



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:50 PM GMT

PDB ID : 1CQZ  
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE.  
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Deposited on : 1999-08-12  
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

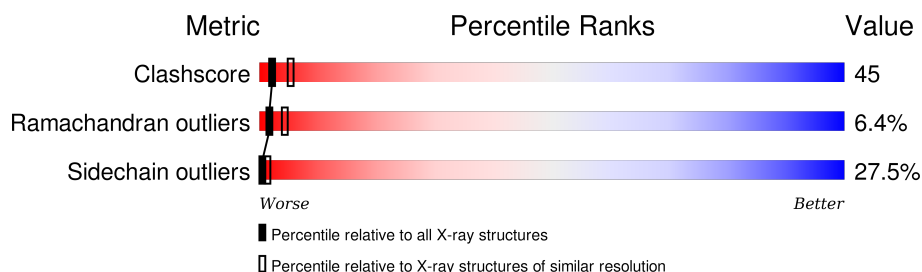
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

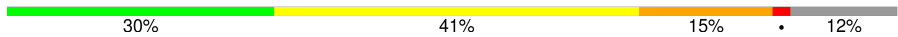
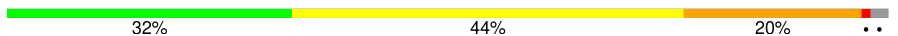
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

There are 2 unique types of molecules in this entry. The entry contains 8218 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 water.

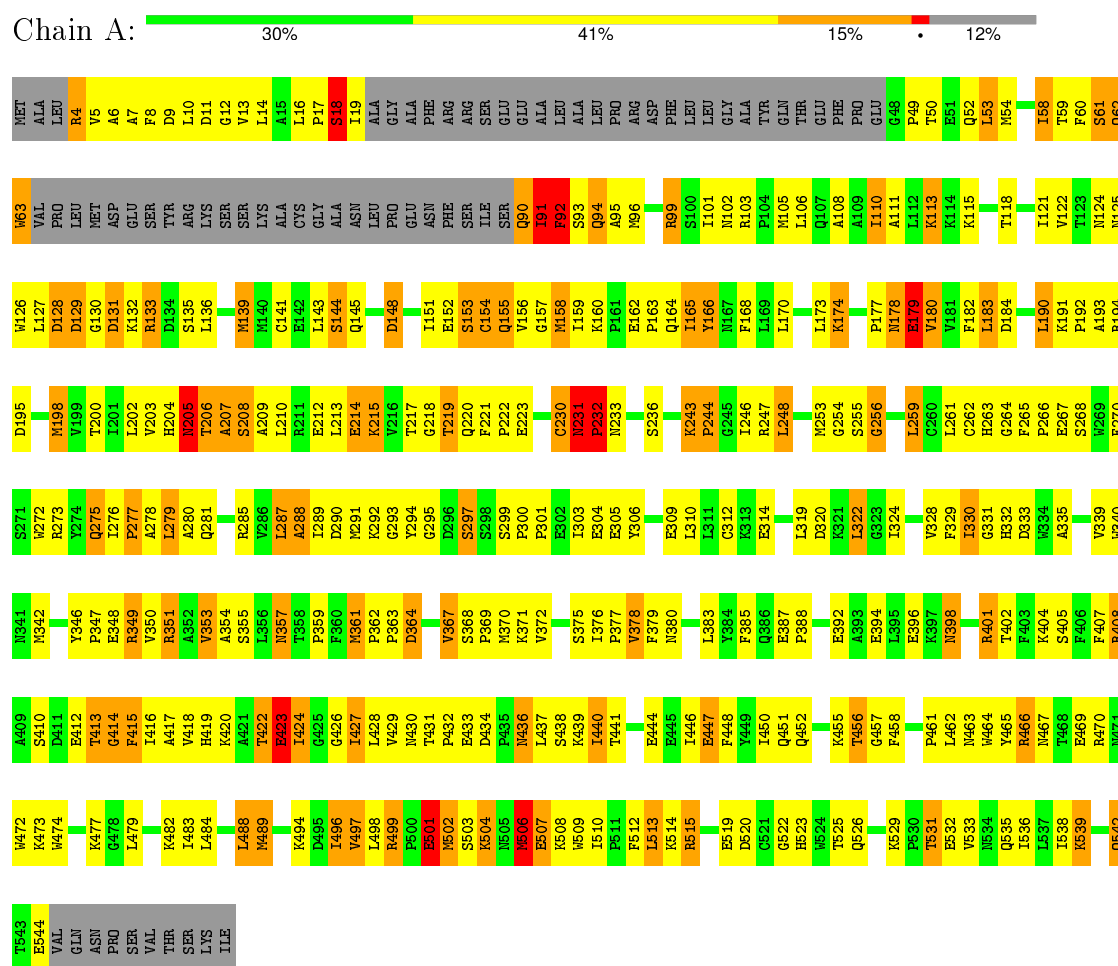
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	22	Total	O	0	0
			22	22		

### 3 Residue-property plots

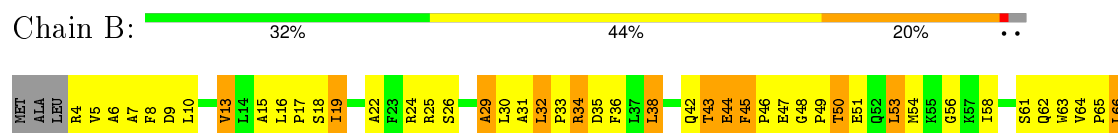
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



#### • Molecule 1: EPOXIDE HYDROLASE





## 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)	94.6 (20.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.214 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.66	0/3981	0.87	6/5397 (0.1%)
1	B	0.68	0/4413	0.86	8/5984 (0.1%)
All	All	0.67	0/8394	0.87	14/11381 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ASN	C-N-CD	-15.19	87.18	120.60
1	A	231	ASN	C-N-CA	8.88	159.29	122.00
1	B	231	ASN	C-N-CD	-8.27	102.40	120.60
1	B	231	ASN	N-CA-C	5.43	125.67	111.00
1	B	231	ASN	C-N-CA	5.36	144.53	122.00
1	A	436	ASN	N-CA-C	-5.32	96.65	111.00
1	B	436	ASN	N-CA-C	-5.26	96.79	111.00
1	B	457	GLY	N-CA-C	-5.24	99.99	113.10
1	B	66	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	232	PRO	CA-N-CD	-5.20	104.22	111.50
1	A	488	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	457	GLY	N-CA-C	-5.09	100.37	113.10
1	B	488	LEU	CA-CB-CG	5.05	126.92	115.30
1	B	183	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3879	0	3863	335	0
1	B	4299	0	4270	398	0
2	A	18	0	0	4	0
2	B	22	0	0	1	0
All	All	8218	0	8133	715	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 45.

All (715) 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:122:VAL:HG12	1:B:151:ILE:HG13	1.26	1.17
1:A:348:GLU:HA	1:B:133:ARG:HG3	1.33	1.11
1:A:5:VAL:HG22	1:A:118:THR:HB	1.33	1.08
1:B:232:PRO:HD2	1:B:233:ASN:H	1.16	1.03
1:A:58:ILE:HG22	1:A:62:GLN:HG3	1.44	1.00
1:B:204:HIS:O	1:B:205:ASN:HB2	1.58	0.99
1:B:19:ILE:HD11	1:B:96:MET:HA	1.41	0.99
1:B:127:LEU:HD12	1:B:127:LEU:H	1.29	0.98
1:B:122:VAL:CG1	1:B:151:ILE:HG13	1.93	0.97
1:B:125:ASN:HD22	1:B:152:GLU:HB3	1.28	0.97
1:B:5:VAL:HG21	1:B:173:LEU:HD21	1.45	0.97
1:A:205:ASN:ND2	1:A:207:ALA:H	1.63	0.96
1:A:193:ALA:O	1:A:198:MET:HG3	1.65	0.96
1:A:484:LEU:HD13	1:B:61:SER:HB2	1.44	0.94
1:B:322:LEU:HB3	1:B:324:ILE:HD12	1.50	0.93
1:A:205:ASN:HD22	1:A:207:ALA:H	0.97	0.92
1:A:422:THR:O	1:A:423:GLU:HB2	1.66	0.92
1:B:5:VAL:HG21	1:B:173:LEU:CD2	1.99	0.91
1:B:44:GLU:O	1:B:46:PRO:HD3	1.69	0.91
1:B:259:LEU:HD21	1:B:279:LEU:HD13	1.52	0.91
1:A:158:MET:HG2	1:A:164:GLN:HG3	1.51	0.91
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.52	0.91
1:B:190:LEU:HD22	1:B:200:THR:HB	1.51	0.90
1:A:259:LEU:HD21	1:A:279:LEU:HD13	1.54	0.90
1:B:127:LEU:HD12	1:B:127:LEU:N	1.88	0.89
1:B:26:SER:HA	1:B:29:ALA:HB3	1.54	0.89
1:A:320:ASP:OD1	1:A:349:ARG:NH2	2.06	0.89
1:B:230:CYS:HB3	1:B:277:PRO:HD3	1.55	0.89
1:A:133:ARG:HG3	1:B:348:GLU:HA	1.55	0.88
1:B:320:ASP:OD1	1:B:349:ARG:NH2	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HB3	1:A:324:ILE:HD12	1.55	0.88
1:A:339:VAL:HG13	1:A:353:VAL:HG12	1.55	0.87
1:B:339:VAL:HG13	1:B:353:VAL:HG12	1.57	0.87
1:A:342:MET:HE2	1:A:346:TYR:HD2	1.38	0.87
1:A:369:PRO:O	1:A:372:VAL:HG22	1.74	0.87
1:B:19:ILE:HD11	1:B:96:MET:CA	2.04	0.86
1:B:369:PRO:O	1:B:372:VAL:HG22	1.75	0.86
1:B:342:MET:HE2	1:B:346:TYR:HD2	1.38	0.86
1:A:158:MET:HB3	1:A:165:ILE:HG12	1.58	0.85
1:B:231:ASN:HD22	1:B:231:ASN:N	1.73	0.84
1:A:263:HIS:CD2	1:A:291:MET:HG2	2.12	0.84
1:B:180:VAL:HG11	1:B:198:MET:HE3	1.57	0.84
1:B:155:GLN:HA	1:B:155:GLN:OE1	1.78	0.84
1:A:155:GLN:OE1	1:A:155:GLN:HA	1.75	0.83
1:B:263:HIS:CD2	1:B:291:MET:HG2	2.13	0.83
1:A:106:LEU:O	1:A:106:LEU:HD23	1.79	0.83
1:A:378:VAL:HG11	2:A:1015:HOH:O	1.78	0.82
1:B:531:THR:HG23	1:B:532:GLU:OE2	1.79	0.82
1:B:232:PRO:CD	1:B:233:ASN:H	1.91	0.82
1:A:52:GLN:CG	1:A:58:ILE:HD11	2.09	0.82
1:A:193:ALA:HB1	1:A:198:MET:SD	2.20	0.82
1:B:5:VAL:HG23	1:B:118:THR:O	1.80	0.82
1:B:62:GLN:O	1:B:65:PRO:HD2	1.79	0.81
1:B:529:LYS:HB3	1:B:532:GLU:CG	2.09	0.81
1:A:531:THR:HG23	1:A:532:GLU:OE2	1.79	0.81
1:A:484:LEU:HD13	1:B:61:SER:CB	2.11	0.81
1:B:446:ILE:O	1:B:450:ILE:HD12	1.80	0.81
1:A:243:LYS:HG2	1:A:244:PRO:HD2	1.62	0.81
1:A:446:ILE:O	1:A:450:ILE:HD12	1.79	0.81
1:B:515:ARG:HH11	1:B:515:ARG:HG2	1.45	0.81
1:A:166:TYR:O	1:A:170:LEU:HD12	1.80	0.80
1:A:529:LYS:HB3	1:A:532:GLU:HG3	1.62	0.80
1:B:194:ARG:HB2	1:B:200:THR:HG21	1.63	0.80
1:B:529:LYS:HB3	1:B:532:GLU:HG3	1.61	0.80
1:A:535:GLN:O	1:A:539:LYS:HD3	1.82	0.80
1:A:13:VAL:HG22	1:A:203:VAL:HG21	1.64	0.79
1:A:52:GLN:HG2	1:A:58:ILE:HD11	1.65	0.79
1:A:484:LEU:CD1	1:B:61:SER:HB2	2.12	0.79
1:B:535:GLN:O	1:B:539:LYS:HD3	1.83	0.79
1:B:232:PRO:HD2	1:B:233:ASN:N	1.97	0.78
1:A:515:ARG:HH11	1:A:515:ARG:HG2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD21	1:A:110:ILE:HD11	1.63	0.78
1:A:529:LYS:HB3	1:A:532:GLU:CG	2.12	0.78
1:B:259:LEU:HB2	1:B:328:VAL:HG22	1.66	0.77
1:B:243:LYS:HG2	1:B:244:PRO:HD2	1.64	0.77
1:B:215:LYS:HA	1:B:219:THR:O	1.84	0.77
1:B:183:LEU:HD13	1:B:201:ILE:HB	1.68	0.76
1:A:177:PRO:O	1:A:198:MET:HA	1.86	0.76
1:A:190:LEU:HD22	1:A:200:THR:HB	1.66	0.76
1:B:50:THR:HG23	1:B:63:TRP:HE1	1.50	0.76
1:B:230:CYS:HB3	1:B:277:PRO:CD	2.15	0.75
1:B:231:ASN:ND2	1:B:231:ASN:N	2.34	0.75
1:A:166:TYR:HD1	1:A:166:TYR:H	1.35	0.74
1:A:108:ALA:O	1:A:111:ALA:HB3	1.87	0.74
1:B:71:TYR:O	1:B:75:SER:HB3	1.87	0.74
1:A:483:ILE:HB	1:A:510:ILE:HG12	1.70	0.74
1:A:259:LEU:HB2	1:A:328:VAL:HG22	1.70	0.73
1:B:300:PRO:HG2	1:B:305:GLU:HG2	1.71	0.73
1:B:127:LEU:H	1:B:127:LEU:CD1	2.02	0.73
1:B:141:CYS:O	1:B:144:SER:HB3	1.89	0.73
1:B:158:MET:CE	1:B:164:GLN:HB2	2.19	0.73
1:B:230:CYS:SG	1:B:230:CYS:O	2.47	0.73
1:B:19:ILE:CD1	1:B:96:MET:HA	2.17	0.73
1:B:330:ILE:HB	1:B:354:ALA:HB3	1.70	0.73
1:B:106:LEU:HD21	1:B:146:HIS:HD2	1.53	0.72
1:A:300:PRO:HG2	1:A:305:GLU:HG2	1.70	0.72
1:B:259:LEU:O	1:B:259:LEU:HD12	1.90	0.72
1:A:60:PHE:O	1:A:63:TRP:HB2	1.90	0.72
1:A:124:ASN:HA	1:A:153:SER:HB3	1.72	0.72
1:B:483:ILE:HB	1:B:510:ILE:HG12	1.70	0.72
1:A:299:SER:CB	1:A:456:THR:HG22	2.19	0.71
1:A:330:ILE:HB	1:A:354:ALA:HB3	1.72	0.71
1:B:230:CYS:HB3	1:B:277:PRO:CG	2.20	0.71
1:A:13:VAL:CG2	1:A:203:VAL:HG21	2.20	0.71
1:A:513:LEU:HD22	1:A:514:LYS:O	1.90	0.71
1:B:158:MET:HG2	1:B:164:GLN:HG3	1.72	0.70
1:A:58:ILE:HG22	1:A:62:GLN:CG	2.19	0.70
1:B:215:LYS:HZ3	1:B:221:PHE:H	1.39	0.70
1:A:342:MET:HE2	1:A:346:TYR:CD2	2.24	0.70
1:B:291:MET:HA	1:B:291:MET:HE3	1.72	0.70
1:B:158:MET:HE2	1:B:164:GLN:HB2	1.74	0.70
1:B:190:LEU:HD13	1:B:202:LEU:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:SER:HB3	1:B:484:LEU:HD13	1.71	0.70
1:A:259:LEU:O	1:A:259:LEU:HD12	1.92	0.70
1:B:75:SER:O	1:B:77:ALA:N	2.25	0.70
1:B:180:VAL:HG13	1:B:198:MET:HG2	1.73	0.69
1:A:496:ILE:HD12	1:A:496:ILE:H	1.56	0.69
1:A:434:ASP:CG	1:A:434:ASP:O	2.29	0.69
1:A:446:ILE:HG22	1:A:450:ILE:HD11	1.75	0.69
1:B:513:LEU:HD22	1:B:514:LYS:O	1.93	0.69
1:A:328:VAL:HG12	1:A:351:ARG:HB3	1.74	0.69
1:A:53:LEU:HA	1:A:58:ILE:HD12	1.74	0.69
1:B:299:SER:CB	1:B:456:THR:HG22	2.22	0.68
1:A:426:GLY:O	1:A:429:VAL:HG23	1.92	0.68
1:B:75:SER:OG	1:B:76:LYS:N	2.23	0.68
1:A:173:LEU:O	1:A:174:LYS:HB2	1.91	0.68
1:B:342:MET:HE2	1:B:346:TYR:CD2	2.26	0.68
1:B:211:ARG:O	1:B:215:LYS:HG2	1.93	0.68
1:B:376:ILE:HD12	1:B:379:PHE:CE2	2.28	0.68
1:B:230:CYS:HB3	1:B:277:PRO:HG3	1.74	0.68
1:B:328:VAL:HG12	1:B:351:ARG:HB3	1.75	0.68
1:A:148:ASP:OD1	1:A:148:ASP:N	2.26	0.68
1:A:348:GLU:HA	1:B:133:ARG:CG	2.19	0.67
1:A:106:LEU:CD2	1:A:110:ILE:HD11	2.23	0.67
1:A:210:LEU:O	1:A:214:GLU:HB2	1.94	0.67
1:B:223:GLU:H	1:B:223:GLU:CD	1.97	0.67
1:B:215:LYS:C	1:B:217:THR:H	1.96	0.67
1:A:52:GLN:HG3	1:A:58:ILE:HD11	1.76	0.67
1:B:194:ARG:HB2	1:B:200:THR:CG2	2.24	0.67
1:B:158:MET:HG2	1:B:164:GLN:CG	2.25	0.67
1:A:207:ALA:O	1:A:210:LEU:HB3	1.95	0.66
1:A:291:MET:HA	1:A:291:MET:HE3	1.76	0.66
1:B:112:LEU:O	1:B:117:PHE:HB2	1.94	0.66
1:B:529:LYS:O	1:B:533:VAL:HG23	1.95	0.66
1:B:270:PHE:CE1	1:B:273:ARG:HD3	2.30	0.66
1:A:205:ASN:ND2	1:A:207:ALA:N	2.39	0.66
1:B:496:ILE:H	1:B:496:ILE:HD12	1.58	0.66
1:A:248:LEU:HA	1:A:297:SER:HB3	1.77	0.66
1:B:467:ASN:OD1	1:B:470:ARG:HD2	1.96	0.66
1:B:204:HIS:O	1:B:205:ASN:CB	2.39	0.66
1:B:46:PRO:HG2	1:B:159:ILE:CD1	2.26	0.66
1:B:446:ILE:HG22	1:B:450:ILE:HD11	1.77	0.65
1:B:248:LEU:HA	1:B:297:SER:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HA	1:A:62:GLN:OE1	1.97	0.65
1:A:50:THR:HA	1:A:63:TRP:HZ2	1.61	0.65
1:B:124:ASN:HA	1:B:153:SER:HB3	1.77	0.65
1:A:309:GLU:HB2	1:A:474:TRP:CD2	2.32	0.65
1:A:166:TYR:HD1	1:A:166:TYR:N	1.94	0.65
1:B:106:LEU:HD21	1:B:146:HIS:CD2	2.31	0.65
1:B:309:GLU:HB2	1:B:474:TRP:CD2	2.31	0.65
1:A:166:TYR:CD1	1:A:166:TYR:N	2.62	0.64
1:B:276:ILE:HD11	1:B:288:ALA:CB	2.27	0.64
1:A:376:ILE:HD12	1:A:379:PHE:CE2	2.33	0.64
1:B:293:GLY:HA2	1:B:299:SER:HA	1.78	0.64
1:B:232:PRO:HD2	1:B:233:ASN:HD22	1.62	0.64
1:A:529:LYS:O	1:A:533:VAL:HG23	1.97	0.64
1:A:145:GLN:HA	1:A:145:GLN:NE2	2.13	0.64
1:B:535:GLN:HG2	1:B:539:LYS:NZ	2.13	0.64
1:A:293:GLY:HA2	1:A:299:SER:HA	1.79	0.64
1:B:159:ILE:O	1:B:162:GLU:HB2	1.97	0.63
1:B:510:ILE:HG22	1:B:513:LEU:HB2	1.80	0.63
1:B:13:VAL:HB	1:B:203:VAL:HG11	1.80	0.63
1:A:177:PRO:O	1:A:198:MET:HB3	1.97	0.63
1:B:75:SER:HB2	1:B:82:LEU:CB	2.29	0.63
1:A:427:ILE:HG12	1:A:427:ILE:O	1.98	0.63
1:A:446:ILE:HG22	1:A:450:ILE:CD1	2.28	0.63
1:A:467:ASN:OD1	1:A:470:ARG:HD2	1.98	0.63
1:A:122:VAL:HG12	1:A:151:ILE:HB	1.79	0.63
1:A:158:MET:CG	1:A:164:GLN:HG3	2.26	0.63
1:B:124:ASN:HA	1:B:153:SER:CB	2.29	0.62
1:A:106:LEU:C	1:A:106:LEU:HD23	2.19	0.62
1:B:38:LEU:HD13	1:B:42:GLN:HB3	1.81	0.62
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.65	0.62
1:A:276:ILE:HD11	1:A:288:ALA:CB	2.30	0.62
1:B:139:MET:O	1:B:143:LEU:HD12	1.99	0.61
1:B:426:GLY:HA3	1:B:429:VAL:CG2	2.29	0.61
1:B:8:PHE:O	1:B:121:ILE:HG23	2.00	0.61
1:B:9:ASP:O	1:B:13:VAL:HG22	2.01	0.61
1:A:394:GLU:OE2	1:A:428:LEU:HB2	2.00	0.61
1:A:270:PHE:CE1	1:A:273:ARG:HD3	2.35	0.61
1:B:264:GLY:HA3	1:B:333:ASP:HB3	1.83	0.61
1:B:259:LEU:HD21	1:B:279:LEU:CD1	2.29	0.61
1:B:394:GLU:OE2	1:B:428:LEU:HB2	2.01	0.61
1:A:535:GLN:HG2	1:A:539:LYS:NZ	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:PRO:HD2	1:B:233:ASN:ND2	2.16	0.60
1:A:497:VAL:HA	2:A:1015:HOH:O	2.00	0.60
1:A:416:ILE:CG2	1:A:427:ILE:HD11	2.30	0.60
1:A:359:PRO:HA	1:A:489:MET:CE	2.30	0.60
1:A:378:VAL:HG21	2:A:1015:HOH:O	2.00	0.60
1:B:146:HIS:N	1:B:146:HIS:ND1	2.50	0.60
1:A:264:GLY:HA3	1:A:333:ASP:HB3	1.83	0.60
1:B:16:LEU:HD13	1:B:206:THR:HG22	1.83	0.60
1:A:329:PHE:HB3	1:A:339:VAL:HG22	1.84	0.60
1:A:159:ILE:O	1:A:165:ILE:HD11	2.02	0.60
1:A:180:VAL:HG13	1:A:198:MET:HB3	1.83	0.60
1:B:259:LEU:C	1:B:259:LEU:HD12	2.23	0.59
1:B:268:SER:HB2	2:B:1004:HOH:O	2.02	0.59
1:A:398:ASN:OD1	1:A:398:ASN:C	2.39	0.59
1:B:187:GLY:HA2	1:B:202:LEU:HD11	1.83	0.59
1:A:322:LEU:HD22	1:A:324:ILE:HD11	1.84	0.59
1:B:529:LYS:HB3	1:B:532:GLU:HG2	1.83	0.59
1:B:446:ILE:HG22	1:B:450:ILE:CD1	2.31	0.59
1:B:215:LYS:NZ	1:B:221:PHE:H	1.99	0.59
1:B:322:LEU:HD22	1:B:324:ILE:HD11	1.83	0.59
1:B:424:ILE:HD13	1:B:424:ILE:N	2.17	0.59
1:A:94:GLN:H	1:A:94:GLN:CD	2.04	0.59
1:B:230:CYS:CB	1:B:277:PRO:HG3	2.33	0.59
1:B:447:GLU:HA	1:B:450:ILE:HD13	1.84	0.59
1:B:74:SER:O	1:B:75:SER:O	2.21	0.59
1:B:359:PRO:HA	1:B:489:MET:CE	2.33	0.59
1:B:270:PHE:HB2	1:B:448:PHE:CE2	2.38	0.58
1:B:398:ASN:C	1:B:398:ASN:OD1	2.39	0.58
1:B:329:PHE:HB3	1:B:339:VAL:HG22	1.85	0.58
1:A:5:VAL:CG1	1:A:6:ALA:N	2.67	0.58
1:A:510:ILE:HG22	1:A:513:LEU:HB2	1.84	0.58
1:A:474:TRP:O	1:A:477:LYS:HG3	2.04	0.58
1:B:538:ILE:O	1:B:542:GLN:HG2	2.04	0.58
1:B:125:ASN:ND2	1:B:152:GLU:HB3	2.10	0.58
1:A:270:PHE:HB2	1:A:448:PHE:CE2	2.39	0.58
1:A:310:LEU:O	1:A:314:GLU:HG3	2.03	0.58
1:A:496:ILE:N	1:A:496:ILE:HD12	2.18	0.58
1:A:7:ALA:O	1:A:183:LEU:HD23	2.04	0.58
1:A:159:ILE:O	1:A:159:ILE:HD12	2.04	0.58
1:A:404:LYS:O	1:A:408:ARG:HD2	2.04	0.58
1:B:424:ILE:H	1:B:424:ILE:CD1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ILE:CD1	1:A:496:ILE:H	2.17	0.57
1:A:177:PRO:O	1:A:198:MET:CA	2.52	0.57
1:B:160:LYS:HA	1:B:165:ILE:HD11	1.86	0.57
1:B:203:VAL:O	1:B:203:VAL:HG12	2.04	0.57
1:A:431:THR:HG23	1:A:432:PRO:HD2	1.86	0.57
1:A:538:ILE:O	1:A:542:GLN:HG2	2.03	0.57
1:B:187:GLY:HA2	1:B:190:LEU:HB2	1.86	0.57
1:B:75:SER:C	1:B:77:ALA:N	2.56	0.57
1:B:404:LYS:O	1:B:408:ARG:HD2	2.05	0.57
1:B:122:VAL:HG21	1:B:182:PHE:CE2	2.40	0.57
1:A:447:GLU:HA	1:A:450:ILE:HD13	1.86	0.57
1:B:75:SER:HB2	1:B:82:LEU:HB2	1.86	0.57
1:B:232:PRO:O	1:B:235:VAL:HG22	2.04	0.57
1:B:291:MET:HA	1:B:291:MET:CE	2.35	0.57
1:B:36:PHE:HZ	1:B:75:SER:HA	1.69	0.57
1:B:26:SER:HA	1:B:29:ALA:CB	2.29	0.56
1:A:159:ILE:C	1:A:165:ILE:HD11	2.25	0.56
1:B:22:ALA:HA	1:B:25:ARG:HD3	1.86	0.56
1:A:61:SER:HB2	1:A:129:ASP:OD1	2.06	0.56
1:B:427:ILE:HG13	1:B:428:LEU:HD13	1.87	0.56
1:B:36:PHE:HE2	1:B:82:LEU:HD13	1.71	0.56
1:B:346:TYR:O	1:B:350:VAL:HG23	2.06	0.56
1:A:291:MET:CE	1:A:291:MET:HA	2.36	0.56
1:B:193:ALA:O	1:B:198:MET:HB2	2.06	0.56
1:A:294:TYR:CZ	1:A:461:PRO:HB3	2.41	0.56
1:A:206:THR:O	1:A:207:ALA:CB	2.54	0.56
1:A:4:ARG:HG3	1:A:179:GLU:HB3	1.88	0.56
1:B:178:ASN:N	1:B:178:ASN:ND2	2.53	0.56
1:B:474:TRP:O	1:B:477:LYS:HG3	2.05	0.56
1:A:17:PRO:O	1:A:18:SER:O	2.24	0.56
1:B:180:VAL:O	1:B:199:VAL:HG23	2.06	0.55
1:A:529:LYS:HB3	1:A:532:GLU:HG2	1.87	0.55
1:B:532:GLU:O	1:B:536:ILE:HG13	2.07	0.55
1:B:73:LYS:O	1:B:77:ALA:HB3	2.05	0.55
1:A:8:PHE:O	1:A:121:ILE:HA	2.06	0.55
1:A:532:GLU:O	1:A:536:ILE:HG13	2.06	0.55
1:B:440:ILE:HG22	1:B:441:THR:HG23	1.88	0.55
1:A:231:ASN:N	1:A:231:ASN:HD22	2.04	0.55
1:A:52:GLN:HE21	1:A:58:ILE:HG12	1.71	0.55
1:A:259:LEU:HD12	1:A:259:LEU:C	2.26	0.55
1:B:434:ASP:H	1:B:435:PRO:HD3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASP:O	1:B:133:ARG:HD3	2.07	0.55
1:B:496:ILE:H	1:B:496:ILE:CD1	2.19	0.55
1:B:496:ILE:N	1:B:496:ILE:HD12	2.21	0.55
1:A:262:CYS:HB2	1:A:335:ALA:HB1	1.89	0.55
1:A:346:TYR:O	1:A:350:VAL:HG23	2.07	0.55
1:B:215:LYS:C	1:B:217:THR:N	2.59	0.55
1:A:231:ASN:N	1:A:231:ASN:ND2	2.53	0.55
1:B:49:PRO:HD2	1:B:67:MET:HE2	1.88	0.55
1:A:156:VAL:HG11	1:A:168:PHE:HE2	1.72	0.55
1:A:463:ASN:HA	1:A:466:ARG:HG3	1.88	0.54
1:A:215:LYS:HB2	1:A:219:THR:O	2.06	0.54
1:B:159:ILE:O	1:B:165:ILE:HD11	2.07	0.54
1:A:497:VAL:O	1:A:498:LEU:HB2	2.07	0.54
1:B:497:VAL:O	1:B:498:LEU:HB2	2.08	0.54
1:A:304:GLU:CD	1:A:304:GLU:H	2.10	0.54
1:B:5:VAL:HG21	1:B:173:LEU:HD23	1.86	0.54
1:A:299:SER:HB2	1:A:456:THR:HG22	1.89	0.54
1:B:310:LEU:O	1:B:314:GLU:HG3	2.07	0.54
1:B:202:LEU:HD23	1:B:204:HIS:CD2	2.42	0.54
1:A:264:GLY:O	1:A:267:GLU:HG3	2.06	0.54
1:A:428:LEU:O	1:A:431:THR:HB	2.07	0.54
1:B:292:LYS:NZ	1:B:305:GLU:HG3	2.23	0.54
1:A:256:GLY:N	1:A:285:ARG:HB2	2.23	0.54
1:A:159:ILE:O	1:A:162:GLU:HB2	2.07	0.54
1:B:100:SER:HA	1:B:139:MET:HE1	1.89	0.54
1:B:434:ASP:N	1:B:435:PRO:HD3	2.22	0.54
1:A:416:ILE:HG21	1:A:427:ILE:HD11	1.89	0.54
1:A:92:PHE:C	1:A:92:PHE:CD1	2.80	0.54
1:B:53:LEU:HD22	1:B:126:TRP:HB2	1.90	0.54
1:B:205:ASN:HB3	1:B:207:ALA:H	1.73	0.54
1:B:421:ALA:HA	1:B:424:ILE:HD11	1.90	0.54
1:B:256:GLY:N	1:B:285:ARG:HB2	2.23	0.54
1:A:166:TYR:O	1:A:170:LEU:CD1	2.54	0.54
1:B:309:GLU:HB2	1:B:474:TRP:CE2	2.43	0.54
1:A:182:PHE:HD1	1:A:183:LEU:H	1.56	0.54
1:A:205:ASN:OD1	1:A:209:ALA:N	2.40	0.53
1:A:287:LEU:O	1:A:289:ILE:HG13	2.08	0.53
1:A:131:ASP:OD1	1:A:131:ASP:N	2.42	0.53
1:B:498:LEU:HD12	1:B:523:HIS:CE1	2.43	0.53
1:B:380:ASN:HB3	1:B:418:VAL:O	2.09	0.53
1:A:62:GLN:OE1	1:B:481:ARG:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:HB2	1:A:200:THR:HG21	1.90	0.53
1:B:426:GLY:C	1:B:429:VAL:HG23	2.28	0.53
1:B:463:ASN:HA	1:B:466:ARG:HG3	1.91	0.53
1:B:47:GLU:HG2	1:B:48:GLY:H	1.71	0.53
1:B:304:GLU:H	1:B:304:GLU:CD	2.12	0.53
1:B:395:LEU:HD21	1:B:427:ILE:HD11	1.90	0.53
1:A:230:CYS:HB3	1:A:277:PRO:HG3	1.89	0.53
1:B:342:MET:CE	1:B:346:TYR:HD2	2.15	0.53
1:B:424:ILE:CD1	1:B:424:ILE:N	2.70	0.53
1:A:303:ILE:HD13	1:A:463:ASN:CG	2.29	0.53
1:B:107:GLN:HG3	1:B:225:PRO:HG2	1.91	0.53
1:B:299:SER:HB2	1:B:456:THR:HG22	1.90	0.53
1:A:125:ASN:HD22	1:A:152:GLU:HB2	1.73	0.53
1:B:206:THR:O	1:B:207:ALA:HB2	2.09	0.53
1:A:292:LYS:NZ	1:A:305:GLU:HG3	2.24	0.53
1:A:416:ILE:HG23	1:A:427:ILE:HG12	1.91	0.53
1:A:503:SER:O	1:A:506:MET:HB2	2.09	0.53
1:A:255:SER:O	1:A:256:GLY:O	2.28	0.53
1:A:501:GLU:O	1:A:504:LYS:HG2	2.09	0.53
1:A:9:ASP:OD1	1:A:160:LYS:NZ	2.37	0.52
1:B:255:SER:O	1:B:256:GLY:O	2.27	0.52
1:A:5:VAL:CG2	1:A:118:THR:HB	2.24	0.52
1:A:5:VAL:HG12	1:A:6:ALA:N	2.24	0.52
1:A:259:LEU:HD21	1:A:279:LEU:CD1	2.32	0.52
1:B:515:ARG:NH1	1:B:515:ARG:HG2	2.21	0.52
1:A:182:PHE:CD1	1:A:183:LEU:N	2.76	0.52
1:A:192:PRO:O	1:A:195:ASP:HB2	2.10	0.52
1:A:275:GLN:O	1:A:279:LEU:HB2	2.10	0.52
1:B:183:LEU:CD1	1:B:201:ILE:HB	2.37	0.52
1:B:141:CYS:O	1:B:144:SER:CB	2.58	0.52
1:A:440:ILE:HG22	1:A:441:THR:HG23	1.91	0.52
1:A:380:ASN:HB3	1:A:418:VAL:O	2.09	0.52
1:B:49:PRO:HG2	1:B:67:MET:HG2	1.91	0.52
1:A:422:THR:O	1:A:423:GLU:CB	2.47	0.52
1:A:498:LEU:HD12	1:A:523:HIS:CE1	2.44	0.52
1:A:141:CYS:O	1:A:144:SER:HB3	2.09	0.52
1:B:6:ALA:O	1:B:119:THR:HA	2.10	0.52
1:A:16:LEU:HA	1:A:17:PRO:C	2.31	0.52
1:B:222:PRO:HG2	1:B:225:PRO:HG3	1.90	0.52
1:B:187:GLY:CA	1:B:202:LEU:HD11	2.40	0.52
1:B:16:LEU:HB3	1:B:17:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ASP:N	1:B:435:PRO:CD	2.72	0.52
1:A:293:GLY:O	1:A:456:THR:HG21	2.10	0.51
1:B:501:GLU:O	1:B:504:LYS:HG2	2.10	0.51
1:B:158:MET:HE2	1:B:164:GLN:C	2.30	0.51
1:A:212:GLU:HA	1:A:215:LYS:HD2	1.92	0.51
1:B:294:TYR:CZ	1:B:461:PRO:HB3	2.45	0.51
1:B:498:LEU:HD12	1:B:523:HIS:HE1	1.76	0.51
1:A:469:GLU:HA	1:A:469:GLU:OE1	2.10	0.51
1:A:91:ILE:H	1:A:91:ILE:HD13	1.75	0.51
1:B:216:VAL:HG13	1:B:216:VAL:O	2.11	0.51
1:A:380:ASN:ND2	1:A:422:THR:OG1	2.43	0.51
1:A:190:LEU:CD2	1:A:200:THR:HB	2.39	0.51
1:B:49:PRO:HD2	1:B:67:MET:CE	2.41	0.51
1:A:173:LEU:O	1:A:174:LYS:CB	2.59	0.51
1:A:49:PRO:O	1:A:52:GLN:HG2	2.11	0.51
1:A:309:GLU:HB2	1:A:474:TRP:CE2	2.46	0.51
1:B:102:ASN:ND2	1:B:105:MET:HG3	2.26	0.51
1:A:515:ARG:HH11	1:A:515:ARG:CG	2.23	0.51
1:B:161:PRO:O	1:B:162:GLU:C	2.49	0.51
1:B:162:GLU:O	1:B:165:ILE:CD1	2.59	0.51
1:B:45:PHE:O	1:B:45:PHE:CG	2.63	0.51
1:B:56:GLY:HA2	1:B:127:LEU:HD11	1.92	0.51
1:A:101:ILE:HG22	1:A:102:ASN:N	2.25	0.51
1:A:497:VAL:HG22	1:A:498:LEU:HG	1.93	0.51
1:B:262:CYS:HB2	1:B:335:ALA:HB1	1.93	0.51
1:A:156:VAL:HG11	1:A:168:PHE:CE2	2.47	0.50
1:B:229:PRO:O	1:B:231:ASN:ND2	2.44	0.50
1:A:10:LEU:HD12	1:A:14:LEU:HB2	1.92	0.50
1:B:149:PHE:CD2	1:B:173:LEU:HD12	2.46	0.50
1:A:178:ASN:O	1:A:180:VAL:N	2.42	0.50
1:B:276:ILE:HD11	1:B:288:ALA:HB2	1.93	0.50
1:A:499:ARG:O	1:A:502:MET:HG3	2.12	0.50
1:B:232:PRO:CD	1:B:233:ASN:N	2.59	0.50
1:A:498:LEU:HD12	1:A:523:HIS:HE1	1.76	0.50
1:B:499:ARG:O	1:B:502:MET:HG3	2.11	0.50
1:B:180:VAL:HG11	1:B:198:MET:CE	2.36	0.50
1:A:16:LEU:HD23	1:A:18:SER:N	2.27	0.50
1:A:52:GLN:HE21	1:A:58:ILE:CG1	2.24	0.50
1:A:515:ARG:NH1	1:A:515:ARG:HG2	2.23	0.50
1:A:392:GLU:HG3	1:A:462:LEU:HD12	1.93	0.50
1:B:121:ILE:O	1:B:151:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:HB2	1:B:165:ILE:HG23	1.94	0.50
1:B:264:GLY:O	1:B:267:GLU:HG3	2.11	0.50
1:B:303:ILE:HD13	1:B:463:ASN:CG	2.31	0.50
1:B:275:GLN:O	1:B:279:LEU:HB2	2.10	0.50
1:B:101:ILE:HG22	1:B:102:ASN:N	2.26	0.50
1:B:428:LEU:HA	1:B:431:THR:OG1	2.12	0.50
1:A:289:ILE:HG22	1:A:290:ASP:N	2.27	0.50
1:B:289:ILE:HG22	1:B:290:ASP:N	2.27	0.50
1:B:54:MET:HA	1:B:125:ASN:O	2.12	0.49
1:B:426:GLY:CA	1:B:429:VAL:CG2	2.89	0.49
1:B:469:GLU:HA	1:B:469:GLU:OE1	2.11	0.49
1:B:158:MET:HE3	1:B:164:GLN:HB2	1.91	0.49
1:B:330:ILE:O	1:B:330:ILE:HG13	2.12	0.49
1:A:10:LEU:C	1:A:12:GLY:N	2.65	0.49
1:B:434:ASP:O	1:B:435:PRO:C	2.51	0.49
1:A:125:ASN:HD22	1:A:152:GLU:CB	2.25	0.49
1:A:128:ASP:O	1:A:133:ARG:HD3	2.11	0.49
1:A:193:ALA:CB	1:A:198:MET:SD	2.96	0.49
1:A:153:SER:HB2	1:A:158:MET:O	2.12	0.49
1:B:216:VAL:CG1	1:B:216:VAL:O	2.60	0.49
1:A:165:ILE:O	1:A:168:PHE:HB3	2.12	0.49
1:B:177:PRO:O	1:B:198:MET:HA	2.11	0.49
1:B:535:GLN:HG2	1:B:539:LYS:HZ1	1.76	0.49
1:B:367:VAL:O	1:B:368:SER:C	2.51	0.49
1:A:93:SER:O	1:A:96:MET:HB3	2.13	0.49
1:B:144:SER:OG	1:B:145:GLN:N	2.44	0.49
1:B:287:LEU:O	1:B:289:ILE:HG13	2.13	0.49
1:B:30:LEU:O	1:B:31:ALA:HB3	2.13	0.49
1:A:439:LYS:HG2	1:A:440:ILE:HD13	1.94	0.49
1:A:424:ILE:O	1:A:424:ILE:HG13	2.13	0.49
1:A:263:HIS:NE2	1:A:291:MET:HG2	2.28	0.48
1:B:270:PHE:CZ	1:B:273:ARG:HD3	2.47	0.48
1:A:342:MET:CE	1:A:346:TYR:HD2	2.17	0.48
1:B:82:LEU:O	1:B:83:PRO:C	2.52	0.48
1:B:309:GLU:HB2	1:B:474:TRP:CG	2.48	0.48
1:B:340:TRP:CZ2	1:B:355:SER:HB2	2.49	0.48
1:B:4:ARG:HE	1:B:179:GLU:HA	1.78	0.48
1:A:319:LEU:HB3	1:A:324:ILE:O	2.14	0.48
1:A:162:GLU:O	1:A:165:ILE:HD12	2.14	0.48
1:B:4:ARG:HB3	1:B:4:ARG:CZ	2.42	0.48
1:B:150:LEU:HG	1:B:152:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:HA	1:B:148:ASP:OD2	2.13	0.48
1:B:497:VAL:HG22	1:B:498:LEU:HG	1.96	0.48
1:B:64:VAL:CB	1:B:65:PRO:HD3	2.32	0.48
1:A:276:ILE:HD11	1:A:288:ALA:HB2	1.96	0.48
1:A:90:GLN:O	1:A:92:PHE:N	2.45	0.48
1:B:151:ILE:H	1:B:151:ILE:HG12	1.34	0.48
1:A:375:SER:OG	1:A:376:ILE:N	2.47	0.48
1:A:330:ILE:HG13	1:A:330:ILE:O	2.11	0.48
1:A:407:PHE:C	1:A:408:ARG:HG2	2.34	0.48
1:B:103:ARG:O	1:B:107:GLN:HB2	2.14	0.48
1:A:270:PHE:CZ	1:A:273:ARG:HD3	2.49	0.48
1:A:54:MET:SD	1:A:124:ASN:HB3	2.55	0.47
1:B:223:GLU:N	1:B:223:GLU:CD	2.66	0.47
1:B:93:SER:OG	1:B:132:LYS:NZ	2.47	0.47
1:B:503:SER:O	1:B:506:MET:HB2	2.13	0.47
1:B:300:PRO:CG	1:B:305:GLU:HG2	2.42	0.47
1:A:92:PHE:N	1:A:94:GLN:OE1	2.47	0.47
1:B:7:ALA:HB2	1:B:120:CYS:SG	2.54	0.47
1:A:265:PHE:C	1:A:265:PHE:CD1	2.87	0.47
1:B:182:PHE:HE1	1:B:184:ASP:HB2	1.78	0.47
1:A:122:VAL:O	1:A:122:VAL:HG23	2.14	0.47
1:A:179:GLU:HG3	1:A:179:GLU:H	1.39	0.47
1:B:439:LYS:HG2	1:B:440:ILE:HD13	1.95	0.47
1:A:53:LEU:HD23	1:A:58:ILE:O	2.13	0.47
1:A:124:ASN:HA	1:A:153:SER:CB	2.43	0.47
1:A:92:PHE:O	1:A:95:ALA:HB3	2.14	0.47
1:B:319:LEU:HB3	1:B:324:ILE:O	2.14	0.47
1:B:160:LYS:HG2	1:B:165:ILE:HD13	1.95	0.47
1:B:222:PRO:HG2	1:B:225:PRO:HB3	1.97	0.47
1:A:254:GLY:H	1:B:323:GLY:HA3	1.79	0.47
1:A:380:ASN:OD1	1:A:422:THR:N	2.45	0.47
1:B:36:PHE:CE2	1:B:82:LEU:HD13	2.50	0.47
1:B:364:ASP:N	1:B:364:ASP:OD1	2.48	0.47
1:A:177:PRO:O	1:A:198:MET:CB	2.62	0.47
1:A:101:ILE:CG2	1:A:102:ASN:N	2.78	0.47
1:B:58:ILE:HD12	1:B:63:TRP:HB2	1.96	0.47
1:B:64:VAL:HB	1:B:65:PRO:CD	2.36	0.47
1:A:309:GLU:HB2	1:A:474:TRP:CG	2.50	0.47
1:A:10:LEU:O	1:A:12:GLY:N	2.47	0.47
1:A:212:GLU:C	1:A:214:GLU:N	2.67	0.47
1:B:270:PHE:CD2	1:B:448:PHE:CD2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:C	1:B:92:PHE:CD1	2.87	0.47
1:B:413:THR:HB	1:B:414:GLY:H	1.51	0.47
1:A:340:TRP:CZ2	1:A:355:SER:HB2	2.50	0.47
1:B:10:LEU:HD11	1:B:15:ALA:HB2	1.97	0.47
1:A:62:GLN:HE22	1:B:482:LYS:N	2.13	0.46
1:A:165:ILE:H	1:A:165:ILE:HG13	1.49	0.46
1:A:9:ASP:CG	1:A:10:LEU:H	2.18	0.46
1:B:124:ASN:HA	1:B:153:SER:OG	2.14	0.46
1:A:328:VAL:O	1:A:328:VAL:CG2	2.63	0.46
1:B:407:PHE:C	1:B:408:ARG:HG2	2.35	0.46
1:B:107:GLN:NE2	1:B:107:GLN:HA	2.29	0.46
1:A:364:ASP:OD1	1:A:364:ASP:N	2.47	0.46
1:B:106:LEU:HD23	1:B:106:LEU:O	2.16	0.46
1:B:145:GLN:HB2	1:B:146:HIS:CE1	2.51	0.46
1:A:367:VAL:O	1:A:368:SER:C	2.54	0.46
1:A:507:GLU:HG2	1:A:507:GLU:H	1.36	0.46
1:A:165:ILE:HD12	1:A:166:TYR:HE1	1.80	0.46
1:A:106:LEU:O	1:A:110:ILE:HG13	2.15	0.46
1:A:50:THR:HG1	1:A:63:TRP:HZ2	1.50	0.46
1:B:13:VAL:CB	1:B:203:VAL:HG11	2.44	0.46
1:A:413:THR:HB	1:A:414:GLY:H	1.48	0.46
1:A:469:GLU:O	1:A:472:TRP:HB3	2.15	0.46
1:B:206:THR:O	1:B:207:ALA:CB	2.64	0.46
1:A:416:ILE:HG23	1:A:427:ILE:HD11	1.97	0.46
1:A:54:MET:O	1:A:154:CYS:HA	2.16	0.46
1:B:178:ASN:H	1:B:178:ASN:ND2	2.12	0.46
1:B:359:PRO:HG2	1:B:361:MET:HG2	1.98	0.46
1:B:149:PHE:HD2	1:B:173:LEU:CD1	2.29	0.46
1:B:293:GLY:O	1:B:456:THR:HG21	2.16	0.46
1:B:434:ASP:H	1:B:435:PRO:CD	2.29	0.46
1:A:347:PRO:O	1:B:133:ARG:HD2	2.15	0.46
1:B:36:PHE:CZ	1:B:75:SER:HA	2.51	0.46
1:B:160:LYS:HA	1:B:165:ILE:CD1	2.46	0.46
1:A:126:TRP:NE1	1:A:128:ASP:OD1	2.32	0.45
1:A:159:ILE:C	1:A:165:ILE:CD1	2.85	0.45
1:B:75:SER:C	1:B:77:ALA:H	2.18	0.45
1:A:359:PRO:HA	1:A:489:MET:HE2	1.97	0.45
1:B:46:PRO:O	1:B:51:GLU:OE1	2.33	0.45
1:B:170:LEU:HD11	1:B:198:MET:HE3	1.98	0.45
1:A:535:GLN:HG2	1:A:539:LYS:HZ1	1.80	0.45
2:A:1028:HOH:O	1:B:285:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HB	1:B:150:LEU:HD12	1.98	0.45
1:A:127:LEU:N	1:A:127:LEU:HD12	2.31	0.45
1:B:265:PHE:C	1:B:265:PHE:CD1	2.90	0.45
1:B:535:GLN:CB	1:B:539:LYS:HZ2	2.29	0.45
1:B:75:SER:HB2	1:B:82:LEU:HB3	1.98	0.45
1:B:149:PHE:HD2	1:B:173:LEU:HD12	1.82	0.45
1:B:158:MET:HE2	1:B:164:GLN:CB	2.45	0.45
1:B:76:LYS:HB2	1:B:81:ASN:HD22	1.81	0.45
1:A:416:ILE:HG23	1:A:427:ILE:CD1	2.47	0.45
1:B:392:GLU:HG3	1:B:462:LEU:HD12	1.96	0.45
1:B:178:ASN:C	1:B:180:VAL:H	2.19	0.45
1:A:145:GLN:NE2	1:A:145:GLN:CA	2.80	0.45
1:B:113:LYS:O	1:B:116:GLY:N	2.49	0.45
1:A:362:PRO:HG3	1:A:509:TRP:CE2	2.52	0.45
1:B:342:MET:CE	1:B:346:TYR:CD2	2.95	0.45
1:A:396:GLU:OE2	1:A:458:PHE:N	2.47	0.45
1:B:362:PRO:HG3	1:B:509:TRP:CE2	2.52	0.45
1:A:153:SER:OG	1:A:154:CYS:N	2.49	0.45
1:B:180:VAL:CG1	1:B:198:MET:HG2	2.45	0.45
1:B:77:ALA:O	1:B:78:CYS:CB	2.65	0.45
1:B:306:TYR:CD1	1:B:306:TYR:N	2.84	0.45
1:B:153:SER:OG	1:B:154:CYS:N	2.50	0.44
1:A:312:CYS:O	1:A:342:MET:HE1	2.17	0.44
1:B:263:HIS:NE2	1:B:291:MET:HG2	2.31	0.44
1:A:434:ASP:OD1	1:A:434:ASP:O	2.35	0.44
1:B:333:ASP:OD2	1:B:523:HIS:NE2	2.41	0.44
1:B:261:LEU:HB3	1:B:272:TRP:CE2	2.53	0.44
1:B:33:PRO:O	1:B:34:ARG:C	2.55	0.44
1:B:26:SER:CA	1:B:29:ALA:HB3	2.38	0.44
1:B:312:CYS:O	1:B:342:MET:HE1	2.17	0.44
1:B:19:ILE:HD11	1:B:96:MET:CB	2.47	0.44
1:A:243:LYS:O	1:A:244:PRO:C	2.55	0.44
1:A:416:ILE:HG23	1:A:427:ILE:CG1	2.46	0.44
1:A:405:SER:OG	1:A:431:THR:HG21	2.17	0.44
1:A:270:PHE:CD2	1:A:448:PHE:CD2	3.04	0.44
1:B:158:MET:CG	1:B:164:GLN:HG3	2.45	0.44
1:B:243:LYS:O	1:B:244:PRO:C	2.55	0.44
1:B:32:LEU:HA	1:B:33:PRO:HD3	1.79	0.44
1:A:482:LYS:HG3	1:B:62:GLN:HE21	1.82	0.44
1:B:329:PHE:O	1:B:353:VAL:HA	2.18	0.44
1:A:535:GLN:CB	1:A:539:LYS:HZ2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HB3	1:A:272:TRP:CE2	2.53	0.44
1:B:469:GLU:O	1:B:472:TRP:HB3	2.17	0.44
1:A:306:TYR:N	1:A:306:TYR:CD1	2.85	0.44
1:B:8:PHE:N	1:B:8:PHE:CD1	2.85	0.44
1:A:53:LEU:HA	1:A:58:ILE:CD1	2.43	0.44
1:A:162:GLU:O	1:A:165:ILE:CD1	2.65	0.44
1:B:230:CYS:O	1:B:231:ASN:CB	2.63	0.44
1:B:375:SER:OG	1:B:376:ILE:N	2.50	0.44
1:A:359:PRO:HG2	1:A:361:MET:HG2	1.99	0.44
1:B:158:MET:HG2	1:B:164:GLN:HG2	2.00	0.44
1:A:54:MET:O	1:A:154:CYS:CA	2.66	0.44
1:B:180:VAL:CG1	1:B:198:MET:HE3	2.38	0.44
1:A:8:PHE:CD2	1:A:105:MET:HE1	2.53	0.44
1:B:331:GLY:N	1:B:339:VAL:HG21	2.33	0.44
1:B:170:LEU:HD11	1:B:198:MET:CE	2.48	0.44
1:A:101:ILE:HG21	1:A:106:LEU:HD12	2.00	0.44
1:B:363:PRO:HD2	1:B:479:LEU:HD21	1.99	0.44
1:B:122:VAL:HG12	1:B:151:ILE:CG1	2.19	0.44
1:A:136:LEU:HD23	1:B:348:GLU:HG2	2.00	0.44
1:B:75:SER:O	1:B:76:LYS:C	2.55	0.44
1:B:119:THR:O	1:B:120:CYS:HB3	2.17	0.44
1:B:278:ALA:HA	1:B:281:GLN:HE21	1.83	0.44
1:B:410:SER:HB3	1:B:522:GLY:N	2.33	0.44
1:A:5:VAL:HG11	1:A:173:LEU:HD21	1.99	0.43
1:B:5:VAL:HG11	1:B:173:LEU:HD23	1.99	0.43
1:B:73:LYS:O	1:B:74:SER:C	2.56	0.43
1:B:268:SER:OG	1:B:269:TRP:N	2.51	0.43
1:B:458:PHE:C	1:B:461:PRO:HD2	2.38	0.43
1:A:52:GLN:HG3	1:A:58:ILE:CD1	2.47	0.43
1:B:43:THR:HB	1:B:44:GLU:H	1.50	0.43
1:A:106:LEU:C	1:A:106:LEU:CD2	2.86	0.43
1:B:74:SER:O	1:B:78:CYS:HB2	2.17	0.43
1:A:385:PHE:HD2	1:A:465:TYR:CD2	2.36	0.43
1:B:253:MET:HG2	1:B:280:ALA:CB	2.47	0.43
1:A:8:PHE:CE2	1:A:105:MET:HE1	2.54	0.43
1:B:396:GLU:OE2	1:B:458:PHE:N	2.49	0.43
1:B:402:THR:O	1:B:406:PHE:HD1	2.02	0.43
1:B:17:PRO:O	1:B:18:SER:C	2.55	0.43
1:A:205:ASN:HD22	1:A:207:ALA:N	1.82	0.43
1:B:291:MET:CE	1:B:291:MET:CA	2.95	0.43
1:A:194:ARG:HB2	1:A:200:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PRO:HA	1:B:489:MET:HE3	2.00	0.43
1:B:507:GLU:H	1:B:507:GLU:HG2	1.36	0.43
1:A:413:THR:O	1:A:415:PHE:N	2.51	0.43
1:B:33:PRO:HD3	1:B:80:ALA:CB	2.48	0.43
1:B:357:ASN:N	1:B:357:ASN:OD1	2.51	0.43
1:B:125:ASN:N	1:B:153:SER:OG	2.51	0.43
1:A:184:ASP:HB3	1:A:190:LEU:CD1	2.48	0.43
1:B:91:ILE:HG12	1:B:92:PHE:N	2.34	0.43
1:B:125:ASN:HD22	1:B:152:GLU:CB	2.13	0.43
1:A:482:LYS:HG3	1:B:62:GLN:NE2	2.34	0.43
1:A:380:ASN:CB	1:A:419:HIS:O	2.66	0.43
1:A:281:GLN:HE21	1:A:281:GLN:HB2	1.59	0.43
1:A:53:LEU:HD22	1:A:126:TRP:HB2	2.01	0.43
1:A:133:ARG:NH1	1:B:350:VAL:O	2.52	0.43
1:B:158:MET:CB	1:B:165:ILE:HG23	2.49	0.43
1:B:328:VAL:CG2	1:B:328:VAL:O	2.65	0.43
1:A:331:GLY:N	1:A:339:VAL:HG21	2.33	0.43
1:B:253:MET:HG2	1:B:280:ALA:HB2	2.01	0.43
1:A:410:SER:HB3	1:A:522:GLY:N	2.34	0.43
1:B:162:GLU:O	1:B:165:ILE:HD11	2.18	0.42
1:B:228:VAL:O	1:B:277:PRO:HG2	2.19	0.42
1:A:300:PRO:CG	1:A:305:GLU:HG2	2.41	0.42
1:A:182:PHE:C	1:A:183:LEU:HD22	2.39	0.42
1:A:342:MET:CE	1:A:346:TYR:CD2	2.98	0.42
1:B:230:CYS:C	1:B:231:ASN:ND2	2.72	0.42
1:B:432:PRO:HB2	1:B:434:ASP:OD1	2.20	0.42
1:B:103:ARG:HB2	1:B:104:PRO:CD	2.49	0.42
1:B:462:LEU:C	1:B:464:TRP:H	2.22	0.42
1:A:357:ASN:N	1:A:357:ASN:OD1	2.52	0.42
1:B:537:LEU:HD23	1:B:537:LEU:HA	1.85	0.42
1:A:378:VAL:O	1:A:378:VAL:HG13	2.17	0.42
1:B:413:THR:O	1:B:415:PHE:N	2.52	0.42
1:B:414:GLY:O	1:B:415:PHE:O	2.37	0.42
1:A:387:GLU:HA	1:A:388:PRO:HD3	1.75	0.42
1:A:13:VAL:HG21	1:A:203:VAL:HG21	2.01	0.42
1:A:359:PRO:HA	1:A:489:MET:HE3	1.98	0.42
1:A:212:GLU:O	1:A:215:LYS:N	2.50	0.42
1:A:162:GLU:HB3	1:A:164:GLN:HE21	1.84	0.42
1:A:262:CYS:O	1:A:272:TRP:HZ2	2.03	0.42
1:A:417:ALA:HB2	1:A:430:ASN:OD1	2.20	0.42
1:B:291:MET:HE2	1:B:291:MET:HB3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:SER:OG	1:A:145:GLN:N	2.53	0.42
1:A:332:HIS:ND1	1:A:333:ASP:HB2	2.35	0.42
1:B:462:LEU:C	1:B:464:TRP:N	2.73	0.42
1:B:401:ARG:O	1:B:402:THR:C	2.58	0.42
1:A:278:ALA:HA	1:A:281:GLN:HE21	1.85	0.42
1:A:243:LYS:NZ	1:A:246:ILE:HD13	2.35	0.42
1:A:401:ARG:O	1:A:402:THR:C	2.57	0.42
1:B:385:PHE:HD2	1:B:465:TYR:CD2	2.38	0.42
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.69	0.42
1:A:232:PRO:HD2	1:A:233:ASN:N	2.34	0.42
1:B:178:ASN:O	1:B:180:VAL:N	2.53	0.42
1:A:497:VAL:CG2	1:A:498:LEU:N	2.83	0.42
1:A:529:LYS:O	1:A:532:GLU:HG2	2.20	0.42
1:B:359:PRO:HA	1:B:489:MET:HE2	2.01	0.42
1:A:363:PRO:HD2	1:A:479:LEU:HD21	2.01	0.42
1:B:387:GLU:HA	1:B:388:PRO:HD3	1.75	0.41
1:B:165:ILE:H	1:B:165:ILE:HG13	1.34	0.41
1:B:276:ILE:HG22	1:B:277:PRO:N	2.35	0.41
1:A:458:PHE:C	1:A:461:PRO:HD2	2.40	0.41
1:B:440:ILE:HD12	1:B:440:ILE:HA	1.79	0.41
1:A:253:MET:HG2	1:A:280:ALA:CB	2.51	0.41
1:A:350:VAL:O	1:B:133:ARG:NH1	2.53	0.41
1:B:318:PHE:O	1:B:322:LEU:HB2	2.19	0.41
1:B:131:ASP:OD1	1:B:131:ASP:N	2.52	0.41
1:A:484:LEU:HD12	1:B:129:ASP:OD2	2.19	0.41
1:A:376:ILE:HG22	1:A:378:VAL:HG12	2.03	0.41
1:B:34:ARG:O	1:B:35:ASP:HB2	2.19	0.41
1:A:433:GLU:HA	1:A:433:GLU:OE1	2.20	0.41
1:A:91:ILE:CD1	1:A:91:ILE:H	2.33	0.41
1:B:33:PRO:HD3	1:B:80:ALA:HB3	2.02	0.41
1:A:162:GLU:HA	1:A:163:PRO:HD2	1.69	0.41
1:A:54:MET:HB2	1:A:159:ILE:HG21	2.01	0.41
1:A:339:VAL:HG13	1:A:353:VAL:CG1	2.39	0.41
1:A:364:ASP:HB2	1:A:367:VAL:HG23	2.02	0.41
1:A:291:MET:HB3	1:A:291:MET:HE2	1.79	0.41
1:B:515:ARG:NH1	1:B:515:ARG:CG	2.83	0.41
1:A:133:ARG:CG	1:B:348:GLU:HA	2.38	0.41
1:B:61:SER:OG	1:B:129:ASP:OD1	2.35	0.41
1:B:61:SER:O	1:B:65:PRO:HD3	2.20	0.41
1:B:22:ALA:CB	1:B:95:ALA:HB2	2.51	0.41
1:B:125:ASN:HB3	1:B:154:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:HB	1:B:118:THR:HB	2.01	0.41
1:A:205:ASN:ND2	1:A:207:ALA:CA	2.84	0.41
1:B:177:PRO:O	1:B:197:GLY:O	2.39	0.41
1:A:448:PHE:O	1:A:452:GLN:HG2	2.21	0.41
1:B:417:ALA:HB3	1:B:427:ILE:HA	2.02	0.41
1:A:230:CYS:O	1:A:231:ASN:HB3	2.20	0.41
1:A:139:MET:O	1:A:143:LEU:HD12	2.21	0.41
1:B:184:ASP:OD1	1:B:185:ASP:N	2.53	0.41
1:B:529:LYS:O	1:B:532:GLU:HG2	2.21	0.41
1:B:398:ASN:O	1:B:398:ASN:OD1	2.39	0.41
1:B:526:GLN:HG3	1:B:526:GLN:H	1.62	0.41
1:B:61:SER:H	1:B:61:SER:HG	1.48	0.40
1:A:376:ILE:HA	1:A:377:PRO:HD2	1.96	0.40
1:B:82:LEU:O	1:B:83:PRO:O	2.38	0.40
1:A:53:LEU:HD21	1:A:59:THR:O	2.21	0.40
1:B:376:ILE:HG22	1:B:378:VAL:HG12	2.02	0.40
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.34	0.40
1:A:17:PRO:HD2	1:A:99:ARG:HA	2.03	0.40
1:B:420:LYS:O	1:B:422:THR:N	2.55	0.40
1:B:166:TYR:O	1:B:169:LEU:HB3	2.21	0.40
1:A:59:THR:H	1:A:62:GLN:HG2	1.86	0.40
1:A:205:ASN:ND2	1:A:207:ALA:C	2.75	0.40
1:A:462:LEU:C	1:A:464:TRP:H	2.25	0.40
1:A:414:GLY:O	1:A:415:PHE:O	2.39	0.40
1:B:158:MET:HE2	1:B:164:GLN:O	2.21	0.40
1:A:332:HIS:CE1	1:A:333:ASP:HB2	2.56	0.40
1:A:398:ASN:OD1	1:A:398:ASN:O	2.39	0.40
1:A:8:PHE:HB2	1:A:14:LEU:HD11	2.04	0.40
1:B:462:LEU:O	1:B:464:TRP:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/554 (87%)	390 (81%)	59 (12%)	32 (7%)	1	4
1	B	539/554 (97%)	438 (81%)	68 (13%)	33 (6%)	2	5
All	All	1020/1108 (92%)	828 (81%)	127 (12%)	65 (6%)	2	4

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	208	SER
1	A	232	PRO
1	A	256	GLY
1	A	415	PHE
1	A	423	GLU
1	B	44	GLU
1	B	75	SER
1	B	76	LYS
1	B	78	CYS
1	B	205	ASN
1	B	207	ALA
1	B	208	SER
1	B	232	PRO
1	B	256	GLY
1	B	415	PHE
1	B	421	ALA
1	A	174	LYS
1	A	205	ASN
1	A	207	ALA
1	A	414	GLY
1	A	501	GLU
1	A	520	ASP
1	B	73	LYS
1	B	179	GLU
1	B	414	GLY
1	B	501	GLU
1	B	520	ASP
1	A	130	GLY
1	A	244	PRO
1	A	295	GLY
1	B	29	ALA
1	B	83	PRO
1	B	206	THR
1	B	244	PRO

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Mol	Chain	Res	Type
1	A	92	PHE
1	A	179	GLU
1	A	367	VAL
1	A	438	SER
1	A	506	MET
1	B	74	SER
1	B	214	GLU
1	B	295	GLY
1	B	434	ASP
1	B	438	SER
1	B	506	MET
1	A	11	ASP
1	A	91	ILE
1	B	111	ALA
1	B	203	VAL
1	B	367	VAL
1	A	222	PRO
1	A	266	PRO
1	A	277	PRO
1	A	288	ALA
1	A	496	ILE
1	B	266	PRO
1	B	277	PRO
1	A	218	GLY
1	A	301	PRO
1	B	496	ILE
1	B	301	PRO
1	A	231	ASN
1	A	157	GLY
1	A	180	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	424/480 (88%)	308 (73%)	116 (27%)	<b>0</b> <b>1</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	468/480 (98%)	339 (72%)	129 (28%)	0	1
All	All	892/960 (93%)	647 (72%)	245 (28%)	0	1

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	SER
1	A	19	ILE
1	A	53	LEU
1	A	58	ILE
1	A	61	SER
1	A	62	GLN
1	A	63	TRP
1	A	90	GLN
1	A	91	ILE
1	A	92	PHE
1	A	94	GLN
1	A	99	ARG
1	A	103	ARG
1	A	110	ILE
1	A	113	LYS
1	A	115	LYS
1	A	128	ASP
1	A	129	ASP
1	A	131	ASP
1	A	132	LYS
1	A	133	ARG
1	A	135	SER
1	A	139	MET
1	A	144	SER
1	A	148	ASP
1	A	153	SER
1	A	154	CYS
1	A	155	GLN
1	A	158	MET
1	A	165	ILE
1	A	166	TYR
1	A	178	ASN
1	A	179	GLU
1	A	183	LEU
1	A	190	LEU

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Mol	Chain	Res	Type
1	A	191	LYS
1	A	198	MET
1	A	202	LEU
1	A	204	HIS
1	A	205	ASN
1	A	206	THR
1	A	208	SER
1	A	213	LEU
1	A	214	GLU
1	A	215	LYS
1	A	217	THR
1	A	219	THR
1	A	220	GLN
1	A	221	PHE
1	A	223	GLU
1	A	230	CYS
1	A	231	ASN
1	A	236	SER
1	A	243	LYS
1	A	247	ARG
1	A	248	LEU
1	A	259	LEU
1	A	268	SER
1	A	275	GLN
1	A	279	LEU
1	A	287	LEU
1	A	297	SER
1	A	322	LEU
1	A	330	ILE
1	A	349	ARG
1	A	351	ARG
1	A	353	VAL
1	A	357	ASN
1	A	361	MET
1	A	364	ASP
1	A	370	MET
1	A	371	LYS
1	A	378	VAL
1	A	383	LEU
1	A	398	ASN
1	A	401	ARG
1	A	408	ARG

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Mol	Chain	Res	Type
1	A	412	GLU
1	A	413	THR
1	A	420	LYS
1	A	422	THR
1	A	423	GLU
1	A	424	ILE
1	A	427	ILE
1	A	436	ASN
1	A	437	LEU
1	A	440	ILE
1	A	444	GLU
1	A	447	GLU
1	A	451	GLN
1	A	455	LYS
1	A	456	THR
1	A	466	ARG
1	A	473	LYS
1	A	488	LEU
1	A	489	MET
1	A	494	LYS
1	A	497	VAL
1	A	499	ARG
1	A	501	GLU
1	A	502	MET
1	A	504	LYS
1	A	506	MET
1	A	507	GLU
1	A	508	LYS
1	A	512	PHE
1	A	513	LEU
1	A	515	ARG
1	A	519	GLU
1	A	525	THR
1	A	526	GLN
1	A	531	THR
1	A	539	LYS
1	A	542	GLN
1	A	544	GLU
1	B	13	VAL
1	B	19	ILE
1	B	24	ARG
1	B	32	LEU

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Mol	Chain	Res	Type
1	B	34	ARG
1	B	38	LEU
1	B	43	THR
1	B	45	PHE
1	B	50	THR
1	B	53	LEU
1	B	66	LEU
1	B	67	MET
1	B	69	GLU
1	B	72	ARG
1	B	73	LYS
1	B	74	SER
1	B	75	SER
1	B	81	ASN
1	B	84	GLU
1	B	85	ASN
1	B	91	ILE
1	B	101	ILE
1	B	103	ARG
1	B	106	LEU
1	B	107	GLN
1	B	110	ILE
1	B	122	VAL
1	B	127	LEU
1	B	128	ASP
1	B	131	ASP
1	B	132	LYS
1	B	133	ARG
1	B	140	MET
1	B	146	HIS
1	B	148	ASP
1	B	151	ILE
1	B	152	GLU
1	B	154	CYS
1	B	155	GLN
1	B	158	MET
1	B	164	GLN
1	B	165	ILE
1	B	173	LEU
1	B	178	ASN
1	B	179	GLU
1	B	181	VAL

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Mol	Chain	Res	Type
1	B	190	LEU
1	B	191	LYS
1	B	199	VAL
1	B	200	THR
1	B	202	LEU
1	B	204	HIS
1	B	206	THR
1	B	208	SER
1	B	212	GLU
1	B	213	LEU
1	B	214	GLU
1	B	215	LYS
1	B	216	VAL
1	B	217	THR
1	B	219	THR
1	B	228	VAL
1	B	230	CYS
1	B	231	ASN
1	B	236	SER
1	B	243	LYS
1	B	247	ARG
1	B	248	LEU
1	B	259	LEU
1	B	268	SER
1	B	275	GLN
1	B	279	LEU
1	B	287	LEU
1	B	297	SER
1	B	322	LEU
1	B	330	ILE
1	B	349	ARG
1	B	351	ARG
1	B	353	VAL
1	B	357	ASN
1	B	361	MET
1	B	364	ASP
1	B	370	MET
1	B	371	LYS
1	B	378	VAL
1	B	383	LEU
1	B	398	ASN
1	B	401	ARG

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Mol	Chain	Res	Type
1	B	408	ARG
1	B	412	GLU
1	B	413	THR
1	B	420	LYS
1	B	422	THR
1	B	423	GLU
1	B	424	ILE
1	B	427	ILE
1	B	428	LEU
1	B	431	THR
1	B	436	ASN
1	B	437	LEU
1	B	440	ILE
1	B	444	GLU
1	B	447	GLU
1	B	451	GLN
1	B	455	LYS
1	B	456	THR
1	B	466	ARG
1	B	473	LYS
1	B	488	LEU
1	B	489	MET
1	B	494	LYS
1	B	497	VAL
1	B	499	ARG
1	B	501	GLU
1	B	502	MET
1	B	504	LYS
1	B	506	MET
1	B	507	GLU
1	B	508	LYS
1	B	512	PHE
1	B	513	LEU
1	B	515	ARG
1	B	519	GLU
1	B	525	THR
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 (22) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	125	ASN
1	A	145	GLN
1	A	164	GLN
1	A	205	ASN
1	A	220	GLN
1	A	231	ASN
1	A	281	GLN
1	A	451	GLN
1	B	81	ASN
1	B	85	ASN
1	B	107	GLN
1	B	125	ASN
1	B	145	GLN
1	B	146	HIS
1	B	178	ASN
1	B	204	HIS
1	B	231	ASN
1	B	233	ASN
1	B	281	GLN
1	B	451	GLN
1	B	526	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.