



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2017 – 12:18 PM EDT

PDB ID : 5GZZ  
Title : Crystal Structure of FIN219-SjGST complex with JA  
Authors : Chen, C.Y.; Cheng, Y.S.  
Deposited on : 2016-10-02  
Resolution : 2.39 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029077



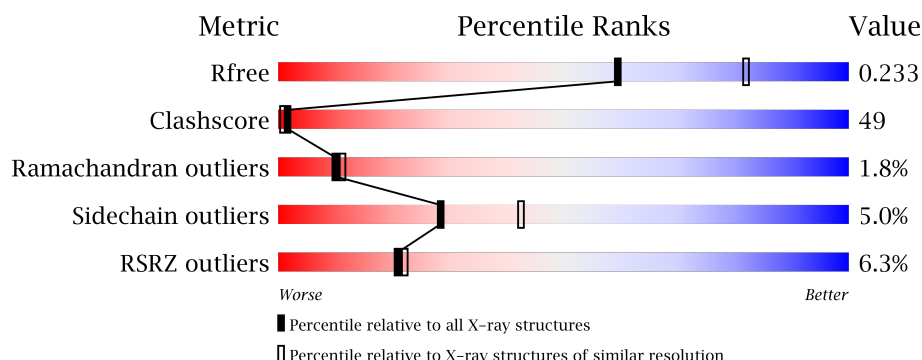
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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  $\geq 3$ , 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>5%</div> <div>34%</div> <div>60%</div> <div>5%</div> </div>
2	B	218	<div> <div>7%</div> <div>33%</div> <div>59%</div> <div>7%</div> </div>
2	C	218	<div> <div>4%</div> <div>30%</div> <div>65%</div> <div>• •</div> </div>
2	D	218	<div> <div>6%</div> <div>38%</div> <div>57%</div> <div>5%</div> </div>
2	E	218	<div> <div>6%</div> <div>29%</div> <div>64%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	218	
2	G	218	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JAA	A	601	-	-	-	X
4	GSH	B	301	-	-	X	-



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16243 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.

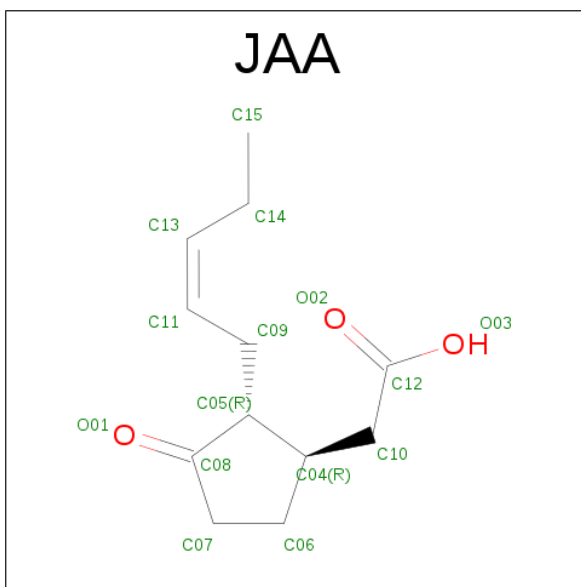
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4479	2859	748	850	22			

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1778	1158	288	319	13			
2	C	216	Total	C	N	O	S	0	0	0
			1778	1158	288	319	13			
2	D	216	Total	C	N	O	S	0	0	0
			1778	1158	288	319	13			
2	E	216	Total	C	N	O	S	0	0	0
			1778	1158	288	319	13			
2	F	216	Total	C	N	O	S	0	0	0
			1778	1158	288	319	13			
2	G	216	Total	C	N	O	S	0	0	0
			1778	1158	288	319	13			

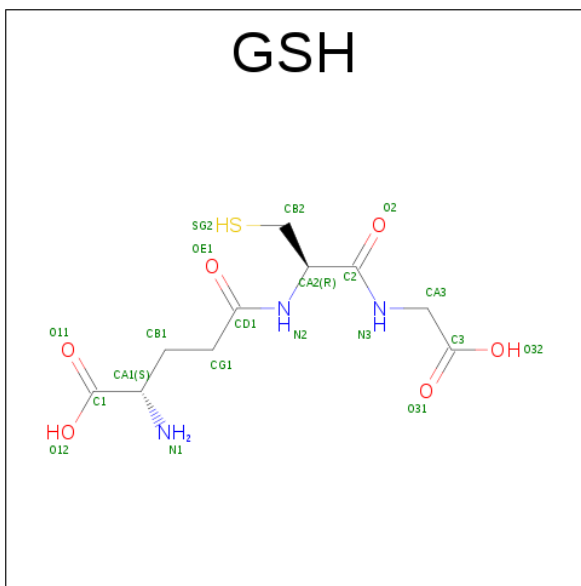
- Molecule 3 is {(1R,2R)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetic acid (three-letter code: JAA) (formula: C<sub>12</sub>H<sub>18</sub>O<sub>3</sub>).





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

- Molecule 4 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



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

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

- Molecule 5 is water.

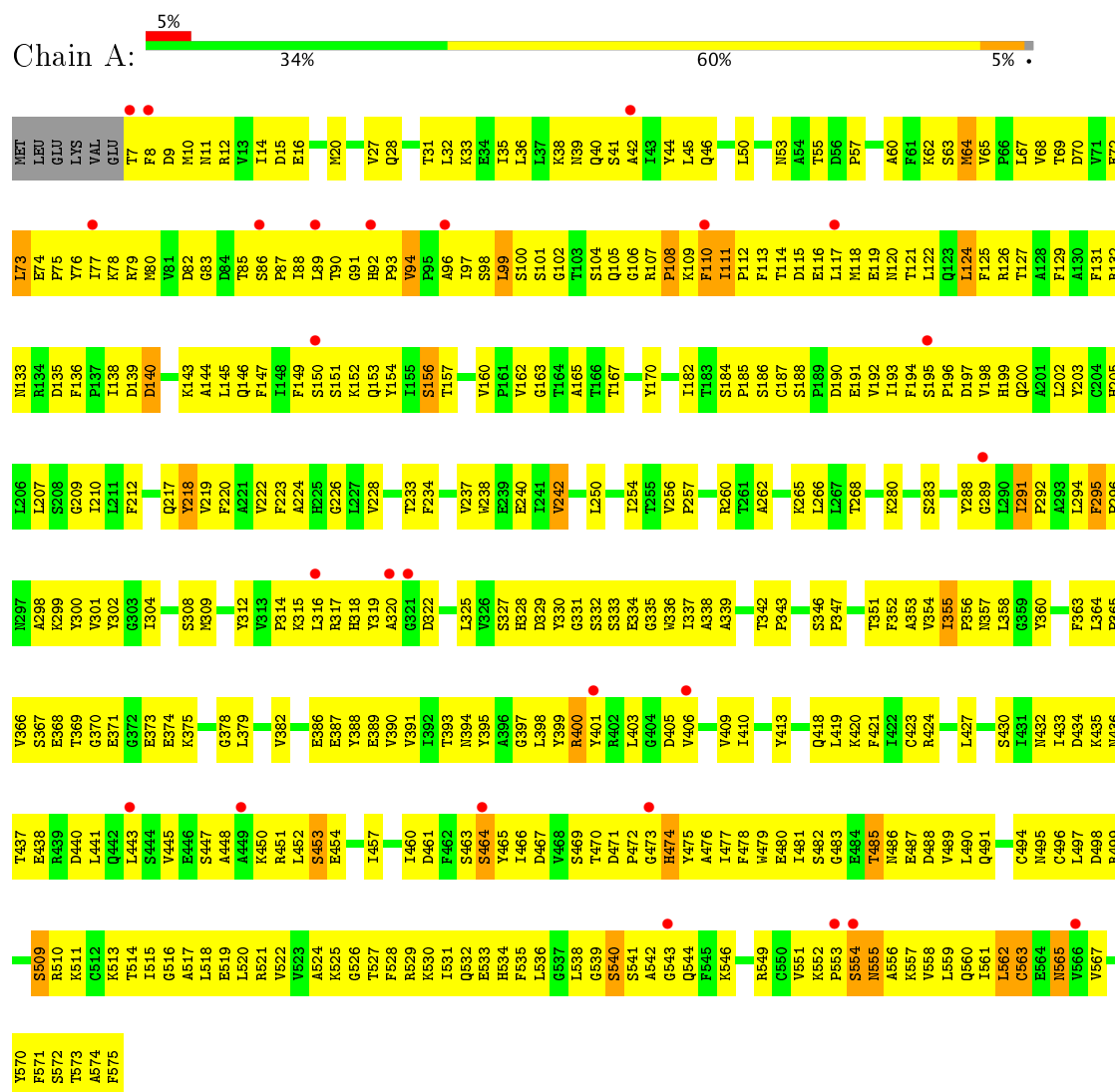
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	257	Total	O	0	0
			257	257		
5	B	110	Total	O	0	0
			110	110		
5	C	81	Total	O	0	0
			81	81		
5	D	123	Total	O	0	0
			123	123		
5	E	113	Total	O	0	0
			113	113		
5	F	161	Total	O	0	0
			161	161		
5	G	116	Total	O	0	0
			116	116		



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

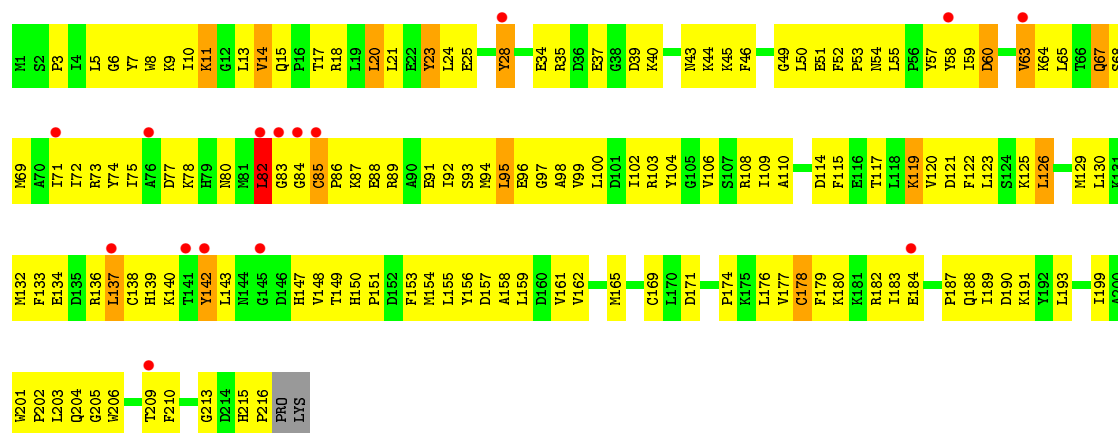
#### • Molecule 1: Jasmonic acid-amido synthetase JAR1



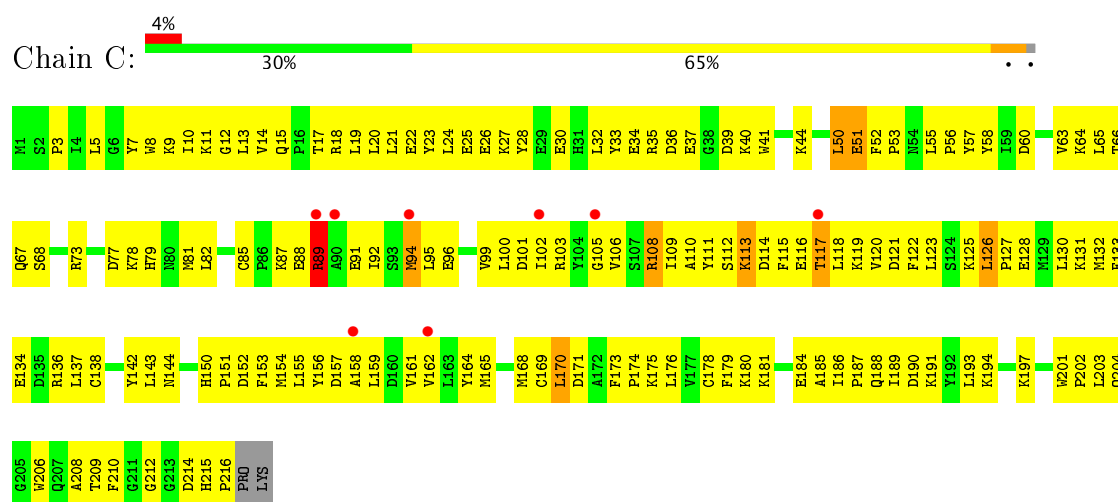
#### • Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme



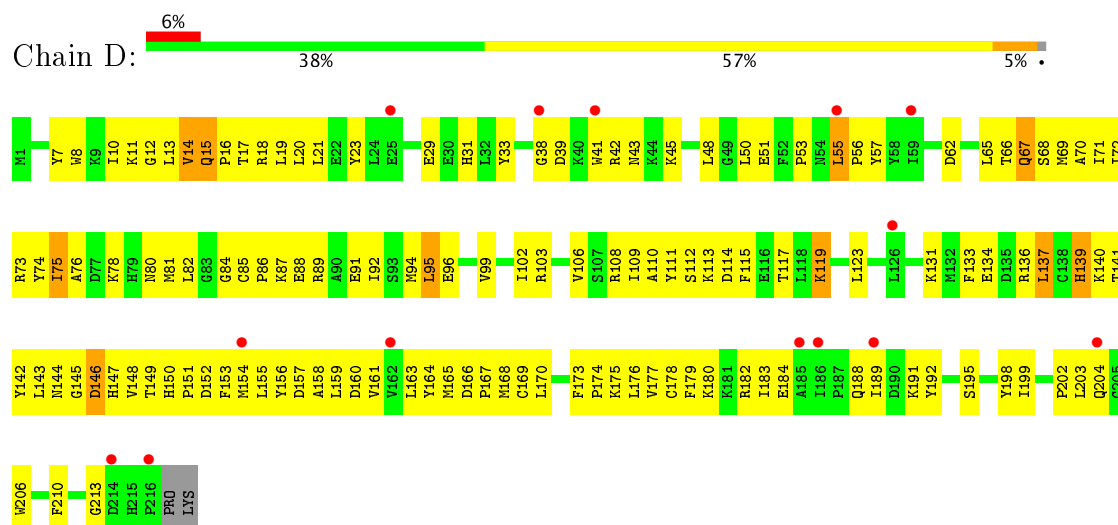




• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme



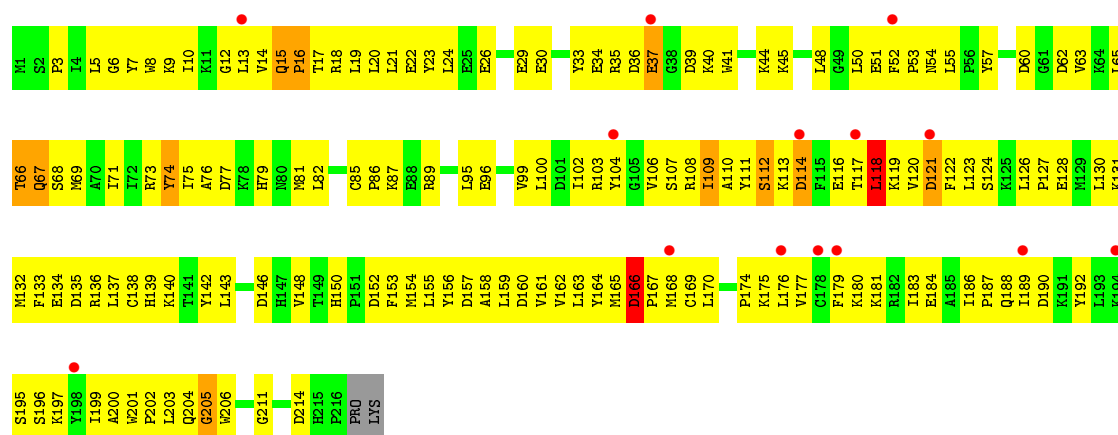
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme



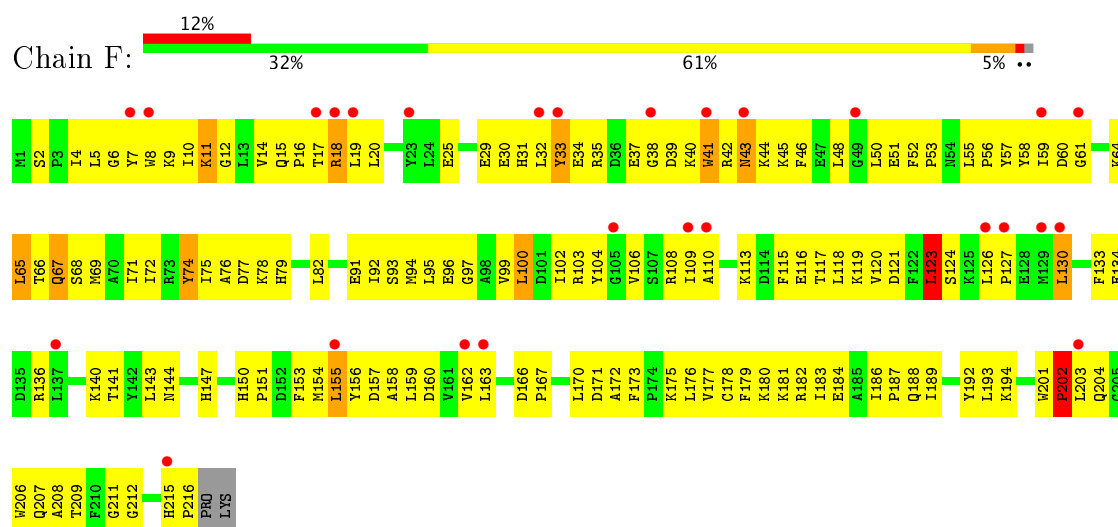
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme



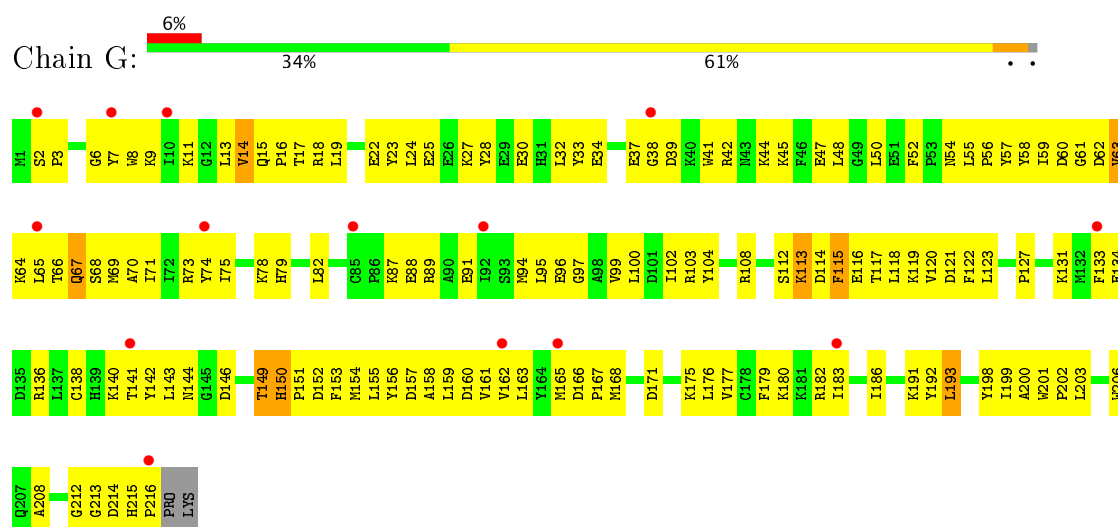




- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme



- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.27Å 91.80Å 91.73Å 89.99° 89.99° 89.93°	Depositor
Resolution (Å)	26.21 – 2.39 26.21 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.1 (26.21-2.39) 99.1 (26.21-2.39)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.204 , 0.234 0.204 , 0.233	Depositor DCC
$R_{free}$ test set	7450 reflections (10.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 354.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.046 for h,-l,k 0.046 for h,l,-k 0.067 for h,-k,-l 0.067 for -h,-k,l 0.041 for -h,k,-l 0.055 for -h,l,k 0.064 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	16243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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, 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	0.40	2/4581 (0.0%)	0.66	3/6219 (0.0%)
2	B	0.42	0/1826	0.79	6/2464 (0.2%)
2	C	0.38	0/1826	0.72	4/2464 (0.2%)
2	D	0.31	0/1826	0.62	1/2464 (0.0%)
2	E	0.43	0/1826	0.81	6/2464 (0.2%)
2	F	0.42	1/1826 (0.1%)	0.77	2/2464 (0.1%)
2	G	0.34	0/1826	0.59	0/2464
All	All	0.39	3/15537 (0.0%)	0.70	22/21003 (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	1
2	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	PHE	CB-CG	-7.24	1.39	1.51
1	A	110	PHE	CD1-CE1	-6.40	1.26	1.39
2	F	33	TYR	CD1-CE1	-5.10	1.31	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	137	LEU	CA-CB-CG	8.61	135.09	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	LEU	CA-CB-CG	7.67	132.94	115.30
1	A	110	PHE	CB-CA-C	-6.44	97.51	110.40
1	A	110	PHE	CB-CG-CD1	-6.43	116.30	120.80
1	A	562	LEU	CA-CB-CG	6.19	129.53	115.30
2	F	123	LEU	CA-CB-CG	6.09	129.31	115.30
2	B	126	LEU	CA-CB-CG	6.00	129.10	115.30
2	B	82	LEU	CA-CB-CG	5.89	128.84	115.30
2	C	170	LEU	CA-CB-CG	5.73	128.48	115.30
2	E	74	TYR	CB-CG-CD1	5.72	124.43	121.00
2	C	50	LEU	CB-CG-CD2	-5.70	101.31	111.00
2	C	89	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	E	121	ASP	CB-CG-OD2	-5.53	113.33	118.30
2	E	74	TYR	CB-CG-CD2	-5.45	117.73	121.00
2	B	142	TYR	CB-CG-CD2	-5.42	117.75	121.00
2	B	23	TYR	CB-CG-CD1	5.40	124.24	121.00
2	F	202	PRO	CA-C-N	5.38	129.03	117.20
2	E	37	GLU	CA-CB-CG	5.35	125.17	113.40
2	D	137	LEU	CA-CB-CG	5.34	127.59	115.30
2	E	166	ASP	C-N-CD	-5.34	108.86	120.60
2	C	89	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	E	118	LEU	CB-CG-CD2	-5.22	102.12	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	554	SER	Mainchain
2	D	31	HIS	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4479	0	4434	467	1
2	B	1778	0	1776	183	6
2	C	1778	0	1776	213	1
2	D	1778	0	1776	169	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1778	0	1776	198	5
2	F	1778	0	1776	175	0
2	G	1778	0	1776	167	0
3	A	15	0	0	5	0
4	B	20	0	15	8	0
4	C	20	0	15	2	0
4	D	20	0	15	2	0
4	E	20	0	15	2	0
4	F	20	0	15	5	0
4	G	20	0	15	3	0
5	A	257	0	0	34	2
5	B	110	0	0	6	0
5	C	81	0	0	14	0
5	D	123	0	0	18	1
5	E	113	0	0	13	0
5	F	161	0	0	25	0
5	G	116	0	0	16	1
All	All	16243	0	15180	1483	10

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 49.

All (1483) 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:260:ARG:HB3	2:F:194:LYS:HZ1	1.14	1.07
1:A:552:LYS:HB2	1:A:554:SER:HB3	1.41	1.02
2:E:131:LYS:NZ	2:E:135:ASP:OD2	1.94	1.00
1:A:199:HIS:HB3	1:A:525:LYS:H	1.26	0.97
2:F:18:ARG:NH2	2:F:30:GLU:OE2	1.97	0.97
2:B:9:LYS:NZ	2:B:34:GLU:OE2	2.00	0.95
4:F:301:GSH:O11	5:F:401:HOH:O	1.86	0.93
2:G:7:TYR:OH	2:G:30:GLU:OE2	1.84	0.93
2:E:137:LEU:HA	2:E:140:LYS:HE2	1.50	0.93
2:D:95:LEU:HD21	2:D:144:ASN:HB3	1.52	0.92
2:B:10:ILE:O	2:B:18:ARG:NH2	2.03	0.90
2:B:114:ASP:OD2	2:B:117:THR:OG1	1.89	0.90
2:E:103:ARG:NH1	2:E:107:SER:OG	2.03	0.90
2:B:34:GLU:H	2:B:37:GLU:HG3	1.37	0.89
2:F:11:LYS:NZ	2:F:160:ASP:OD2	2.05	0.89
1:A:490:LEU:HD13	1:A:522:VAL:HG21	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:44:LYS:NZ	2:F:57:TYR:OH	2.05	0.88
2:E:22:GLU:OE2	5:E:401:HOH:O	1.91	0.88
2:G:103:ARG:NH2	2:G:154:MET:O	2.07	0.88
2:D:39:ASP:OD2	5:D:401:HOH:O	1.92	0.87
2:D:91:GLU:OE2	2:D:136:ARG:NH2	2.08	0.87
1:A:28:GLN:NE2	1:A:356:PRO:O	2.07	0.87
1:A:40:GLN:NE2	2:D:146:ASP:OD1	2.07	0.87
1:A:108:PRO:HG2	1:A:552:LYS:HG3	1.55	0.87
2:D:146:ASP:O	2:D:147:HIS:ND1	2.08	0.87
1:A:268:THR:HG21	2:F:163:LEU:HD13	1.57	0.87
1:A:405:ASP:HB2	1:A:541:SER:HB3	1.56	0.87
1:A:149:PHE:H	1:A:530:LYS:HE3	1.40	0.86
1:A:403:LEU:HD22	1:A:538:LEU:HD22	1.57	0.86
2:E:170:LEU:HB2	2:E:176:LEU:HD11	1.57	0.85
2:F:202:PRO:HB2	2:F:203:LEU:HA	1.57	0.85
2:C:159:LEU:HD22	2:C:176:LEU:HD21	1.55	0.85
2:E:108:ARG:O	2:E:110:ALA:N	2.10	0.84
2:F:116:GLU:OE2	5:F:403:HOH:O	1.94	0.84
2:C:95:LEU:HD21	2:C:143:LEU:HD13	1.59	0.84
2:C:109:ILE:HG21	2:C:118:LEU:HD12	1.57	0.84
2:F:25:GLU:OE2	5:F:402:HOH:O	1.94	0.84
1:A:150:SER:HB2	1:A:170:TYR:HD2	1.42	0.84
2:E:102:ILE:HD13	2:E:158:ALA:HB1	1.58	0.83
2:B:54:ASN:ND2	4:B:301:GSH:O11	2.11	0.83
2:B:17:THR:HA	2:B:20:LEU:HG	1.61	0.82
2:E:54:ASN:HB3	2:E:66:THR:HG21	1.60	0.82
1:A:351:THR:HB	1:A:410:ILE:HD12	1.60	0.82
1:A:250:LEU:HD22	1:A:260:ARG:HG3	1.61	0.82
1:A:102:GLY:HA2	1:A:546:LYS:HE3	1.60	0.81
2:D:143:LEU:HD11	2:D:155:LEU:HB2	1.60	0.81
2:B:77:ASP:OD2	2:C:89:ARG:NH2	2.14	0.81
2:E:159:LEU:HD13	2:E:180:LYS:HE2	1.63	0.81
2:G:149:THR:HB	2:G:151:PRO:HD2	1.62	0.81
1:A:476:ALA:HB1	1:A:521:ARG:HH21	1.45	0.81
2:B:161:VAL:HG22	2:B:203:LEU:HD22	1.63	0.81
2:D:103:ARG:NH1	5:D:403:HOH:O	2.14	0.81
2:B:20:LEU:HD13	2:B:75:ILE:HG21	1.63	0.81
2:G:71:ILE:HA	2:G:74:TYR:CE2	2.16	0.80
1:A:50:LEU:HB3	2:D:146:ASP:OD2	1.82	0.80
1:A:365:PRO:HA	1:A:388:TYR:HD1	1.45	0.80
2:B:157:ASP:OD2	5:B:401:HOH:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:LEU:HA	2:D:140:LYS:HB3	1.64	0.80
2:E:69:MET:HG3	2:E:100:LEU:HD21	1.62	0.80
2:E:17:THR:HA	2:E:20:LEU:HD13	1.62	0.80
2:E:150:HIS:HA	2:E:153:PHE:HD2	1.46	0.80
1:A:9:ASP:HB3	1:A:12:ARG:HB3	1.65	0.79
1:A:322:ASP:OD2	5:A:701:HOH:O	2.01	0.79
1:A:551:VAL:HG12	1:A:555:ASN:HD22	1.45	0.79
2:B:103:ARG:HH21	2:B:154:MET:HB2	1.46	0.79
2:C:66:THR:HG23	2:C:67:GLN:HG3	1.63	0.79
2:C:77:ASP:OD1	2:C:78:LYS:N	2.16	0.79
1:A:90:THR:HG23	1:A:397:GLY:HA3	1.64	0.79
2:C:22:GLU:OE2	5:C:401:HOH:O	2.00	0.79
2:G:44:LYS:NZ	2:G:47:GLU:OE2	2.15	0.79
1:A:99:LEU:HB3	1:A:557:LYS:H	1.47	0.79
2:F:154:MET:SD	5:F:480:HOH:O	2.41	0.78
1:A:92:HIS:HA	2:D:182:ARG:NH2	1.98	0.78
2:B:82:LEU:C	2:B:84:GLY:H	1.86	0.78
2:E:146:ASP:OD2	5:E:402:HOH:O	2.01	0.78
2:B:60:ASP:H	2:B:63:VAL:HG12	1.49	0.78
1:A:53:ASN:HD22	2:D:87:LYS:HD3	1.49	0.78
2:G:156:TYR:CZ	2:G:183:ILE:HG12	2.18	0.78
2:D:20:LEU:HD22	2:D:150:HIS:HB2	1.66	0.78
2:E:107:SER:O	2:E:204:GLN:NE2	2.17	0.78
2:G:162:VAL:HA	2:G:165:MET:HB3	1.64	0.77
1:A:475:TYR:HB3	1:A:510:ARG:HH22	1.49	0.77
2:G:114:ASP:O	2:G:116:GLU:N	2.15	0.77
2:E:118:LEU:HD23	2:E:122:PHE:HB2	1.65	0.77
2:B:88:GLU:O	2:B:92:ILE:N	2.13	0.77
2:B:13:LEU:HB3	2:B:68:SER:HB2	1.65	0.77
2:E:134:GLU:OE1	5:E:403:HOH:O	2.02	0.77
1:A:226:GLY:HA3	1:A:529:ARG:HE	1.49	0.77
1:A:410:ILE:HD11	1:A:420:LYS:HB2	1.67	0.77
1:A:157:THR:HG22	1:A:469:SER:HB3	1.68	0.76
2:E:26:GLU:O	5:E:401:HOH:O	2.04	0.76
2:B:87:LYS:O	2:B:91:GLU:N	2.19	0.76
2:G:113:LYS:O	5:G:402:HOH:O	2.04	0.76
2:G:47:GLU:OE2	5:G:401:HOH:O	2.01	0.76
2:F:68:SER:OG	4:F:301:GSH:O12	2.04	0.76
1:A:480:GLU:OE2	1:A:527:THR:N	2.18	0.76
2:D:18:ARG:NH2	5:D:404:HOH:O	2.17	0.76
1:A:90:THR:HG22	1:A:91:GLY:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:VAL:HG13	2:B:203:LEU:HD13	1.66	0.75
2:E:162:VAL:O	2:E:166:ASP:N	2.19	0.75
1:A:67:LEU:HA	1:A:400:ARG:HB3	1.68	0.75
1:A:33:LYS:NZ	1:A:53:ASN:OD1	2.18	0.75
2:B:54:ASN:HD21	4:B:301:GSH:HG12	1.51	0.75
2:B:99:VAL:O	2:B:103:ARG:N	2.17	0.75
2:G:103:ARG:HH22	2:G:157:ASP:HB3	1.51	0.75
2:E:20:LEU:HD11	2:E:153:PHE:HB3	1.69	0.75
1:A:108:PRO:O	5:A:702:HOH:O	2.05	0.74
2:F:11:LYS:HA	2:F:15:GLN:HB2	1.68	0.74
2:F:18:ARG:HH22	2:F:30:GLU:CD	1.88	0.74
2:B:82:LEU:HD22	2:B:89:ARG:HH21	1.50	0.74
1:A:199:HIS:H	1:A:524:ALA:HB1	1.52	0.74
2:E:112:SER:OG	5:E:404:HOH:O	2.05	0.74
1:A:443:LEU:O	1:A:447:SER:OG	2.06	0.74
2:B:89:ARG:NE	2:C:73:ARG:HH21	1.86	0.74
1:A:521:ARG:NH1	5:A:705:HOH:O	2.18	0.74
2:E:67:GLN:O	2:E:71:ILE:HG23	1.88	0.74
2:F:134:GLU:HB2	2:F:175:LYS:HE2	1.70	0.74
1:A:332:SER:HB2	1:A:538:LEU:HA	1.70	0.74
2:E:108:ARG:HB3	2:E:111:TYR:HE1	1.53	0.74
2:F:33:TYR:HE1	2:F:40:LYS:HB3	1.52	0.74
2:B:73:ARG:NH2	2:B:96:GLU:OE1	2.21	0.74
2:B:153:PHE:HA	2:B:156:TYR:HB2	1.70	0.73
2:D:50:LEU:HD21	2:D:66:THR:HB	1.70	0.73
1:A:461:ASP:HB3	1:A:528:PHE:HD2	1.53	0.73
2:C:105:GLY:O	2:C:108:ARG:HG3	1.88	0.73
2:G:41:TRP:HB2	2:G:45:LYS:HE2	1.70	0.73
1:A:89:LEU:O	5:A:703:HOH:O	2.06	0.73
2:E:164:TYR:OH	2:E:200:ALA:O	2.07	0.73
2:D:41:TRP:HB3	2:D:45:LYS:HE2	1.69	0.73
2:E:112:SER:OG	2:E:113:LYS:N	2.22	0.73
1:A:192:VAL:O	1:A:195:SER:OG	2.05	0.72
1:A:556:ALA:HA	1:A:559:LEU:HG	1.70	0.72
1:A:517:ALA:HB1	1:A:572:SER:HB3	1.71	0.72
2:E:138:CYS:HA	2:E:175:LYS:HG2	1.69	0.72
2:F:123:LEU:HA	2:F:126:LEU:HD23	1.70	0.72
2:C:58:TYR:HB3	2:C:65:LEU:HB2	1.70	0.72
2:E:104:TYR:HB3	2:E:108:ARG:HH12	1.52	0.72
1:A:101:SER:OG	1:A:544:GLN:HB3	1.90	0.72
1:A:7:THR:O	1:A:12:ARG:NH2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:176:LEU:O	2:G:180:LYS:N	2.22	0.72
1:A:165:ALA:HB2	1:A:333:SER:HB3	1.71	0.72
1:A:487:GLU:OE1	1:A:570:TYR:OH	2.05	0.72
1:A:540:SER:OG	1:A:541:SER:N	2.22	0.72
2:F:99:VAL:HG11	2:F:154:MET:HG3	1.72	0.72
1:A:289:GLY:HA2	1:A:319:TYR:O	1.88	0.72
2:G:14:VAL:HG22	2:G:56:PRO:HG3	1.70	0.72
1:A:332:SER:OG	1:A:334:GLU:OE1	2.06	0.72
2:E:136:ARG:HG2	2:E:140:LYS:HZ3	1.55	0.72
2:C:33:TYR:HB2	2:C:37:GLU:HB2	1.72	0.72
2:C:89:ARG:CZ	2:C:89:ARG:HB2	2.18	0.72
2:D:191:LYS:O	2:D:195:SER:OG	2.08	0.72
2:D:139:HIS:O	5:D:402:HOH:O	2.08	0.71
2:E:116:GLU:OE2	2:E:119:LYS:HB2	1.89	0.71
1:A:331:GLY:HA3	1:A:336:TRP:CE3	2.26	0.71
1:A:390:VAL:HG11	1:A:540:SER:HA	1.72	0.71
1:A:153:GLN:HA	1:A:560:GLN:HG2	1.73	0.71
2:D:161:VAL:HG13	2:D:203:LEU:HD13	1.72	0.71
2:F:8:TRP:H	2:F:55:LEU:HD23	1.54	0.71
1:A:534:HIS:O	5:A:704:HOH:O	2.09	0.71
2:F:159:LEU:HD13	2:F:176:LEU:HD21	1.72	0.71
2:D:157:ASP:OD1	2:D:158:ALA:N	2.24	0.71
2:E:174:PRO:HG2	2:E:175:LYS:HD2	1.72	0.71
2:E:177:VAL:HA	2:E:180:LYS:HD2	1.73	0.71
2:F:7:TYR:HE1	2:F:10:ILE:H	1.39	0.71
2:F:96:GLU:OE2	2:F:150:HIS:NE2	2.18	0.71
2:G:192:TYR:O	2:G:198:TYR:HB2	1.90	0.71
1:A:467:ASP:OD2	1:A:470:THR:OG1	2.08	0.71
1:A:465:TYR:HB3	1:A:476:ALA:HB3	1.71	0.71
2:E:34:GLU:N	2:E:37:GLU:OE1	2.22	0.71
1:A:101:SER:OG	1:A:544:GLN:NE2	2.23	0.71
1:A:76:TYR:CD2	1:A:89:LEU:HB3	2.26	0.71
2:D:67:GLN:OE1	4:D:301:GSH:N1	2.24	0.71
2:D:10:ILE:HG12	2:D:202:PRO:HG2	1.72	0.70
2:F:6:GLY:HA3	2:F:57:TYR:CE2	2.26	0.70
2:E:140:LYS:HZ2	2:E:143:LEU:HA	1.56	0.70
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.73	0.70
2:B:67:GLN:O	2:B:71:ILE:HG23	1.90	0.70
2:F:40:LYS:NZ	5:F:415:HOH:O	2.23	0.70
2:D:67:GLN:HE21	2:D:69:MET:H	1.37	0.70
1:A:132:ARG:HA	1:A:343:PRO:HG3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:GLU:OE1	5:B:402:HOH:O	2.09	0.70
1:A:574:ALA:HA	2:C:174:PRO:HB2	1.71	0.70
2:C:41:TRP:HZ3	2:C:55:LEU:HD21	1.56	0.70
1:A:200:GLN:HA	1:A:203:TYR:CE2	2.26	0.70
2:G:9:LYS:HA	2:G:32:LEU:HD22	1.72	0.70
1:A:513:LYS:HE2	1:A:517:ALA:HB2	1.74	0.70
2:F:15:GLN:HA	2:F:18:ARG:HG3	1.74	0.70
2:F:2:SER:OG	2:F:29:GLU:OE1	2.08	0.70
2:F:37:GLU:O	2:F:40:LYS:N	2.23	0.70
2:G:201:TRP:CD2	2:G:202:PRO:HA	2.26	0.70
1:A:198:VAL:HG22	1:A:524:ALA:HB3	1.72	0.70
2:D:156:TYR:O	2:D:160:ASP:N	2.22	0.70
1:A:451:ARG:HE	1:A:489:VAL:HA	1.57	0.69
2:C:13:LEU:HD13	2:C:68:SER:HB3	1.74	0.69
2:D:143:LEU:HD21	2:D:155:LEU:HD22	1.73	0.69
1:A:105:GLN:NE2	5:A:722:HOH:O	2.23	0.69
1:A:220:PHE:HD1	1:A:302:TYR:HB3	1.58	0.69
2:F:182:ARG:NH1	5:F:416:HOH:O	2.26	0.69
1:A:546:LYS:O	5:A:706:HOH:O	2.11	0.69
2:G:136:ARG:O	5:G:403:HOH:O	2.10	0.69
2:C:77:ASP:HB3	2:C:82:LEU:HB2	1.75	0.69
2:D:179:PHE:HD2	2:D:182:ARG:HH11	1.41	0.69
2:D:99:VAL:HG12	2:D:103:ARG:HE	1.58	0.69
2:G:67:GLN:HE21	2:G:69:MET:HG2	1.57	0.69
1:A:457:ILE:HD12	1:A:485:THR:HG23	1.73	0.69
2:C:150:HIS:HA	2:C:153:PHE:CD2	2.28	0.69
2:C:28:TYR:OH	5:C:401:HOH:O	2.10	0.69
2:G:11:LYS:HZ3	2:G:200:ALA:HA	1.58	0.69
1:A:325:LEU:HB2	1:A:347:PRO:HD3	1.74	0.69
2:G:60:ASP:OD1	2:G:61:GLY:N	2.23	0.69
1:A:521:ARG:O	5:A:705:HOH:O	2.10	0.68
2:B:82:LEU:C	2:B:84:GLY:N	2.47	0.68
2:E:50:LEU:HD23	2:E:53:PRO:HA	1.76	0.68
1:A:454:GLU:OE2	5:A:707:HOH:O	2.12	0.68
2:B:99:VAL:HG12	2:B:103:ARG:HG3	1.75	0.68
2:B:133:PHE:O	2:B:137:LEU:HD12	1.93	0.68
1:A:316:LEU:O	1:A:320:ALA:N	2.26	0.68
2:B:82:LEU:HD12	2:B:83:GLY:H	1.58	0.68
2:B:143:LEU:HD11	2:B:155:LEU:HD22	1.74	0.68
2:E:116:GLU:HG2	2:E:119:LYS:HD3	1.75	0.68
2:G:119:LYS:HE3	2:G:123:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:HB2	5:A:708:HOH:O	1.94	0.68
2:C:111:TYR:HA	2:C:209:THR:H	1.58	0.68
2:D:13:LEU:O	5:D:403:HOH:O	2.12	0.68
2:C:44:LYS:NZ	2:C:57:TYR:OH	2.25	0.68
2:F:115:PHE:HB2	2:F:119:LYS:HE2	1.76	0.68
1:A:365:PRO:HA	1:A:388:TYR:CD1	2.27	0.68
2:C:103:ARG:HH22	2:C:162:VAL:HG23	1.58	0.68
2:B:15:GLN:OE1	2:B:18:ARG:NH1	2.27	0.67
2:G:182:ARG:NH2	5:G:411:HOH:O	2.26	0.67
1:A:219:VAL:HG21	1:A:295:PHE:CZ	2.29	0.67
2:B:58:TYR:CZ	2:B:65:LEU:HB2	2.29	0.67
2:E:134:GLU:OE2	5:E:405:HOH:O	2.11	0.67
2:B:93:SER:O	2:B:97:GLY:N	2.26	0.67
2:C:137:LEU:HD11	2:C:143:LEU:HG	1.75	0.67
1:A:450:LYS:HG3	2:C:190:ASP:HA	1.77	0.67
2:E:10:ILE:HA	2:E:199:ILE:HG21	1.77	0.67
2:G:152:ASP:OD1	2:G:153:PHE:N	2.28	0.67
1:A:478:PHE:CZ	1:A:562:LEU:HB3	2.30	0.67
2:B:100:LEU:HD12	2:B:103:ARG:NH1	2.10	0.67
2:B:52:PHE:CE2	2:C:94:MET:HG2	2.30	0.67
2:E:140:LYS:NZ	2:E:143:LEU:HA	2.10	0.67
1:A:151:SER:O	1:A:565:ASN:ND2	2.28	0.67
2:E:102:ILE:HD12	2:E:126:LEU:HD11	1.76	0.67
2:F:50:LEU:HD11	2:F:65:LEU:HA	1.76	0.67
5:F:456:HOH:O	2:G:94:MET:SD	2.52	0.67
2:B:74:TYR:O	2:B:78:LYS:HG2	1.94	0.67
2:G:97:GLY:HA2	2:G:100:LEU:HD12	1.77	0.67
2:E:22:GLU:HB3	2:E:192:TYR:CE2	2.30	0.67
2:B:119:LYS:O	2:B:123:LEU:N	2.27	0.67
2:C:165:MET:HA	2:C:210:PHE:HZ	1.60	0.67
2:D:76:ALA:HB1	2:D:81:MET:HB2	1.74	0.67
2:F:116:GLU:HA	2:F:119:LYS:HG2	1.77	0.66
1:A:447:SER:O	5:A:709:HOH:O	2.12	0.66
2:D:136:ARG:NH1	2:E:51:GLU:OE1	2.29	0.66
2:D:96:GLU:OE2	2:D:150:HIS:HE1	1.78	0.66
2:D:42:ARG:NH1	5:D:416:HOH:O	2.28	0.66
2:G:32:LEU:HD11	2:G:199:ILE:HD11	1.77	0.66
2:G:103:ARG:NH2	2:G:157:ASP:HB3	2.09	0.66
1:A:147:PHE:HB3	1:A:529:ARG:HH22	1.58	0.66
2:E:195:SER:OG	2:E:196:SER:N	2.27	0.66
1:A:129:PHE:HA	1:A:132:ARG:HD3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:SER:O	1:A:543:GLY:N	2.28	0.66
2:F:102:ILE:O	5:F:405:HOH:O	2.13	0.66
2:B:89:ARG:NH1	2:C:82:LEU:HD23	2.10	0.66
2:E:103:ARG:HH12	2:E:107:SER:HG	1.41	0.66
2:F:170:LEU:HD12	2:F:173:PHE:HB2	1.78	0.66
1:A:448:ALA:O	2:C:181:LYS:NZ	2.29	0.66
2:C:159:LEU:HD12	2:C:180:LYS:HB2	1.77	0.66
2:B:122:PHE:HA	2:B:125:LYS:HE3	1.77	0.66
2:B:153:PHE:CZ	2:B:189:ILE:HG12	2.30	0.65
2:C:188:GLN:NE2	5:C:408:HOH:O	2.29	0.65
2:F:192:TYR:O	5:F:404:HOH:O	2.13	0.65
2:G:18:ARG:HD2	2:G:19:LEU:HD13	1.77	0.65
1:A:207:LEU:HA	1:A:210:ILE:HD12	1.76	0.65
2:D:177:VAL:HA	2:D:180:LYS:HE2	1.78	0.65
2:F:163:LEU:HD11	2:F:170:LEU:HD23	1.77	0.65
1:A:461:ASP:HB3	1:A:528:PHE:CD2	2.31	0.65
1:A:92:HIS:HA	2:D:182:ARG:HH22	1.61	0.65
2:B:88:GLU:HG3	2:B:92:ILE:HG13	1.78	0.65
2:C:128:GLU:O	2:C:132:MET:HG2	1.96	0.65
2:D:189:ILE:HA	2:D:192:TYR:CD2	2.31	0.65
2:E:140:LYS:HE3	2:E:143:LEU:HA	1.78	0.65
2:B:156:TYR:CZ	2:B:183:ILE:HG12	2.32	0.65
2:B:67:GLN:HA	4:B:301:GSH:O11	1.96	0.65
2:B:68:SER:O	2:B:71:ILE:HG12	1.97	0.65
2:E:160:ASP:HA	2:E:163:LEU:HB2	1.77	0.65
1:A:154:TYR:O	5:A:711:HOH:O	2.14	0.65
1:A:522:VAL:HB	1:A:567:VAL:HB	1.79	0.65
2:G:156:TYR:O	2:G:160:ASP:N	2.29	0.65
1:A:465:TYR:HD1	1:A:551:VAL:HG23	1.62	0.65
1:A:563:CYS:N	5:A:708:HOH:O	2.12	0.65
2:D:51:GLU:OE1	2:E:136:ARG:NH1	2.29	0.65
2:E:140:LYS:HZ1	2:E:143:LEU:HD23	1.62	0.65
1:A:31:THR:HG21	1:A:357:ASN:HA	1.79	0.65
2:G:59:ILE:HG23	2:G:64:LYS:HE3	1.79	0.65
2:F:16:PRO:HG3	2:F:154:MET:HA	1.79	0.64
2:F:66:THR:HG23	2:F:67:GLN:HG2	1.79	0.64
1:A:450:LYS:HE3	2:C:189:ILE:HG13	1.78	0.64
2:D:153:PHE:HE1	2:D:183:ILE:HB	1.60	0.64
2:G:79:HIS:NE2	2:G:150:HIS:HE1	1.94	0.64
1:A:552:LYS:C	1:A:554:SER:N	2.48	0.64
1:A:93:PRO:HB2	2:D:178:CYS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HD3	2:F:184:GLU:HG2	1.79	0.64
2:B:3:PRO:HB3	2:B:60:ASP:HA	1.80	0.64
1:A:114:THR:O	5:A:712:HOH:O	2.14	0.64
1:A:120:ASN:HB3	1:A:358:LEU:HD21	1.79	0.64
1:A:511:LYS:O	5:A:713:HOH:O	2.15	0.64
2:C:20:LEU:HA	2:C:23:TYR:HD2	1.62	0.64
2:F:92:ILE:O	2:F:96:GLU:HG3	1.97	0.64
1:A:365:PRO:HB2	1:A:374:GLU:HB3	1.79	0.64
1:A:60:ALA:O	1:A:64:MET:HB3	1.98	0.64
2:E:13:LEU:O	2:E:68:SER:OG	2.15	0.64
2:C:96:GLU:OE2	2:C:150:HIS:HE1	1.81	0.64
2:C:18:ARG:HA	2:C:21:LEU:HD12	1.80	0.64
2:D:192:TYR:O	2:D:198:TYR:HB2	1.98	0.64
1:A:474:HIS:HB2	1:A:475:TYR:CD2	2.32	0.64
2:D:141:THR:HA	2:D:182:ARG:NH2	2.13	0.64
1:A:355:ILE:HD12	1:A:358:LEU:HD13	1.80	0.64
2:B:74:TYR:CZ	2:B:78:LYS:HE2	2.33	0.64
1:A:100:SER:HG	1:A:401:TYR:HH	1.44	0.64
2:F:67:GLN:NE2	5:F:420:HOH:O	2.31	0.64
1:A:552:LYS:C	1:A:554:SER:H	1.98	0.63
2:C:206:TRP:HZ3	2:C:214:ASP:HA	1.61	0.63
1:A:16:GLU:O	1:A:20:MET:HB2	1.99	0.63
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.79	0.63
1:A:552:LYS:HE2	1:A:554:SER:HB3	1.80	0.63
2:B:156:TYR:OH	2:B:179:PHE:O	2.12	0.63
2:G:159:LEU:O	2:G:163:LEU:N	2.31	0.63
2:G:18:ARG:HH21	2:G:198:TYR:HE1	1.46	0.63
2:F:40:LYS:HA	2:F:43:ASN:HB3	1.81	0.63
2:F:48:LEU:HD23	2:F:50:LEU:HD13	1.80	0.63
2:G:19:LEU:O	2:G:23:TYR:N	2.29	0.63
1:A:99:LEU:N	1:A:556:ALA:HB3	2.12	0.63
2:B:153:PHE:HZ	2:B:189:ILE:HG12	1.64	0.63
2:E:150:HIS:HA	2:E:153:PHE:CD2	2.32	0.63
2:G:11:LYS:HB2	2:G:203:LEU:HA	1.79	0.63
1:A:117:LEU:O	1:A:121:THR:N	2.30	0.63
1:A:64:MET:HG2	1:A:65:VAL:N	2.11	0.63
2:B:20:LEU:HB2	2:B:23:TYR:CE2	2.34	0.63
2:D:50:LEU:HD23	2:D:53:PRO:HA	1.81	0.63
2:F:204:GLN:O	5:F:407:HOH:O	2.16	0.63
1:A:364:LEU:HD22	1:A:389:GLU:OE2	1.97	0.63
2:E:8:TRP:HD1	2:E:33:TYR:O	1.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:O	1:A:572:SER:N	2.32	0.63
2:D:149:THR:HB	2:D:151:PRO:HD2	1.81	0.63
2:G:7:TYR:CE1	2:G:32:LEU:HD21	2.34	0.63
2:E:140:LYS:CE	2:E:143:LEU:HA	2.29	0.63
2:F:201:TRP:CE2	2:F:202:PRO:HB3	2.33	0.63
2:C:115:PHE:CG	2:C:210:PHE:HB2	2.33	0.62
2:F:75:ILE:O	2:F:79:HIS:ND1	2.31	0.62
1:A:450:LYS:HD2	2:C:184:GLU:HB3	1.80	0.62
2:E:23:TYR:HB2	2:E:189:ILE:HG23	1.79	0.62
1:A:438:GLU:HG2	1:A:549:ARG:HD2	1.81	0.62
2:E:82:LEU:HD23	2:E:89:ARG:HH11	1.62	0.62
1:A:135:ASP:OD2	1:A:343:PRO:HG2	2.00	0.62
1:A:122:LEU:O	1:A:126:ARG:HB2	2.00	0.62
1:A:150:SER:HB2	1:A:170:TYR:CD2	2.32	0.62
2:E:60:ASP:OD1	2:E:63:VAL:N	2.24	0.62
2:G:22:GLU:HB3	2:G:192:TYR:CZ	2.34	0.62
2:B:132:MET:O	2:B:136:ARG:HG2	1.99	0.62
2:E:106:VAL:HG11	2:E:161:VAL:HG11	1.80	0.62
2:F:7:TYR:HB3	2:F:56:PRO:HA	1.80	0.62
2:G:74:TYR:O	2:G:78:LYS:HG2	1.99	0.62
2:C:155:LEU:HD21	2:C:179:PHE:HE2	1.65	0.62
1:A:32:LEU:O	1:A:36:LEU:HG	2.00	0.62
2:C:35:ARG:NH2	2:C:36:ASP:OD1	2.33	0.62
2:D:99:VAL:HG11	2:D:154:MET:HB3	1.82	0.62
2:B:99:VAL:HA	2:B:102:ILE:HB	1.81	0.62
2:B:159:LEU:HD22	2:B:176:LEU:HD21	1.80	0.62
1:A:467:ASP:O	1:A:473:GLY:HA2	2.00	0.62
2:B:14:VAL:HB	2:B:18:ARG:HH21	1.65	0.62
2:C:165:MET:HA	2:C:210:PHE:CZ	2.35	0.62
2:C:8:TRP:NE1	4:C:301:GSH:HB22	2.14	0.62
2:G:138:CYS:SG	2:G:175:LYS:NZ	2.72	0.62
2:G:42:ARG:NH1	5:G:414:HOH:O	2.32	0.62
2:F:52:PHE:H	2:F:65:LEU:HD21	1.64	0.61
2:D:94:MET:HG3	2:E:65:LEU:HD22	1.80	0.61
2:E:79:HIS:CE1	2:E:81:MET:HG3	2.35	0.61
1:A:116:GLU:O	1:A:120:ASN:N	2.31	0.61
2:D:146:ASP:N	2:D:146:ASP:OD1	2.33	0.61
2:D:110:ALA:HB1	2:D:204:GLN:HE22	1.64	0.61
2:C:101:ASP:OD1	2:C:102:ILE:N	2.33	0.61
2:G:39:ASP:OD1	2:G:42:ARG:NH2	2.33	0.61
1:A:441:LEU:HD23	1:A:549:ARG:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TYR:O	2:B:108:ARG:HG3	1.99	0.61
1:A:196:PRO:HA	1:A:565:ASN:ND2	2.16	0.61
2:B:156:TYR:HA	2:B:159:LEU:HG	1.82	0.61
1:A:129:PHE:CZ	1:A:182:ILE:HB	2.36	0.61
1:A:145:LEU:O	1:A:220:PHE:N	2.33	0.61
2:C:9:LYS:HB3	2:C:206:TRP:HE1	1.65	0.61
2:B:74:TYR:CE2	2:B:78:LYS:HE2	2.36	0.61
2:D:87:LYS:NZ	5:D:414:HOH:O	2.27	0.61
2:G:201:TRP:NE1	2:G:213:GLY:O	2.34	0.61
1:A:329:ASP:HB3	1:A:339:ALA:HA	1.83	0.61
1:A:93:PRO:HD3	2:D:182:ARG:HD3	1.83	0.61
2:B:139:HIS:HB2	2:B:140:LYS:HD2	1.83	0.61
2:E:109:ILE:HD12	2:E:110:ALA:HB2	1.82	0.61
2:G:201:TRP:HE1	2:G:213:GLY:C	2.04	0.61
1:A:199:HIS:CE1	1:A:200:GLN:HG3	2.36	0.61
2:B:49:GLY:O	2:B:64:LYS:NZ	2.30	0.61
2:C:127:PRO:HD3	5:C:404:HOH:O	2.01	0.61
4:F:301:GSH:OE1	5:F:408:HOH:O	2.16	0.61
2:G:159:LEU:HD13	2:G:176:LEU:HD21	1.83	0.61
1:A:188:SER:HB3	1:A:205:HIS:HB2	1.83	0.60
1:A:76:TYR:CZ	1:A:89:LEU:HD22	2.36	0.60
2:D:189:ILE:HA	2:D:192:TYR:CE2	2.36	0.60
2:E:156:TYR:O	2:E:160:ASP:N	2.32	0.60
2:F:65:LEU:HB3	2:G:94:MET:SD	2.41	0.60
1:A:150:SER:HA	1:A:167:THR:HG22	1.83	0.60
1:A:333:SER:OG	5:A:714:HOH:O	2.16	0.60
2:B:201:TRP:CE2	2:B:216:PRO:HA	2.36	0.60
2:F:11:LYS:HE3	2:F:157:ASP:OD1	2.02	0.60
2:F:40:LYS:O	2:F:44:LYS:N	2.33	0.60
1:A:312:TYR:HD2	1:A:315:LYS:HE2	1.65	0.60
2:E:76:ALA:HB2	2:E:150:HIS:CD2	2.35	0.60
2:F:171:ASP:OD2	5:F:406:HOH:O	2.15	0.60
2:C:120:VAL:HA	2:C:123:LEU:HG	1.83	0.60
2:E:163:LEU:HD23	2:E:166:ASP:OD2	2.01	0.60
2:E:68:SER:O	2:E:71:ILE:HG13	2.01	0.60
2:G:68:SER:HA	2:G:71:ILE:HB	1.82	0.60
1:A:143:LYS:HB2	1:A:212:PHE:CE2	2.36	0.60
2:C:206:TRP:CZ3	2:C:214:ASP:HA	2.36	0.60
2:E:114:ASP:N	5:E:404:HOH:O	2.34	0.60
2:E:122:PHE:O	2:E:126:LEU:HB2	2.01	0.60
2:F:202:PRO:HD2	2:F:203:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:PHE:O	5:F:410:HOH:O	2.16	0.60
2:G:34:GLU:HB2	2:G:37:GLU:HG3	1.84	0.60
1:A:76:TYR:HE2	1:A:90:THR:HG1	1.47	0.60
1:A:92:HIS:NE2	2:D:175:LYS:O	2.30	0.60
1:A:39:ASN:OD1	5:D:402:HOH:O	2.15	0.60
2:D:142:TYR:HB3	2:D:152:ASP:CG	2.21	0.60
2:D:94:MET:HE3	2:E:65:LEU:HB3	1.84	0.60
1:A:250:LEU:HD21	1:A:254:ILE:HB	1.84	0.60
2:E:153:PHE:HA	2:E:156:TYR:CE2	2.37	0.60
1:A:308:SER:HA	1:A:424:ARG:HE	1.67	0.59
1:A:92:HIS:CD2	1:A:93:PRO:HD2	2.37	0.59
1:A:38:LYS:O	2:D:140:LYS:HG3	2.02	0.59
2:D:82:LEU:HD11	2:E:73:ARG:HH22	1.67	0.59
1:A:111:ILE:HB	1:A:398:LEU:HD21	1.84	0.59
1:A:389:GLU:HB3	1:A:406:VAL:HG22	1.84	0.59
1:A:65:VAL:O	1:A:400:ARG:NH1	2.35	0.59
1:A:552:LYS:HE2	1:A:554:SER:CB	2.32	0.59
2:F:11:LYS:HE2	2:F:203:LEU:H	1.66	0.59
2:G:11:LYS:N	2:G:202:PRO:O	2.24	0.59
2:E:15:GLN:HG2	2:E:157:ASP:OD2	2.03	0.59
1:A:423:CYS:SG	1:A:541:SER:OG	2.59	0.59
2:F:69:MET:SD	2:F:100:LEU:HD11	2.43	0.59
1:A:217:GLN:HA	1:A:298:ALA:HA	1.84	0.59
2:D:108:ARG:O	5:D:405:HOH:O	2.17	0.59
2:C:99:VAL:HG23	2:C:158:ALA:HB2	1.83	0.59
2:D:15:GLN:HG3	2:D:16:PRO:HD3	1.85	0.59
1:A:92:HIS:HE2	2:D:175:LYS:C	2.05	0.59
2:E:112:SER:HG	2:E:113:LYS:H	1.50	0.59
2:E:71:ILE:HA	2:E:74:TYR:CD2	2.37	0.59
2:D:159:LEU:HD13	2:D:176:LEU:HD21	1.85	0.59
2:E:158:ALA:O	2:E:162:VAL:HG23	2.02	0.59
2:E:176:LEU:HD13	2:E:180:LYS:HE3	1.84	0.59
1:A:339:ALA:O	1:A:353:ALA:N	2.20	0.59
2:C:103:ARG:HH12	2:C:162:VAL:HG23	1.67	0.59
1:A:98:SER:N	5:A:734:HOH:O	2.35	0.58
1:A:265:LYS:HG3	2:F:193:LEU:HD11	1.84	0.58
2:C:89:ARG:NH1	2:C:89:ARG:HB2	2.17	0.58
2:E:15:GLN:HB3	2:E:16:PRO:HD2	1.84	0.58
2:B:174:PRO:O	2:B:177:VAL:HG22	2.03	0.58
2:D:11:LYS:HE2	2:D:199:ILE:O	2.04	0.58
2:F:202:PRO:HB2	2:F:203:LEU:CA	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:PHE:CD2	1:A:541:SER:HA	2.39	0.58
2:C:26:GLU:O	5:C:403:HOH:O	2.17	0.58
2:D:38:GLY:O	5:D:407:HOH:O	2.17	0.58
1:A:525:LYS:NZ	5:A:720:HOH:O	2.32	0.58
2:B:115:PHE:CD2	2:B:209:THR:HB	2.38	0.58
2:B:77:ASP:OD1	2:B:78:LYS:N	2.37	0.58
2:C:126:LEU:HG	2:C:130:LEU:HG	1.85	0.58
2:G:62:ASP:O	2:G:63:VAL:HB	2.02	0.58
1:A:64:MET:O	5:A:715:HOH:O	2.17	0.58
2:B:20:LEU:HB2	2:B:23:TYR:CD2	2.39	0.58
2:D:80:ASN:OD1	5:D:406:HOH:O	2.17	0.58
1:A:50:LEU:HD21	1:A:65:VAL:HG21	1.86	0.58
2:C:41:TRP:CZ3	2:C:55:LEU:HD21	2.38	0.58
2:G:87:LYS:O	2:G:91:GLU:HG2	2.04	0.58
1:A:144:ALA:HB1	1:A:218:TYR:HB2	1.84	0.58
1:A:325:LEU:HD12	1:A:347:PRO:HG3	1.85	0.58
1:A:35:ILE:O	1:A:39:ASN:N	2.36	0.58
1:A:99:LEU:HD13	1:A:555:ASN:OD1	2.04	0.58
2:D:33:TYR:CG	2:D:41:TRP:HH2	2.22	0.58
1:A:191:GLU:OE2	2:F:187:PRO:HD3	2.04	0.57
2:B:123:LEU:O	2:B:126:LEU:HG	2.04	0.57
2:G:6:GLY:HA3	2:G:57:TYR:CZ	2.38	0.57
1:A:140:ASP:OD1	1:A:140:ASP:N	2.29	0.57
2:F:35:ARG:NE	5:F:419:HOH:O	2.29	0.57
2:G:121:ASP:OD1	2:G:122:PHE:N	2.37	0.57
2:G:56:PRO:HG2	2:G:71:ILE:CD1	2.33	0.57
1:A:551:VAL:HB	1:A:555:ASN:CB	2.33	0.57
2:F:207:GLN:NE2	5:F:412:HOH:O	2.22	0.57
1:A:97:ILE:HG12	1:A:162:VAL:HB	1.86	0.57
2:F:30:GLU:OE1	2:F:32:LEU:HD11	2.04	0.57
2:G:138:CYS:HA	2:G:175:LYS:NZ	2.19	0.57
1:A:77:ILE:HB	1:A:110:PHE:HD2	1.70	0.57
2:D:170:LEU:HD13	2:D:176:LEU:HB3	1.87	0.57
2:D:87:LYS:HE2	2:E:62:ASP:OD1	2.05	0.57
2:F:97:GLY:HA3	2:G:67:GLN:HG2	1.86	0.57
1:A:99:LEU:HB3	1:A:557:LYS:HG2	1.86	0.57
1:A:62:LYS:HG3	1:A:63:SER:N	2.20	0.57
2:G:22:GLU:HB3	2:G:192:TYR:CE2	2.40	0.57
2:C:126:LEU:N	5:C:404:HOH:O	2.34	0.57
2:D:166:ASP:OD1	2:D:168:MET:HG2	2.04	0.57
2:F:115:PHE:HB2	2:F:119:LYS:CE	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HG13	1:A:295:PHE:CZ	2.39	0.57
1:A:367:SER:O	5:A:716:HOH:O	2.17	0.57
2:B:82:LEU:HD22	2:B:89:ARG:NH2	2.17	0.57
2:D:163:LEU:HD12	2:D:167:PRO:HA	1.87	0.57
2:E:6:GLY:HA3	2:E:57:TYR:CE2	2.40	0.57
2:C:11:LYS:HD3	2:C:18:ARG:HH11	1.70	0.57
2:B:89:ARG:HE	2:C:73:ARG:HH21	1.52	0.57
2:E:143:LEU:N	2:E:152:ASP:OD1	2.30	0.57
2:G:24:LEU:O	2:G:25:GLU:HG2	2.05	0.57
2:C:110:ALA:HB3	2:C:204:GLN:OE1	2.05	0.57
1:A:92:HIS:CD2	2:D:175:LYS:HB3	2.40	0.57
2:G:168:MET:HA	2:G:171:ASP:OD2	2.05	0.57
1:A:268:THR:O	5:A:717:HOH:O	2.17	0.56
1:A:337:ILE:O	1:A:354:VAL:HA	2.05	0.56
1:A:386:GLU:OE1	1:A:388:TYR:OH	2.17	0.56
1:A:486:ASN:OD1	1:A:487:GLU:N	2.35	0.56
2:D:142:TYR:HB3	2:D:152:ASP:OD2	2.05	0.56
2:E:104:TYR:HB3	2:E:108:ARG:NH1	2.19	0.56
2:E:119:LYS:O	2:E:123:LEU:HB2	2.05	0.56
1:A:336:TRP:HB2	1:A:358:LEU:HD22	1.87	0.56
1:A:99:LEU:HG	1:A:535:PHE:HZ	1.70	0.56
2:D:161:VAL:HG22	2:D:203:LEU:HD22	1.87	0.56
1:A:197:ASP:N	1:A:197:ASP:OD1	2.39	0.56
1:A:421:PHE:HD2	1:A:541:SER:HA	1.69	0.56
1:A:147:PHE:CB	1:A:529:ARG:HH22	2.18	0.56
1:A:80:MET:HA	1:A:85:THR:HA	1.86	0.56
2:B:110:ALA:HB1	2:B:204:GLN:HG2	1.87	0.56
2:E:155:LEU:O	2:E:159:LEU:HG	2.05	0.56
2:F:201:TRP:CD1	2:F:216:PRO:HG3	2.41	0.56
2:F:8:TRP:O	2:F:10:ILE:HG23	2.05	0.56
2:B:136:ARG:NH2	2:C:51:GLU:OE1	2.39	0.56
2:D:157:ASP:O	2:D:161:VAL:HG23	2.05	0.56
2:D:188:GLN:N	2:D:188:GLN:OE1	2.38	0.56
1:A:199:HIS:CE1	1:A:200:GLN:HE21	2.23	0.56
2:C:168:MET:HB3	2:C:171:ASP:OD2	2.04	0.56
1:A:77:ILE:HB	1:A:110:PHE:CD2	2.40	0.56
2:B:115:PHE:HD2	2:B:209:THR:HB	1.70	0.56
2:G:74:TYR:CE1	2:G:75:ILE:HG13	2.40	0.56
1:A:393:THR:HG23	1:A:399:TYR:CD1	2.41	0.56
1:A:53:ASN:ND2	2:D:87:LYS:HD3	2.17	0.56
1:A:41:SER:CB	2:D:142:TYR:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LEU:HG	2:D:192:TYR:HD2	1.70	0.56
2:F:71:ILE:HA	2:F:74:TYR:HD2	1.71	0.56
1:A:73:LEU:HD22	5:A:798:HOH:O	2.06	0.56
2:C:155:LEU:O	2:C:159:LEU:HG	2.06	0.56
2:C:21:LEU:O	2:C:26:GLU:N	2.39	0.56
2:F:202:PRO:CB	2:F:211:GLY:HA2	2.36	0.56
1:A:118:MET:O	1:A:121:THR:OG1	2.21	0.56
1:A:199:HIS:HA	1:A:525:LYS:HG2	1.87	0.56
2:B:126:LEU:HD13	2:B:130:LEU:HD12	1.87	0.56
2:C:9:LYS:HD3	2:C:206:TRP:HZ2	1.70	0.56
2:D:108:ARG:HG3	2:E:108:ARG:NE	2.21	0.56
2:E:39:ASP:O	2:E:41:TRP:HD1	1.89	0.56
2:E:74:TYR:HA	2:E:77:ASP:OD1	2.06	0.56
2:B:39:ASP:O	2:B:43:ASN:ND2	2.38	0.56
2:G:99:VAL:HG22	2:G:155:LEU:HD13	1.88	0.56
1:A:146:GLN:HE21	1:A:186:SER:HB2	1.70	0.55
1:A:530:LYS:O	1:A:533:GLU:HB2	2.06	0.55
2:C:123:LEU:O	5:C:404:HOH:O	2.18	0.55
2:C:103:ARG:HH12	2:C:162:VAL:CG2	2.18	0.55
2:D:110:ALA:HB1	2:D:204:GLN:NE2	2.21	0.55
2:D:48:LEU:HD22	2:D:50:LEU:HD22	1.88	0.55
2:D:68:SER:OG	5:D:403:HOH:O	2.09	0.55
2:E:23:TYR:CD1	2:E:188:GLN:HB2	2.41	0.55
2:G:67:GLN:O	2:G:71:ILE:N	2.37	0.55
1:A:93:PRO:HD3	2:D:182:ARG:NH2	2.21	0.55
2:F:7:TYR:CZ	2:F:14:VAL:HG11	2.40	0.55
1:A:76:TYR:HE2	1:A:90:THR:OG1	1.90	0.55
2:E:162:VAL:C	2:E:166:ASP:OD1	2.45	0.55
2:F:208:ALA:O	2:F:212:GLY:HA3	2.06	0.55
2:F:5:LEU:HB2	2:F:30:GLU:OE2	2.06	0.55
1:A:117:LEU:HD21	1:A:335:GLY:HA2	1.89	0.55
2:B:64:LYS:O	2:B:65:LEU:HD23	2.07	0.55
2:C:116:GLU:HA	2:C:119:LYS:HD3	1.89	0.55
2:E:158:ALA:O	2:E:161:VAL:HG12	2.06	0.55
2:G:52:PHE:HZ	2:G:64:LYS:O	1.89	0.55
1:A:200:GLN:OE1	1:A:254:ILE:HG23	2.06	0.55
2:B:50:LEU:HA	2:B:64:LYS:HE3	1.89	0.55
2:F:52:PHE:HE1	2:G:136:ARG:HB2	1.72	0.55
1:A:154:TYR:HB3	1:A:560:GLN:HA	1.88	0.55
1:A:478:PHE:O	1:A:479:TRP:HD1	1.89	0.55
1:A:499:ARG:NH1	5:C:405:HOH:O	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:CYS:HG	1:A:541:SER:HG	1.46	0.55
1:A:41:SER:OG	2:D:145:GLY:O	2.22	0.55
2:E:120:VAL:O	2:E:124:SER:N	2.40	0.55
2:F:39:ASP:HA	2:F:42:ARG:HD3	1.87	0.55
2:G:155:LEU:HG	2:G:159:LEU:HD12	1.87	0.55
1:A:250:LEU:HG	1:A:254:ILE:HD12	1.89	0.55
1:A:475:TYR:HD2	1:A:510:ARG:HH12	1.55	0.55
2:B:13:LEU:O	2:B:68:SER:OG	2.24	0.55
2:C:10:ILE:HG22	2:C:202:PRO:HG2	1.88	0.55
2:C:91:GLU:HA	2:C:94:MET:HE2	1.89	0.55
2:G:214:ASP:O	5:G:404:HOH:O	2.18	0.55
2:G:9:LYS:O	2:G:202:PRO:HD2	2.07	0.55
1:A:46:GLN:O	1:A:46:GLN:NE2	2.40	0.55
1:A:92:HIS:HB2	2:D:137:LEU:O	2.07	0.55
2:D:155:LEU:HG	2:D:159:LEU:HD11	1.89	0.55
2:D:62:ASP:O	5:D:408:HOH:O	2.18	0.55
2:G:52:PHE:CZ	2:G:65:LEU:HA	2.41	0.55
1:A:357:ASN:OD1	1:A:358:LEU:HD12	2.06	0.55
2:B:204:GLN:HG3	2:B:205:GLY:N	2.22	0.55
2:B:59:ILE:HD12	5:B:479:HOH:O	2.07	0.55
2:F:104:TYR:O	2:F:108:ARG:HG2	2.07	0.55
2:G:131:LYS:HA	2:G:134:GLU:OE2	2.07	0.55
1:A:478:PHE:HZ	1:A:562:LEU:HB3	1.70	0.54
2:B:54:ASN:ND2	4:B:301:GSH:HG12	2.20	0.54
1:A:260:ARG:CB	2:F:194:LYS:HZ1	2.04	0.54
1:A:132:ARG:NH1	1:A:300:TYR:OH	2.41	0.54
1:A:46:GLN:OE1	2:D:147:HIS:HB3	2.06	0.54
1:A:472:PRO:HG3	1:A:514:THR:O	2.07	0.54
2:C:150:HIS:CD2	2:C:151:PRO:HD3	2.43	0.54
2:G:8:TRP:HA	2:G:33:TYR:HB2	1.88	0.54
1:A:117:LEU:O	1:A:121:THR:HG23	2.08	0.54
2:B:58:TYR:CE1	2:B:71:ILE:HG22	2.43	0.54
2:D:7:TYR:OH	2:D:18:ARG:NH1	2.40	0.54
2:E:15:GLN:NE2	2:E:103:ARG:HG2	2.23	0.54
2:F:153:PHE:O	2:F:156:TYR:HB3	2.06	0.54
1:A:460:ILE:N	1:A:480:GLU:O	2.30	0.54
1:A:494:CYS:O	1:A:518:LEU:HD23	2.07	0.54
2:B:40:LYS:HE2	2:B:44:LYS:HB2	1.90	0.54
2:D:164:TYR:CE2	2:D:203:LEU:HD21	2.43	0.54
2:E:140:LYS:NZ	2:E:143:LEU:HD23	2.23	0.54
2:E:79:HIS:HD1	2:E:79:HIS:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ALA:O	1:A:266:LEU:HG	2.08	0.54
1:A:494:CYS:HB2	1:A:520:LEU:HB2	1.90	0.54
2:E:156:TYR:HA	2:E:159:LEU:HD12	1.89	0.54
2:E:176:LEU:HD12	2:E:177:VAL:N	2.23	0.54
1:A:363:PHE:CE2	1:A:390:VAL:HG23	2.43	0.54
2:B:156:TYR:HE1	2:B:180:LYS:HA	1.73	0.54
2:B:8:TRP:CH2	4:B:301:GSH:HB22	2.41	0.54
2:B:82:LEU:HD12	2:B:83:GLY:N	2.22	0.54
2:E:136:ARG:CG	2:E:140:LYS:HZ3	2.20	0.54
2:F:9:LYS:CE	2:F:32:LEU:HD13	2.38	0.54
2:F:76:ALA:HA	2:F:79:HIS:CE1	2.43	0.54
2:G:100:LEU:HD21	2:G:154:MET:HE1	1.90	0.54
1:A:197:ASP:OD2	1:A:200:GLN:HB2	2.08	0.54
1:A:220:PHE:CD1	1:A:302:TYR:HB3	2.42	0.54
1:A:432:ASN:ND2	1:A:434:ASP:OD1	2.38	0.54
1:A:199:HIS:HB2	1:A:525:LYS:HE3	1.90	0.54
2:B:184:GLU:O	2:B:190:ASP:HB3	2.08	0.54
2:E:23:TYR:HB2	2:E:189:ILE:CG2	2.37	0.54
1:A:11:ASN:HA	1:A:14:ILE:HG12	1.89	0.53
2:D:96:GLU:OE2	2:D:150:HIS:CE1	2.58	0.53
2:G:120:VAL:HA	2:G:123:LEU:HG	1.90	0.53
1:A:413:TYR:CE2	1:A:418:GLN:HB3	2.43	0.53
1:A:454:GLU:OE1	5:A:719:HOH:O	2.19	0.53
1:A:491:GLN:HB3	1:A:573:THR:OG1	2.08	0.53
2:C:33:TYR:HD1	5:C:402:HOH:O	1.91	0.53
2:G:119:LYS:O	2:G:123:LEU:HG	2.08	0.53
1:A:121:THR:HG22	1:A:336:TRP:CZ2	2.43	0.53
1:A:366:VAL:HG13	1:A:371:GLU:HG3	1.91	0.53
1:A:92:HIS:CE1	2:D:179:PHE:HB2	2.44	0.53
2:B:165:MET:HB3	2:B:210:PHE:HE2	1.73	0.53
2:D:82:LEU:HD11	2:E:73:ARG:NH2	2.23	0.53
2:F:188:GLN:NE2	5:F:414:HOH:O	2.27	0.53
1:A:115:ASP:O	1:A:118:MET:HG2	2.08	0.53
1:A:77:ILE:HG23	1:A:80:MET:HE2	1.91	0.53
2:D:141:THR:HA	2:D:182:ARG:HH22	1.74	0.53
2:B:109:ILE:HG22	2:B:115:PHE:CD1	2.44	0.53
2:B:178:CYS:O	2:B:182:ARG:N	2.42	0.53
2:C:12:GLY:O	2:C:15:GLN:HG3	2.09	0.53
2:B:51:GLU:HG3	2:B:52:PHE:CD1	2.43	0.53
2:E:95:LEU:O	2:E:99:VAL:HG23	2.09	0.53
2:F:7:TYR:CE1	2:F:9:LYS:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:NH2	1:A:434:ASP:HB3	2.24	0.53
1:A:65:VAL:HB	1:A:400:ARG:HH22	1.73	0.53
2:F:34:GLU:HB2	2:F:37:GLU:CD	2.29	0.53
1:A:222:VAL:O	1:A:304:ILE:N	2.40	0.53
2:E:134:GLU:HG2	2:E:135:ASP:N	2.23	0.53
2:D:94:MET:CE	2:E:65:LEU:HB3	2.38	0.53
2:E:17:THR:HG21	2:E:71:ILE:HD11	1.89	0.53
2:G:95:LEU:HD13	2:G:143:LEU:HB3	1.91	0.53
2:B:8:TRP:CZ3	4:B:301:GSH:HB22	2.44	0.52
1:A:510:ARG:NH1	1:A:516:GLY:O	2.41	0.52
1:A:70:ASP:OD2	1:A:109:LYS:HE2	2.09	0.52
2:C:201:TRP:CD1	2:C:203:LEU:HG	2.43	0.52
2:D:140:LYS:HG2	2:D:142:TYR:O	2.09	0.52
2:B:72:ILE:HG21	2:B:154:MET:HE1	1.90	0.52
2:C:152:ASP:O	2:C:156:TYR:N	2.43	0.52
2:E:8:TRP:HZ2	2:E:206:TRP:HD1	1.57	0.52
1:A:291:ILE:HG13	1:A:295:PHE:CE1	2.44	0.52
1:A:364:LEU:HB3	1:A:389:GLU:HG2	1.92	0.52
1:A:434:ASP:O	1:A:436:ASN:HB2	2.10	0.52
1:A:475:TYR:HD1	1:A:476:ALA:N	2.08	0.52
2:B:17:THR:CA	2:B:20:LEU:HG	2.38	0.52
2:E:157:ASP:O	2:E:161:VAL:N	2.37	0.52
2:F:109:ILE:HG21	2:F:118:LEU:HB3	1.92	0.52
1:A:228:VAL:HG13	1:A:319:TYR:HE2	1.73	0.52
1:A:450:LYS:HE2	2:C:193:LEU:HG	1.91	0.52
2:C:157:ASP:O	2:C:161:VAL:HG23	2.10	0.52
2:D:19:LEU:HG	2:D:192:TYR:CD2	2.45	0.52
2:F:144:ASN:ND2	5:F:423:HOH:O	2.38	0.52
2:G:119:LYS:O	2:G:123:LEU:N	2.43	0.52
2:G:59:ILE:HG12	2:G:64:LYS:HD3	1.91	0.52
1:A:110:PHE:CZ	1:A:554:SER:O	2.63	0.52
1:A:224:ALA:HB1	1:A:316:LEU:HB2	1.91	0.52
1:A:363:PHE:CZ	1:A:379:LEU:HD13	2.45	0.52
1:A:76:TYR:CE2	1:A:89:LEU:HB3	2.44	0.52
2:C:7:TYR:CG	2:C:14:VAL:HG11	2.45	0.52
2:D:165:MET:HG3	2:D:210:PHE:CE1	2.44	0.52
2:F:104:TYR:HB3	2:G:108:ARG:HH12	1.75	0.52
1:A:452:LEU:HD21	1:A:490:LEU:HD21	1.92	0.52
2:C:102:ILE:O	2:C:106:VAL:HG13	2.10	0.52
2:C:131:LYS:HA	2:C:134:GLU:HG2	1.92	0.52
2:C:20:LEU:HA	2:C:23:TYR:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:TYR:HE2	2:B:74:TYR:CG	2.27	0.52
2:C:87:LYS:O	2:C:91:GLU:HG2	2.10	0.52
2:D:103:ARG:NH2	2:D:154:MET:SD	2.82	0.52
2:D:73:ARG:CZ	2:E:73:ARG:HH21	2.23	0.52
2:E:8:TRP:CZ2	2:E:206:TRP:HD1	2.28	0.52
2:E:12:GLY:O	2:E:15:GLN:HG3	2.10	0.52
2:E:23:TYR:CE1	2:E:186:ILE:HD12	2.45	0.52
1:A:126:ARG:HA	1:A:129:PHE:CZ	2.45	0.52
1:A:132:ARG:O	1:A:136:PHE:N	2.41	0.52
1:A:228:VAL:HG21	1:A:315:LYS:HE3	1.92	0.52
1:A:363:PHE:O	1:A:365:PRO:HD3	2.10	0.52
2:B:171:ASP:O	5:B:403:HOH:O	2.18	0.52
2:B:95:LEU:HD11	2:B:143:LEU:HD13	1.92	0.52
2:D:8:TRP:HA	2:D:33:TYR:HB2	1.91	0.52
2:E:34:GLU:HG2	2:E:35:ARG:H	1.74	0.52
2:G:198:TYR:CE2	2:G:200:ALA:HB2	2.45	0.52
2:G:88:GLU:N	2:G:88:GLU:OE1	2.43	0.52
1:A:288:TYR:CE2	1:A:318:HIS:HA	2.45	0.51
2:D:206:TRP:O	5:D:409:HOH:O	2.18	0.51
2:E:201:TRP:NE1	5:E:414:HOH:O	2.34	0.51
2:F:12:GLY:HA2	2:F:103:ARG:NH2	2.25	0.51
2:F:180:LYS:HG2	2:F:184:GLU:OE2	2.09	0.51
2:C:130:LEU:HA	2:C:133:PHE:CE2	2.46	0.51
2:D:20:LEU:HD21	2:D:72:ILE:HD11	1.93	0.51
2:B:149:THR:HB	2:B:151:PRO:HD2	1.91	0.51
2:F:9:LYS:HE3	2:F:32:LEU:HD13	1.92	0.51
1:A:302:TYR:CE1	1:A:328:HIS:HA	2.46	0.51
1:A:69:THR:N	1:A:72:GLU:OE2	2.40	0.51
2:G:100:LEU:HB3	2:G:104:TYR:CE2	2.45	0.51
2:G:215:HIS:ND1	2:G:216:PRO:HD2	2.26	0.51
2:G:55:LEU:HB2	4:G:301:GSH:O2	2.11	0.51
1:A:265:LYS:HG3	2:F:193:LEU:CD1	2.41	0.51
2:C:175:LYS:HG3	5:C:419:HOH:O	2.10	0.51
2:C:15:GLN:HA	2:C:18:ARG:HG2	1.92	0.51
2:D:48:LEU:HD22	2:D:50:LEU:HB2	1.92	0.51
2:G:176:LEU:HA	2:G:179:PHE:HB3	1.93	0.51
2:F:110:ALA:HB1	2:F:208:ALA:CB	2.41	0.51
2:B:7:TYR:HB2	2:B:14:VAL:HG21	1.92	0.51
2:E:130:LEU:HA	2:E:133:PHE:HD2	1.76	0.51
1:A:314:PRO:O	1:A:318:HIS:N	2.43	0.51
1:A:38:LYS:HB3	5:D:402:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:TYR:HD1	5:A:798:HOH:O	1.93	0.51
2:D:114:ASP:HB3	2:D:117:THR:OG1	2.11	0.51
2:F:202:PRO:HD2	2:F:203:LEU:HD23	1.93	0.51
2:F:110:ALA:HB1	2:F:208:ALA:HB2	1.92	0.51
2:G:54:ASN:HB3	2:G:66:THR:HG21	1.93	0.51
1:A:152:LYS:HD3	1:A:561:ILE:HG23	1.92	0.51
2:C:11:LYS:HB3	2:C:15:GLN:HG2	1.91	0.51
2:E:76:ALA:HB2	2:E:150:HIS:HD2	1.76	0.51
2:E:68:SER:HA	2:E:71:ILE:HG12	1.93	0.51
2:F:52:PHE:CE1	2:G:136:ARG:HB2	2.46	0.51
1:A:465:TYR:CE2	1:A:467:ASP:HB2	2.46	0.51
1:A:482:SER:O	5:A:720:HOH:O	2.20	0.51
1:A:403:LEU:HD23	1:A:540:SER:OG	2.10	0.51
2:B:130:LEU:O	2:B:134:GLU:N	2.40	0.51
2:B:50:LEU:HA	2:B:64:LYS:CE	2.41	0.51
2:C:103:ARG:NH2	2:C:162:VAL:HG23	2.24	0.51
2:F:17:THR:HG22	2:F:72:ILE:HA	1.93	0.51
1:A:551:VAL:HB	1:A:555:ASN:HB2	1.93	0.50
1:A:99:LEU:HB2	1:A:556:ALA:H	1.76	0.50
2:D:113:LYS:HG3	2:D:114:ASP:N	2.26	0.50
2:E:126:LEU:HG	2:E:130:LEU:HD13	1.92	0.50
1:A:334:GLU:O	1:A:394:ASN:ND2	2.44	0.50
2:C:64:LYS:O	2:C:65:LEU:HD23	2.11	0.50
2:D:65:LEU:HD11	2:D:70:ALA:HB1	1.93	0.50
2:E:162:VAL:O	2:E:166:ASP:OD1	2.29	0.50
2:F:51:GLU:C	2:F:52:PHE:HD1	2.14	0.50
2:F:58:TYR:CD2	2:F:71:ILE:HG22	2.46	0.50
2:G:116:GLU:HA	2:G:119:LYS:HB2	1.93	0.50
2:G:183:ILE:O	2:G:186:ILE:HG22	2.10	0.50
2:G:56:PRO:O	2:G:66:THR:HG23	2.11	0.50
1:A:10:MET:SD	1:A:133:ASN:HB3	2.51	0.50
1:A:209:GLY:HA2	1:A:212:PHE:CE1	2.47	0.50
2:C:152:ASP:HA	2:C:155:LEU:HB3	1.93	0.50
2:D:71:ILE:O	2:D:75:ILE:HG23	2.11	0.50
2:G:193:LEU:HG	2:G:198:TYR:CZ	2.47	0.50
2:C:17:THR:HA	2:C:20:LEU:HG	1.92	0.50
2:C:63:VAL:HG13	2:C:65:LEU:HG	1.93	0.50
2:D:159:LEU:HD22	2:D:176:LEU:HD21	1.93	0.50
2:F:202:PRO:CD	2:F:203:LEU:HB3	2.42	0.50
2:B:17:THR:HA	2:B:20:LEU:CG	2.38	0.50
2:C:102:ILE:HD12	2:C:122:PHE:HZ	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:191:LYS:HA	2:C:194:LYS:HD2	1.94	0.50
2:E:166:ASP:OD2	2:E:170:LEU:HD21	2.11	0.50
2:F:10:ILE:HD12	2:F:12:GLY:HA3	1.94	0.50
2:F:71:ILE:O	2:F:75:ILE:HD12	2.12	0.50
2:G:66:THR:HG22	2:G:67:GLN:H	1.76	0.50
1:A:475:TYR:CD1	1:A:476:ALA:N	2.80	0.50
2:C:111:TYR:HB2	2:C:208:ALA:HA	1.94	0.50
2:B:6:GLY:HA3	2:B:57:TYR:CZ	2.46	0.50
2:C:82:LEU:O	2:C:92:ILE:HD12	2.11	0.50
2:E:181:LYS:O	2:E:184:GLU:HG2	2.11	0.50
2:G:67:GLN:NE2	4:G:301:GSH:O12	2.45	0.50
2:C:18:ARG:HG3	2:C:19:LEU:N	2.27	0.50
2:C:165:MET:HE2	2:C:210:PHE:HE2	1.77	0.50
2:G:97:GLY:O	2:G:100:LEU:HB2	2.12	0.50
1:A:39:ASN:HB2	1:A:399:TYR:OH	2.12	0.50
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.93	0.50
2:B:155:LEU:HD23	2:B:179:PHE:CE2	2.46	0.50
2:B:23:TYR:OH	2:B:75:ILE:HG22	2.11	0.50
2:C:184:GLU:HA	2:C:189:ILE:HD11	1.94	0.50
2:C:35:ARG:HB3	2:C:35:ARG:CZ	2.42	0.50
1:A:126:ARG:HA	1:A:129:PHE:CE2	2.47	0.49
1:A:136:PHE:CE2	1:A:343:PRO:HB2	2.47	0.49
2:D:94:MET:HE2	2:E:65:LEU:HD13	1.94	0.49
2:F:130:LEU:HA	2:F:133:PHE:HD2	1.76	0.49
1:A:441:LEU:CD2	1:A:549:ARG:HB3	2.42	0.49
2:B:51:GLU:HG2	2:B:64:LYS:HE2	1.94	0.49
2:C:22:GLU:OE2	2:C:28:TYR:OH	2.29	0.49
2:E:50:LEU:HD21	2:E:66:THR:HB	1.92	0.49
1:A:44:TYR:HD1	1:A:45:LEU:HD12	1.78	0.49
2:C:35:ARG:HB3	2:C:35:ARG:NH1	2.27	0.49
2:C:56:PRO:O	2:C:66:THR:OG1	2.14	0.49
2:C:99:VAL:O	2:C:102:ILE:HG22	2.12	0.49
2:E:30:GLU:HG2	2:E:197:LYS:NZ	2.27	0.49
2:E:67:GLN:NE2	2:E:69:MET:H	2.10	0.49
2:F:77:ASP:OD1	2:F:78:LYS:N	2.46	0.49
1:A:143:LYS:HA	1:A:185:PRO:HD2	1.94	0.49
1:A:491:GLN:O	1:A:494:CYS:HB3	2.12	0.49
2:D:11:LYS:HG2	2:D:15:GLN:HB3	1.93	0.49
2:E:123:LEU:HD21	2:E:162:VAL:CG1	2.42	0.49
2:E:142:TYR:CE1	2:E:148:VAL:HG13	2.47	0.49
2:F:50:LEU:HD23	2:F:53:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG22	3:A:601:JAA:C07	2.41	0.49
1:A:409:VAL:HA	1:A:419:LEU:HD23	1.95	0.49
1:A:534:HIS:CE1	1:A:557:LYS:HE3	2.47	0.49
2:C:73:ARG:HD2	2:C:82:LEU:HD11	1.93	0.49
2:D:85:CYS:SG	2:D:87:LYS:HG2	2.53	0.49
2:G:95:LEU:HD13	2:G:143:LEU:HD22	1.95	0.49
1:A:317:ARG:HA	1:A:320:ALA:HB3	1.94	0.49
1:A:498:ASP:OD1	1:A:510:ARG:HD2	2.12	0.49
2:E:12:GLY:O	2:E:103:ARG:NH2	2.45	0.49
2:E:79:HIS:NE2	2:E:81:MET:HG3	2.26	0.49
1:A:346:SER:N	5:A:747:HOH:O	2.46	0.49
1:A:107:ARG:HH12	1:A:433:ILE:HG13	1.77	0.49
1:A:475:TYR:HD1	1:A:476:ALA:H	1.58	0.49
1:A:495:ASN:HD21	1:A:573:THR:N	2.11	0.49
2:C:27:LYS:HD2	2:C:28:TYR:H	1.77	0.49
2:F:215:HIS:ND1	2:F:216:PRO:HD2	2.28	0.49
2:B:69:MET:HG3	2:B:100:LEU:HD21	1.93	0.49
2:B:39:ASP:OD1	2:B:39:ASP:N	2.46	0.49
2:E:137:LEU:HD23	2:E:140:LYS:CE	2.42	0.49
2:F:136:ARG:O	2:F:140:LYS:HG2	2.12	0.49
2:G:191:LYS:HE3	2:G:192:TYR:CZ	2.48	0.49
1:A:108:PRO:HB3	1:A:555:ASN:OD1	2.12	0.49
1:A:94:VAL:HG21	1:A:113:PHE:H	1.78	0.49
2:B:162:VAL:HG12	2:B:169:CYS:SG	2.53	0.49
2:F:155:LEU:O	2:F:159:LEU:HG	2.13	0.49
2:G:66:THR:HG22	2:G:67:GLN:N	2.28	0.49
2:G:118:LEU:HD12	2:G:118:LEU:H	1.78	0.48
1:A:114:THR:OG1	1:A:115:ASP:N	2.46	0.48
1:A:80:MET:SD	1:A:87:PRO:HB3	2.53	0.48
2:E:20:LEU:HD11	2:E:153:PHE:CB	2.40	0.48
1:A:74:GLU:O	1:A:78:LYS:HB2	2.12	0.48
2:C:159:LEU:HB2	2:C:180:LYS:HE3	1.95	0.48
1:A:257:PRO:HA	2:F:194:LYS:NZ	2.27	0.48
2:F:77:ASP:HB2	2:G:89:ARG:HH21	1.78	0.48
2:B:103:ARG:O	2:B:106:VAL:HG12	2.13	0.48
2:C:155:LEU:HD21	2:C:179:PHE:CE2	2.47	0.48
2:D:133:PHE:O	2:D:137:LEU:HG	2.14	0.48
1:A:145:LEU:HA	1:A:187:CYS:SG	2.53	0.48
1:A:452:LEU:HD11	1:A:479:TRP:HZ3	1.78	0.48
2:B:45:LYS:HE3	2:B:55:LEU:HD11	1.95	0.48
2:E:23:TYR:HD1	2:E:188:GLN:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:LYS:HZ3	2:F:143:LEU:HA	1.78	0.48
2:F:95:LEU:HD22	2:F:143:LEU:HD23	1.96	0.48
1:A:124:LEU:HD12	1:A:355:ILE:HD13	1.96	0.48
1:A:107:ARG:HB3	1:A:552:LYS:NZ	2.28	0.48
1:A:317:ARG:NH1	5:A:750:HOH:O	2.47	0.48
1:A:464:SER:O	1:A:551:VAL:HG22	2.14	0.48
1:A:162:VAL:HG21	1:A:559:LEU:HB2	1.96	0.48
2:B:123:LEU:HA	2:B:126:LEU:HD23	1.96	0.48
2:B:120:VAL:HA	2:B:123:LEU:HB3	1.95	0.48
2:B:202:PRO:HG3	2:B:206:TRP:CD1	2.48	0.48
2:C:117:THR:O	2:C:120:VAL:HG12	2.14	0.48
2:C:8:TRP:CD1	2:C:33:TYR:HE2	2.32	0.48
2:D:23:TYR:OH	2:D:148:VAL:HG11	2.13	0.48
2:D:69:MET:O	2:D:72:ILE:HG22	2.13	0.48
2:D:7:TYR:CE1	2:D:14:VAL:HG11	2.49	0.48
2:E:15:GLN:HE21	2:E:103:ARG:HG2	1.78	0.48
2:F:58:TYR:HD2	2:F:71:ILE:HG22	1.78	0.48
2:B:46:PHE:HZ	2:C:132:MET:SD	2.35	0.48
2:E:99:VAL:HG11	2:E:154:MET:HB3	1.93	0.48
2:F:99:VAL:HA	2:F:102:ILE:HG12	1.95	0.48
2:F:103:ARG:NH1	5:F:409:HOH:O	2.16	0.48
2:F:11:LYS:H	2:F:203:LEU:HD11	1.79	0.48
2:G:16:PRO:HB3	2:G:154:MET:HA	1.96	0.48
2:G:2:SER:O	5:G:405:HOH:O	2.19	0.48
2:G:71:ILE:HA	2:G:74:TYR:HE2	1.74	0.48
1:A:106:GLY:O	1:A:107:ARG:HD2	2.14	0.48
1:A:317:ARG:HG2	1:A:325:LEU:HD11	1.95	0.48
2:E:23:TYR:CZ	2:E:186:ILE:HD12	2.49	0.48
2:F:96:GLU:O	2:F:100:LEU:HD12	2.14	0.48
2:F:103:ARG:O	2:F:106:VAL:HG12	2.14	0.48
2:E:143:LEU:H	2:E:152:ASP:CG	2.14	0.48
2:E:162:VAL:HG22	5:E:470:HOH:O	2.13	0.48
2:F:117:THR:O	2:F:120:VAL:HG12	2.13	0.48
2:F:183:ILE:O	2:F:189:ILE:HD11	2.14	0.48
2:F:59:ILE:HG23	2:F:64:LYS:HG2	1.96	0.48
1:A:100:SER:OG	1:A:401:TYR:OH	2.23	0.47
1:A:558:VAL:HA	1:A:561:ILE:HD12	1.96	0.47
1:A:74:GLU:OE2	1:A:552:LYS:HE3	2.14	0.47
2:B:120:VAL:HG23	2:B:123:LEU:HD23	1.96	0.47
2:C:142:TYR:HD1	2:C:144:ASN:H	1.60	0.47
2:B:94:MET:HE1	2:C:51:GLU:CD	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:THR:O	2:E:67:GLN:HB2	2.13	0.47
2:F:115:PHE:CE1	2:F:209:THR:HG21	2.49	0.47
1:A:138:ILE:HG12	1:A:139:ASP:N	2.30	0.47
1:A:478:PHE:CE1	1:A:558:VAL:HG13	2.49	0.47
1:A:220:PHE:HZ	3:A:601:JAA:C07	2.27	0.47
2:B:10:ILE:HD12	2:B:205:GLY:HA2	1.95	0.47
1:A:36:LEU:O	1:A:40:GLN:HG2	2.14	0.47
1:A:528:PHE:O	1:A:531:ILE:HG13	2.13	0.47
1:A:551:VAL:HB	1:A:555:ASN:HB3	1.95	0.47
2:C:103:ARG:O	2:C:106:VAL:HG22	2.14	0.47
2:C:103:ARG:HE	2:C:158:ALA:HB1	1.79	0.47
2:E:67:GLN:HA	4:E:301:GSH:O12	2.14	0.47
2:F:115:PHE:CD1	2:F:209:THR:HG21	2.49	0.47
2:G:102:ILE:HG23	2:G:158:ALA:HB1	1.95	0.47
2:G:2:SER:HB3	2:G:27:LYS:O	2.13	0.47
2:G:91:GLU:O	2:G:95:LEU:HG	2.14	0.47
2:D:141:THR:O	2:D:182:ARG:CZ	2.63	0.47
2:D:163:LEU:HD22	2:D:180:LYS:HE3	1.95	0.47
2:D:183:ILE:HG13	2:D:184:GLU:N	2.29	0.47
2:E:34:GLU:CG	2:E:35:ARG:H	2.27	0.47
2:F:19:LEU:HG	2:F:189:ILE:HG22	1.96	0.47
2:G:167:PRO:O	5:G:406:HOH:O	2.20	0.47
2:G:201:TRP:CE3	2:G:202:PRO:HA	2.49	0.47
1:A:336:TRP:HH2	3:A:601:JAA:C09	2.27	0.47
1:A:336:TRP:HB2	1:A:358:LEU:CD2	2.45	0.47
1:A:62:LYS:NZ	1:A:375:LYS:HG2	2.29	0.47
1:A:65:VAL:HB	1:A:400:ARG:HH12	1.79	0.47
2:B:85:CYS:O	2:B:89:ARG:HB2	2.14	0.47
2:C:105:GLY:O	2:C:108:ARG:CZ	2.62	0.47
2:C:111:TYR:CB	2:C:208:ALA:HA	2.44	0.47
2:C:115:PHE:CD2	2:C:210:PHE:HB2	2.48	0.47
2:D:151:PRO:HA	2:D:154:MET:HG3	1.95	0.47
2:E:13:LEU:HB3	2:E:68:SER:CB	2.44	0.47
2:E:14:VAL:HG11	2:E:18:ARG:CZ	2.44	0.47
2:G:140:LYS:HB3	2:G:142:TYR:O	2.15	0.47
1:A:82:ASP:HA	1:A:157:THR:OG1	2.14	0.47
2:C:155:LEU:O	2:C:158:ALA:HB3	2.14	0.47
2:C:190:ASP:O	2:C:194:LYS:HG3	2.15	0.47
2:C:8:TRP:CD1	2:C:55:LEU:HD22	2.49	0.47
2:F:118:LEU:HD23	2:F:121:ASP:OD2	2.14	0.47
1:A:156:SER:HB3	1:A:160:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:HB3	2:F:194:LYS:NZ	2.03	0.47
2:C:103:ARG:HE	2:C:158:ALA:CB	2.28	0.47
2:C:73:ARG:O	2:C:82:LEU:HD22	2.15	0.47
2:E:203:LEU:HG	2:E:211:GLY:HA3	1.95	0.47
2:F:202:PRO:HB2	2:F:211:GLY:HA2	1.95	0.47
1:A:353:ALA:HB2	1:A:413:TYR:CE2	2.50	0.47
2:B:142:TYR:HB2	2:B:179:PHE:CE1	2.50	0.47
2:D:156:TYR:HA	2:D:159:LEU:HD12	1.95	0.47
2:F:7:TYR:HA	2:F:55:LEU:HG	1.96	0.47
2:G:156:TYR:OH	2:G:180:LYS:HA	2.15	0.47
1:A:117:LEU:HA	1:A:120:ASN:HB2	1.96	0.47
1:A:124:LEU:HD21	1:A:329:ASP:HB2	1.96	0.47
1:A:76:TYR:HB2	1:A:88:ILE:HG13	1.97	0.47
2:C:10:ILE:HD13	2:C:12:GLY:HA3	1.95	0.47
2:E:7:TYR:OH	2:E:12:GLY:HA3	2.14	0.47
2:F:41:TRP:CH2	2:F:45:LYS:HG3	2.50	0.47
2:G:116:GLU:HG2	2:G:119:LYS:HE2	1.97	0.47
2:G:15:GLN:O	5:G:409:HOH:O	2.21	0.47
1:A:50:LEU:HD21	1:A:65:VAL:CG2	2.45	0.47
2:B:176:LEU:O	2:B:179:PHE:HB3	2.14	0.47
2:C:108:ARG:C	2:C:109:ILE:HG13	2.35	0.47
2:C:142:TYR:HB3	2:C:179:PHE:HE1	1.79	0.47
2:C:165:MET:HE2	2:C:165:MET:HB2	1.53	0.47
2:E:45:LYS:HG3	2:E:53:PRO:HB3	1.96	0.47
2:E:6:GLY:HA3	2:E:57:TYR:CZ	2.50	0.47
2:F:37:GLU:O	2:F:39:ASP:N	2.48	0.47
2:C:9:LYS:HD3	2:C:206:TRP:CZ2	2.50	0.47
2:F:115:PHE:HB2	2:F:119:LYS:HZ3	1.80	0.47
2:F:20:LEU:HD11	2:F:150:HIS:HB2	1.97	0.47
1:A:144:ALA:HB2	1:A:184:SER:OG	2.15	0.46
1:A:330:TYR:HB3	1:A:338:ALA:HB3	1.97	0.46
1:A:451:ARG:CB	2:C:181:LYS:HZ2	2.28	0.46
2:D:137:LEU:HA	2:D:140:LYS:HE2	1.96	0.46
2:D:160:ASP:OD1	2:D:164:TYR:OH	2.27	0.46
2:G:114:ASP:OD1	5:G:408:HOH:O	2.20	0.46
1:A:465:TYR:CD1	1:A:551:VAL:HG23	2.47	0.46
2:C:130:LEU:HD22	2:C:133:PHE:HE2	1.80	0.46
2:C:33:TYR:HB3	2:C:41:TRP:CH2	2.50	0.46
2:D:174:PRO:O	2:D:177:VAL:HG12	2.15	0.46
2:E:75:ILE:O	2:E:79:HIS:ND1	2.48	0.46
2:F:33:TYR:OH	2:F:41:TRP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:THR:O	1:A:237:VAL:HG22	2.14	0.46
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.58	0.46
1:A:378:GLY:O	1:A:382:VAL:HG23	2.15	0.46
2:B:132:MET:SD	2:C:53:PRO:HD2	2.55	0.46
2:B:119:LYS:HD3	2:B:165:MET:SD	2.55	0.46
2:B:58:TYR:CE1	2:B:65:LEU:HB2	2.49	0.46
2:C:33:TYR:HA	2:C:37:GLU:OE1	2.16	0.46
2:E:30:GLU:OE2	2:E:197:LYS:HD3	2.16	0.46
2:F:95:LEU:HD13	2:F:143:LEU:HB3	1.98	0.46
2:G:112:SER:OG	2:G:115:PHE:HA	2.15	0.46
1:A:238:TRP:O	1:A:242:VAL:HG13	2.15	0.46
1:A:42:ALA:HB3	1:A:45:LEU:HD13	1.98	0.46
1:A:481:ILE:HD13	1:A:483:GLY:O	2.15	0.46
1:A:520:LEU:N	1:A:570:TYR:O	2.36	0.46
2:C:102:ILE:HD12	2:C:122:PHE:CZ	2.51	0.46
2:C:95:LEU:O	2:C:99:VAL:HG12	2.16	0.46
2:D:14:VAL:HG22	2:D:56:PRO:HG3	1.96	0.46
2:E:16:PRO:CG	2:E:157:ASP:HB2	2.45	0.46
2:E:19:LEU:HD23	2:E:156:TYR:OH	2.15	0.46
2:F:184:GLU:HA	2:F:189:ILE:HD11	1.97	0.46
1:A:135:ASP:HB2	1:A:343:PRO:HG2	1.97	0.46
1:A:552:LYS:HB3	1:A:553:PRO:HD2	1.98	0.46
2:B:51:GLU:HG2	2:B:64:LYS:HZ3	1.80	0.46
1:A:187:CYS:HG	1:A:212:PHE:HE1	1.63	0.46
2:C:25:GLU:HG3	2:C:188:GLN:HG2	1.97	0.46
2:C:8:TRP:HZ2	4:C:301:GSH:HN3	1.64	0.46
2:D:50:LEU:HD11	2:D:65:LEU:C	2.36	0.46
2:E:183:ILE:O	2:E:189:ILE:HD11	2.15	0.46
2:F:67:GLN:HA	4:F:301:GSH:O11	2.16	0.46
1:A:217:GLN:HB3	1:A:299:LYS:HE2	1.96	0.46
1:A:400:ARG:HB2	1:A:400:ARG:HE	1.45	0.46
2:B:206:TRP:HD1	2:B:213:GLY:O	1.97	0.46
2:F:68:SER:N	5:F:401:HOH:O	2.49	0.46
2:G:133:PHE:O	2:G:136:ARG:HB3	2.16	0.46
2:G:162:VAL:O	2:G:166:ASP:N	2.29	0.46
1:A:190:ASP:O	1:A:193:ILE:HG12	2.15	0.46
1:A:31:THR:HG21	1:A:357:ASN:CA	2.45	0.46
1:A:110:PHE:HZ	1:A:554:SER:CA	2.29	0.46
1:A:574:ALA:HA	2:C:174:PRO:CB	2.43	0.46
1:A:75:PRO:O	1:A:79:ARG:HG3	2.16	0.46
2:B:155:LEU:HD23	2:B:179:PHE:HE2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:PRO:O	2:B:191:LYS:HB3	2.15	0.46
2:E:85:CYS:SG	2:E:86:PRO:HD2	2.56	0.46
2:E:16:PRO:HG2	2:E:157:ASP:HB2	1.98	0.46
2:E:52:PHE:HE1	2:E:66:THR:O	1.99	0.46
2:F:93:SER:HB2	2:G:70:ALA:HA	1.97	0.46
1:A:405:ASP:N	1:A:405:ASP:OD1	2.49	0.46
1:A:535:PHE:HB3	1:A:544:GLN:O	2.15	0.46
2:C:114:ASP:HB3	2:C:117:THR:OG1	2.15	0.46
2:C:150:HIS:CG	2:C:151:PRO:HD3	2.50	0.46
2:C:159:LEU:HD13	2:C:176:LEU:HG	1.98	0.46
2:F:33:TYR:OH	2:F:41:TRP:N	2.35	0.46
2:F:7:TYR:CE2	2:F:14:VAL:HG11	2.51	0.46
2:F:6:GLY:O	2:F:7:TYR:HB3	2.16	0.46
2:G:58:TYR:HE1	2:G:65:LEU:HB2	1.81	0.46
2:B:98:ALA:N	2:C:67:GLN:HE22	2.14	0.45
2:C:103:ARG:NH1	2:C:162:VAL:HG23	2.31	0.45
2:C:122:PHE:CD1	2:C:125:LYS:HD3	2.50	0.45
2:D:106:VAL:HA	2:D:109:ILE:HG12	1.97	0.45
2:E:7:TYR:CG	2:E:8:TRP:N	2.84	0.45
2:F:115:PHE:HB2	2:F:119:LYS:NZ	2.31	0.45
2:G:54:ASN:C	2:G:66:THR:HG21	2.35	0.45
1:A:237:VAL:O	1:A:240:GLU:HB3	2.16	0.45
2:B:5:LEU:HG	2:B:7:TYR:CD1	2.51	0.45
2:C:134:GLU:OE2	2:C:173:PHE:HB3	2.17	0.45
2:C:133:PHE:CE1	2:C:176:LEU:HD13	2.51	0.45
2:C:21:LEU:HD13	2:C:28:TYR:CG	2.51	0.45
1:A:101:SER:HB3	1:A:535:PHE:CD1	2.51	0.45
2:D:213:GLY:N	5:D:427:HOH:O	2.45	0.45
2:E:40:LYS:HD2	2:E:40:LYS:HA	1.75	0.45
2:E:55:LEU:HG	4:E:301:GSH:O2	2.17	0.45
1:A:463:SER:HB3	1:A:478:PHE:HB2	1.98	0.45
2:B:95:LEU:O	2:B:99:VAL:HG23	2.16	0.45
2:D:67:GLN:NE2	5:D:430:HOH:O	2.49	0.45
1:A:14:ILE:HG13	1:A:15:ASP:N	2.30	0.45
1:A:328:HIS:CE1	3:A:601:JAA:C04	2.99	0.45
2:C:170:LEU:HA	2:C:173:PHE:CE1	2.52	0.45
2:B:82:LEU:HD21	2:C:89:ARG:CZ	2.47	0.45
2:D:50:LEU:HD12	2:D:50:LEU:HA	1.84	0.45
2:E:10:ILE:HD13	2:E:204:GLN:HA	1.98	0.45
2:F:10:ILE:HB	2:F:203:LEU:HD11	1.99	0.45
2:F:147:HIS:ND1	5:F:422:HOH:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:202:PRO:CG	2:F:203:LEU:HB3	2.47	0.45
2:F:4:ILE:HA	2:F:29:GLU:O	2.15	0.45
2:G:201:TRP:CG	2:G:216:PRO:HD3	2.52	0.45
2:B:150:HIS:O	2:B:154:MET:HE2	2.17	0.45
2:C:170:LEU:HA	2:C:173:PHE:CZ	2.52	0.45
2:C:179:PHE:HB2	5:C:419:HOH:O	2.17	0.45
2:C:5:LEU:HG	2:C:7:TYR:CD1	2.52	0.45
2:E:137:LEU:HD23	2:E:140:LYS:HE2	1.98	0.45
2:E:44:LYS:O	2:E:48:LEU:HG	2.17	0.45
2:F:126:LEU:N	2:F:127:PRO:HD2	2.32	0.45
2:F:150:HIS:CG	2:F:151:PRO:HD3	2.51	0.45
2:F:8:TRP:HD1	2:F:55:LEU:HD23	1.81	0.45
1:A:117:LEU:HD22	1:A:336:TRP:CD1	2.52	0.45
1:A:495:ASN:HB3	2:C:178:CYS:HB3	1.98	0.45
2:D:73:ARG:NH2	2:E:73:ARG:HH21	2.14	0.45
2:G:95:LEU:HB3	5:G:450:HOH:O	2.16	0.45
1:A:111:ILE:HD13	1:A:334:GLU:HA	1.99	0.45
2:B:18:ARG:HD3	2:B:199:ILE:HD12	1.99	0.45
2:B:99:VAL:HB	2:B:103:ARG:CZ	2.46	0.45
5:A:709:HOH:O	2:C:185:ALA:HA	2.17	0.45
2:C:73:ARG:HE	2:C:82:LEU:HD21	1.82	0.45
2:D:75:ILE:O	2:D:78:LYS:HB2	2.17	0.45
2:F:160:ASP:OD1	5:F:411:HOH:O	2.21	0.45
2:F:6:GLY:HA3	2:F:57:TYR:CZ	2.51	0.45
2:G:96:GLU:O	2:G:100:LEU:HG	2.16	0.45
2:G:119:LYS:HG2	2:G:123:LEU:HD21	1.97	0.45
2:G:159:LEU:HD11	2:G:176:LEU:HD11	1.98	0.45
1:A:188:SER:HB3	1:A:205:HIS:CB	2.47	0.45
1:A:309:MET:HG2	1:A:536:LEU:CD2	2.46	0.45
1:A:32:LEU:O	1:A:35:ILE:HG13	2.16	0.45
1:A:509:SER:HB3	1:A:515:ILE:HG12	1.99	0.45
1:A:521:ARG:NE	5:A:749:HOH:O	2.46	0.45
2:B:5:LEU:HD22	2:B:21:LEU:HD11	1.99	0.45
2:D:92:ILE:O	2:D:96:GLU:HG3	2.17	0.45
2:E:121:ASP:HA	2:E:124:SER:OG	2.17	0.45
1:A:401:TYR:OH	1:A:403:LEU:HD13	2.17	0.45
1:A:480:GLU:OE2	1:A:526:GLY:N	2.50	0.45
1:A:526:GLY:O	1:A:530:LYS:N	2.45	0.45
1:A:86:SER:O	1:A:86:SER:OG	2.33	0.45
2:B:59:ILE:HG22	2:B:60:ASP:O	2.16	0.45
2:D:140:LYS:NZ	2:D:143:LEU:O	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:GLN:O	2:D:191:LYS:HB3	2.17	0.45
2:E:170:LEU:HB2	2:E:176:LEU:CD1	2.39	0.45
2:F:136:ARG:HB2	2:F:140:LYS:HE3	1.99	0.45
2:F:60:ASP:OD1	2:F:61:GLY:N	2.48	0.45
2:F:7:TYR:HE1	2:F:10:ILE:N	2.11	0.45
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.70	0.44
1:A:14:ILE:HB	1:A:131:PHE:CZ	2.52	0.44
1:A:233:THR:O	1:A:237:VAL:N	2.41	0.44
1:A:44:TYR:OH	5:A:721:HOH:O	2.21	0.44
2:D:119:LYS:O	2:D:123:LEU:N	2.34	0.44
2:D:95:LEU:HD22	2:D:143:LEU:HB3	1.98	0.44
1:A:403:LEU:HD23	1:A:405:ASP:OD2	2.16	0.44
2:B:71:ILE:O	2:B:74:TYR:HB3	2.17	0.44
2:B:129:MET:HG2	2:C:52:PHE:HE1	1.83	0.44
2:G:114:ASP:HB2	2:G:117:THR:OG1	2.17	0.44
1:A:162:VAL:N	5:A:711:HOH:O	2.32	0.44
1:A:355:ILE:HD12	1:A:358:LEU:HD22	1.99	0.44
2:C:106:VAL:O	2:C:110:ALA:HB2	2.17	0.44
2:C:123:LEU:C	5:C:404:HOH:O	2.55	0.44
2:D:8:TRP:CD1	2:D:55:LEU:HD13	2.52	0.44
2:E:5:LEU:O	2:E:30:GLU:HA	2.17	0.44
2:G:117:THR:HG21	5:G:464:HOH:O	2.17	0.44
2:G:3:PRO:HA	2:G:59:ILE:O	2.16	0.44
1:A:228:VAL:HA	1:A:319:TYR:CE2	2.52	0.44
1:A:464:SER:HA	1:A:476:ALA:O	2.18	0.44
1:A:452:LEU:HD22	1:A:481:ILE:HG21	1.99	0.44
2:C:106:VAL:HG21	2:C:161:VAL:HG11	1.99	0.44
2:E:22:GLU:HB3	2:E:192:TYR:CZ	2.51	0.44
1:A:265:LYS:HB3	2:F:184:GLU:CD	2.38	0.44
2:C:103:ARG:NE	2:C:158:ALA:HA	2.33	0.44
2:C:109:ILE:HG22	2:C:109:ILE:O	2.18	0.44
2:C:161:VAL:HA	2:C:164:TYR:CD1	2.52	0.44
1:A:466:ILE:HB	1:A:553:PRO:HD3	2.00	0.44
2:E:166:ASP:OD2	2:E:167:PRO:HA	2.17	0.44
2:E:33:TYR:HE2	2:E:55:LEU:HD13	1.82	0.44
1:A:50:LEU:HA	1:A:50:LEU:HD23	1.72	0.44
2:B:88:GLU:HA	2:B:91:GLU:HB3	1.98	0.44
2:F:17:THR:HG23	2:F:72:ILE:HG22	2.00	0.44
2:F:30:GLU:HB3	2:F:32:LEU:HD11	2.00	0.44
2:G:193:LEU:HA	2:G:198:TYR:CD1	2.53	0.44
1:A:125:PHE:HB2	3:A:601:JAA:C15	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:PRO:HB3	2:B:60:ASP:OD1	2.18	0.44
2:E:162:VAL:O	2:E:165:MET:N	2.50	0.44
2:E:186:ILE:HA	2:E:187:PRO:HD3	1.81	0.44
2:E:87:LYS:NZ	5:E:422:HOH:O	2.42	0.44
2:G:100:LEU:HA	2:G:103:ARG:HG2	2.00	0.44
2:G:52:PHE:CD1	2:G:52:PHE:N	2.86	0.44
1:A:105:GLN:HA	1:A:430:SER:HB3	2.00	0.44
1:A:111:ILE:HD13	1:A:334:GLU:HG3	1.99	0.44
1:A:519:GLU:HA	1:A:571:PHE:HA	2.00	0.44
1:A:87:PRO:HG3	1:A:93:PRO:HG3	1.99	0.44
1:A:8:PHE:CZ	1:A:10:MET:HA	2.53	0.44
2:B:100:LEU:HD12	2:B:103:ARG:HH12	1.79	0.44
2:B:139:HIS:CB	2:B:140:LYS:HD2	2.47	0.44
2:B:59:ILE:HG21	2:B:59:ILE:HD13	1.68	0.44
2:C:92:ILE:HD13	2:C:150:HIS:NE2	2.33	0.44
2:E:142:TYR:CE1	2:E:183:ILE:HD13	2.53	0.44
2:E:17:THR:HG21	2:E:71:ILE:CD1	2.48	0.44
2:G:156:TYR:CE2	2:G:183:ILE:HG21	2.53	0.44
2:G:52:PHE:HZ	2:G:65:LEU:HA	1.82	0.44
1:A:234:PHE:O	1:A:238:TRP:HB3	2.18	0.43
1:A:440:ASP:O	1:A:443:LEU:HG	2.18	0.43
1:A:110:PHE:HZ	1:A:554:SER:HA	1.82	0.43
2:B:58:TYR:OH	2:B:71:ILE:HA	2.17	0.43
2:C:133:PHE:O	2:C:137:LEU:HD13	2.18	0.43
2:C:208:ALA:HB3	2:C:212:GLY:CA	2.48	0.43
2:B:65:LEU:HD22	2:C:94:MET:HE1	2.00	0.43
2:D:89:ARG:O	2:D:92:ILE:HG13	2.17	0.43
2:E:13:LEU:HD21	2:E:104:TYR:CZ	2.53	0.43
2:E:24:LEU:HD13	2:E:79:HIS:NE2	2.33	0.43
2:E:30:GLU:HG2	2:E:197:LYS:HZ3	1.82	0.43
2:F:37:GLU:HB3	2:F:40:LYS:HB3	1.99	0.43
2:G:38:GLY:HA2	2:G:41:TRP:CD1	2.53	0.43
1:A:360:TYR:N	5:A:755:HOH:O	2.50	0.43
2:B:52:PHE:HA	2:B:53:PRO:HD3	1.79	0.43
2:C:110:ALA:O	2:C:210:PHE:N	2.44	0.43
2:E:161:VAL:HG23	2:E:203:LEU:HD13	2.00	0.43
2:G:32:LEU:HA	2:G:32:LEU:HD23	1.82	0.43
1:A:133:ASN:HA	1:A:136:PHE:O	2.18	0.43
1:A:435:LYS:HA	1:A:436:ASN:C	2.38	0.43
1:A:149:PHE:HE2	1:A:529:ARG:HH12	1.66	0.43
2:B:103:ARG:HE	2:B:154:MET:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:GLN:OE1	4:B:301:GSH:N1	2.51	0.43
2:D:15:GLN:HG3	2:D:16:PRO:CD	2.47	0.43
2:E:14:VAL:HG12	2:E:17:THR:HG22	1.98	0.43
2:F:19:LEU:HD23	2:F:153:PHE:CD1	2.54	0.43
2:F:206:TRP:HD1	2:F:212:GLY:C	2.21	0.43
1:A:109:LYS:C	1:A:110:PHE:HD1	2.22	0.43
1:A:197:ASP:OD1	1:A:256:VAL:HG11	2.18	0.43
1:A:320:ALA:HB1	1:A:325:LEU:HD21	2.00	0.43
2:B:35:ARG:HB2	2:B:206:TRP:CE3	2.53	0.43
2:D:12:GLY:N	2:D:203:LEU:O	2.31	0.43
2:G:146:ASP:N	5:G:413:HOH:O	2.50	0.43
1:A:529:ARG:O	1:A:533:GLU:HG3	2.19	0.43
1:A:487:GLU:HB3	1:A:570:TYR:HE2	1.83	0.43
2:B:150:HIS:CD2	2:B:151:PRO:HD3	2.52	0.43
2:C:85:CYS:SG	2:C:87:LYS:HE3	2.58	0.43
2:E:159:LEU:HB3	2:E:180:LYS:NZ	2.33	0.43
2:E:176:LEU:O	2:E:180:LYS:HG3	2.19	0.43
1:A:494:CYS:HA	1:A:497:LEU:HD12	2.00	0.43
1:A:92:HIS:HE1	2:D:179:PHE:HB2	1.84	0.43
2:B:158:ALA:O	2:B:162:VAL:HG23	2.19	0.43
2:B:156:TYR:CE2	2:B:183:ILE:HG21	2.53	0.43
2:C:161:VAL:HA	2:C:164:TYR:HD1	1.84	0.43
2:D:112:SER:N	2:D:115:PHE:CZ	2.86	0.43
1:A:91:GLY:HA3	2:D:139:HIS:C	2.39	0.43
2:E:81:MET:N	5:E:420:HOH:O	2.50	0.43
2:G:155:LEU:HB2	5:G:433:HOH:O	2.19	0.43
1:A:494:CYS:HB2	1:A:520:LEU:CB	2.48	0.43
1:A:496:CYS:SG	5:C:435:HOH:O	2.61	0.43
2:C:112:SER:OG	2:C:113:LYS:HG3	2.19	0.43
2:F:37:GLU:C	2:F:39:ASP:N	2.72	0.43
2:F:75:ILE:HG22	2:F:79:HIS:CE1	2.54	0.43
2:G:206:TRP:HA	2:G:213:GLY:H	1.82	0.43
2:G:54:ASN:HD21	4:G:301:GSH:CB1	2.32	0.43
1:A:288:TYR:HD2	1:A:318:HIS:ND1	2.16	0.43
1:A:351:THR:HG23	1:A:413:TYR:OH	2.18	0.43
1:A:427:LEU:HA	1:A:546:LYS:NZ	2.34	0.43
2:B:51:GLU:OE1	2:C:136:ARG:NE	2.52	0.43
2:C:186:ILE:HA	2:C:187:PRO:HD3	1.88	0.43
2:D:50:LEU:CD2	2:D:66:THR:HB	2.45	0.43
2:F:12:GLY:O	2:F:157:ASP:OD2	2.36	0.43
2:F:91:GLU:O	2:F:94:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:47:GLU:HG2	2:G:48:LEU:HD12	2.01	0.43
2:G:69:MET:HE1	2:G:100:LEU:HD21	2.00	0.43
1:A:346:SER:HB2	1:A:347:PRO:HD2	2.01	0.43
2:B:94:MET:SD	2:C:66:THR:HG22	2.59	0.43
2:C:82:LEU:HA	2:C:82:LEU:HD12	1.66	0.43
1:A:38:LYS:HB3	2:D:139:HIS:CD2	2.53	0.43
2:D:14:VAL:O	2:D:17:THR:HG22	2.19	0.43
2:F:158:ALA:O	2:F:162:VAL:HG12	2.19	0.43
2:G:144:ASN:HB2	2:G:149:THR:HG23	1.99	0.43
4:B:301:GSH:HN12	2:C:101:ASP:HB3	1.84	0.43
2:C:109:ILE:HA	2:C:112:SER:HB3	2.01	0.43
2:C:13:LEU:HD11	2:C:56:PRO:HD3	1.99	0.43
2:C:133:PHE:CZ	2:C:176:LEU:HD22	2.54	0.43
2:E:96:GLU:OE2	5:E:406:HOH:O	2.21	0.43
1:A:280:LYS:HZ3	1:A:294:LEU:HD23	1.83	0.42
1:A:320:ALA:CB	1:A:325:LEU:HD21	2.48	0.42
1:A:40:GLN:CD	2:D:145:GLY:HA2	2.38	0.42
1:A:40:GLN:HB3	2:D:146:ASP:OD1	2.19	0.42
1:A:432:ASN:OD1	1:A:433:ILE:N	2.52	0.42
2:B:21:LEU:HD13	2:B:28:TYR:CD1	2.54	0.42
2:C:15:GLN:HE22	2:C:203:LEU:CD2	2.32	0.42
1:A:50:LEU:O	2:D:146:ASP:HB2	2.19	0.42
2:E:143:LEU:HD12	2:E:152:ASP:N	2.34	0.42
2:F:97:GLY:HA3	2:G:67:GLN:CG	2.49	0.42
2:G:48:LEU:HD21	2:G:57:TYR:CG	2.54	0.42
1:A:391:VAL:HG12	1:A:400:ARG:HA	2.01	0.42
2:B:58:TYR:HE2	2:B:74:TYR:CD1	2.37	0.42
2:F:113:LYS:HE3	2:G:113:LYS:HB2	2.01	0.42
2:G:52:PHE:HE2	2:G:66:THR:N	2.17	0.42
2:G:82:LEU:HD11	2:G:89:ARG:HG3	2.01	0.42
1:A:151:SER:HB3	1:A:195:SER:O	2.18	0.42
2:B:156:TYR:CE1	2:B:180:LYS:HA	2.53	0.42
2:C:17:THR:O	2:C:21:LEU:HG	2.19	0.42
2:C:23:TYR:HE1	2:C:81:MET:SD	2.43	0.42
2:D:134:GLU:OE2	2:D:173:PHE:CE1	2.72	0.42
2:E:15:GLN:HB3	2:E:16:PRO:CD	2.48	0.42
2:E:137:LEU:HD22	2:E:179:PHE:CD1	2.53	0.42
2:F:204:GLN:NE2	2:F:208:ALA:HB2	2.34	0.42
1:A:315:LYS:O	1:A:318:HIS:HB3	2.19	0.42
1:A:354:VAL:N	5:A:759:HOH:O	2.51	0.42
2:C:100:LEU:HD11	2:C:154:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:ARG:NH2	2:C:122:PHE:CG	2.87	0.42
2:D:131:LYS:O	2:D:134:GLU:HB3	2.18	0.42
2:G:67:GLN:HB3	2:G:70:ALA:HB3	2.02	0.42
2:B:34:GLU:N	2:B:37:GLU:HG3	2.18	0.42
2:C:119:LYS:HB3	2:C:119:LYS:HE2	1.71	0.42
2:C:197:LYS:HE2	2:C:197:LYS:HB2	1.71	0.42
2:C:3:PRO:HA	2:C:60:ASP:OD1	2.20	0.42
2:D:109:ILE:O	2:D:115:PHE:CE1	2.73	0.42
2:E:153:PHE:HA	2:E:156:TYR:CD2	2.54	0.42
2:E:164:TYR:HE1	2:E:201:TRP:CE2	2.37	0.42
2:F:130:LEU:HD12	2:F:133:PHE:CD2	2.53	0.42
2:F:166:ASP:HA	2:F:167:PRO:HD2	1.87	0.42
2:F:17:THR:CG2	2:F:72:ILE:HG22	2.50	0.42
2:F:82:LEU:HD11	2:G:89:ARG:NE	2.35	0.42
2:G:73:ARG:HD2	2:G:82:LEU:HD22	2.02	0.42
1:A:147:PHE:CE2	1:A:205:HIS:HE1	2.37	0.42
1:A:403:LEU:HD23	1:A:540:SER:HG	1.84	0.42
1:A:107:ARG:HH21	1:A:552:LYS:HG2	1.84	0.42
1:A:80:MET:HA	1:A:86:SER:H	1.84	0.42
2:C:159:LEU:HB2	2:C:180:LYS:CE	2.48	0.42
2:D:67:GLN:HA	4:D:301:GSH:O12	2.20	0.42
2:E:164:TYR:CE2	2:E:203:LEU:HD21	2.53	0.42
2:D:86:PRO:HB3	2:E:77:ASP:OD2	2.20	0.42
2:G:7:TYR:CZ	2:G:30:GLU:OE2	2.70	0.42
1:A:387:GLU:HB3	1:A:406:VAL:HG12	2.02	0.42
1:A:555:ASN:O	1:A:559:LEU:HG	2.20	0.42
2:C:109:ILE:HG23	2:C:113:LYS:HG3	2.01	0.42
2:D:99:VAL:O	2:D:102:ILE:HG22	2.19	0.42
2:E:128:GLU:O	2:E:132:MET:HG3	2.20	0.42
2:G:18:ARG:HG3	2:G:19:LEU:H	1.84	0.42
2:G:22:GLU:HG3	2:G:28:TYR:HE1	1.84	0.42
2:B:120:VAL:HG13	2:B:121:ASP:OD1	2.19	0.42
2:B:5:LEU:HD13	2:B:58:TYR:HB3	2.02	0.42
2:B:6:GLY:HA3	2:B:57:TYR:CE2	2.55	0.42
2:C:118:LEU:HD23	2:C:118:LEU:HA	1.85	0.42
2:C:11:LYS:C	2:C:15:GLN:HG2	2.40	0.42
2:D:8:TRP:NE1	2:D:55:LEU:HD13	2.35	0.42
2:G:103:ARG:HB3	2:G:158:ALA:HB2	2.00	0.42
2:E:137:LEU:HD22	2:E:179:PHE:CG	2.55	0.42
2:G:25:GLU:HG3	5:G:439:HOH:O	2.19	0.42
1:A:197:ASP:HB3	1:A:256:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HG12	1:A:292:PRO:HD3	2.02	0.42
1:A:312:TYR:CD2	1:A:315:LYS:HE2	2.50	0.42
1:A:351:THR:OG1	1:A:419:LEU:N	2.52	0.42
1:A:513:LYS:HE3	1:A:575:PHE:HB2	2.01	0.42
2:B:149:THR:CB	2:B:151:PRO:HD2	2.49	0.42
1:A:499:ARG:HD3	2:C:175:LYS:HE3	2.02	0.42
2:C:186:ILE:HG22	2:C:189:ILE:HG12	2.02	0.42
2:C:215:HIS:HA	2:C:216:PRO:HD3	1.94	0.42
2:C:73:ARG:HA	2:C:82:LEU:CD1	2.50	0.42
2:D:48:LEU:HD11	2:D:57:TYR:CZ	2.54	0.42
2:F:68:SER:HA	2:F:71:ILE:HG12	2.01	0.42
1:A:70:ASP:CB	1:A:104:SER:HB2	2.48	0.41
2:C:37:GLU:N	5:C:402:HOH:O	2.12	0.41
2:C:85:CYS:SG	2:C:88:GLU:OE2	2.73	0.41
2:E:102:ILE:HA	2:E:122:PHE:HZ	1.85	0.41
2:G:67:GLN:NE2	2:G:69:MET:HG2	2.32	0.41
1:A:226:GLY:CA	1:A:529:ARG:HE	2.26	0.41
2:B:150:HIS:CG	2:B:151:PRO:HD3	2.56	0.41
2:B:189:ILE:O	2:B:193:LEU:HG	2.20	0.41
2:B:11:LYS:HA	2:B:18:ARG:HH12	1.85	0.41
2:B:77:ASP:HB3	2:B:82:LEU:CD2	2.51	0.41
2:C:19:LEU:HD23	2:C:153:PHE:HB3	2.01	0.41
2:C:30:GLU:OE1	2:C:32:LEU:HD11	2.20	0.41
2:F:172:ALA:O	5:F:413:HOH:O	2.22	0.41
2:G:52:PHE:CE2	2:G:65:LEU:HA	2.55	0.41
2:B:69:MET:SD	2:B:100:LEU:HD11	2.61	0.41
2:C:143:LEU:HD12	2:C:152:ASP:OD1	2.20	0.41
2:E:29:GLU:N	2:E:29:GLU:OE1	2.54	0.41
2:E:67:GLN:CD	2:E:69:MET:H	2.24	0.41
2:G:66:THR:O	2:G:67:GLN:HB3	2.20	0.41
1:A:212:PHE:CG	1:A:212:PHE:O	2.73	0.41
1:A:475:TYR:CE1	1:A:519:GLU:HB3	2.55	0.41
1:A:490:LEU:HB3	1:A:520:LEU:HD21	2.02	0.41
1:A:162:VAL:O	1:A:560:GLN:HG3	2.20	0.41
2:B:102:ILE:HD13	2:B:122:PHE:CZ	2.54	0.41
2:B:165:MET:HB3	2:B:210:PHE:CE2	2.55	0.41
2:B:75:ILE:O	5:B:404:HOH:O	2.22	0.41
2:C:94:MET:HE2	2:C:94:MET:HB2	1.39	0.41
2:E:126:LEU:HD21	2:E:162:VAL:HG21	2.02	0.41
2:F:179:PHE:CZ	2:F:183:ILE:HD12	2.55	0.41
2:F:186:ILE:HG23	2:F:187:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:LEU:HB2	2:B:23:TYR:HE2	1.84	0.41
2:B:77:ASP:HB3	2:B:82:LEU:HD23	2.02	0.41
2:C:40:LYS:HA	2:C:40:LYS:HD2	1.55	0.41
2:D:21:LEU:HD21	2:D:75:ILE:HG21	2.02	0.41
2:F:202:PRO:HB3	2:F:211:GLY:HA2	2.03	0.41
4:F:301:GSH:HG12	5:F:420:HOH:O	2.19	0.41
2:G:103:ARG:HG3	2:G:104:TYR:N	2.35	0.41
2:G:157:ASP:O	2:G:161:VAL:HG23	2.20	0.41
1:A:295:PHE:HA	1:A:296:PRO:HD2	1.69	0.41
1:A:327:SER:HB2	1:A:352:PHE:HE1	1.86	0.41
1:A:351:THR:OG1	1:A:418:GLN:HB2	2.19	0.41
1:A:451:ARG:HB3	2:C:181:LYS:HZ2	1.85	0.41
1:A:482:SER:O	1:A:525:LYS:NZ	2.46	0.41
2:B:7:TYR:CG	2:B:14:VAL:HG11	2.55	0.41
1:A:41:SER:HB3	2:D:142:TYR:CD2	2.55	0.41
2:D:156:TYR:CD1	2:D:180:LYS:HG2	2.55	0.41
2:D:176:LEU:O	2:D:176:LEU:HD23	2.21	0.41
2:F:110:ALA:O	2:F:208:ALA:HA	2.21	0.41
2:G:74:TYR:CD1	2:G:75:ILE:HG13	2.55	0.41
1:A:150:SER:O	1:A:194:PHE:HD1	2.04	0.41
1:A:339:ALA:N	1:A:353:ALA:O	2.53	0.41
1:A:453:SER:HB2	2:C:194:LYS:HZ3	1.86	0.41
2:B:165:MET:HG2	2:B:165:MET:H	1.70	0.41
2:C:23:TYR:CD2	2:C:153:PHE:CE2	3.09	0.41
2:E:8:TRP:HZ3	2:E:205:GLY:H	1.69	0.41
1:A:127:THR:O	1:A:131:PHE:HD2	2.04	0.41
1:A:410:ILE:CD1	1:A:420:LYS:HB2	2.44	0.41
1:A:471:ASP:HA	1:A:472:PRO:HA	1.76	0.41
1:A:202:LEU:HD22	1:A:525:LYS:HD2	2.03	0.41
1:A:68:VAL:HA	1:A:72:GLU:OE2	2.21	0.41
1:A:73:LEU:HG	1:A:76:TYR:HE1	1.85	0.41
1:A:92:HIS:HB3	5:D:433:HOH:O	2.21	0.41
2:C:116:GLU:O	2:C:119:LYS:HB2	2.20	0.41
2:C:39:ASP:OD1	2:C:40:LYS:N	2.54	0.41
1:A:93:PRO:CD	2:D:182:ARG:HD3	2.50	0.41
2:D:84:GLY:N	2:D:88:GLU:OE2	2.53	0.41
2:E:10:ILE:HG22	2:E:202:PRO:HD2	2.01	0.41
2:E:174:PRO:HG2	2:E:175:LYS:CD	2.48	0.41
1:A:111:ILE:HG13	1:A:111:ILE:O	2.21	0.41
1:A:308:SER:HA	1:A:424:ARG:NE	2.34	0.41
1:A:99:LEU:HD12	1:A:100:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:PHE:HA	2:B:125:LYS:HG2	2.03	0.41
2:C:186:ILE:HG13	2:C:187:PRO:HD2	2.02	0.41
2:E:123:LEU:O	2:E:127:PRO:HD3	2.21	0.41
2:E:35:ARG:NH2	2:E:214:ASP:HB3	2.36	0.41
2:E:8:TRP:CD1	2:E:9:LYS:N	2.89	0.41
1:A:198:VAL:HG23	1:A:525:LYS:O	2.21	0.41
1:A:199:HIS:NE2	1:A:200:GLN:HG3	2.36	0.41
2:B:98:ALA:HB3	2:B:133:PHE:CZ	2.56	0.41
2:B:24:LEU:HD22	5:B:404:HOH:O	2.20	0.41
2:B:58:TYR:CZ	2:B:71:ILE:HA	2.55	0.41
2:B:58:TYR:CE2	2:B:74:TYR:CD1	3.09	0.41
2:C:8:TRP:HB2	2:C:10:ILE:HG13	2.02	0.41
2:C:73:ARG:HB3	2:C:82:LEU:HD21	2.02	0.41
2:D:112:SER:OG	2:D:113:LYS:N	2.52	0.41
2:D:142:TYR:HB3	2:D:152:ASP:OD1	2.20	0.41
2:D:73:ARG:NH2	2:E:89:ARG:HG3	2.36	0.41
2:G:127:PRO:O	2:G:131:LYS:HB2	2.21	0.41
1:A:165:ALA:HB2	1:A:333:SER:CB	2.48	0.41
1:A:280:LYS:O	1:A:283:SER:OG	2.35	0.41
1:A:42:ALA:HB2	2:D:141:THR:OG1	2.21	0.41
1:A:466:ILE:HB	1:A:552:LYS:HA	2.03	0.41
1:A:445:VAL:HG13	1:A:479:TRP:NE1	2.35	0.41
1:A:69:THR:O	1:A:72:GLU:HG2	2.21	0.41
2:C:85:CYS:HB2	2:C:88:GLU:HG2	2.03	0.41
2:C:88:GLU:HG2	2:C:88:GLU:H	1.77	0.41
2:G:191:LYS:HE2	2:G:191:LYS:HB3	1.76	0.41
2:G:73:ARG:HA	2:G:73:ARG:HD3	1.76	0.41
1:A:119:GLU:O	1:A:122:LEU:HG	2.21	0.40
1:A:266:LEU:HD13	2:F:181:LYS:NZ	2.35	0.40
2:B:95:LEU:HD11	2:B:143:LEU:HD22	2.03	0.40
2:B:215:HIS:ND1	2:B:216:PRO:HD2	2.36	0.40
2:B:37:GLU:O	2:B:40:LYS:HB3	2.21	0.40
2:G:208:ALA:N	5:G:424:HOH:O	2.54	0.40
1:A:96:ALA:HB1	1:A:163:GLY:N	2.36	0.40
1:A:107:ARG:NH2	1:A:552:LYS:HG2	2.36	0.40
2:C:102:ILE:HG23	2:C:103:ARG:NE	2.36	0.40
2:C:121:ASP:OD1	2:C:122:PHE:N	2.55	0.40
2:C:11:LYS:HB3	2:C:15:GLN:CD	2.41	0.40
2:C:22:GLU:HB2	2:C:189:ILE:HG22	2.04	0.40
2:D:66:THR:O	2:D:67:GLN:HB3	2.20	0.40
2:D:73:ARG:HH21	2:E:89:ARG:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:LYS:HD2	2:E:142:TYR:O	2.22	0.40
2:F:109:ILE:HA	5:F:459:HOH:O	2.21	0.40
2:F:66:THR:O	2:F:67:GLN:HB2	2.21	0.40
1:A:117:LEU:HA	1:A:117:LEU:HD23	1.85	0.40
1:A:572:SER:OG	1:A:574:ALA:HB3	2.21	0.40
2:C:35:ARG:HH21	2:C:36:ASP:CG	2.25	0.40
2:D:113:LYS:HE2	2:D:114:ASP:OD1	2.21	0.40
2:E:139:HIS:CE1	2:E:140:LYS:HD3	2.56	0.40
2:E:21:LEU:HA	2:E:21:LEU:HD12	1.85	0.40
2:F:51:GLU:OE1	2:G:136:ARG:HD2	2.21	0.40
2:G:13:LEU:N	2:G:13:LEU:HD12	2.37	0.40
2:G:14:VAL:HG12	2:G:17:THR:HB	2.03	0.40
1:A:143:LYS:HD2	1:A:212:PHE:CD2	2.56	0.40
1:A:38:LYS:HG2	2:D:139:HIS:NE2	2.36	0.40
1:A:68:VAL:HG23	1:A:401:TYR:HA	2.03	0.40
2:B:25:GLU:OE2	2:B:188:GLN:NE2	2.54	0.40
2:B:190:ASP:N	2:B:190:ASP:OD1	2.54	0.40
2:B:77:ASP:O	2:B:80:ASN:N	2.55	0.40
2:D:137:LEU:CA	2:D:140:LYS:HE2	2.51	0.40
2:D:74:TYR:OH	2:D:78:LYS:HE2	2.22	0.40
2:E:3:PRO:HD2	5:E:425:HOH:O	2.21	0.40
2:G:11:LYS:HD2	2:G:203:LEU:HD23	2.04	0.40
2:G:206:TRP:HA	2:G:212:GLY:CA	2.51	0.40
1:A:487:GLU:HB3	1:A:570:TYR:CE2	2.57	0.40
1:A:477:ILE:O	1:A:521:ARG:NH1	2.55	0.40
1:A:532:GLN:HG3	5:A:773:HOH:O	2.20	0.40
1:A:108:PRO:HD2	1:A:552:LYS:HZ3	1.86	0.40
2:B:115:PHE:HE2	2:B:209:THR:H	1.70	0.40
2:C:73:ARG:O	2:C:77:ASP:OD2	2.38	0.40
2:C:24:LEU:HD21	2:C:79:HIS:CB	2.51	0.40
2:E:155:LEU:HD23	2:E:179:PHE:CE2	2.57	0.40
2:G:141:THR:C	2:G:142:TYR:HD1	2.24	0.40

All (10) 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)
2:B:142:TYR:OH	2:E:121:ASP:OD2[1_566]	1.93	0.27
2:B:147:HIS:N	2:E:121:ASP:OD2[1_566]	1.99	0.21
2:B:182:ARG:NH1	2:D:111:TYR:O[1_566]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:440:HOH:O	5:G:464:HOH:O[1_645]	2.13	0.07
2:C:175:LYS:NZ	5:A:710:HOH:O[1_655]	2.15	0.05
5:A:710:HOH:O	5:A:713:HOH:O[1_455]	2.17	0.03
2:B:85:CYS:SG	2:E:169:CYS:CB[1_566]	2.17	0.03
2:B:136:ARG:O	2:E:117:THR:OG1[1_566]	2.17	0.03
1:A:67:LEU:N	2:B:121:ASP:OD2[1_545]	2.18	0.02
2:D:29:GLU:OE1	2:E:44:LYS:NZ[1_655]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/575 (99%)	532 (94%)	28 (5%)	7 (1%)	15	20
2	B	214/218 (98%)	198 (92%)	9 (4%)	7 (3%)	4	3
2	C	214/218 (98%)	202 (94%)	10 (5%)	2 (1%)	20	27
2	D	214/218 (98%)	203 (95%)	10 (5%)	1 (0%)	32	44
2	E	214/218 (98%)	196 (92%)	10 (5%)	8 (4%)	4	3
2	F	214/218 (98%)	199 (93%)	10 (5%)	5 (2%)	7	7
2	G	214/218 (98%)	204 (95%)	6 (3%)	4 (2%)	9	10
All	All	1851/1883 (98%)	1734 (94%)	83 (4%)	34 (2%)	10	11

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	A	540	SER
1	A	542	ALA
2	B	148	VAL
2	E	67	GLN
2	E	109	ILE

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Mol	Chain	Res	Type
2	E	168	MET
2	F	202	PRO
2	G	113	LYS
2	G	115	PHE
2	B	82	LEU
2	E	15	GLN
2	E	205	GLY
2	G	63	VAL
1	A	57	PRO
2	B	138	CYS
2	C	113	LYS
2	E	166	ASP
2	F	11	LYS
2	F	65	LEU
2	F	67	GLN
2	G	67	GLN
1	A	474	HIS
1	A	539	GLY
2	B	85	CYS
2	B	86	PRO
2	E	16	PRO
2	F	38	GLY
2	C	34	GLU
2	D	67	GLN
2	B	11	LYS
2	B	67	GLN
2	E	112	SER
1	A	83	GLY

### 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%)	467 (94%)	32 (6%)	20	29
2	B	192/194 (99%)	185 (96%)	7 (4%)	40	58
2	C	192/194 (99%)	183 (95%)	9 (5%)	30	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	192/194 (99%)	182 (95%)	10 (5%)	27	40
2	E	192/194 (99%)	187 (97%)	5 (3%)	51	70
2	F	192/194 (99%)	179 (93%)	13 (7%)	18	27
2	G	192/194 (99%)	186 (97%)	6 (3%)	45	64
All	All	1651/1669 (99%)	1569 (95%)	82 (5%)	28	42

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	55	THR
1	A	64	MET
1	A	73	LEU
1	A	94	VAL
1	A	99	LEU
1	A	108	PRO
1	A	111	ILE
1	A	124	LEU
1	A	140	ASP
1	A	156	SER
1	A	218	TYR
1	A	223	PHE
1	A	242	VAL
1	A	291	ILE
1	A	295	PHE
1	A	301	VAL
1	A	342	THR
1	A	355	ILE
1	A	369	THR
1	A	373	GLU
1	A	395	TYR
1	A	400	ARG
1	A	437	THR
1	A	453	SER
1	A	464	SER
1	A	485	THR
1	A	488	ASP
1	A	509	SER
1	A	555	ASN
1	A	563	CYS
1	A	565	ASN

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Mol	Chain	Res	Type
2	B	14	VAL
2	B	28	TYR
2	B	60	ASP
2	B	63	VAL
2	B	95	LEU
2	B	119	LYS
2	B	178	CYS
2	C	50	LEU
2	C	51	GLU
2	C	89	ARG
2	C	94	MET
2	C	108	ARG
2	C	117	THR
2	C	126	LEU
2	C	138	CYS
2	C	169	CYS
2	D	14	VAL
2	D	15	GLN
2	D	43	ASN
2	D	55	LEU
2	D	75	ILE
2	D	95	LEU
2	D	119	LYS
2	D	139	HIS
2	D	146	ASP
2	D	169	CYS
2	E	36	ASP
2	E	66	THR
2	E	114	ASP
2	E	118	LEU
2	E	190	ASP
2	F	18	ARG
2	F	31	HIS
2	F	41	TRP
2	F	43	ASN
2	F	74	TYR
2	F	100	LEU
2	F	123	LEU
2	F	124	SER
2	F	130	LEU
2	F	141	THR
2	F	155	LEU

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Mol	Chain	Res	Type
2	F	177	VAL
2	F	178	CYS
2	G	14	VAL
2	G	50	LEU
2	G	149	THR
2	G	150	HIS
2	G	177	VAL
2	G	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	200	GLN
1	A	565	ASN
2	B	54	ASN
2	B	150	HIS
2	C	15	GLN
2	C	150	HIS
2	D	80	ASN
2	D	150	HIS
2	E	150	HIS
2	F	204	GLN
2	G	15	GLN
2	G	67	GLN
2	G	150	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	JAA	A	601	-	12,15,15	1.04	0	12,19,19	2.53	7 (58%)
4	GSH	B	301	-	11,19,19	2.07	3 (27%)	14,24,24	2.26	3 (21%)
4	GSH	C	301	-	11,19,19	2.02	2 (18%)	14,24,24	2.33	6 (42%)
4	GSH	D	301	-	11,19,19	2.01	2 (18%)	14,24,24	2.11	3 (21%)
4	GSH	E	301	-	11,19,19	2.09	2 (18%)	14,24,24	1.68	4 (28%)
4	GSH	F	301	-	11,19,19	2.05	2 (18%)	14,24,24	2.29	6 (42%)
4	GSH	G	301	-	11,19,19	2.05	2 (18%)	14,24,24	1.85	5 (35%)

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	GSH	B	301	-	-	0/18/24/24	0/0/0/0
4	GSH	C	301	-	-	0/18/24/24	0/0/0/0
4	GSH	D	301	-	-	0/18/24/24	0/0/0/0
4	GSH	E	301	-	-	0/18/24/24	0/0/0/0
4	GSH	F	301	-	-	0/18/24/24	0/0/0/0
4	GSH	G	301	-	-	0/18/24/24	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	GSH	CA2-N2	-2.01	1.41	1.45
4	F	301	GSH	CD1-N2	3.67	1.41	1.34
4	B	301	GSH	CD1-N2	3.73	1.41	1.34
4	D	301	GSH	CD1-N2	3.75	1.41	1.34
4	C	301	GSH	CD1-N2	3.98	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	GSH	C2-N3	4.13	1.42	1.33
4	E	301	GSH	CD1-N2	4.14	1.42	1.34
4	G	301	GSH	CD1-N2	4.14	1.42	1.34
4	C	301	GSH	C2-N3	4.17	1.42	1.33
4	B	301	GSH	C2-N3	4.23	1.42	1.33
4	G	301	GSH	C2-N3	4.27	1.42	1.33
4	E	301	GSH	C2-N3	4.33	1.42	1.33
4	F	301	GSH	C2-N3	4.42	1.42	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	GSH	CB2-CA2-N2	-5.78	103.02	111.39
4	D	301	GSH	CA2-CB2-SG2	-5.66	107.54	114.15
4	F	301	GSH	CB2-CA2-N2	-5.21	103.85	111.39
4	C	301	GSH	CB2-CA2-N2	-4.61	104.71	111.39
4	C	301	GSH	CA3-N3-C2	-4.07	116.89	122.39
4	G	301	GSH	CA2-CB2-SG2	-3.97	109.52	114.15
4	B	301	GSH	CA2-CB2-SG2	-3.94	109.56	114.15
3	A	601	JAA	C06-C04-C05	-3.69	98.07	103.37
4	F	301	GSH	CG1-CB1-CA1	-3.68	105.27	113.84
4	B	301	GSH	CG1-CB1-CA1	-3.37	105.97	113.84
4	C	301	GSH	O2-C2-N3	-3.26	116.78	123.07
4	C	301	GSH	CA2-CB2-SG2	-2.95	110.71	114.15
4	E	301	GSH	CA2-CB2-SG2	-2.92	110.74	114.15
4	E	301	GSH	CB2-CA2-N2	-2.83	107.29	111.39
3	A	601	JAA	C06-C07-C08	-2.83	102.44	105.42
4	D	301	GSH	CG1-CB1-CA1	-2.39	108.28	113.84
4	G	301	GSH	CB1-CG1-CD1	-2.37	107.81	113.18
4	F	301	GSH	CA3-N3-C2	-2.36	119.19	122.39
4	D	301	GSH	CB1-CG1-CD1	-2.29	108.00	113.18
4	G	301	GSH	CA3-N3-C2	-2.29	119.30	122.39
3	A	601	JAA	C07-C06-C04	-2.27	102.20	104.49
4	G	301	GSH	CB2-CA2-N2	-2.22	108.18	111.39
4	E	301	GSH	CA3-N3-C2	-2.18	119.44	122.39
4	F	301	GSH	CB1-CG1-CD1	-2.07	108.51	113.18
4	C	301	GSH	CG1-CB1-CA1	-2.06	109.05	113.84
3	A	601	JAA	C10-C04-C05	2.18	119.78	114.74
4	G	301	GSH	CA2-C2-N3	2.21	121.03	116.51
4	F	301	GSH	CG1-CD1-N2	2.23	119.75	115.82
4	E	301	GSH	CA2-C2-N3	2.36	121.32	116.51
4	F	301	GSH	CA2-C2-N3	2.80	122.23	116.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	GSH	CA2-C2-N3	2.85	122.33	116.51
3	A	601	JAA	O01-C08-C05	2.96	129.52	125.58
3	A	601	JAA	C12-C10-C04	3.20	120.77	114.63
3	A	601	JAA	C05-C09-C11	4.61	122.77	112.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	JAA	5	0
4	B	301	GSH	8	0
4	C	301	GSH	2	0
4	D	301	GSH	2	0
4	E	301	GSH	2	0
4	F	301	GSH	5	0
4	G	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	569/575 (98%)	0.32	26 (4%)	33 35	5, 12, 17, 24	0
2	B	216/218 (99%)	0.62	15 (6%)	18 18	9, 17, 24, 30	0
2	C	216/218 (99%)	0.40	8 (3%)	42 45	9, 17, 23, 28	0
2	D	216/218 (99%)	0.48	14 (6%)	20 20	11, 19, 27, 53	0
2	E	216/218 (99%)	0.64	14 (6%)	20 20	9, 18, 26, 53	0
2	F	216/218 (99%)	0.71	27 (12%)	4 5	9, 17, 25, 36	0
2	G	216/218 (99%)	0.52	14 (6%)	20 20	9, 17, 23, 37	0
All	All	1865/1883 (99%)	0.49	118 (6%)	21 22	5, 16, 24, 53	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	84	GLY	11.0
2	B	145	GLY	7.9
2	B	85	CYS	7.0
2	E	178	CYS	5.1
2	F	110	ALA	4.8
2	G	7	TYR	4.4
2	B	83	GLY	4.4
2	F	155	LEU	4.2
2	E	121	ASP	4.1
2	F	59	ILE	4.1
2	F	17	THR	4.0
2	E	168	MET	3.9
2	F	41	TRP	3.9
2	F	105	GLY	3.9
2	B	82	LEU	3.9
1	A	554	SER	3.9
1	A	401	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	110	PHE	3.8
2	D	185	ALA	3.8
1	A	117	LEU	3.8
2	B	63	VAL	3.6
2	D	55	LEU	3.5
2	F	215	HIS	3.5
1	A	406	VAL	3.4
2	E	114	ASP	3.3
1	A	464	SER	3.3
2	F	8	TRP	3.3
1	A	96	ALA	3.3
2	E	176	LEU	3.3
2	G	2	SER	3.3
2	C	102	ILE	3.2
1	A	566	VAL	3.2
2	F	38	GLY	3.2
2	E	194	LYS	3.2
2	F	203	LEU	3.1
2	G	133	PHE	3.1
2	G	74	TYR	3.0
2	F	43	ASN	3.0
1	A	553	PRO	3.0
2	C	105	GLY	3.0
2	D	189	ILE	3.0
2	F	61	GLY	3.0
2	E	117	THR	2.9
2	F	32	LEU	2.9
2	F	109	ILE	2.9
2	G	85	CYS	2.9
2	G	92	ILE	2.9
2	F	126	LEU	2.9
2	B	142	TYR	2.9
1	A	543	GLY	2.9
1	A	449	ALA	2.9
2	G	65	LEU	2.9
2	E	37	GLU	2.8
2	F	18	ARG	2.8
2	D	186	ILE	2.8
2	F	33	TYR	2.8
2	C	117	THR	2.8
2	B	58	TYR	2.8
2	E	52	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	G	38	GLY	2.7
2	B	137	LEU	2.7
1	A	289	GLY	2.7
2	F	127	PRO	2.7
2	C	94	MET	2.7
2	F	130	LEU	2.7
2	E	198	TYR	2.6
2	G	165	MET	2.6
1	A	443	LEU	2.5
1	A	42	ALA	2.5
2	D	126	LEU	2.5
2	E	189	ILE	2.5
1	A	150	SER	2.5
2	B	28	TYR	2.5
2	F	162	VAL	2.4
2	G	216	PRO	2.4
2	F	23	TYR	2.4
2	D	59	ILE	2.4
1	A	195	SER	2.4
2	E	179	PHE	2.4
2	B	76	ALA	2.4
2	D	162	VAL	2.4
1	A	316	LEU	2.4
2	D	38	GLY	2.4
2	B	141	THR	2.3
2	D	204	GLN	2.3
2	G	183	ILE	2.3
2	F	7	TYR	2.3
2	F	163	LEU	2.3
1	A	473	GLY	2.2
2	B	71	ILE	2.2
2	B	209	THR	2.2
2	F	129	MET	2.2
2	C	162	VAL	2.2
1	A	86	SER	2.2
2	D	214	ASP	2.2
1	A	77	ILE	2.2
2	C	158	ALA	2.2
1	A	320	ALA	2.1
2	C	90	ALA	2.1
2	B	184	GLU	2.1
1	A	7	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	141	THR	2.1
2	G	10	ILE	2.1
2	E	13	LEU	2.1
2	E	104	TYR	2.1
1	A	92	HIS	2.1
2	D	25	GLU	2.1
2	D	216	PRO	2.1
2	F	137	LEU	2.1
1	A	321	GLY	2.1
2	F	19	LEU	2.1
2	D	41	TRP	2.1
2	F	49	GLY	2.1
1	A	89	LEU	2.0
2	G	162	VAL	2.0
1	A	8	PHE	2.0
2	D	154	MET	2.0
2	C	89	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	JAA	A	601	15/15	0.68	0.38	6.33	20,20,20,20	0
4	GSH	F	301	20/20	0.89	0.16	-0.47	6,7,7,7	0
4	GSH	D	301	20/20	0.93	0.13	-0.57	6,7,7,7	0
4	GSH	C	301	20/20	0.92	0.14	-0.61	6,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GSH	B	301	20/20	0.91	0.13	-1.55	6,7,7,7	0
4	GSH	E	301	20/20	0.96	0.09	-1.74	6,7,7,7	0
4	GSH	G	301	20/20	0.94	0.11	-2.04	6,7,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.