



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:51 PM GMT

PDB ID : 1CR6  
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE  
COMPLEXED WITH CPU INHIBITOR  
Authors : Argiriadi, M.A.; Morisseau, C.; Hammock, B.D.; Christianson, D.W.  
Deposited on : 1999-08-13  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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 (RC4), CSD as536be (2015)  
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) : trunk26865

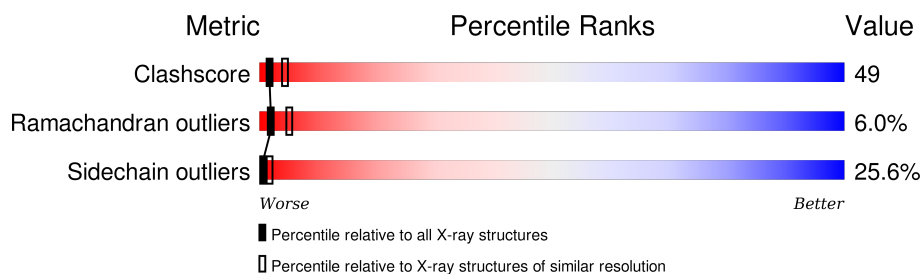
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

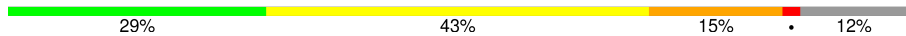

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	
1	B	554	

## 2 Entry composition [i](#)

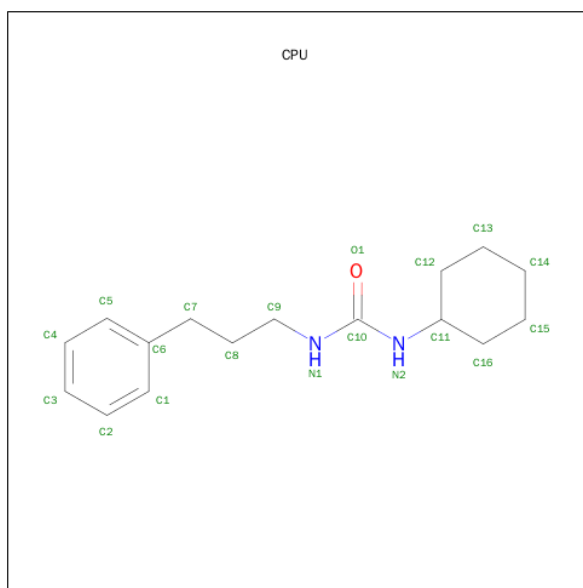
There are 3 unique types of molecules in this entry. The entry contains 8237 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EPOXIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	61	0	0
			3879	2501	648	701	29			
1	B	541	Total	C	N	O	S	71	0	0
			4299	2766	719	783	31			

- Molecule 2 is N-CYCLOHEXYL-N'-(PROPYL)PHENYL UREA (three-letter code: CPU) (formula: C<sub>16</sub>H<sub>24</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	16	2	1		
2	B	1	Total	C	N	O	0	0
			19	16	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	9	Total 9	O 9	0	0



Q535 I536 I537 I538 K639	W471 W472 W473 W474 W475 S476 S477 G478 L479 G480 B481 K482 L483 L484 V485	T402 F403 K404 S405 F406 R407 F408	G323 I324 P325  V328 F329  H332 D333 K334 V337 P338 V339  K342	L289  Q262 Q263 Q264 P265 P266 Q267 S268 P269 P270 S271 W272 R273  Q274 Q275 L276 P277 A278 L279 A280 V280 Q281	L190 K191 P192 A193 R194 D195 L196 M198 L199 T200 L201 L202 W203 H204 M205 T206 A207 S208 A209 L210 R211 R212 L213 E214 K215 V216 T217 G218 G219 Q220 P221 P222 V223 S224 Q225	M125 L126 P127 D128 D129 G130 L131 D132 K133 L134 M135 L136 A137 Q138 M139 M140	W63 V64 P65 L66 M67 D68 E69 S70 S71 R133 R134 R135 S74 S75 K76 K77 G78 G79 A80 N81 L82 P83 E84 N85 P86 S87 I88 S89 Q90 I91 P92 S93 Q94 A95 M96																																																																
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.90 Å   143.00 Å   60.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	91.0 (20.00-2.80)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.201 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.60	0/3981	0.79	1/5397 (0.0%)
1	B	0.60	0/4413	0.80	3/5984 (0.1%)
All	All	0.60	0/8394	0.80	4/11381 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ASN	C-N-CD	-11.76	94.72	120.60
1	B	231	ASN	C-N-CA	7.25	152.46	122.00
1	A	488	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	488	LEU	CA-CB-CG	5.32	127.53	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3879	0	3863	370	0
1	B	4299	0	4270	434	0
2	A	19	0	24	5	0
2	B	19	0	24	5	0
3	A	12	0	0	0	0

*Continued on next page...*



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	0	0	0
All	All	8237	0	8181	786	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 49.

All (786) 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:232:PRO:HD2	1:B:233:ASN:H	1.11	1.11
1:B:5:VAL:HG21	1:B:173:LEU:HD21	1.35	1.08
1:A:101:ILE:HG21	1:A:106:LEU:HD12	1.38	1.06
1:B:300:PRO:HG2	1:B:305:GLU:HG2	1.36	1.05
1:B:496:ILE:H	1:B:496:ILE:HD12	1.19	1.04
1:B:424:ILE:HD13	1:B:424:ILE:H	1.19	1.04
1:A:300:PRO:HG2	1:A:305:GLU:HG2	1.36	1.02
1:A:90:GLN:HG3	1:A:91:ILE:HD13	1.37	1.02
1:A:496:ILE:HD12	1:A:496:ILE:H	1.20	1.01
1:A:193:ALA:HA	1:A:198:MET:HE3	1.44	1.00
1:A:232:PRO:HD2	1:A:233:ASN:H	1.27	0.99
1:A:166:TYR:O	1:A:170:LEU:HD12	1.60	0.98
1:A:52:GLN:HG3	1:A:58:ILE:HD11	1.44	0.98
1:B:19:ILE:HD11	1:B:96:MET:HA	1.45	0.98
1:B:263:HIS:CD2	1:B:291:MET:HG2	2.00	0.96
1:A:430:ASN:HD22	1:A:430:ASN:H	1.06	0.94
1:A:263:HIS:CD2	1:A:291:MET:HG2	2.01	0.94
1:A:193:ALA:O	1:A:198:MET:HB2	1.68	0.94
1:A:13:VAL:HG22	1:A:203:VAL:HG21	1.48	0.94
1:B:155:GLN:HA	1:B:155:GLN:OE1	1.69	0.93
1:A:155:GLN:OE1	1:A:155:GLN:HA	1.69	0.92
1:A:447:GLU:HA	1:A:450:ILE:HD13	1.51	0.92
1:B:447:GLU:HA	1:B:450:ILE:HD13	1.51	0.92
1:A:322:LEU:HB3	1:A:324:ILE:CD1	2.00	0.92
1:B:106:LEU:HD21	1:B:146:HIS:CD2	2.06	0.91
1:A:205:ASN:ND2	1:A:209:ALA:H	1.69	0.91
1:B:322:LEU:HB3	1:B:324:ILE:CD1	2.00	0.90
1:A:205:ASN:HD21	1:A:209:ALA:HB3	1.36	0.90
1:B:13:VAL:HB	1:B:203:VAL:HG11	1.54	0.88
1:B:72:ARG:HA	1:B:75:SER:HB3	1.53	0.88
1:A:17:PRO:HD2	1:A:99:ARG:HA	1.54	0.88
1:B:232:PRO:CD	1:B:233:ASN:H	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PRO:CD	1:A:233:ASN:H	1.87	0.87
1:B:424:ILE:H	1:B:424:ILE:CD1	1.87	0.86
1:B:158:MET:HE3	1:B:165:ILE:HA	1.57	0.86
1:B:127:LEU:HD12	1:B:127:LEU:H	1.40	0.86
1:B:5:VAL:HG23	1:B:118:THR:O	1.75	0.85
1:A:230:CYS:O	1:A:231:ASN:HB3	1.75	0.85
1:B:122:VAL:HB	1:B:151:ILE:HG13	1.56	0.85
1:A:211:ARG:HA	1:A:214:GLU:HB2	1.59	0.85
1:A:48:GLY:N	1:A:51:GLU:HB2	1.91	0.85
1:A:102:ASN:HD22	1:A:104:PRO:HD2	1.41	0.84
1:B:496:ILE:H	1:B:496:ILE:CD1	1.90	0.84
1:A:529:LYS:O	1:A:533:VAL:HG23	1.78	0.84
1:B:404:LYS:O	1:B:408:ARG:HD2	1.77	0.84
1:B:232:PRO:O	1:B:235:VAL:HG22	1.78	0.83
1:A:404:LYS:O	1:A:408:ARG:HD2	1.78	0.83
1:A:422:THR:O	1:A:423:GLU:HB2	1.77	0.83
1:A:94:GLN:H	1:A:94:GLN:CD	1.82	0.82
1:A:215:LYS:HG2	1:A:220:GLN:HA	1.61	0.82
1:A:496:ILE:CD1	1:A:496:ILE:H	1.91	0.82
1:B:424:ILE:HD13	1:B:424:ILE:N	1.95	0.81
1:B:322:LEU:HB3	1:B:324:ILE:HD13	1.61	0.81
1:B:529:LYS:O	1:B:533:VAL:HG23	1.81	0.81
1:B:5:VAL:HG13	1:B:180:VAL:HB	1.61	0.81
1:B:339:VAL:HG13	1:B:353:VAL:HG12	1.62	0.81
1:A:140:MET:HE3	1:A:140:MET:HA	1.62	0.81
1:B:232:PRO:HD2	1:B:233:ASN:N	1.92	0.81
1:A:369:PRO:O	1:A:372:VAL:HG22	1.80	0.81
1:B:58:ILE:HD12	1:B:63:TRP:HB2	1.64	0.80
1:B:369:PRO:O	1:B:372:VAL:HG22	1.80	0.80
1:A:463:ASN:HA	1:A:466:ARG:HG3	1.62	0.80
1:B:463:ASN:HA	1:B:466:ARG:HG3	1.62	0.80
1:A:446:ILE:O	1:A:450:ILE:HD12	1.81	0.80
1:A:96:MET:SD	1:A:136:LEU:HD23	2.21	0.80
1:A:535:GLN:O	1:A:539:LYS:HD3	1.82	0.80
1:B:50:THR:CG2	1:B:63:TRP:HE1	1.95	0.80
1:B:270:PHE:CE1	1:B:273:ARG:HD3	2.17	0.80
1:A:62:GLN:O	1:A:63:TRP:HD1	1.64	0.80
1:A:102:ASN:ND2	1:A:104:PRO:HD2	1.97	0.79
1:A:133:ARG:HG2	1:B:348:GLU:HA	1.63	0.79
1:A:339:VAL:HG13	1:A:353:VAL:HG12	1.63	0.79
1:B:5:VAL:HG21	1:B:173:LEU:CD2	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:O	1:B:165:ILE:HG12	1.82	0.79
1:A:205:ASN:HD21	1:A:209:ALA:CB	1.94	0.79
1:B:535:GLN:O	1:B:539:LYS:HD3	1.83	0.79
1:B:431:THR:HG22	1:B:432:PRO:HD2	1.63	0.78
1:A:270:PHE:CE1	1:A:273:ARG:HD3	2.19	0.78
1:A:124:ASN:HA	1:A:153:SER:HB3	1.65	0.77
1:B:529:LYS:HB3	1:B:532:GLU:HG3	1.66	0.77
1:A:497:VAL:O	1:A:498:LEU:HB2	1.84	0.77
1:B:300:PRO:CG	1:B:305:GLU:HG2	2.13	0.77
1:B:112:LEU:O	1:B:117:PHE:HB2	1.85	0.77
1:A:159:ILE:O	1:A:159:ILE:HD12	1.85	0.76
1:B:50:THR:HG23	1:B:63:TRP:HE1	1.49	0.76
1:A:13:VAL:CG2	1:A:203:VAL:HG21	2.15	0.76
1:B:320:ASP:OD1	1:B:349:ARG:NH2	2.19	0.76
1:B:483:ILE:HB	1:B:510:ILE:HG12	1.67	0.76
1:B:446:ILE:O	1:B:450:ILE:HD12	1.86	0.76
1:A:322:LEU:HB3	1:A:324:ILE:HD13	1.66	0.75
1:A:52:GLN:CG	1:A:58:ILE:HD11	2.17	0.75
1:B:424:ILE:HB	1:B:429:VAL:HG11	1.67	0.75
1:A:91:ILE:C	1:A:94:GLN:HE22	1.90	0.75
1:A:529:LYS:HB3	1:A:532:GLU:HG3	1.66	0.75
1:A:162:GLU:HB3	1:A:164:GLN:HE21	1.51	0.75
1:A:292:LYS:NZ	1:A:305:GLU:HG3	2.03	0.74
1:B:292:LYS:NZ	1:B:305:GLU:HG3	2.02	0.74
1:A:446:ILE:HG22	1:A:450:ILE:HD11	1.68	0.74
1:B:446:ILE:HG22	1:B:450:ILE:HD11	1.69	0.74
1:B:9:ASP:O	1:B:13:VAL:HG22	1.87	0.74
1:A:499:ARG:O	1:A:502:MET:HG3	1.88	0.74
1:A:320:ASP:OD1	1:A:349:ARG:NH2	2.19	0.73
1:B:177:PRO:O	1:B:198:MET:HA	1.89	0.73
1:A:300:PRO:CG	1:A:305:GLU:HG2	2.14	0.73
1:A:231:ASN:HB2	1:A:232:PRO:HA	1.69	0.73
1:A:205:ASN:ND2	1:A:209:ALA:HB3	2.03	0.73
1:A:483:ILE:HB	1:A:510:ILE:HG12	1.69	0.73
1:B:73:LYS:HZ2	1:B:73:LYS:HA	1.53	0.73
1:B:127:LEU:HD12	1:B:127:LEU:N	2.03	0.73
1:B:497:VAL:O	1:B:498:LEU:HB2	1.86	0.73
1:B:177:PRO:O	1:B:198:MET:HG3	1.87	0.72
1:B:510:ILE:HG22	1:B:513:LEU:HB2	1.71	0.72
1:B:499:ARG:O	1:B:502:MET:HG3	1.89	0.72
1:B:64:VAL:HB	1:B:65:PRO:CD	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:CD1	1:B:63:TRP:HB2	2.19	0.72
1:B:8:PHE:N	1:B:8:PHE:CD1	2.57	0.72
1:B:121:ILE:O	1:B:151:ILE:HG12	1.89	0.71
1:B:83:PRO:HG2	1:B:86:PHE:HB2	1.69	0.71
1:A:348:GLU:HA	1:B:133:ARG:CG	2.19	0.71
1:B:201:ILE:HD12	1:B:201:ILE:N	2.05	0.71
1:B:420:LYS:HB3	1:B:424:ILE:HD12	1.72	0.71
1:A:159:ILE:O	1:A:165:ILE:HD11	1.91	0.71
1:B:8:PHE:CE1	1:B:147:PHE:HE2	2.08	0.71
1:A:162:GLU:O	1:A:165:ILE:HG13	1.90	0.71
1:A:10:LEU:O	1:A:12:GLY:N	2.24	0.70
1:B:232:PRO:HD2	1:B:233:ASN:HD22	1.55	0.70
1:B:531:THR:HG23	1:B:532:GLU:OE2	1.90	0.70
1:B:103:ARG:O	1:B:107:GLN:HB2	1.92	0.70
1:A:58:ILE:HG22	1:A:62:GLN:HB3	1.73	0.70
1:B:5:VAL:HG11	1:B:173:LEU:HD23	1.74	0.70
1:B:158:MET:CE	1:B:165:ILE:HA	2.22	0.70
1:B:496:ILE:N	1:B:496:ILE:HD12	2.01	0.69
1:A:136:LEU:O	1:A:140:MET:HG2	1.92	0.69
1:A:324:ILE:HD12	1:A:324:ILE:N	2.08	0.69
1:B:181:VAL:HG23	1:B:201:ILE:CD1	2.22	0.69
1:B:7:ALA:HA	1:B:120:CYS:O	1.91	0.69
1:B:128:ASP:O	1:B:133:ARG:HG3	1.92	0.69
1:B:259:LEU:O	1:B:259:LEU:HD12	1.92	0.69
1:B:497:VAL:HG13	2:B:1200:CPU:C12	2.21	0.69
1:A:187:GLY:HA2	1:A:190:LEU:HD12	1.74	0.69
1:A:416:ILE:HG23	1:A:427:ILE:CG1	2.23	0.69
1:B:77:ALA:O	1:B:78:CYS:HB2	1.92	0.69
1:B:229:PRO:HB2	1:B:231:ASN:HD21	1.56	0.69
1:B:124:ASN:HA	1:B:153:SER:HB3	1.75	0.69
1:B:529:LYS:HB3	1:B:532:GLU:CG	2.22	0.69
1:A:348:GLU:HA	1:B:133:ARG:HG2	1.72	0.69
1:A:510:ILE:HG22	1:A:513:LEU:HB2	1.74	0.69
1:A:216:VAL:CG1	1:A:217:THR:N	2.56	0.68
1:B:49:PRO:HB2	1:B:67:MET:HG2	1.74	0.68
1:B:103:ARG:HB2	1:B:104:PRO:HD3	1.75	0.68
1:A:52:GLN:HG3	1:A:58:ILE:CD1	2.22	0.68
1:A:430:ASN:ND2	1:A:430:ASN:H	1.84	0.68
1:B:159:ILE:O	1:B:165:ILE:HD11	1.92	0.68
1:B:222:PRO:HG2	1:B:225:PRO:HG3	1.73	0.68
1:A:496:ILE:N	1:A:496:ILE:HD12	2.03	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:CD1	1:A:147:PHE:HE2	2.11	0.68
1:B:427:ILE:HG13	1:B:428:LEU:HD13	1.75	0.68
1:A:214:GLU:OE1	1:A:214:GLU:HA	1.91	0.68
1:A:5:VAL:HB	1:A:118:THR:HB	1.76	0.68
1:B:93:SER:HB2	1:B:132:LYS:HE2	1.76	0.68
1:A:92:PHE:N	1:A:94:GLN:HE22	1.90	0.67
1:A:158:MET:HE3	1:A:165:ILE:HA	1.76	0.67
1:A:529:LYS:HB3	1:A:532:GLU:CG	2.23	0.67
1:A:157:GLY:O	1:A:158:MET:HG2	1.95	0.67
1:B:72:ARG:HD3	1:B:73:LYS:HZ1	1.59	0.67
1:B:72:ARG:CA	1:B:75:SER:HB3	2.25	0.67
1:A:206:THR:O	1:A:207:ALA:HB3	1.95	0.67
1:A:159:ILE:C	1:A:159:ILE:HD12	2.15	0.67
1:A:223:GLU:O	1:A:225:PRO:HD3	1.94	0.67
1:A:513:LEU:HD22	1:A:514:LYS:O	1.93	0.67
1:A:205:ASN:ND2	1:A:209:ALA:N	2.43	0.67
1:A:216:VAL:HG12	1:A:217:THR:HG23	1.76	0.67
1:A:5:VAL:HG22	1:A:180:VAL:HB	1.77	0.66
1:B:19:ILE:HD11	1:B:96:MET:CA	2.23	0.66
1:B:513:LEU:HD22	1:B:514:LYS:O	1.95	0.66
1:A:531:THR:HG23	1:A:532:GLU:OE2	1.95	0.66
1:B:181:VAL:HA	1:B:199:VAL:HB	1.76	0.66
1:A:124:ASN:HD21	1:A:160:LYS:HB2	1.60	0.66
1:A:259:LEU:O	1:A:259:LEU:HD12	1.96	0.66
1:B:532:GLU:O	1:B:536:ILE:HG13	1.96	0.65
1:A:137:ALA:O	1:A:141:CYS:N	2.27	0.65
1:A:15:ALA:O	1:A:16:LEU:HD23	1.97	0.65
1:B:499:ARG:HB3	1:B:501:GLU:HG3	1.79	0.65
1:A:108:ALA:O	1:A:111:ALA:HB3	1.96	0.65
1:B:497:VAL:HG13	2:B:1200:CPU:H121	1.79	0.65
1:A:272:TRP:HA	1:A:275:GLN:HE21	1.60	0.65
1:B:272:TRP:HA	1:B:275:GLN:HE21	1.61	0.65
1:B:324:ILE:HD12	1:B:324:ILE:N	2.10	0.65
1:A:264:GLY:HA3	1:A:333:ASP:HB3	1.78	0.65
1:B:25:ARG:O	1:B:29:ALA:HB2	1.97	0.64
1:A:532:GLU:O	1:A:536:ILE:HG13	1.97	0.64
1:A:416:ILE:HG23	1:A:427:ILE:HG13	1.77	0.64
1:B:264:GLY:HA3	1:B:333:ASP:HB3	1.78	0.64
1:A:177:PRO:O	1:A:198:MET:HG3	1.97	0.64
1:A:211:ARG:CA	1:A:214:GLU:HB2	2.26	0.64
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:SER:O	1:A:256:GLY:O	2.16	0.64
1:A:101:ILE:CG2	1:A:106:LEU:HD12	2.21	0.64
1:A:499:ARG:HB3	1:A:501:GLU:HG3	1.80	0.64
1:B:255:SER:O	1:B:256:GLY:O	2.16	0.64
1:B:420:LYS:C	1:B:424:ILE:HD11	2.18	0.64
1:A:169:LEU:O	1:A:173:LEU:HB2	1.97	0.64
1:A:193:ALA:CA	1:A:198:MET:HE3	2.22	0.64
1:B:119:THR:HG23	1:B:148:ASP:H	1.61	0.63
1:B:469:GLU:O	1:B:472:TRP:HB3	1.98	0.63
1:B:212:GLU:C	1:B:214:GLU:H	2.00	0.63
1:A:5:VAL:HG21	1:A:173:LEU:CD2	2.28	0.63
1:A:190:LEU:HD22	1:A:200:THR:HG22	1.79	0.63
1:B:458:PHE:C	1:B:461:PRO:HD2	2.19	0.63
1:B:72:ARG:HD3	1:B:73:LYS:NZ	2.13	0.63
1:A:9:ASP:OD1	1:A:11:ASP:HB2	1.98	0.63
1:B:248:LEU:HA	1:B:297:SER:HB3	1.79	0.63
1:A:458:PHE:C	1:A:461:PRO:HD2	2.19	0.63
1:A:106:LEU:HD22	1:A:110:ILE:HD11	1.80	0.63
1:B:292:LYS:CE	1:B:305:GLU:HG3	2.28	0.63
1:B:124:ASN:HA	1:B:153:SER:CB	2.29	0.63
1:A:205:ASN:ND2	1:A:209:ALA:CB	2.61	0.63
1:A:248:LEU:HA	1:A:297:SER:HB3	1.79	0.63
1:A:214:GLU:HB3	1:A:221:PHE:CZ	2.33	0.63
1:A:125:ASN:OD1	1:A:152:GLU:HB3	1.99	0.63
1:A:292:LYS:CE	1:A:305:GLU:HG3	2.29	0.62
1:B:535:GLN:HB3	1:B:539:LYS:HZ2	1.64	0.62
1:A:158:MET:O	1:A:165:ILE:HG12	1.99	0.62
1:B:32:LEU:HB3	1:B:33:PRO:HD2	1.82	0.62
1:A:433:GLU:HA	1:A:433:GLU:OE1	1.99	0.62
1:A:232:PRO:CD	1:A:233:ASN:N	2.60	0.62
1:A:497:VAL:HG13	2:A:1100:CPU:H122	1.81	0.62
1:B:232:PRO:HG2	1:B:233:ASN:ND2	2.14	0.62
1:B:26:SER:HA	1:B:29:ALA:HB3	1.81	0.62
1:B:75:SER:OG	1:B:76:LYS:N	2.31	0.62
1:B:181:VAL:HG23	1:B:201:ILE:HD13	1.80	0.62
1:B:180:VAL:HG22	1:B:198:MET:CG	2.30	0.62
1:A:62:GLN:HE22	1:B:481:ARG:HA	1.63	0.62
1:A:230:CYS:HB3	1:A:277:PRO:HG3	1.82	0.62
1:A:216:VAL:HG12	1:A:217:THR:N	2.14	0.62
1:A:276:ILE:HD11	1:A:288:ALA:CB	2.29	0.61
1:A:206:THR:O	1:A:207:ALA:CB	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:CD2	1:A:200:THR:HG22	2.30	0.61
1:A:157:GLY:C	1:A:158:MET:HG2	2.20	0.61
1:A:124:ASN:ND2	1:A:160:LYS:HB2	2.14	0.61
1:A:205:ASN:HD21	1:A:209:ALA:N	1.98	0.61
1:B:524:TRP:HB3	1:B:527:ILE:HD12	1.81	0.61
1:A:205:ASN:C	1:A:207:ALA:H	2.04	0.61
1:B:32:LEU:HD22	1:B:36:PHE:CD2	2.35	0.61
1:B:380:ASN:ND2	1:B:422:THR:OG1	2.32	0.61
1:A:183:LEU:HD13	1:A:201:ILE:HB	1.82	0.61
1:A:163:PRO:O	1:A:167:ASN:ND2	2.34	0.61
1:B:119:THR:HG23	1:B:147:PHE:HA	1.83	0.61
1:B:62:GLN:O	1:B:65:PRO:HD2	2.01	0.61
1:A:294:TYR:CZ	1:A:461:PRO:HB3	2.36	0.61
1:B:276:ILE:HD11	1:B:288:ALA:CB	2.30	0.61
1:A:339:VAL:CG1	1:A:353:VAL:HG12	2.30	0.60
1:A:469:GLU:O	1:A:472:TRP:HB3	2.01	0.60
1:A:153:SER:OG	1:A:154:CYS:N	2.31	0.60
1:A:205:ASN:HD21	1:A:209:ALA:H	1.48	0.60
1:B:339:VAL:CG1	1:B:353:VAL:HG12	2.31	0.60
1:A:524:TRP:HB3	1:A:527:ILE:HD12	1.84	0.60
1:B:194:ARG:HB2	1:B:200:THR:HG21	1.84	0.60
1:B:39:GLY:HA2	1:B:43:THR:CG2	2.31	0.60
1:B:107:GLN:HA	1:B:107:GLN:NE2	2.17	0.60
1:B:119:THR:HG21	1:B:146:HIS:O	2.01	0.60
1:B:122:VAL:CB	1:B:151:ILE:HG13	2.31	0.60
1:A:4:ARG:HA	1:A:179:GLU:O	2.01	0.60
1:B:122:VAL:HG11	1:B:182:PHE:HE1	1.67	0.60
1:A:201:ILE:HD13	1:A:213:LEU:HB3	1.84	0.60
1:A:287:LEU:O	1:A:289:ILE:HG13	2.02	0.60
1:A:293:GLY:HA2	1:A:299:SER:HA	1.84	0.60
1:B:4:ARG:HB3	1:B:4:ARG:CZ	2.32	0.60
1:A:177:PRO:O	1:A:198:MET:HA	2.02	0.59
1:B:73:LYS:HA	1:B:73:LYS:NZ	2.17	0.59
1:B:421:ALA:N	1:B:424:ILE:HD11	2.18	0.59
1:B:183:LEU:CD1	1:B:201:ILE:HB	2.33	0.59
1:B:72:ARG:HA	1:B:75:SER:CB	2.30	0.59
1:A:216:VAL:HG12	1:A:217:THR:H	1.67	0.59
1:B:467:ASN:OD1	1:B:470:ARG:HD2	2.02	0.59
1:B:20:ALA:O	1:B:23:PHE:HB2	2.03	0.59
1:B:45:PHE:CE1	1:B:47:GLU:HB2	2.36	0.59
1:A:90:GLN:HG3	1:A:91:ILE:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HG3	1:A:221:PHE:CE1	2.38	0.59
1:B:54:MET:HB2	1:B:159:ILE:CG2	2.33	0.58
1:A:232:PRO:HG2	1:A:233:ASN:OD1	2.03	0.58
1:A:213:LEU:O	1:A:216:VAL:HG12	2.03	0.58
1:B:201:ILE:HD12	1:B:201:ILE:H	1.69	0.58
1:A:359:PRO:HD2	1:A:361:MET:HE3	1.86	0.58
1:B:294:TYR:CZ	1:B:461:PRO:HB3	2.38	0.58
1:A:236:SER:HB2	1:B:322:LEU:HD12	1.85	0.58
1:B:8:PHE:CD1	1:B:147:PHE:HE2	2.21	0.58
1:B:293:GLY:HA2	1:B:299:SER:HA	1.83	0.58
1:A:347:PRO:O	1:B:133:ARG:HD2	2.04	0.58
1:A:309:GLU:HB2	1:A:474:TRP:CD2	2.38	0.58
1:B:228:VAL:O	1:B:277:PRO:HG2	2.03	0.57
1:B:420:LYS:HB3	1:B:424:ILE:CD1	2.33	0.57
1:B:158:MET:HE1	1:B:164:GLN:O	2.04	0.57
1:B:309:GLU:HB2	1:B:474:TRP:CD2	2.38	0.57
1:B:432:PRO:HB2	1:B:434:ASP:OD1	2.04	0.57
1:B:287:LEU:O	1:B:289:ILE:HG13	2.03	0.57
1:B:75:SER:HB2	1:B:82:LEU:HB3	1.86	0.57
1:A:535:GLN:HB3	1:A:539:LYS:HZ2	1.68	0.57
1:A:169:LEU:HD11	1:A:173:LEU:HD22	1.85	0.57
1:B:160:LYS:HA	1:B:165:ILE:CD1	2.34	0.57
1:B:272:TRP:HE3	1:B:275:GLN:HG3	1.69	0.57
1:B:417:ALA:HB3	1:B:427:ILE:HA	1.85	0.57
1:B:102:ASN:O	1:B:105:MET:HB2	2.04	0.57
1:B:434:ASP:N	1:B:435:PRO:CD	2.68	0.57
1:B:91:ILE:HG13	1:B:92:PHE:N	2.19	0.56
1:A:467:ASN:OD1	1:A:470:ARG:HD2	2.05	0.56
1:A:53:LEU:HD23	1:A:59:THR:O	2.05	0.56
1:B:46:PRO:HG2	1:B:159:ILE:HD11	1.87	0.56
1:B:44:GLU:O	1:B:46:PRO:HD3	2.05	0.56
1:B:222:PRO:CG	1:B:225:PRO:HG3	2.35	0.56
1:B:102:ASN:OD1	1:B:105:MET:HG3	2.05	0.56
1:B:51:GLU:O	1:B:55:LYS:HG3	2.04	0.56
1:A:106:LEU:HD21	1:A:146:HIS:CD2	2.40	0.56
1:B:458:PHE:HB3	1:B:462:LEU:HD12	1.87	0.56
1:B:270:PHE:CZ	1:B:273:ARG:HD3	2.40	0.56
1:A:272:TRP:HE3	1:A:275:GLN:HG3	1.70	0.56
1:A:510:ILE:O	1:A:513:LEU:HB2	2.05	0.56
1:B:426:GLY:HA3	1:B:429:VAL:HG23	1.88	0.56
1:A:230:CYS:O	1:A:231:ASN:CB	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LYS:HZ3	1:A:305:GLU:HG3	1.68	0.56
1:A:214:GLU:HB3	1:A:221:PHE:HZ	1.69	0.56
1:A:192:PRO:O	1:A:195:ASP:HB2	2.05	0.56
1:B:292:LYS:HE2	1:B:305:GLU:HG3	1.88	0.56
1:A:270:PHE:CZ	1:A:273:ARG:HD3	2.41	0.56
1:A:307:ALA:O	1:A:311:LEU:HG	2.05	0.56
1:B:8:PHE:O	1:B:121:ILE:HG23	2.05	0.56
1:B:421:ALA:HA	1:B:426:GLY:O	2.05	0.56
1:A:426:GLY:HA3	1:A:429:VAL:CG2	2.36	0.56
1:B:232:PRO:CD	1:B:233:ASN:HD22	2.19	0.55
1:A:446:ILE:HG22	1:A:450:ILE:CD1	2.36	0.55
1:B:535:GLN:CB	1:B:539:LYS:HZ2	2.19	0.55
1:B:292:LYS:HZ3	1:B:305:GLU:HG3	1.70	0.55
1:A:230:CYS:HB3	1:A:277:PRO:CG	2.36	0.55
1:B:26:SER:O	1:B:30:LEU:HB2	2.06	0.55
1:B:170:LEU:O	1:B:174:LYS:N	2.39	0.55
1:B:337:VAL:HG21	2:B:1200:CPU:H4	1.88	0.55
1:B:529:LYS:O	1:B:532:GLU:HG2	2.06	0.55
1:B:50:THR:O	1:B:54:MET:HG2	2.06	0.55
1:A:186:PHE:O	1:A:188:SER:N	2.39	0.55
1:A:426:GLY:HA3	1:A:429:VAL:HG23	1.89	0.55
1:B:359:PRO:HD2	1:B:361:MET:HE3	1.88	0.55
1:B:181:VAL:HG23	1:B:201:ILE:HD11	1.88	0.55
1:A:231:ASN:HB2	1:A:232:PRO:CA	2.36	0.55
1:B:446:ILE:HG22	1:B:450:ILE:CD1	2.37	0.55
1:A:351:ARG:O	1:A:351:ARG:HD2	2.07	0.55
1:B:37:LEU:C	1:B:39:GLY:H	2.09	0.54
1:B:222:PRO:HB2	1:B:225:PRO:HG3	1.89	0.54
1:B:351:ARG:HD2	1:B:351:ARG:O	2.06	0.54
1:A:292:LYS:HE2	1:A:305:GLU:HG3	1.89	0.54
1:B:510:ILE:O	1:B:513:LEU:HB2	2.06	0.54
1:B:203:VAL:O	1:B:203:VAL:HG12	2.06	0.54
1:B:372:VAL:CG2	1:B:373:ILE:HD12	2.37	0.54
1:B:186:PHE:HB2	1:B:189:ASN:HD22	1.71	0.54
1:A:264:GLY:HA3	1:A:333:ASP:CB	2.38	0.54
1:A:458:PHE:HB3	1:A:462:LEU:HD12	1.89	0.54
1:A:359:PRO:HD2	1:A:361:MET:CE	2.38	0.54
1:A:484:LEU:HD13	1:B:61:SER:OG	2.08	0.54
1:A:304:GLU:CD	1:A:304:GLU:H	2.12	0.54
1:A:398:ASN:C	1:A:398:ASN:OD1	2.45	0.54
1:B:136:LEU:O	1:B:140:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:MET:O	1:A:154:CYS:CA	2.56	0.53
1:B:264:GLY:HA3	1:B:333:ASP:CB	2.38	0.53
1:B:134:ASP:O	1:B:137:ALA:N	2.41	0.53
1:A:170:LEU:HD23	1:A:175:ALA:O	2.07	0.53
1:B:9:ASP:OD1	1:B:11:ASP:O	2.26	0.53
1:B:106:LEU:O	1:B:110:ILE:HG13	2.08	0.53
1:B:24:ARG:C	1:B:26:SER:H	2.11	0.53
1:B:30:LEU:HB3	1:B:32:LEU:CD1	2.39	0.53
1:A:211:ARG:C	1:A:214:GLU:HB2	2.28	0.53
1:A:497:VAL:CG1	2:A:1100:CPU:H122	2.38	0.53
1:B:359:PRO:HD2	1:B:361:MET:CE	2.38	0.53
1:A:5:VAL:HG21	1:A:173:LEU:HD21	1.89	0.53
1:B:497:VAL:CG1	2:B:1200:CPU:H122	2.38	0.53
1:B:497:VAL:HG13	2:B:1200:CPU:H122	1.90	0.53
1:B:125:ASN:HB2	1:B:152:GLU:HB3	1.89	0.53
1:A:529:LYS:O	1:A:532:GLU:HG2	2.08	0.53
1:A:140:MET:CE	1:A:140:MET:HA	2.34	0.53
1:A:535:GLN:CB	1:A:539:LYS:HZ2	2.21	0.53
1:B:212:GLU:C	1:B:214:GLU:N	2.61	0.53
1:B:304:GLU:CD	1:B:304:GLU:H	2.12	0.53
1:B:187:GLY:HA2	1:B:190:LEU:HD12	1.89	0.53
1:B:212:GLU:HA	1:B:215:LYS:HG3	1.89	0.53
1:A:48:GLY:O	1:A:52:GLN:HG2	2.09	0.53
1:A:334:TRP:CZ3	2:A:1100:CPU:H4	2.44	0.53
1:B:45:PHE:CZ	1:B:47:GLU:HB2	2.44	0.53
1:B:375:SER:OG	1:B:376:ILE:N	2.42	0.53
1:B:20:ALA:O	1:B:23:PHE:N	2.42	0.52
1:A:156:VAL:HG23	1:A:158:MET:HG3	1.91	0.52
1:A:122:VAL:HG22	1:A:122:VAL:O	2.08	0.52
1:B:441:THR:OG1	1:B:446:ILE:HD11	2.09	0.52
1:A:236:SER:HB2	1:B:322:LEU:CD1	2.39	0.52
1:B:511:PRO:C	1:B:513:LEU:H	2.12	0.52
1:B:11:ASP:HB2	1:B:99:ARG:NH1	2.24	0.52
1:B:86:PHE:CD1	1:B:87:SER:N	2.77	0.52
1:A:372:VAL:CG2	1:A:373:ILE:HD12	2.39	0.52
1:B:398:ASN:C	1:B:398:ASN:OD1	2.48	0.52
1:A:159:ILE:O	1:A:162:GLU:HB2	2.09	0.52
1:A:441:THR:OG1	1:A:446:ILE:HD11	2.10	0.52
1:A:300:PRO:HG2	1:A:305:GLU:CG	2.26	0.52
1:A:160:LYS:HA	1:A:165:ILE:CD1	2.39	0.52
1:B:75:SER:HB2	1:B:82:LEU:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:VAL:HG22	1:B:352:ALA:HB3	1.92	0.52
1:A:301:PRO:HG2	1:A:302:GLU:OE1	2.10	0.52
1:A:538:ILE:O	1:A:542:GLN:HG2	2.10	0.52
1:A:54:MET:O	1:A:154:CYS:HA	2.09	0.52
1:A:211:ARG:HA	1:A:214:GLU:CB	2.37	0.52
1:A:458:PHE:O	1:A:461:PRO:HD2	2.10	0.52
1:B:356:LEU:O	1:B:357:ASN:HB2	2.10	0.52
1:B:332:HIS:CD2	1:B:333:ASP:HB2	2.45	0.52
1:B:276:ILE:HB	1:B:277:PRO:HD3	1.90	0.52
1:A:246:ILE:HD12	1:A:246:ILE:N	2.25	0.52
1:A:375:SER:OG	1:A:376:ILE:N	2.39	0.51
1:B:301:PRO:HG2	1:B:302:GLU:OE1	2.10	0.51
1:A:91:ILE:HA	1:A:94:GLN:OE1	2.09	0.51
1:B:77:ALA:O	1:B:78:CYS:CB	2.58	0.51
1:A:381:TYR:CE1	1:A:382:GLN:HG3	2.45	0.51
1:B:479:LEU:O	1:B:509:TRP:HZ3	1.94	0.51
1:B:64:VAL:CG1	1:B:89:SER:HB2	2.41	0.51
1:A:112:LEU:HD23	1:A:117:PHE:CD2	2.45	0.51
1:A:62:GLN:NE2	1:B:481:ARG:HA	2.25	0.51
1:B:458:PHE:O	1:B:461:PRO:HD2	2.11	0.51
1:B:322:LEU:C	1:B:324:ILE:HD12	2.30	0.51
1:B:37:LEU:C	1:B:39:GLY:N	2.63	0.51
1:B:381:TYR:CE1	1:B:382:GLN:HG3	2.46	0.51
1:B:39:GLY:HA2	1:B:43:THR:HG23	1.91	0.51
1:A:289:ILE:HG22	1:A:290:ASP:N	2.25	0.51
1:A:91:ILE:H	1:A:91:ILE:HD13	1.75	0.51
1:B:33:PRO:O	1:B:34:ARG:C	2.48	0.51
1:A:407:PHE:C	1:A:408:ARG:HG2	2.30	0.51
1:B:434:ASP:H	1:B:435:PRO:CD	2.24	0.51
1:A:363:PRO:HB2	1:A:472:TRP:CD1	2.46	0.51
1:B:299:SER:HB2	1:B:456:THR:HG22	1.93	0.51
1:A:192:PRO:HA	1:A:195:ASP:HB2	1.92	0.51
1:A:158:MET:SD	1:A:164:GLN:HB2	2.51	0.51
1:B:11:ASP:HB2	1:B:99:ARG:HH12	1.75	0.51
1:B:50:THR:HA	1:B:53:LEU:HB2	1.92	0.51
1:B:34:ARG:O	1:B:35:ASP:HB2	2.11	0.51
1:A:5:VAL:HG21	1:A:173:LEU:HD23	1.91	0.50
1:B:122:VAL:HA	1:B:151:ILE:HG13	1.92	0.50
1:B:36:PHE:HE2	1:B:82:LEU:HD13	1.75	0.50
1:A:191:LYS:CB	1:A:192:PRO:HD3	2.41	0.50
1:B:307:ALA:O	1:B:311:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:HB	1:A:277:PRO:HD3	1.92	0.50
1:B:8:PHE:CE1	1:B:147:PHE:CE2	2.96	0.50
1:B:72:ARG:HG2	1:B:72:ARG:O	2.11	0.50
1:A:485:VAL:HB	1:B:133:ARG:NH1	2.26	0.50
1:A:332:HIS:CD2	1:A:333:ASP:HB2	2.45	0.50
1:B:363:PRO:HB2	1:B:472:TRP:CD1	2.46	0.50
1:A:159:ILE:CD1	1:A:159:ILE:C	2.79	0.50
1:A:60:PHE:C	1:A:62:GLN:N	2.64	0.50
1:A:128:ASP:O	1:A:133:ARG:HG3	2.10	0.50
1:B:155:GLN:CA	1:B:155:GLN:OE1	2.51	0.50
1:B:372:VAL:HG22	1:B:373:ILE:HD12	1.93	0.50
1:A:511:PRO:C	1:A:513:LEU:H	2.14	0.50
1:B:246:ILE:HD12	1:B:246:ILE:N	2.25	0.50
1:A:328:VAL:HG22	1:A:352:ALA:HB3	1.94	0.50
1:B:160:LYS:HA	1:B:165:ILE:HD11	1.94	0.50
1:A:90:GLN:CG	1:A:91:ILE:HD13	2.26	0.50
1:B:21:GLY:O	1:B:25:ARG:HD3	2.11	0.50
1:A:231:ASN:CB	1:A:232:PRO:HA	2.34	0.50
1:B:157:GLY:C	1:B:158:MET:HG2	2.33	0.50
1:A:299:SER:HB2	1:A:456:THR:HG22	1.94	0.50
1:A:62:GLN:O	1:A:63:TRP:CD1	2.55	0.50
1:A:61:SER:C	1:A:63:TRP:H	2.15	0.50
1:B:180:VAL:HG23	1:B:181:VAL:N	2.26	0.49
1:A:325:PRO:O	1:A:349:ARG:NH1	2.45	0.49
1:B:43:THR:O	1:B:44:GLU:CB	2.60	0.49
1:B:229:PRO:O	1:B:231:ASN:ND2	2.33	0.49
1:A:121:ILE:HG13	1:A:147:PHE:CD2	2.46	0.49
1:A:124:ASN:HA	1:A:153:SER:CB	2.37	0.49
1:B:63:TRP:O	1:B:67:MET:HB2	2.12	0.49
1:B:194:ARG:HB2	1:B:200:THR:CG2	2.42	0.49
1:B:402:THR:O	1:B:406:PHE:HD2	1.96	0.49
1:A:92:PHE:C	1:A:92:PHE:CD2	2.86	0.49
1:A:61:SER:HB2	1:B:484:LEU:HD13	1.95	0.49
1:B:20:ALA:O	1:B:21:GLY:C	2.51	0.49
1:A:106:LEU:CD2	1:A:110:ILE:HD11	2.41	0.49
1:A:55:LYS:HG3	1:A:159:ILE:HG23	1.93	0.49
1:B:106:LEU:HD22	1:B:110:ILE:HD11	1.94	0.49
1:B:192:PRO:O	1:B:196:MET:HB2	2.12	0.49
1:B:125:ASN:CB	1:B:152:GLU:HB3	2.43	0.49
1:B:229:PRO:C	1:B:231:ASN:HD22	2.13	0.49
1:B:278:ALA:HA	1:B:281:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:GLN:HB3	1:B:539:LYS:NZ	2.27	0.49
1:B:325:PRO:O	1:B:349:ARG:NH1	2.45	0.49
1:A:9:ASP:OD2	1:A:160:LYS:NZ	2.44	0.48
1:B:229:PRO:HA	1:B:273:ARG:O	2.13	0.48
1:A:501:GLU:O	1:A:504:LYS:HD3	2.13	0.48
1:A:53:LEU:HA	1:A:58:ILE:HD12	1.95	0.48
1:A:322:LEU:C	1:A:324:ILE:HD12	2.33	0.48
1:B:186:PHE:C	1:B:188:SER:H	2.15	0.48
1:B:407:PHE:C	1:B:408:ARG:HG2	2.32	0.48
1:B:428:LEU:CD1	1:B:428:LEU:N	2.76	0.48
1:B:186:PHE:HB3	1:B:188:SER:OG	2.12	0.48
1:B:8:PHE:H	1:B:8:PHE:HD1	1.61	0.48
1:A:356:LEU:O	1:A:357:ASN:HB2	2.13	0.48
1:A:15:ALA:HA	1:A:100:SER:O	2.14	0.48
1:B:339:VAL:O	1:B:342:MET:HB2	2.13	0.48
1:B:534:ASN:O	1:B:535:GLN:C	2.52	0.48
1:A:479:LEU:O	1:A:509:TRP:HZ3	1.97	0.48
1:B:182:PHE:HD2	1:B:190:LEU:HD23	1.78	0.48
1:A:205:ASN:HD21	1:A:209:ALA:CA	2.26	0.48
1:B:267:GLU:HB3	1:B:271:SER:OG	2.13	0.48
1:A:339:VAL:O	1:A:342:MET:HB2	2.13	0.48
1:A:231:ASN:CB	1:A:232:PRO:CA	2.91	0.48
1:B:434:ASP:O	1:B:435:PRO:C	2.51	0.48
1:A:17:PRO:O	1:A:18:SER:O	2.32	0.48
1:A:256:GLY:N	1:A:285:ARG:HB2	2.29	0.48
1:B:238:GLY:HA3	1:B:250:PHE:CE1	2.49	0.48
1:B:215:LYS:NZ	1:B:221:PHE:O	2.47	0.48
1:B:290:ASP:HB3	1:B:297:SER:OG	2.14	0.48
1:A:474:TRP:O	1:A:477:LYS:HG3	2.14	0.48
1:B:160:LYS:HB3	1:B:189:ASN:OD1	2.14	0.47
1:B:431:THR:CG2	1:B:432:PRO:HD2	2.41	0.47
1:A:193:ALA:O	1:A:198:MET:CB	2.51	0.47
1:A:290:ASP:HB3	1:A:297:SER:OG	2.14	0.47
1:B:210:LEU:O	1:B:214:GLU:HB2	2.13	0.47
1:A:278:ALA:HA	1:A:281:GLN:HE21	1.79	0.47
1:B:538:ILE:O	1:B:542:GLN:HG2	2.15	0.47
1:B:491:THR:OG1	1:B:517:HIS:HD2	1.98	0.47
1:A:9:ASP:O	1:A:13:VAL:HB	2.15	0.47
1:B:125:ASN:C	1:B:154:CYS:HB3	2.35	0.47
1:B:270:PHE:HB2	1:B:448:PHE:CE2	2.50	0.47
1:B:102:ASN:HB3	1:B:105:MET:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASN:H	1:B:233:ASN:HD22	1.61	0.47
1:B:124:ASN:HA	1:B:153:SER:OG	2.14	0.47
1:B:329:PHE:O	1:B:353:VAL:HA	2.15	0.47
1:A:372:VAL:HG22	1:A:373:ILE:HD12	1.95	0.47
1:B:474:TRP:O	1:B:477:LYS:HG3	2.14	0.47
1:B:232:PRO:CD	1:B:233:ASN:N	2.55	0.47
1:B:5:VAL:HB	1:B:118:THR:HB	1.95	0.47
1:B:501:GLU:O	1:B:504:LYS:HD3	2.14	0.47
1:B:64:VAL:HG11	1:B:89:SER:HB2	1.97	0.47
1:A:8:PHE:HD1	1:A:147:PHE:HE2	1.58	0.47
1:B:204:HIS:O	1:B:205:ASN:CB	2.62	0.47
1:A:7:ALA:HA	1:A:120:CYS:O	2.15	0.47
1:A:402:THR:O	1:A:406:PHE:HD2	1.97	0.47
1:B:229:PRO:HB2	1:B:231:ASN:ND2	2.25	0.47
1:B:428:LEU:HA	1:B:431:THR:OG1	2.15	0.47
1:A:270:PHE:HB2	1:A:448:PHE:CE2	2.50	0.47
1:B:483:ILE:HD12	1:B:510:ILE:HD11	1.97	0.47
1:A:301:PRO:HA	1:A:459:ARG:HD3	1.96	0.47
1:A:262:CYS:O	1:A:272:TRP:HZ2	1.98	0.47
1:B:256:GLY:N	1:B:285:ARG:HB2	2.30	0.47
1:B:201:ILE:N	1:B:201:ILE:CD1	2.74	0.47
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.67	0.47
1:B:524:TRP:O	1:B:528:GLU:HB2	2.15	0.47
1:B:45:PHE:O	1:B:45:PHE:CG	2.68	0.47
1:B:38:LEU:HD23	1:B:38:LEU:O	2.15	0.47
1:A:230:CYS:CB	1:A:277:PRO:HG3	2.44	0.46
1:B:24:ARG:O	1:B:26:SER:N	2.48	0.46
1:B:4:ARG:HB2	1:B:117:PHE:CE2	2.50	0.46
1:B:107:GLN:CA	1:B:107:GLN:NE2	2.78	0.46
1:B:7:ALA:HB2	1:B:120:CYS:SG	2.55	0.46
1:B:207:ALA:O	1:B:210:LEU:N	2.46	0.46
1:A:512:PHE:CD2	1:A:512:PHE:N	2.82	0.46
1:A:182:PHE:HD2	1:A:190:LEU:CD2	2.28	0.46
1:A:186:PHE:C	1:A:188:SER:H	2.18	0.46
1:A:91:ILE:CD1	1:A:91:ILE:H	2.28	0.46
1:B:52:GLN:HB3	1:B:58:ILE:HG12	1.98	0.46
1:B:289:ILE:HG22	1:B:290:ASP:N	2.28	0.46
1:B:301:PRO:HA	1:B:459:ARG:HD3	1.96	0.46
1:B:50:THR:HG22	1:B:63:TRP:HE1	1.79	0.46
1:B:5:VAL:HG13	1:B:180:VAL:CB	2.37	0.46
1:A:497:VAL:HG13	2:A:1100:CPU:C12	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:O	1:A:112:LEU:HD12	2.16	0.46
1:A:524:TRP:O	1:A:528:GLU:HB2	2.14	0.46
1:B:101:ILE:HG22	1:B:102:ASN:N	2.31	0.46
1:B:312:CYS:O	1:B:315:MET:HB2	2.15	0.46
1:B:428:LEU:HD13	1:B:428:LEU:N	2.31	0.46
1:B:170:LEU:HD23	1:B:175:ALA:O	2.16	0.46
1:A:378:VAL:HG13	1:A:378:VAL:O	2.15	0.46
1:B:22:ALA:HA	1:B:25:ARG:HD3	1.97	0.46
1:B:106:LEU:O	1:B:106:LEU:HD23	2.16	0.45
1:A:182:PHE:CE2	1:A:184:ASP:HB2	2.51	0.45
1:B:119:THR:HG23	1:B:148:ASP:N	2.29	0.45
1:B:49:PRO:O	1:B:52:GLN:HB2	2.17	0.45
1:A:535:GLN:HB3	1:A:539:LYS:NZ	2.31	0.45
1:A:312:CYS:O	1:A:315:MET:HB2	2.16	0.45
1:B:43:THR:O	1:B:44:GLU:HB2	2.16	0.45
1:B:50:THR:CG2	1:B:63:TRP:NE1	2.72	0.45
1:A:115:LYS:NZ	1:A:219:THR:HG23	2.30	0.45
1:A:267:GLU:HB3	1:A:271:SER:OG	2.16	0.45
1:B:39:GLY:HA2	1:B:43:THR:HG21	1.98	0.45
1:B:30:LEU:HB3	1:B:32:LEU:HD11	1.98	0.45
1:B:61:SER:O	1:B:65:PRO:HD2	2.16	0.45
1:B:84:GLU:HG3	1:B:84:GLU:H	1.42	0.45
1:A:58:ILE:HG22	1:A:62:GLN:OE1	2.17	0.45
1:B:125:ASN:N	1:B:153:SER:OG	2.50	0.45
1:B:25:ARG:O	1:B:29:ALA:CB	2.63	0.45
1:A:325:PRO:HB3	1:B:138:GLN:HA	1.99	0.45
1:B:125:ASN:O	1:B:154:CYS:HB3	2.16	0.45
1:A:19:ILE:HD12	1:A:126:TRP:HH2	1.82	0.45
1:B:364:ASP:HA	1:B:365:PRO:HD3	1.76	0.45
1:B:26:SER:CA	1:B:29:ALA:HB3	2.46	0.45
1:A:491:THR:OG1	1:A:517:HIS:HD2	2.00	0.45
1:B:17:PRO:O	1:B:18:SER:C	2.53	0.45
1:A:60:PHE:C	1:A:62:GLN:H	2.20	0.45
1:B:112:LEU:HD23	1:B:117:PHE:CE1	2.51	0.45
1:A:484:LEU:HD12	1:B:129:ASP:OD1	2.16	0.45
1:A:507:GLU:H	1:A:507:GLU:HG2	1.41	0.45
1:A:238:GLY:HA3	1:A:250:PHE:CE1	2.51	0.45
1:A:430:ASN:HD22	1:A:430:ASN:N	1.87	0.45
1:A:52:GLN:HA	1:A:55:LYS:HB2	1.99	0.44
1:A:215:LYS:HA	1:A:219:THR:O	2.17	0.44
1:A:381:TYR:HB2	1:A:427:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:HB2	1:A:14:LEU:HD11	1.99	0.44
1:A:275:GLN:NE2	1:A:526:GLN:HB3	2.32	0.44
1:B:275:GLN:NE2	1:B:526:GLN:HB3	2.32	0.44
1:B:334:TRP:O	1:B:337:VAL:HB	2.17	0.44
1:A:183:LEU:CD1	1:A:201:ILE:HB	2.46	0.44
1:A:139:MET:HG2	1:A:143:LEU:HD12	1.98	0.44
1:A:155:GLN:CA	1:A:155:GLN:OE1	2.51	0.44
1:A:322:LEU:HD12	1:B:236:SER:HB2	1.99	0.44
1:A:380:ASN:CB	1:A:419:HIS:O	2.65	0.44
1:A:127:LEU:N	1:A:127:LEU:HD12	2.32	0.44
1:B:216:VAL:HG12	1:B:217:THR:OG1	2.17	0.44
1:B:71:TYR:HE1	1:B:88:ILE:HD13	1.83	0.44
1:A:165:ILE:H	1:A:165:ILE:HG13	1.33	0.44
1:B:54:MET:HB2	1:B:159:ILE:HG21	1.99	0.44
1:A:133:ARG:CG	1:B:348:GLU:HA	2.42	0.44
1:B:162:GLU:O	1:B:165:ILE:CD1	2.66	0.44
1:B:30:LEU:HD11	1:B:83:PRO:CG	2.48	0.44
1:B:262:CYS:O	1:B:272:TRP:HZ2	2.00	0.44
1:B:206:THR:O	1:B:207:ALA:CB	2.66	0.44
1:A:125:ASN:O	1:A:126:TRP:HB3	2.16	0.44
1:B:230:CYS:HB3	1:B:277:PRO:HG3	2.00	0.44
1:B:144:SER:OG	1:B:145:GLN:NE2	2.44	0.44
1:B:121:ILE:HB	1:B:150:LEU:HD12	2.00	0.44
1:B:154:CYS:SG	1:B:154:CYS:O	2.76	0.44
1:B:190:LEU:HD11	1:B:202:LEU:HA	2.00	0.44
1:B:76:LYS:HE2	1:B:76:LYS:O	2.17	0.44
1:A:381:TYR:CB	1:A:427:ILE:HD12	2.48	0.44
1:B:512:PHE:N	1:B:512:PHE:CD2	2.84	0.44
1:A:346:TYR:O	1:A:350:VAL:HG23	2.17	0.44
1:A:210:LEU:C	1:A:212:GLU:H	2.22	0.44
1:B:210:LEU:O	1:B:214:GLU:CB	2.66	0.44
1:B:68:ASP:O	1:B:71:TYR:HB2	2.18	0.44
1:A:420:LYS:O	1:A:424:ILE:HG12	2.17	0.44
1:B:5:VAL:CG1	1:B:180:VAL:HB	2.41	0.44
1:A:534:ASN:O	1:A:535:GLN:C	2.54	0.44
1:B:107:GLN:CA	1:B:107:GLN:HE21	2.30	0.44
1:A:122:VAL:HG13	1:A:182:PHE:HE1	1.82	0.44
1:A:394:GLU:OE1	1:A:427:ILE:HG22	2.17	0.44
1:B:300:PRO:HG2	1:B:305:GLU:CG	2.26	0.43
1:A:5:VAL:HG23	1:A:6:ALA:N	2.32	0.43
1:B:19:ILE:HD13	1:B:19:ILE:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:SER:C	1:A:210:LEU:N	2.66	0.43
1:A:16:LEU:HB3	1:A:17:PRO:HA	1.99	0.43
1:A:334:TRP:O	1:A:337:VAL:HB	2.18	0.43
1:B:183:LEU:HD13	1:B:201:ILE:HB	2.00	0.43
1:A:158:MET:HB3	1:A:164:GLN:HG3	2.00	0.43
1:A:102:ASN:HD22	1:A:102:ASN:C	2.22	0.43
1:B:466:ARG:H	1:B:466:ARG:HG2	1.49	0.43
1:A:60:PHE:O	1:A:62:GLN:N	2.50	0.43
1:A:209:ALA:HA	1:A:212:GLU:HB2	2.01	0.43
1:B:215:LYS:O	1:B:219:THR:O	2.37	0.43
1:B:50:THR:HG22	1:B:63:TRP:NE1	2.33	0.43
1:A:329:PHE:O	1:A:353:VAL:HA	2.18	0.43
1:A:365:PRO:HG3	1:A:479:LEU:HD13	2.00	0.43
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.86	0.43
1:A:276:ILE:HD11	1:A:288:ALA:HB2	1.99	0.43
1:B:119:THR:CG2	1:B:147:PHE:HA	2.46	0.43
1:A:426:GLY:CA	1:A:429:VAL:HG23	2.49	0.43
1:B:41:TYR:HB3	1:B:42:GLN:H	1.63	0.43
1:B:5:VAL:CG2	1:B:6:ALA:N	2.81	0.43
1:A:230:CYS:HB3	1:A:277:PRO:HD3	2.01	0.43
1:B:263:HIS:HD2	1:B:291:MET:HG2	1.74	0.43
1:A:8:PHE:HB2	1:A:14:LEU:CD1	2.49	0.43
1:A:222:PRO:HG2	1:A:225:PRO:HB3	1.99	0.43
1:B:276:ILE:CB	1:B:277:PRO:HD3	2.49	0.43
1:B:105:MET:O	1:B:108:ALA:HB3	2.19	0.43
1:B:373:ILE:HG22	1:B:383:LEU:HD11	2.00	0.43
1:B:278:ALA:HA	1:B:281:GLN:NE2	2.34	0.43
1:A:207:ALA:HA	1:A:210:LEU:HB3	2.00	0.43
1:B:511:PRO:C	1:B:513:LEU:N	2.72	0.43
1:B:222:PRO:CB	1:B:225:PRO:HG3	2.47	0.43
1:B:358:THR:HG22	1:B:359:PRO:O	2.19	0.43
1:A:481:ARG:HG2	1:B:57:LYS:O	2.19	0.43
1:B:265:PHE:HA	1:B:266:PRO:HA	1.87	0.43
1:A:373:ILE:HG22	1:A:383:LEU:HD11	2.00	0.42
1:B:222:PRO:HA	1:B:223:GLU:OE2	2.19	0.42
1:B:6:ALA:HA	1:B:181:VAL:HG13	2.01	0.42
1:A:220:GLN:HB2	1:A:220:GLN:HE21	1.58	0.42
1:A:107:GLN:O	1:A:108:ALA:C	2.57	0.42
1:A:127:LEU:HD12	1:A:127:LEU:H	1.84	0.42
1:A:50:THR:HA	1:A:63:TRP:HZ2	1.83	0.42
1:A:60:PHE:O	1:A:63:TRP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PRO:HG3	1:B:80:ALA:HB2	2.01	0.42
1:A:483:ILE:HD12	1:A:510:ILE:HD11	2.01	0.42
1:A:111:ALA:O	1:A:114:LYS:N	2.53	0.42
1:A:303:ILE:C	1:A:305:GLU:N	2.72	0.42
1:A:90:GLN:CG	1:A:91:ILE:N	2.82	0.42
1:A:205:ASN:O	1:A:207:ALA:N	2.52	0.42
1:B:30:LEU:HD11	1:B:83:PRO:HG3	2.01	0.42
1:B:119:THR:HG22	1:B:148:ASP:OD1	2.20	0.42
1:B:122:VAL:HG22	1:B:160:LYS:HE2	2.01	0.42
1:B:187:GLY:HA2	1:B:190:LEU:HB2	2.01	0.42
1:B:8:PHE:HD1	1:B:120:CYS:O	2.03	0.42
1:A:226:LEU:CD2	1:A:226:LEU:N	2.82	0.42
1:A:490:VAL:HA	1:A:516:GLY:O	2.20	0.42
1:B:13:VAL:CG2	1:B:14:LEU:N	2.83	0.42
1:B:36:PHE:CE2	1:B:82:LEU:HD13	2.54	0.42
1:B:64:VAL:CB	1:B:65:PRO:CD	2.88	0.42
1:A:181:VAL:HG22	1:A:181:VAL:O	2.19	0.42
1:A:232:PRO:HD2	1:A:233:ASN:N	2.11	0.42
1:B:63:TRP:CE2	1:B:67:MET:HG3	2.55	0.42
1:A:243:LYS:O	1:A:244:PRO:C	2.58	0.42
1:B:112:LEU:HA	1:B:115:LYS:HB3	2.02	0.42
1:B:367:VAL:O	1:B:368:SER:C	2.58	0.42
1:B:180:VAL:HG22	1:B:198:MET:HG2	2.01	0.42
1:B:187:GLY:O	1:B:190:LEU:HB2	2.19	0.42
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.84	0.42
1:B:511:PRO:O	1:B:513:LEU:N	2.52	0.42
1:B:214:GLU:HG3	1:B:221:PHE:CE1	2.54	0.42
1:B:303:ILE:C	1:B:305:GLU:N	2.73	0.42
1:A:276:ILE:CB	1:A:277:PRO:HD3	2.50	0.42
1:B:369:PRO:O	1:B:373:ILE:CD1	2.68	0.42
1:A:8:PHE:O	1:A:121:ILE:HA	2.20	0.42
1:B:350:VAL:HG13	1:B:352:ALA:O	2.20	0.42
1:A:92:PHE:O	1:A:95:ALA:HB3	2.20	0.41
1:A:277:PRO:O	1:A:280:ALA:N	2.53	0.41
1:A:61:SER:C	1:A:63:TRP:N	2.73	0.41
1:A:422:THR:O	1:A:423:GLU:CB	2.56	0.41
1:B:490:VAL:HA	1:B:516:GLY:O	2.20	0.41
1:A:180:VAL:HG22	1:A:198:MET:HG2	2.02	0.41
1:B:122:VAL:HG22	1:B:122:VAL:O	2.20	0.41
1:B:21:GLY:C	1:B:25:ARG:HD3	2.40	0.41
1:A:380:ASN:OD1	1:A:422:THR:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ALA:HB1	1:B:325:PRO:O	2.20	0.41
1:B:207:ALA:O	1:B:209:ALA:N	2.53	0.41
1:B:243:LYS:O	1:B:244:PRO:C	2.58	0.41
1:B:303:ILE:HG21	1:B:466:ARG:HB2	2.03	0.41
1:B:481:ARG:HH11	1:B:481:ARG:HD2	1.70	0.41
1:B:122:VAL:CA	1:B:151:ILE:HG13	2.50	0.41
1:A:511:PRO:C	1:A:513:LEU:N	2.74	0.41
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.80	0.41
1:B:380:ASN:HB3	1:B:418:VAL:O	2.20	0.41
1:B:230:CYS:SG	1:B:230:CYS:O	2.77	0.41
1:B:346:TYR:O	1:B:350:VAL:HG23	2.19	0.41
1:A:380:ASN:HB3	1:A:418:VAL:O	2.20	0.41
1:A:358:THR:HG22	1:A:359:PRO:O	2.19	0.41
1:B:167:ASN:O	1:B:171:ASP:OD2	2.39	0.41
1:B:263:HIS:HE1	1:B:294:TYR:CD2	2.38	0.41
1:A:205:ASN:C	1:A:207:ALA:N	2.70	0.41
1:B:198:MET:HE2	1:B:198:MET:HB2	2.00	0.41
1:A:303:ILE:HG21	1:A:466:ARG:HB2	2.03	0.41
1:B:54:MET:HA	1:B:125:ASN:O	2.21	0.41
1:B:378:VAL:O	1:B:378:VAL:HG13	2.20	0.41
1:A:228:VAL:HA	1:A:229:PRO:HD3	1.79	0.41
1:A:280:ALA:HA	1:A:284:PHE:O	2.20	0.41
1:B:56:GLY:HA2	1:B:127:LEU:HD11	2.03	0.41
1:B:206:THR:O	1:B:207:ALA:HB3	2.20	0.41
1:B:199:VAL:HG12	1:B:201:ILE:HD11	2.03	0.41
1:B:281:GLN:HE21	1:B:281:GLN:HB2	1.62	0.41
1:A:110:ILE:HD13	1:A:228:VAL:HG12	2.03	0.41
1:B:420:LYS:O	1:B:421:ALA:C	2.59	0.41
1:B:396:GLU:OE1	1:B:458:PHE:N	2.54	0.41
1:A:484:LEU:CD1	1:B:61:SER:OG	2.69	0.41
1:B:71:TYR:CE1	1:B:88:ILE:HD13	2.55	0.41
1:B:20:ALA:HA	1:B:23:PHE:HB2	2.03	0.41
1:A:170:LEU:HD21	1:A:177:PRO:HA	2.03	0.40
1:B:11:ASP:OD2	1:B:19:ILE:HG12	2.22	0.40
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.77	0.40
1:B:73:LYS:O	1:B:77:ALA:HB3	2.20	0.40
1:A:289:ILE:CG2	1:A:290:ASP:N	2.84	0.40
1:B:380:ASN:CB	1:B:419:HIS:O	2.69	0.40
1:A:191:LYS:CB	1:A:192:PRO:CD	2.99	0.40
1:A:191:LYS:HB2	1:A:192:PRO:HD3	2.03	0.40
1:A:58:ILE:HG22	1:A:62:GLN:CB	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.94	0.40
1:B:54:MET:HB2	1:B:159:ILE:HG22	2.03	0.40
1:B:408:ARG:HA	1:B:438:SER:OG	2.21	0.40
1:B:280:ALA:HA	1:B:284:PHE:O	2.20	0.40
1:A:278:ALA:O	1:A:282:ALA:N	2.53	0.40
1:B:303:ILE:CG2	1:B:466:ARG:HB2	2.52	0.40
1:A:4:ARG:HH11	1:A:4:ARG:HB2	1.86	0.40
1:A:496:ILE:N	1:A:496:ILE:CD1	2.70	0.40
1:B:538:ILE:O	1:B:539:LYS:C	2.59	0.40
1:A:334:TRP:CE3	2:A:1100:CPU:H4	2.55	0.40
1:B:277:PRO:O	1:B:280:ALA:N	2.54	0.40
1:A:278:ALA:HA	1:A:281:GLN:NE2	2.36	0.40
1:A:493:GLU:HG2	1:A:494:LYS:HG2	2.03	0.40
1:A:303:ILE:CG2	1:A:466:ARG:HB2	2.52	0.40
1:A:511:PRO:O	1:A:513:LEU:N	2.55	0.40
1:A:401:ARG:O	1:A:402:THR:C	2.60	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	481/554 (87%)	392 (82%)	59 (12%)	30 (6%)	2	5
1	B	539/554 (97%)	431 (80%)	77 (14%)	31 (6%)	2	5
All	All	1020/1108 (92%)	823 (81%)	136 (13%)	61 (6%)	2	5

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	207	ALA

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Mol	Chain	Res	Type
1	A	231	ASN
1	A	244	PRO
1	A	256	GLY
1	A	415	PHE
1	A	423	GLU
1	B	41	TYR
1	B	75	SER
1	B	78	CYS
1	B	207	ALA
1	B	208	SER
1	B	222	PRO
1	B	232	PRO
1	B	244	PRO
1	B	256	GLY
1	B	415	PHE
1	B	421	ALA
1	A	18	SER
1	A	98	ALA
1	A	158	MET
1	A	466	ARG
1	A	520	ASP
1	B	25	ARG
1	B	44	GLU
1	B	80	ALA
1	B	205	ASN
1	B	386	GLN
1	B	466	ARG
1	B	520	ASP
1	A	154	CYS
1	A	288	ALA
1	A	402	THR
1	B	63	TRP
1	A	126	TRP
1	A	210	LEU
1	A	232	PRO
1	A	386	GLN
1	A	496	ILE
1	B	288	ALA
1	B	402	THR
1	B	434	ASP
1	A	125	ASN
1	A	206	THR

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Mol	Chain	Res	Type
1	A	230	CYS
1	A	277	PRO
1	B	34	ARG
1	B	203	VAL
1	B	219	THR
1	B	277	PRO
1	B	432	PRO
1	B	496	ILE
1	A	187	GLY
1	A	295	GLY
1	B	295	GLY
1	A	229	PRO
1	A	12	GLY
1	B	216	VAL
1	A	91	ILE
1	A	266	PRO
1	B	266	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/480 (88%)	322 (76%)	102 (24%)	1	2
1	B	468/480 (98%)	342 (73%)	126 (27%)	0	1
All	All	892/960 (93%)	664 (74%)	228 (26%)	0	2

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	VAL
1	A	18	SER
1	A	19	ILE
1	A	53	LEU
1	A	55	LYS

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Mol	Chain	Res	Type
1	A	58	ILE
1	A	61	SER
1	A	90	GLN
1	A	91	ILE
1	A	92	PHE
1	A	93	SER
1	A	94	GLN
1	A	99	ARG
1	A	102	ASN
1	A	103	ARG
1	A	119	THR
1	A	122	VAL
1	A	125	ASN
1	A	128	ASP
1	A	129	ASP
1	A	131	ASP
1	A	136	LEU
1	A	152	GLU
1	A	154	CYS
1	A	155	GLN
1	A	158	MET
1	A	164	GLN
1	A	165	ILE
1	A	169	LEU
1	A	170	LEU
1	A	174	LYS
1	A	181	VAL
1	A	184	ASP
1	A	200	THR
1	A	202	LEU
1	A	204	HIS
1	A	208	SER
1	A	213	LEU
1	A	214	GLU
1	A	216	VAL
1	A	220	GLN
1	A	221	PHE
1	A	223	GLU
1	A	226	LEU
1	A	230	CYS
1	A	231	ASN
1	A	247	ARG

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Mol	Chain	Res	Type
1	A	248	LEU
1	A	268	SER
1	A	275	GLN
1	A	290	ASP
1	A	297	SER
1	A	299	SER
1	A	310	LEU
1	A	313	LYS
1	A	315	MET
1	A	322	LEU
1	A	349	ARG
1	A	351	ARG
1	A	353	VAL
1	A	361	MET
1	A	366	ASP
1	A	368	SER
1	A	370	MET
1	A	371	LYS
1	A	378	VAL
1	A	383	LEU
1	A	398	ASN
1	A	404	LYS
1	A	408	ARG
1	A	412	GLU
1	A	413	THR
1	A	420	LYS
1	A	422	THR
1	A	423	GLU
1	A	430	ASN
1	A	439	LYS
1	A	440	ILE
1	A	447	GLU
1	A	451	GLN
1	A	466	ARG
1	A	468	THR
1	A	470	ARG
1	A	475	SER
1	A	485	VAL
1	A	488	LEU
1	A	494	LYS
1	A	497	VAL
1	A	501	GLU

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Mol	Chain	Res	Type
1	A	502	MET
1	A	504	LYS
1	A	505	ASN
1	A	507	GLU
1	A	512	PHE
1	A	513	LEU
1	A	519	GLU
1	A	526	GLN
1	A	531	THR
1	A	539	LYS
1	A	542	GLN
1	A	544	GLU
1	B	4	ARG
1	B	5	VAL
1	B	8	PHE
1	B	10	LEU
1	B	13	VAL
1	B	16	LEU
1	B	23	PHE
1	B	24	ARG
1	B	25	ARG
1	B	30	LEU
1	B	35	ASP
1	B	41	TYR
1	B	42	GLN
1	B	43	THR
1	B	47	GLU
1	B	53	LEU
1	B	61	SER
1	B	67	MET
1	B	69	GLU
1	B	70	SER
1	B	71	TYR
1	B	72	ARG
1	B	73	LYS
1	B	74	SER
1	B	76	LYS
1	B	78	CYS
1	B	81	ASN
1	B	84	GLU
1	B	85	ASN
1	B	91	ILE

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Mol	Chain	Res	Type
1	B	94	GLN
1	B	99	ARG
1	B	100	SER
1	B	101	ILE
1	B	102	ASN
1	B	103	ARG
1	B	106	LEU
1	B	107	GLN
1	B	110	ILE
1	B	118	THR
1	B	122	VAL
1	B	125	ASN
1	B	127	LEU
1	B	131	ASP
1	B	132	LYS
1	B	133	ARG
1	B	135	SER
1	B	136	LEU
1	B	151	ILE
1	B	154	CYS
1	B	155	GLN
1	B	158	MET
1	B	159	ILE
1	B	164	GLN
1	B	165	ILE
1	B	180	VAL
1	B	181	VAL
1	B	183	LEU
1	B	198	MET
1	B	200	THR
1	B	201	ILE
1	B	202	LEU
1	B	206	THR
1	B	208	SER
1	B	210	LEU
1	B	213	LEU
1	B	217	THR
1	B	219	THR
1	B	228	VAL
1	B	233	ASN
1	B	247	ARG
1	B	248	LEU

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Mol	Chain	Res	Type
1	B	268	SER
1	B	275	GLN
1	B	290	ASP
1	B	297	SER
1	B	299	SER
1	B	310	LEU
1	B	313	LYS
1	B	315	MET
1	B	322	LEU
1	B	349	ARG
1	B	351	ARG
1	B	353	VAL
1	B	361	MET
1	B	366	ASP
1	B	368	SER
1	B	370	MET
1	B	371	LYS
1	B	378	VAL
1	B	383	LEU
1	B	398	ASN
1	B	404	LYS
1	B	408	ARG
1	B	412	GLU
1	B	413	THR
1	B	422	THR
1	B	424	ILE
1	B	427	ILE
1	B	428	LEU
1	B	431	THR
1	B	439	LYS
1	B	440	ILE
1	B	447	GLU
1	B	451	GLN
1	B	466	ARG
1	B	468	THR
1	B	470	ARG
1	B	475	SER
1	B	485	VAL
1	B	488	LEU
1	B	494	LYS
1	B	497	VAL
1	B	501	GLU

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Mol	Chain	Res	Type
1	B	502	MET
1	B	504	LYS
1	B	505	ASN
1	B	507	GLU
1	B	512	PHE
1	B	513	LEU
1	B	519	GLU
1	B	526	GLN
1	B	531	THR
1	B	539	LYS
1	B	542	GLN
1	B	544	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	102	ASN
1	A	107	GLN
1	A	125	ASN
1	A	146	HIS
1	A	164	GLN
1	A	205	ASN
1	A	220	GLN
1	A	275	GLN
1	A	281	GLN
1	A	332	HIS
1	A	386	GLN
1	A	430	ASN
1	A	517	HIS
1	B	81	ASN
1	B	90	GLN
1	B	107	GLN
1	B	146	HIS
1	B	167	ASN
1	B	178	ASN
1	B	204	HIS
1	B	231	ASN
1	B	233	ASN
1	B	275	GLN
1	B	281	GLN
1	B	332	HIS

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Mol	Chain	Res	Type
1	B	517	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 ⓘ

2 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	$\# Z  > 2$
2	CPU	A	1100	-	20,20,20	1.72	8 (40%)	24,24,24	1.53	3 (12%)
2	CPU	B	1200	-	20,20,20	1.88	8 (40%)	24,24,24	1.67	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPU	A	1100	-	-	0/11/19/19	0/2/2/2
2	CPU	B	1200	-	-	0/11/19/19	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1100	CPU	C11-N2	2.01	1.50	1.46
2	A	1100	CPU	C14-C13	2.01	1.59	1.51
2	B	1200	CPU	C5-C6	2.04	1.43	1.38
2	B	1200	CPU	C4-C5	2.11	1.43	1.38
2	B	1200	CPU	C15-C14	2.13	1.60	1.51
2	B	1200	CPU	C16-C11	2.17	1.57	1.51
2	A	1100	CPU	C13-C12	2.19	1.59	1.53
2	B	1200	CPU	C13-C12	2.22	1.59	1.53
2	A	1100	CPU	C15-C16	2.22	1.59	1.53
2	A	1100	CPU	C12-C11	2.24	1.57	1.51
2	A	1100	CPU	C16-C11	2.31	1.57	1.51
2	B	1200	CPU	C12-C11	2.35	1.57	1.51
2	B	1200	CPU	C4-C3	2.64	1.44	1.38
2	A	1100	CPU	C4-C5	2.67	1.44	1.38
2	A	1100	CPU	C1-C6	3.20	1.45	1.38
2	B	1200	CPU	C1-C6	3.68	1.46	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1100	CPU	C9-C8-C7	-4.09	100.41	113.22
2	B	1200	CPU	O1-C10-N1	-3.88	115.55	122.75
2	A	1100	CPU	O1-C10-N1	-3.60	116.06	122.75
2	B	1200	CPU	C9-C8-C7	-3.58	102.02	113.22
2	B	1200	CPU	C8-C7-C6	2.14	121.85	113.71
2	B	1200	CPU	C11-N2-C10	2.40	129.44	123.28
2	A	1100	CPU	C8-C7-C6	2.74	124.15	113.71
2	B	1200	CPU	C13-C12-C11	2.87	115.56	111.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	CPU	5	0
2	B	1200	CPU	5	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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