Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:06 AM GMT

PDB ID	:	1ZQ1
Title	:	Structure of GatDE tRNA-Dependent Amidotransferase from Pyrococcus abyssi
Authors	:	Schmitt, E.; Panvert, M.; Blanquet, S.; Mechulam, Y.
Deposited on	:	2005-05-18
Resolution	:	3.00 Å(reported)

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

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

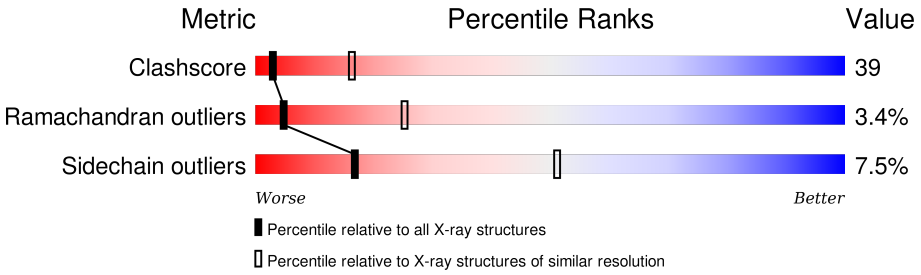
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	438	41% 52% 6%
1	B	438	41% 51% 8%
2	C	633	37% 38% 5% 20%
2	D	633	37% 39% • 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ASP	A	1000	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14869 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 Glutamyl-tRNA(Gln) amidotransferase subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	Se	0	0	0
			3406	2159	578	650	5	14			
1	B	437	Total	C	N	O	S	Se	0	0	0
			3406	2162	575	650	5	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	36	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	127	LEU	VAL	CONFLICT	UNP Q9V0T9
A	149	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	181	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	191	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	217	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	225	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	234	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	237	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	257	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	362	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	393	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	403	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	418	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	419	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	36	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	127	LEU	VAL	CONFLICT	UNP Q9V0T9
B	149	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	181	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	191	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	217	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	225	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	234	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9

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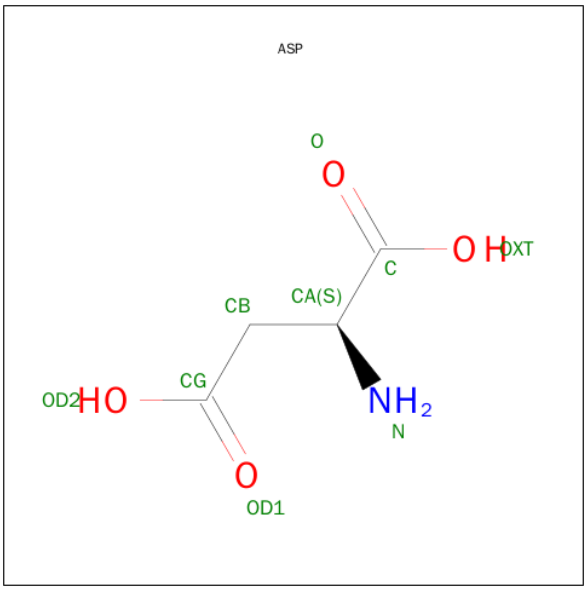
Chain	Residue	Modelled	Actual	Comment	Reference
B	237	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	257	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	362	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	393	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	403	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	418	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	419	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9

- Molecule 2 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	508	Total	C	N	O	S	0	0	0
			4005	2543	700	755	7			
2	D	508	Total	C	N	O	S	0	0	0
			3966	2523	693	743	7			

- Molecule 3 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		
3	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	24	Total O 24 24	0	0
4	C	22	Total O 22 22	0	0
4	D	10	Total O 10 10	0	0

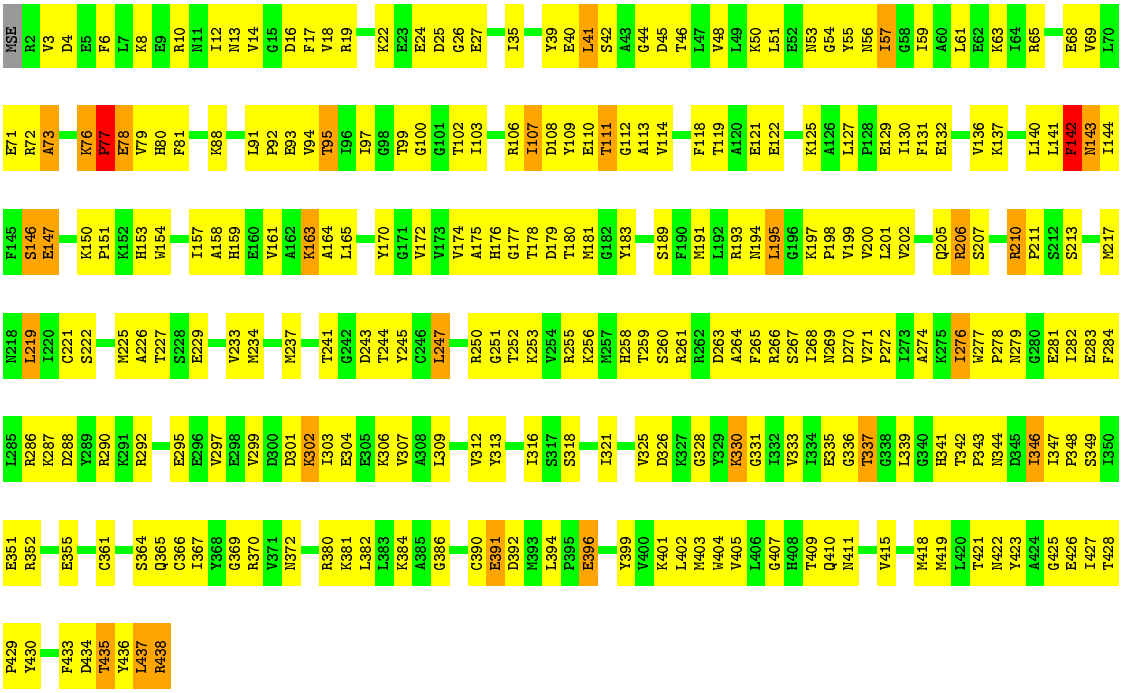
3 Residue-property plots (i)

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

Note EDS was not executed.

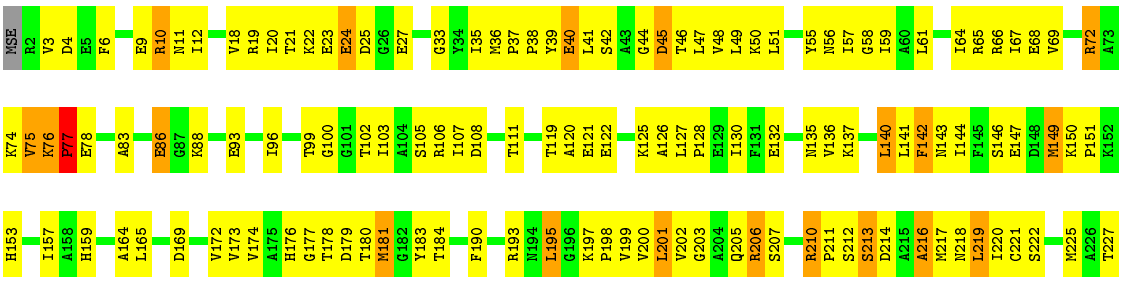
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit D

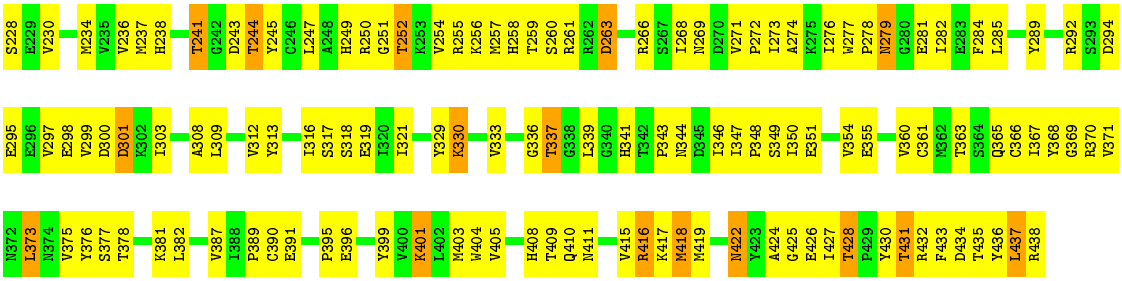
Chain A:



- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit D

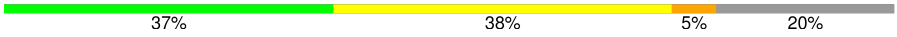
Chain B:

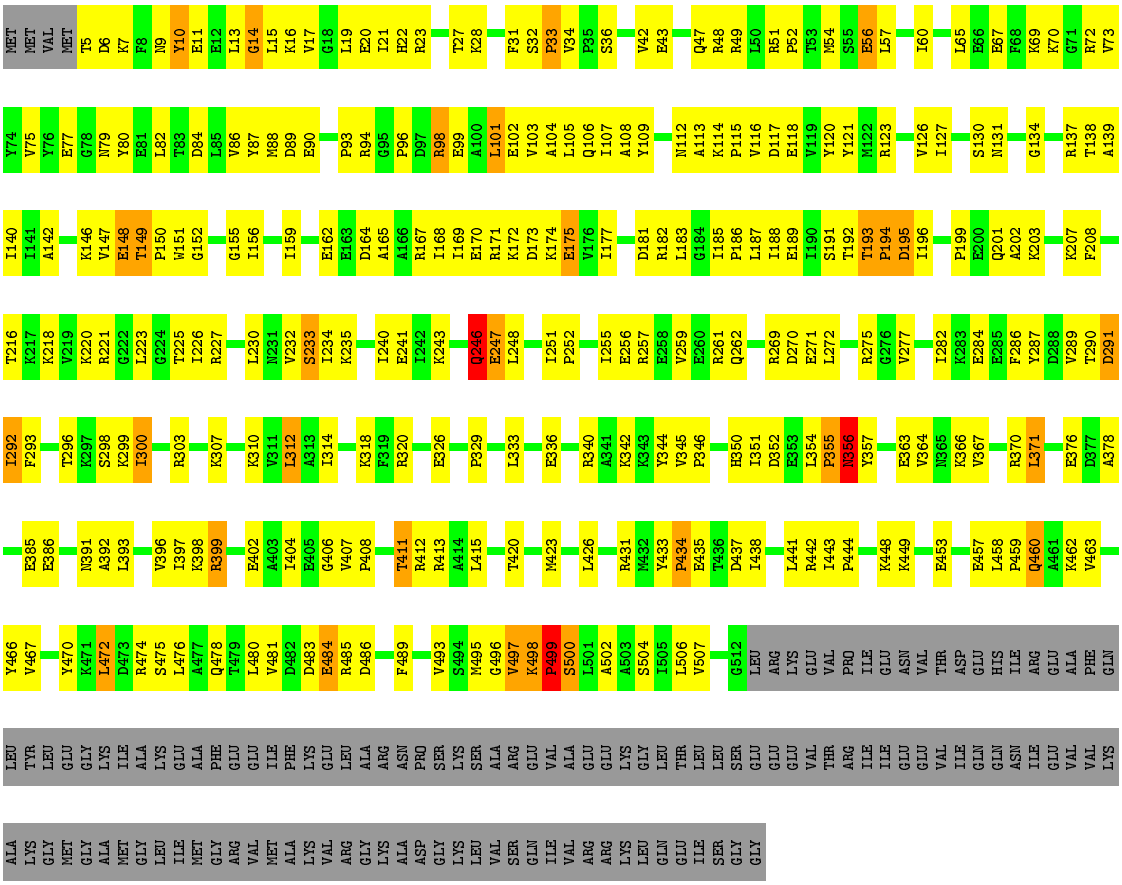




• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit E

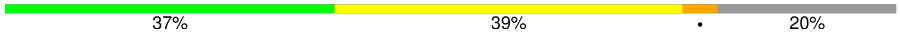
Chain C:

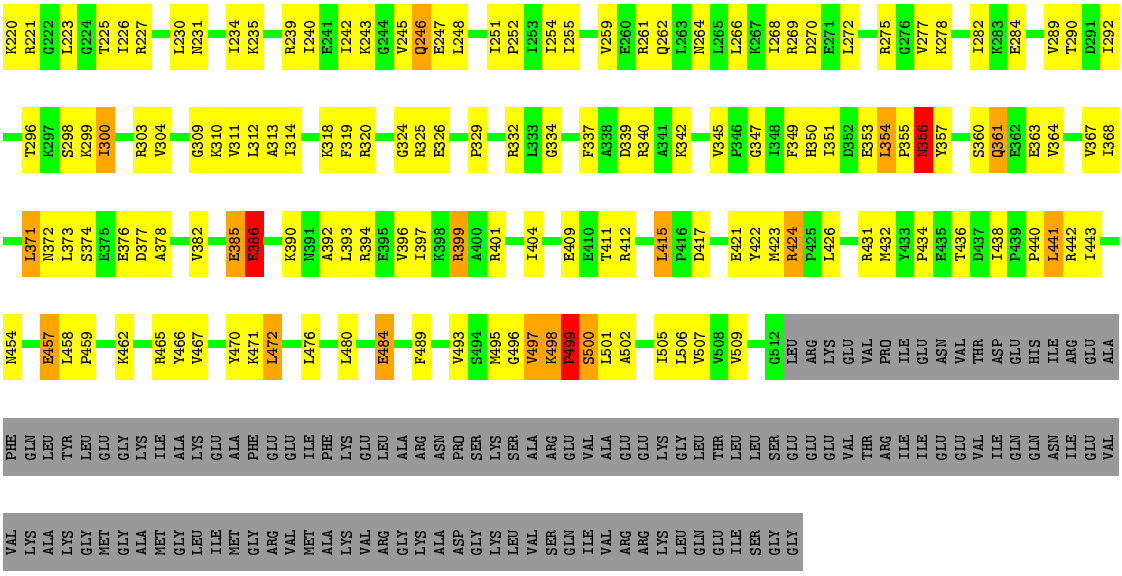




• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit E

Chain D:




K220 R221 G222 L223 G224 T225 I226 R227 L230 N231 I234 K235 R239 I240 E241 I242 K243 G244 V245 Q246 E247 L248 I251 P252 I253 I254 I255 V259 E260 R261 Q262 L263 N264 L265 L266 K267 I268 R269 D270 E271 L272 R275 G276 V277 K278 I282 K283 E284 V289 T290 D291 I292
T296 K297 S298 K299 I300 R303 V304 G309 K310 V311 L312 A313 I314 K318 F319 R320 G324 R325 E326 P329 R332 L333 G334 F337 A338 D339 R340 A341 K342 V345 P346 G347 I348 F349 H350 I351 D352 E353 L354 P355 N356 Y357 S360 Q361 E362 E363 V364 V367 I368
L371 N372 L373 S374 E375 E376 D377 A378 V382 E385 E386 K390 N391 A392 L393 R394 E395 V396 I397 K398 R399 A400 R401 I404 E409 E410 T411 R412 L415 P416 D417 E421 Y422 M423 R424 P425 L426 R431 M432 Y433 P434 E435 T436 D437 I438 P439 P440 L441 R442 I443
N454 E457 L458 P459 K462 R465 Y466 V467 Y470 K471 L472 L476 L480 E484 F489 V493 S494 M495 G496 V497 K498 P499 S500 L501 A502 I505 L506 V507 V508 V509 G512
LEU ARG LYS GLU VAL PRO ILE GLU ASN VAL THR ASP GLU HIS ILE ARG GLU ALA
PHE GLN LEU TYR LEU GLU GLY LYS ILE ALA LYS GLU ALA PHE GLU GLU ILE PHE LYS GLU LEU ALA ARG ASN PRO SER LYS SER ALA ARG GLU VAL ALA GLU GLU LYS GLY LEU THR LEU LEU SER GLU GLU GLU VAL THR ARG ILE ILE GLU GLU VAL ILE GLN GLN ASN ILE GLU VAL
VAL LYS ALA LYS GLY MET GLY ALA MET GLY LEU ILE MET GLY ARG VAL MET ALA LYS VAL ARG GLY LYS ALA ASP GLY LYS LEU SER VAL SER GLN ILE VAL ARG ARG LYS LEU GLN GLU ILE SER GLY GLY

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.70Å 138.20Å 134.40Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.9 (50.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14869	wwPDB-VP
Average B, all atoms (Å^2)	67.0	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	0.41	0/3455	0.72	2/4651 (0.0%)
1	B	0.42	0/3455	0.73	0/4652
2	C	0.39	0/4070	0.69	0/5497
2	D	0.33	0/4031	0.62	0/5450
All	All	0.39	0/15011	0.69	2/20250 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	PRO	N-CA-C	5.26	125.78	112.10
1	A	45	ASP	N-CA-C	-5.25	96.82	111.00

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	3406	0	3410	355	0
1	B	3406	0	3417	335	0
2	C	4005	0	4058	287	0
2	D	3966	0	4003	279	0
3	A	9	0	3	4	0
3	B	9	0	3	1	0
4	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	0	0
4	C	22	0	0	0	0
4	D	10	0	0	0	0
All	All	14869	0	14894	1160	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 39.

All (1160) 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)
2:C:192:THR:HG22	2:C:193:THR:H	1.02	1.12
2:D:192:THR:HG22	2:D:193:THR:H	1.00	1.11
1:B:276:ILE:HG22	1:B:282:ILE:HG12	1.27	1.09
1:A:266:ARG:HD2	1:B:437:LEU:HD21	1.36	1.07
1:A:409:THR:HG22	1:A:411:ASN:H	1.18	1.05
1:A:76:LYS:HB2	1:A:77:PRO:CD	1.89	1.02
1:B:3:VAL:HA	1:B:61:LEU:HD11	1.40	1.02
1:A:76:LYS:CB	1:A:77:PRO:HD2	1.90	1.01
2:C:72:ARG:HG2	2:C:174:LYS:HA	1.39	1.01
1:A:221:CYS:HB3	1:A:276:ILE:HD12	1.40	1.00
1:A:76:LYS:HB2	1:A:77:PRO:HD2	1.01	0.99
1:A:380:ARG:HD2	1:B:40:GLU:HG2	1.45	0.97
1:A:3:VAL:HG22	1:A:61:LEU:HD11	1.46	0.96
1:A:402:LEU:HA	1:A:419:MSE:CE	1.97	0.95
2:C:149:THR:HG22	2:C:152:GLY:O	1.67	0.95
2:C:411:THR:HG22	2:C:426:LEU:HD23	1.48	0.95
2:C:192:THR:HG22	2:C:193:THR:N	1.80	0.95
2:C:20:GLU:OE2	2:C:191:SER:HB3	1.66	0.95
1:A:402:LEU:HA	1:A:419:MSE:HE3	1.48	0.94
2:C:192:THR:CG2	2:C:193:THR:H	1.82	0.93
1:A:77:PRO:O	1:A:78:GLU:HB3	1.67	0.93
2:D:192:THR:HG22	2:D:193:THR:N	1.83	0.92
1:B:3:VAL:HG13	1:B:61:LEU:HD21	1.50	0.92
2:D:368:ILE:HG23	2:D:373:LEU:HB2	1.51	0.91
1:B:217:MSE:HE1	1:B:243:ASP:HB3	1.51	0.91
1:A:3:VAL:HG23	1:A:44:GLY:O	1.71	0.90
1:A:202:VAL:HG21	1:A:222:SER:CB	2.02	0.90
1:B:250:ARG:HD3	1:B:425:GLY:HA3	1.50	0.90
2:D:207:LYS:HB2	2:D:248:LEU:HD21	1.55	0.88
2:C:98:ARG:CD	2:C:98:ARG:H	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:HG21	1:B:367:ILE:HG22	1.56	0.88
1:B:409:THR:HG22	1:B:411:ASN:H	1.37	0.88
2:D:502:ALA:O	2:D:506:LEU:HG	1.73	0.88
2:C:293:PHE:HA	2:C:296:THR:HG23	1.52	0.88
1:A:95:THR:HG21	1:A:164:ALA:HB1	1.55	0.88
1:B:103:ILE:HG21	1:B:219:LEU:HG	1.56	0.87
1:A:202:VAL:HG21	1:A:222:SER:HB3	1.55	0.87
1:A:50:LYS:HE3	1:A:56:ASN:HD21	1.38	0.87
1:A:108:ASP:OD1	1:A:110:GLU:HG2	1.75	0.87
2:C:106:GLN:HE21	2:C:216:THR:HG22	1.40	0.86
2:C:463:VAL:HG11	2:C:478:GLN:HE21	1.41	0.86
2:D:211:ASP:HB3	2:D:459:PRO:HD2	1.58	0.86
1:A:217:MSE:HE2	2:C:49:ARG:HH22	1.41	0.85
1:A:241:THR:O	2:C:48:ARG:NH1	2.08	0.85
2:D:411:THR:HG22	2:D:424:ARG:O	1.76	0.85
1:A:337:THR:HG22	1:A:341:HIS:HB2	1.57	0.84
1:B:165:LEU:HD13	1:B:172:VAL:HG23	1.58	0.84
1:A:165:LEU:HD23	1:A:297:VAL:HG21	1.59	0.84
1:B:119:THR:HG22	1:B:121:GLU:H	1.43	0.84
1:B:150:LYS:H	1:B:153:HIS:HD2	1.20	0.84
2:D:409:GLU:HG2	2:D:426:LEU:HD22	1.60	0.84
1:B:241:THR:HG22	2:D:48:ARG:HH12	1.41	0.84
1:A:150:LYS:H	1:A:153:HIS:HD2	1.24	0.84
2:D:72:ARG:HG2	2:D:174:LYS:HA	1.59	0.84
1:A:125:LYS:HE3	2:C:60:ILE:HG12	1.60	0.84
2:C:149:THR:HG23	2:C:151:TRP:H	1.43	0.83
2:C:257:ARG:HH11	2:C:257:ARG:HG3	1.41	0.83
2:D:340:ARG:NH1	2:D:399:ARG:HG2	1.94	0.83
1:B:344:ASN:HD22	1:B:381:LYS:NZ	1.75	0.83
1:A:409:THR:HG22	1:A:411:ASN:N	1.94	0.83
1:B:127:LEU:HD22	1:B:219:LEU:HD12	1.61	0.83
1:A:401:LYS:HD2	1:A:419:MSE:SE	2.28	0.83
2:D:193:THR:HB	2:D:195:ASP:OD1	1.79	0.82
2:D:355:PRO:HG2	2:D:361:GLN:HG2	1.59	0.82
2:D:138:THR:HG23	2:D:162:GLU:HB3	1.60	0.82
2:D:289:VAL:HG13	2:D:292:ILE:HD12	1.61	0.82
1:B:69:VAL:HG11	1:B:72:ARG:HH11	1.44	0.82
1:A:78:GLU:O	1:A:78:GLU:HG3	1.81	0.81
2:D:472:LEU:HD23	2:D:472:LEU:H	1.45	0.81
2:C:72:ARG:HG2	2:C:174:LYS:CA	2.09	0.81
1:B:241:THR:HG23	2:D:90:GLU:OE2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:ILE:HD12	2:D:262:GLN:HE21	1.44	0.81
1:B:313:TYR:H	1:B:316:ILE:HD11	1.45	0.81
1:B:217:MSE:HG3	1:B:278:PRO:HG3	1.64	0.80
1:B:100:GLY:HA2	1:B:143:ASN:HD22	1.46	0.80
2:D:192:THR:CG2	2:D:193:THR:H	1.86	0.80
1:B:59:ILE:HG21	1:B:64:ILE:HD11	1.62	0.80
2:C:22:HIS:HB2	2:C:227:ARG:HB2	1.61	0.80
1:A:313:TYR:CE1	1:A:316:ILE:HG12	2.15	0.80
1:A:18:VAL:HG13	1:A:68:GLU:O	1.82	0.80
1:A:336:GLY:O	1:A:365:GLN:HG3	1.81	0.80
1:B:303:ILE:HG22	1:B:404:TRP:HA	1.64	0.79
1:B:241:THR:O	2:D:48:ARG:NH1	2.15	0.79
2:D:149:THR:HG22	2:D:152:GLY:O	1.83	0.79
2:C:98:ARG:H	2:C:98:ARG:HD3	1.48	0.79
2:D:65:LEU:HD22	2:D:69:LYS:HE3	1.65	0.79
2:C:164:ASP:HB2	2:C:187:LEU:HD13	1.65	0.79
1:B:3:VAL:HG23	1:B:44:GLY:HA2	1.64	0.78
1:B:257:MSE:HE2	1:B:268:ILE:HD12	1.64	0.78
1:A:179:ASP:OD2	3:A:1000:ASP:HB3	1.84	0.78
2:C:292:ILE:HD13	2:C:366:LYS:HB3	1.65	0.78
1:A:179:ASP:OD1	1:B:337:THR:HG23	1.84	0.78
1:A:3:VAL:HG22	1:A:61:LEU:CD1	2.14	0.77
2:C:463:VAL:HG11	2:C:478:GLN:NE2	1.98	0.77
1:B:258:HIS:HD2	1:B:260:SER:H	1.29	0.77
1:A:258:HIS:HD2	1:A:261:ARG:H	1.30	0.77
2:C:293:PHE:HA	2:C:296:THR:CG2	2.15	0.76
2:D:138:THR:HG22	2:D:139:ALA:H	1.51	0.76
2:D:480:LEU:HD21	2:D:489:PHE:CG	2.21	0.76
1:A:193:ARG:HA	1:A:193:ARG:NE	2.01	0.76
2:C:287:TYR:CD2	2:C:371:LEU:HD22	2.20	0.76
1:B:337:THR:HG22	1:B:341:HIS:HB2	1.66	0.76
1:B:221:CYS:HB3	1:B:276:ILE:CD1	2.16	0.75
1:A:217:MSE:HG3	1:A:278:PRO:HG3	1.67	0.75
2:C:502:ALA:O	2:C:506:LEU:HG	1.86	0.75
1:B:375:VAL:HG13	2:C:437:ASP:OD1	1.86	0.75
1:B:74:LYS:O	1:B:76:LYS:HG3	1.85	0.75
1:A:370:ARG:HH11	1:A:391:GLU:HG3	1.51	0.75
2:D:277:VAL:HG22	2:D:318:LYS:HD2	1.67	0.75
1:B:88:LYS:H	1:B:135:ASN:HD21	1.31	0.75
1:A:312:VAL:HA	1:A:316:ILE:HD11	1.67	0.75
1:B:318:SER:HB2	1:B:349:SER:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:HB2	1:A:180:THR:H	1.51	0.75
2:C:14:GLY:H	2:C:235:LYS:HB2	1.50	0.75
1:B:126:ALA:HB2	2:D:54:MET:CE	2.16	0.75
1:A:217:MSE:HE1	1:A:243:ASP:HB3	1.68	0.74
1:B:179:ASP:OD2	3:B:5000:ASP:HB3	1.87	0.74
1:B:344:ASN:HD22	1:B:381:LYS:HZ3	1.34	0.74
2:D:22:HIS:HB2	2:D:227:ARG:HB2	1.69	0.74
1:A:193:ARG:HE	1:A:193:ARG:HA	1.52	0.74
1:A:51:LEU:HD21	1:A:57:ILE:HD12	1.69	0.74
1:A:437:LEU:HD21	1:B:266:ARG:HD2	1.70	0.74
2:D:342:LYS:HA	2:D:345:VAL:O	1.87	0.74
1:B:165:LEU:HD23	1:B:297:VAL:HG21	1.69	0.74
2:D:394:ARG:HA	2:D:397:ILE:HD12	1.69	0.74
2:C:221:ARG:HH22	2:C:484:GLU:CB	2.00	0.74
1:B:150:LYS:H	1:B:153:HIS:CD2	2.05	0.73
2:C:193:THR:HB	2:C:195:ASP:OD1	1.88	0.73
1:A:180:THR:HG23	1:A:183:TYR:HB2	1.68	0.73
2:D:498:LYS:CB	2:D:502:ALA:HB3	2.18	0.73
2:C:326:GLU:OE2	2:C:329:PRO:HA	1.88	0.73
1:B:433:PHE:HB2	2:C:88:MET:CE	2.19	0.73
1:B:313:TYR:N	1:B:316:ILE:HD11	2.03	0.73
2:C:36:SER:HB2	2:C:185:ILE:HG12	1.69	0.73
2:C:314:ILE:HG12	2:C:393:LEU:HD22	1.71	0.73
1:B:244:THR:HG22	1:B:277:TRP:CZ3	2.25	0.72
1:A:153:HIS:O	1:A:157:ILE:HG12	1.90	0.72
2:D:411:THR:HG21	2:D:424:ARG:HD2	1.70	0.71
1:A:12:ILE:HG21	1:A:35:ILE:HD12	1.72	0.71
2:D:234:ILE:HD11	2:D:259:VAL:HA	1.70	0.71
1:B:126:ALA:HB2	2:D:54:MET:HE1	1.73	0.71
1:B:119:THR:HG22	1:B:121:GLU:N	2.05	0.71
2:D:324:GLY:O	2:D:332:ARG:HD3	1.89	0.71
1:A:100:GLY:HA2	1:A:143:ASN:HD22	1.54	0.71
1:A:422:ASN:ND2	1:A:426:GLU:HG2	2.06	0.71
2:C:103:VAL:HG22	2:C:218:LYS:HD2	1.73	0.71
2:C:138:THR:HG23	2:C:162:GLU:HB3	1.72	0.71
1:A:405:VAL:HB	1:A:419:MSE:CE	2.20	0.71
1:A:409:THR:CG2	1:A:411:ASN:H	2.01	0.70
1:B:126:ALA:C	1:B:127:LEU:HD12	2.10	0.70
1:B:141:LEU:HD23	1:B:157:ILE:HD13	1.73	0.70
2:D:465:ARG:HH21	2:D:466:TYR:HE2	1.37	0.70
2:D:54:MET:HG2	2:D:58:GLY:HA2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:GLU:OE1	2:C:172:LYS:HE3	1.92	0.70
2:D:457:GLU:H	2:D:457:GLU:CD	1.93	0.70
1:B:422:ASN:ND2	1:B:426:GLU:HG2	2.05	0.70
1:A:303:ILE:HG13	1:A:303:ILE:O	1.91	0.70
1:A:103:ILE:HG21	1:A:219:LEU:HG	1.73	0.70
2:C:70:LYS:HD2	2:C:72:ARG:HH21	1.56	0.70
2:D:207:LYS:CB	2:D:248:LEU:HD21	2.22	0.70
2:D:200:GLU:O	2:D:204:VAL:HG23	1.92	0.70
2:C:466:TYR:HB3	2:C:472:LEU:HD21	1.72	0.70
2:C:234:ILE:HD11	2:C:259:VAL:HG13	1.74	0.69
2:D:14:GLY:HA3	2:D:235:LYS:HG3	1.73	0.69
1:B:271:VAL:HG23	1:B:272:PRO:O	1.93	0.69
1:A:409:THR:HG22	1:A:410:GLN:N	2.07	0.69
1:A:165:LEU:HD13	1:A:172:VAL:HG23	1.74	0.69
1:B:258:HIS:CD2	1:B:260:SER:H	2.10	0.69
2:D:106:GLN:HE21	2:D:216:THR:HG22	1.58	0.69
2:D:393:LEU:O	2:D:397:ILE:HG13	1.92	0.69
1:B:176:HIS:HB3	1:B:181:MSE:HE2	1.73	0.69
1:B:18:VAL:HG12	1:B:19:ARG:N	2.08	0.69
1:B:127:LEU:HD21	1:B:216:ALA:HA	1.75	0.69
1:A:313:TYR:CD1	1:A:316:ILE:HG12	2.28	0.69
1:B:299:VAL:HG12	1:B:300:ASP:N	2.08	0.69
2:D:65:LEU:CD2	2:D:69:LYS:HE3	2.23	0.68
1:A:176:HIS:HB3	1:A:181:MSE:HE2	1.75	0.68
2:D:96:PRO:HD2	2:D:441:LEU:HD12	1.74	0.68
1:A:174:VAL:HB	1:A:201:LEU:HD13	1.75	0.68
2:D:282:ILE:HD11	2:D:404:ILE:HD11	1.75	0.68
2:D:28:LYS:HE3	2:D:33:PRO:HA	1.75	0.68
2:D:314:ILE:HG12	2:D:393:LEU:HD22	1.76	0.68
1:B:257:MSE:HE2	1:B:268:ILE:CD1	2.22	0.68
1:A:312:VAL:HA	1:A:316:ILE:CD1	2.24	0.68
2:D:149:THR:HG21	2:D:201:GLN:HG3	1.75	0.68
1:A:259:THR:CG2	1:B:339:LEU:HD23	2.23	0.68
1:A:88:LYS:HB2	1:A:91:LEU:HD12	1.74	0.68
2:D:23:ARG:NE	2:D:226:ILE:HG12	2.09	0.68
1:A:279:ASN:ND2	1:A:281:GLU:HG3	2.08	0.68
1:A:258:HIS:CD2	1:A:261:ARG:H	2.13	0.67
1:B:227:THR:HG22	1:B:227:THR:O	1.94	0.67
2:D:296:THR:HG22	2:D:298:SER:H	1.60	0.67
2:D:23:ARG:HD3	2:D:226:ILE:HG23	1.75	0.67
1:B:77:PRO:O	1:B:78:GLU:HB3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LYS:CB	1:B:77:PRO:CD	2.72	0.67
1:B:433:PHE:HB2	2:C:88:MET:HE2	1.75	0.67
1:A:370:ARG:O	1:B:259:THR:HG21	1.93	0.67
2:D:392:ALA:O	2:D:396:VAL:HG23	1.93	0.67
1:A:422:ASN:HD21	1:A:427:ILE:H	1.40	0.67
1:A:244:THR:HG22	1:A:245:TYR:CD2	2.30	0.67
1:A:313:TYR:O	1:A:316:ILE:HG13	1.95	0.67
1:A:259:THR:HG22	1:B:339:LEU:HD23	1.75	0.67
1:A:266:ARG:HD3	1:A:438:ARG:O	1.95	0.67
1:A:108:ASP:CG	2:C:56:GLU:HG2	2.15	0.67
2:D:89:ASP:HB2	2:D:132:VAL:HG12	1.75	0.67
1:A:158:ALA:HB2	1:A:191:MSE:HE3	1.77	0.66
2:C:19:LEU:H	2:C:192:THR:HB	1.58	0.66
2:D:320:ARG:HH21	2:D:351:ILE:HD11	1.58	0.66
1:B:405:VAL:HA	1:B:418:MSE:CE	2.25	0.66
2:C:314:ILE:CG1	2:C:393:LEU:HD22	2.25	0.66
1:A:127:LEU:HD22	1:A:130:ILE:HG12	1.77	0.66
1:B:125:LYS:HE3	2:D:60:ILE:HG12	1.76	0.66
1:A:111:THR:HG22	1:A:113:ALA:H	1.60	0.66
1:B:432:ARG:O	1:B:435:THR:HG22	1.96	0.66
2:C:476:LEU:O	2:C:480:LEU:HG	1.95	0.66
1:B:434:ASP:HB3	2:C:80:TYR:CD2	2.31	0.66
1:A:225:MSE:HG2	1:A:276:ILE:HD13	1.79	0.65
1:A:301:ASP:O	1:A:303:ILE:HG23	1.96	0.65
1:A:405:VAL:CB	1:A:419:MSE:HE2	2.26	0.65
2:C:356:ASN:HB3	2:C:357:TYR:CD1	2.31	0.65
1:B:151:PRO:CG	1:B:403:MSE:HE1	2.26	0.65
1:A:434:ASP:HA	1:A:438:ARG:NH1	2.11	0.65
1:A:312:VAL:HG11	1:A:343:PRO:HD3	1.78	0.65
2:D:149:THR:HG23	2:D:151:TRP:H	1.61	0.65
1:A:401:LYS:C	1:A:419:MSE:HE1	2.17	0.65
2:C:463:VAL:HG21	2:C:478:GLN:NE2	2.12	0.65
1:B:69:VAL:HG11	1:B:72:ARG:NH1	2.12	0.65
1:A:402:LEU:HA	1:A:419:MSE:HE1	1.76	0.65
2:C:234:ILE:HD11	2:C:259:VAL:HA	1.77	0.65
1:A:50:LYS:HE2	1:A:54:GLY:O	1.96	0.65
2:C:28:LYS:HE3	2:C:33:PRO:HA	1.78	0.65
1:B:6:PHE:CE2	1:B:61:LEU:HD22	2.32	0.65
1:A:405:VAL:CG2	1:A:419:MSE:HE2	2.27	0.65
1:B:195:LEU:HD11	1:B:199:VAL:HG23	1.79	0.65
1:B:146:SER:HB2	1:B:180:THR:HB	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:VAL:HB	1:A:419:MSE:HE2	1.77	0.65
2:D:13:LEU:HB3	2:D:234:ILE:HG23	1.78	0.65
1:A:266:ARG:NH1	1:A:438:ARG:OXT	2.30	0.64
2:D:363:GLU:O	2:D:367:VAL:HG23	1.97	0.64
1:B:405:VAL:HA	1:B:418:MSE:HE3	1.78	0.64
1:A:158:ALA:HB2	1:A:191:MSE:CE	2.27	0.64
2:D:349:PHE:HA	2:D:353:GLU:OE2	1.97	0.64
1:B:313:TYR:CE1	1:B:316:ILE:HG12	2.31	0.64
1:A:344:ASN:HD21	1:A:381:LYS:HD2	1.62	0.64
1:A:427:ILE:HG22	1:A:428:THR:N	2.12	0.64
2:C:299:LYS:O	2:C:303:ARG:HG3	1.98	0.64
1:B:409:THR:HG22	1:B:410:GLN:N	2.12	0.64
1:B:178:THR:HG21	1:B:205:GLN:OE1	1.97	0.64
2:C:314:ILE:HD12	2:C:397:ILE:HD11	1.79	0.64
2:C:356:ASN:HB3	2:C:357:TYR:CE1	2.32	0.64
2:C:9:ASN:O	2:C:11:GLU:N	2.30	0.64
1:B:18:VAL:HG12	1:B:19:ARG:H	1.63	0.64
1:B:50:LYS:CE	1:B:56:ASN:HD21	2.10	0.64
1:A:146:SER:HB3	1:A:176:HIS:CE1	2.32	0.64
1:A:339:LEU:HD23	1:B:259:THR:CG2	2.28	0.64
2:C:277:VAL:HG21	2:C:318:LYS:HB2	1.78	0.64
2:D:353:GLU:HG2	2:D:354:LEU:HD23	1.80	0.64
1:B:76:LYS:HB2	1:B:77:PRO:HD3	1.79	0.64
1:A:6:PHE:HE1	1:A:10:ARG:HE	1.45	0.64
2:C:246:GLN:HG2	2:C:247:GLU:H	1.62	0.64
2:C:240:ILE:HD12	2:C:262:GLN:NE2	2.13	0.64
1:B:252:THR:CB	1:B:425:GLY:O	2.46	0.63
1:B:103:ILE:O	1:B:103:ILE:HG22	1.98	0.63
1:B:76:LYS:CB	1:B:77:PRO:HD3	2.28	0.63
1:A:22:LYS:NZ	1:A:24:GLU:HG2	2.13	0.63
1:B:217:MSE:HE2	2:D:49:ARG:NH2	2.13	0.63
1:B:344:ASN:HA	1:B:347:ILE:HG12	1.80	0.63
2:C:310:LYS:HD2	2:C:386:GLU:HG3	1.80	0.63
1:B:225:MSE:SE	1:B:276:ILE:HG21	2.49	0.63
1:A:51:LEU:N	1:A:51:LEU:HD12	2.14	0.63
1:A:422:ASN:ND2	1:A:427:ILE:H	1.96	0.63
2:C:103:VAL:O	2:C:107:ILE:HG13	1.98	0.63
2:C:240:ILE:HD12	2:C:262:GLN:HE21	1.64	0.63
2:D:350:HIS:CE1	2:D:353:GLU:HB3	2.34	0.63
2:D:126:VAL:HG21	2:D:131:ASN:ND2	2.14	0.63
1:B:252:THR:HB	1:B:425:GLY:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:O	1:A:355:GLU:HG3	1.98	0.63
1:A:93:GLU:HB3	1:A:137:LYS:HE3	1.80	0.63
1:A:270:ASP:OD2	1:A:286:ARG:NH2	2.32	0.62
1:A:92:PRO:HB3	1:A:170:TYR:CD2	2.34	0.62
2:C:98:ARG:NE	2:C:98:ARG:H	1.96	0.62
2:D:167:ARG:HG3	2:D:182:ARG:HD3	1.81	0.62
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.64	0.62
1:A:405:VAL:HG21	1:A:419:MSE:HE2	1.81	0.62
1:B:303:ILE:O	1:B:303:ILE:HG13	1.99	0.62
1:B:274:ALA:HB2	1:B:284:PHE:HA	1.81	0.62
1:A:244:THR:HG22	1:A:245:TYR:HD2	1.62	0.62
1:A:347:ILE:HD12	1:A:382:LEU:HG	1.81	0.62
1:B:50:LYS:HE2	1:B:56:ASN:HD21	1.64	0.62
1:A:205:GLN:HE22	1:A:256:LYS:CE	2.12	0.62
1:A:344:ASN:HA	1:A:347:ILE:HG12	1.82	0.62
1:B:409:THR:HG22	1:B:411:ASN:N	2.13	0.62
2:D:261:ARG:NH1	2:D:412:ARG:NE	2.48	0.62
1:B:12:ILE:CG2	1:B:35:ILE:HD12	2.30	0.62
2:D:167:ARG:NH1	2:D:181:ASP:OD2	2.33	0.62
1:B:405:VAL:HG22	1:B:418:MSE:HE3	1.82	0.62
1:A:69:VAL:HG11	1:A:72:ARG:NH1	2.14	0.62
1:B:108:ASP:CG	2:D:56:GLU:HG2	2.20	0.62
2:D:251:ILE:HB	2:D:252:PRO:HD3	1.80	0.61
2:D:14:GLY:H	2:D:235:LYS:H	1.47	0.61
1:B:108:ASP:HA	2:D:56:GLU:HG2	1.81	0.61
1:B:347:ILE:HB	1:B:348:PRO:HD3	1.80	0.61
1:A:259:THR:HG23	1:B:339:LEU:HA	1.81	0.61
1:A:225:MSE:HB3	1:A:234:MSE:HE1	1.82	0.61
1:A:195:LEU:HD22	1:A:197:LYS:O	2.00	0.61
1:B:217:MSE:CE	1:B:243:ASP:HB3	2.26	0.61
2:D:326:GLU:HA	2:D:332:ARG:HG2	1.81	0.61
1:B:312:VAL:HA	1:B:316:ILE:CD1	2.30	0.61
1:B:76:LYS:HB2	1:B:77:PRO:CD	2.30	0.61
2:C:65:LEU:CD2	2:C:69:LYS:HE3	2.29	0.61
2:C:289:VAL:HG11	2:C:367:VAL:HG22	1.82	0.61
2:D:93:PRO:HG3	2:D:137:ARG:NH1	2.14	0.61
1:A:225:MSE:CG	1:A:276:ILE:HD13	2.31	0.61
2:D:240:ILE:HD13	2:D:261:ARG:NH2	2.16	0.61
2:C:284:GLU:HG3	2:C:284:GLU:O	2.01	0.61
1:B:221:CYS:HB3	1:B:276:ILE:HD11	1.81	0.60
1:B:252:THR:OG1	1:B:425:GLY:O	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:ARG:NH1	2:C:181:ASP:OD2	2.34	0.60
1:A:99:THR:HG23	1:A:142:PHE:HE1	1.66	0.60
2:D:221:ARG:HH22	2:D:484:GLU:CB	2.14	0.60
2:C:130:SER:HB2	2:C:165:ALA:HB1	1.81	0.60
1:A:259:THR:HB	1:B:369:GLY:HA3	1.82	0.60
2:D:354:LEU:HB2	2:D:355:PRO:HA	1.83	0.60
1:B:214:ASP:HB2	1:B:238:HIS:CE1	2.36	0.60
1:A:205:GLN:HA	1:A:205:GLN:OE1	2.02	0.60
1:A:109:TYR:CD2	2:C:431:ARG:HB3	2.37	0.60
2:C:208:PHE:HE1	2:C:458:LEU:HD21	1.65	0.60
1:A:99:THR:HG22	1:A:99:THR:O	2.02	0.60
2:C:23:ARG:NE	2:C:226:ILE:HG12	2.16	0.60
1:A:266:ARG:HD2	1:B:437:LEU:CD2	2.22	0.60
1:A:433:PHE:HB2	2:D:88:MET:HE2	1.83	0.60
2:C:257:ARG:NH1	2:C:257:ARG:HG3	2.14	0.60
2:D:354:LEU:HD12	2:D:364:VAL:HG22	1.84	0.60
2:C:72:ARG:CG	2:C:174:LYS:HA	2.25	0.60
2:C:293:PHE:CD2	2:C:296:THR:HG21	2.36	0.59
2:C:272:LEU:HD13	2:C:404:ILE:HG12	1.83	0.59
2:C:261:ARG:NH1	2:C:412:ARG:CZ	2.65	0.59
1:B:3:VAL:CA	1:B:61:LEU:HD11	2.23	0.59
1:A:200:VAL:HG12	1:A:202:VAL:HG23	1.84	0.59
2:C:393:LEU:O	2:C:397:ILE:HG13	2.02	0.59
2:C:138:THR:HG22	2:C:139:ALA:N	2.18	0.59
1:B:195:LEU:HD11	1:B:199:VAL:CG2	2.32	0.59
1:B:312:VAL:HA	1:B:316:ILE:HD11	1.84	0.59
2:D:96:PRO:HG3	2:D:121:TYR:CE1	2.37	0.59
1:A:39:TYR:O	1:A:41:LEU:N	2.34	0.59
1:A:205:GLN:HE22	1:A:256:LYS:HE3	1.66	0.59
1:B:176:HIS:HE2	1:B:184:THR:HG1	1.48	0.59
2:D:105:LEU:HD21	2:D:443:ILE:HD13	1.84	0.59
1:B:140:LEU:HD12	1:B:140:LEU:C	2.23	0.59
2:D:85:LEU:HD23	2:D:88:MET:CE	2.33	0.59
1:A:18:VAL:CG1	1:A:19:ARG:N	2.65	0.59
1:A:159:HIS:CE1	1:A:299:VAL:HG11	2.37	0.59
2:C:15:LEU:HD12	2:C:16:LYS:N	2.18	0.59
1:B:86:GLU:CD	1:B:86:GLU:H	2.05	0.59
1:B:313:TYR:CD1	1:B:316:ILE:HG12	2.37	0.59
1:B:96:ILE:HA	1:B:173:VAL:O	2.03	0.59
1:A:274:ALA:HB2	1:A:284:PHE:HA	1.85	0.59
1:A:342:THR:HG23	1:A:343:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HG21	1:A:35:ILE:CD1	2.32	0.58
2:D:356:ASN:HB3	2:D:357:TYR:CD1	2.38	0.58
2:C:31:PHE:CE2	2:C:438:ILE:HG13	2.38	0.58
1:A:151:PRO:HG3	1:A:403:MSE:HE1	1.85	0.58
2:D:231:ASN:HA	2:D:240:ILE:O	2.03	0.58
2:D:32:SER:O	2:D:34:VAL:N	2.33	0.58
2:C:155:GLY:O	2:C:156:ILE:HD12	2.02	0.58
1:B:99:THR:O	1:B:99:THR:HG22	2.04	0.58
1:A:411:ASN:O	1:A:415:VAL:HG23	2.03	0.58
1:A:217:MSE:HE2	2:C:49:ARG:NH2	2.12	0.58
2:D:31:PHE:CE2	2:D:438:ILE:HG12	2.39	0.58
2:C:168:ILE:HD11	2:C:171:ARG:HG2	1.85	0.58
2:C:27:THR:OG1	2:C:186:PRO:HG2	2.03	0.58
2:D:27:THR:HG21	2:D:100:ALA:N	2.19	0.58
2:C:87:TYR:CD2	2:C:183:LEU:HG	2.39	0.58
2:C:77:GLU:OE1	2:C:169:ILE:HG13	2.03	0.58
1:A:250:ARG:HD3	1:A:425:GLY:HA3	1.85	0.58
1:B:3:VAL:HG23	1:B:44:GLY:CA	2.32	0.58
2:C:49:ARG:HG2	2:C:73:VAL:HG23	1.85	0.58
1:A:380:ARG:HD2	1:B:40:GLU:CG	2.28	0.58
1:B:125:LYS:HE2	2:D:58:GLY:O	2.03	0.58
2:C:47:GLN:HE21	2:C:73:VAL:HG21	1.68	0.58
2:C:43:GLU:OE1	2:C:79:ASN:HB2	2.04	0.58
2:D:138:THR:HG22	2:D:139:ALA:N	2.17	0.58
2:D:282:ILE:HD12	2:D:401:ARG:HG2	1.85	0.58
1:A:146:SER:OG	3:A:1000:ASP:O	2.21	0.58
1:A:229:GLU:HA	1:A:292:ARG:HG2	1.86	0.58
1:A:435:THR:HG23	1:A:435:THR:O	2.03	0.58
1:B:347:ILE:HD12	1:B:382:LEU:HG	1.86	0.57
2:D:48:ARG:NH2	2:D:88:MET:O	2.37	0.57
2:C:470:TYR:N	2:C:470:TYR:HD1	2.02	0.57
2:C:126:VAL:HG11	2:C:131:ASN:HD22	1.68	0.57
1:B:250:ARG:O	1:B:254:VAL:HG23	2.04	0.57
2:D:167:ARG:HD3	2:D:181:ASP:OD1	2.04	0.57
1:A:195:LEU:CB	1:A:290:ARG:HH12	2.17	0.57
1:B:217:MSE:HG3	1:B:278:PRO:CG	2.34	0.57
2:C:289:VAL:O	2:C:289:VAL:HG12	2.05	0.57
1:A:433:PHE:HB2	2:D:88:MET:CE	2.35	0.57
2:C:350:HIS:HD2	2:C:352:ASP:H	1.52	0.57
1:A:225:MSE:HE3	1:A:234:MSE:HE1	1.87	0.57
1:B:127:LEU:HD22	1:B:219:LEU:CD1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:LEU:HD23	2:D:88:MET:HE3	1.87	0.57
2:C:402:GLU:HB3	2:C:408:PRO:HG3	1.87	0.57
1:B:86:GLU:N	1:B:86:GLU:CD	2.58	0.57
1:A:333:VAL:HG21	1:A:399:TYR:HA	1.85	0.57
1:B:3:VAL:HG22	1:B:61:LEU:HG	1.87	0.57
1:A:50:LYS:HE3	1:A:56:ASN:ND2	2.14	0.57
2:C:470:TYR:N	2:C:470:TYR:CD1	2.73	0.57
1:B:218:ASN:ND2	1:B:237:MSE:HE1	2.20	0.57
1:A:95:THR:HG21	1:A:164:ALA:CB	2.31	0.56
2:D:314:ILE:CG1	2:D:393:LEU:HD22	2.35	0.56
1:A:384:LYS:HD2	1:B:41:LEU:HD13	1.87	0.56
1:B:99:THR:O	1:B:99:THR:CG2	2.53	0.56
1:A:81:PHE:HB2	1:A:119:THR:HG21	1.85	0.56
1:A:195:LEU:HB3	1:A:290:ARG:NH1	2.21	0.56
1:A:342:THR:HG21	1:A:346:ILE:HG22	1.88	0.56
1:A:269:ASN:ND2	1:A:392:ASP:HB2	2.20	0.56
2:D:325:ARG:O	2:D:332:ARG:HB3	2.06	0.56
2:C:481:VAL:HA	2:C:486:ASP:HB3	1.86	0.56
2:C:293:PHE:CA	2:C:296:THR:HG23	2.32	0.56
1:B:225:MSE:HG2	1:B:276:ILE:HD13	1.88	0.56
1:B:316:ILE:HB	1:B:346:ILE:HD11	1.88	0.56
1:B:153:HIS:O	1:B:157:ILE:HG12	2.06	0.56
1:B:205:GLN:OE1	1:B:205:GLN:HA	2.06	0.56
2:D:79:ASN:OD1	2:D:82:LEU:HB2	2.06	0.56
1:B:350:ILE:O	1:B:354:VAL:HG23	2.06	0.56
1:A:189:SER:HA	1:A:233:VAL:HG21	1.88	0.56
2:C:149:THR:HG21	2:C:201:GLN:HG3	1.88	0.55
2:D:495:MET:C	2:D:497:VAL:H	2.09	0.55
1:A:312:VAL:HG12	1:A:313:TYR:N	2.21	0.55
2:C:67:GLU:HG2	2:C:127:ILE:HG22	1.88	0.55
2:C:98:ARG:O	2:C:102:GLU:HG3	2.07	0.55
2:D:296:THR:HG22	2:D:298:SER:N	2.20	0.55
2:C:234:ILE:CD1	2:C:259:VAL:HG13	2.36	0.55
2:C:412:ARG:HH11	2:C:412:ARG:HG2	1.71	0.55
2:C:354:LEU:HD13	2:C:364:VAL:HG22	1.88	0.55
1:B:299:VAL:CG1	1:B:300:ASP:N	2.70	0.55
2:C:32:SER:O	2:C:34:VAL:N	2.35	0.55
1:A:3:VAL:CG2	1:A:61:LEU:HD11	2.31	0.55
1:A:202:VAL:HG21	1:A:222:SER:HB2	1.87	0.55
2:C:79:ASN:HD21	2:C:82:LEU:HG	1.71	0.55
2:D:181:ASP:OD1	2:D:182:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:ASP:HB3	2:C:10:TYR:HE1	1.71	0.55
1:B:44:GLY:O	1:B:46:THR:N	2.40	0.55
1:B:409:THR:HG22	1:B:410:GLN:H	1.70	0.55
1:A:141:LEU:O	1:A:141:LEU:HD12	2.06	0.55
2:C:476:LEU:HD13	2:C:504:SER:CB	2.37	0.55
1:A:106:ARG:HD3	1:A:122:GLU:OE2	2.06	0.55
1:A:421:THR:HB	1:A:423:TYR:HE1	1.72	0.55
2:C:19:LEU:HD12	2:C:230:LEU:HD23	1.88	0.55
2:C:196:ILE:HG23	2:C:201:GLN:HG2	1.88	0.55
1:A:312:VAL:HG12	1:A:313:TYR:H	1.70	0.55
2:D:466:TYR:HB3	2:D:472:LEU:HD21	1.88	0.55
2:C:181:ASP:OD1	2:C:182:ARG:N	2.40	0.55
1:B:9:GLU:C	1:B:11:ASN:H	2.09	0.55
1:A:3:VAL:HG22	1:A:61:LEU:CG	2.37	0.55
1:A:18:VAL:HG12	1:A:19:ARG:N	2.20	0.55
1:B:279:ASN:OD1	1:B:281:GLU:HG3	2.07	0.55
1:B:106:ARG:HB3	2:D:55:SER:O	2.07	0.55
2:D:326:GLU:CA	2:D:332:ARG:HG2	2.36	0.55
1:B:433:PHE:HB2	2:C:88:MET:HE1	1.88	0.54
3:A:1000:ASP:HB2	1:B:376:TYR:CE1	2.42	0.54
1:B:159:HIS:CE1	1:B:299:VAL:HG11	2.41	0.54
1:B:363:THR:HG21	1:B:395:PRO:HA	1.90	0.54
1:B:205:GLN:HE22	1:B:256:LYS:HE3	1.72	0.54
2:C:155:GLY:C	2:C:156:ILE:HD12	2.27	0.54
1:B:24:GLU:O	1:B:27:GLU:HB2	2.07	0.54
1:A:430:TYR:CD2	2:D:34:VAL:HG22	2.42	0.54
1:B:274:ALA:CB	1:B:284:PHE:HA	2.37	0.54
1:B:214:ASP:O	1:B:218:ASN:ND2	2.40	0.54
1:B:416:ARG:O	1:B:417:LYS:C	2.46	0.54
1:A:158:ALA:CB	1:A:191:MSE:HE3	2.36	0.54
2:D:261:ARG:NH1	2:D:412:ARG:CZ	2.70	0.54
2:D:166:ALA:HB2	2:D:183:LEU:HB2	1.88	0.54
2:C:84:ASP:OD2	2:C:86:VAL:HB	2.07	0.54
1:A:179:ASP:HB3	1:B:337:THR:HG23	1.89	0.54
2:C:42:VAL:HG13	2:C:77:GLU:HB3	1.89	0.54
1:A:258:HIS:CD2	1:A:260:SER:H	2.26	0.54
1:B:64:ILE:HG21	1:B:67:ILE:HD11	1.89	0.54
2:D:312:LEU:HB2	2:D:393:LEU:HD11	1.89	0.54
1:A:402:LEU:N	1:A:419:MSE:HE1	2.23	0.54
2:C:16:LYS:HB3	2:C:194:PRO:O	2.07	0.54
2:D:23:ARG:O	2:D:188:ILE:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:VAL:CG2	2:C:318:LYS:HD2	2.38	0.54
1:A:195:LEU:CB	1:A:290:ARG:NH1	2.71	0.54
2:D:498:LYS:O	2:D:499:PRO:C	2.46	0.54
2:C:65:LEU:HD22	2:C:69:LYS:HE3	1.89	0.54
1:A:342:THR:HG22	1:A:343:PRO:O	2.08	0.54
1:A:179:ASP:HB3	1:B:337:THR:CG2	2.38	0.54
2:C:355:PRO:O	2:C:356:ASN:HB2	2.08	0.54
2:D:505:ILE:O	2:D:509:VAL:HB	2.08	0.54
1:B:217:MSE:HE2	2:D:49:ARG:HH22	1.73	0.54
2:C:96:PRO:HG3	2:C:121:TYR:CE1	2.44	0.54
2:D:19:LEU:HB3	2:D:192:THR:OG1	2.08	0.53
2:C:460:GLN:OE1	2:C:478:GLN:NE2	2.41	0.53
1:A:339:LEU:HD23	1:B:259:THR:HG22	1.90	0.53
1:A:178:THR:HG23	1:A:265:PHE:CE1	2.44	0.53
1:A:263:ASP:CB	1:B:436:TYR:HE2	2.21	0.53
1:A:179:ASP:OD1	1:B:337:THR:CG2	2.55	0.53
2:C:75:VAL:HB	2:C:177:ILE:HG12	1.89	0.53
2:D:299:LYS:O	2:D:303:ARG:HG3	2.08	0.53
2:D:275:ARG:HD3	2:D:318:LYS:HB3	1.89	0.53
1:A:57:ILE:HD11	2:C:140:ILE:HG21	1.90	0.53
1:B:361:CYS:HB3	1:B:390:CYS:SG	2.48	0.53
1:B:51:LEU:HD11	1:B:57:ILE:HD12	1.89	0.53
1:B:3:VAL:HG22	1:B:61:LEU:CD1	2.39	0.53
1:A:437:LEU:CD2	1:B:266:ARG:HD2	2.37	0.53
2:C:398:LYS:HE2	2:C:402:GLU:OE1	2.08	0.53
2:C:87:TYR:HD2	2:C:183:LEU:HG	1.74	0.53
1:A:227:THR:O	1:A:227:THR:CG2	2.55	0.53
1:A:409:THR:HG22	1:A:410:GLN:H	1.71	0.53
1:B:268:ILE:O	1:B:269:ASN:HB2	2.08	0.53
2:C:312:LEU:N	2:C:312:LEU:HD23	2.24	0.53
1:A:195:LEU:HB2	1:A:290:ARG:HH12	1.73	0.53
1:B:200:VAL:HG22	1:B:234:MSE:HE3	1.89	0.53
1:A:402:LEU:CA	1:A:419:MSE:HE1	2.38	0.53
2:C:296:THR:HG22	2:C:363:GLU:CD	2.29	0.53
1:A:405:VAL:HG22	1:A:418:MSE:HE2	1.91	0.53
2:D:394:ARG:O	2:D:397:ILE:HB	2.07	0.53
1:A:205:GLN:HG2	1:A:261:ARG:O	2.08	0.53
1:B:93:GLU:OE1	1:B:137:LYS:HE3	2.09	0.53
2:D:147:VAL:HG23	2:D:156:ILE:HD11	1.91	0.53
2:D:157:PRO:HD2	2:D:191:SER:O	2.09	0.53
2:D:19:LEU:HD13	2:D:230:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:411:THR:O	2:C:423:MET:HB3	2.08	0.52
2:C:88:MET:O	2:C:89:ASP:HB3	2.09	0.52
2:C:277:VAL:HG22	2:C:318:LYS:HD2	1.91	0.52
1:A:307:VAL:HG13	1:A:331:GLY:O	2.09	0.52
2:C:15:LEU:HD11	2:C:17:VAL:HG23	1.90	0.52
1:B:274:ALA:HA	1:B:285:LEU:HG	1.91	0.52
1:B:159:HIS:NE2	1:B:301:ASP:OD2	2.38	0.52
1:A:6:PHE:CE1	1:A:10:ARG:NE	2.77	0.52
1:B:21:THR:OG1	1:B:66:ARG:HB2	2.09	0.52
1:A:206:ARG:HG3	1:A:210:ARG:HD3	1.91	0.52
2:D:150:PRO:HB2	2:D:151:TRP:CE3	2.43	0.52
1:B:69:VAL:HG21	1:B:72:ARG:HH12	1.75	0.52
1:B:258:HIS:CE1	1:B:261:ARG:HD2	2.44	0.52
1:A:51:LEU:N	1:A:51:LEU:CD1	2.73	0.52
1:A:263:ASP:HB2	1:B:436:TYR:HE2	1.74	0.52
1:B:344:ASN:ND2	1:B:381:LYS:NZ	2.53	0.52
2:D:29:LYS:HE2	2:D:183:LEU:O	2.10	0.52
2:D:29:LYS:HD2	2:D:34:VAL:HB	1.92	0.52
1:A:142:PHE:HD1	1:A:142:PHE:O	1.93	0.52
2:C:467:VAL:HG21	2:C:474:ARG:HG2	1.90	0.52
1:A:326:ASP:OD1	1:A:352:ARG:NH2	2.43	0.52
1:A:258:HIS:HD2	1:A:260:SER:H	1.56	0.52
2:D:394:ARG:HA	2:D:397:ILE:CD1	2.40	0.52
1:A:330:LYS:HA	1:A:330:LYS:HE3	1.90	0.52
2:D:231:ASN:HD22	2:D:239:ARG:HE	1.56	0.52
1:B:261:ARG:HH11	1:B:263:ASP:CB	2.23	0.52
1:A:51:LEU:C	1:A:53:ASN:H	2.13	0.52
2:C:246:GLN:H	2:C:246:GLN:CD	2.12	0.52
2:D:310:LYS:HD2	2:D:386:GLU:HG2	1.91	0.52
1:A:409:THR:CG2	1:A:410:GLN:N	2.72	0.52
1:B:83:ALA:HA	1:B:119:THR:HG23	1.92	0.52
1:A:180:THR:CG2	1:A:180:THR:O	2.58	0.52
2:D:36:SER:HB2	2:D:220:LYS:NZ	2.25	0.52
1:B:22:LYS:HE2	1:B:24:GLU:HG2	1.91	0.52
2:D:284:GLU:HG3	2:D:284:GLU:O	2.10	0.52
1:A:51:LEU:HD11	1:A:57:ILE:HB	1.92	0.52
1:A:303:ILE:HG22	1:A:404:TRP:HA	1.91	0.52
1:B:176:HIS:ND1	1:B:177:GLY:N	2.58	0.52
2:D:27:THR:OG1	2:D:186:PRO:HG2	2.10	0.52
2:D:7:LYS:HG2	2:D:8:PHE:CE1	2.45	0.52
2:D:360:SER:OG	2:D:363:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:HG22	1:B:404:TRP:CA	2.39	0.52
1:A:347:ILE:N	1:A:348:PRO:CD	2.73	0.52
1:A:271:VAL:HG22	1:A:272:PRO:HD2	1.91	0.52
1:A:76:LYS:CB	1:A:77:PRO:CD	2.66	0.51
1:A:3:VAL:HG13	1:A:61:LEU:HD21	1.92	0.51
1:B:165:LEU:CD1	1:B:172:VAL:HG23	2.37	0.51
1:A:141:LEU:HD23	1:A:157:ILE:HD13	1.93	0.51
2:D:72:ARG:HG2	2:D:174:LYS:CA	2.36	0.51
1:A:51:LEU:CD2	1:A:57:ILE:HD12	2.38	0.51
2:D:101:LEU:O	2:D:104:ALA:HB3	2.10	0.51
2:D:123:ARG:O	2:D:432:MET:HA	2.10	0.51
1:B:411:ASN:O	1:B:415:VAL:HG23	2.09	0.51
1:A:130:ILE:HG13	1:A:131:PHE:CD1	2.45	0.51
1:A:6:PHE:HE1	1:A:10:ARG:NE	2.08	0.51
1:B:249:HIS:HB3	1:B:254:VAL:HG22	1.93	0.51
2:C:257:ARG:HH11	2:C:257:ARG:CG	2.19	0.51
2:C:271:GLU:O	2:C:275:ARG:HG3	2.10	0.51
1:B:351:GLU:O	1:B:355:GLU:HG3	2.10	0.51
1:A:14:VAL:HG13	1:A:14:VAL:O	2.11	0.51
2:D:203:LYS:HD2	2:D:252:PRO:HG2	1.92	0.51
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.26	0.51
2:C:269:ARG:HG3	2:C:404:ILE:O	2.09	0.51
1:B:39:TYR:O	1:B:40:GLU:C	2.48	0.51
2:C:101:LEU:O	2:C:104:ALA:HB3	2.11	0.51
1:B:317:SER:C	1:B:319:GLU:H	2.14	0.51
1:A:402:LEU:CA	1:A:419:MSE:CE	2.82	0.51
1:A:100:GLY:HA2	1:A:143:ASN:ND2	2.24	0.51
2:C:275:ARG:HB3	2:C:318:LYS:HD3	1.92	0.51
1:B:221:CYS:HB3	1:B:276:ILE:HD12	1.88	0.51
1:B:165:LEU:HD13	1:B:172:VAL:CG2	2.37	0.51
1:B:130:ILE:HD12	1:B:136:VAL:HG21	1.92	0.51
1:A:330:LYS:HD3	1:A:410:GLN:OE1	2.11	0.51
1:A:107:ILE:HG22	1:A:114:VAL:HG13	1.92	0.51
1:B:39:TYR:HD2	1:B:42:SER:OG	1.94	0.51
1:B:249:HIS:CB	1:B:254:VAL:HG22	2.40	0.51
1:B:330:LYS:HE2	1:B:410:GLN:OE1	2.11	0.51
1:A:369:GLY:HA3	1:B:259:THR:HB	1.92	0.51
2:D:123:ARG:HD3	2:D:135:PHE:CE2	2.46	0.51
2:D:495:MET:C	2:D:497:VAL:N	2.64	0.50
2:C:48:ARG:NH2	2:C:88:MET:O	2.44	0.50
2:D:242:ILE:HA	2:D:412:ARG:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:O	1:A:180:THR:HB	2.11	0.50
2:C:13:LEU:O	2:C:15:LEU:N	2.42	0.50
2:D:156:ILE:HD12	2:D:156:ILE:N	2.25	0.50
1:A:307:VAL:HG13	1:A:331:GLY:C	2.32	0.50
2:D:320:ARG:HB2	2:D:376:GLU:O	2.11	0.50
2:C:93:PRO:HG3	2:C:137:ARG:NH1	2.26	0.50
1:A:312:VAL:CA	1:A:316:ILE:HD11	2.40	0.50
2:D:166:ALA:HB1	2:D:179:ARG:O	2.12	0.50
2:D:248:LEU:HD12	2:D:251:ILE:HD12	1.94	0.50
1:A:103:ILE:HD11	1:A:175:ALA:HB1	1.94	0.50
1:A:423:TYR:CD1	1:A:423:TYR:N	2.79	0.50
1:B:33:GLY:C	1:B:49:LEU:HD11	2.32	0.50
2:C:98:ARG:N	2:C:98:ARG:CD	2.63	0.50
1:B:119:THR:HG22	1:B:120:ALA:N	2.26	0.50
2:D:476:LEU:O	2:D:480:LEU:HB2	2.12	0.50
2:D:345:VAL:HG12	2:D:347:GLY:H	1.76	0.50
2:D:311:VAL:O	2:D:312:LEU:HD23	2.12	0.50
1:A:22:LYS:HZ2	1:A:24:GLU:HG2	1.74	0.50
2:C:156:ILE:HG22	2:C:156:ILE:O	2.11	0.50
1:A:372:ASN:ND2	2:D:92:PRO:HB2	2.27	0.50
1:B:190:PHE:CZ	1:B:401:LYS:HG3	2.47	0.50
2:C:109:TYR:OH	2:C:448:LYS:HB3	2.11	0.50
2:C:495:MET:C	2:C:497:VAL:H	2.13	0.50
2:D:498:LYS:O	2:D:500:SER:N	2.45	0.50
1:B:150:LYS:N	1:B:153:HIS:HD2	1.98	0.50
1:A:253:LYS:O	1:A:267:SER:HA	2.12	0.50
2:D:390:LYS:O	2:D:394:ARG:HG3	2.12	0.50
1:B:408:HIS:HB2	1:B:418:MSE:HE2	1.93	0.50
2:D:231:ASN:ND2	2:D:239:ARG:HE	2.09	0.50
1:A:309:LEU:HB3	1:B:313:TYR:CD2	2.46	0.50
1:B:181:MSE:HE1	1:B:203:GLY:N	2.27	0.50
1:B:279:ASN:C	1:B:279:ASN:OD1	2.50	0.50
2:D:415:LEU:HD11	2:D:421:GLU:HB2	1.94	0.50
1:A:259:THR:HG21	1:B:370:ARG:O	2.11	0.50
1:B:140:LEU:HD12	1:B:141:LEU:N	2.27	0.50
2:D:231:ASN:HD22	2:D:239:ARG:NE	2.10	0.50
1:A:227:THR:O	1:A:227:THR:HG22	2.10	0.50
1:A:427:ILE:HG22	1:A:428:THR:H	1.76	0.50
1:B:51:LEU:HD21	1:B:57:ILE:HD12	1.93	0.50
1:B:174:VAL:HB	1:B:201:LEU:HD13	1.93	0.50
1:A:210:ARG:NH2	2:C:123:ARG:NH2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:O	1:A:165:LEU:HB2	2.12	0.49
2:D:149:THR:HG23	2:D:151:TRP:HE3	1.77	0.49
2:D:167:ARG:HG3	2:D:182:ARG:HB2	1.94	0.49
1:B:430:TYR:CD2	2:C:34:VAL:HG22	2.47	0.49
2:D:498:LYS:CA	2:D:502:ALA:HB3	2.41	0.49
1:B:100:GLY:HA2	1:B:143:ASN:ND2	2.22	0.49
2:C:9:ASN:C	2:C:11:GLU:H	2.16	0.49
2:D:147:VAL:HG11	2:D:205:VAL:HA	1.94	0.49
2:C:47:GLN:NE2	2:C:73:VAL:HG21	2.28	0.49
2:D:411:THR:O	2:D:411:THR:HG23	2.11	0.49
2:D:289:VAL:HG11	2:D:367:VAL:HG22	1.94	0.49
2:D:13:LEU:HB3	2:D:234:ILE:CG2	2.42	0.49
1:B:47:LEU:HD12	1:B:48:VAL:N	2.26	0.49
1:A:154:TRP:C	1:A:191:MSE:HE1	2.33	0.49
2:C:13:LEU:HB3	2:C:234:ILE:HG23	1.93	0.49
1:A:402:LEU:HD12	1:A:419:MSE:HE3	1.93	0.49
1:B:258:HIS:HD2	1:B:261:ARG:H	1.60	0.49
1:B:373:LEU:HD22	1:B:389:PRO:HB3	1.95	0.49
2:C:112:ASN:O	2:C:114:LYS:HE3	2.12	0.49
2:D:66:GLU:HG2	2:D:70:LYS:HE3	1.94	0.49
2:D:355:PRO:HG3	2:D:364:VAL:HG21	1.94	0.49
1:A:53:ASN:HB3	1:A:55:TYR:HD1	1.77	0.49
1:A:127:LEU:HD13	1:A:219:LEU:CD1	2.43	0.49
1:B:195:LEU:HD22	1:B:197:LYS:H	1.78	0.49
1:A:39:TYR:HD2	1:A:42:SER:HB2	1.77	0.49
1:B:247:LEU:HD23	1:B:249:HIS:HE1	1.77	0.49
2:D:289:VAL:HG12	2:D:289:VAL:O	2.12	0.49
2:D:167:ARG:HG3	2:D:182:ARG:CB	2.42	0.49
2:C:149:THR:HG23	2:C:151:TRP:N	2.22	0.49
1:B:428:THR:CG2	1:B:430:TYR:O	2.60	0.49
1:B:250:ARG:CD	1:B:425:GLY:HA3	2.34	0.49
1:B:126:ALA:O	2:D:51:ARG:NH2	2.46	0.49
2:D:275:ARG:O	2:D:318:LYS:HD3	2.12	0.49
2:C:413:ARG:HB3	2:C:423:MET:HE1	1.95	0.49
1:A:427:ILE:CG2	1:A:428:THR:N	2.76	0.49
1:B:210:ARG:NH2	2:D:123:ARG:NH2	2.60	0.49
2:D:67:GLU:HA	2:D:70:LYS:HD2	1.94	0.49
2:D:261:ARG:HH12	2:D:412:ARG:CZ	2.26	0.49
1:B:18:VAL:CG1	1:B:19:ARG:N	2.75	0.49
2:C:240:ILE:HD13	2:C:261:ARG:NH2	2.27	0.49
1:B:12:ILE:HG21	1:B:35:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:HG22	1:B:61:LEU:CG	2.43	0.48
1:A:125:LYS:HB3	2:C:54:MET:HE3	1.94	0.48
1:A:176:HIS:HD1	1:A:177:GLY:N	2.11	0.48
1:B:18:VAL:HG13	1:B:68:GLU:O	2.12	0.48
2:D:264:ASN:O	2:D:268:ILE:HG13	2.13	0.48
2:D:467:VAL:O	2:D:471:LYS:HA	2.13	0.48
2:C:19:LEU:CD1	2:C:230:LEU:HD23	2.43	0.48
1:B:9:GLU:HG2	1:B:10:ARG:N	2.27	0.48
2:C:241:GLU:CD	2:C:243:LYS:HE2	2.34	0.48
1:A:217:MSE:HE2	1:A:278:PRO:HG2	1.95	0.48
1:A:421:THR:HB	1:A:423:TYR:CE1	2.48	0.48
1:B:333:VAL:HG21	1:B:399:TYR:HA	1.95	0.48
2:D:457:GLU:N	2:D:457:GLU:CD	2.65	0.48
2:D:220:LYS:HB2	2:D:225:THR:HG21	1.95	0.48
1:A:423:TYR:HD1	1:A:423:TYR:H	1.61	0.48
2:D:385:GLU:O	2:D:386:GLU:C	2.52	0.48
1:B:33:GLY:O	1:B:49:LEU:HD11	2.13	0.48
1:B:436:TYR:CE1	1:B:437:LEU:HD13	2.48	0.48
1:B:370:ARG:HH11	2:C:94:ARG:CZ	2.26	0.48
1:B:3:VAL:HG23	1:B:44:GLY:C	2.33	0.48
2:C:292:ILE:HG22	2:C:292:ILE:O	2.13	0.48
2:C:208:PHE:CE1	2:C:458:LEU:HD21	2.47	0.48
2:C:495:MET:C	2:C:497:VAL:N	2.66	0.48
2:C:457:GLU:CD	2:C:462:LYS:HG2	2.34	0.48
1:A:181:MSE:SE	1:A:237:MSE:HE2	2.64	0.48
2:D:480:LEU:HD21	2:D:489:PHE:CD1	2.49	0.48
2:C:42:VAL:CG1	2:C:77:GLU:HB3	2.43	0.48
1:B:225:MSE:HA	1:B:228:SER:OG	2.12	0.48
2:C:173:ASP:O	2:C:174:LYS:HB2	2.11	0.48
2:D:240:ILE:HD12	2:D:262:GLN:NE2	2.19	0.48
1:A:313:TYR:CZ	1:A:316:ILE:HG12	2.49	0.48
1:B:422:ASN:ND2	1:B:424:ALA:O	2.47	0.48
1:A:245:TYR:HE1	1:A:247:LEU:CD1	2.26	0.48
1:A:195:LEU:HD11	1:A:199:VAL:HG21	1.95	0.48
1:A:17:PHE:HB3	1:A:71:GLU:HB2	1.96	0.48
2:C:207:LYS:HB2	2:C:248:LEU:HD21	1.96	0.48
2:D:19:LEU:HD13	2:D:230:LEU:CD2	2.44	0.48
1:B:258:HIS:CD2	1:B:261:ARG:H	2.31	0.48
1:B:197:LYS:HG2	1:B:292:ARG:NH1	2.28	0.48
2:C:113:ALA:O	2:C:115:PRO:HD3	2.14	0.48
2:C:342:LYS:HA	2:C:345:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:TYR:CD1	2:C:391:ASN:HB3	2.48	0.48
2:D:107:ILE:HD13	2:D:213:LEU:CD2	2.44	0.48
1:A:176:HIS:ND1	1:A:177:GLY:N	2.62	0.47
2:D:290:THR:HA	2:D:311:VAL:HB	1.96	0.47
2:C:195:ASP:O	2:C:196:ILE:C	2.52	0.47
2:C:106:GLN:HE21	2:C:216:THR:CG2	2.21	0.47
2:D:311:VAL:C	2:D:312:LEU:HD23	2.35	0.47
2:D:371:LEU:HD23	2:D:371:LEU:N	2.29	0.47
1:A:217:MSE:CE	2:C:49:ARG:NH2	2.76	0.47
1:B:55:TYR:OH	2:D:138:THR:HG21	2.14	0.47
1:A:339:LEU:HA	1:B:259:THR:HG23	1.94	0.47
1:B:432:ARG:O	1:B:435:THR:CG2	2.61	0.47
1:A:22:LYS:HB2	1:A:63:LYS:O	2.14	0.47
1:B:206:ARG:HG3	1:B:210:ARG:HD2	1.96	0.47
1:B:317:SER:C	1:B:319:GLU:N	2.67	0.47
2:C:320:ARG:HB2	2:C:376:GLU:O	2.13	0.47
1:A:337:THR:HG23	1:B:179:ASP:HB3	1.95	0.47
1:B:119:THR:HB	1:B:122:GLU:HG3	1.95	0.47
1:A:282:ILE:HG12	1:A:283:GLU:N	2.29	0.47
2:C:493:VAL:O	2:C:496:GLY:N	2.47	0.47
2:C:99:GLU:O	2:C:103:VAL:HG23	2.15	0.47
2:D:345:VAL:HG23	2:D:392:ALA:HB2	1.96	0.47
2:C:65:LEU:HD23	2:C:65:LEU:O	2.14	0.47
1:B:48:VAL:HG22	2:D:120:TYR:CZ	2.48	0.47
1:B:230:VAL:HG22	1:B:289:TYR:CE1	2.50	0.47
1:A:429:PRO:O	2:D:94:ARG:NH2	2.48	0.47
1:A:361:CYS:HB3	1:A:390:CYS:SG	2.54	0.47
1:A:258:HIS:CD2	1:A:261:ARG:HG3	2.49	0.47
1:A:108:ASP:O	1:A:112:GLY:N	2.42	0.47
1:A:147:GLU:OE2	3:A:1000:ASP:N	2.48	0.47
1:A:279:ASN:ND2	1:A:281:GLU:OE2	2.47	0.47
1:A:337:THR:CG2	1:B:179:ASP:HB3	2.44	0.47
1:A:146:SER:HB3	1:A:176:HIS:HE1	1.76	0.47
1:B:57:ILE:CG2	1:B:58:GLY:N	2.77	0.47
1:B:234:MSE:HG2	1:B:273:ILE:HD12	1.96	0.47
2:D:107:ILE:HD13	2:D:213:LEU:HD22	1.97	0.47
2:D:334:GLY:O	2:D:337:PHE:HB2	2.15	0.47
2:D:374:SER:H	2:D:377:ASP:HB2	1.78	0.47
2:C:411:THR:CG2	2:C:426:LEU:HA	2.45	0.47
1:A:125:LYS:HE3	2:C:60:ILE:CG1	2.39	0.47
1:A:127:LEU:HD13	1:A:219:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PHE:CB	1:A:119:THR:HG21	2.45	0.47
1:B:422:ASN:HD22	1:B:426:GLU:HG2	1.80	0.47
2:D:167:ARG:CG	2:D:182:ARG:HD3	2.43	0.47
1:A:144:ILE:CD1	1:A:153:HIS:CE1	2.97	0.47
2:D:272:LEU:HD22	2:D:319:PHE:CE1	2.49	0.47
1:A:111:THR:HG22	1:A:113:ALA:N	2.30	0.47
1:A:255:ARG:HB2	1:A:394:LEU:HD21	1.97	0.47
1:A:211:PRO:HB2	2:C:134:GLY:HA3	1.97	0.47
2:C:199:PRO:O	2:C:202:ALA:HB3	2.15	0.46
2:C:291:ASP:C	2:C:293:PHE:H	2.19	0.46
2:C:232:VAL:HG12	2:C:233:SER:H	1.79	0.46
1:B:3:VAL:HG22	1:B:61:LEU:HD11	1.98	0.46
2:D:457:GLU:OE1	2:D:462:LYS:HE3	2.15	0.46
1:A:16:ASP:OD2	1:A:73:ALA:N	2.42	0.46
1:B:193:ARG:HB2	1:B:298:GLU:O	2.15	0.46
1:A:306:LYS:HD2	1:A:328:GLY:O	2.15	0.46
2:C:116:VAL:O	2:C:443:ILE:HD12	2.16	0.46
1:A:409:THR:CG2	1:A:410:GLN:H	2.28	0.46
2:D:27:THR:HG21	2:D:100:ALA:CA	2.46	0.46
1:A:337:THR:HG23	1:B:179:ASP:OD1	2.15	0.46
2:C:170:GLU:CD	2:C:172:LYS:HE3	2.35	0.46
2:D:351:ILE:CG2	2:D:378:ALA:HB1	2.45	0.46
2:D:126:VAL:HG21	2:D:131:ASN:HD22	1.77	0.46
1:B:12:ILE:HG22	1:B:35:ILE:HD12	1.97	0.46
1:A:107:ILE:HD11	1:A:109:TYR:CZ	2.51	0.46
2:D:154:VAL:HG12	2:D:192:THR:HG23	1.97	0.46
1:A:263:ASP:HB2	1:B:436:TYR:CE2	2.50	0.46
1:B:370:ARG:NH1	2:C:94:ARG:CZ	2.78	0.46
2:D:124:LYS:HA	2:D:432:MET:HG2	1.97	0.46
2:D:245:VAL:HG13	2:D:254:ILE:HD12	1.98	0.46
1:A:25:ASP:O	1:A:25:ASP:OD1	2.32	0.46
1:A:244:THR:CG2	1:A:245:TYR:HD2	2.29	0.46
2:C:449:LYS:O	2:C:453:GLU:HG3	2.16	0.46
2:D:497:VAL:O	2:D:499:PRO:N	2.49	0.46
2:C:312:LEU:HB2	2:C:393:LEU:CD1	2.45	0.46
2:D:14:GLY:N	2:D:235:LYS:H	2.14	0.46
1:B:299:VAL:CG1	1:B:300:ASP:H	2.28	0.46
2:C:351:ILE:HG21	2:C:378:ALA:HB1	1.97	0.46
1:B:127:LEU:O	1:B:128:PRO:C	2.54	0.46
1:A:147:GLU:OE1	1:B:378:THR:OG1	2.27	0.46
1:A:428:THR:CG2	1:A:430:TYR:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:THR:CG2	1:A:245:TYR:CD2	2.97	0.46
2:D:180:LEU:O	2:D:181:ASP:C	2.54	0.46
1:B:147:GLU:H	1:B:147:GLU:HG3	1.44	0.46
1:A:154:TRP:O	1:A:157:ILE:HB	2.16	0.46
1:B:164:ALA:HB1	1:B:169:ASP:OD2	2.16	0.46
1:B:225:MSE:O	1:B:228:SER:OG	2.34	0.46
2:D:497:VAL:O	2:D:498:LYS:C	2.54	0.46
2:D:353:GLU:CG	2:D:354:LEU:HD23	2.45	0.46
1:B:261:ARG:NH1	1:B:263:ASP:CB	2.79	0.46
2:D:234:ILE:HG22	2:D:235:LYS:N	2.31	0.46
1:B:151:PRO:HG2	1:B:403:MSE:HE1	1.97	0.46
1:B:176:HIS:NE2	1:B:184:THR:OG1	2.43	0.45
1:A:69:VAL:HG11	1:A:72:ARG:HH11	1.81	0.45
2:D:415:LEU:HD11	2:D:421:GLU:CB	2.46	0.45
1:A:259:THR:HG22	1:B:339:LEU:CD2	2.46	0.45
1:B:257:MSE:HE3	1:B:368:TYR:CE1	2.51	0.45
1:B:257:MSE:CE	1:B:368:TYR:CE1	2.98	0.45
1:A:428:THR:HG22	1:A:430:TYR:H	1.81	0.45
2:C:251:ILE:O	2:C:255:ILE:HG13	2.16	0.45
1:B:313:TYR:H	1:B:316:ILE:CD1	2.24	0.45
1:A:12:ILE:CG2	1:A:35:ILE:HD12	2.44	0.45
1:A:88:LYS:NZ	1:A:132:GLU:OE2	2.49	0.45
2:D:23:ARG:CD	2:D:226:ILE:HG12	2.46	0.45
1:B:408:HIS:HB2	1:B:418:MSE:CE	2.47	0.45
2:C:65:LEU:HD21	2:C:69:LYS:HE3	1.99	0.45
2:C:220:LYS:CB	2:C:225:THR:HG21	2.47	0.45
1:B:20:ILE:HA	1:B:66:ARG:O	2.16	0.45
2:D:374:SER:H	2:D:377:ASP:CG	2.20	0.45
1:A:210:ARG:HH21	2:C:123:ARG:NH2	2.14	0.45
2:D:423:MET:HB3	2:D:424:ARG:HG3	1.98	0.45
2:D:354:LEU:HB2	2:D:355:PRO:CA	2.45	0.45
2:C:234:ILE:HD11	2:C:259:VAL:CA	2.45	0.45
2:C:262:GLN:HG2	2:C:407:VAL:HG11	1.99	0.45
2:C:497:VAL:O	2:C:499:PRO:N	2.49	0.45
1:B:336:GLY:O	1:B:365:GLN:HG3	2.16	0.45
2:C:442:ARG:O	2:C:444:PRO:HD3	2.16	0.45
2:D:300:ILE:H	2:D:300:ILE:HG13	1.54	0.45
1:A:271:VAL:HG13	1:A:272:PRO:O	2.16	0.45
1:A:206:ARG:NH2	1:A:260:SER:O	2.40	0.45
2:C:15:LEU:HD11	2:C:17:VAL:CG2	2.46	0.45
1:B:217:MSE:CE	2:D:49:ARG:NH2	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ALA:HB2	2:D:54:MET:HE3	1.98	0.45
1:B:50:LYS:HE3	1:B:56:ASN:HD21	1.79	0.45
1:B:409:THR:CG2	1:B:410:GLN:N	2.80	0.45
1:A:198:PRO:HB2	1:A:226:ALA:HA	1.98	0.45
1:B:36:MSE:HE1	1:B:111:THR:O	2.17	0.45
2:D:22:HIS:CE1	2:D:189:GLU:HG3	2.52	0.45
2:D:255:ILE:O	2:D:259:VAL:HG23	2.17	0.45
2:D:272:LEU:HD12	2:D:404:ILE:HA	1.99	0.45
2:D:198:HIS:ND1	2:D:199:PRO:HD2	2.32	0.45
2:C:257:ARG:NH1	2:C:257:ARG:CG	2.79	0.45
1:A:147:GLU:HG3	1:A:147:GLU:H	1.30	0.45
1:A:428:THR:HG22	1:A:430:TYR:N	2.32	0.45
2:D:269:ARG:HG3	2:D:404:ILE:O	2.17	0.45
2:C:355:PRO:O	2:C:356:ASN:CB	2.65	0.45
1:A:22:LYS:HZ1	1:A:24:GLU:HG2	1.80	0.45
2:C:459:PRO:O	2:C:462:LYS:HB2	2.16	0.45
2:D:19:LEU:H	2:D:192:THR:HB	1.82	0.44
2:C:123:ARG:HE	2:C:435:GLU:HA	1.82	0.44
2:C:292:ILE:CD1	2:C:366:LYS:HB3	2.40	0.44
1:A:97:ILE:HD12	1:A:161:VAL:HG22	1.99	0.44
2:C:282:ILE:HG22	2:C:397:ILE:HG23	1.99	0.44
1:A:245:TYR:HE1	1:A:247:LEU:HD13	1.81	0.44
2:C:480:LEU:HD13	2:C:489:PHE:CG	2.52	0.44
2:D:27:THR:O	2:D:36:SER:OG	2.33	0.44
2:C:67:GLU:HG2	2:C:127:ILE:CG2	2.46	0.44
1:A:304:GLU:OE2	1:A:306:LYS:HB2	2.17	0.44
2:C:196:ILE:HD13	2:C:202:ALA:HA	1.98	0.44
1:A:225:MSE:SE	1:A:276:ILE:HG21	2.67	0.44
1:B:216:ALA:O	1:B:220:ILE:HG13	2.18	0.44
2:D:73:VAL:HG12	2:D:174:LYS:O	2.17	0.44
1:A:143:ASN:HA	1:A:143:ASN:HD22	1.59	0.44
2:D:35:PRO:C	2:D:37:GLU:H	2.20	0.44
2:C:240:ILE:CD1	2:C:261:ARG:HH21	2.30	0.44
1:A:119:THR:HG22	1:A:121:GLU:H	1.81	0.44
2:C:232:VAL:HG12	2:C:233:SER:N	2.32	0.44
1:B:217:MSE:HE2	1:B:278:PRO:HG2	1.99	0.44
1:B:245:TYR:HE1	1:B:247:LEU:HD13	1.82	0.44
1:B:247:LEU:HD23	1:B:249:HIS:CE1	2.51	0.44
1:B:344:ASN:ND2	1:B:381:LYS:HD2	2.32	0.44
2:D:24:GLN:HG3	2:D:225:THR:HG23	1.99	0.44
2:C:203:LYS:HB2	2:C:252:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:VAL:HA	1:B:247:LEU:O	2.18	0.44
2:D:411:THR:O	2:D:423:MET:HB2	2.17	0.44
1:A:109:TYR:CE2	2:C:431:ARG:HB3	2.52	0.44
2:D:219:VAL:HG12	2:D:220:LYS:N	2.32	0.44
1:B:193:ARG:NE	1:B:193:ARG:HA	2.32	0.44
1:A:46:THR:HG21	2:C:118:GLU:OE1	2.16	0.44
2:C:411:THR:HG22	2:C:426:LEU:HA	1.99	0.44
2:C:20:GLU:OE2	2:C:191:SER:CB	2.53	0.44
1:A:39:TYR:C	1:A:41:LEU:H	2.20	0.44
1:A:250:ARG:CD	1:A:425:GLY:HA3	2.47	0.44
2:D:266:LEU:C	2:D:268:ILE:N	2.71	0.44
1:A:118:PHE:HD2	1:A:140:LEU:HD23	1.82	0.44
2:D:193:THR:C	2:D:195:ASP:H	2.20	0.44
1:B:146:SER:HB2	1:B:180:THR:H	1.82	0.44
1:B:180:THR:HG23	1:B:183:TYR:HB2	2.00	0.44
1:A:286:ARG:HG2	1:A:287:LYS:N	2.32	0.44
2:C:220:LYS:HB2	2:C:225:THR:HG21	2.00	0.44
1:B:45:ASP:OD2	2:D:442:ARG:NH1	2.51	0.44
1:B:142:PHE:O	1:B:142:PHE:HD1	2.00	0.44
2:C:70:LYS:HD2	2:C:72:ARG:NH2	2.30	0.44
2:D:203:LYS:HB2	2:D:252:PRO:HG3	1.98	0.44
1:A:366:CYS:O	1:A:367:ILE:C	2.54	0.44
2:D:339:ASP:HB3	2:D:422:TYR:HB3	2.00	0.44
2:D:154:VAL:CG1	2:D:192:THR:HG23	2.47	0.44
1:A:206:ARG:HB3	1:A:213:SER:HA	1.99	0.44
2:C:216:THR:O	2:C:218:LYS:HG2	2.18	0.44
2:C:47:GLN:HE21	2:C:73:VAL:CG2	2.31	0.44
1:A:268:ILE:O	1:A:269:ASN:HB2	2.16	0.44
2:D:56:GLU:HG3	2:D:56:GLU:H	1.45	0.44
1:A:99:THR:CG2	1:A:99:THR:O	2.65	0.44
2:C:147:VAL:HG22	2:C:208:PHE:CD2	2.52	0.44
1:A:207:SER:O	1:A:210:ARG:HG3	2.17	0.44
2:C:31:PHE:HB3	2:C:93:PRO:HB2	1.99	0.44
1:A:144:ILE:HD13	1:A:153:HIS:CE1	2.53	0.44
2:D:34:VAL:HA	2:D:35:PRO:HD3	1.75	0.44
2:C:406:GLY:O	2:C:408:PRO:HD3	2.18	0.44
2:C:105:LEU:O	2:C:108:ALA:HB3	2.17	0.44
1:A:321:ILE:O	1:A:325:VAL:HG23	2.18	0.44
1:B:370:ARG:HB2	1:B:370:ARG:HE	1.45	0.43
1:B:312:VAL:HG11	1:B:343:PRO:HD3	2.00	0.43
1:B:59:ILE:HG21	1:B:64:ILE:CD1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:TYR:N	1:A:316:ILE:HD11	2.32	0.43
2:C:14:GLY:O	2:C:16:LYS:HG2	2.18	0.43
2:C:240:ILE:CD1	2:C:261:ARG:NH2	2.80	0.43
2:C:108:ALA:HA	2:C:159:ILE:CD1	2.48	0.43
2:C:33:PRO:HD2	2:C:94:ARG:HH21	1.83	0.43
2:C:174:LYS:O	2:C:175:GLU:HB2	2.18	0.43
2:C:413:ARG:HB3	2:C:423:MET:CE	2.48	0.43
2:C:291:ASP:C	2:C:293:PHE:N	2.71	0.43
1:A:391:GLU:HB3	1:A:392:ASP:H	1.51	0.43
2:D:93:PRO:HG2	2:D:438:ILE:HD13	2.00	0.43
1:A:286:ARG:HG3	1:A:288:ASP:OD1	2.18	0.43
1:A:433:PHE:HD1	2:D:88:MET:HE1	1.83	0.43
1:B:234:MSE:HG2	1:B:273:ILE:CD1	2.48	0.43
2:C:113:ALA:HB1	2:C:142:ALA:HB1	2.00	0.43
1:A:318:SER:HB2	1:A:349:SER:HB3	2.00	0.43
1:B:217:MSE:HE1	1:B:243:ASP:CB	2.35	0.43
1:A:250:ARG:O	1:A:252:THR:N	2.51	0.43
2:C:207:LYS:CB	2:C:248:LEU:HD21	2.49	0.43
2:C:351:ILE:CG2	2:C:378:ALA:HB1	2.48	0.43
1:B:23:GLU:CD	1:B:65:ARG:NH1	2.71	0.43
1:A:259:THR:HG21	1:B:370:ARG:C	2.38	0.43
2:D:313:ALA:O	2:D:314:ILE:HD13	2.19	0.43
2:D:225:THR:O	2:D:225:THR:HG22	2.17	0.43
1:A:271:VAL:HG22	1:A:272:PRO:CD	2.48	0.43
1:B:198:PRO:HG3	1:B:230:VAL:O	2.19	0.43
1:B:360:VAL:HG12	1:B:387:VAL:HG13	2.01	0.43
1:A:178:THR:HG21	1:A:205:GLN:OE1	2.19	0.43
2:D:368:ILE:HA	2:D:373:LEU:HD12	2.00	0.43
2:C:412:ARG:NH1	2:C:412:ARG:HG2	2.33	0.43
2:C:168:ILE:O	2:C:168:ILE:HG23	2.17	0.43
2:D:36:SER:HB3	2:D:185:ILE:HG12	2.00	0.43
1:A:384:LYS:C	1:A:386:GLY:H	2.22	0.43
2:C:354:LEU:HD13	2:C:364:VAL:CG2	2.48	0.43
2:C:5:THR:O	2:C:5:THR:HG23	2.18	0.43
1:B:276:ILE:HG22	1:B:282:ILE:CG1	2.20	0.43
1:A:194:ASN:OD1	1:A:295:GLU:HB3	2.18	0.43
2:D:296:THR:HG23	2:D:363:GLU:OE2	2.19	0.43
2:D:465:ARG:NH2	2:D:466:TYR:HE2	2.09	0.43
2:C:314:ILE:HG13	2:C:393:LEU:HD22	2.00	0.43
1:A:427:ILE:CG2	1:A:428:THR:H	2.31	0.43
1:B:292:ARG:HH11	1:B:292:ARG:CG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:ARG:NH2	2:C:270:ASP:OD1	2.43	0.43
1:A:46:THR:HA	1:A:59:ILE:O	2.19	0.43
2:C:51:ARG:HA	2:C:52:PRO:HD3	1.92	0.43
1:A:178:THR:HG23	1:A:265:PHE:HE1	1.83	0.43
1:A:12:ILE:HG22	1:A:13:ASN:N	2.34	0.43
1:B:108:ASP:HA	2:D:56:GLU:CG	2.45	0.43
2:D:266:LEU:C	2:D:268:ILE:H	2.22	0.43
2:D:130:SER:HB2	2:D:165:ALA:HB1	2.01	0.43
2:D:9:ASN:O	2:D:11:GLU:N	2.52	0.43
1:A:225:MSE:CE	1:A:234:MSE:HE1	2.48	0.43
1:A:200:VAL:HG12	1:A:202:VAL:CG2	2.49	0.43
2:C:292:ILE:HD13	2:C:366:LYS:CB	2.41	0.43
1:A:346:ILE:CG2	1:A:346:ILE:O	2.66	0.43
1:B:177:GLY:O	1:B:181:MSE:HB2	2.19	0.43
2:D:385:GLU:OE1	2:D:385:GLU:C	2.57	0.43
2:C:98:ARG:N	2:C:98:ARG:HD3	2.24	0.43
2:C:291:ASP:O	2:C:293:PHE:N	2.52	0.43
1:A:194:ASN:O	1:A:297:VAL:HA	2.19	0.43
2:D:470:TYR:HB2	2:D:472:LEU:HD22	2.01	0.43
2:D:240:ILE:HD13	2:D:261:ARG:HH21	1.84	0.43
2:D:345:VAL:HG21	2:D:382:VAL:CG1	2.49	0.42
2:D:351:ILE:HG21	2:D:378:ALA:CB	2.49	0.42
1:B:206:ARG:O	1:B:207:SER:C	2.56	0.42
1:B:244:THR:HG22	1:B:277:TRP:CH2	2.54	0.42
2:C:21:ILE:HA	2:C:227:ARG:O	2.19	0.42
1:A:253:LYS:NZ	1:A:392:ASP:OD2	2.53	0.42
2:D:93:PRO:HG2	2:D:438:ILE:CD1	2.49	0.42
2:C:303:ARG:O	2:C:307:LYS:HG3	2.20	0.42
1:B:37:PRO:HA	1:B:38:PRO:HD3	1.80	0.42
1:A:65:ARG:HA	1:A:65:ARG:HD3	1.87	0.42
1:B:50:LYS:HE2	1:B:56:ASN:ND2	2.33	0.42
1:B:6:PHE:CE1	1:B:10:ARG:NE	2.87	0.42
1:A:401:LYS:CD	1:A:419:MSE:SE	3.12	0.42
1:B:247:LEU:HB3	1:B:249:HIS:CE1	2.54	0.42
2:C:292:ILE:HD13	2:C:366:LYS:C	2.38	0.42
1:A:163:LYS:O	1:A:164:ALA:C	2.57	0.42
2:C:103:VAL:HG22	2:C:218:LYS:CD	2.46	0.42
1:B:313:TYR:O	1:B:316:ILE:HG13	2.19	0.42
1:A:342:THR:CG2	1:A:346:ILE:HG22	2.48	0.42
2:C:277:VAL:CG2	2:C:318:LYS:HB2	2.46	0.42
2:C:116:VAL:HG12	2:C:117:ASP:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:PHE:HA	2:C:94:ARG:O	2.18	0.42
1:A:125:LYS:HB3	2:C:54:MET:CE	2.49	0.42
1:B:144:ILE:CG2	1:B:149:MSE:HE3	2.50	0.42
1:B:18:VAL:CG1	1:B:19:ARG:H	2.28	0.42
1:A:307:VAL:HG22	1:A:331:GLY:HA3	2.01	0.42
2:C:345:VAL:HA	2:C:346:PRO:HD3	1.70	0.42
2:C:344:TYR:CE1	2:C:391:ASN:HB3	2.55	0.42
1:A:4:ASP:OD1	1:A:8:LYS:HE3	2.19	0.42
2:D:5:THR:O	2:D:5:THR:HG23	2.20	0.42
2:D:57:LEU:HD12	2:D:57:LEU:H	1.85	0.42
2:D:164:ASP:HB2	2:D:187:LEU:HD13	2.02	0.42
2:C:483:ASP:O	2:C:485:ARG:N	2.53	0.42
1:A:261:ARG:O	1:A:264:ALA:HB2	2.19	0.42
1:B:126:ALA:O	1:B:127:LEU:HD12	2.20	0.42
2:D:67:GLU:HG2	2:D:127:ILE:CG2	2.50	0.42
1:B:74:LYS:O	1:B:75:VAL:C	2.58	0.42
1:A:428:THR:HG21	1:A:430:TYR:O	2.20	0.42
2:C:23:ARG:HD3	2:C:226:ILE:HG23	2.01	0.42
1:B:210:ARG:O	1:B:212:SER:N	2.52	0.42
1:B:130:ILE:C	1:B:132:GLU:H	2.23	0.42
1:B:230:VAL:HG22	1:B:289:TYR:CD1	2.55	0.42
2:C:433:TYR:HA	2:C:434:PRO:HD3	1.92	0.42
2:D:141:ILE:HD12	2:D:161:LEU:HB2	2.01	0.42
1:A:94:VAL:HG23	1:A:94:VAL:O	2.19	0.42
2:D:170:GLU:OE1	2:D:172:LYS:HE3	2.20	0.42
2:C:340:ARG:HG3	2:C:399:ARG:HG2	2.01	0.42
2:C:289:VAL:C	2:C:291:ASP:N	2.73	0.42
2:D:466:TYR:O	2:D:472:LEU:HD23	2.20	0.42
1:B:321:ILE:HD12	1:B:346:ILE:CG2	2.49	0.42
1:A:436:TYR:CE1	1:B:258:HIS:HB2	2.55	0.42
1:A:48:VAL:HG22	2:C:120:TYR:CZ	2.55	0.42
2:D:140:ILE:HG12	2:D:158:THR:CG2	2.49	0.42
1:B:225:MSE:CG	1:B:276:ILE:HD13	2.50	0.42
1:A:260:SER:HB3	1:B:339:LEU:HD21	2.02	0.42
1:B:370:ARG:NH1	2:C:94:ARG:NH1	2.68	0.42
1:B:218:ASN:ND2	1:B:237:MSE:CE	2.83	0.42
2:D:107:ILE:O	2:D:111:LEU:HG	2.20	0.42
2:D:493:VAL:O	2:D:496:GLY:N	2.48	0.42
2:D:304:VAL:HG12	2:D:309:GLY:HA3	2.01	0.42
2:C:289:VAL:HG13	2:C:292:ILE:HD12	2.01	0.42
1:A:309:LEU:HB3	1:B:313:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:TRP:N	1:A:277:TRP:CD1	2.87	0.42
2:C:300:ILE:H	2:C:300:ILE:HG13	1.33	0.42
1:B:202:VAL:O	1:B:202:VAL:HG13	2.20	0.42
1:A:261:ARG:NH2	1:B:436:TYR:HB3	2.35	0.41
1:B:250:ARG:HD3	1:B:425:GLY:CA	2.35	0.41
1:B:401:LYS:HD3	1:B:419:MSE:SE	2.69	0.41
1:A:79:VAL:HG12	1:A:80:HIS:N	2.35	0.41
1:A:258:HIS:NE2	1:A:261:ARG:HG3	2.36	0.41
2:D:345:VAL:HG21	2:D:382:VAL:HG11	2.02	0.41
2:D:14:GLY:CA	2:D:235:LYS:HG3	2.47	0.41
2:C:470:TYR:HB2	2:C:472:LEU:HD23	2.02	0.41
1:B:431:THR:HG22	1:B:435:THR:HG21	2.02	0.41
1:A:170:TYR:CZ	1:A:292:ARG:NH2	2.88	0.41
2:D:219:VAL:CG1	2:D:220:LYS:N	2.82	0.41
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.85	0.41
1:A:103:ILE:HG22	1:A:103:ILE:O	2.20	0.41
2:C:356:ASN:HD22	2:C:357:TYR:H	1.69	0.41
2:C:474:ARG:O	2:C:475:SER:C	2.59	0.41
1:B:210:ARG:NH2	2:D:123:ARG:HH22	2.18	0.41
2:C:423:MET:HB2	2:C:423:MET:HE2	1.94	0.41
1:A:183:TYR:CE2	1:A:396:GLU:HB3	2.56	0.41
2:D:31:PHE:HE2	2:D:438:ILE:HG12	1.83	0.41
1:B:272:PRO:HB2	1:B:285:LEU:HD12	2.01	0.41
2:C:310:LYS:NZ	2:C:386:GLU:OE2	2.48	0.41
2:D:501:LEU:O	2:D:505:ILE:CB	2.69	0.41
1:A:302:LYS:HB3	1:A:407:GLY:O	2.21	0.41
1:A:154:TRP:O	1:A:191:MSE:HE1	2.20	0.41
2:D:70:LYS:HD3	2:D:72:ARG:NH2	2.36	0.41
1:B:205:GLN:HG2	1:B:261:ARG:O	2.21	0.41
1:A:279:ASN:HD22	1:A:281:GLU:HG3	1.82	0.41
2:C:277:VAL:O	2:C:404:ILE:HG21	2.20	0.41
1:B:12:ILE:HG21	1:B:35:ILE:CD1	2.50	0.41
2:D:208:PHE:HE1	2:D:458:LEU:CD2	2.34	0.41
2:C:150:PRO:HB2	2:C:151:TRP:CE3	2.55	0.41
1:A:206:ARG:NH1	2:C:90:GLU:HA	2.35	0.41
1:A:150:LYS:H	1:A:153:HIS:CD2	2.16	0.41
1:A:154:TRP:HZ3	1:A:403:MSE:CE	2.32	0.41
1:B:100:GLY:HA3	1:B:144:ILE:H	1.85	0.41
2:C:21:ILE:O	2:C:189:GLU:HA	2.21	0.41
1:A:277:TRP:HD1	1:A:281:GLU:O	2.02	0.41
1:A:270:ASP:CG	1:A:286:ARG:HH22	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ALA:CB	1:A:284:PHE:HA	2.48	0.41
1:B:318:SER:HB2	1:B:349:SER:CB	2.43	0.41
2:D:31:PHE:O	2:D:32:SER:HB2	2.20	0.41
2:C:9:ASN:C	2:C:11:GLU:N	2.74	0.41
2:C:310:LYS:HD2	2:C:386:GLU:HB2	2.02	0.41
2:C:497:VAL:O	2:C:498:LYS:C	2.59	0.41
2:C:498:LYS:O	2:C:500:SER:N	2.54	0.41
2:C:392:ALA:O	2:C:396:VAL:HG23	2.21	0.41
1:B:244:THR:HB	1:B:245:TYR:H	1.34	0.41
2:D:277:VAL:CG2	2:D:318:LYS:HB2	2.51	0.41
2:D:277:VAL:HG12	2:D:278:LYS:N	2.35	0.41
2:C:6:ASP:HB3	2:C:10:TYR:CE1	2.53	0.41
2:D:116:VAL:HG12	2:D:118:GLU:H	1.84	0.41
1:A:210:ARG:HH21	2:C:123:ARG:CZ	2.33	0.41
1:A:259:THR:HG23	1:B:339:LEU:HD23	1.99	0.41
2:C:32:SER:HA	2:C:33:PRO:HD3	1.88	0.41
2:C:243:LYS:HB2	2:C:423:MET:HE1	2.02	0.41
2:C:289:VAL:O	2:C:291:ASP:N	2.53	0.41
2:C:291:ASP:OD2	2:C:370:ARG:NH1	2.54	0.41
1:B:344:ASN:ND2	1:B:381:LYS:CD	2.83	0.41
2:D:149:THR:CG2	2:D:152:GLY:O	2.63	0.41
2:D:32:SER:HA	2:D:33:PRO:HD3	1.88	0.41
1:B:426:GLU:HG2	1:B:427:ILE:H	1.86	0.41
2:C:43:GLU:HB3	2:C:80:TYR:CE1	2.56	0.41
1:A:22:LYS:HZ1	1:A:24:GLU:CG	2.34	0.41
2:C:169:ILE:HB	2:C:177:ILE:HG22	2.03	0.41
1:B:51:LEU:HD21	1:B:57:ILE:CD1	2.51	0.41
2:C:298:SER:OG	2:C:300:ILE:HD12	2.21	0.41
2:D:17:VAL:O	2:D:196:ILE:HB	2.20	0.41
1:B:25:ASP:OD1	1:B:25:ASP:O	2.39	0.41
2:C:7:LYS:HD2	2:C:256:GLU:OE2	2.21	0.41
2:D:243:LYS:HB2	2:D:423:MET:HE1	2.03	0.41
1:A:370:ARG:HB2	1:A:392:ASP:HB3	2.03	0.41
2:D:188:ILE:O	2:D:188:ILE:HG23	2.21	0.41
1:A:229:GLU:HA	1:A:292:ARG:CG	2.51	0.41
2:C:23:ARG:HD2	2:C:225:THR:O	2.22	0.41
2:C:333:LEU:O	2:C:336:GLU:HB2	2.22	0.41
2:C:188:ILE:HG23	2:C:188:ILE:O	2.21	0.41
2:C:463:VAL:HG11	2:C:478:GLN:HG2	2.03	0.40
1:B:165:LEU:HA	1:B:165:LEU:HD12	1.75	0.40
2:D:85:LEU:HA	2:D:88:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:THR:HG23	1:A:343:PRO:CD	2.51	0.40
1:B:430:TYR:CE2	2:C:34:VAL:HG22	2.55	0.40
1:B:9:GLU:C	1:B:11:ASN:N	2.75	0.40
1:B:39:TYR:HB2	2:D:440:PRO:HG2	2.02	0.40
2:C:147:VAL:HG22	2:C:208:PHE:HD2	1.86	0.40
1:B:294:ASP:O	1:B:295:GLU:C	2.59	0.40
1:B:241:THR:CG2	2:D:90:GLU:OE2	2.62	0.40
1:A:151:PRO:HA	1:A:154:TRP:CE3	2.57	0.40
1:A:170:TYR:CE1	1:A:292:ARG:CZ	3.04	0.40
2:D:374:SER:H	2:D:377:ASP:CB	2.35	0.40
2:D:208:PHE:HE1	2:D:458:LEU:HD21	1.87	0.40
1:B:308:ALA:HB2	1:B:329:TYR:CE2	2.56	0.40
1:B:396:GLU:H	1:B:396:GLU:CD	2.22	0.40
1:A:313:TYR:CD2	1:B:309:LEU:HB3	2.57	0.40
1:A:179:ASP:CB	1:B:337:THR:HG23	2.51	0.40
2:C:138:THR:HG22	2:C:139:ALA:H	1.86	0.40
1:A:219:LEU:HA	1:A:219:LEU:HD23	1.86	0.40
1:B:206:ARG:HB3	1:B:213:SER:HA	2.03	0.40
2:C:146:LYS:HE3	2:C:148:GLU:OE1	2.21	0.40
2:D:261:ARG:HH12	2:D:412:ARG:NE	2.16	0.40
2:D:25:LEU:HD21	2:D:188:ILE:HB	2.04	0.40
1:A:244:THR:HG22	1:A:245:TYR:N	2.37	0.40
2:D:125:ILE:HG12	2:D:431:ARG:O	2.21	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	435/438 (99%)	374 (86%)	49 (11%)	12 (3%)	6 30
1	B	435/438 (99%)	366 (84%)	56 (13%)	13 (3%)	5 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	506/633 (80%)	434 (86%)	54 (11%)	18 (4%)	4 24
2	D	506/633 (80%)	428 (85%)	57 (11%)	21 (4%)	3 20
All	All	1882/2142 (88%)	1602 (85%)	216 (12%)	64 (3%)	5 25

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	77	PRO
1	A	78	GLU
1	A	163	LYS
1	A	251	GLY
1	B	40	GLU
1	B	45	ASP
1	B	75	VAL
1	B	76	LYS
1	B	77	PRO
2	C	10	TYR
2	C	499	PRO
2	D	246	GLN
2	D	386	GLU
2	D	499	PRO
1	A	27	GLU
1	A	41	LEU
1	B	251	GLY
2	C	175	GLU
2	C	223	LEU
2	C	484	GLU
2	C	500	SER
2	C	507	VAL
2	D	10	TYR
2	D	372	ASN
2	D	497	VAL
2	D	500	SER
1	A	73	ALA
1	A	302	LYS
1	B	10	ARG
1	B	181	MSE
1	B	213	SER
1	B	416	ARG
2	C	33	PRO

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Mol	Chain	Res	Type
2	C	356	ASN
2	C	498	LYS
2	D	217	LYS
2	D	223	LEU
2	D	484	GLU
2	D	498	LYS
1	A	26	GLY
1	A	142	PHE
1	B	211	PRO
2	C	14	GLY
2	C	290	THR
2	C	355	PRO
2	C	434	PRO
2	C	497	VAL
2	D	33	PRO
2	D	128	ASP
2	D	300	ILE
2	D	356	ASN
2	D	454	ASN
2	D	507	VAL
1	B	216	ALA
1	B	418	MSE
2	C	246	GLN
2	D	144	ASP
1	A	129	GLU
2	C	194	PRO
2	C	292	ILE
2	D	434	PRO
2	D	194	PRO
2	D	329	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	366/357 (102%)	338 (92%)	28 (8%)	16 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	367/357 (103%)	331 (90%)	36 (10%)	10 36
2	C	421/548 (77%)	395 (94%)	26 (6%)	23 60
2	D	412/548 (75%)	384 (93%)	28 (7%)	20 56
All	All	1566/1810 (86%)	1448 (92%)	118 (8%)	17 51

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	76	LYS
1	A	77	PRO
1	A	95	THR
1	A	102	THR
1	A	107	ILE
1	A	111	THR
1	A	136	VAL
1	A	142	PHE
1	A	143	ASN
1	A	146	SER
1	A	147	GLU
1	A	195	LEU
1	A	206	ARG
1	A	210	ARG
1	A	219	LEU
1	A	247	LEU
1	A	276	ILE
1	A	330	LYS
1	A	335	GLU
1	A	337	THR
1	A	346	ILE
1	A	364	SER
1	A	391	GLU
1	A	396	GLU
1	A	435	THR
1	A	437	LEU
1	A	438	ARG
1	B	4	ASP
1	B	24	GLU
1	B	72	ARG
1	B	77	PRO
1	B	86	GLU

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Mol	Chain	Res	Type
1	B	102	THR
1	B	105	SER
1	B	107	ILE
1	B	140	LEU
1	B	142	PHE
1	B	149	MSE
1	B	195	LEU
1	B	201	LEU
1	B	206	ARG
1	B	210	ARG
1	B	219	LEU
1	B	222	SER
1	B	241	THR
1	B	244	THR
1	B	252	THR
1	B	263	ASP
1	B	279	ASN
1	B	301	ASP
1	B	330	LYS
1	B	337	THR
1	B	366	CYS
1	B	371	VAL
1	B	373	LEU
1	B	377	SER
1	B	391	GLU
1	B	401	LYS
1	B	422	ASN
1	B	428	THR
1	B	431	THR
1	B	437	LEU
1	B	438	ARG
2	C	56	GLU
2	C	57	LEU
2	C	98	ARG
2	C	101	LEU
2	C	148	GLU
2	C	149	THR
2	C	193	THR
2	C	195	ASP
2	C	233	SER
2	C	246	GLN
2	C	247	GLU

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Mol	Chain	Res	Type
2	C	286	PHE
2	C	291	ASP
2	C	300	ILE
2	C	312	LEU
2	C	356	ASN
2	C	371	LEU
2	C	385	GLU
2	C	399	ARG
2	C	411	THR
2	C	415	LEU
2	C	420	THR
2	C	441	LEU
2	C	460	GLN
2	C	472	LEU
2	C	499	PRO
2	D	36	SER
2	D	48	ARG
2	D	56	GLU
2	D	57	LEU
2	D	65	LEU
2	D	79	ASN
2	D	110	LEU
2	D	148	GLU
2	D	149	THR
2	D	158	THR
2	D	246	GLN
2	D	247	GLU
2	D	270	ASP
2	D	354	LEU
2	D	356	ASN
2	D	361	GLN
2	D	371	LEU
2	D	385	GLU
2	D	386	GLU
2	D	399	ARG
2	D	415	LEU
2	D	417	ASP
2	D	424	ARG
2	D	436	THR
2	D	441	LEU
2	D	457	GLU
2	D	472	LEU

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Mol	Chain	Res	Type
2	D	499	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	135	ASN
1	A	143	ASN
1	A	153	HIS
1	A	218	ASN
1	A	258	HIS
1	A	279	ASN
1	A	344	ASN
1	A	422	ASN
1	B	56	ASN
1	B	135	ASN
1	B	143	ASN
1	B	153	HIS
1	B	194	ASN
1	B	218	ASN
1	B	258	HIS
1	B	344	ASN
1	B	408	HIS
1	B	422	ASN
2	C	22	HIS
2	C	47	GLN
2	C	79	ASN
2	C	106	GLN
2	C	131	ASN
2	C	231	ASN
2	C	262	GLN
2	C	350	HIS
2	C	356	ASN
2	C	478	GLN
2	D	22	HIS
2	D	106	GLN
2	D	131	ASN
2	D	262	GLN
2	D	350	HIS
2	D	356	ASN
2	D	361	GLN
2	D	478	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ASP	A	1000	-	2,8,8	0.52	0	0,10,10	0.00	-
3	ASP	B	5000	-	2,8,8	0.62	0	0,10,10	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASP	A	1000	-	-	0/2/8/8	0/0/0/0
3	ASP	B	5000	-	-	0/2/8/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	ASP	4	0
3	B	5000	ASP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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