	3.2
2	F	132	VAL	3.2
1	D	516	GLY	3.2
2	B	32	TYR	3.2
1	A	214	ASP	3.2
1	A	355	ILE	3.2
1	D	187	CYS	3.2
1	A	103	THR	3.2
1	A	271	PRO	3.2
1	D	314	PRO	3.2
2	F	216	ASN	3.2
1	A	54	ALA	3.2
1	D	208	SER	3.2
2	E	90	TYR	3.2
2	E	91	GLY	3.2
2	E	124	GLY	3.2
1	A	412	PHE	3.2
1	D	110	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	412	PHE	3.2
1	D	421	PHE	3.2
2	F	157	LEU	3.2
1	D	43	ILE	3.2
1	A	341	VAL	3.2
1	D	122	LEU	3.2
1	D	222	VAL	3.2
2	E	44	LEU	3.2
2	C	170	PHE	3.2
2	E	10	TYR	3.2
1	A	109	LYS	3.1
1	A	93	PRO	3.1
1	A	127	THR	3.1
1	A	316	LEU	3.1
1	D	558	VAL	3.1
1	A	464	SER	3.1
1	D	399	TYR	3.1
2	E	73	TYR	3.1
2	B	134	ILE	3.1
1	D	335	GLY	3.1
1	A	81	VAL	3.1
2	E	30	PHE	3.1
1	A	337	ILE	3.1
2	F	135	LEU	3.1
2	F	153	VAL	3.1
1	D	311	PRO	3.1
1	A	321	GLY	3.1
2	E	210	ALA	3.1
1	A	465	TYR	3.1
1	A	561	ILE	3.1
2	B	158	ILE	3.1
1	A	445	VAL	3.1
2	B	206	VAL	3.1
2	E	22	ALA	3.1
1	D	573	THR	3.0
2	E	54	ILE	3.0
1	A	269	PRO	3.0
1	D	289	GLY	3.0
1	A	518	LEU	3.0
2	F	102	VAL	3.0
2	F	217	LEU	3.0
1	D	431	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	390	VAL	3.0
1	D	277	ILE	3.0
1	A	181	SER	3.0
1	A	273	LEU	3.0
1	A	358	LEU	3.0
1	A	508	SER	3.0
2	B	180	PRO	3.0
1	D	124	LEU	3.0
1	D	495	ASN	3.0
2	B	207	ALA	3.0
1	A	148	ILE	3.0
1	D	337	ILE	3.0
2	C	32	TYR	3.0
1	A	501	PHE	3.0
2	F	171	GLY	3.0
1	D	121	THR	2.9
1	A	560	GLN	2.9
1	D	360	TYR	2.9
1	D	433	ILE	2.9
1	D	570	TYR	2.9
1	D	494	CYS	2.9
1	A	98	SER	2.9
1	A	472	PRO	2.9
1	D	465	TYR	2.9
1	D	45	LEU	2.9
1	D	403	LEU	2.9
1	A	277	ILE	2.9
2	E	6	ILE	2.9
2	E	50	ILE	2.9
1	A	83	GLY	2.9
1	A	302	TYR	2.9
2	F	10	TYR	2.9
1	A	361	PHE	2.9
1	D	220	PHE	2.9
1	D	363	PHE	2.9
2	C	49	PRO	2.9
2	C	83	PRO	2.9
2	B	102	VAL	2.9
2	E	28	VAL	2.9
1	A	322	ASP	2.9
1	A	422	ILE	2.9
1	D	259	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	390	VAL	2.8
1	D	489	VAL	2.8
1	D	538	LEU	2.8
1	A	106	GLY	2.8
1	A	289	GLY	2.8
1	D	47	ASN	2.8
2	E	14	MET	2.8
1	A	96	ALA	2.8
1	A	128	ALA	2.8
2	C	183	ILE	2.8
1	D	413	TYR	2.8
2	E	32	TYR	2.8
1	A	505	GLY	2.8
1	D	178	GLY	2.8
1	A	421	PHE	2.8
1	D	125	PHE	2.8
1	D	535	PHE	2.8
1	D	575	PHE	2.8
2	E	43	LEU	2.8
1	D	112	PRO	2.8
2	E	12	PRO	2.8
1	D	165	ALA	2.8
1	A	91	GLY	2.8
1	D	148	ILE	2.8
1	D	477	ILE	2.8
1	A	124	LEU	2.8
1	D	366	VAL	2.8
1	A	223	PHE	2.8
2	B	164	PHE	2.8
2	E	160	PHE	2.8
2	F	97	PHE	2.8
1	A	512	CYS	2.8
1	D	496	CYS	2.8
1	D	510	ARG	2.8
2	B	129	ILE	2.8
2	B	167	TYR	2.8
1	A	259	VAL	2.8
1	D	427	LEU	2.8
1	D	567	VAL	2.8
2	B	56	VAL	2.8
1	D	541	SER	2.8
2	B	93	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	553	PRO	2.8
1	A	276	THR	2.7
2	E	7	LEU	2.7
1	A	476	ALA	2.7
2	E	93	ALA	2.7
1	D	568	SER	2.7
2	B	174	SER	2.7
1	D	69	THR	2.7
1	D	268	THR	2.7
2	E	205	ILE	2.7
1	D	169	VAL	2.7
1	D	198	VAL	2.7
1	D	207	LEU	2.7
1	D	216	VAL	2.7
2	E	166	ALA	2.7
1	D	562	LEU	2.7
2	B	182	LEU	2.7
2	C	44	LEU	2.7
1	D	417	PRO	2.7
1	A	61	PHE	2.7
1	A	21	THR	2.7
1	A	90	THR	2.7
1	A	410	ILE	2.7
2	B	186	ALA	2.7
1	D	336	TRP	2.7
2	C	185	TRP	2.7
2	C	68	LEU	2.7
2	E	47	SER	2.7
2	E	64	VAL	2.7
1	A	328	HIS	2.7
2	E	150	PHE	2.7
1	D	504	ALA	2.7
1	A	502	ILE	2.7
1	A	99	LEU	2.7
1	A	562	LEU	2.7
1	D	545	PHE	2.7
2	F	72	GLN	2.7
1	D	60	ALA	2.6
1	A	550	CYS	2.6
1	A	68	VAL	2.6
1	A	222	VAL	2.6
1	D	445	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	31	THR	2.6
1	D	205	HIS	2.6
1	A	194	PHE	2.6
1	A	212	PHE	2.6
1	A	478	PHE	2.6
2	B	101	PHE	2.6
2	B	173	PHE	2.6
1	D	392	ILE	2.6
1	D	103	THR	2.6
1	D	470	THR	2.6
1	D	249	VAL	2.6
1	A	300	TYR	2.6
1	D	37	LEU	2.6
1	A	516	GLY	2.6
1	A	144	ALA	2.6
2	B	98	TRP	2.6
2	C	98	TRP	2.6
1	A	528	PHE	2.6
1	D	8	PHE	2.6
1	D	17	PHE	2.6
1	D	55	THR	2.6
1	D	255	THR	2.6
1	D	492	ASP	2.6
1	A	97	ILE	2.6
2	E	155	ILE	2.6
1	A	398	LEU	2.6
1	D	170	TYR	2.6
1	D	464	SER	2.6
1	A	261	THR	2.6
1	A	372	GLY	2.6
1	D	501	PHE	2.6
1	A	350	ALA	2.6
1	D	221	ALA	2.6
2	C	70	VAL	2.6
1	D	218	TYR	2.6
1	A	453	SER	2.6
2	B	137	SER	2.6
1	A	342	THR	2.5
2	F	164	PHE	2.5
1	A	92	HIS	2.5
1	A	10	MET	2.5
1	A	195	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	481	ILE	2.5
1	A	108	PRO	2.5
1	A	376	PRO	2.5
1	D	518	LEU	2.5
2	E	45	LEU	2.5
1	A	44	TYR	2.5
1	A	413	TYR	2.5
1	D	44	TYR	2.5
1	D	163	GLY	2.5
1	D	359	GLY	2.5
2	C	73	TYR	2.5
1	A	573	THR	2.5
1	D	48	CYS	2.5
1	A	236	GLN	2.5
1	A	462	PHE	2.5
2	F	145	PHE	2.5
2	E	55	PRO	2.5
1	D	88	ILE	2.5
1	D	67	LEU	2.5
2	C	139	LEU	2.5
1	A	395	TYR	2.5
1	A	570	TYR	2.5
1	D	300	TYR	2.5
1	A	499	ARG	2.5
1	A	204	CYS	2.5
1	D	96	ALA	2.5
1	D	137	PRO	2.5
2	F	15	PHE	2.5
2	F	106	PHE	2.5
2	C	11	TRP	2.5
1	A	32	LEU	2.5
1	A	206	LEU	2.5
1	D	482	SER	2.5
2	B	177	SER	2.5
2	E	151	GLY	2.5
1	D	500	ALA	2.5
1	A	534	HIS	2.5
2	E	149	SER	2.5
2	C	30	PHE	2.5
1	A	111	ILE	2.5
2	E	113	VAL	2.5
1	D	73	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	142	GLY	2.5
2	B	163	TRP	2.5
1	A	288	TYR	2.4
1	D	321	GLY	2.4
1	A	120	ASN	2.4
1	A	94	VAL	2.4
1	A	304	ILE	2.4
1	D	175	PHE	2.4
1	D	502	ILE	2.4
2	B	160	PHE	2.4
2	F	111	PHE	2.4
2	E	209	ALA	2.4
1	A	63	SER	2.4
1	D	127	THR	2.4
2	E	65	CYS	2.4
2	B	113	VAL	2.4
1	A	504	ALA	2.4
1	A	544	GLN	2.4
2	C	128	PHE	2.4
2	C	207	ALA	2.4
1	A	232	ARG	2.4
1	A	209	GLY	2.4
2	C	212	TYR	2.4
2	E	27	GLY	2.4
1	A	189	PRO	2.4
1	A	449	ALA	2.4
1	A	357	ASN	2.4
2	C	102	VAL	2.4
1	A	73	LEU	2.4
1	A	245	ILE	2.4
1	A	427	LEU	2.4
1	D	485	THR	2.4
1	D	527	THR	2.4
1	D	559	LEU	2.4
1	A	359	GLY	2.4
1	A	292	PRO	2.4
2	C	5	PRO	2.4
2	F	86	PRO	2.4
1	A	76	TYR	2.4
2	E	78	TRP	2.4
2	B	215	ASN	2.4
1	D	351	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	229	HIS	2.4
1	A	207	LEU	2.3
1	A	452	LEU	2.3
1	D	99	LEU	2.3
1	D	129	PHE	2.3
2	B	37	PHE	2.3
1	D	80	MET	2.3
1	A	360	TYR	2.3
2	E	144	TYR	2.3
1	D	521	ARG	2.3
2	B	166	ALA	2.3
2	B	209	ALA	2.3
2	C	163	TRP	2.3
1	D	90	THR	2.3
1	D	459	VAL	2.3
1	A	227	LEU	2.3
1	D	36	LEU	2.3
1	D	50	LEU	2.3
1	D	254	ILE	2.3
2	F	129	ILE	2.3
1	A	298	ALA	2.3
1	D	312	TYR	2.3
2	B	90	TYR	2.3
1	A	440	ASP	2.3
1	A	426	ASN	2.3
1	A	308	SER	2.3
1	D	27	VAL	2.3
1	A	266	LEU	2.3
1	A	335	GLY	2.3
2	B	120	GLU	2.3
1	A	329	ASP	2.3
1	D	223	PHE	2.3
1	D	295	PHE	2.3
2	B	84	PHE	2.3
1	A	7	THR	2.3
2	B	172	ASN	2.3
1	D	330	TYR	2.3
1	A	215	GLN	2.3
1	A	163	GLY	2.3
2	C	64	VAL	2.3
1	A	559	LEU	2.3
1	D	486	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	548	PRO	2.3
1	A	380	THR	2.3
1	A	485	THR	2.3
1	D	574	ALA	2.3
2	C	166	ALA	2.3
1	D	309	MET	2.3
1	A	278	ARG	2.2
1	A	264	SER	2.2
1	D	184	SER	2.2
1	D	347	PRO	2.2
2	C	162	SER	2.2
2	F	70	VAL	2.2
1	A	167	THR	2.2
1	A	293	ALA	2.2
1	D	183	THR	2.2
1	D	97	ILE	2.2
1	D	231	PHE	2.2
2	E	170	PHE	2.2
1	D	296	PRO	2.2
1	D	324	PRO	2.2
1	A	351	THR	2.2
2	F	195	VAL	2.2
1	D	379	LEU	2.2
1	A	11	ASN	2.2
1	A	133	ASN	2.2
1	D	532	GLN	2.2
2	E	163	TRP	2.2
2	E	13	SER	2.2
1	A	75	PRO	2.2
1	D	87	PRO	2.2
1	D	116	GLU	2.2
1	D	196	PRO	2.2
2	B	86	PRO	2.2
2	C	12	PRO	2.2
2	C	84	PHE	2.2
2	E	85	PHE	2.2
2	E	106	PHE	2.2
2	E	164	PHE	2.2
2	C	152	TYR	2.2
1	D	201	ALA	2.2
2	F	215	ASN	2.2
1	A	409	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	94	VAL	2.2
2	C	135	LEU	2.2
2	B	136	GLU	2.2
1	D	245	ILE	2.2
1	D	291	ILE	2.2
1	A	479	TRP	2.2
1	A	394	ASN	2.2
1	A	363	PHE	2.2
1	D	24	ALA	2.2
2	C	85	PHE	2.2
2	C	95	ALA	2.2
2	E	101	PHE	2.2
1	D	557	LYS	2.2
1	A	20	MET	2.2
1	A	213	ARG	2.2
2	B	74	VAL	2.2
2	E	58	VAL	2.2
2	E	72	GLN	2.2
1	D	57	PRO	2.2
2	E	182	LEU	2.2
1	A	138	ILE	2.2
1	D	378	GLY	2.2
1	A	114	THR	2.2
1	D	306	THR	2.2
1	A	201	ALA	2.2
2	E	11	TRP	2.2
2	F	185	TRP	2.2
1	A	12	ARG	2.1
1	D	101	SER	2.1
2	C	33	ARG	2.1
2	C	179	SER	2.1
1	D	212	PHE	2.1
2	E	84	PHE	2.1
1	A	192	VAL	2.1
1	A	117	LEU	2.1
1	A	492	ASP	2.1
1	D	140	ASP	2.1
2	C	209	ALA	2.1
2	E	53	LYS	2.1
2	C	78	TRP	2.1
1	A	575	PHE	2.1
1	A	228	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	423	CYS	2.1
2	E	153	VAL	2.1
1	A	29	LYS	2.1
1	D	270	ASN	2.1
2	B	19	ALA	2.1
2	F	184	ALA	2.1
1	A	417	PRO	2.1
2	B	16	GLY	2.1
2	C	167	TYR	2.1
2	F	32	TYR	2.1
2	B	114	TRP	2.1
2	C	101	PHE	2.1
1	A	47	ASN	2.1
1	A	382	VAL	2.1
1	D	267	LEU	2.1
1	D	339	ALA	2.1
2	C	23	LEU	2.1
1	D	66	PRO	2.1
2	B	133	LYS	2.1
1	A	509	SER	2.1
1	A	255	THR	2.1
1	D	261	THR	2.1
2	B	152	TYR	2.1
2	B	30	PHE	2.1
2	B	145	PHE	2.1
2	C	106	PHE	2.1
2	F	85	PHE	2.1
2	F	101	PHE	2.1
1	A	130	ALA	2.1
1	A	216	VAL	2.1
1	D	326	VAL	2.1
1	D	341	VAL	2.1
2	F	11	TRP	2.1
2	F	207	ALA	2.1
2	B	43	LEU	2.1
2	C	43	LEU	2.1
1	A	494	CYS	2.1
1	D	14	ILE	2.1
2	C	50	ILE	2.1
1	D	166	THR	2.0
2	F	79	PRO	2.0
1	D	54	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	140	GLY	2.0
1	A	242	VAL	2.0
1	A	256	VAL	2.0
1	D	478	PHE	2.0
2	E	145	PHE	2.0
2	C	4	LEU	2.0
1	A	164	THR	2.0
1	A	183	THR	2.0
1	D	157	THR	2.0
1	D	422	ILE	2.0
1	D	247	ASP	2.0
2	F	83	PRO	2.0
1	D	118	MET	2.0
2	C	190	MET	2.0
2	C	184	ALA	2.0
1	A	123	GLN	2.0
2	E	177	SER	2.0
2	E	152	TYR	2.0
1	D	382	VAL	2.0
1	D	273	LEU	2.0
2	B	157	LEU	2.0
2	E	111	PHE	2.0
2	F	182	LEU	2.0
1	A	226	GLY	2.0
2	B	12	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	603	1/1	0.94	0.21	2.00	19,19,19,19	0
5	GSH	B	301	20/20	0.93	0.18	1.60	5,21,23,28	0
4	VAL	D	602	8/8	0.76	0.21	1.13	12,17,23,28	0
5	GSH	C	301	20/20	0.90	0.16	0.14	4,11,20,27	0
3	JAA	D	601	15/15	0.81	0.18	0.11	7,13,19,20	0
3	JAA	A	601	15/15	0.85	0.20	-0.16	12,15,20,24	0
4	VAL	A	602	8/8	0.71	0.22	-0.28	15,20,22,28	0
5	GSH	F	301	20/20	0.89	0.14	-0.97	6,10,14,19	0
5	GSH	E	301	20/20	0.88	0.14	-1.51	5,13,20,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.