Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:04 PM GMT

PDB ID	:	1GYL
Title	:	INVOLVEMENT OF TYR24 AND TRP108 IN SUBSTRATE BINDING AND SUBSTRATE SPECIFICITY OF GLYCOLATE OXIDASE
Authors	:	Lindqvist, Y.; Stenberg, K.
Deposited on	:	1995-01-30
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

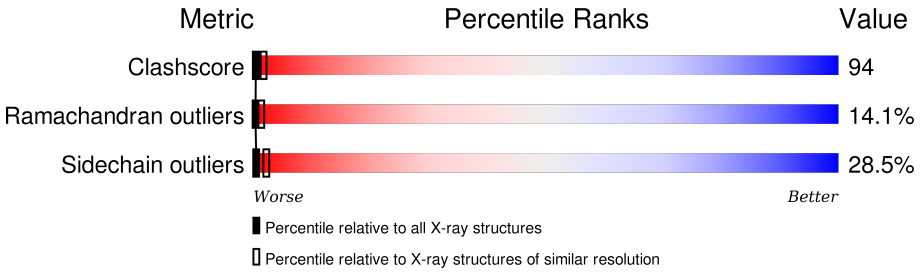
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	369	17% 54% 22% • 5%
1	B	369	11% 51% 26% 6% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5436 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.

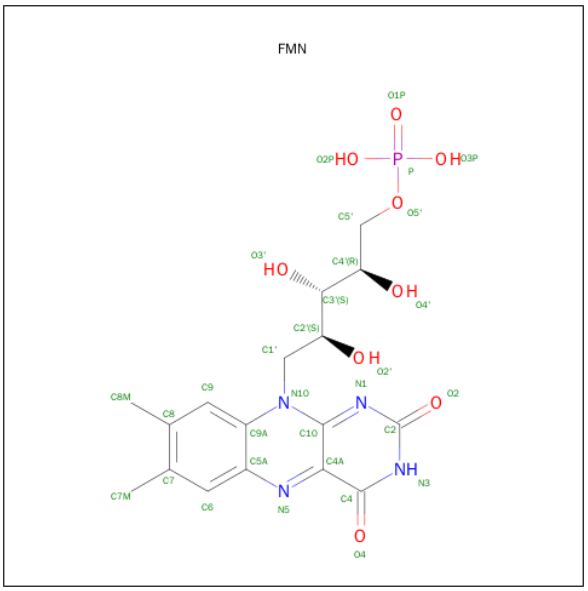
- Molecule 1 is a protein called GLYCOLATE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2708	1726	474	495	13			
1	B	350	Total	C	N	O	S	0	0	0
			2695	1718	471	493	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	PHE	TYR	CONFLICT	UNP P05414
B	24	PHE	TYR	CONFLICT	UNP P05414

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0

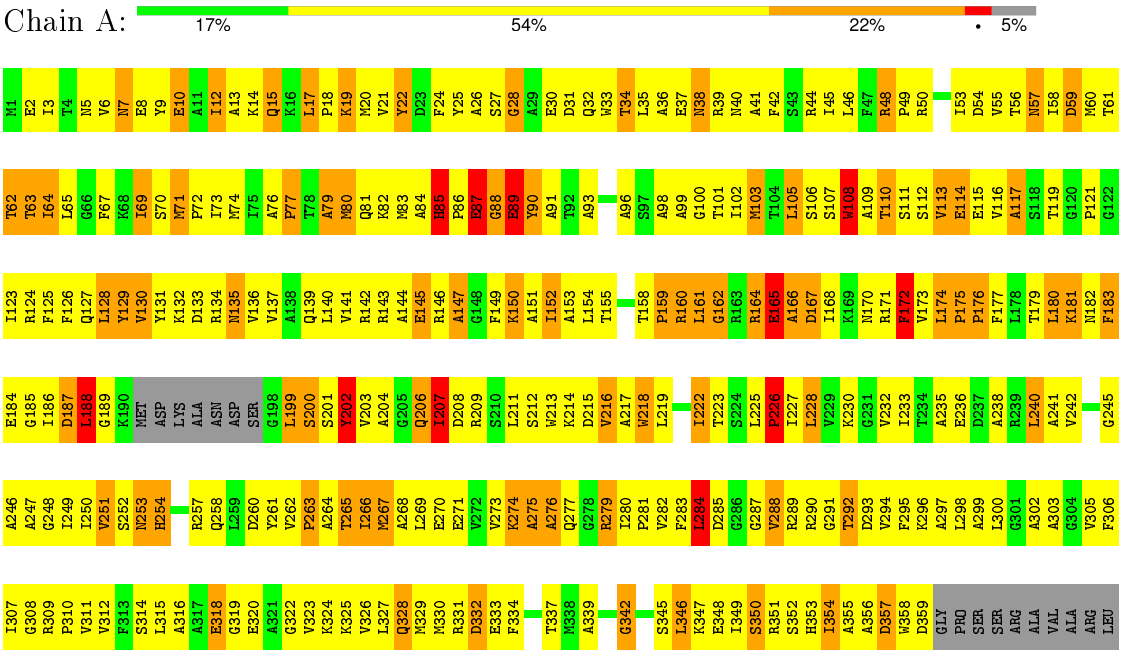
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

Note EDS was not executed.

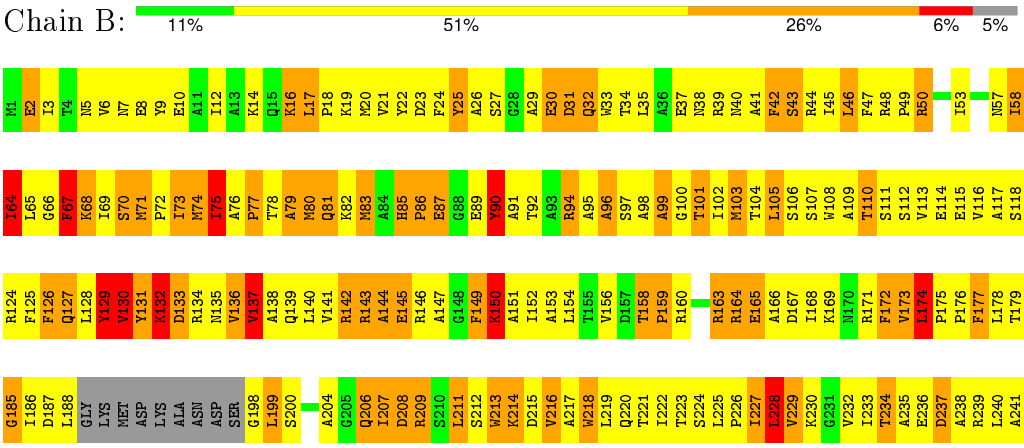
- Molecule 1: GLYCOLATE OXIDASE

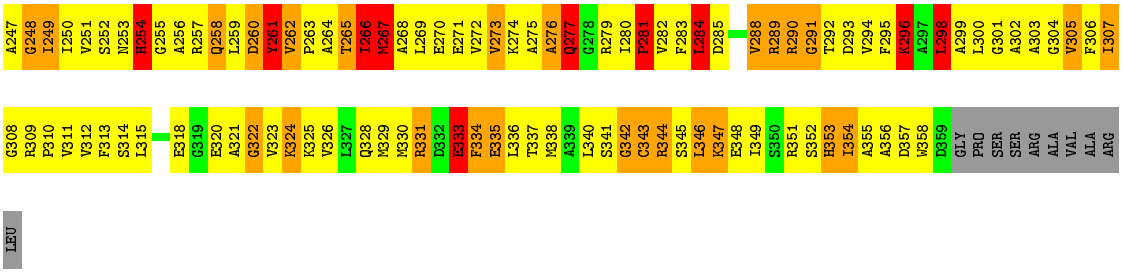
Chain A:



- Molecule 1: GLYCOLATE OXIDASE

Chain B:




A247 G248 I249 I250 V251 S252 N253 H254 G255 A256 R257 Q258 L259 D260 Y261 V262 P263 A264 T265 I266 M267 A268 L269 E270 E271 Y272 Y273 K274 A275 A276 Q277 G278 R279 I280 P281 V282 F283 I284 D285 V288 R289 R290 G291 T292 D293 V294 F295 K296 A297 L298 A299 L300 G301 A302 A303 G304 Y305 F306 I307
G308 R309 P310 V311 V312 F313 S314 L315 E318 G319 E320 A321 G322 V323 K324 K325 V326 L327 Q328 M329 M330 R331 D332 E333 F334 E335 L336 T337 M338 A339 L340 S341 G342 C343 R344 S345 L346 K347 E348 I349 S350 R351 S352 H353 I354 A355 A356 D357 W358 D359 GLY PRO SER SER ARG ALA VAL ALA ARG
LEU

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	145.50Å 145.50Å 100.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.254 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5436	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

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	0.75	1/2756 (0.0%)	1.09	13/3729 (0.3%)
1	B	0.78	0/2743	1.15	11/3713 (0.3%)
All	All	0.77	1/5499 (0.0%)	1.12	24/7442 (0.3%)

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
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	GLU	CG-CD	5.40	1.60	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	LEU	CA-CB-CG	7.61	132.80	115.30
1	B	228	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	160	ARG	N-CA-C	-6.48	93.51	111.00
1	A	147	ALA	N-CA-C	-6.45	93.57	111.00
1	B	298	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	202	TYR	N-CA-C	-6.18	94.31	111.00
1	A	170	ASN	N-CA-C	-5.90	95.07	111.00
1	A	188	LEU	N-CA-C	-5.86	95.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	ILE	N-CA-C	-5.73	95.54	111.00
1	B	60	MET	N-CA-C	-5.70	95.61	111.00
1	B	150	LYS	N-CA-C	5.51	125.89	111.00
1	B	354	ILE	N-CA-C	-5.50	96.15	111.00
1	B	284	LEU	CA-CB-CG	5.46	127.85	115.30
1	B	99	ALA	N-CA-C	-5.43	96.33	111.00
1	A	188	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	183	PHE	N-CA-C	-5.35	96.56	111.00
1	A	50	ARG	N-CA-C	-5.30	96.70	111.00
1	B	132	LYS	N-CA-C	5.22	125.09	111.00
1	A	128	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	342	GLY	N-CA-C	5.09	125.83	113.10
1	A	89	GLU	N-CA-C	-5.08	97.28	111.00
1	A	28	GLY	N-CA-C	-5.07	100.43	113.10
1	B	166	ALA	N-CA-C	-5.01	97.47	111.00
1	B	281	PRO	N-CA-C	5.00	125.10	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	TYR	Sidechain
1	B	90	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2708	0	2771	408	0
1	B	2695	0	2755	681	0
2	A	31	0	19	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	5436	0	5545	1032	0

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 94.

All (1032) 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:B:235:ALA:HA	1:B:238:ALA:HB3	1.18	1.14
1:A:80:MET:HG2	1:A:110:THR:HG23	1.27	1.14
1:B:82:LYS:HB2	1:B:178:LEU:HD11	1.22	1.13
1:B:227:ILE:HB	1:B:246:ALA:HB1	1.17	1.09
1:B:165:GLU:HA	1:B:168:ILE:HB	1.16	1.09
1:B:144:ALA:HA	1:B:149:PHE:HB3	1.35	1.08
1:B:132:LYS:HG3	1:B:208:ASP:HB2	1.37	1.06
1:A:146:ARG:HB2	1:B:114:GLU:HA	1.31	1.04
1:B:47:PHE:HA	1:B:355:ALA:H	1.24	1.02
1:A:142:ARG:NH1	1:B:184:GLU:HG3	1.74	1.01
1:A:181:LYS:HA	1:A:184:GLU:HB2	1.45	0.98
1:A:143:ARG:NE	1:B:142:ARG:HA	1.79	0.97
1:B:25:TYR:HE2	1:B:81:GLN:HB3	1.28	0.97
1:A:112:SER:HB2	1:A:181:LYS:O	1.66	0.96
1:B:229:VAL:HG22	1:B:246:ALA:HB3	1.47	0.95
1:B:131:TYR:HB3	1:B:136:VAL:HB	1.46	0.95
1:B:307:ILE:HB	1:B:310:PRO:HG3	1.47	0.94
1:B:228:LEU:HA	1:B:247:ALA:O	1.68	0.94
1:A:5:ASN:HB3	1:A:8:GLU:HB2	1.48	0.94
1:B:74:MET:HB2	1:B:102:ILE:HB	1.49	0.94
1:B:82:LYS:HD3	1:B:178:LEU:HD21	1.49	0.93
1:A:60:MET:O	1:A:72:PRO:HD3	1.68	0.93
1:B:248:GLY:HA2	1:B:281:PRO:HB2	1.47	0.93
1:B:41:ALA:O	1:B:44:ARG:HB3	1.67	0.93
1:B:98:ALA:HB1	1:B:324:LYS:HE2	1.50	0.93
1:B:45:ILE:HG13	1:B:357:ASP:H	1.32	0.93
1:B:74:MET:CB	1:B:102:ILE:HB	1.99	0.93
1:B:24:PHE:HA	1:B:164:ARG:HH21	1.33	0.92
1:B:300:LEU:HD21	1:B:354:ILE:HG21	1.52	0.92
1:B:232:VAL:H	1:B:251:VAL:HA	1.33	0.91
1:A:28:GLY:HA3	1:A:35:LEU:HD11	1.52	0.91
1:B:298:LEU:HA	1:B:302:ALA:HB3	1.48	0.91
1:B:247:ALA:HA	1:B:280:ILE:HB	1.53	0.90
1:B:291:GLY:HA2	1:B:330:MET:SD	2.11	0.90
1:B:67:PHE:HA	1:B:68:LYS:HZ1	1.37	0.90
1:B:132:LYS:HB2	1:B:206:GLN:HA	1.55	0.89
1:A:82:LYS:HB3	1:A:110:THR:HG21	1.55	0.89
1:A:48:ARG:HB2	1:A:354:ILE:HA	1.53	0.89
1:A:114:GLU:HG3	1:A:115:GLU:HG3	1.56	0.88
1:B:229:VAL:HG23	1:B:249:ILE:HG12	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HA	1:B:139:GLN:HG3	1.54	0.88
1:A:152:ILE:HD12	1:A:227:ILE:HD11	1.56	0.88
1:B:30:GLU:HG3	1:B:259:LEU:HA	1.56	0.87
1:B:61:THR:HG23	1:B:70:SER:HA	1.56	0.87
1:B:268:ALA:O	1:B:272:VAL:HG22	1.75	0.87
1:B:31:ASP:O	1:B:260:ASP:HB3	1.74	0.87
1:A:12:ILE:O	1:A:15:GLN:HG3	1.74	0.87
1:B:37:GLU:HG3	1:B:264:ALA:HB2	1.54	0.87
1:A:45:ILE:HD11	1:A:266:ILE:HD11	1.57	0.87
1:A:87:GLU:O	1:A:90:TYR:HB2	1.75	0.87
1:B:346:LEU:HA	1:B:349:ILE:HG12	1.57	0.86
1:B:73:ILE:HA	1:B:305:VAL:HB	1.57	0.86
1:A:151:ALA:HA	1:A:225:LEU:O	1.76	0.86
1:B:152:ILE:HD11	1:B:225:LEU:HD12	1.56	0.86
1:B:283:PHE:HE1	1:B:303:ALA:HB3	1.39	0.86
1:B:283:PHE:CE1	1:B:303:ALA:HB3	2.11	0.85
1:A:186:ILE:HG12	1:B:142:ARG:NH1	1.90	0.85
1:B:273:VAL:HA	1:B:282:VAL:HG21	1.56	0.85
1:B:235:ALA:CA	1:B:238:ALA:HB3	2.05	0.85
1:B:152:ILE:HB	1:B:226:PRO:O	1.76	0.85
1:B:29:ALA:HA	1:B:164:ARG:HB3	1.55	0.85
1:A:74:MET:O	1:A:307:ILE:HG12	1.75	0.85
1:B:22:TYR:HA	1:B:25:TYR:CD1	2.12	0.85
1:B:264:ALA:O	1:B:267:MET:SD	2.35	0.85
1:A:284:LEU:HD11	1:A:297:ALA:HB1	1.59	0.84
1:A:60:MET:SD	1:A:331:ARG:HG3	2.18	0.84
1:A:143:ARG:CZ	1:B:142:ARG:HA	2.06	0.84
1:B:233:ILE:HA	1:B:251:VAL:HG13	1.60	0.84
1:A:64:ILE:HG13	1:A:283:PHE:CE1	2.12	0.84
1:A:146:ARG:HB2	1:B:114:GLU:CA	2.09	0.83
1:A:274:LYS:HE2	1:A:274:LYS:HA	1.58	0.83
1:A:354:ILE:HG12	1:A:355:ALA:H	1.42	0.83
1:B:230:LYS:HG2	1:B:250:ILE:CG2	2.09	0.83
1:A:63:THR:HA	1:A:67:PHE:O	1.79	0.83
1:A:88:GLY:O	1:A:89:GLU:HB2	1.79	0.83
1:B:270:GLU:HA	1:B:273:VAL:HG12	1.59	0.82
1:B:186:ILE:HG13	1:B:188:LEU:HB3	1.61	0.82
1:B:23:ASP:HB2	1:B:167:ASP:HB3	1.62	0.82
1:A:116:VAL:O	1:A:119:THR:HG23	1.80	0.81
1:A:39:ARG:HD3	1:A:289:ARG:HH21	1.45	0.81
1:B:131:TYR:CD1	1:B:206:GLN:HG2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:CG2	1:A:143:ARG:HD3	2.10	0.80
1:A:188:LEU:HD12	1:B:135:ASN:ND2	1.96	0.80
1:B:141:VAL:HG22	1:B:223:THR:HB	1.64	0.80
1:B:269:LEU:HD21	1:B:300:LEU:HB3	1.64	0.80
1:B:53:ILE:HG13	1:B:342:GLY:HA3	1.63	0.80
1:B:237:ASP:HA	1:B:240:LEU:HD12	1.64	0.79
1:B:20:MET:HG2	1:B:172:PHE:HB2	1.65	0.79
1:B:184:GLU:O	1:B:186:ILE:HG12	1.82	0.79
1:B:295:PHE:HA	1:B:298:LEU:HG	1.64	0.79
1:B:71:MET:HG2	1:B:73:ILE:HG13	1.64	0.79
1:B:24:PHE:HA	1:B:164:ARG:NH2	1.97	0.79
1:B:266:ILE:HG23	1:B:267:MET:SD	2.23	0.79
1:A:106:SER:HA	1:A:127:GLN:HB3	1.62	0.79
1:A:164:ARG:NH1	1:A:257:ARG:HB3	1.98	0.79
1:A:222:ILE:HG22	1:B:185:GLY:HA3	1.63	0.78
1:B:25:TYR:CE2	1:B:81:GLN:HB3	2.16	0.78
1:B:125:PHE:CZ	1:B:151:ALA:HB3	2.18	0.78
1:A:48:ARG:CB	1:A:354:ILE:HA	2.14	0.78
1:B:333:GLU:O	1:B:336:LEU:HB2	1.83	0.78
1:A:300:LEU:HA	1:A:351:ARG:HD3	1.66	0.78
1:B:91:ALA:CA	1:B:320:GLU:HA	2.14	0.78
1:B:307:ILE:HB	1:B:310:PRO:CG	2.12	0.78
1:A:131:TYR:HD1	1:A:207:ILE:HA	1.48	0.78
1:B:188:LEU:HD13	1:B:198:GLY:HA2	1.66	0.78
1:A:291:GLY:HA2	1:A:294:VAL:HB	1.66	0.77
1:B:35:LEU:HD13	1:B:256:ALA:HB3	1.66	0.77
1:B:26:ALA:HA	1:B:309:ARG:CZ	2.15	0.77
1:B:75:ILE:HA	1:B:307:ILE:HG13	1.67	0.77
1:A:273:VAL:HG22	1:A:282:VAL:HG21	1.65	0.77
1:B:267:MET:N	1:B:267:MET:SD	2.57	0.77
1:B:298:LEU:HA	1:B:302:ALA:CB	2.15	0.77
1:B:209:ARG:HE	1:B:209:ARG:H	1.31	0.77
1:B:24:PHE:CD2	1:B:80:MET:HB2	2.20	0.77
1:B:110:THR:HB	1:B:181:LYS:HB2	1.67	0.76
1:B:143:ARG:O	1:B:145:GLU:HG2	1.85	0.76
1:B:251:VAL:HG12	1:B:265:THR:HG22	1.66	0.76
1:A:201:SER:HA	1:A:204:ALA:HB3	1.65	0.76
1:A:131:TYR:HA	1:A:207:ILE:HA	1.65	0.76
1:A:267:MET:SD	1:A:358:TRP:CZ3	2.79	0.76
1:B:96:ALA:C	1:B:100:GLY:HA2	2.06	0.76
1:B:269:LEU:HD23	1:B:270:GLU:HG3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PHE:HD1	1:B:127:GLN:N	1.82	0.76
1:B:75:ILE:HG22	1:B:308:GLY:N	2.01	0.76
1:A:39:ARG:NH2	1:A:289:ARG:HB2	2.01	0.76
1:A:142:ARG:HH12	1:B:184:GLU:HG3	1.50	0.75
1:A:64:ILE:HG13	1:A:283:PHE:HE1	1.49	0.75
1:A:128:LEU:HD21	1:A:130:VAL:HG23	1.68	0.75
1:B:164:ARG:HD2	1:B:164:ARG:O	1.86	0.75
1:A:284:LEU:O	1:A:305:VAL:HG23	1.85	0.75
1:B:235:ALA:HB2	1:B:271:GLU:O	1.87	0.75
1:A:146:ARG:HH11	1:B:117:ALA:HB1	1.50	0.75
1:A:73:ILE:O	1:A:101:THR:HG21	1.87	0.75
1:B:75:ILE:HG22	1:B:308:GLY:CA	2.16	0.75
1:B:26:ALA:HB2	1:B:309:ARG:HD3	1.69	0.75
1:B:106:SER:HA	1:B:127:GLN:HB3	1.69	0.74
1:B:250:ILE:HB	1:B:283:PHE:HB2	1.67	0.74
1:B:300:LEU:HD22	1:B:300:LEU:H	1.51	0.74
1:A:80:MET:CG	1:A:110:THR:HG23	2.13	0.74
1:A:143:ARG:HA	1:B:143:ARG:HG2	1.69	0.74
1:B:199:LEU:HD12	1:B:199:LEU:H	1.52	0.74
1:B:47:PHE:HA	1:B:355:ALA:N	2.00	0.74
1:A:285:ASP:HB3	1:A:306:PHE:HB2	1.69	0.74
1:B:18:PRO:HG2	1:B:21:VAL:HB	1.68	0.74
1:B:136:VAL:HG11	1:B:206:GLN:NE2	2.03	0.74
1:A:132:LYS:HB3	1:A:132:LYS:NZ	2.02	0.74
1:B:134:ARG:HD2	1:B:218:TRP:HH2	1.53	0.74
1:B:242:VAL:HG21	1:B:276:ALA:HB2	1.70	0.73
1:B:331:ARG:HA	1:B:334:PHE:CE1	2.23	0.73
1:A:143:ARG:HA	1:B:143:ARG:HA	1.70	0.73
1:B:27:SER:O	1:B:257:ARG:HD2	1.87	0.73
1:B:91:ALA:CB	1:B:320:GLU:HA	2.19	0.73
1:B:131:TYR:HB2	1:B:137:VAL:HG22	1.70	0.73
1:B:22:TYR:HA	1:B:25:TYR:CE1	2.24	0.73
1:B:75:ILE:HG22	1:B:308:GLY:HA2	1.69	0.73
1:A:103:MET:SD	1:A:103:MET:C	2.67	0.73
1:B:309:ARG:O	1:B:312:VAL:HB	1.89	0.73
1:B:346:LEU:HD12	1:B:349:ILE:HG13	1.69	0.73
1:B:108:TRP:CH2	1:B:129:TYR:HE2	2.07	0.72
1:B:146:ARG:HH21	1:B:225:LEU:HA	1.55	0.72
1:B:254:HIS:HB2	1:B:258:GLN:HB2	1.70	0.72
1:B:153:ALA:HB1	1:B:228:LEU:O	1.88	0.72
1:B:184:GLU:HA	1:B:199:LEU:HD23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:HB3	1:A:345:SER:HB3	1.71	0.72
1:A:113:VAL:HG21	1:A:143:ARG:HD3	1.70	0.72
1:B:2:GLU:HG2	1:B:3:ILE:N	2.05	0.72
1:B:139:GLN:HA	1:B:142:ARG:HD2	1.72	0.72
1:B:209:ARG:H	1:B:209:ARG:NE	1.87	0.72
1:B:294:VAL:HG21	1:B:330:MET:HG3	1.71	0.71
1:B:91:ALA:HB1	1:B:320:GLU:HA	1.72	0.71
1:A:269:LEU:HD23	1:A:300:LEU:HB2	1.71	0.71
1:A:135:ASN:O	1:A:139:GLN:HG3	1.89	0.71
1:A:184:GLU:O	1:A:199:LEU:HB3	1.89	0.71
1:B:248:GLY:HA2	1:B:281:PRO:CB	2.20	0.71
1:B:229:VAL:CG2	1:B:246:ALA:HB3	2.20	0.71
1:A:58:ILE:HG22	1:A:59:ASP:H	1.54	0.71
1:B:308:GLY:C	1:B:310:PRO:HD2	2.11	0.71
1:B:20:MET:SD	1:B:172:PHE:HD1	2.13	0.71
1:A:189:GLY:HA3	1:B:133:ASP:HA	1.72	0.70
1:A:142:ARG:HB2	1:B:143:ARG:NE	2.06	0.70
1:B:183:PHE:O	1:B:186:ILE:HG23	1.92	0.70
1:B:236:GLU:HA	1:B:239:ARG:NH1	2.06	0.70
1:A:143:ARG:HB2	1:B:142:ARG:O	1.91	0.70
1:A:144:ALA:HB1	1:A:149:PHE:HB2	1.73	0.70
1:B:91:ALA:HA	1:B:320:GLU:HA	1.71	0.70
1:A:159:PRO:HG2	1:A:160:ARG:H	1.54	0.70
1:B:215:ASP:HA	1:B:218:TRP:CD2	2.27	0.70
1:B:239:ARG:HG3	1:B:240:LEU:HG	1.74	0.69
1:A:101:THR:HG22	1:A:102:ILE:H	1.57	0.69
1:B:329:MET:O	1:B:333:GLU:HB2	1.93	0.69
1:B:266:ILE:HA	1:B:284:LEU:CD1	2.21	0.69
1:B:63:THR:HA	1:B:67:PHE:O	1.93	0.69
1:B:61:THR:HG22	1:B:68:LYS:O	1.92	0.69
1:A:152:ILE:HD12	1:A:227:ILE:CD1	2.22	0.69
1:B:249:ILE:HD11	1:B:280:ILE:HD12	1.75	0.69
1:B:64:ILE:CD1	1:B:69:ILE:HG12	2.22	0.69
1:B:233:ILE:CA	1:B:251:VAL:HG13	2.22	0.69
1:B:30:GLU:HB2	1:B:260:ASP:HB2	1.75	0.69
1:A:110:THR:O	1:A:181:LYS:HE2	1.92	0.68
1:A:82:LYS:HD2	1:A:110:THR:HB	1.75	0.68
1:B:260:ASP:O	1:B:261:TYR:HB2	1.92	0.68
1:B:39:ARG:HG2	1:B:289:ARG:HD2	1.74	0.68
1:B:61:THR:HG23	1:B:70:SER:CA	2.22	0.68
1:B:144:ALA:HA	1:B:149:PHE:CB	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ILE:HA	1:B:305:VAL:CB	2.22	0.68
1:A:222:ILE:HG13	1:A:222:ILE:O	1.93	0.68
1:B:74:MET:HB3	1:B:102:ILE:HB	1.74	0.68
1:B:130:VAL:O	1:B:130:VAL:HG13	1.94	0.68
1:B:50:ARG:H	1:B:341:SER:HB3	1.59	0.68
1:B:144:ALA:O	1:B:225:LEU:HD13	1.94	0.68
1:B:132:LYS:HB2	1:B:206:GLN:CA	2.24	0.68
1:A:59:ASP:CB	1:A:345:SER:HB3	2.23	0.67
1:A:186:ILE:HB	1:A:202:TYR:CE2	2.29	0.67
1:A:222:ILE:CG2	1:B:185:GLY:HA3	2.23	0.67
1:B:163:ARG:HG3	1:B:163:ARG:HH11	1.59	0.67
1:B:345:SER:O	1:B:349:ILE:HG12	1.95	0.67
1:A:31:ASP:HB2	1:A:261:TYR:OH	1.95	0.67
1:A:126:PHE:HB2	1:A:149:PHE:CD2	2.30	0.67
1:B:6:VAL:HG22	1:B:329:MET:SD	2.34	0.67
1:B:49:PRO:HB3	1:B:341:SER:OG	1.94	0.67
1:A:273:VAL:HG22	1:A:282:VAL:CG2	2.24	0.67
1:B:35:LEU:HD13	1:B:256:ALA:CB	2.24	0.67
1:A:136:VAL:HG11	1:A:186:ILE:HG21	1.77	0.67
1:B:232:VAL:N	1:B:251:VAL:HA	2.09	0.67
1:B:238:ALA:O	1:B:242:VAL:HG23	1.95	0.67
1:B:219:LEU:O	1:B:222:ILE:HB	1.96	0.66
1:A:162:GLY:O	1:A:164:ARG:HD3	1.95	0.66
1:B:124:ARG:HB3	1:B:149:PHE:CD1	2.30	0.66
1:A:288:VAL:HG11	1:A:305:VAL:HG21	1.75	0.66
1:B:242:VAL:HG21	1:B:275:ALA:O	1.95	0.66
1:B:232:VAL:O	1:B:251:VAL:HG22	1.95	0.66
1:B:307:ILE:CB	1:B:310:PRO:HG3	2.24	0.66
1:A:180:LEU:HD11	1:A:200:SER:HA	1.77	0.66
1:B:289:ARG:NH1	1:B:289:ARG:HB3	2.09	0.66
1:A:267:MET:SD	1:A:358:TRP:HZ3	2.19	0.66
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.60	0.66
1:A:312:VAL:O	1:A:315:LEU:HD23	1.95	0.66
1:B:212:SER:HB2	1:B:214:LYS:HD3	1.78	0.66
1:B:318:GLU:HB2	1:B:322:GLY:CA	2.26	0.66
1:A:114:GLU:HA	1:B:145:GLU:HB3	1.78	0.66
1:B:22:TYR:HA	1:B:25:TYR:HD1	1.60	0.66
1:B:152:ILE:HG22	1:B:153:ALA:N	2.11	0.66
1:B:134:ARG:HD2	1:B:218:TRP:CH2	2.31	0.66
1:A:128:LEU:HD13	1:A:154:LEU:HD13	1.77	0.66
1:B:131:TYR:HD1	1:B:206:GLN:HG2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:N	1:B:209:ARG:NE	2.45	0.65
1:B:58:ILE:HA	1:B:344:ARG:HB3	1.78	0.65
1:B:29:ALA:O	1:B:260:ASP:HB2	1.96	0.65
1:B:288:VAL:HG12	1:B:293:ASP:CB	2.26	0.65
1:A:113:VAL:HG23	1:A:143:ARG:HD3	1.79	0.65
1:A:114:GLU:HB2	1:B:225:LEU:HD21	1.78	0.65
1:B:138:ALA:O	1:B:141:VAL:HB	1.97	0.65
1:B:232:VAL:O	1:B:232:VAL:HG13	1.97	0.65
1:B:311:VAL:O	1:B:315:LEU:N	2.30	0.65
1:B:5:ASN:HA	1:B:290:ARG:NH1	2.12	0.65
1:A:227:ILE:HG22	1:A:227:ILE:O	1.97	0.65
1:A:69:ILE:HB	1:A:101:THR:HG23	1.79	0.65
1:B:126:PHE:HD2	1:B:144:ALA:HB2	1.62	0.65
1:B:252:SER:HA	1:B:265:THR:HG21	1.78	0.65
1:B:45:ILE:HG13	1:B:357:ASP:N	2.09	0.65
1:A:39:ARG:HD3	1:A:289:ARG:NH2	2.11	0.65
1:A:98:ALA:HB3	1:A:324:LYS:NZ	2.12	0.65
1:B:108:TRP:O	1:B:110:THR:HG23	1.97	0.65
1:A:146:ARG:NH1	1:B:117:ALA:HB1	2.11	0.65
1:B:266:ILE:HA	1:B:284:LEU:HD11	1.78	0.65
1:B:74:MET:SD	1:B:305:VAL:N	2.70	0.65
1:B:288:VAL:HB	1:B:294:VAL:HG13	1.79	0.64
1:A:293:ASP:HA	1:A:296:LYS:HD2	1.78	0.64
1:B:105:LEU:O	1:B:127:GLN:HB2	1.97	0.64
1:B:45:ILE:HG23	1:B:356:ALA:HA	1.79	0.64
1:A:274:LYS:HE2	1:A:274:LYS:CA	2.26	0.64
1:A:64:ILE:O	1:A:67:PHE:HB2	1.97	0.64
1:B:188:LEU:HB2	1:B:198:GLY:C	2.18	0.64
1:A:232:VAL:O	1:A:251:VAL:HG12	1.97	0.64
1:B:48:ARG:O	1:B:353:HIS:HD2	1.81	0.64
1:B:106:SER:HA	1:B:127:GLN:CB	2.27	0.64
1:B:291:GLY:HA3	1:B:333:GLU:HB3	1.79	0.64
1:B:108:TRP:CH2	1:B:129:TYR:CE2	2.86	0.64
1:B:104:THR:HG22	1:B:125:PHE:CB	2.28	0.63
1:A:249:ILE:CG2	1:A:251:VAL:HG22	2.28	0.63
1:B:178:LEU:HD23	1:B:181:LYS:HE3	1.80	0.63
1:B:208:ASP:HA	1:B:209:ARG:CZ	2.28	0.63
1:A:80:MET:HG2	1:A:110:THR:CG2	2.17	0.63
1:B:227:ILE:HB	1:B:246:ALA:CB	2.12	0.63
1:A:273:VAL:CG2	1:A:282:VAL:HG21	2.28	0.63
1:A:44:ARG:HD3	1:A:357:ASP:CG	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLN:O	1:A:279:ARG:HD2	1.98	0.63
1:A:107:SER:HB3	1:A:183:PHE:HE1	1.63	0.63
1:A:62:THR:HG22	1:A:63:THR:H	1.64	0.63
1:A:300:LEU:HD23	1:A:351:ARG:HD2	1.81	0.62
1:A:32:GLN:HB3	1:A:35:LEU:HD13	1.80	0.62
1:B:321:ALA:HB1	1:B:325:LYS:HE3	1.80	0.62
1:B:47:PHE:CA	1:B:355:ALA:H	2.06	0.62
1:A:242:VAL:HG11	1:A:279:ARG:HG2	1.81	0.62
1:B:321:ALA:HA	1:B:324:LYS:HG2	1.81	0.62
1:A:33:TRP:CE3	1:A:261:TYR:HA	2.33	0.62
1:A:139:GLN:HB2	1:B:139:GLN:HB3	1.82	0.62
1:A:20:MET:SD	1:A:172:PHE:CD1	2.92	0.62
1:A:20:MET:SD	1:A:173:VAL:O	2.58	0.62
1:A:179:THR:OG1	1:A:181:LYS:HG3	1.99	0.62
1:B:6:VAL:HG23	1:B:290:ARG:HD3	1.80	0.62
1:A:276:ALA:HA	1:A:279:ARG:NE	2.14	0.62
1:A:84:ALA:HB1	1:A:316:ALA:HB2	1.82	0.62
1:A:186:ILE:HD11	1:B:139:GLN:HE21	1.64	0.62
1:B:233:ILE:HG22	1:B:251:VAL:CG1	2.29	0.62
1:B:311:VAL:HB	1:B:323:VAL:HG12	1.82	0.62
1:B:9:TYR:HA	1:B:12:ILE:HD12	1.82	0.62
1:A:265:THR:CG2	1:A:284:LEU:HB2	2.30	0.62
1:B:156:VAL:HG22	1:B:230:LYS:O	1.99	0.61
1:B:334:PHE:CD1	1:B:335:GLU:N	2.68	0.61
1:A:248:GLY:N	1:A:280:ILE:HD13	2.15	0.61
1:A:199:LEU:O	1:A:201:SER:N	2.33	0.61
1:A:218:TRP:NE1	1:A:222:ILE:HG21	2.14	0.61
1:B:254:HIS:HB3	1:B:257:ARG:HG2	1.80	0.61
1:B:237:ASP:O	1:B:240:LEU:HB2	2.00	0.61
1:B:336:LEU:O	1:B:340:LEU:HB2	2.00	0.61
1:A:285:ASP:CB	1:A:306:PHE:HB2	2.31	0.61
1:B:131:TYR:HE2	1:B:140:LEU:HD21	1.66	0.61
1:A:60:MET:HB3	1:A:72:PRO:HD2	1.81	0.61
1:B:273:VAL:HG23	1:B:282:VAL:CB	2.30	0.61
1:B:251:VAL:HG12	1:B:265:THR:CG2	2.30	0.61
1:B:270:GLU:HA	1:B:273:VAL:CG1	2.28	0.61
1:B:123:ILE:HB	1:B:150:LYS:HB2	1.83	0.61
1:B:102:ILE:HG22	1:B:104:THR:HG23	1.82	0.61
1:B:25:TYR:OH	1:B:83:MET:SD	2.59	0.61
1:B:35:LEU:HD22	1:B:256:ALA:O	2.00	0.61
1:A:115:GLU:OE2	1:A:181:LYS:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HA	1:A:208:ASP:OD1	2.01	0.60
1:A:102:ILE:HG23	1:A:124:ARG:HA	1.82	0.60
1:A:142:ARG:HB2	1:B:143:ARG:HE	1.64	0.60
1:B:318:GLU:HB2	1:B:322:GLY:HA3	1.82	0.60
1:B:269:LEU:HD21	1:B:300:LEU:CB	2.30	0.60
1:A:151:ALA:HB1	1:A:228:LEU:HD21	1.82	0.60
1:B:253:ASN:HB2	1:B:262:VAL:HG21	1.82	0.60
1:B:324:LYS:HG3	1:B:325:LYS:HG3	1.83	0.60
1:B:240:LEU:HA	1:B:243:GLN:HB3	1.82	0.60
1:A:45:ILE:CD1	1:A:266:ILE:HD11	2.30	0.60
1:B:27:SER:HB3	1:B:164:ARG:HD3	1.84	0.60
1:B:233:ILE:HG22	1:B:251:VAL:HG12	1.83	0.60
1:B:324:LYS:HG3	1:B:325:LYS:N	2.17	0.60
1:B:234:THR:HA	1:B:271:GLU:OE1	2.02	0.60
1:B:110:THR:HG22	1:B:180:LEU:HA	1.83	0.60
1:A:226:PRO:O	1:A:228:LEU:HD22	2.02	0.60
1:A:228:LEU:HD22	1:A:228:LEU:H	1.66	0.60
1:B:248:GLY:CA	1:B:281:PRO:HB2	2.28	0.60
1:A:275:ALA:O	1:A:277:GLN:HG3	2.01	0.60
1:A:328:GLN:O	1:A:332:ASP:HB2	2.01	0.60
1:B:62:THR:O	1:B:68:LYS:HA	2.01	0.59
1:A:76:ALA:HB1	2:A:370:FMN:H3'	1.84	0.59
1:A:114:GLU:HB3	1:B:145:GLU:OE2	2.01	0.59
1:B:20:MET:SD	1:B:172:PHE:CD1	2.94	0.59
1:B:331:ARG:O	1:B:335:GLU:HB2	2.03	0.59
1:B:273:VAL:HG23	1:B:282:VAL:HB	1.83	0.59
1:A:161:LEU:HA	1:A:258:GLN:HE22	1.67	0.59
1:A:110:THR:O	1:A:181:LYS:HB2	2.02	0.59
1:B:21:VAL:HG22	1:B:172:PHE:CZ	2.36	0.59
1:B:250:ILE:HG12	1:B:251:VAL:O	2.02	0.59
1:A:202:TYR:C	1:A:202:TYR:CD1	2.76	0.59
1:B:146:ARG:NH2	1:B:224:SER:O	2.35	0.59
1:B:20:MET:CE	1:B:171:ARG:HB3	2.33	0.59
1:B:228:LEU:O	1:B:228:LEU:HD12	2.03	0.59
1:B:230:LYS:HG2	1:B:250:ILE:HG21	1.84	0.59
1:A:128:LEU:CD2	1:A:130:VAL:HG23	2.33	0.59
1:B:213:TRP:CH2	1:B:240:LEU:HB3	2.38	0.58
1:B:216:VAL:CG1	1:B:217:ALA:N	2.65	0.58
1:B:242:VAL:HG11	1:B:276:ALA:HA	1.84	0.58
1:B:321:ALA:O	1:B:324:LYS:N	2.35	0.58
1:B:64:ILE:HD11	1:B:69:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:CE	1:A:274:LYS:HA	2.32	0.58
1:A:111:SER:HB2	1:A:116:VAL:HG22	1.85	0.58
1:A:347:LYS:HD3	1:A:348:GLU:HG3	1.85	0.58
1:B:90:TYR:CD1	1:B:116:VAL:HA	2.36	0.58
1:A:312:VAL:HA	1:A:315:LEU:CD2	2.34	0.58
1:B:139:GLN:HA	1:B:142:ARG:CD	2.32	0.58
1:A:186:ILE:HG12	1:B:142:ARG:HH11	1.63	0.58
1:B:253:ASN:ND2	1:B:263:PRO:O	2.36	0.58
1:B:82:LYS:CB	1:B:178:LEU:HD11	2.15	0.58
1:B:186:ILE:HG13	1:B:188:LEU:CB	2.32	0.58
1:A:254:HIS:O	1:A:257:ARG:HB2	2.03	0.58
1:B:188:LEU:HB2	1:B:198:GLY:CA	2.34	0.58
1:A:90:TYR:HA	1:A:116:VAL:HG13	1.86	0.58
1:A:18:PRO:HD2	1:A:21:VAL:HG21	1.84	0.58
1:A:98:ALA:HB3	1:A:324:LYS:HZ3	1.69	0.58
1:B:126:PHE:HB2	1:B:144:ALA:HB2	1.86	0.58
1:B:154:LEU:H	1:B:227:ILE:HG22	1.68	0.58
1:B:279:ARG:HG2	1:B:280:ILE:HG12	1.85	0.58
1:B:61:THR:HA	1:B:70:SER:HA	1.85	0.58
1:B:142:ARG:NH2	1:B:222:ILE:HG23	2.19	0.58
1:B:9:TYR:HB3	1:B:313:PHE:HB3	1.85	0.58
1:A:267:MET:SD	1:A:358:TRP:CE3	2.97	0.58
1:A:39:ARG:HH21	1:A:289:ARG:HB2	1.69	0.58
1:A:187:ASP:O	1:B:134:ARG:HB2	2.04	0.58
1:B:299:ALA:HB3	1:B:300:LEU:HD22	1.85	0.58
1:B:6:VAL:HG13	1:B:329:MET:CE	2.34	0.58
1:B:309:ARG:N	1:B:310:PRO:HD2	2.20	0.57
1:B:64:ILE:HD13	1:B:67:PHE:O	2.04	0.57
1:B:68:LYS:HZ2	1:B:68:LYS:N	2.02	0.57
1:A:17:LEU:HD21	1:A:316:ALA:HB1	1.86	0.57
1:B:295:PHE:O	1:B:298:LEU:HG	2.03	0.57
1:B:17:LEU:HB2	1:B:18:PRO:HD2	1.85	0.57
1:B:83:MET:HB3	1:B:175:PRO:HG3	1.86	0.57
1:A:103:MET:HE1	1:A:105:LEU:HD22	1.86	0.57
1:B:266:ILE:HG13	1:B:267:MET:N	2.19	0.57
1:B:219:LEU:HD23	1:B:219:LEU:O	2.04	0.57
1:B:251:VAL:HG11	1:B:268:ALA:HB3	1.87	0.57
1:B:46:LEU:HB2	1:B:355:ALA:HB3	1.86	0.57
1:B:75:ILE:HG13	1:B:103:MET:CE	2.34	0.57
1:A:172:PHE:C	1:A:172:PHE:CD1	2.78	0.57
1:A:213:TRP:HA	1:A:216:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:THR:HG22	1:B:125:PHE:HB3	1.86	0.57
1:A:246:ALA:O	1:A:280:ILE:HG21	2.05	0.57
1:B:259:LEU:O	1:B:262:VAL:HG22	2.04	0.56
1:A:131:TYR:O	1:A:134:ARG:HD3	2.04	0.56
1:B:240:LEU:O	1:B:244:HIS:HD2	1.87	0.56
1:B:34:THR:HA	1:B:37:GLU:OE2	2.06	0.56
1:A:64:ILE:HG23	1:A:65:LEU:HD13	1.86	0.56
1:B:110:THR:HG22	1:B:181:LYS:H	1.70	0.56
1:B:156:VAL:HG13	1:B:229:VAL:HG12	1.86	0.56
1:B:288:VAL:HG12	1:B:293:ASP:HB3	1.86	0.56
1:A:162:GLY:HA3	1:A:258:GLN:HA	1.88	0.56
1:A:131:TYR:HA	1:A:207:ILE:CA	2.34	0.56
1:A:247:ALA:HA	1:A:280:ILE:HG21	1.85	0.56
1:B:125:PHE:CE2	1:B:151:ALA:HB3	2.40	0.56
1:B:232:VAL:HG12	1:B:251:VAL:N	2.19	0.56
1:A:107:SER:HB3	1:A:183:PHE:CE1	2.41	0.56
1:B:126:PHE:CD2	1:B:144:ALA:HB2	2.40	0.56
1:B:320:GLU:O	1:B:323:VAL:HG22	2.05	0.56
1:B:294:VAL:HG21	1:B:330:MET:CG	2.36	0.56
1:A:164:ARG:CD	1:A:164:ARG:H	2.19	0.56
1:A:103:MET:CE	1:A:105:LEU:HD22	2.36	0.56
1:B:132:LYS:CG	1:B:208:ASP:HB2	2.24	0.56
1:B:174:LEU:HG	1:B:175:PRO:CD	2.35	0.56
1:A:265:THR:HG21	1:A:284:LEU:HB2	1.88	0.56
1:A:323:VAL:HA	1:A:326:VAL:HB	1.88	0.56
1:B:227:ILE:CB	1:B:246:ALA:HB1	2.11	0.56
1:B:75:ILE:HG22	1:B:308:GLY:H	1.70	0.56
1:A:228:LEU:HD22	1:A:228:LEU:N	2.21	0.56
1:B:101:THR:HG23	1:B:102:ILE:N	2.21	0.56
1:B:77:PRO:HD2	1:B:230:LYS:NZ	2.21	0.56
1:B:67:PHE:HA	1:B:68:LYS:NZ	2.17	0.56
1:A:46:LEU:O	1:A:354:ILE:HG12	2.05	0.56
1:B:126:PHE:CD1	1:B:127:GLN:N	2.71	0.56
1:B:6:VAL:HG21	1:B:289:ARG:O	2.06	0.56
1:B:34:THR:O	1:B:38:ASN:OD1	2.24	0.56
1:B:69:ILE:HD12	1:B:72:PRO:HA	1.88	0.56
1:B:72:PRO:O	1:B:74:MET:N	2.39	0.56
1:A:164:ARG:H	1:A:164:ARG:HD3	1.69	0.56
1:A:55:VAL:HG12	1:A:55:VAL:O	2.06	0.56
1:B:141:VAL:HG21	1:B:222:ILE:HG22	1.87	0.55
1:B:288:VAL:H	1:B:289:ARG:HH21	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HA	1:A:356:ALA:HA	1.88	0.55
1:A:263:PRO:HB2	1:A:268:ALA:HB2	1.87	0.55
1:B:131:TYR:CB	1:B:136:VAL:HB	2.29	0.55
1:B:300:LEU:HD22	1:B:300:LEU:N	2.21	0.55
1:B:99:ALA:CB	1:B:324:LYS:HA	2.36	0.55
1:A:18:PRO:O	1:A:21:VAL:N	2.38	0.55
1:A:113:VAL:HG12	1:A:149:PHE:CZ	2.42	0.55
1:A:139:GLN:HB2	1:B:139:GLN:OE1	2.06	0.55
1:A:61:THR:O	1:A:346:LEU:HD21	2.06	0.55
1:B:246:ALA:O	1:B:247:ALA:HB2	2.06	0.55
1:B:32:GLN:OE1	1:B:35:LEU:HB2	2.07	0.55
1:B:159:PRO:CG	1:B:211:LEU:HD21	2.37	0.55
1:A:3:ILE:HD12	1:A:8:GLU:OE1	2.07	0.55
1:B:53:ILE:HG21	1:B:342:GLY:CA	2.37	0.55
1:A:69:ILE:O	1:A:69:ILE:HG13	2.07	0.55
1:A:38:ASN:O	1:A:42:PHE:HE1	1.89	0.55
1:A:146:ARG:CB	1:B:114:GLU:HA	2.21	0.55
1:A:188:LEU:HD12	1:B:135:ASN:CG	2.27	0.55
1:B:73:ILE:HG23	1:B:305:VAL:HB	1.88	0.55
1:A:172:PHE:HD1	1:A:172:PHE:C	2.09	0.55
1:B:174:LEU:HG	1:B:175:PRO:N	2.22	0.55
1:B:64:ILE:HD12	1:B:69:ILE:HG12	1.87	0.55
1:B:73:ILE:HD13	1:B:330:MET:HB3	1.89	0.55
1:B:104:THR:HG22	1:B:125:PHE:HB2	1.89	0.54
1:B:279:ARG:CG	1:B:280:ILE:HG12	2.37	0.54
1:A:171:ARG:NH1	1:A:171:ARG:HG2	2.22	0.54
1:B:263:PRO:HB2	1:B:267:MET:HE2	1.89	0.54
1:B:216:VAL:HG12	1:B:217:ALA:H	1.73	0.54
1:B:45:ILE:HG13	1:B:356:ALA:HA	1.90	0.54
1:B:318:GLU:HB2	1:B:322:GLY:HA2	1.88	0.54
1:A:139:GLN:HE22	1:B:140:LEU:HD12	1.72	0.54
1:B:145:GLU:HA	1:B:225:LEU:HD22	1.89	0.54
1:A:358:TRP:CD1	1:A:359:ASP:N	2.75	0.54
1:B:239:ARG:HG3	1:B:240:LEU:N	2.22	0.54
1:B:242:VAL:CG2	1:B:276:ALA:HB2	2.36	0.54
1:A:158:THR:HG23	1:A:258:GLN:NE2	2.23	0.54
1:B:216:VAL:CG1	1:B:217:ALA:H	2.21	0.54
1:B:289:ARG:HB3	1:B:289:ARG:HH11	1.71	0.54
1:A:219:LEU:O	1:A:223:THR:HG22	2.08	0.54
1:B:239:ARG:O	1:B:243:GLN:N	2.39	0.53
1:B:188:LEU:HB2	1:B:198:GLY:HA2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:O	1:B:20:MET:C	2.47	0.53
1:B:152:ILE:HG22	1:B:227:ILE:HG23	1.90	0.53
1:B:288:VAL:CG2	1:B:294:VAL:HG12	2.38	0.53
1:B:61:THR:CG2	1:B:70:SER:HA	2.34	0.53
1:A:84:ALA:O	1:A:85:HIS:HB3	2.08	0.53
1:A:105:LEU:HG	1:A:126:PHE:HD1	1.72	0.53
1:A:139:GLN:CB	1:B:139:GLN:HB3	2.39	0.53
1:B:346:LEU:CD1	1:B:349:ILE:HG13	2.37	0.53
1:A:99:ALA:CB	1:A:327:LEU:HD13	2.38	0.53
1:B:21:VAL:HG11	1:B:83:MET:HG2	1.90	0.53
1:B:326:VAL:O	1:B:329:MET:N	2.41	0.53
1:A:126:PHE:CZ	1:A:182:ASN:ND2	2.76	0.53
1:B:295:PHE:CA	1:B:298:LEU:HG	2.36	0.53
1:A:213:TRP:O	1:A:216:VAL:HG12	2.09	0.53
1:B:218:TRP:CE3	1:B:219:LEU:HB2	2.44	0.53
1:B:291:GLY:HA3	1:B:333:GLU:CB	2.38	0.53
1:A:158:THR:HG23	1:A:258:GLN:CD	2.28	0.53
1:B:24:PHE:CE2	1:B:80:MET:HB2	2.42	0.53
1:B:34:THR:HG21	1:B:262:VAL:HG23	1.90	0.53
1:B:78:THR:O	1:B:79:ALA:HB2	2.09	0.53
1:B:23:ASP:O	1:B:164:ARG:NE	2.42	0.53
1:A:59:ASP:HB3	1:A:345:SER:CB	2.38	0.53
1:B:106:SER:O	1:B:109:ALA:HB3	2.09	0.53
1:A:131:TYR:HB3	1:A:206:GLN:CD	2.29	0.53
1:B:20:MET:O	1:B:23:ASP:HB2	2.09	0.53
1:B:251:VAL:CG1	1:B:265:THR:HG22	2.38	0.53
1:B:324:LYS:HG3	1:B:325:LYS:H	1.72	0.53
1:B:6:VAL:HA	1:B:329:MET:SD	2.49	0.53
1:A:329:MET:O	1:A:333:GLU:HG3	2.09	0.52
1:A:143:ARG:CA	1:B:143:ARG:HG2	2.39	0.52
1:B:71:MET:HB3	1:B:331:ARG:HG3	1.90	0.52
1:A:270:GLU:O	1:A:274:LYS:HB2	2.09	0.52
1:A:247:ALA:HA	1:A:280:ILE:CG2	2.39	0.52
1:B:128:LEU:HG	1:B:140:LEU:HD23	1.91	0.52
1:B:220:GLN:NE2	1:B:246:ALA:HA	2.24	0.52
1:B:5:ASN:HA	1:B:290:ARG:HH12	1.74	0.52
1:A:249:ILE:HG21	1:A:251:VAL:HG22	1.91	0.52
1:A:82:LYS:CB	1:A:110:THR:HG21	2.36	0.52
1:A:142:ARG:HB2	1:B:143:ARG:CZ	2.39	0.52
1:A:143:ARG:HG3	1:B:143:ARG:HA	1.91	0.52
1:B:247:ALA:HA	1:B:280:ILE:CB	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:HD3	1:B:117:ALA:HB3	1.91	0.52
1:B:165:GLU:O	1:B:169:LYS:HB3	2.09	0.52
1:B:111:SER:HB3	1:B:116:VAL:CG2	2.39	0.52
1:B:111:SER:HB3	1:B:116:VAL:HG23	1.91	0.52
1:B:266:ILE:HA	1:B:284:LEU:HD12	1.91	0.52
1:A:42:PHE:HB3	1:A:296:LYS:HZ2	1.74	0.52
1:B:110:THR:HG22	1:B:181:LYS:N	2.23	0.52
1:B:152:ILE:CG2	1:B:153:ALA:N	2.73	0.52
1:B:307:ILE:CG2	1:B:310:PRO:HG3	2.40	0.52
1:A:314:SER:OG	1:A:326:VAL:HG21	2.09	0.52
1:A:71:MET:HG2	1:A:73:ILE:HD12	1.91	0.52
1:B:23:ASP:HB2	1:B:167:ASP:CB	2.36	0.52
1:B:265:THR:OG1	1:B:285:ASP:O	2.27	0.52
1:B:330:MET:O	1:B:334:PHE:CD1	2.63	0.52
1:B:253:ASN:HD22	1:B:262:VAL:HG23	1.75	0.51
1:B:60:MET:HB3	1:B:338:MET:HE1	1.92	0.51
1:B:45:ILE:HA	1:B:357:ASP:OD1	2.10	0.51
1:A:296:LYS:O	1:A:299:ALA:N	2.42	0.51
1:B:95:ALA:O	1:B:97:SER:N	2.41	0.51
1:B:76:ALA:N	1:B:104:THR:OG1	2.43	0.51
1:A:117:ALA:CB	1:B:147:ALA:HB3	2.41	0.51
1:B:20:MET:HE1	1:B:171:ARG:HB3	1.93	0.51
1:B:103:MET:HE2	1:B:104:THR:H	1.74	0.51
1:B:291:GLY:CA	1:B:330:MET:SD	2.92	0.51
1:B:126:PHE:HD1	1:B:127:GLN:H	1.55	0.51
1:B:60:MET:HG2	1:B:61:THR:H	1.75	0.51
1:B:63:THR:HG23	1:B:66:GLY:O	2.11	0.51
1:B:75:ILE:HB	1:B:104:THR:HG1	1.75	0.51
1:A:39:ARG:C	1:A:41:ALA:H	2.14	0.51
1:B:152:ILE:HG22	1:B:153:ALA:H	1.75	0.51
1:A:136:VAL:O	1:B:139:GLN:OE1	2.29	0.51
1:A:290:ARG:O	1:A:294:VAL:HG23	2.11	0.51
1:A:34:THR:HG21	1:A:262:VAL:O	2.10	0.51
1:B:40:ASN:HA	1:B:43:SER:OG	2.11	0.51
1:B:30:GLU:HB2	1:B:260:ASP:CB	2.40	0.51
1:A:218:TRP:HE1	1:B:185:GLY:C	2.13	0.51
1:B:171:ARG:HG3	1:B:171:ARG:O	2.10	0.51
1:B:73:ILE:HA	1:B:305:VAL:O	2.11	0.51
1:A:67:PHE:CZ	1:A:150:LYS:HG3	2.45	0.51
1:B:71:MET:SD	1:B:100:GLY:O	2.69	0.51
1:B:209:ARG:N	1:B:209:ARG:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:O	1:B:244:HIS:CD2	2.63	0.50
1:B:112:SER:O	1:B:115:GLU:N	2.44	0.50
1:B:232:VAL:HG13	1:B:251:VAL:HG22	1.93	0.50
1:B:38:ASN:O	1:B:42:PHE:HE1	1.94	0.50
1:B:89:GLU:OE2	1:B:105:LEU:HD23	2.11	0.50
1:A:132:LYS:HB3	1:A:132:LYS:HZ3	1.76	0.50
1:B:108:TRP:HA	1:B:180:LEU:HG	1.92	0.50
1:B:266:ILE:O	1:B:269:LEU:HB2	2.12	0.50
1:B:68:LYS:NZ	1:B:68:LYS:N	2.58	0.50
1:B:71:MET:O	1:B:71:MET:SD	2.69	0.50
1:A:159:PRO:CG	1:A:160:ARG:H	2.23	0.50
1:A:295:PHE:HB2	1:A:337:THR:HG21	1.93	0.50
1:A:64:ILE:HG23	1:A:65:LEU:CD1	2.41	0.50
1:A:28:GLY:HA3	1:A:35:LEU:CD1	2.36	0.50
1:A:235:ALA:HB1	1:A:275:ALA:HB2	1.92	0.50
1:A:184:GLU:OE2	1:B:222:ILE:HA	2.11	0.50
1:B:68:LYS:H	1:B:68:LYS:HZ2	1.59	0.50
1:A:186:ILE:HG22	1:A:187:ASP:N	2.26	0.50
1:B:250:ILE:CB	1:B:283:PHE:HB2	2.38	0.50
1:B:311:VAL:O	1:B:315:LEU:HB2	2.12	0.50
1:B:8:GLU:O	1:B:12:ILE:HD12	2.12	0.50
1:B:294:VAL:HG23	1:B:295:PHE:N	2.26	0.50
1:A:186:ILE:O	1:A:187:ASP:HB2	2.12	0.50
1:A:202:TYR:CD1	1:A:203:VAL:N	2.80	0.50
1:A:283:PHE:HB2	1:A:306:PHE:HE1	1.77	0.50
1:B:145:GLU:O	1:B:150:LYS:N	2.46	0.49
1:B:20:MET:O	1:B:167:ASP:HB3	2.12	0.49
1:B:264:ALA:HB3	1:B:266:ILE:HG22	1.93	0.49
1:B:288:VAL:HG21	1:B:294:VAL:HG12	1.94	0.49
1:B:74:MET:SD	1:B:304:GLY:HA3	2.52	0.49
1:A:131:TYR:HB3	1:A:206:GLN:NE2	2.27	0.49
1:B:239:ARG:O	1:B:242:VAL:HB	2.12	0.49
1:B:20:MET:CG	1:B:172:PHE:HB2	2.39	0.49
1:B:33:TRP:CD2	1:B:261:TYR:HA	2.47	0.49
1:A:6:VAL:O	1:A:7:ASN:HB2	2.11	0.49
1:A:280:ILE:HB	1:A:281:PRO:HD2	1.93	0.49
1:B:74:MET:CE	1:B:304:GLY:HA3	2.42	0.49
1:B:82:LYS:HG3	1:B:110:THR:OG1	2.12	0.49
1:A:71:MET:HE3	1:A:331:ARG:HB2	1.94	0.49
1:B:269:LEU:O	1:B:273:VAL:HB	2.12	0.49
1:A:312:VAL:C	1:A:314:SER:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HB3	1:A:357:ASP:HB3	1.94	0.49
1:A:186:ILE:CD1	1:B:139:GLN:HE21	2.25	0.49
1:A:42:PHE:HB3	1:A:296:LYS:NZ	2.28	0.49
1:A:32:GLN:O	1:A:35:LEU:HB2	2.13	0.49
1:B:214:LYS:N	1:B:214:LYS:HD2	2.27	0.49
1:B:95:ALA:C	1:B:97:SER:H	2.14	0.49
1:B:129:TYR:O	1:B:137:VAL:HG13	2.13	0.49
1:B:175:PRO:HG2	1:B:178:LEU:HD12	1.94	0.49
1:B:300:LEU:CD2	1:B:300:LEU:H	2.23	0.49
1:B:60:MET:HG2	1:B:61:THR:N	2.28	0.49
1:A:56:THR:C	1:A:57:ASN:HD22	2.15	0.49
1:B:176:PRO:HG2	1:B:177:PHE:H	1.78	0.49
1:B:131:TYR:N	1:B:137:VAL:HG22	2.28	0.49
1:B:60:MET:HB3	1:B:335:GLU:HG2	1.95	0.49
1:B:73:ILE:CD1	1:B:330:MET:HB3	2.42	0.49
1:B:53:ILE:CG1	1:B:342:GLY:HA3	2.39	0.49
1:A:173:VAL:O	1:A:175:PRO:HD3	2.13	0.49
1:B:141:VAL:CG2	1:B:219:LEU:HD21	2.43	0.49
1:B:72:PRO:C	1:B:305:VAL:HG23	2.33	0.49
1:A:131:TYR:HD1	1:A:207:ILE:CA	2.24	0.49
1:B:159:PRO:HG3	1:B:211:LEU:HD21	1.95	0.49
1:B:107:SER:HA	1:B:182:ASN:CG	2.33	0.49
1:A:145:GLU:C	1:A:147:ALA:H	2.16	0.49
1:B:20:MET:HE2	1:B:171:ARG:HB3	1.95	0.49
1:A:32:GLN:HB3	1:A:35:LEU:HD22	1.95	0.49
1:B:159:PRO:HG3	1:B:211:LEU:HD11	1.94	0.49
1:A:53:ILE:HG22	1:A:54:ASP:H	1.78	0.49
1:B:238:ALA:C	1:B:241:ALA:H	2.16	0.48
1:B:152:ILE:O	1:B:227:ILE:HA	2.13	0.48
1:A:222:ILE:O	1:A:223:THR:HB	2.13	0.48
1:A:62:THR:OG1	1:A:69:ILE:HG13	2.13	0.48
1:A:160:ARG:HG3	1:A:209:ARG:NE	2.28	0.48
1:A:61:THR:HA	1:A:70:SER:O	2.13	0.48
1:B:207:ILE:HG13	1:B:207:ILE:O	2.13	0.48
1:A:140:LEU:HD11	1:A:182:ASN:OD1	2.13	0.48
1:B:80:MET:HG3	1:B:108:TRP:HB3	1.95	0.48
1:B:123:ILE:HB	1:B:150:LYS:CB	2.41	0.48
1:B:128:LEU:HD11	1:B:152:ILE:HG23	1.94	0.48
1:B:334:PHE:O	1:B:337:THR:HB	2.14	0.48
1:B:295:PHE:HE2	1:B:338:MET:HG3	1.79	0.48
1:B:94:ARG:HD3	1:B:119:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ALA:HB1	1:A:320:GLU:HG2	1.95	0.48
1:B:75:ILE:HG13	1:B:103:MET:HE3	1.94	0.48
1:B:295:PHE:HA	1:B:298:LEU:CG	2.40	0.48
1:A:39:ARG:NH1	1:A:287:GLY:O	2.47	0.48
1:B:236:GLU:HA	1:B:239:ARG:HH12	1.75	0.48
1:B:184:GLU:O	1:B:186:ILE:N	2.46	0.48
1:B:333:GLU:HA	1:B:336:LEU:HD12	1.95	0.48
1:B:83:MET:N	1:B:83:MET:SD	2.82	0.48
1:A:277:GLN:H	1:A:279:ARG:CZ	2.26	0.48
1:A:117:ALA:HB1	1:B:147:ALA:HB3	1.95	0.48
1:A:342:GLY:O	1:A:353:HIS:HE1	1.96	0.48
1:A:250:ILE:HA	1:A:283:PHE:O	2.13	0.48
1:B:112:SER:HB3	1:B:115:GLU:HB2	1.94	0.48
1:A:25:TYR:HE2	1:A:84:ALA:HB2	1.79	0.48
1:A:207:ILE:HG23	1:A:208:ASP:N	2.29	0.48
1:B:240:LEU:C	1:B:242:VAL:H	2.15	0.48
1:A:103:MET:O	1:A:124:ARG:HB2	2.13	0.48
1:B:131:TYR:CB	1:B:137:VAL:HG22	2.40	0.48
1:B:145:GLU:O	1:B:150:LYS:HA	2.13	0.48
1:B:215:ASP:HA	1:B:218:TRP:CG	2.48	0.48
1:B:24:PHE:HE2	1:B:79:ALA:C	2.17	0.48
1:A:81:GLN:O	1:A:315:LEU:HD11	2.14	0.48
1:B:35:LEU:CD1	1:B:256:ALA:HB3	2.40	0.48
1:B:270:GLU:O	1:B:274:LYS:HG3	2.14	0.48
1:B:90:TYR:CE2	1:B:115:GLU:O	2.67	0.48
1:B:134:ARG:O	1:B:138:ALA:HB3	2.14	0.48
1:B:152:ILE:CG2	1:B:153:ALA:H	2.26	0.48
1:B:204:ALA:O	1:B:206:GLN:N	2.43	0.48
1:B:253:ASN:O	1:B:255:GLY:N	2.47	0.48
1:A:165:GLU:HB3	1:A:166:ALA:H	1.53	0.48
1:A:318:GLU:O	1:A:322:GLY:N	2.45	0.48
1:B:22:TYR:CA	1:B:25:TYR:HD1	2.26	0.47
1:A:111:SER:HB2	1:A:116:VAL:CG2	2.43	0.47
1:A:289:ARG:HH12	2:A:370:FMN:P	2.37	0.47
1:A:62:THR:HB	1:A:69:ILE:HG12	1.96	0.47
1:B:34:THR:HG21	1:B:253:ASN:ND2	2.28	0.47
1:B:10:GLU:HG2	1:B:313:PHE:HE2	1.79	0.47
1:A:300:LEU:HD23	1:A:351:ARG:CD	2.42	0.47
1:A:354:ILE:HG23	1:A:355:ALA:N	2.29	0.47
1:A:103:MET:O	1:A:103:MET:SD	2.72	0.47
1:A:125:PHE:CE1	1:A:150:LYS:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:SER:HB2	1:B:127:GLN:OE1	2.14	0.47
1:B:144:ALA:CA	1:B:149:PHE:HB3	2.26	0.47
1:B:294:VAL:O	1:B:298:LEU:HB3	2.14	0.47
1:A:81:GLN:O	1:A:88:GLY:HA3	2.15	0.47
1:B:2:GLU:HG2	1:B:3:ILE:H	1.80	0.47
1:A:188:LEU:O	1:B:134:ARG:HB2	2.15	0.47
1:B:218:TRP:HE3	1:B:219:LEU:HB2	1.78	0.47
1:B:254:HIS:HB2	1:B:257:ARG:O	2.13	0.47
1:A:25:TYR:CE2	1:A:84:ALA:HB2	2.50	0.47
1:B:137:VAL:O	1:B:139:GLN:N	2.43	0.47
1:B:250:ILE:O	1:B:250:ILE:HG23	2.15	0.47
1:B:58:ILE:N	1:B:58:ILE:HD13	2.29	0.47
1:A:146:ARG:CZ	1:B:117:ALA:O	2.62	0.47
1:B:16:LYS:HB3	1:B:17:LEU:HD23	1.96	0.47
1:B:250:ILE:HD12	1:B:306:PHE:CE2	2.49	0.47
1:A:101:THR:HG22	1:A:102:ILE:N	2.25	0.47
1:B:151:ALA:HA	1:B:226:PRO:HD2	1.96	0.47
1:A:9:TYR:HA	1:A:12:ILE:CG1	2.45	0.47
1:A:265:THR:HG22	1:A:284:LEU:HB2	1.95	0.47
1:B:80:MET:SD	1:B:108:TRP:HD1	2.38	0.47
1:B:5:ASN:O	1:B:8:GLU:HB2	2.15	0.47
1:A:172:PHE:HE1	1:A:174:LEU:HA	1.79	0.47
1:A:60:MET:HB3	1:A:72:PRO:CD	2.45	0.47
1:A:188:LEU:O	1:B:134:ARG:N	2.48	0.47
1:B:110:THR:HG21	1:B:179:THR:O	2.15	0.47
1:A:131:TYR:CD1	1:A:207:ILE:HA	2.39	0.47
1:A:188:LEU:O	1:B:134:ARG:CB	2.64	0.47
1:A:18:PRO:O	1:A:19:LYS:C	2.52	0.47
1:A:155:THR:HA	1:A:230:LYS:HB3	1.97	0.47
1:B:213:TRP:CH2	1:B:240:LEU:CB	2.98	0.46
1:B:230:LYS:HG2	1:B:250:ILE:HG23	1.94	0.46
1:B:298:LEU:HD12	1:B:299:ALA:N	2.30	0.46
1:B:154:LEU:O	1:B:229:VAL:HG12	2.15	0.46
1:B:252:SER:HA	1:B:265:THR:CG2	2.44	0.46
1:B:289:ARG:NE	1:B:289:ARG:N	2.63	0.46
1:B:31:ASP:O	1:B:33:TRP:N	2.48	0.46
1:B:234:THR:O	1:B:238:ALA:HB2	2.15	0.46
1:B:7:ASN:O	1:B:10:GLU:HB2	2.16	0.46
1:B:295:PHE:CE2	1:B:338:MET:HG3	2.51	0.46
1:A:284:LEU:HD12	1:A:302:ALA:CB	2.46	0.46
1:A:130:VAL:HG22	1:A:137:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:O	1:B:353:HIS:CD2	2.65	0.46
1:B:244:HIS:CD2	1:B:244:HIS:N	2.83	0.46
1:B:105:LEU:N	1:B:105:LEU:HD12	2.30	0.46
1:A:146:ARG:NH1	1:B:117:ALA:O	2.49	0.46
1:B:129:TYR:HB2	1:B:131:TYR:CZ	2.50	0.46
1:B:6:VAL:HG21	1:B:290:ARG:HA	1.97	0.46
1:B:30:GLU:HB2	1:B:260:ASP:N	2.31	0.46
1:A:21:VAL:HG12	1:A:25:TYR:CE2	2.49	0.46
1:A:27:SER:HB2	1:A:164:ARG:HB2	1.97	0.46
1:B:42:PHE:CE2	1:B:288:VAL:CG1	2.98	0.46
1:B:238:ALA:HA	1:B:241:ALA:CB	2.46	0.46
1:B:308:GLY:O	1:B:311:VAL:HG22	2.16	0.46
1:B:78:THR:O	1:B:79:ALA:CB	2.63	0.46
1:A:265:THR:HB	1:A:284:LEU:HD23	1.97	0.46
1:A:107:SER:HB2	1:A:129:TYR:HD2	1.80	0.46
1:A:34:THR:HA	1:A:37:GLU:HB3	1.98	0.46
1:A:80:MET:HB3	1:A:83:MET:HG3	1.97	0.46
1:B:273:VAL:O	1:B:277:GLN:HB3	2.16	0.46
1:A:108:TRP:CE3	1:A:108:TRP:HA	2.51	0.46
1:A:55:VAL:HG11	1:A:339:ALA:CB	2.45	0.46
1:B:216:VAL:HG13	1:B:217:ALA:N	2.31	0.46
1:B:235:ALA:CB	1:B:271:GLU:O	2.61	0.46
1:B:292:THR:O	1:B:295:PHE:N	2.49	0.46
1:B:345:SER:OG	1:B:348:GLU:HG2	2.15	0.46
1:B:62:THR:C	1:B:68:LYS:HA	2.36	0.46
1:A:9:TYR:O	1:A:12:ILE:N	2.48	0.46
1:A:254:HIS:CE1	2:A:370:FMN:C2	2.98	0.46
1:A:82:LYS:HB2	1:A:110:THR:OG1	2.16	0.46
1:B:326:VAL:O	1:B:329:MET:HB3	2.16	0.46
1:B:90:TYR:HA	1:B:116:VAL:HG13	1.98	0.46
1:A:214:LYS:HG3	1:A:215:ASP:N	2.30	0.46
1:B:186:ILE:CG1	1:B:188:LEU:HB3	2.37	0.45
1:B:269:LEU:CD2	1:B:270:GLU:HG3	2.42	0.45
1:A:289:ARG:HG2	1:A:310:PRO:HG3	1.98	0.45
1:A:55:VAL:HG11	1:A:339:ALA:HB1	1.98	0.45
1:B:131:TYR:O	1:B:137:VAL:CG2	2.65	0.45
1:B:77:PRO:HD2	1:B:230:LYS:HZ3	1.82	0.45
1:A:7:ASN:C	1:A:9:TYR:N	2.68	0.45
1:A:24:PHE:CD1	1:A:172:PHE:HE2	2.34	0.45
1:B:235:ALA:HB1	1:B:275:ALA:CB	2.46	0.45
1:B:144:ALA:C	1:B:149:PHE:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ARG:N	1:B:344:ARG:HD3	2.31	0.45
1:B:89:GLU:C	1:B:91:ALA:H	2.17	0.45
1:A:143:ARG:C	1:A:145:GLU:H	2.20	0.45
1:B:75:ILE:HG13	1:B:103:MET:HE2	1.97	0.45
1:A:142:ARG:CB	1:B:143:ARG:NE	2.77	0.45
1:B:18:PRO:HG2	1:B:21:VAL:CB	2.43	0.45
1:B:125:PHE:CE2	1:B:228:LEU:HD23	2.51	0.45
1:A:254:HIS:CG	1:A:258:GLN:HG2	2.51	0.45
1:A:133:ASP:HB3	1:B:187:ASP:OD2	2.17	0.45
1:B:131:TYR:HB3	1:B:206:GLN:HG3	1.99	0.45
1:B:150:LYS:HD2	1:B:151:ALA:HB2	1.99	0.45
1:B:172:PHE:CZ	1:B:174:LEU:HA	2.51	0.45
1:B:233:ILE:CD1	1:B:263:PRO:HD2	2.46	0.45
1:B:298:LEU:CA	1:B:302:ALA:HB3	2.32	0.45
1:A:235:ALA:CB	1:A:275:ALA:HB2	2.46	0.45
1:A:158:THR:HA	1:A:258:GLN:NE2	2.32	0.45
1:A:103:MET:SD	1:A:105:LEU:HD22	2.57	0.45
1:B:10:GLU:CG	1:B:313:PHE:HE2	2.30	0.45
1:A:59:ASP:HB2	1:A:345:SER:HB3	1.96	0.45
1:A:202:TYR:HD1	1:A:203:VAL:N	2.14	0.45
1:A:151:ALA:HB1	1:A:228:LEU:CD2	2.47	0.45
1:B:208:ASP:HA	1:B:209:ARG:NH2	2.31	0.45
1:B:25:TYR:HB3	1:B:312:VAL:HG11	1.99	0.45
1:B:213:TRP:HA	1:B:216:VAL:HB	1.98	0.45
1:B:238:ALA:O	1:B:241:ALA:N	2.49	0.45
1:B:213:TRP:CE3	1:B:244:HIS:HB2	2.52	0.45
1:A:146:ARG:HH11	1:B:117:ALA:CB	2.23	0.45
1:B:186:ILE:HB	1:B:187:ASP:H	1.55	0.45
1:B:41:ALA:C	1:B:44:ARG:HB3	2.33	0.45
1:A:150:LYS:O	1:A:225:LEU:HA	2.17	0.45
1:B:23:ASP:O	1:B:164:ARG:NH2	2.50	0.45
1:A:183:PHE:C	1:A:185:GLY:H	2.20	0.45
1:B:158:THR:HA	1:B:159:PRO:HD3	1.37	0.45
1:B:89:GLU:OE1	1:B:116:VAL:HG21	2.16	0.45
1:B:94:ARG:CA	1:B:119:THR:HG21	2.47	0.45
1:B:290:ARG:O	1:B:292:THR:N	2.44	0.45
1:B:90:TYR:HD1	1:B:90:TYR:N	2.14	0.45
1:A:236:GLU:OE1	1:A:236:GLU:N	2.50	0.45
1:B:131:TYR:O	1:B:133:ASP:N	2.46	0.44
1:A:143:ARG:HG3	1:B:143:ARG:N	2.32	0.44
1:B:270:GLU:CA	1:B:273:VAL:HG12	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG23	1:B:282:VAL:HG11	1.99	0.44
1:A:277:GLN:N	1:A:279:ARG:CD	2.80	0.44
1:A:77:PRO:HB2	1:A:106:SER:HB2	1.99	0.44
1:A:132:LYS:HB2	1:A:206:GLN:OE1	2.17	0.44
1:B:131:TYR:CE2	1:B:140:LEU:HD11	2.51	0.44
1:B:42:PHE:HB3	1:B:296:LYS:HG2	1.97	0.44
1:A:108:TRP:HZ3	1:A:131:TYR:OH	2.00	0.44
1:A:98:ALA:CB	1:A:324:LYS:HZ1	2.30	0.44
1:A:62:THR:HG21	1:A:69:ILE:HD11	2.00	0.44
1:B:131:TYR:CA	1:B:137:VAL:HG22	2.48	0.44
1:B:99:ALA:HB2	1:B:324:LYS:HA	1.99	0.44
1:B:90:TYR:N	1:B:90:TYR:CD1	2.85	0.44
1:A:296:LYS:O	1:A:299:ALA:HB3	2.17	0.44
1:A:96:ALA:O	1:A:100:GLY:N	2.51	0.44
1:B:238:ALA:HA	1:B:241:ALA:HB3	1.97	0.44
1:B:126:PHE:CD1	1:B:127:GLN:O	2.70	0.44
1:B:127:GLN:NE2	1:B:131:TYR:OH	2.50	0.44
1:B:47:PHE:HD2	1:B:296:LYS:NZ	2.16	0.44
1:B:334:PHE:HD1	1:B:335:GLU:H	1.65	0.44
1:A:315:LEU:HG	1:A:316:ALA:N	2.33	0.44
1:A:114:GLU:OE1	1:B:225:LEU:HG	2.18	0.44
1:A:105:LEU:HD21	1:A:149:PHE:HE2	1.82	0.44
1:B:132:LYS:HB2	1:B:206:GLN:C	2.37	0.44
1:B:76:ALA:HB3	1:B:307:ILE:O	2.18	0.44
1:B:61:THR:HA	1:B:70:SER:CA	2.45	0.44
1:A:277:GLN:H	1:A:279:ARG:NH1	2.14	0.44
1:A:326:VAL:O	1:A:330:MET:HB2	2.18	0.44
1:B:40:ASN:HA	1:B:43:SER:CB	2.48	0.44
1:B:259:LEU:HB3	1:B:262:VAL:HG13	2.00	0.44
1:B:294:VAL:CG2	1:B:330:MET:HG3	2.44	0.44
1:B:90:TYR:CG	1:B:116:VAL:HA	2.53	0.44
1:B:229:VAL:O	1:B:249:ILE:HG23	2.17	0.44
1:B:253:ASN:HD22	1:B:262:VAL:CG2	2.31	0.44
1:B:46:LEU:HG	1:B:355:ALA:O	2.18	0.44
1:B:248:GLY:HA2	1:B:281:PRO:CA	2.47	0.44
1:A:53:ILE:HG22	1:A:54:ASP:N	2.32	0.44
1:A:250:ILE:HG22	1:A:285:ASP:OD1	2.18	0.44
1:B:288:VAL:HG12	1:B:293:ASP:HB2	1.97	0.44
1:B:94:ARG:O	1:B:94:ARG:HG3	2.18	0.44
1:A:269:LEU:HD23	1:A:300:LEU:CB	2.44	0.44
1:A:18:PRO:HD2	1:A:21:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:VAL:O	1:B:130:VAL:CG1	2.63	0.44
1:B:20:MET:SD	1:B:172:PHE:HA	2.58	0.44
1:B:323:VAL:O	1:B:326:VAL:HB	2.18	0.44
1:B:98:ALA:CB	1:B:324:LYS:HE2	2.36	0.44
1:A:274:LYS:NZ	1:A:277:GLN:HG2	2.32	0.44
1:A:358:TRP:NE1	1:A:359:ASP:OD2	2.51	0.44
1:B:353:HIS:CD2	1:B:353:HIS:O	2.71	0.44
1:A:142:ARG:HD3	1:A:222:ILE:O	2.18	0.43
1:B:33:TRP:CD1	1:B:261:TYR:CE1	3.06	0.43
1:B:295:PHE:HD2	1:B:334:PHE:HB2	1.83	0.43
1:B:334:PHE:HD1	1:B:335:GLU:N	2.16	0.43
1:B:42:PHE:HD1	1:B:42:PHE:H	1.61	0.43
1:B:312:VAL:CG1	1:B:312:VAL:O	2.66	0.43
1:B:290:ARG:C	1:B:292:THR:H	2.21	0.43
1:A:325:LYS:HB3	1:A:329:MET:HE2	2.01	0.43
1:B:112:SER:O	1:B:114:GLU:N	2.51	0.43
1:B:175:PRO:CG	1:B:178:LEU:HD12	2.48	0.43
1:B:325:LYS:O	1:B:329:MET:N	2.52	0.43
1:A:248:GLY:HA2	1:A:281:PRO:O	2.18	0.43
1:A:214:LYS:O	1:A:217:ALA:HB3	2.19	0.43
1:A:200:SER:O	1:A:203:VAL:HG23	2.18	0.43
1:A:274:LYS:HE2	1:A:274:LYS:O	2.19	0.43
1:A:252:SER:OG	1:A:253:ASN:N	2.51	0.43
1:B:253:ASN:C	1:B:255:GLY:H	2.21	0.43
1:B:273:VAL:HG23	1:B:282:VAL:CG1	2.48	0.43
1:B:344:ARG:HD3	1:B:344:ARG:H	1.84	0.43
1:B:90:TYR:OH	1:B:115:GLU:HB3	2.19	0.43
1:A:36:ALA:HB1	1:A:40:ASN:ND2	2.34	0.43
1:A:105:LEU:O	1:A:126:PHE:HA	2.18	0.43
1:A:189:GLY:CA	1:B:133:ASP:HA	2.46	0.43
1:A:188:LEU:CD1	1:B:135:ASN:ND2	2.75	0.43
1:B:71:MET:CG	1:B:73:ILE:HG13	2.43	0.43
1:A:39:ARG:HH11	1:A:39:ARG:HA	1.83	0.43
1:B:50:ARG:HD2	1:B:53:ILE:HD11	2.00	0.43
1:A:22:TYR:O	1:A:26:ALA:N	2.48	0.43
1:A:67:PHE:CE1	1:A:150:LYS:HG3	2.53	0.43
1:B:131:TYR:HB3	1:B:206:GLN:CG	2.48	0.43
1:B:215:ASP:O	1:B:218:TRP:CE3	2.72	0.43
1:B:233:ILE:HA	1:B:251:VAL:CG1	2.40	0.43
1:B:64:ILE:HD12	1:B:69:ILE:CG1	2.49	0.43
1:A:42:PHE:CD2	1:A:293:ASP:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:O	1:A:329:MET:HG3	2.19	0.43
1:B:232:VAL:H	1:B:251:VAL:CA	2.16	0.43
1:B:295:PHE:HE2	1:B:338:MET:CG	2.32	0.43
1:B:86:PRO:HB2	1:B:87:GLU:H	1.65	0.43
1:B:150:LYS:HD2	1:B:151:ALA:N	2.33	0.43
1:B:288:VAL:HB	1:B:294:VAL:CG1	2.47	0.43
1:B:98:ALA:HB1	1:B:324:LYS:CE	2.35	0.43
1:A:9:TYR:O	1:A:10:GLU:C	2.57	0.43
2:A:370:FMN:H1'2	2:A:370:FMN:H9	1.61	0.43
1:A:350:SER:C	1:A:352:SER:H	2.21	0.43
1:B:91:ALA:HA	1:B:320:GLU:CA	2.44	0.42
1:B:128:LEU:O	1:B:129:TYR:CG	2.72	0.42
1:B:129:TYR:HB2	1:B:131:TYR:CE1	2.53	0.42
1:B:78:THR:H	1:B:105:LEU:HA	1.84	0.42
1:B:131:TYR:CE2	1:B:140:LEU:HD21	2.50	0.42
1:B:229:VAL:CG2	1:B:249:ILE:HG12	2.36	0.42
1:A:13:ALA:O	1:A:17:LEU:HG	2.19	0.42
1:A:84:ALA:O	1:A:85:HIS:CB	2.67	0.42
1:A:249:ILE:HG23	1:A:251:VAL:HG22	2.01	0.42
1:A:236:GLU:O	1:A:240:LEU:HD23	2.19	0.42
1:B:16:LYS:C	1:B:17:LEU:HD23	2.40	0.42
1:A:266:ILE:HG23	1:A:267:MET:H	1.83	0.42
1:A:58:ILE:HG22	1:A:59:ASP:N	2.27	0.42
1:A:292:THR:O	1:A:295:PHE:HB3	2.19	0.42
1:B:309:ARG:O	1:B:312:VAL:N	2.43	0.42
1:B:59:ASP:OD1	1:B:62:THR:HB	2.19	0.42
1:A:42:PHE:HA	1:A:266:ILE:HD12	2.02	0.42
1:A:96:ALA:O	1:A:99:ALA:N	2.52	0.42
1:A:127:GLN:HA	1:A:153:ALA:O	2.20	0.42
1:A:289:ARG:HH11	1:A:310:PRO:HD3	1.84	0.42
1:A:107:SER:C	1:A:109:ALA:H	2.23	0.42
1:A:57:ASN:HD22	1:A:57:ASN:N	2.18	0.42
1:A:155:THR:O	1:A:155:THR:HG22	2.19	0.42
1:A:188:LEU:HB3	1:A:189:GLY:H	1.69	0.42
1:A:142:ARG:HH11	1:B:184:GLU:HG3	1.71	0.42
1:A:131:TYR:H	1:A:137:VAL:HG21	1.85	0.42
1:B:100:GLY:O	1:B:101:THR:HB	2.19	0.42
1:A:143:ARG:NE	1:B:145:GLU:OE2	2.53	0.42
1:B:75:ILE:N	1:B:75:ILE:HD13	2.34	0.42
1:A:270:GLU:OE2	1:A:351:ARG:NE	2.53	0.42
1:A:308:GLY:O	1:A:309:ARG:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ARG:HD2	1:B:142:ARG:H	1.85	0.42
1:A:235:ALA:HB1	1:A:275:ALA:CB	2.50	0.42
1:B:214:LYS:H	1:B:214:LYS:HD2	1.83	0.42
1:A:112:SER:OG	1:A:113:VAL:N	2.53	0.42
1:A:35:LEU:O	1:A:38:ASN:HB2	2.20	0.42
1:A:247:ALA:HA	1:A:280:ILE:CB	2.50	0.42
1:A:14:LYS:HA	1:A:22:TYR:CD1	2.55	0.42
1:A:143:ARG:HG3	1:B:143:ARG:CA	2.50	0.41
1:A:151:ALA:HB1	1:A:226:PRO:O	2.20	0.41
1:B:117:ALA:C	1:B:119:THR:H	2.23	0.41
1:B:220:GLN:HE21	1:B:246:ALA:HA	1.85	0.41
1:B:346:LEU:HD12	1:B:349:ILE:CG1	2.44	0.41
1:B:59:ASP:HB3	1:B:345:SER:HA	2.03	0.41
1:B:71:MET:HB3	1:B:331:ARG:CG	2.50	0.41
1:B:213:TRP:HH2	1:B:240:LEU:CB	2.33	0.41
1:B:172:PHE:CG	1:B:173:VAL:N	2.89	0.41
1:B:85:HIS:HE2	1:B:315:LEU:HD23	1.84	0.41
1:A:354:ILE:HG12	1:A:355:ALA:N	2.22	0.41
1:A:161:LEU:HD12	1:A:161:LEU:H	1.85	0.41
1:A:27:SER:OG	1:A:257:ARG:NH1	2.53	0.41
1:A:44:ARG:O	1:A:357:ASP:N	2.54	0.41
1:B:159:PRO:HG2	1:B:211:LEU:HD21	2.01	0.41
1:A:228:LEU:CD2	1:A:228:LEU:H	2.31	0.41
1:B:126:PHE:HB2	1:B:144:ALA:CB	2.50	0.41
1:B:309:ARG:N	1:B:310:PRO:CD	2.84	0.41
1:A:299:ALA:O	1:A:351:ARG:N	2.54	0.41
1:B:163:ARG:CG	1:B:163:ARG:NH1	2.82	0.41
1:B:234:THR:O	1:B:238:ALA:CB	2.68	0.41
1:B:233:ILE:HG22	1:B:251:VAL:HG13	2.00	0.41
1:B:73:ILE:N	1:B:305:VAL:HG23	2.35	0.41
1:B:64:ILE:N	1:B:64:ILE:HD13	2.35	0.41
1:B:133:ASP:HB2	1:B:136:VAL:HG22	2.02	0.41
1:B:295:PHE:O	1:B:296:LYS:C	2.59	0.41
1:B:343:CYS:HB3	1:B:349:ILE:HD13	2.03	0.41
1:B:70:SER:HB2	1:B:71:MET:HE3	2.03	0.41
1:B:91:ALA:HA	1:B:320:GLU:HG2	2.01	0.41
1:B:271:GLU:O	1:B:271:GLU:HG2	2.20	0.41
1:A:80:MET:HE3	1:A:80:MET:HB2	1.99	0.41
1:B:306:PHE:O	1:B:307:ILE:HG23	2.20	0.41
1:B:38:ASN:O	1:B:42:PHE:CE1	2.72	0.41
1:B:81:GLN:HE21	1:B:81:GLN:HB2	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG13	1:A:134:ARG:HE	1.86	0.41
1:A:37:GLU:O	1:A:264:ALA:HB2	2.20	0.41
1:A:238:ALA:O	1:A:241:ALA:N	2.52	0.41
1:B:59:ASP:HB3	1:B:344:ARG:O	2.21	0.41
1:A:323:VAL:O	1:A:327:LEU:HG	2.20	0.41
1:A:175:PRO:HA	1:A:176:PRO:HD2	1.50	0.41
1:A:24:PHE:HE2	1:A:79:ALA:HB3	1.85	0.41
1:B:14:LYS:HD3	1:B:14:LYS:HA	1.77	0.41
1:A:142:ARG:HE	1:B:143:ARG:NH2	2.19	0.41
1:B:92:THR:HA	1:B:323:VAL:HG21	2.03	0.41
1:B:328:GLN:NE2	1:B:331:ARG:HB3	2.35	0.41
1:B:75:ILE:HB	1:B:104:THR:OG1	2.20	0.41
1:B:128:LEU:HD13	1:B:153:ALA:O	2.21	0.41
1:B:76:ALA:O	1:B:77:PRO:C	2.59	0.41
1:A:183:PHE:O	1:A:185:GLY:N	2.47	0.41
1:A:24:PHE:CD1	1:A:172:PHE:CE2	3.09	0.41
1:B:134:ARG:NH1	1:B:218:TRP:CH2	2.88	0.41
1:B:146:ARG:NH2	1:B:225:LEU:HA	2.31	0.41
1:B:37:GLU:CG	1:B:264:ALA:HB2	2.39	0.41
1:A:162:GLY:HA3	1:A:257:ARG:O	2.20	0.41
1:A:162:GLY:O	1:A:164:ARG:CD	2.66	0.41
1:A:39:ARG:CZ	1:A:287:GLY:O	2.69	0.41
1:A:127:GLN:NE2	2:A:370:FMN:HN3	2.19	0.41
1:A:165:GLU:O	1:A:166:ALA:C	2.58	0.41
1:B:266:ILE:O	1:B:269:LEU:N	2.47	0.40
2:A:370:FMN:C10	2:A:370:FMN:HO2'	2.33	0.40
1:A:179:THR:O	1:A:181:LYS:NZ	2.51	0.40
1:B:128:LEU:HG	1:B:140:LEU:CD2	2.50	0.40
1:B:131:TYR:HE2	1:B:140:LEU:HD11	1.87	0.40
1:B:266:ILE:C	1:B:266:ILE:HD12	2.42	0.40
1:B:311:VAL:HG11	1:B:323:VAL:HB	2.02	0.40
1:A:24:PHE:CE2	1:A:79:ALA:HB3	2.57	0.40
1:A:117:ALA:O	1:B:147:ALA:CB	2.69	0.40
1:A:331:ARG:C	1:A:333:GLU:H	2.25	0.40
1:B:45:ILE:CG2	1:B:356:ALA:HA	2.47	0.40
1:A:165:GLU:O	1:A:167:ASP:N	2.54	0.40
1:A:93:ALA:HA	1:A:103:MET:HG3	2.02	0.40
1:B:311:VAL:HB	1:B:323:VAL:CG1	2.50	0.40
1:B:72:PRO:HB2	1:B:304:GLY:HA2	2.03	0.40
1:A:269:LEU:HA	1:A:269:LEU:HD12	1.92	0.40
1:B:107:SER:O	1:B:182:ASN:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLN:HB3	1:B:244:HIS:CD2	2.56	0.40
1:A:141:VAL:HG11	1:A:222:ILE:HD11	2.04	0.40
1:A:186:ILE:HD11	1:B:139:GLN:NE2	2.33	0.40
1:B:73:ILE:CA	1:B:305:VAL:HB	2.39	0.40
1:B:307:ILE:HG13	1:B:308:GLY:H	1.86	0.40
1:B:64:ILE:HG12	1:B:67:PHE:CD1	2.56	0.40
1:B:77:PRO:HB3	1:B:127:GLN:HB2	2.03	0.40
1:B:163:ARG:HG3	1:B:163:ARG:NH1	2.31	0.40

There are no symmetry-related clashes.

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	348/369 (94%)	238 (68%)	64 (18%)	46 (13%)	0 1
1	B	346/369 (94%)	203 (59%)	91 (26%)	52 (15%)	0 1
All	All	694/738 (94%)	441 (64%)	155 (22%)	98 (14%)	0 1

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	19	LYS
1	A	89	GLU
1	A	150	LYS
1	A	165	GLU
1	A	166	ALA
1	A	200	SER
1	A	207	ILE
1	A	226	PRO
1	A	303	ALA

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Mol	Chain	Res	Type
1	A	357	ASP
1	B	25	TYR
1	B	30	GLU
1	B	67	PHE
1	B	86	PRO
1	B	113	VAL
1	B	132	LYS
1	B	133	ASP
1	B	144	ALA
1	B	150	LYS
1	B	159	PRO
1	B	184	GLU
1	B	237	ASP
1	B	254	HIS
1	B	261	TYR
1	B	277	GLN
1	B	281	PRO
1	B	291	GLY
1	B	307	ILE
1	A	63	THR
1	A	85	HIS
1	A	87	GLU
1	A	159	PRO
1	A	175	PRO
1	A	181	LYS
1	A	245	GLY
1	A	254	HIS
1	A	275	ALA
1	A	288	VAL
1	A	350	SER
1	A	354	ILE
1	B	79	ALA
1	B	80	MET
1	B	96	ALA
1	B	101	THR
1	B	118	SER
1	B	143	ARG
1	B	181	LYS
1	B	182	ASN
1	B	185	GLY
1	B	249	ILE
1	B	258	GLN

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Mol	Chain	Res	Type
1	B	322	GLY
1	B	347	LYS
1	A	30	GLU
1	A	77	PRO
1	A	79	ALA
1	A	80	MET
1	A	121	PRO
1	A	145	GLU
1	A	162	GLY
1	A	176	PRO
1	A	263	PRO
1	B	64	ILE
1	B	129	TYR
1	B	227	ILE
1	B	267	MET
1	B	301	GLY
1	B	333	GLU
1	B	353	HIS
1	A	108	TRP
1	A	117	ALA
1	A	188	LEU
1	A	233	ILE
1	A	276	ALA
1	B	73	ILE
1	B	110	THR
1	B	131	TYR
1	B	266	ILE
1	B	276	ALA
1	B	296	LYS
1	B	343	CYS
1	A	86	PRO
1	A	88	GLY
1	A	172	PHE
1	A	332	ASP
1	A	342	GLY
1	A	349	ILE
1	B	207	ILE
1	B	248	GLY
1	A	10	GLU
1	B	75	ILE
1	B	174	LEU
1	B	137	VAL

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Mol	Chain	Res	Type
1	A	319	GLY
1	B	173	VAL
1	A	168	ILE
1	B	130	VAL

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	281/294 (96%)	216 (77%)	65 (23%)	1 5
1	B	280/294 (95%)	185 (66%)	95 (34%)	0 1
All	All	561/588 (95%)	401 (72%)	160 (28%)	0 2

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	12	ILE
1	A	15	GLN
1	A	17	LEU
1	A	34	THR
1	A	38	ASN
1	A	48	ARG
1	A	49	PRO
1	A	57	ASN
1	A	59	ASP
1	A	62	THR
1	A	64	ILE
1	A	71	MET
1	A	85	HIS
1	A	87	GLU
1	A	89	GLU
1	A	90	TYR
1	A	103	MET
1	A	105	LEU

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Mol	Chain	Res	Type
1	A	108	TRP
1	A	110	THR
1	A	113	VAL
1	A	123	ILE
1	A	129	TYR
1	A	130	VAL
1	A	135	ASN
1	A	152	ILE
1	A	161	LEU
1	A	164	ARG
1	A	165	GLU
1	A	167	ASP
1	A	172	PHE
1	A	174	LEU
1	A	177	PHE
1	A	180	LEU
1	A	187	ASP
1	A	199	LEU
1	A	202	TYR
1	A	206	GLN
1	A	207	ILE
1	A	211	LEU
1	A	212	SER
1	A	216	VAL
1	A	218	TRP
1	A	222	ILE
1	A	226	PRO
1	A	228	LEU
1	A	240	LEU
1	A	251	VAL
1	A	253	ASN
1	A	260	ASP
1	A	265	THR
1	A	266	ILE
1	A	267	MET
1	A	271	GLU
1	A	274	LYS
1	A	279	ARG
1	A	284	LEU
1	A	292	THR
1	A	298	LEU
1	A	311	VAL

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Mol	Chain	Res	Type
1	A	318	GLU
1	A	328	GLN
1	A	334	PHE
1	A	346	LEU
1	B	2	GLU
1	B	16	LYS
1	B	17	LEU
1	B	31	ASP
1	B	32	GLN
1	B	42	PHE
1	B	43	SER
1	B	46	LEU
1	B	50	ARG
1	B	57	ASN
1	B	58	ILE
1	B	60	MET
1	B	61	THR
1	B	64	ILE
1	B	65	LEU
1	B	67	PHE
1	B	68	LYS
1	B	70	SER
1	B	71	MET
1	B	74	MET
1	B	75	ILE
1	B	77	PRO
1	B	81	GLN
1	B	83	MET
1	B	85	HIS
1	B	87	GLU
1	B	90	TYR
1	B	94	ARG
1	B	103	MET
1	B	105	LEU
1	B	121	PRO
1	B	126	PHE
1	B	127	GLN
1	B	129	TYR
1	B	130	VAL
1	B	132	LYS
1	B	136	VAL
1	B	137	VAL

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Mol	Chain	Res	Type
1	B	142	ARG
1	B	145	GLU
1	B	149	PHE
1	B	158	THR
1	B	160	ARG
1	B	163	ARG
1	B	164	ARG
1	B	165	GLU
1	B	172	PHE
1	B	174	LEU
1	B	177	PHE
1	B	180	LEU
1	B	181	LYS
1	B	199	LEU
1	B	200	SER
1	B	206	GLN
1	B	208	ASP
1	B	209	ARG
1	B	211	LEU
1	B	213	TRP
1	B	214	LYS
1	B	216	VAL
1	B	218	TRP
1	B	221	THR
1	B	228	LEU
1	B	229	VAL
1	B	234	THR
1	B	244	HIS
1	B	254	HIS
1	B	260	ASP
1	B	261	TYR
1	B	262	VAL
1	B	265	THR
1	B	266	ILE
1	B	267	MET
1	B	273	VAL
1	B	277	GLN
1	B	281	PRO
1	B	284	LEU
1	B	288	VAL
1	B	289	ARG
1	B	290	ARG

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Mol	Chain	Res	Type
1	B	296	LYS
1	B	298	LEU
1	B	305	VAL
1	B	314	SER
1	B	324	LYS
1	B	331	ARG
1	B	333	GLU
1	B	334	PHE
1	B	335	GLU
1	B	344	ARG
1	B	346	LEU
1	B	347	LYS
1	B	351	ARG
1	B	352	SER
1	B	358	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	57	ASN
1	A	139	GLN
1	A	244	HIS
1	A	254	HIS
1	B	7	ASN
1	B	38	ASN
1	B	40	ASN
1	B	81	GLN
1	B	206	GLN
1	B	244	HIS
1	B	353	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
2	FMN	A	370	-	32,33,33	3.42	13 (40%)	34,50,50	2.99	14 (41%)

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
2	FMN	A	370	-	-	0/18/18/18	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	370	FMN	C1'-N10	-8.92	1.38	1.48
2	A	370	FMN	C6-C5A	-3.26	1.36	1.41
2	A	370	FMN	C6-C7	2.05	1.43	1.37
2	A	370	FMN	O4'-C4'	2.38	1.48	1.43
2	A	370	FMN	C9A-N10	2.42	1.42	1.38
2	A	370	FMN	C2-N1	2.65	1.43	1.38
2	A	370	FMN	P-O5'	3.97	1.71	1.59
2	A	370	FMN	C10-N1	4.12	1.42	1.35
2	A	370	FMN	C10-N10	4.37	1.44	1.39
2	A	370	FMN	C4A-N5	4.41	1.40	1.33
2	A	370	FMN	C4'-C3'	5.08	1.63	1.53
2	A	370	FMN	C4-N3	5.31	1.42	1.33
2	A	370	FMN	C5'-C4'	11.09	1.68	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	370	FMN	N3-C2-N1	-8.04	114.16	127.69
2	A	370	FMN	C4A-C4-N3	-4.44	117.72	123.52
2	A	370	FMN	O2P-P-O5'	-2.51	99.39	106.72
2	A	370	FMN	C7M-C7-C8	-2.20	115.99	120.73
2	A	370	FMN	O3P-P-O2P	2.16	115.38	107.44
2	A	370	FMN	O4'-C4'-C3'	2.31	114.89	108.96
2	A	370	FMN	O4'-C4'-C5'	2.63	115.83	110.09
2	A	370	FMN	C5A-C9A-N10	3.16	119.95	117.58
2	A	370	FMN	O2'-C2'-C3'	3.20	117.20	108.96
2	A	370	FMN	C4A-C10-N10	3.22	122.86	120.52
2	A	370	FMN	C4-C4A-C10	4.14	122.59	119.94
2	A	370	FMN	C4A-N5-C5A	4.28	121.77	116.72
2	A	370	FMN	O2'-C2'-C1'	5.12	122.58	109.93
2	A	370	FMN	C4-N3-C2	9.02	122.68	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	370	FMN	6	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.