



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:23 am BST

PDB ID : 1M3J
Title : CRYSTAL form II of perfringolysin O
Authors : Rossjohn, J.; Parker, M.; Polekhina, G.; Feil, S.; Tweten, R.
Deposited on : 2002-06-28
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

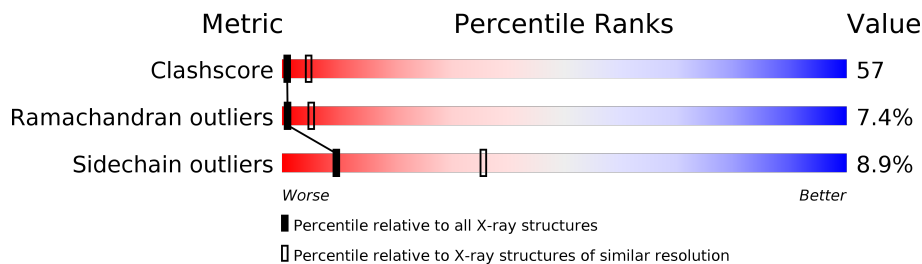
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7467 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 perfringolysin o.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	471	Total	C	N	O	S	0	0	0
			3705	2332	622	746	5			
1	B	471	Total	C	N	O	S	0	0	0
			3705	2332	622	746	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	LEU	PHE	see remark 999	UNP P19995
B	114	LEU	PHE	see remark 999	UNP P19995

- Molecule 2 is water.

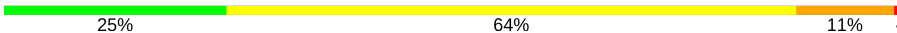
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	31	Total	O	0	0
			31	31		

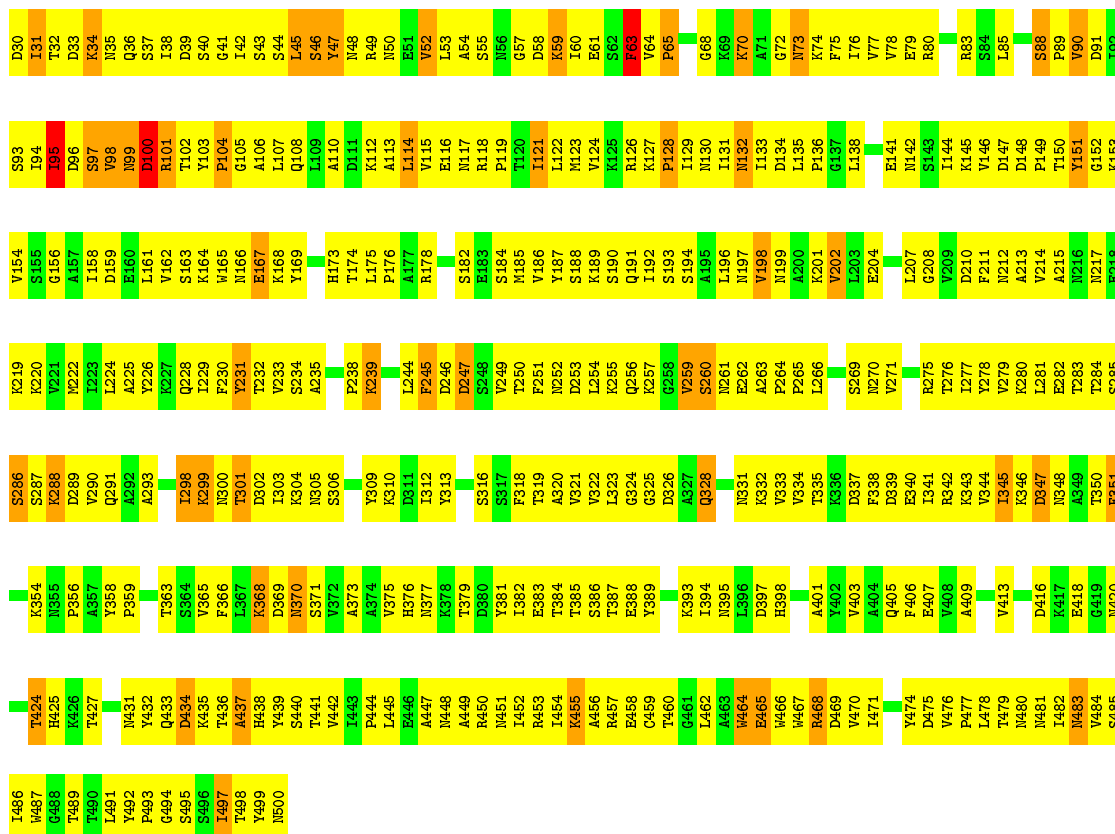
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

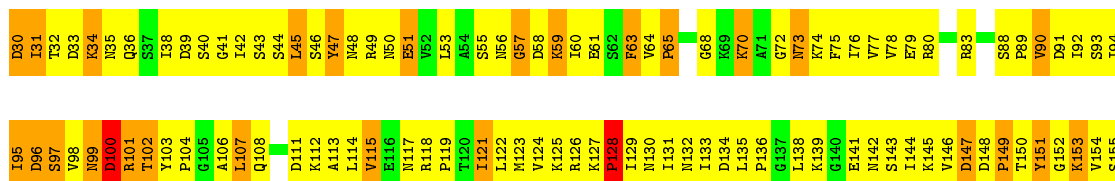
- Molecule 1: perfringolysin o

Chain A: 



- Molecule 1: perfringolysin o

Chain B: 



T490	H425	K855	A283	G156
L491	K426	P386	F294	A187
Y492	K427	A357	K295	I158
P493	T427	Y358	A296	D159
G494		P359	L297	
		I360	I298	V162
		S361	K299	S163
		Y362	N300	K164
		T363	T301	V165
		S364	D302	N166
		V365	I303	E167
		F366	K304	K168
		L367	N305	Y169
		K368	S306	
		D369	Q307	
		N370	Q308	T172
		S371	Y309	H173
		A372	K310	
		A373	D311	R178
		V374	E312	
		V375	Y313	S182
			E314	E183
		T379	N315	S184
		D380	S316	M185
		Y381	S317	V186
		L382	F318	Y187
		E383	T319	S188
		T384	A320	K189
		T385	V321	S190
		S386	V322	Q191
		T387	L323	I192
		E388	G324	S193
		Y389	G325	
		S390	D326	L196
		K391	A327	N197
		G392	Q328	V198
		K393	E329	N199
		L394	H330	
		N395	N331	V202
		L396	K332	L203
		D397	V333	E204
		H398	V334	
			T335	L207
		A401	K336	G208
		Y402	D337	V209
		V403	F338	D210
		A404	D339	F211
		Q405	E340	N212
		E406	I341	A213
		E407	R342	V214
		V408	K343	A215
		A409	V344	R216
			I345	L276
		E412	K346	L277
		V413	D347	Y278
			N348	V279
		K417	F351	K280
		E418		A213
		G419		L281
		T489		F282
				T283
				T284
				S285
				K219
				K220
				V221
				M222
				L223
				L224
				A225

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.00Å 214.11Å 47.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.00)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , 0.337	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7467	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/3776	0.70	0/5127
1	B	0.48	0/3776	0.70	0/5127
All	All	0.47	0/7552	0.70	0/10254

There are no bond length outliers.

There are no bond angle outliers.

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	3705	0	3656	427	0
1	B	3705	0	3656	418	0
2	A	26	0	0	3	0
2	B	31	0	0	0	0
All	All	7467	0	7312	845	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 57.

All (845) 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:96:ASP:HB2	1:B:100:ASP:HB2	1.22	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:HB2	1:A:100:ASP:HB2	1.23	1.16
1:A:481:ASN:HB2	1:A:500:ASN:ND2	1.62	1.12
1:B:70:LYS:H	1:B:70:LYS:HD3	1.08	1.10
1:A:70:LYS:HD3	1:A:70:LYS:H	1.15	1.09
1:A:96:ASP:HB3	1:A:99:ASN:HB2	1.30	1.08
1:B:163:SER:HA	1:B:166:ASN:HD22	1.20	1.06
1:A:305:ASN:HA	1:A:310:LYS:HE2	1.41	1.02
1:B:339:ASP:HA	1:B:342:ARG:HD2	1.37	1.02
1:B:53:LEU:HD21	1:B:114:LEU:HD23	1.41	1.01
1:A:468:ARG:HH11	1:A:468:ARG:HB3	1.25	1.01
1:A:226:TYR:HB2	1:A:277:ILE:HB	1.42	1.01
1:A:481:ASN:HB2	1:A:500:ASN:HD22	0.87	1.00
1:A:38:ILE:HA	1:A:251:PHE:HB2	1.42	1.00
1:A:462:LEU:HD22	1:A:466:TRP:HZ3	1.27	0.99
1:A:335:THR:HG22	1:A:337:ASP:H	1.27	0.98
1:A:449:ALA:C	1:A:450:ARG:HD2	1.84	0.97
1:B:59:LYS:HB2	1:B:59:LYS:HZ2	1.29	0.97
1:B:393:LYS:HD2	1:B:442:VAL:HG11	1.45	0.97
1:B:130:ASN:HD21	1:B:145:LYS:HE2	1.31	0.96
1:A:182:SER:HB2	1:A:225:ALA:HB3	1.48	0.95
1:A:277:ILE:CD1	1:A:345:ILE:HA	1.97	0.94
1:B:335:THR:HG22	1:B:337:ASP:H	1.30	0.94
1:A:59:LYS:HZ2	1:A:59:LYS:HB2	1.34	0.93
1:B:96:ASP:CB	1:B:100:ASP:H	1.82	0.92
1:B:226:TYR:HB2	1:B:277:ILE:HB	1.48	0.92
1:A:96:ASP:HB3	1:A:100:ASP:H	1.33	0.92
1:A:479:THR:HG21	1:A:499:TYR:HB3	1.50	0.92
1:A:462:LEU:HD22	1:A:466:TRP:CZ3	2.05	0.90
1:A:96:ASP:CB	1:A:100:ASP:H	1.83	0.90
1:A:418:GLU:HB2	1:A:420:ASN:ND2	1.88	0.88
1:A:394:ILE:HD11	1:A:445:LEU:HD11	1.54	0.88
1:A:96:ASP:HB2	1:A:100:ASP:CB	2.04	0.87
1:B:107:LEU:HD11	1:B:126:ARG:HH11	1.37	0.87
1:B:186:VAL:O	1:B:214:VAL:HG11	1.73	0.86
1:B:96:ASP:HB2	1:B:100:ASP:CB	2.03	0.86
1:A:343:LYS:HG2	1:A:347:ASP:OD2	1.75	0.86
1:B:277:ILE:HD13	1:B:345:ILE:HA	1.58	0.86
1:B:128:PRO:HG3	1:B:147:ASP:HA	1.59	0.84
1:B:182:SER:HB2	1:B:225:ALA:HB3	1.57	0.84
1:B:343:LYS:HA	1:B:346:LYS:HE3	1.58	0.84
1:B:90:VAL:O	1:B:363:THR:HG22	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HG3	1:A:50:ASN:ND2	1.93	0.84
1:B:412:GLU:HG3	1:B:426:LYS:HD2	1.60	0.84
1:B:79:GLU:HB2	1:B:385:THR:OG1	1.77	0.83
1:A:277:ILE:HD13	1:A:345:ILE:HA	1.60	0.83
1:B:277:ILE:HG12	1:B:322:VAL:HG22	1.60	0.83
1:B:239:LYS:H	1:B:239:LYS:HD2	1.42	0.83
1:B:403:VAL:HG11	1:B:434:ASP:OD2	1.78	0.83
1:B:398:HIS:HA	1:B:486:ILE:HD11	1.59	0.83
1:B:43:SER:HA	1:B:368:LYS:HG3	1.60	0.82
1:A:103:TYR:CD1	1:A:154:VAL:HG21	2.14	0.82
1:A:95:ILE:HG22	1:A:96:ASP:N	1.95	0.82
1:A:220:LYS:HD2	1:A:290:VAL:HG21	1.62	0.82
1:B:104:PRO:HB2	1:B:235:ALA:HB2	1.61	0.82
1:B:96:ASP:HB2	1:B:100:ASP:H	1.43	0.82
1:A:224:LEU:HB2	1:A:279:VAL:HB	1.60	0.82
1:B:456:ALA:HB3	1:B:471:ILE:HG22	1.60	0.81
1:A:70:LYS:HD3	1:A:70:LYS:N	1.94	0.81
1:A:101:ARG:NE	1:A:101:ARG:H	1.79	0.81
1:A:232:THR:HB	1:A:271:VAL:O	1.81	0.81
1:B:70:LYS:N	1:B:70:LYS:HD3	1.91	0.81
1:B:95:ILE:HG12	1:B:117:ASN:HB2	1.63	0.80
1:A:33:ASP:O	1:A:34:LYS:HG3	1.82	0.80
1:A:398:HIS:ND1	1:A:486:ILE:HD11	1.97	0.80
1:B:224:LEU:HB2	1:B:279:VAL:HB	1.64	0.79
1:B:107:LEU:HD11	1:B:126:ARG:NH1	1.98	0.79
1:B:38:ILE:HA	1:B:251:PHE:HB2	1.64	0.79
1:A:491:LEU:HD22	1:A:492:TYR:CE1	2.18	0.79
1:B:95:ILE:HG12	1:B:117:ASN:CB	2.13	0.79
1:A:178:ARG:HB2	1:A:229:ILE:HB	1.62	0.78
1:A:59:LYS:NZ	1:A:59:LYS:HB2	1.95	0.78
1:B:148:ASP:O	1:B:153:LYS:HG2	1.83	0.78
1:B:402:TYR:HB3	1:B:490:THR:OG1	1.84	0.78
1:A:104:PRO:HG3	1:A:233:VAL:CG1	2.14	0.78
1:B:449:ALA:C	1:B:450:ARG:HD2	2.03	0.78
1:A:124:VAL:HG21	1:A:245:PHE:HD2	1.48	0.78
1:A:413:VAL:HG11	1:A:450:ARG:NH1	1.99	0.78
1:A:150:THR:O	1:A:154:VAL:HG23	1.83	0.77
1:A:80:ARG:HG3	1:A:80:ARG:HH11	1.48	0.77
1:A:458:GLU:O	1:A:467:TRP:HB3	1.84	0.77
1:B:457:ARG:HD3	1:B:469:ASP:OD2	1.84	0.77
1:A:418:GLU:HB2	1:A:420:ASN:HD22	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ILE:HG21	1:A:484:VAL:HG21	1.67	0.77
1:A:306:SER:O	1:A:310:LYS:HG2	1.85	0.76
1:A:49:ARG:HG3	1:A:50:ASN:HD22	1.49	0.76
1:B:129:ILE:HG12	1:B:130:ASN:H	1.49	0.76
1:B:96:ASP:HB3	1:B:100:ASP:H	1.50	0.76
1:A:98:VAL:HG12	1:A:325:GLY:HA2	1.67	0.76
1:B:135:LEU:HD23	1:B:136:PRO:HD2	1.66	0.76
1:B:96:ASP:HB3	1:B:99:ASN:HB2	1.67	0.76
1:A:101:ARG:HE	1:A:101:ARG:H	1.31	0.76
1:A:104:PRO:HG3	1:A:233:VAL:HG11	1.68	0.76
1:A:305:ASN:HA	1:A:310:LYS:CE	2.15	0.75
1:A:210:ASP:OD2	1:A:213:ALA:HB2	1.87	0.75
1:A:339:ASP:HA	1:A:342:ARG:HD2	1.69	0.74
1:A:263:ALA:N	1:A:264:PRO:HD3	2.02	0.74
1:B:306:SER:O	1:B:310:LYS:HG2	1.88	0.74
1:A:144:ILE:HG13	1:A:145:LYS:H	1.52	0.74
1:A:144:ILE:HB	1:A:161:LEU:HD21	1.67	0.74
1:A:491:LEU:HD22	1:A:492:TYR:CD1	2.23	0.74
1:A:465:GLU:CD	1:A:465:GLU:H	1.89	0.74
1:B:457:ARG:NH2	1:B:465:GLU:HA	2.03	0.73
1:B:103:TYR:CD1	1:B:154:VAL:HG21	2.23	0.73
1:B:163:SER:HA	1:B:166:ASN:ND2	1.99	0.73
1:B:263:ALA:N	1:B:264:PRO:HD3	2.03	0.73
1:A:96:ASP:HB3	1:A:99:ASN:CB	2.14	0.73
1:B:335:THR:HG22	1:B:337:ASP:N	2.04	0.73
1:B:49:ARG:HG3	1:B:50:ASN:N	2.03	0.73
1:B:91:ASP:OD1	1:B:361:SER:OG	2.06	0.73
1:A:335:THR:HG21	1:A:340:GLU:HG3	1.69	0.73
1:B:112:LYS:HA	1:B:115:VAL:HG23	1.70	0.73
1:B:70:LYS:CD	1:B:70:LYS:H	1.93	0.73
1:B:130:ASN:ND2	1:B:145:LYS:HE2	2.04	0.72
1:A:121:ILE:HD13	1:A:122:LEU:H	1.54	0.72
1:B:365:VAL:HG13	1:B:371:SER:O	1.88	0.72
1:A:158:ILE:O	1:A:162:VAL:HG23	1.89	0.72
1:B:398:HIS:ND1	1:B:486:ILE:HD11	2.04	0.72
1:A:196:LEU:HD22	1:A:225:ALA:HB2	1.72	0.72
1:A:133:ILE:HG13	1:A:232:THR:O	1.89	0.72
1:A:123:MET:H	1:A:257:LYS:HE2	1.51	0.72
1:B:230:PHE:HZ	1:B:275:ARG:NH1	1.88	0.72
1:B:55:SER:HB3	1:B:115:VAL:HG11	1.70	0.72
1:B:95:ILE:HG22	1:B:96:ASP:N	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASP:OD1	1:A:420:ASN:HB2	1.90	0.71
1:B:98:VAL:HG12	1:B:358:TYR:HD1	1.56	0.71
1:B:230:PHE:HB3	1:B:351:PHE:CE1	2.25	0.71
1:A:41:GLY:HA3	1:A:251:PHE:CE2	2.25	0.71
1:A:98:VAL:HG12	1:A:358:TYR:CD1	2.25	0.71
1:A:403:VAL:HG11	1:A:434:ASP:OD2	1.91	0.71
1:B:417:LYS:NZ	1:B:417:LYS:HB2	2.06	0.71
1:A:213:ALA:HB1	1:A:219:LYS:HG3	1.71	0.71
1:A:266:LEU:HD23	1:A:366:PHE:HA	1.73	0.71
1:A:468:ARG:CB	1:A:468:ARG:HH11	2.04	0.70
1:B:104:PRO:HG3	1:B:233:VAL:HG12	1.73	0.70
1:A:259:VAL:HG13	1:A:265:PRO:HD3	1.72	0.70
1:B:476:VAL:HG13	1:B:499:TYR:OH	1.91	0.70
1:B:366:PHE:CE1	1:B:373:ALA:HA	2.26	0.70
1:B:458:GLU:O	1:B:467:TRP:HB3	1.92	0.70
1:B:324:GLY:O	1:B:358:TYR:HB2	1.91	0.70
1:B:129:ILE:HG12	1:B:130:ASN:N	2.06	0.70
1:B:96:ASP:HB3	1:B:99:ASN:CB	2.22	0.70
1:B:393:LYS:HD2	1:B:442:VAL:CG1	2.22	0.70
1:A:393:LYS:HD2	1:A:442:VAL:HG11	1.74	0.69
1:B:178:ARG:HB2	1:B:229:ILE:HB	1.73	0.69
1:A:107:LEU:O	1:A:121:ILE:HD13	1.92	0.69
1:B:53:LEU:HD21	1:B:114:LEU:CD2	2.20	0.69
1:B:339:ASP:HA	1:B:342:ARG:CD	2.20	0.69
1:A:158:ILE:HD13	1:A:233:VAL:HG21	1.73	0.69
1:B:123:MET:H	1:B:257:LYS:HE2	1.57	0.69
1:B:287:SER:O	1:B:290:VAL:HG23	1.93	0.69
1:B:31:ILE:HD11	1:B:35:ASN:O	1.92	0.69
1:A:114:LEU:HA	1:A:119:PRO:HB3	1.74	0.68
1:B:199:ASN:HB3	1:B:202:VAL:HG23	1.72	0.68
1:B:398:HIS:HA	1:B:486:ILE:CD1	2.23	0.68
1:A:144:ILE:HG13	1:A:145:LYS:N	2.07	0.68
1:B:452:ILE:HD11	1:B:478:LEU:HD13	1.75	0.68
1:A:185:MET:SD	1:A:222:MET:HG3	2.34	0.68
1:A:34:LYS:HE2	1:A:34:LYS:C	2.14	0.68
1:B:192:ILE:HG12	1:B:223:ILE:HD12	1.76	0.68
1:A:228:GLN:HA	1:A:228:GLN:HE21	1.57	0.68
1:A:409:ALA:HB2	1:A:427:THR:HG22	1.75	0.67
1:B:46:SER:O	1:B:47:TYR:HB3	1.93	0.67
1:B:38:ILE:HG23	1:B:39:ASP:H	1.59	0.67
1:A:98:VAL:CG1	1:A:325:GLY:HA2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:THR:HB	1:A:431:ASN:ND2	2.10	0.67
1:B:96:ASP:CB	1:B:100:ASP:HB2	2.13	0.67
1:B:30:ASP:CA	1:B:36:GLN:HG2	2.25	0.67
1:B:479:THR:HG21	1:B:499:TYR:HB3	1.77	0.67
1:A:85:LEU:HD23	1:A:194:SER:HB3	1.75	0.67
1:A:110:ALA:HB2	1:A:266:LEU:HD11	1.77	0.66
1:A:107:LEU:HD11	1:A:126:ARG:HH11	1.59	0.66
1:A:94:ILE:HD12	1:A:359:PRO:HB2	1.76	0.66
1:A:46:SER:O	1:A:47:TYR:HB3	1.95	0.66
1:A:462:LEU:HB3	1:A:466:TRP:CE3	2.29	0.66
1:B:449:ALA:O	1:B:450:ARG:HD2	1.95	0.66
1:B:480:ASN:HB2	1:B:500:ASN:O	1.96	0.66
1:B:394:ILE:HG12	1:B:482:ILE:HB	1.78	0.66
1:A:131:ILE:HG23	1:A:233:VAL:HG13	1.78	0.66
1:A:144:ILE:HD11	2:A:506:HOH:O	1.96	0.66
1:B:133:ILE:HD11	1:B:231:TYR:CD2	2.30	0.66
1:B:230:PHE:CE1	1:B:351:PHE:HB2	2.31	0.66
1:B:391:LYS:HG2	1:B:447:ALA:H	1.60	0.66
1:A:124:VAL:HG21	1:A:245:PHE:CD2	2.31	0.66
1:A:457:ARG:HG2	1:A:467:TRP:HB2	1.76	0.65
1:A:452:ILE:CD1	1:A:478:LEU:HD13	2.26	0.65
1:A:452:ILE:HD11	1:A:478:LEU:HD13	1.78	0.65
1:B:277:ILE:CD1	1:B:345:ILE:HA	2.27	0.65
1:A:312:ILE:HA	2:A:524:HOH:O	1.95	0.65
1:A:318:PHE:HD1	1:A:335:THR:O	1.79	0.65
1:A:134:ASP:OD1	1:A:232:THR:HG23	1.97	0.65
1:A:97:SER:HB3	1:A:324:GLY:HA2	1.79	0.65
1:A:68:GLY:HA2	1:A:76:ILE:O	1.97	0.64
1:B:413:VAL:HG11	1:B:450:ARG:NH1	2.12	0.64
1:B:49:ARG:HG3	1:B:50:ASN:H	1.62	0.64
1:A:98:VAL:HG12	1:A:358:TYR:HD1	1.62	0.64
1:A:96:ASP:HB2	1:A:100:ASP:H	1.62	0.64
1:A:366:PHE:CE1	1:A:373:ALA:HA	2.32	0.64
1:B:30:ASP:HA	1:B:36:GLN:HG2	1.80	0.64
1:A:199:ASN:HB3	1:A:202:VAL:HG23	1.79	0.64
1:A:309:TYR:HB3	1:A:313:TYR:CE1	2.32	0.64
1:B:135:LEU:CD2	1:B:136:PRO:HD2	2.26	0.64
1:B:128:PRO:HA	1:B:146:VAL:O	1.98	0.64
1:B:96:ASP:HB2	1:B:100:ASP:N	2.10	0.64
1:A:477:PRO:O	1:A:482:ILE:HD11	1.98	0.64
1:B:275:ARG:HD2	1:B:322:VAL:CG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG13	1:B:265:PRO:HD3	1.79	0.64
1:A:337:ASP:OD2	1:A:339:ASP:HB2	1.99	0.64
1:A:182:SER:HB2	1:A:225:ALA:CB	2.24	0.63
1:B:98:VAL:HG12	1:B:358:TYR:CD1	2.33	0.63
1:A:305:ASN:CA	1:A:310:LYS:HE2	2.25	0.63
1:A:95:ILE:HG12	1:A:117:ASN:CB	2.29	0.63
1:B:305:ASN:HA	1:B:310:LYS:HE2	1.81	0.63
1:B:45:LEU:O	1:B:368:LYS:NZ	2.22	0.63
1:B:212:ASN:HA	1:B:215:ALA:HB3	1.80	0.63
1:A:449:ALA:O	1:A:450:ARG:HD2	1.99	0.63
1:A:339:ASP:HA	1:A:342:ARG:CD	2.29	0.63
1:A:394:ILE:HG23	1:A:482:ILE:O	1.98	0.63
1:B:457:ARG:HH21	1:B:465:GLU:HA	1.63	0.63
1:A:134:ASP:CG	1:A:178:ARG:HH22	2.02	0.62
1:A:31:ILE:HD11	1:A:35:ASN:O	1.98	0.62
1:A:75:PHE:HB3	1:A:389:TYR:HB2	1.81	0.62
1:B:291:GLN:O	1:B:295:LYS:HG3	2.00	0.62
1:A:107:LEU:HD12	1:A:107:LEU:N	2.15	0.62
1:A:187:TYR:HD1	1:A:381:TYR:HE1	1.46	0.62
1:A:409:ALA:HB1	1:A:425:HIS:CE1	2.34	0.62
1:B:60:ILE:HG12	1:B:61:GLU:N	2.14	0.62
1:A:138:LEU:CD1	1:A:141:GLU:HG3	2.30	0.62
1:B:319:THR:HA	1:B:333:VAL:O	2.00	0.62
1:A:103:TYR:OH	1:A:150:THR:HA	2.00	0.62
1:B:369:ASP:OD2	1:B:371:SER:HB3	1.99	0.62
1:A:269:SER:HB3	1:A:365:VAL:HG23	1.82	0.61
1:A:95:ILE:CG2	1:A:96:ASP:N	2.62	0.61
1:A:129:ILE:C	1:A:130:ASN:HD22	2.02	0.61
1:A:130:ASN:HD21	1:A:145:LYS:HE2	1.65	0.61
1:A:138:LEU:HD12	1:A:141:GLU:HG3	1.82	0.61
1:A:222:MET:O	1:A:281:LEU:HD12	2.00	0.61
1:A:413:VAL:HG12	1:A:448:ASN:O	2.00	0.61
1:B:394:ILE:HA	1:B:482:ILE:O	2.00	0.61
1:B:486:ILE:O	1:B:486:ILE:HD12	2.01	0.61
1:B:73:ASN:C	1:B:74:LYS:HG3	2.20	0.61
1:A:89:PRO:HD2	1:A:375:VAL:O	2.01	0.60
1:A:90:VAL:O	1:A:363:THR:HG22	2.00	0.60
1:B:48:ASN:HD22	1:B:51:GLU:HB2	1.66	0.60
1:B:230:PHE:CD1	1:B:351:PHE:HB2	2.36	0.60
1:B:89:PRO:HD2	1:B:375:VAL:O	2.01	0.60
1:A:107:LEU:HD11	1:A:126:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LYS:HD2	1:B:290:VAL:HG21	1.83	0.60
1:B:263:ALA:N	1:B:264:PRO:CD	2.62	0.60
1:B:401:ALA:HB3	1:B:489:THR:HA	1.84	0.60
1:A:53:LEU:O	1:A:375:VAL:HA	2.02	0.59
1:B:154:VAL:O	1:B:158:ILE:HG13	2.02	0.59
1:B:198:VAL:HG11	1:B:278:TYR:OH	2.01	0.59
1:B:291:GLN:HE21	1:B:295:LYS:HD2	1.65	0.59
1:A:130:ASN:C	1:A:131:ILE:HD12	2.22	0.59
1:A:397:ASP:HB3	1:A:485:SER:OG	2.02	0.59
1:B:125:LYS:HD3	1:B:246:ASP:OD2	2.01	0.59
1:A:30:ASP:CA	1:A:36:GLN:HG2	2.32	0.59
1:B:263:ALA:H	1:B:264:PRO:HD3	1.67	0.59
1:B:33:ASP:O	1:B:34:LYS:HG3	2.01	0.59
1:B:462:LEU:HD23	1:B:462:LEU:O	2.02	0.59
1:B:454:ILE:HG21	1:B:484:VAL:HG21	1.83	0.59
1:B:259:VAL:HG12	1:B:260:SER:N	2.18	0.59
1:A:104:PRO:HG3	1:A:233:VAL:HG12	1.85	0.59
1:A:95:ILE:HG22	1:A:96:ASP:H	1.66	0.59
1:B:189:LYS:HG2	1:B:211:PHE:CZ	2.38	0.59
1:B:293:ALA:HB1	1:B:313:TYR:CE2	2.38	0.59
1:B:133:ILE:HD13	1:B:135:LEU:HD12	1.85	0.59
1:B:207:LEU:HD22	1:B:280:LYS:HB2	1.85	0.59
1:B:461:GLY:C	1:B:467:TRP:HE1	2.06	0.59
1:A:319:THR:HA	1:A:333:VAL:O	2.03	0.59
1:A:462:LEU:O	1:A:462:LEU:HD23	2.03	0.59
1:A:49:ARG:CG	1:A:50:ASN:ND2	2.64	0.59
1:B:124:VAL:HG21	1:B:245:PHE:HD2	1.68	0.59
1:B:68:GLY:HA2	1:B:76:ILE:O	2.03	0.59
1:A:228:GLN:HA	1:A:228:GLN:NE2	2.17	0.58
1:B:134:ASP:OD1	1:B:232:THR:HG23	2.03	0.58
1:B:30:ASP:CG	1:B:36:GLN:HB3	2.23	0.58
1:B:391:LYS:HG2	1:B:447:ALA:N	2.18	0.58
1:B:491:LEU:HD22	1:B:492:TYR:CE1	2.38	0.58
1:A:41:GLY:HA3	1:A:251:PHE:CD2	2.39	0.58
1:A:114:LEU:O	1:A:114:LEU:HD12	2.04	0.58
1:A:254:LEU:O	1:A:259:VAL:HG23	2.03	0.58
1:B:60:ILE:CD1	1:B:382:ILE:HD11	2.34	0.58
1:A:263:ALA:N	1:A:264:PRO:CD	2.67	0.58
1:A:275:ARG:HB2	1:A:323:LEU:O	2.04	0.58
1:B:275:ARG:HB2	1:B:323:LEU:O	2.04	0.58
1:A:222:MET:HE1	1:A:281:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD21	1:A:278:TYR:O	2.02	0.58
1:A:79:GLU:HB2	1:A:385:THR:OG1	2.04	0.58
1:B:83:ARG:NE	1:B:383:GLU:OE2	2.37	0.58
1:A:275:ARG:HH21	1:A:348:ASN:CA	2.16	0.57
1:A:48:ASN:O	1:A:52:VAL:HG13	2.03	0.57
1:B:111:ASP:O	1:B:114:LEU:HB3	2.04	0.57
1:A:30:ASP:CB	1:A:36:GLN:HG2	2.35	0.57
1:A:239:LYS:HD2	1:A:239:LYS:H	1.69	0.57
1:A:38:ILE:HG23	1:A:39:ASP:H	1.69	0.57
1:A:80:ARG:CG	1:A:80:ARG:HH11	2.17	0.57
1:A:230:PHE:CE1	1:A:351:PHE:HB2	2.40	0.57
1:A:413:VAL:HG11	1:A:450:ARG:CZ	2.35	0.57
1:A:484:VAL:CG2	1:A:497:ILE:HD12	2.34	0.57
1:A:133:ILE:HD11	1:A:231:TYR:CD2	2.40	0.57
1:A:432:TYR:O	1:A:433:GLN:HG3	2.04	0.57
1:B:77:VAL:O	1:B:386:SER:HA	2.05	0.57
1:B:284:THR:OG1	1:B:315:ASN:HB3	2.04	0.57
1:A:287:SER:O	1:A:290:VAL:HG23	2.04	0.57
1:A:409:ALA:CB	1:A:427:THR:HG22	2.34	0.57
1:A:98:VAL:HA	1:A:358:TYR:CD1	2.39	0.57
1:B:104:PRO:CB	1:B:235:ALA:HB2	2.34	0.56
1:B:486:ILE:C	1:B:486:ILE:HD12	2.25	0.56
1:A:471:ILE:HD13	1:A:495:SER:HB2	1.85	0.56
1:B:103:TYR:HB2	1:B:104:PRO:HD2	1.87	0.56
1:A:365:VAL:HG13	1:A:371:SER:O	2.05	0.56
1:A:394:ILE:HA	1:A:482:ILE:O	2.05	0.56
1:B:95:ILE:CG1	1:B:117:ASN:HB2	2.35	0.56
1:A:158:ILE:CD1	1:A:233:VAL:HG21	2.35	0.56
1:B:230:PHE:CE2	1:B:274:GLY:HA2	2.40	0.56
1:A:298:ILE:HG22	1:A:299:LYS:N	2.20	0.56
1:B:468:ARG:HH11	1:B:468:ARG:HB3	1.69	0.56
1:A:134:ASP:OD2	1:A:231:TYR:HB2	2.04	0.56
1:A:31:ILE:H	1:A:31:ILE:HD12	1.70	0.56
1:B:465:GLU:CD	1:B:465:GLU:H	2.08	0.56
1:B:96:ASP:HB3	1:B:99:ASN:OD1	2.04	0.56
1:A:226:TYR:CB	1:A:277:ILE:HB	2.27	0.56
1:A:298:ILE:C	1:A:300:ASN:H	2.09	0.56
1:A:491:LEU:C	1:A:493:PRO:HD3	2.25	0.56
1:A:401:ALA:HB3	1:A:489:THR:HA	1.87	0.56
1:B:104:PRO:HG3	1:B:233:VAL:CG1	2.34	0.56
1:B:230:PHE:CD2	1:B:274:GLY:HA2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ILE:HD11	1:B:382:ILE:HD11	1.88	0.56
1:B:150:THR:O	1:B:154:VAL:HG23	2.06	0.55
1:B:101:ARG:NE	1:B:101:ARG:H	2.04	0.55
1:A:275:ARG:HH21	1:A:348:ASN:C	2.09	0.55
1:B:293:ALA:HB1	1:B:313:TYR:HE2	1.71	0.55
1:B:369:ASP:CG	1:B:371:SER:HB3	2.27	0.55
1:A:189:LYS:O	1:A:193:SER:HB2	2.06	0.55
1:A:238:PRO:HB3	1:A:244:LEU:HD21	1.88	0.55
1:A:481:ASN:CB	1:A:500:ASN:ND2	2.54	0.55
1:B:207:LEU:HD21	1:B:278:TYR:O	2.07	0.55
1:A:230:PHE:HZ	1:A:275:ARG:NH1	2.05	0.55
1:B:209:VAL:HG12	1:B:211:PHE:H	1.72	0.55
1:A:186:VAL:O	1:A:214:VAL:HG11	2.07	0.54
1:B:138:LEU:HD12	1:B:141:GLU:HG3	1.89	0.54
1:B:94:ILE:HD13	1:B:359:PRO:HB2	1.88	0.54
1:A:407:GLU:HA	1:A:431:ASN:OD1	2.08	0.54
1:B:452:ILE:O	1:B:476:VAL:N	2.37	0.54
1:A:163:SER:HA	1:A:166:ASN:ND2	2.22	0.54
1:B:226:TYR:CE1	1:B:345:ILE:HD13	2.42	0.54
1:B:464:TRP:HA	1:B:467:TRP:CE3	2.42	0.54
1:B:189:LYS:HG2	1:B:211:PHE:CE1	2.42	0.54
1:B:456:ALA:H	1:B:471:ILE:HG23	1.72	0.54
1:A:452:ILE:O	1:A:476:VAL:N	2.33	0.54
1:B:259:VAL:O	1:B:260:SER:HB3	2.08	0.54
1:B:72:GLY:O	1:B:74:LYS:N	2.38	0.54
1:A:156:GLY:O	1:A:159:ASP:HB2	2.08	0.53
1:A:214:VAL:HA	1:A:219:LYS:O	2.09	0.53
1:A:281:LEU:N	1:A:281:LEU:HD12	2.23	0.53
1:B:304:LYS:HA	1:B:309:TYR:HD2	1.74	0.53
1:B:38:ILE:HG23	1:B:39:ASP:N	2.22	0.53
1:B:457:ARG:CD	1:B:469:ASP:OD2	2.55	0.53
1:A:42:ILE:O	1:A:45:LEU:HB2	2.09	0.53
1:A:97:SER:C	1:A:99:ASN:H	2.11	0.53
1:A:186:VAL:HG22	1:A:192:ILE:HD13	1.89	0.53
1:B:107:LEU:HB2	1:B:122:LEU:HB2	1.90	0.53
1:B:276:THR:CG2	1:B:278:TYR:CE1	2.92	0.53
1:B:59:LYS:HB2	1:B:59:LYS:NZ	2.10	0.53
1:A:187:TYR:HD1	1:A:381:TYR:CE1	2.25	0.53
1:B:346:LYS:C	1:B:348:ASN:H	2.12	0.53
1:B:83:ARG:CB	1:B:381:TYR:CZ	2.91	0.53
1:B:456:ALA:HB3	1:B:471:ILE:CG2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:N	1:A:167:GLU:OE2	2.41	0.53
1:A:259:VAL:O	1:A:260:SER:HB3	2.09	0.53
1:A:259:VAL:HG12	1:A:260:SER:N	2.23	0.53
1:A:394:ILE:HG23	1:A:482:ILE:HG22	1.89	0.53
1:B:58:ASP:OD2	1:B:190:SER:CB	2.56	0.53
1:B:207:LEU:HD11	1:B:278:TYR:HB3	1.90	0.53
1:A:99:ASN:OD1	1:A:99:ASN:N	2.42	0.53
1:B:391:LYS:HG3	1:B:447:ALA:HB2	1.90	0.53
1:B:491:LEU:HD22	1:B:492:TYR:CD1	2.44	0.53
1:A:113:ALA:HA	1:A:118:ARG:NH1	2.24	0.52
1:A:129:ILE:HG12	1:A:130:ASN:H	1.74	0.52
1:A:335:THR:HG22	1:A:337:ASP:N	2.10	0.52
1:A:41:GLY:HA3	1:A:251:PHE:CZ	2.44	0.52
1:A:457:ARG:HD3	1:A:469:ASP:OD2	2.08	0.52
1:B:253:ASP:O	1:B:257:LYS:HG3	2.08	0.52
1:B:189:LYS:O	1:B:193:SER:HB2	2.08	0.52
1:B:491:LEU:O	1:B:493:PRO:HD3	2.09	0.52
1:B:96:ASP:HB3	1:B:99:ASN:CG	2.30	0.52
1:A:188:SER:O	1:A:192:ILE:HG22	2.09	0.52
1:A:107:LEU:HB2	1:A:122:LEU:HB2	1.91	0.52
1:A:346:LYS:C	1:A:348:ASN:H	2.13	0.52
1:B:366:PHE:CZ	1:B:373:ALA:HA	2.44	0.52
1:B:464:TRP:C	1:B:466:TRP:H	2.13	0.52
1:A:30:ASP:HA	1:A:36:GLN:HG2	1.90	0.52
1:B:48:ASN:ND2	1:B:51:GLU:HB2	2.24	0.52
1:B:93:SER:O	1:B:117:ASN:ND2	2.40	0.52
1:A:480:ASN:HB2	1:A:500:ASN:O	2.10	0.52
1:B:224:LEU:HD11	1:B:281:LEU:HD11	1.92	0.52
1:B:427:THR:HB	1:B:431:ASN:ND2	2.25	0.52
1:B:433:GLN:O	1:B:435:LYS:NZ	2.41	0.52
1:A:103:TYR:CE1	1:A:154:VAL:HG21	2.45	0.52
1:A:325:GLY:HA3	1:A:358:TYR:CD1	2.45	0.52
1:B:150:THR:HB	1:B:153:LYS:HB2	1.92	0.52
1:B:230:PHE:HB3	1:B:351:PHE:CZ	2.43	0.52
1:A:96:ASP:CB	1:A:99:ASN:HB2	2.22	0.52
1:B:224:LEU:CD1	1:B:281:LEU:HD11	2.39	0.52
1:B:269:SER:OG	1:B:365:VAL:HG23	2.09	0.52
1:B:441:THR:CG2	1:B:442:VAL:N	2.72	0.52
1:A:77:VAL:O	1:A:386:SER:HA	2.09	0.52
1:B:434:ASP:O	1:B:435:LYS:HD3	2.10	0.52
1:A:275:ARG:HD2	1:A:322:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HD12	1:A:345:ILE:HA	1.89	0.52
1:B:365:VAL:HG13	1:B:371:SER:C	2.29	0.52
1:A:85:LEU:CD2	1:A:194:SER:HB3	2.40	0.51
1:B:130:ASN:HB2	1:B:236:ASP:OD1	2.10	0.51
1:B:144:ILE:HG13	1:B:145:LYS:H	1.75	0.51
1:B:112:LYS:O	1:B:113:ALA:C	2.47	0.51
1:A:298:ILE:O	1:A:300:ASN:N	2.43	0.51
1:A:60:ILE:HD11	1:A:382:ILE:HD11	1.92	0.51
1:A:450:ARG:HD2	1:A:450:ARG:N	2.25	0.51
1:B:403:VAL:CG1	1:B:434:ASP:OD2	2.55	0.51
1:B:78:VAL:HG11	1:B:80:ARG:HE	1.74	0.51
1:A:103:TYR:HB2	1:A:104:PRO:HD2	1.92	0.51
1:A:133:ILE:HD13	1:A:135:LEU:HD12	1.93	0.51
1:A:57:GLY:HA3	1:A:379:THR:HB	1.93	0.51
1:B:219:LYS:HA	1:B:283:THR:O	2.11	0.51
1:B:318:PHE:O	1:B:341:ILE:HD11	2.11	0.51
1:A:228:GLN:CA	1:A:228:GLN:HE21	2.18	0.51
1:A:340:GLU:O	1:A:344:VAL:HG23	2.10	0.51
1:B:254:LEU:O	1:B:259:VAL:HG23	2.10	0.51
1:B:481:ASN:HB2	1:B:500:ASN:HD22	1.74	0.51
1:A:343:LYS:HA	1:A:346:LYS:HE3	1.93	0.51
1:A:394:ILE:O	1:A:442:VAL:HA	2.11	0.51
1:B:101:ARG:HB2	1:B:151:TYR:CE1	2.45	0.51
1:B:131:ILE:HG23	1:B:233:VAL:HG13	1.93	0.51
1:A:497:ILE:O	1:A:497:ILE:HG23	2.10	0.51
1:B:112:LYS:HA	1:B:115:VAL:CG2	2.39	0.51
1:A:83:ARG:NE	1:A:383:GLU:OE2	2.44	0.51
1:A:409:ALA:HB1	1:A:425:HIS:HE1	1.76	0.51
1:B:214:VAL:HA	1:B:219:LYS:O	2.11	0.51
1:B:95:ILE:O	1:B:97:SER:N	2.44	0.51
1:A:366:PHE:O	1:A:370:ASN:HA	2.11	0.51
1:A:462:LEU:HB3	1:A:466:TRP:HE3	1.76	0.51
1:B:128:PRO:HG3	1:B:147:ASP:CA	2.36	0.51
1:B:222:MET:CE	1:B:224:LEU:HD21	2.41	0.51
1:A:298:ILE:C	1:A:300:ASN:N	2.64	0.50
1:A:318:PHE:O	1:A:341:ILE:HD11	2.11	0.50
1:B:126:ARG:HB3	1:B:149:PRO:HD2	1.92	0.50
1:B:256:GLN:HA	1:B:256:GLN:OE1	2.11	0.50
1:A:104:PRO:HB2	1:A:235:ALA:HB2	1.93	0.50
1:A:324:GLY:O	1:A:358:TYR:HB2	2.11	0.50
1:B:42:ILE:O	1:B:45:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:GLU:O	1:B:448:ASN:N	2.43	0.50
1:A:458:GLU:OE1	1:A:460:THR:HB	2.12	0.50
1:B:114:LEU:HA	1:B:119:PRO:HB3	1.93	0.50
1:B:45:LEU:HD11	1:B:259:VAL:HG12	1.92	0.50
1:A:134:ASP:OD1	1:A:178:ARG:NH2	2.45	0.50
1:B:107:LEU:N	1:B:107:LEU:HD12	2.27	0.50
1:B:232:THR:HB	1:B:271:VAL:O	2.12	0.50
1:B:226:TYR:CB	1:B:277:ILE:HB	2.33	0.50
1:A:130:ASN:N	1:A:130:ASN:HD22	2.08	0.50
1:B:98:VAL:HG12	1:B:325:GLY:HA2	1.93	0.50
1:B:409:ALA:HB1	1:B:425:HIS:CE1	2.46	0.50
1:A:132:ASN:OD1	1:A:234:SER:O	2.30	0.50
1:A:304:LYS:HA	1:A:309:TYR:HD2	1.76	0.50
1:A:319:THR:OG1	1:A:334:VAL:HG13	2.12	0.50
1:B:30:ASP:CB	1:B:36:GLN:HG2	2.41	0.50
1:A:94:ILE:CD1	1:A:359:PRO:HB2	2.42	0.50
1:A:133:ILE:HG23	1:A:135:LEU:H	1.77	0.49
1:B:151:TYR:O	1:B:152:GLY:C	2.47	0.49
1:B:185:MET:SD	1:B:291:GLN:HG3	2.52	0.49
1:B:30:ASP:HA	1:B:36:GLN:CG	2.41	0.49
1:A:112:LYS:HA	1:A:115:VAL:HG23	1.94	0.49
1:A:186:VAL:HG13	1:A:192:ILE:HB	1.93	0.49
1:B:417:LYS:HZ2	1:B:417:LYS:HB2	1.74	0.49
1:B:277:ILE:HD11	1:B:348:ASN:HB2	1.94	0.49
1:B:63:PHE:HD1	1:B:64:VAL:N	2.10	0.49
1:B:441:THR:HG22	1:B:442:VAL:N	2.26	0.49
1:A:131:ILE:N	1:A:131:ILE:HD12	2.27	0.49
1:A:464:TRP:O	1:A:466:TRP:N	2.46	0.49
1:B:166:ASN:O	1:B:169:TYR:C	2.51	0.49
1:B:138:LEU:HG	1:B:142:ASN:HB3	1.93	0.49
1:B:224:LEU:HD12	1:B:279:VAL:HB	1.95	0.49
1:B:343:LYS:HG2	1:B:347:ASP:OD2	2.12	0.49
1:A:182:SER:HB3	1:A:196:LEU:HD23	1.94	0.49
1:A:63:PHE:CD1	1:A:63:PHE:C	2.85	0.49
1:A:96:ASP:CB	1:A:100:ASP:HB2	2.16	0.49
1:A:127:LYS:HD2	1:A:246:ASP:HA	1.94	0.49
1:A:464:TRP:C	1:A:466:TRP:H	2.16	0.49
1:B:228:GLN:HA	1:B:228:GLN:NE2	2.28	0.49
1:B:232:THR:O	1:B:233:VAL:HG23	2.12	0.49
1:B:335:THR:HG21	1:B:340:GLU:HG3	1.94	0.49
1:B:407:GLU:HG3	1:B:432:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:MET:CE	1:A:281:LEU:HD13	2.43	0.49
1:A:61:GLU:HG3	1:A:61:GLU:O	2.13	0.49
1:B:129:ILE:CG1	1:B:130:ASN:N	2.76	0.49
1:B:320:ALA:HB2	1:B:341:ILE:HD12	1.94	0.49
1:B:150:THR:O	1:B:154:VAL:N	2.39	0.49
1:B:92:ILE:O	1:B:361:SER:HA	2.13	0.49
1:A:441:THR:HG22	1:A:442:VAL:N	2.27	0.48
1:A:457:ARG:NH2	1:A:464:TRP:CE2	2.81	0.48
1:B:265:PRO:CG	1:B:367:LEU:HD12	2.43	0.48
1:A:219:LYS:HA	1:A:283:THR:O	2.12	0.48
1:A:454:ILE:HD11	1:A:482:ILE:HG21	1.94	0.48
1:A:98:VAL:HG12	1:A:358:TYR:CE1	2.47	0.48
1:B:112:LYS:O	1:B:115:VAL:HG23	2.13	0.48
1:B:265:PRO:HG2	1:B:367:LEU:HD12	1.95	0.48
1:B:457:ARG:HG2	1:B:467:TRP:HB2	1.94	0.48
1:A:168:LYS:HD3	1:A:169:TYR:HE1	1.77	0.48
1:A:433:GLN:HB3	1:A:435:LYS:NZ	2.28	0.48
1:A:480:ASN:CB	1:A:500:ASN:O	2.61	0.48
1:B:158:ILE:O	1:B:162:VAL:HG23	2.13	0.48
1:A:491:LEU:O	1:A:493:PRO:HD3	2.13	0.48
1:A:275:ARG:HD2	1:A:322:VAL:HG13	1.95	0.48
1:A:318:PHE:CD1	1:A:335:THR:O	2.64	0.48
1:A:74:LYS:HA	1:A:389:TYR:O	2.13	0.48
1:B:356:PRO:HB2	1:B:358:TYR:CE2	2.49	0.48
1:A:230:PHE:CD1	1:A:351:PHE:HB2	2.48	0.48
1:B:41:GLY:HA3	1:B:251:PHE:CE1	2.49	0.48
1:B:259:VAL:HG12	1:B:260:SER:H	1.75	0.48
1:B:275:ARG:HA	1:B:324:GLY:HA3	1.94	0.48
1:B:217:ASN:HB2	1:B:384:THR:HG21	1.94	0.48
1:A:135:LEU:CD2	1:A:136:PRO:HD2	2.43	0.48
1:A:261:ASN:HB2	1:A:262:GLU:OE2	2.14	0.48
1:B:281:LEU:N	1:B:281:LEU:HD12	2.28	0.48
1:B:398:HIS:NE2	1:B:435:LYS:O	2.46	0.48
1:B:427:THR:HB	1:B:431:ASN:HD21	1.79	0.48
1:A:101:ARG:N	1:A:101:ARG:CD	2.77	0.48
1:A:453:ARG:HG2	1:A:453:ARG:HH11	1.78	0.48
1:B:156:GLY:O	1:B:159:ASP:HB2	2.14	0.48
1:A:114:LEU:HD12	1:A:114:LEU:C	2.34	0.47
1:A:163:SER:HA	1:A:166:ASN:HD22	1.77	0.47
1:A:196:LEU:HD22	1:A:225:ALA:CB	2.43	0.47
1:A:328:GLN:O	1:A:331:ASN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:NZ	1:A:388:GLU:HB3	2.27	0.47
1:A:456:ALA:HB3	1:A:471:ILE:HG22	1.96	0.47
1:B:230:PHE:CZ	1:B:275:ARG:NH1	2.77	0.47
1:B:83:ARG:O	1:B:380:ASP:HA	2.13	0.47
1:A:453:ARG:HD2	1:A:474:TYR:HE2	1.78	0.47
1:A:63:PHE:C	1:A:63:PHE:HD1	2.18	0.47
1:A:70:LYS:H	1:A:70:LYS:CD	2.01	0.47
1:B:307:GLN:O	1:B:311:ASP:OD1	2.32	0.47
1:B:226:TYR:CZ	1:B:345:ILE:HD13	2.48	0.47
1:A:483:ASN:OD1	1:A:498:THR:O	2.32	0.47
1:A:88:SER:HA	1:A:375:VAL:O	2.14	0.47
1:A:33:ASP:C	1:A:34:LYS:HG3	2.35	0.47
1:A:60:ILE:CD1	1:A:382:ILE:HD11	2.43	0.47
1:A:212:ASN:HA	1:A:215:ALA:HB3	1.96	0.47
1:A:286:SER:HB2	1:A:388:GLU:HG2	1.96	0.47
1:A:290:VAL:O	1:A:291:GLN:C	2.51	0.47
1:B:332:LYS:HG2	1:B:333:VAL:N	2.30	0.47
1:B:72:GLY:C	1:B:74:LYS:H	2.16	0.47
1:A:31:ILE:HD12	1:A:31:ILE:N	2.30	0.47
1:A:464:TRP:HA	1:A:467:TRP:CE3	2.50	0.47
1:B:259:VAL:O	1:B:260:SER:CB	2.62	0.47
1:B:287:SER:O	1:B:289:ASP:N	2.47	0.47
1:B:297:LEU:HD13	1:B:313:TYR:CZ	2.50	0.47
1:B:56:ASN:HD21	1:B:59:LYS:NZ	2.13	0.47
1:A:96:ASP:HB2	1:A:100:ASP:N	2.30	0.47
1:B:325:GLY:HA3	1:B:358:TYR:CD1	2.50	0.47
1:A:31:ILE:HG13	1:A:252:ASN:CG	2.36	0.46
1:A:253:ASP:O	1:A:257:LYS:HG3	2.14	0.46
1:B:133:ILE:HG13	1:B:232:THR:O	2.14	0.46
1:B:297:LEU:HD12	1:B:304:LYS:HD2	1.97	0.46
1:B:30:ASP:OD2	1:B:36:GLN:HB3	2.15	0.46
1:B:328:GLN:O	1:B:331:ASN:HB3	2.15	0.46
1:B:266:LEU:HD23	1:B:366:PHE:HA	1.96	0.46
1:A:124:VAL:HG11	1:A:254:LEU:CD2	2.45	0.46
1:A:168:LYS:HG2	1:A:169:TYR:CE1	2.50	0.46
1:A:174:THR:HB	1:A:350:THR:HG23	1.97	0.46
1:B:480:ASN:CB	1:B:500:ASN:O	2.63	0.46
1:A:343:LYS:HA	1:A:346:LYS:CE	2.45	0.46
1:A:416:ASP:OD2	1:A:420:ASN:N	2.37	0.46
1:A:457:ARG:HB3	1:A:464:TRP:CZ3	2.50	0.46
1:B:78:VAL:HG12	1:B:79:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:HA	1:A:376:HIS:HB2	1.96	0.46
1:B:168:LYS:HD3	1:B:169:TYR:HE1	1.79	0.46
1:B:464:TRP:O	1:B:466:TRP:N	2.48	0.46
1:B:83:ARG:HB2	1:B:381:TYR:CZ	2.50	0.46
1:A:174:THR:HB	1:A:350:THR:CG2	2.45	0.46
1:A:123:MET:N	1:A:257:LYS:HE2	2.25	0.46
1:A:383:GLU:HG2	1:A:383:GLU:O	2.15	0.46
1:A:454:ILE:O	1:A:455:LYS:HB2	2.16	0.46
1:A:405:GLN:HG3	1:A:459:CYS:SG	2.56	0.46
1:A:80:ARG:NH1	1:A:80:ARG:CG	2.78	0.46
1:B:89:PRO:HG2	1:B:375:VAL:HB	1.97	0.46
1:A:281:LEU:H	1:A:281:LEU:HD12	1.80	0.46
1:B:106:ALA:HB1	1:B:121:ILE:HD11	1.97	0.46
1:B:88:SER:HA	1:B:375:VAL:O	2.15	0.46
1:A:491:LEU:O	1:A:491:LEU:HD23	2.16	0.46
1:B:398:HIS:O	1:B:438:HIS:N	2.48	0.46
1:B:453:ARG:O	1:B:453:ARG:HG3	2.15	0.46
1:B:45:LEU:HD11	1:B:259:VAL:CG1	2.46	0.46
1:A:165:TRP:CZ3	1:A:169:TYR:HB2	2.51	0.46
1:A:246:ASP:O	1:A:249:VAL:N	2.36	0.46
1:A:173:HIS:CE1	1:A:354:LYS:NZ	2.83	0.46
1:A:204:GLU:O	1:A:204:GLU:HG2	2.15	0.45
1:A:78:VAL:HG11	1:A:80:ARG:NH2	2.31	0.45
1:B:172:THR:O	1:B:173:HIS:HD2	1.99	0.45
1:B:32:THR:C	1:B:34:LYS:H	2.19	0.45
1:A:318:PHE:O	1:A:334:VAL:HA	2.16	0.45
1:A:436:THR:O	1:A:437:ALA:C	2.55	0.45
1:B:130:ASN:ND2	1:B:145:LYS:HG3	2.31	0.45
1:B:417:LYS:HZ3	1:B:417:LYS:HB2	1.79	0.45
1:B:418:GLU:HB2	1:B:420:ASN:ND2	2.31	0.45
1:A:101:ARG:H	1:A:101:ARG:CD	2.29	0.45
1:A:150:THR:HG22	1:A:151:TYR:N	2.31	0.45
1:A:224:LEU:HD12	1:A:279:VAL:HB	1.98	0.45
1:B:129:ILE:CG1	1:B:130:ASN:H	2.22	0.45
1:A:321:VAL:HG12	1:A:332:LYS:HG3	1.97	0.45
1:A:356:PRO:HB2	1:A:358:TYR:HE2	1.82	0.45
1:A:458:GLU:HB2	1:A:470:VAL:CG2	2.46	0.45
1:A:96:ASP:HB3	1:A:100:ASP:N	2.16	0.45
1:B:476:VAL:CG1	1:B:477:PRO:HD2	2.47	0.45
1:A:38:ILE:HA	1:A:251:PHE:CB	2.30	0.45
1:A:453:ARG:HG2	1:A:453:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LYS:HD3	1:B:246:ASP:CB	2.47	0.45
1:B:228:GLN:HA	1:B:228:GLN:HE21	1.81	0.45
1:A:441:THR:CG2	1:A:442:VAL:N	2.79	0.45
1:B:210:ASP:O	1:B:211:PHE:C	2.55	0.45
1:B:58:ASP:OD2	1:B:190:SER:HB3	2.16	0.45
1:B:73:ASN:O	1:B:74:LYS:HG3	2.16	0.45
1:A:105:GLY:O	1:A:106:ALA:C	2.55	0.45
1:A:30:ASP:HB3	1:A:36:GLN:HG2	1.98	0.45
1:B:102:THR:OG1	1:B:108:GLN:NE2	2.49	0.45
1:B:49:ARG:HG3	1:B:50:ASN:CG	2.36	0.45
1:B:60:ILE:CG1	1:B:61:GLU:N	2.80	0.45
1:A:58:ASP:OD2	1:A:190:SER:CB	2.64	0.45
1:B:40:SER:O	1:B:44:SER:CB	2.65	0.45
1:B:433:GLN:HB3	1:B:435:LYS:HZ1	1.82	0.45
1:B:96:ASP:CB	1:B:100:ASP:N	2.65	0.45
1:A:121:ILE:CD1	1:A:122:LEU:H	2.26	0.45
1:A:269:SER:HB3	1:A:365:VAL:CG2	2.46	0.45
1:A:31:ILE:HG12	1:A:255:LYS:NZ	2.32	0.45
1:A:93:SER:O	1:A:117:ASN:ND2	2.50	0.45
1:B:212:ASN:HA	1:B:215:ALA:CB	2.45	0.45
1:B:389:TYR:O	1:B:447:ALA:HB1	2.16	0.45
1:B:49:ARG:HG3	1:B:50:ASN:ND2	2.32	0.45
1:A:283:THR:OG1	1:A:284:THR:N	2.48	0.45
1:A:73:ASN:C	1:A:74:LYS:HG3	2.36	0.45
1:B:132:ASN:ND2	1:B:143:SER:OG	2.50	0.45
1:B:83:ARG:HB3	1:B:381:TYR:CZ	2.52	0.45
1:B:446:GLU:C	1:B:448:ASN:H	2.21	0.45
1:B:187:TYR:HD1	1:B:381:TYR:CE1	2.36	0.44
1:B:182:SER:HB3	1:B:196:LEU:CD2	2.48	0.44
1:B:292:ALA:O	1:B:293:ALA:C	2.55	0.44
1:B:40:SER:O	1:B:44:SER:HB3	2.17	0.44
1:B:432:TYR:CD2	1:B:432:TYR:N	2.84	0.44
1:A:192:ILE:HD11	1:A:196:LEU:HD12	2.00	0.44
1:B:214:VAL:HG22	1:B:221:VAL:HG23	1.99	0.44
1:B:491:LEU:C	1:B:493:PRO:HD3	2.38	0.44
1:B:468:ARG:CZ	1:B:493:PRO:HG2	2.47	0.44
1:B:222:MET:CE	1:B:298:ILE:HD11	2.48	0.44
1:B:277:ILE:HG21	1:B:345:ILE:HG12	1.99	0.44
1:A:189:LYS:O	1:A:193:SER:CB	2.66	0.44
1:B:163:SER:OG	1:B:164:LYS:N	2.50	0.44
1:B:224:LEU:CB	1:B:279:VAL:HB	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:THR:HB	1:B:316:SER:OG	2.18	0.44
1:B:42:ILE:HG22	1:B:368:LYS:HB2	1.99	0.44
1:B:95:ILE:HG12	1:B:117:ASN:HB3	1.95	0.44
1:A:131:ILE:N	1:A:131:ILE:CD1	2.80	0.44
1:A:210:ASP:OD2	1:A:213:ALA:CB	2.60	0.44
1:B:113:ALA:HB1	1:B:118:ARG:O	2.17	0.44
1:B:299:LYS:HB2	1:B:301:THR:HG22	2.00	0.44
1:B:173:HIS:CE1	1:B:354:LYS:HZ1	2.36	0.44
1:A:219:LYS:HD3	1:A:282:GLU:OE2	2.17	0.44
1:B:150:THR:O	1:B:153:LYS:HB3	2.17	0.44
1:B:155:SER:O	1:B:159:ASP:OD2	2.36	0.44
1:B:189:LYS:NZ	1:B:204:GLU:OE1	2.40	0.44
1:B:319:THR:OG1	1:B:334:VAL:HG22	2.18	0.44
1:A:132:ASN:HA	1:A:142:ASN:O	2.17	0.44
1:A:341:ILE:O	1:A:344:VAL:HB	2.17	0.44
1:A:427:THR:HB	1:A:431:ASN:HD22	1.81	0.44
1:B:118:ARG:HH11	1:B:118:ARG:HG3	1.81	0.44
1:B:126:ARG:CB	1:B:149:PRO:HD2	2.46	0.44
1:B:239:LYS:HE3	1:B:239:LYS:HB3	1.83	0.44
1:B:113:ALA:HA	1:B:118:ARG:NH1	2.33	0.44
1:B:138:LEU:CG	1:B:142:ASN:HB3	2.47	0.44
1:B:173:HIS:CD2	1:B:354:LYS:HZ1	2.35	0.44
1:B:49:ARG:NH2	1:B:369:ASP:OD2	2.51	0.44
1:B:96:ASP:HB2	1:B:100:ASP:CA	2.48	0.44
1:A:366:PHE:HB2	1:A:369:ASP:OD1	2.18	0.44
1:B:78:VAL:HA	1:B:385:THR:O	2.17	0.44
1:A:163:SER:CA	1:A:166:ASN:HD22	2.30	0.43
1:A:175:LEU:HD22	1:A:176:PRO:HD2	2.00	0.43
1:A:198:VAL:HG11	1:A:278:TYR:OH	2.18	0.43
1:A:285:SER:OG	1:A:286:SER:N	2.51	0.43
1:A:49:ARG:HB2	1:A:366:PHE:CZ	2.53	0.43
1:A:487:TRP:O	1:A:494:GLY:N	2.51	0.43
1:B:122:LEU:HA	1:B:122:LEU:HD23	1.82	0.43
1:B:148:ASP:HB3	1:B:153:LYS:HE2	1.98	0.43
1:B:276:THR:N	1:B:323:LEU:O	2.46	0.43
1:B:405:GLN:HG2	1:B:433:GLN:C	2.38	0.43
1:A:129:ILE:HG12	1:A:130:ASN:N	2.32	0.43
1:A:144:ILE:CG1	1:A:145:LYS:H	2.27	0.43
1:A:277:ILE:HD11	1:A:348:ASN:HB2	2.00	0.43
1:A:301:THR:O	1:A:303:ILE:N	2.51	0.43
1:B:124:VAL:HG12	1:B:257:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:HD13	1:B:364:SER:OG	2.17	0.43
1:B:327:ALA:O	1:B:328:GLN:C	2.56	0.43
1:B:433:GLN:CB	1:B:435:LYS:HZ1	2.31	0.43
1:B:436:THR:O	1:B:437:ALA:C	2.56	0.43
1:A:128:PRO:HA	1:A:146:VAL:O	2.18	0.43
1:B:150:THR:O	1:B:151:TYR:C	2.57	0.43
1:B:453:ARG:NH1	1:B:453:ARG:HG2	2.33	0.43
1:A:103:TYR:CE2	1:A:151:TYR:N	2.87	0.43
1:A:89:PRO:HG2	1:A:375:VAL:HB	2.01	0.43
1:A:64:VAL:HA	1:A:65:PRO:HD2	1.65	0.43
1:B:39:ASP:OD1	1:B:241:PRO:HD2	2.18	0.43
1:B:398:HIS:CA	1:B:486:ILE:HD11	2.40	0.43
1:A:134:ASP:OD1	1:A:178:ARG:NH1	2.50	0.43
1:A:293:ALA:HB1	1:A:313:TYR:CE2	2.54	0.43
1:B:114:LEU:HD11	1:B:362:TYR:OH	2.19	0.43
1:B:132:ASN:HA	1:B:142:ASN:O	2.17	0.43
1:A:134:ASP:N	1:A:134:ASP:OD2	2.49	0.43
1:A:83:ARG:HG3	1:A:383:GLU:HB2	2.01	0.43
1:B:296:ALA:HA	1:B:301:THR:HG23	2.00	0.43
1:A:252:ASN:ND2	1:A:255:LYS:HD2	2.34	0.43
1:B:101:ARG:HE	1:B:101:ARG:H	1.67	0.43
1:B:346:LYS:O	1:B:348:ASN:N	2.52	0.43
1:A:151:TYR:O	1:A:152:GLY:C	2.56	0.43
1:A:434:ASP:O	1:A:435:LYS:HD3	2.18	0.43
1:A:288:LYS:HE3	1:A:387:THR:HG23	2.01	0.43
1:A:358:TYR:HB3	1:A:359:PRO:HD2	1.99	0.43
1:B:42:ILE:O	1:B:45:LEU:N	2.52	0.43
1:B:483:ASN:OD1	1:B:498:THR:O	2.37	0.43
1:A:104:PRO:HD3	1:A:271:VAL:CG2	2.49	0.42
1:A:338:PHE:O	1:A:342:ARG:HG3	2.19	0.42
1:B:283:THR:OG1	1:B:284:THR:N	2.52	0.42
1:B:407:GLU:HG3	1:B:432:TYR:HE2	1.83	0.42
1:B:458:GLU:OE2	1:B:460:THR:N	2.52	0.42
1:A:118:ARG:HG3	1:A:118:ARG:O	2.19	0.42
1:A:95:ILE:HG12	1:A:117:ASN:HB2	2.01	0.42
1:B:125:LYS:HD3	1:B:246:ASP:HB3	2.00	0.42
1:B:343:LYS:HA	1:B:346:LYS:CE	2.38	0.42
1:B:452:ILE:HB	1:B:476:VAL:O	2.19	0.42
1:A:130:ASN:ND2	1:A:145:LYS:HE2	2.33	0.42
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.74	0.42
1:A:199:ASN:OD1	1:A:201:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD22	1:A:280:LYS:HB2	2.01	0.42
1:A:95:ILE:HA	1:A:95:ILE:HD13	1.78	0.42
1:B:413:VAL:HG11	1:B:450:ARG:CZ	2.49	0.42
1:B:64:VAL:HA	1:B:65:PRO:HD2	1.60	0.42
1:A:457:ARG:NH2	1:A:464:TRP:NE1	2.68	0.42
1:A:484:VAL:HG23	1:A:497:ILE:HD12	2.00	0.42
1:A:128:PRO:HG3	1:A:147:ASP:HA	2.02	0.42
1:A:32:THR:HG21	2:A:517:HOH:O	2.19	0.42
1:B:209:VAL:HG12	1:B:211:PHE:N	2.33	0.42
1:B:276:THR:HB	1:B:278:TYR:HE1	1.82	0.42
1:B:305:ASN:HA	1:B:310:LYS:CE	2.48	0.42
1:A:276:THR:HG21	1:A:278:TYR:CZ	2.55	0.42
1:A:418:GLU:CB	1:A:420:ASN:ND2	2.72	0.42
1:A:50:ASN:N	1:A:50:ASN:HD22	2.17	0.42
1:B:131:ILE:CG2	1:B:132:ASN:N	2.83	0.42
1:B:409:ALA:CB	1:B:427:THR:HG22	2.50	0.42
1:A:38:ILE:HG23	1:A:39:ASP:N	2.34	0.42
1:A:465:GLU:CD	1:A:465:GLU:N	2.65	0.42
1:B:222:MET:HE2	1:B:224:LEU:HD21	2.01	0.42
1:B:227:LYS:HA	1:B:276:THR:HG23	2.01	0.42
1:A:343:LYS:HA	1:A:346:LYS:NZ	2.35	0.42
1:A:34:LYS:HE2	1:A:34:LYS:O	2.19	0.42
1:B:152:GLY:O	1:B:153:LYS:C	2.57	0.42
1:A:165:TRP:O	1:A:168:LYS:N	2.52	0.42
1:A:232:THR:CB	1:A:271:VAL:O	2.61	0.42
1:A:30:ASP:HA	1:A:36:GLN:CG	2.49	0.42
1:A:50:ASN:HA	1:A:376:HIS:NE2	2.35	0.42
1:B:271:VAL:HG12	1:B:273:TYR:CE1	2.55	0.42
1:B:220:LYS:HB2	1:B:283:THR:HG23	2.02	0.42
1:A:150:THR:C	1:A:154:VAL:HG23	2.40	0.42
1:A:275:ARG:NH2	1:A:348:ASN:O	2.52	0.42
1:A:450:ARG:O	1:A:451:ASN:HB2	2.20	0.42
1:A:60:ILE:HG12	1:A:61:GLU:N	2.34	0.42
1:A:83:ARG:CZ	1:A:383:GLU:OE2	2.67	0.42
1:B:43:SER:O	1:B:368:LYS:HE3	2.20	0.42
1:A:433:GLN:HB3	1:A:435:LYS:HZ3	1.85	0.41
1:B:338:PHE:CE1	1:B:341:ILE:HG21	2.54	0.41
1:A:351:PHE:C	1:A:351:PHE:CD1	2.93	0.41
1:A:424:THR:O	1:A:424:THR:HG22	2.19	0.41
1:B:144:ILE:HG13	1:B:145:LYS:N	2.34	0.41
1:B:239:LYS:H	1:B:239:LYS:CD	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:C	1:B:305:ASN:H	2.23	0.41
1:A:449:ALA:O	1:A:478:LEU:HD22	2.21	0.41
1:B:127:LYS:HD2	1:B:246:ASP:HA	2.02	0.41
1:A:287:SER:O	1:A:289:ASP:N	2.53	0.41
1:B:273:TYR:CD1	1:B:273:TYR:N	2.87	0.41
1:B:396:LEU:HA	1:B:484:VAL:O	2.19	0.41
1:A:96:ASP:CB	1:A:100:ASP:N	2.66	0.41
1:B:266:LEU:HA	1:B:365:VAL:O	2.20	0.41
1:B:75:PHE:HB3	1:B:389:TYR:HB2	2.02	0.41
1:B:487:TRP:O	1:B:494:GLY:N	2.53	0.41
1:A:113:ALA:HA	1:A:116:GLU:OE1	2.20	0.41
1:A:182:SER:CB	1:A:225:ALA:HB3	2.35	0.41
1:A:320:ALA:HB2	1:A:341:ILE:HG23	2.02	0.41
1:A:43:SER:HA	1:A:368:LYS:HG3	2.03	0.41
1:B:150:THR:HG22	1:B:151:TYR:N	2.36	0.41
1:B:163:SER:O	1:B:167:GLU:OE1	2.39	0.41
1:B:319:THR:HG23	1:B:333:VAL:O	2.21	0.41
1:B:456:ALA:H	1:B:471:ILE:CG2	2.33	0.41
1:B:461:GLY:CA	1:B:467:TRP:HE1	2.33	0.41
1:B:63:PHE:CD1	1:B:63:PHE:C	2.94	0.41
1:A:103:TYR:CE2	1:A:151:TYR:CA	3.04	0.41
1:A:37:SER:HB3	1:A:40:SER:CB	2.51	0.41
1:A:75:PHE:O	1:A:389:TYR:HD1	2.03	0.41
1:A:398:HIS:HD2	1:A:436:THR:O	2.03	0.41
1:B:462:LEU:C	1:B:462:LEU:HD23	2.41	0.41
1:A:196:LEU:O	1:A:197:ASN:HB3	2.21	0.41
1:A:31:ILE:HG23	1:A:252:ASN:OD1	2.20	0.41
1:A:55:SER:OG	1:A:377:ASN:HA	2.21	0.41
1:B:95:ILE:HD11	1:B:199:ASN:HB2	2.03	0.41
1:B:343:LYS:O	1:B:347:ASP:OD2	2.39	0.41
1:B:398:HIS:HB3	1:B:439:TYR:H	1.86	0.41
1:B:391:LYS:CG	1:B:447:ALA:H	2.29	0.41
1:B:74:LYS:HZ1	1:B:388:GLU:CD	2.24	0.41
1:A:166:ASN:H	1:A:166:ASN:ND2	2.19	0.41
1:A:457:ARG:HD2	1:A:467:TRP:O	2.21	0.41
1:A:107:LEU:HA	1:A:266:LEU:O	2.20	0.41
1:A:148:ASP:O	1:A:153:LYS:HG2	2.20	0.41
1:A:282:GLU:O	1:A:316:SER:HA	2.21	0.41
1:A:32:THR:C	1:A:34:LYS:H	2.25	0.41
1:A:342:ARG:O	1:A:346:LYS:HG2	2.21	0.41
1:A:80:ARG:NH1	1:A:80:ARG:HG3	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:HG3	1:B:383:GLU:HB2	2.03	0.41
1:B:405:GLN:HG2	1:B:434:ASP:N	2.35	0.41
1:B:94:ILE:HD12	1:B:360:ILE:N	2.36	0.41
1:A:230:PHE:O	1:A:231:TYR:HB3	2.21	0.40
1:A:254:LEU:C	1:A:256:GLN:N	2.75	0.40
1:A:191:GLN:HG3	1:A:381:TYR:CD1	2.55	0.40
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.93	0.40
1:A:439:TYR:CG	1:A:440:SER:N	2.90	0.40
1:B:192:ILE:HD11	1:B:196:LEU:CD1	2.51	0.40
1:B:346:LYS:C	1:B:348:ASN:N	2.74	0.40
1:B:38:ILE:HA	1:B:251:PHE:CB	2.44	0.40
1:B:79:GLU:HB2	1:B:385:THR:HG1	1.83	0.40
1:A:161:LEU:O	1:A:164:LYS:HB3	2.22	0.40
1:A:72:GLY:C	1:A:74:LYS:H	2.24	0.40
1:A:90:VAL:HG23	1:A:91:ASP:N	2.37	0.40
1:B:57:GLY:HA3	1:B:379:THR:HB	2.03	0.40
1:B:78:VAL:CG1	1:B:80:ARG:HE	2.34	0.40
1:A:126:ARG:HB3	1:A:149:PRO:HD2	2.04	0.40
1:A:217:ASN:OD1	1:A:384:THR:HG21	2.22	0.40
1:A:406:PHE:CD1	1:A:406:PHE:N	2.89	0.40
1:B:101:ARG:CD	1:B:101:ARG:N	2.85	0.40
1:B:298:ILE:C	1:B:300:ASN:H	2.24	0.40
1:B:318:PHE:CD1	1:B:318:PHE:N	2.89	0.40
1:B:461:GLY:N	1:B:467:TRP:HE1	2.18	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	469/471 (100%)	358 (76%)	77 (16%)	34 (7%)	1 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	469/471 (100%)	358 (76%)	76 (16%)	35 (8%)	1	5
All	All	938/942 (100%)	716 (76%)	153 (16%)	69 (7%)	1	5

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	ILE
1	B	288	LYS
1	B	438	HIS
1	A	151	TYR
1	A	259	VAL
1	A	288	LYS
1	A	438	HIS
1	A	464	TRP
1	A	465	GLU
1	B	47	TYR
1	B	95	ILE
1	B	96	ASP
1	B	151	TYR
1	B	259	VAL
1	B	260	SER
1	B	347	ASP
1	B	447	ALA
1	B	464	TRP
1	B	465	GLU
1	A	47	TYR
1	A	97	SER
1	A	100	ASP
1	A	247	ASP
1	A	299	LYS
1	A	302	ASP
1	A	345	ILE
1	A	347	ASP
1	A	447	ALA
1	B	63	PHE
1	B	65	PRO
1	B	73	ASN
1	B	97	SER
1	B	100	ASP
1	B	128	PRO
1	B	153	LYS
1	B	211	PHE

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Mol	Chain	Res	Type
1	B	302	ASP
1	A	63	PHE
1	A	73	ASN
1	A	211	PHE
1	A	231	TYR
1	A	368	LYS
1	A	437	ALA
1	B	139	LYS
1	B	208	GLY
1	B	437	ALA
1	A	65	PRO
1	A	260	SER
1	A	328	GLN
1	A	455	LYS
1	B	51	GLU
1	B	57	GLY
1	B	327	ALA
1	B	368	LYS
1	A	95	ILE
1	A	208	GLY
1	B	162	VAL
1	B	231	TYR
1	B	310	LYS
1	B	328	GLN
1	B	298	ILE
1	B	345	ILE
1	A	52	VAL
1	A	104	PRO
1	A	202	VAL
1	A	128	PRO
1	A	98	VAL
1	A	497	ILE
1	B	149	PRO

5.3.2 Protein sidechains [i](#)

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	418/418 (100%)	379 (91%)	39 (9%)	9	33
1	B	418/418 (100%)	383 (92%)	35 (8%)	11	38
All	All	836/836 (100%)	762 (91%)	74 (9%)	9	35

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	34	LYS
1	A	44	SER
1	A	45	LEU
1	A	46	SER
1	A	59	LYS
1	A	63	PHE
1	A	70	LYS
1	A	88	SER
1	A	90	VAL
1	A	95	ILE
1	A	99	ASN
1	A	100	ASP
1	A	101	ARG
1	A	102	THR
1	A	108	GLN
1	A	114	LEU
1	A	121	ILE
1	A	132	ASN
1	A	167	GLU
1	A	184	SER
1	A	198	VAL
1	A	239	LYS
1	A	245	PHE
1	A	247	ASP
1	A	250	THR
1	A	270	ASN
1	A	286	SER
1	A	301	THR
1	A	326	ASP
1	A	351	PHE
1	A	370	ASN
1	A	395	ASN
1	A	424	THR
1	A	434	ASP

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Mol	Chain	Res	Type
1	A	444	PRO
1	A	468	ARG
1	A	475	ASP
1	A	483	ASN
1	B	30	ASP
1	B	31	ILE
1	B	34	LYS
1	B	45	LEU
1	B	59	LYS
1	B	70	LYS
1	B	90	VAL
1	B	99	ASN
1	B	100	ASP
1	B	101	ARG
1	B	102	THR
1	B	107	LEU
1	B	115	VAL
1	B	121	ILE
1	B	128	PRO
1	B	147	ASP
1	B	163	SER
1	B	184	SER
1	B	239	LYS
1	B	250	THR
1	B	286	SER
1	B	289	ASP
1	B	301	THR
1	B	326	ASP
1	B	330	HIS
1	B	339	ASP
1	B	351	PHE
1	B	370	ASN
1	B	371	SER
1	B	395	ASN
1	B	453	ARG
1	B	457	ARG
1	B	468	ARG
1	B	475	ASP
1	B	497	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	56	ASN
1	A	130	ASN
1	A	132	ASN
1	A	166	ASN
1	A	173	HIS
1	A	197	ASN
1	A	228	GLN
1	A	252	ASN
1	A	270	ASN
1	A	291	GLN
1	A	308	GLN
1	A	420	ASN
1	A	433	GLN
1	A	451	ASN
1	A	500	ASN
1	B	48	ASN
1	B	50	ASN
1	B	56	ASN
1	B	108	GLN
1	B	130	ASN
1	B	132	ASN
1	B	197	ASN
1	B	205	ASN
1	B	228	GLN
1	B	252	ASN
1	B	291	GLN
1	B	405	GLN
1	B	420	ASN
1	B	433	GLN
1	B	451	ASN
1	B	500	ASN

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.