Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 01:11 pm BST

PDB ID	:	4H02
Title	:	Crystal structure of P. falciparum Lysyl-tRNA synthetase
Authors	:	Khan, S.; Garg, A.; Sharma, A.
Deposited on	:	2012-09-07
Resolution	:	2.90 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 ①) were used in the production of this report:

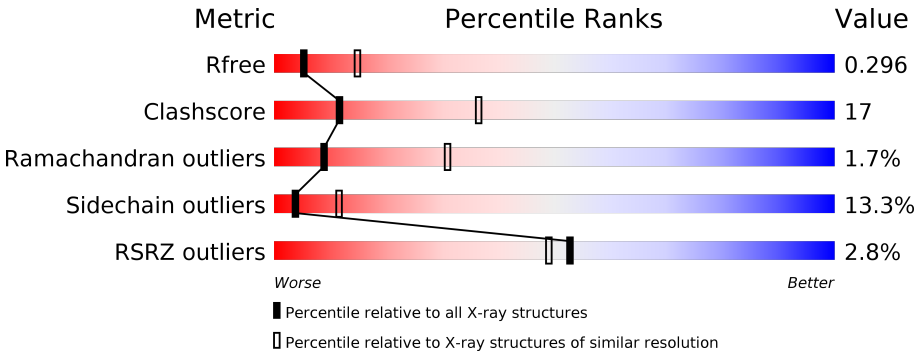
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	507	50% 38% · 7%
1	B	507	2% 52% 33% 8% 7%
1	C	507	2% 51% 35% 6% 7%
1	D	507	4% 51% 35% 7% 7%
1	E	507	3% 54% 33% 6% 7%
1	F	507	4% 51% 34% 8% 7%

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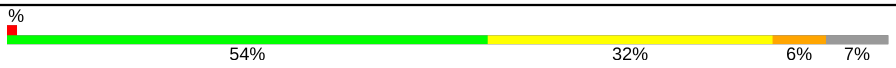
Mol	Chain	Length	Quality of chain
1	G	507	
1	H	507	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30845 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 Lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	3	0
			3848	2488	639	704	17			
1	B	471	Total	C	N	O	S	0	1	0
			3852	2490	640	705	17			
1	C	471	Total	C	N	O	S	0	0	0
			3844	2484	639	705	16			
1	D	471	Total	C	N	O	S	0	0	0
			3849	2488	640	705	16			
1	E	470	Total	C	N	O	S	0	0	0
			3833	2477	638	702	16			
1	F	470	Total	C	N	O	S	0	1	0
			3843	2485	638	704	16			
1	G	470	Total	C	N	O	S	0	0	0
			3840	2483	638	703	16			
1	H	471	Total	C	N	O	S	0	0	0
			3839	2481	639	703	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	14	Total	O	0	0
			14	14		
2	C	13	Total	O	0	0
			13	13		
2	D	16	Total	O	0	0
			16	16		
2	E	9	Total	O	0	0
			9	9		
2	F	8	Total	O	0	0
			8	8		

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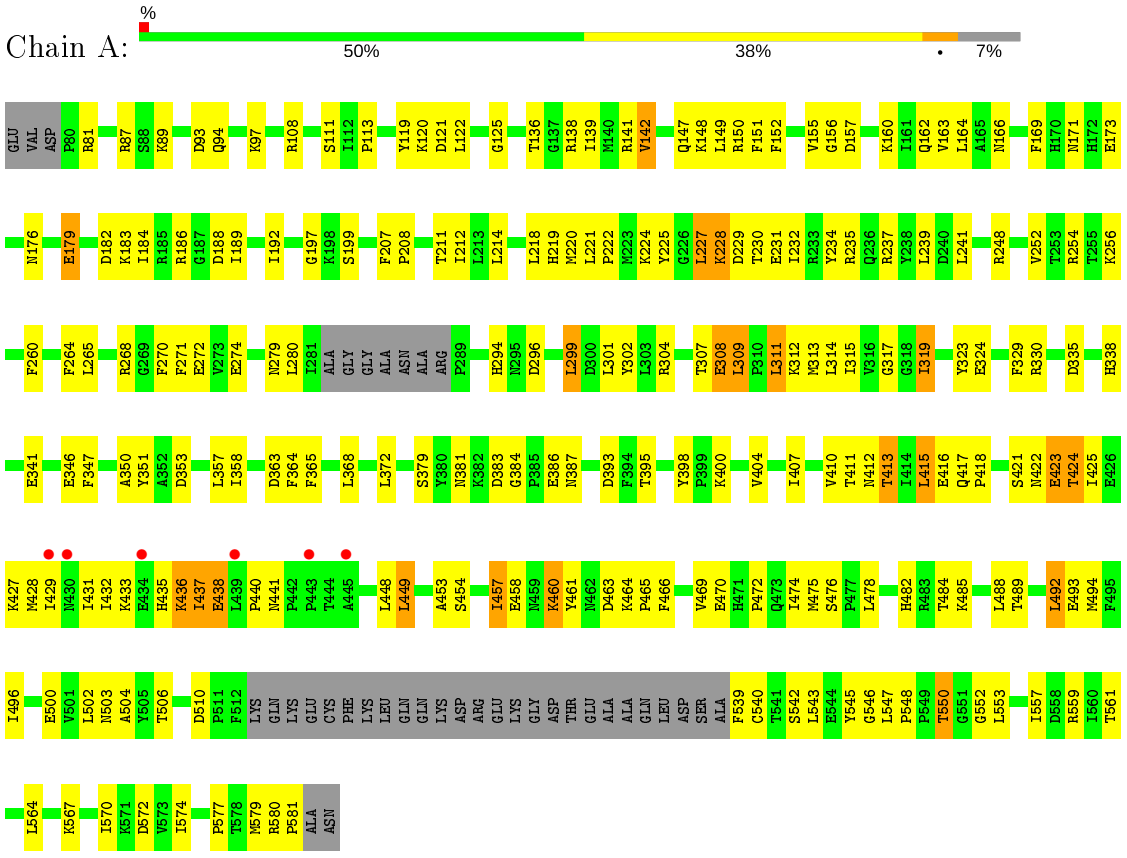
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	9	Total O 9 9	0	0
2	H	18	Total O 18 18	0	0

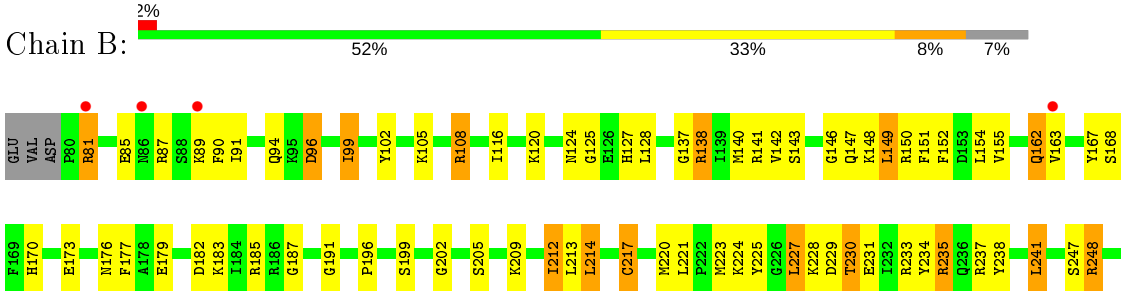
3 Residue-property plots (i)

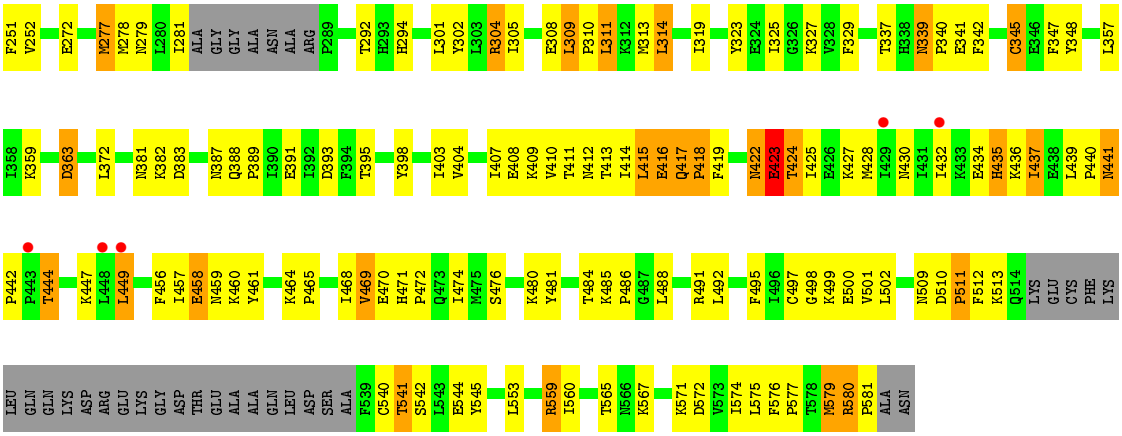
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Lysyl-tRNA synthetase



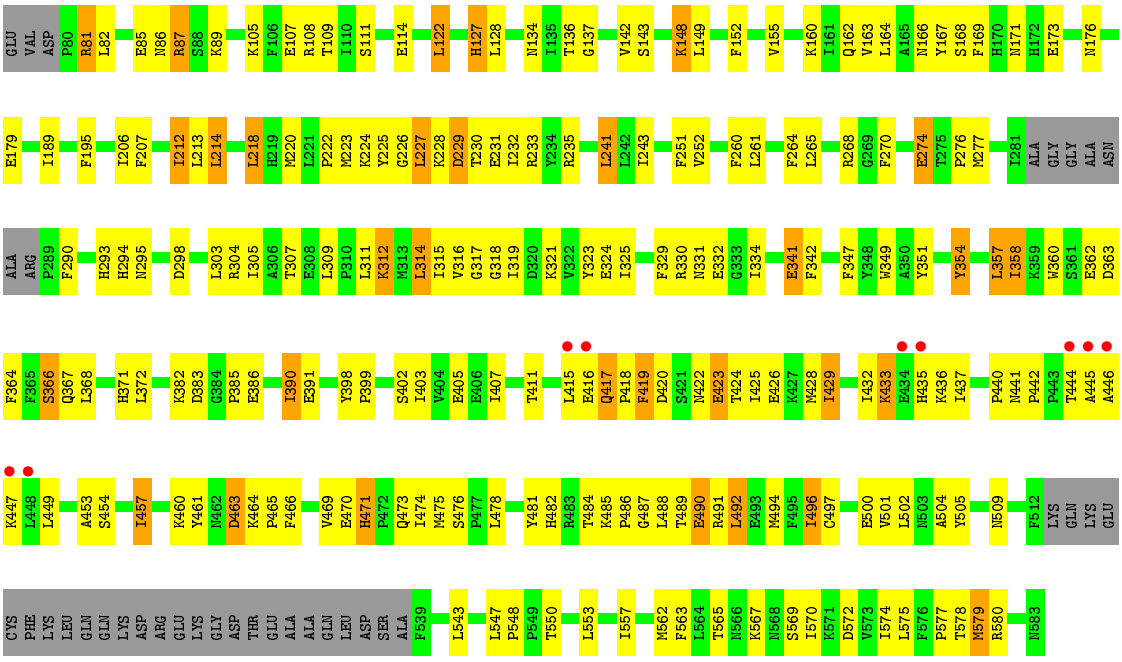
- Molecule 1: Lysyl-tRNA synthetase





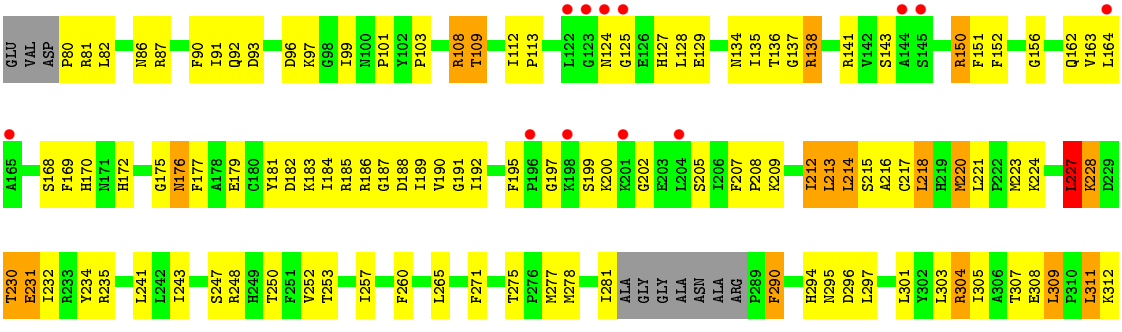
• Molecule 1: Lysyl-tRNA synthetase

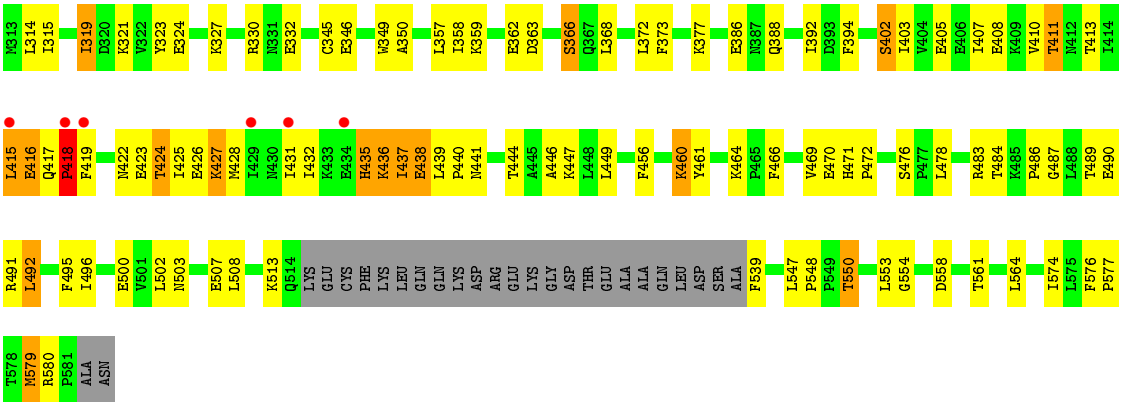
Chain C:



• Molecule 1: Lysyl-tRNA synthetase

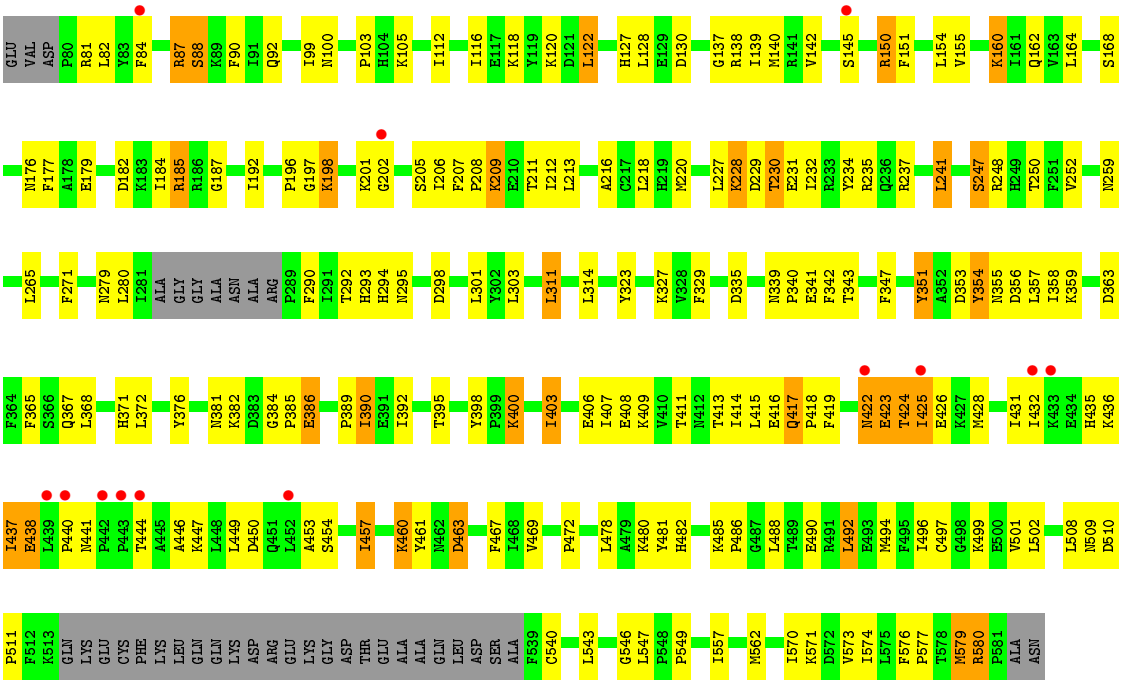
Chain D:





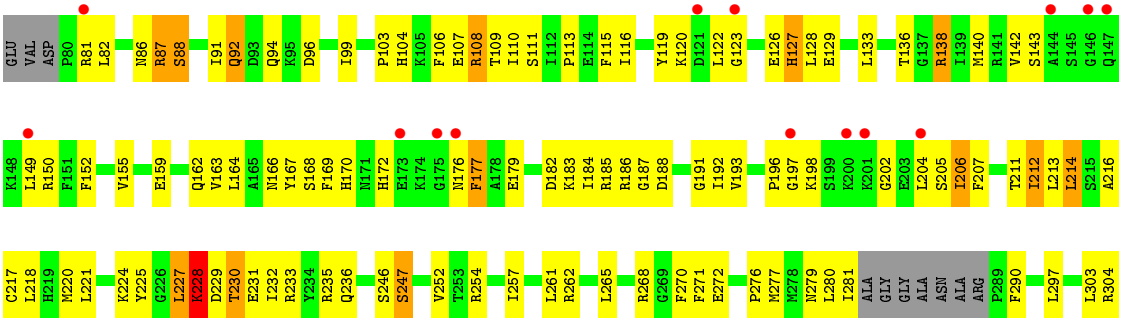
• Molecule 1: Lysyl-tRNA synthetase

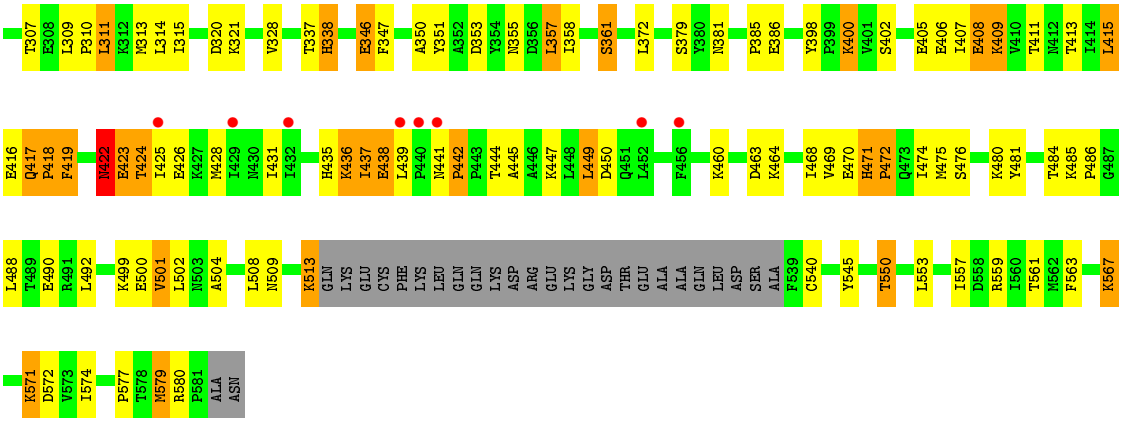
Chain E:



• Molecule 1: Lysyl-tRNA synthetase

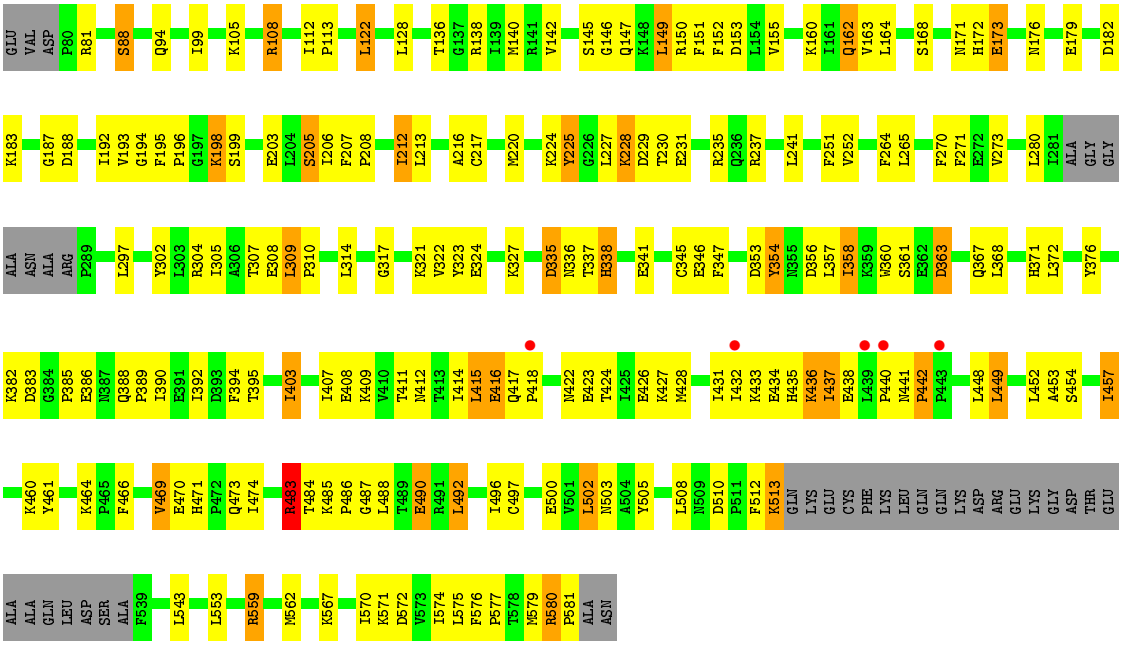
Chain F:





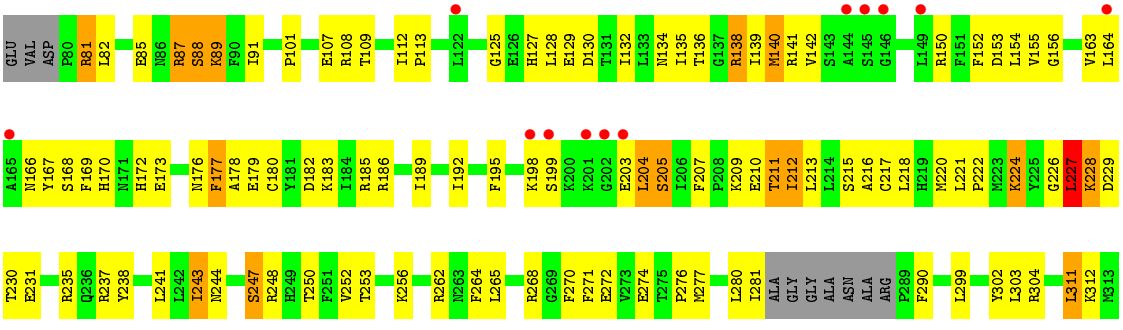
• Molecule 1: Lysyl-tRNA synthetase

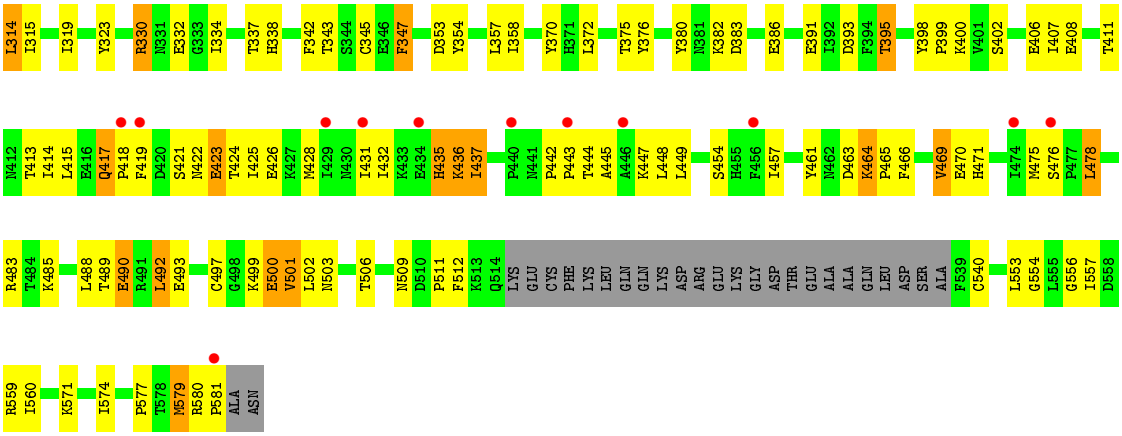
Chain G:



• Molecule 1: Lysyl-tRNA synthetase

Chain H:




L314 I315 I319 Y323 R330 N331 E332 G333 I334 T337 H338 F342 T343 S344 C345 E346 F347 D353 Y354 L357 I358 Y370 H371 L372 T375 Y376 Y380 N381 K382 D383 E386 E391 I392 D393 F394 T395 Y398 P399 K400 V401 S402 E406 I407 E408 T411
N412 T413 I414 L415 E416 Q417 P418 F419 D420 S421 N422 E423 T424 I425 E426 K427 M428 I429 N430 I431 I432 K433 E434 H435 K436 I437 P440 N441 P442 P443 T444 A445 A446 K447 L448 L449 S454 H455 F456 I457 Y461 N462 D463 K464 P465 F466 V469 E470 H471 I474 M475 S476 F477 L478
R483 T484 K485 L488 T489 E490 R491 L492 E493 C497 G498 K499 E500 V501 L502 N503 T506 N509 D510 P511 F512 K513 Q514 LYS GLU CYS PHE LYS LEU GLN GLN LYS ASP ARG GLU LYS GLY ASP THR GLU ALA ALA GLN LEU ASP SER ALA F539 C540 L553 G554 L555 G556 I557 D558
R559 I560 K571 I574 P577 T578 M579 R580 P581 ALA ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	141.33Å 59.14Å 297.22Å 90.00° 97.47° 90.00°	Depositor
Resolution (Å)	48.70 – 2.90 48.70 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.70-2.90) 93.4 (48.70-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.22 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7.1_743, REFMAC	Depositor
R, R_{free}	0.226 , 0.298 0.222 , 0.296	Depositor DCC
R_{free} test set	3110 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	30845	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.49	0/3954	0.63	0/5342
1	B	0.50	0/3952	0.65	0/5339
1	C	0.53	1/3941 (0.0%)	0.68	1/5326 (0.0%)
1	D	0.52	0/3946	0.64	0/5331
1	E	0.53	0/3929	0.65	0/5308
1	F	0.51	0/3943	0.61	0/5327
1	G	0.51	0/3937	0.65	1/5319 (0.0%)
1	H	0.53	0/3935	0.62	0/5316
All	All	0.51	1/31537 (0.0%)	0.64	2/42608 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	3
1	F	0	1
1	G	0	2
1	H	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	360	TRP	NE1-CE2	-5.37	1.30	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	483	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	C	360	TRP	CE2-CD2-CG	-5.12	103.20	107.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	416	GLU	Peptide
1	A	418	PRO	Peptide
1	D	227	LEU	Peptide
1	D	416	GLU	Peptide
1	D	418	PRO	Peptide
1	F	442	PRO	Peptide
1	G	416	GLU	Peptide
1	G	442	PRO	Peptide
1	H	227	LEU	Peptide

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	3848	0	3817	145	0
1	B	3852	0	3819	145	1
1	C	3844	0	3804	138	0
1	D	3849	0	3814	150	0
1	E	3833	0	3799	132	0
1	F	3843	0	3811	139	0
1	G	3840	0	3806	121	1
1	H	3839	0	3803	153	0
2	A	10	0	0	1	0
2	B	14	0	0	1	0
2	C	13	0	0	0	0
2	D	16	0	0	0	0
2	E	9	0	0	1	0
2	F	8	0	0	1	0
2	G	9	0	0	1	0
2	H	18	0	0	1	0
All	All	30845	0	30473	1071	1

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 17.

All (1071) 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:C:547:LEU:HD12	1:C:548:PRO:HD2	1.33	1.09
1:G:469:VAL:HG13	1:G:470:GLU:HG3	1.35	1.05
1:H:417:GLN:O	1:H:419:PHE:N	1.92	1.01
1:D:308:GLU:HG3	1:D:309:LEU:HD13	1.40	1.01
1:B:235:ARG:NH2	1:B:580:ARG:O	2.00	0.95
1:F:213:LEU:HD21	1:F:216:ALA:HB2	1.49	0.94
1:H:150:ARG:NH2	1:H:182:ASP:OD1	2.01	0.94
1:A:268:ARG:HH11	1:A:268:ARG:HG3	1.31	0.93
1:F:109:THR:HG21	1:F:133:LEU:HD22	1.48	0.93
1:E:122:LEU:O	1:E:198:LYS:NZ	2.01	0.92
1:A:150:ARG:NH2	1:A:182:ASP:OD1	2.03	0.91
1:H:186:ARG:NH1	1:H:221:LEU:O	2.05	0.90
1:G:358:ILE:HD13	1:G:492:LEU:HD13	1.54	0.89
1:C:358:ILE:HG12	1:C:492:LEU:HD13	1.55	0.89
1:B:417:GLN:O	1:B:419:PHE:N	2.06	0.88
1:C:417:GLN:O	1:C:419:PHE:N	2.05	0.88
1:D:164:LEU:HD13	1:D:207:PHE:HE1	1.40	0.86
1:A:469:VAL:HG13	1:A:470:GLU:HG3	1.55	0.85
1:C:407:ILE:O	1:C:411:THR:HG22	1.76	0.85
1:D:164:LEU:HD13	1:D:207:PHE:CE1	2.13	0.84
1:F:231:GLU:O	1:F:235:ARG:HG3	1.76	0.84
1:E:358:ILE:HD13	1:E:492:LEU:HD13	1.59	0.83
1:F:176:ASN:HB3	1:F:179:GLU:HB3	1.58	0.83
1:B:277:MET:HA	1:B:304:ARG:HG2	1.60	0.83
1:E:574:ILE:O	1:E:577:PRO:HD3	1.79	0.83
1:F:192:ILE:HG21	1:F:206:ILE:HG12	1.60	0.83
1:A:111:SER:OG	1:A:113:PRO:HD2	1.79	0.82
1:B:388:GLN:HG2	1:B:389:PRO:HD2	1.61	0.82
1:A:268:ARG:NH1	1:A:268:ARG:HG3	1.91	0.82
1:H:574:ILE:O	1:H:577:PRO:HD3	1.80	0.82
1:C:349:TRP:O	1:C:550:THR:HG23	1.79	0.81
1:B:231:GLU:O	1:B:235:ARG:HG3	1.80	0.80
1:B:228:LYS:HG3	1:B:233:ARG:HD3	1.62	0.80
1:E:259:ASN:HA	2:E:605:HOH:O	1.82	0.80
1:D:186:ARG:NH1	1:D:221:LEU:O	2.14	0.79
1:A:350:ALA:HA	1:A:550:THR:HG23	1.64	0.79
1:H:164:LEU:HD13	1:H:207:PHE:HE1	1.48	0.78
1:F:417:GLN:O	1:F:419:PHE:N	2.16	0.78
1:G:140:MET:HG2	1:G:155:VAL:HG22	1.66	0.78
1:D:227:LEU:O	1:D:228:LYS:HB2	1.81	0.78
1:H:224:LYS:NZ	1:H:244:ASN:OD1	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:GLY:O	1:D:217:CYS:HB2	1.84	0.77
1:C:471:HIS:HB3	1:C:475:MET:HE2	1.67	0.77
1:G:502:LEU:HD23	1:G:502:LEU:C	2.05	0.77
1:D:416:GLU:O	1:D:417:GLN:HG2	1.83	0.77
1:F:406:GLU:OE2	1:F:460:LYS:NZ	2.17	0.77
1:B:407:ILE:O	1:B:411:THR:HG22	1.86	0.76
1:E:571:LYS:HD3	1:E:579:MET:HE1	1.66	0.76
1:B:444:THR:HG22	1:B:447:LYS:H	1.51	0.76
1:F:408:GLU:OE2	1:F:415:LEU:N	2.18	0.75
1:H:235:ARG:NH2	1:H:580:ARG:O	2.15	0.75
1:C:567:LYS:HD2	1:C:572:ASP:HB3	1.66	0.75
1:A:138:ARG:NH2	1:A:189:ILE:HD11	2.02	0.75
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.69	0.75
1:B:237:ARG:HG3	1:B:241:LEU:HD22	1.69	0.74
1:C:440:PRO:O	1:C:441:ASN:HB2	1.87	0.74
1:E:444:THR:HB	1:E:447:LYS:HB2	1.69	0.74
1:C:330:ARG:HG3	1:C:342:PHE:HE2	1.52	0.74
1:B:152:PHE:HB2	1:B:163:VAL:HB	1.69	0.74
1:D:417:GLN:O	1:D:419:PHE:N	2.20	0.74
1:G:453:ALA:HA	1:G:457:ILE:HG13	1.70	0.74
1:H:222:PRO:HG2	1:H:243:ILE:HD13	1.69	0.73
1:A:411:THR:HG23	1:A:413:THR:HG23	1.69	0.73
1:B:422:ASN:O	1:B:424:THR:N	2.21	0.73
1:A:235:ARG:NH2	1:A:580:ARG:O	2.18	0.73
1:D:91:ILE:HG23	1:D:101:PRO:HG3	1.71	0.73
1:G:469:VAL:CG1	1:G:470:GLU:HG3	2.18	0.73
1:B:87:ARG:CZ	1:B:185:ARG:HG3	2.17	0.73
1:D:189:ILE:HD13	1:D:215:SER:HB3	1.69	0.73
1:B:567:LYS:HD2	1:B:572:ASP:HB3	1.71	0.72
1:B:150:ARG:NH2	1:B:182:ASP:OD1	2.22	0.72
1:G:224:LYS:O	1:G:225:TYR:HB3	1.87	0.72
1:B:480:LYS:NZ	1:B:509:ASN:OD1	2.21	0.72
1:E:197:GLY:HA3	1:E:207:PHE:HE2	1.54	0.71
1:F:254:ARG:HA	1:F:257:ILE:HD12	1.72	0.71
1:B:187:GLY:O	1:B:217:CYS:HB2	1.89	0.71
1:D:444:THR:HG22	1:D:447:LYS:H	1.55	0.71
1:D:362:GLU:O	1:D:366:SER:HB3	1.90	0.71
1:C:251:PHE:CE1	1:C:575:LEU:HD23	2.25	0.71
1:F:407:ILE:O	1:F:411:THR:HG22	1.90	0.71
1:C:270:PHE:CD1	1:C:321:LYS:HB3	2.26	0.70
1:B:325:ILE:HG12	1:B:345:CYS:HB2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:502:LEU:HD11	1:H:553:LEU:HD11	1.72	0.70
1:D:213:LEU:HD11	1:D:216:ALA:HB2	1.74	0.70
1:E:437:ILE:O	1:E:438:GLU:CB	2.40	0.70
1:B:339:ASN:ND2	1:B:340:PRO:HD2	2.07	0.70
1:B:574:ILE:O	1:B:577:PRO:HD3	1.91	0.69
1:B:440:PRO:O	1:B:441:ASN:HB2	1.90	0.69
1:A:120:LYS:HG3	1:A:121:ASP:N	2.06	0.69
1:C:429:ILE:HG23	1:C:433:LYS:HE3	1.73	0.69
1:D:152:PHE:HB2	1:D:163:VAL:HB	1.74	0.69
1:F:103:PRO:HG3	1:F:212:ILE:HD11	1.75	0.69
1:A:574:ILE:O	1:A:577:PRO:HD3	1.93	0.69
1:D:109:THR:HB	1:D:134:ASN:H	1.56	0.69
1:D:169:PHE:CE2	1:D:195:PHE:HZ	2.09	0.69
1:G:150:ARG:NH2	1:G:182:ASP:OD1	2.25	0.69
1:H:128:LEU:O	1:H:195:PHE:HB2	1.93	0.69
1:B:227:LEU:O	1:B:228:LYS:HB2	1.92	0.69
1:C:329:PHE:C	1:C:330:ARG:HG2	2.13	0.69
1:A:453:ALA:HA	1:A:457:ILE:HG13	1.75	0.68
1:D:152:PHE:CE1	1:D:184:ILE:HG21	2.28	0.68
1:H:382:LYS:HE2	1:H:497:CYS:HB3	1.74	0.68
1:H:112:ILE:HD12	1:H:156:GLY:HA3	1.76	0.68
1:F:123:GLY:N	1:F:126:GLU:OE1	2.27	0.68
1:F:152:PHE:HB2	1:F:163:VAL:HB	1.74	0.67
1:G:484:THR:OG1	1:G:485:LYS:HG3	1.95	0.67
1:G:358:ILE:CD1	1:G:492:LEU:HD13	2.24	0.67
1:G:149:LEU:HD23	1:G:151:PHE:HZ	1.58	0.67
1:B:187:GLY:C	1:B:217:CYS:HB2	2.15	0.67
1:C:315:ILE:HD13	1:C:319:ILE:O	1.95	0.67
1:F:358:ILE:CD1	1:F:492:LEU:HD13	2.25	0.67
1:C:382:LYS:HB2	1:C:390:ILE:HD11	1.77	0.66
1:H:499:LYS:HE3	1:H:559:ARG:HH12	1.60	0.66
1:E:398:TYR:O	1:E:400:LYS:NZ	2.23	0.66
1:B:485:LYS:HB3	1:B:488:LEU:HD22	1.78	0.66
1:C:329:PHE:O	1:C:330:ARG:HG2	1.95	0.66
1:F:230:THR:O	1:F:233:ARG:NE	2.26	0.66
1:A:440:PRO:O	1:A:441:ASN:HB2	1.96	0.66
1:H:152:PHE:HB2	1:H:163:VAL:CG2	2.26	0.65
1:A:559[B]:ARG:HG2	1:A:559[B]:ARG:HH11	1.61	0.65
1:C:231:GLU:OE1	1:C:235:ARG:NH1	2.30	0.65
1:D:150:ARG:NH2	1:D:182:ASP:OD1	2.30	0.65
1:D:321:LYS:HG2	1:D:349:TRP:CD1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:231:GLU:O	1:G:235:ARG:HG3	1.96	0.65
1:G:361:SER:OG	1:G:502:LEU:HD11	1.97	0.65
1:B:571:LYS:HD3	1:B:579:MET:HE1	1.79	0.65
1:G:149:LEU:HD23	1:G:151:PHE:CZ	2.32	0.65
1:C:446:ALA:HB2	1:C:474:ILE:HG13	1.78	0.64
1:B:212:ILE:HG13	1:B:213:LEU:N	2.13	0.64
1:D:290:PHE:HB3	1:D:303:LEU:HD12	1.80	0.64
1:F:435:HIS:O	1:F:436:LYS:C	2.35	0.64
1:D:418:PRO:HB3	1:D:487:GLY:HA3	1.80	0.64
1:E:381:ASN:OD1	1:E:389:PRO:HB3	1.98	0.64
1:A:313:MET:CE	1:B:576:PHE:HE1	2.10	0.63
1:D:417:GLN:C	1:D:419:PHE:H	2.01	0.63
1:E:192:ILE:HG23	1:E:208:PRO:HB3	1.81	0.63
1:H:421:SER:HA	1:H:425:ILE:HG13	1.79	0.63
1:A:186:ARG:NH1	1:A:221:LEU:O	2.31	0.63
1:A:186:ARG:NH1	1:A:222:PRO:O	2.24	0.63
1:A:265:LEU:HD13	1:A:323:TYR:CG	2.34	0.63
1:D:466:PHE:CE2	1:D:495:PHE:HB2	2.34	0.63
1:E:485:LYS:HB3	1:E:488:LEU:HD22	1.80	0.63
1:F:437:ILE:O	1:F:438:GLU:CB	2.47	0.63
1:A:231:GLU:OE1	1:A:235:ARG:NH1	2.31	0.63
1:E:151:PHE:HD1	1:E:162:GLN:HE21	1.46	0.63
1:D:460:LYS:HB3	1:D:461:TYR:CD2	2.34	0.63
1:C:444:THR:HB	1:C:447:LYS:HB2	1.81	0.63
1:D:257:ILE:HD12	1:D:561:THR:HG23	1.79	0.63
1:C:82:LEU:O	1:C:86:ASN:ND2	2.31	0.63
1:F:381:ASN:HD22	1:F:385:PRO:HA	1.64	0.62
1:A:510:ASP:HB2	1:B:102:TYR:CD2	2.34	0.62
1:G:336:ASN:ND2	2:G:603:HOH:O	2.32	0.62
1:A:547:LEU:HD12	1:A:548:PRO:HD2	1.81	0.62
1:C:570:ILE:HG12	1:C:574:ILE:HD12	1.81	0.62
1:E:509:ASN:HB3	1:E:547:LEU:HD23	1.80	0.62
1:F:279:ASN:O	1:F:280:LEU:HG	1.99	0.62
1:G:435:HIS:O	1:G:436:LYS:C	2.37	0.62
1:H:138:ARG:O	1:H:154:LEU:HD12	2.00	0.62
1:D:112:ILE:HD12	1:D:156:GLY:N	2.15	0.62
1:A:138:ARG:CZ	1:A:189:ILE:HD11	2.30	0.62
1:H:222:PRO:HG2	1:H:243:ILE:CD1	2.29	0.62
1:A:299:LEU:HD11	1:B:581:PRO:HG3	1.82	0.62
1:C:547:LEU:HD12	1:C:548:PRO:CD	2.21	0.62
1:F:468:ILE:HG22	1:F:471:HIS:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ARG:O	1:D:152:PHE:HA	1.99	0.62
1:D:103:PRO:HG3	1:D:212:ILE:HD11	1.81	0.62
1:H:81:ARG:O	1:H:85:GLU:HG3	1.99	0.62
1:D:129:GLU:HG2	1:D:195:PHE:CE1	2.35	0.62
1:F:198:LYS:HB3	1:F:202:GLY:HA2	1.80	0.62
1:F:224:LYS:O	1:F:225:TYR:HB3	2.00	0.62
1:A:148:LYS:O	1:A:149:LEU:HD12	2.00	0.61
1:B:339:ASN:HD22	1:B:341:GLU:H	1.47	0.61
1:F:402[B]:SER:OG	1:F:405:GLU:HB3	1.99	0.61
1:G:192:ILE:HG23	1:G:208:PRO:HB3	1.82	0.61
1:E:449:LEU:HD21	1:E:472:PRO:HG2	1.81	0.61
1:C:314:LEU:HB3	1:C:319:ILE:HD12	1.81	0.61
1:A:313:MET:HE1	1:B:576:PHE:HE1	1.64	0.61
1:G:265:LEU:HB3	1:G:270:PHE:HB2	1.82	0.61
1:E:417:GLN:NE2	1:E:424:THR:OG1	2.33	0.61
1:A:268:ARG:HH11	1:A:268:ARG:CG	2.10	0.61
1:H:417:GLN:C	1:H:419:PHE:H	2.00	0.61
1:C:227:LEU:O	1:C:228:LYS:HB2	1.99	0.61
1:C:469:VAL:CG1	1:C:470:GLU:HG3	2.31	0.61
1:E:339:ASN:HD22	1:E:341:GLU:H	1.49	0.61
1:C:290:PHE:HB2	1:C:303:LEU:HB2	1.83	0.61
1:C:362:GLU:O	1:C:366:SER:HB3	2.01	0.60
1:B:410:VAL:HG11	1:B:456:PHE:HD1	1.66	0.60
1:F:472:PRO:HB2	1:F:475:MET:HG3	1.82	0.60
1:A:465:PRO:HB3	1:A:496:ILE:HG12	1.83	0.60
1:D:440:PRO:O	1:D:441:ASN:HB2	2.01	0.60
1:F:310:PRO:HA	1:F:313:MET:HG3	1.81	0.60
1:G:252:VAL:HA	1:H:271:PHE:CZ	2.37	0.60
1:B:90:PHE:CZ	1:B:183:LYS:HB3	2.36	0.60
1:C:252:VAL:HA	1:D:271:PHE:CZ	2.36	0.60
1:E:327:LYS:HD3	1:E:342:PHE:O	2.01	0.60
1:F:321:LYS:NZ	2:F:607:HOH:O	2.33	0.60
1:D:87:ARG:NH1	1:D:185:ARG:HG2	2.17	0.60
1:F:230:THR:HB	1:F:232:ILE:HG12	1.83	0.60
1:A:539:PHE:O	1:A:542:SER:OG	2.14	0.60
1:F:485:LYS:HB3	1:F:488:LEU:HD22	1.84	0.60
1:H:192:ILE:HG12	1:H:211:THR:OG1	2.01	0.60
1:D:162:GLN:O	1:D:205:SER:HA	2.02	0.60
1:A:176:ASN:HB3	1:A:179:GLU:HB2	1.84	0.60
1:G:403:ILE:HG22	1:G:469:VAL:O	2.02	0.60
1:G:473:GLN:HG3	1:G:487:GLY:C	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:PRO:CG	1:F:486:PRO:HB2	2.31	0.59
1:G:176:ASN:HB3	1:G:179:GLU:HB3	1.84	0.59
1:H:212:ILE:HD12	1:H:213:LEU:N	2.17	0.59
1:H:315:ILE:HD13	1:H:319:ILE:O	2.02	0.59
1:A:315:ILE:HD13	1:A:319:ILE:O	2.02	0.59
1:A:411:THR:HG23	1:A:413:THR:H	1.67	0.59
1:B:148:LYS:HG3	1:B:167:TYR:HB3	1.84	0.59
1:C:473:GLN:NE2	1:C:481:TYR:CD1	2.70	0.59
1:D:93:ASP:O	1:D:97:LYS:HB2	2.02	0.59
1:F:277:MET:HA	1:F:304:ARG:HD3	1.83	0.59
1:C:463:ASP:OD1	1:C:463:ASP:N	2.33	0.59
1:E:120:LYS:O	1:E:198:LYS:NZ	2.35	0.59
1:G:171:ASN:O	1:G:173:GLU:N	2.35	0.59
1:H:330:ARG:HG3	1:H:342:PHE:CE2	2.37	0.59
1:A:365:PHE:CE2	1:A:494:MET:HE2	2.37	0.59
1:G:140:MET:HG2	1:G:155:VAL:CG2	2.32	0.59
1:G:153:ASP:HB3	1:G:160:LYS:HD3	1.83	0.59
1:H:141:ARG:HB3	1:H:153:ASP:HB2	1.83	0.59
1:B:441:ASN:HD22	1:B:447:LYS:HE2	1.67	0.59
1:A:428:MET:O	1:A:432:ILE:HG12	2.03	0.59
1:C:252:VAL:HA	1:D:271:PHE:HZ	1.67	0.59
1:D:484:THR:O	1:D:486:PRO:HD3	2.03	0.58
1:G:212:ILE:HG13	1:G:213:LEU:N	2.18	0.58
1:E:376:TYR:CD2	1:E:395:THR:HG23	2.38	0.58
1:H:91:ILE:HG23	1:H:101:PRO:HG3	1.85	0.58
1:D:435:HIS:O	1:D:436:LYS:C	2.41	0.58
1:G:407:ILE:O	1:G:411:THR:HG22	2.02	0.58
1:H:108:ARG:HD2	1:H:136:THR:OG1	2.03	0.58
1:D:359:LYS:NZ	1:D:363:ASP:OD2	2.30	0.58
1:E:363:ASP:O	1:E:367:GLN:HG3	2.04	0.58
1:E:105:LYS:NZ	1:F:351:TYR:O	2.37	0.58
1:G:394:PHE:CZ	1:G:496:ILE:HD13	2.39	0.58
1:C:565:THR:O	1:C:567:LYS:HG2	2.04	0.58
1:D:415:LEU:HD22	1:D:428:MET:HG2	1.84	0.58
1:E:546:GLY:O	1:F:138:ARG:NH2	2.36	0.58
1:D:277:MET:HA	1:D:304:ARG:HG2	1.84	0.58
1:D:411:THR:HG23	1:D:413:THR:HG23	1.85	0.58
1:H:347:PHE:CD1	1:H:347:PHE:C	2.77	0.58
1:C:347:PHE:CZ	1:C:553:LEU:HD13	2.38	0.58
1:D:439:LEU:HD12	1:D:439:LEU:H	1.69	0.58
1:G:280:LEU:HA	1:G:302:TYR:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:HA	1:A:150:ARG:HH11	1.69	0.57
1:D:294:HIS:CE1	1:D:297:LEU:HD13	2.38	0.57
1:H:231:GLU:OE1	1:H:235:ARG:NH1	2.37	0.57
1:C:224:LYS:O	1:C:225:TYR:HB3	2.04	0.57
1:B:182:ASP:O	1:B:185:ARG:NH2	2.37	0.57
1:D:312:LYS:HD2	1:D:507:GLU:OE1	2.04	0.57
1:E:351:TYR:N	1:E:549:PRO:O	2.35	0.57
1:F:559:ARG:HD2	1:F:563:PHE:CE2	2.40	0.57
1:G:385:PRO:HD2	1:G:386:GLU:OE1	2.04	0.57
1:H:469:VAL:HG13	1:H:470:GLU:HG3	1.87	0.57
1:F:358:ILE:HD13	1:F:492:LEU:HD13	1.86	0.57
1:A:502:LEU:HD23	1:A:502:LEU:C	2.25	0.57
1:E:150:ARG:NH2	1:E:182:ASP:OD1	2.38	0.57
1:A:472:PRO:HB2	1:A:474:ILE:HG22	1.87	0.57
1:C:492:LEU:HD23	1:C:492:LEU:H	1.68	0.57
1:D:80:PRO:HA	1:D:220:MET:HE2	1.86	0.57
1:H:501:VAL:HG22	1:H:560:ILE:HG12	1.85	0.57
1:C:562:MET:HE3	1:C:569:SER:C	2.25	0.57
1:E:413:THR:HG21	1:E:431:ILE:HD11	1.87	0.57
1:F:127:HIS:O	1:F:128:LEU:HD23	2.05	0.57
1:H:423:GLU:O	1:H:426:GLU:HB3	2.04	0.57
1:D:416:GLU:O	1:D:417:GLN:CG	2.51	0.57
1:D:90:PHE:CE1	1:D:183:LYS:HB3	2.40	0.57
1:A:429:ILE:HG23	1:A:433:LYS:HE3	1.87	0.57
1:C:334:ILE:HD12	1:D:297:LEU:HD11	1.86	0.57
1:B:128:LEU:HB2	1:B:196:PRO:HG2	1.87	0.56
1:H:173:GLU:N	1:H:173:GLU:OE1	2.28	0.56
1:H:330:ARG:HG3	1:H:342:PHE:HE2	1.70	0.56
1:G:88:SER:HB3	1:H:512:PHE:CZ	2.40	0.56
1:C:316:VAL:C	1:C:318:GLY:H	2.09	0.56
1:F:192:ILE:CG2	1:F:206:ILE:HG12	2.32	0.56
1:G:473:GLN:HG3	1:G:487:GLY:O	2.05	0.56
1:A:410:VAL:O	1:A:412:ASN:ND2	2.38	0.56
1:A:309:LEU:O	1:A:313:MET:HG3	2.06	0.56
1:A:472:PRO:HD2	1:A:475:MET:SD	2.46	0.56
1:A:313:MET:CE	1:B:576:PHE:CE1	2.89	0.56
1:B:359:LYS:NZ	1:B:363:ASP:OD1	2.37	0.56
1:A:280:LEU:HA	1:A:302:TYR:CD2	2.40	0.56
1:B:96:ASP:OD1	1:B:96:ASP:N	2.37	0.56
1:D:230:THR:HB	1:D:232:ILE:HG12	1.87	0.56
1:A:147:GLN:HA	1:A:150:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLY:N	1:B:199:SER:O	2.38	0.56
1:C:265:LEU:HD13	1:C:323:TYR:CG	2.41	0.56
1:E:339:ASN:ND2	1:E:340:PRO:HD2	2.21	0.56
1:G:567:LYS:HD2	1:G:572:ASP:HB3	1.88	0.56
1:G:570:ILE:HG12	1:G:574:ILE:HD12	1.88	0.56
1:B:565:THR:O	1:B:567:LYS:HG2	2.06	0.56
1:F:186:ARG:NH1	1:F:221:LEU:O	2.39	0.56
1:E:290:PHE:HB2	1:E:303:LEU:HB2	1.87	0.56
1:C:471:HIS:O	1:C:489:THR:HG23	2.04	0.55
1:B:469:VAL:HG13	1:B:470:GLU:HG3	1.88	0.55
1:E:480:LYS:HA	1:E:508:LEU:HD13	1.88	0.55
1:C:314:LEU:HG	1:C:319:ILE:HD12	1.87	0.55
1:C:264:PHE:CD2	1:C:364:PHE:HD1	2.24	0.55
1:E:368:LEU:O	1:E:371:HIS:HB3	2.05	0.55
1:H:167:TYR:CZ	1:H:172:HIS:HE1	2.24	0.55
1:H:407:ILE:O	1:H:411:THR:HG22	2.05	0.55
1:B:308:GLU:HG3	1:B:309:LEU:HD13	1.87	0.55
1:B:81:ARG:O	1:B:85:GLU:HG3	2.07	0.55
1:C:429:ILE:O	1:C:433:LYS:HD2	2.07	0.55
1:E:467:PHE:CE1	1:E:494:MET:HB2	2.41	0.55
1:E:562:MET:HG3	1:E:573:VAL:HG21	1.87	0.55
1:G:94:GLN:HE22	1:G:183:LYS:HE2	1.71	0.55
1:H:407:ILE:HG13	1:H:457:ILE:HD11	1.88	0.55
1:C:469:VAL:HG13	1:C:470:GLU:HG3	1.89	0.55
1:E:428:MET:O	1:E:432:ILE:HG13	2.07	0.55
1:D:152:PHE:HE1	1:D:184:ILE:HG21	1.71	0.54
1:C:276:PRO:HD3	1:D:576:PHE:HB2	1.90	0.54
1:F:170:HIS:O	1:F:172:HIS:CD2	2.60	0.54
1:C:578:THR:O	1:C:579:MET:HE3	2.08	0.54
1:D:294:HIS:HB2	1:D:301:LEU:HD12	1.89	0.54
1:E:105:LYS:HE2	1:F:353:ASP:HB3	1.89	0.54
1:E:406:GLU:HG3	1:E:406:GLU:O	2.07	0.54
1:F:402[B]:SER:OG	1:F:405:GLU:OE1	2.19	0.54
1:E:138:ARG:O	1:E:154:LEU:HA	2.07	0.54
1:F:152:PHE:CE1	1:F:184:ILE:HG21	2.42	0.54
1:H:237:ARG:O	1:H:241:LEU:HD13	2.07	0.54
1:A:260:PHE:CD2	1:A:368:LEU:HD13	2.43	0.54
1:A:567:LYS:HD2	1:A:572:ASP:HB3	1.88	0.54
1:B:179:GLU:OE1	1:B:183:LYS:NZ	2.38	0.54
1:C:570:ILE:HG12	1:C:574:ILE:CD1	2.38	0.54
1:C:235:ARG:NH2	1:C:580:ARG:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:LEU:HD21	1:E:216:ALA:HB2	1.89	0.54
1:C:485:LYS:O	1:C:488:LEU:HB2	2.06	0.54
1:G:224:LYS:O	1:G:225:TYR:CB	2.55	0.54
1:B:430:ASN:O	1:B:434:GLU:HG3	2.07	0.54
1:C:453:ALA:HA	1:C:457:ILE:HG13	1.89	0.54
1:D:417:GLN:C	1:D:419:PHE:N	2.60	0.54
1:E:151:PHE:HD1	1:E:162:GLN:NE2	2.04	0.54
1:H:277:MET:HA	1:H:304:ARG:HD3	1.89	0.54
1:G:194:GLY:HA3	1:G:207:PHE:O	2.08	0.54
1:E:440:PRO:O	1:E:441:ASN:HB2	2.08	0.54
1:F:307:THR:OG1	1:F:346:GLU:HG3	2.07	0.54
1:B:422:ASN:O	1:B:425:ILE:N	2.39	0.53
1:F:152:PHE:HE1	1:F:184:ILE:HG21	1.74	0.53
1:A:407:ILE:O	1:A:411:THR:HG22	2.08	0.53
1:F:315:ILE:HD12	1:F:550:THR:HG21	1.90	0.53
1:A:546:GLY:O	1:B:138:ARG:NH2	2.41	0.53
1:B:435:HIS:O	1:B:436:LYS:C	2.45	0.53
1:H:164:LEU:HB3	1:H:207:PHE:CD1	2.44	0.53
1:B:272:GLU:HB2	1:B:323:TYR:CZ	2.43	0.53
1:C:251:PHE:CD1	1:C:575:LEU:HD23	2.43	0.53
1:H:432:ILE:O	1:H:437:ILE:HA	2.08	0.53
1:B:411:THR:HG23	1:B:413:THR:HG23	1.90	0.53
1:D:80:PRO:HA	1:D:220:MET:CE	2.38	0.53
1:H:167:TYR:CZ	1:H:172:HIS:CE1	2.96	0.53
1:C:399:PRO:HB2	1:C:466:PHE:HB2	1.89	0.53
1:G:145:SER:HB3	1:G:151:PHE:HE2	1.74	0.53
1:H:87:ARG:NH2	1:H:185:ARG:HB2	2.23	0.53
1:A:358:ILE:CD1	1:A:492:LEU:HD13	2.39	0.53
1:D:265:LEU:HD13	1:D:323:TYR:CG	2.44	0.53
1:G:448:LEU:O	1:G:452:LEU:HG	2.09	0.53
1:B:279:ASN:O	1:B:301:LEU:HD23	2.09	0.53
1:B:414:ILE:O	1:B:427:LYS:NZ	2.36	0.53
1:F:176:ASN:HB3	1:F:179:GLU:CB	2.35	0.53
1:B:281:ILE:O	1:B:281:ILE:HG23	2.09	0.53
1:E:247:SER:O	1:E:250:THR:N	2.42	0.53
1:F:108:ARG:HD2	1:F:136:THR:OG1	2.09	0.53
1:E:145:SER:HA	1:H:391:GLU:OE2	2.09	0.53
1:B:308:GLU:HB2	1:B:348:TYR:OH	2.09	0.53
1:C:382:LYS:HD2	1:C:497:CYS:HB3	1.91	0.53
1:F:109:THR:HG21	1:F:133:LEU:CD2	2.30	0.53
1:F:162:GLN:O	1:F:205:SER:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:LEU:HB3	1:F:270:PHE:HB2	1.91	0.53
1:F:502:LEU:HD11	1:F:553:LEU:HD11	1.91	0.52
1:B:137:GLY:HA3	1:B:154:LEU:HD11	1.91	0.52
1:B:137:GLY:CA	1:B:154:LEU:HD11	2.39	0.52
1:D:125:GLY:N	1:D:199:SER:O	2.33	0.52
1:D:275:THR:HG23	1:D:324:GLU:OE1	2.09	0.52
1:H:485:LYS:HB3	1:H:488:LEU:HD22	1.91	0.52
1:C:347:PHE:CE2	1:C:553:LEU:HD13	2.44	0.52
1:G:147:GLN:HA	1:G:150:ARG:NH1	2.25	0.52
1:G:460:LYS:HE3	1:G:461:TYR:HE2	1.73	0.52
1:H:471:HIS:HB3	1:H:475:MET:HE2	1.92	0.52
1:A:423:GLU:OE2	1:A:427:LYS:NZ	2.39	0.52
1:A:493:GLU:HG3	1:A:503:ASN:OD1	2.09	0.52
1:C:492:LEU:N	1:C:492:LEU:HD23	2.24	0.52
1:D:408:GLU:OE2	1:D:415:LEU:N	2.40	0.52
1:G:105:LYS:HD3	1:H:353:ASP:HB3	1.92	0.52
1:A:156:GLY:O	1:A:157:ASP:HB2	2.09	0.52
1:A:457:ILE:O	1:A:460:LYS:HB2	2.10	0.52
1:A:506:THR:HA	1:A:550:THR:O	2.09	0.52
1:E:271:PHE:CZ	1:F:252:VAL:HA	2.44	0.52
1:H:204:LEU:HD12	1:H:205:SER:H	1.75	0.52
1:B:410:VAL:HG11	1:B:456:PHE:CD1	2.44	0.52
1:F:109:THR:HG22	1:F:110:ILE:HB	1.92	0.52
1:A:510:ASP:HB2	1:B:102:TYR:CG	2.45	0.52
1:E:265:LEU:HD13	1:E:323:TYR:CG	2.45	0.52
1:E:441:ASN:HB3	1:E:447:LYS:HE2	1.92	0.52
1:C:212:ILE:HG13	1:C:213:LEU:N	2.25	0.52
1:D:170:HIS:NE2	1:D:175:GLY:O	2.41	0.52
1:D:502:LEU:HD23	1:D:503:ASN:N	2.24	0.52
1:G:416:GLU:O	1:G:418:PRO:N	2.43	0.52
1:B:151:PHE:HD1	1:B:162:GLN:HE22	1.57	0.52
1:B:382:LYS:HD2	1:B:497:CYS:HB3	1.91	0.52
1:D:469:VAL:HG13	1:D:470:GLU:HG3	1.92	0.52
1:G:335:ASP:OD1	1:G:338:HIS:N	2.43	0.52
1:G:382:LYS:HD2	1:G:497:CYS:HB3	1.92	0.52
1:C:260:PHE:CD2	1:C:368:LEU:HD13	2.44	0.51
1:B:457:ILE:O	1:B:459:ASN:N	2.44	0.51
1:C:108:ARG:HD2	1:C:136:THR:OG1	2.10	0.51
1:C:578:THR:O	1:C:579:MET:CE	2.58	0.51
1:E:231:GLU:O	1:E:235:ARG:HG3	2.10	0.51
1:E:234:TYR:HB3	1:E:577:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ILE:HD12	1:B:495:PHE:CE2	2.44	0.51
1:D:184:ILE:HG22	1:D:184:ILE:O	2.08	0.51
1:H:375:THR:OG1	1:H:376:TYR:N	2.42	0.51
1:B:314:LEU:HG	1:B:319:ILE:HD12	1.92	0.51
1:C:314:LEU:HD13	1:D:576:PHE:HZ	1.75	0.51
1:H:139:ILE:HD13	1:H:154:LEU:HD13	1.92	0.51
1:E:279:ASN:O	1:E:280:LEU:HG	2.10	0.51
1:F:361:SER:HB3	1:F:502:LEU:HD13	1.92	0.51
1:D:179:GLU:O	1:D:183:LYS:HE3	2.10	0.51
1:F:418:PRO:HG2	1:F:486:PRO:HB2	1.92	0.51
1:E:279:ASN:O	1:E:301:LEU:HD23	2.10	0.51
1:E:425:ILE:HG22	1:E:426:GLU:N	2.25	0.51
1:A:432:ILE:O	1:A:437:ILE:HA	2.10	0.51
1:B:140:MET:HG2	1:B:155:VAL:HG22	1.93	0.51
1:A:264:PHE:CE1	1:A:268:ARG:NH2	2.79	0.51
1:B:416:GLU:O	1:B:417:GLN:C	2.47	0.51
1:C:316:VAL:O	1:C:318:GLY:N	2.43	0.51
1:D:415:LEU:HB3	1:D:427:LYS:HZ2	1.76	0.51
1:F:106:PHE:CE1	1:F:191:GLY:HA3	2.45	0.51
1:F:501:VAL:HG12	1:F:502:LEU:N	2.26	0.51
1:G:502:LEU:CD2	1:G:502:LEU:C	2.78	0.51
1:A:304:ARG:NH1	1:A:324:GLU:OE2	2.36	0.50
1:A:329:PHE:N	1:A:329:PHE:CD2	2.79	0.50
1:D:124:ASN:ND2	1:D:202:GLY:HA3	2.25	0.50
1:D:235:ARG:NH2	1:D:580:ARG:O	2.34	0.50
1:G:271:PHE:CZ	1:H:252:VAL:HA	2.46	0.50
1:F:439:LEU:H	1:F:439:LEU:HD12	1.76	0.50
1:A:279:ASN:O	1:A:280:LEU:HG	2.12	0.50
1:A:358:ILE:HD13	1:A:492:LEU:HD13	1.92	0.50
1:B:411:THR:HG23	1:B:413:THR:H	1.75	0.50
1:D:312:LYS:HE3	1:D:539:PHE:CE1	2.47	0.50
1:C:171:ASN:OD1	1:C:173:GLU:HG2	2.12	0.50
1:F:87:ARG:HH21	1:F:185:ARG:HB2	1.76	0.50
1:G:435:HIS:O	1:G:437:ILE:N	2.44	0.50
1:F:187:GLY:O	1:F:217:CYS:HB2	2.11	0.50
1:F:254:ARG:HB2	1:F:561:THR:HG21	1.92	0.50
1:G:382:LYS:HB2	1:G:390:ILE:HD13	1.94	0.50
1:H:140:MET:HG2	1:H:155:VAL:CG2	2.42	0.50
1:C:164:LEU:HD22	1:C:207:PHE:CE1	2.47	0.50
1:F:94:GLN:HE22	1:F:183:LYS:NZ	2.09	0.50
1:G:195:PHE:O	1:G:206:ILE:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:508:LEU:HD21	1:G:513:LYS:HB2	1.92	0.50
1:H:152:PHE:HB2	1:H:163:VAL:HB	1.93	0.50
1:H:406:GLU:O	1:H:406:GLU:HG3	2.11	0.50
1:H:502:LEU:C	1:H:502:LEU:HD23	2.32	0.50
1:A:485:LYS:HB3	1:A:488:LEU:HD22	1.93	0.50
1:B:329:PHE:N	1:B:329:PHE:CD2	2.80	0.50
1:B:418:PRO:CG	1:B:486:PRO:HB2	2.42	0.50
1:F:472:PRO:HB3	1:F:474:ILE:HG22	1.94	0.50
1:A:346:GLU:HA	1:A:553:LEU:O	2.11	0.50
1:E:329:PHE:CE1	1:E:341:GLU:HG2	2.47	0.50
1:E:460:LYS:HB3	1:E:461:TYR:CD2	2.46	0.50
1:A:280:LEU:HA	1:A:302:TYR:HD2	1.76	0.49
1:D:431:ILE:O	1:D:435:HIS:HB2	2.11	0.49
1:D:444:THR:HB	1:D:447:LYS:HD2	1.94	0.49
1:H:248:ARG:O	1:H:252:VAL:HG23	2.12	0.49
1:H:476:SER:O	1:H:478:LEU:N	2.45	0.49
1:C:385:PRO:HD2	1:C:386:GLU:OE1	2.12	0.49
1:E:543:LEU:HD11	1:E:547:LEU:HD22	1.94	0.49
1:F:140:MET:HG2	1:F:155:VAL:HG22	1.94	0.49
1:H:358:ILE:HD13	1:H:492:LEU:HD13	1.94	0.49
1:H:444:THR:HB	1:H:447:LYS:HG3	1.93	0.49
1:A:347:PHE:C	1:A:347:PHE:CD1	2.86	0.49
1:C:435:HIS:O	1:C:436:LYS:C	2.50	0.49
1:D:508:LEU:HD21	1:D:513:LYS:O	2.13	0.49
1:H:262:ARG:HD2	1:H:272:GLU:OE2	2.12	0.49
1:A:545:TYR:O	1:B:138:ARG:NH1	2.43	0.49
1:A:559[B]:ARG:HG2	1:A:559[B]:ARG:NH1	2.25	0.49
1:B:458:GLU:O	1:B:498:GLY:HA2	2.11	0.49
1:C:347:PHE:C	1:C:347:PHE:CD1	2.85	0.49
1:D:402:SER:HB3	1:D:405:GLU:HB3	1.95	0.49
1:G:376:TYR:HB3	1:G:395:THR:N	2.27	0.49
1:G:394:PHE:HZ	1:G:496:ILE:HD13	1.76	0.49
1:H:502:LEU:HD23	1:H:503:ASN:N	2.28	0.49
1:A:224:LYS:O	1:A:225:TYR:HB3	2.12	0.49
1:G:460:LYS:HE3	1:G:461:TYR:CE2	2.47	0.49
1:H:109:THR:CB	1:H:134:ASN:H	2.25	0.49
1:H:571:LYS:HD3	1:H:579:MET:HE1	1.95	0.49
1:A:353:ASP:HB3	1:B:105:LYS:HD3	1.95	0.49
1:A:461:TYR:HB2	1:A:466:PHE:CD2	2.47	0.49
1:A:119:TYR:O	1:A:122:LEU:HB2	2.12	0.49
1:A:564:LEU:HD23	1:A:564:LEU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:GLN:HG3	1:C:487:GLY:O	2.12	0.49
1:E:271:PHE:HZ	1:F:252:VAL:HA	1.78	0.49
1:G:304:ARG:HG3	1:G:304:ARG:O	2.13	0.49
1:F:422:ASN:H	1:F:425:ILE:HD12	1.78	0.49
1:F:87:ARG:NH2	1:F:188:ASP:OD2	2.46	0.49
1:G:466:PHE:N	1:G:466:PHE:CD2	2.81	0.49
1:C:261:LEU:HD23	1:C:325:ILE:HD11	1.93	0.49
1:D:439:LEU:CD1	1:D:439:LEU:H	2.26	0.49
1:G:304:ARG:NH1	1:G:307:THR:HG22	2.28	0.49
1:G:162:GLN:O	1:G:205:SER:HB3	2.13	0.48
1:C:294:HIS:HE1	1:D:332:GLU:O	1.95	0.48
1:C:460:LYS:HG2	1:C:461:TYR:CE2	2.47	0.48
1:G:280:LEU:HA	1:G:302:TYR:CD2	2.47	0.48
1:H:125:GLY:N	1:H:199:SER:O	2.46	0.48
1:H:425:ILE:HD11	1:H:445:ALA:HB2	1.96	0.48
1:C:363:ASP:O	1:C:367:GLN:HG3	2.13	0.48
1:C:368:LEU:O	1:C:371:HIS:HB3	2.12	0.48
1:D:403:ILE:O	1:D:407:ILE:HG13	2.13	0.48
1:E:228:LYS:HG3	1:E:229:ASP:OD1	2.14	0.48
1:F:166:ASN:HB3	1:F:169:PHE:CD2	2.48	0.48
1:G:237:ARG:HG3	1:G:237:ARG:O	2.11	0.48
1:G:408:GLU:O	1:G:412:ASN:N	2.45	0.48
1:B:251:PHE:CG	1:B:575:LEU:CD2	2.96	0.48
1:C:81:ARG:O	1:C:85:GLU:HG3	2.13	0.48
1:E:453:ALA:HA	1:E:457:ILE:HG13	1.95	0.48
1:F:150:ARG:NH2	1:F:182:ASP:OD1	2.47	0.48
1:G:251:PHE:CE1	1:G:575:LEU:HD23	2.49	0.48
1:C:574:ILE:O	1:C:577:PRO:HD3	2.13	0.48
1:D:311:LEU:HA	1:D:311:LEU:HD12	1.65	0.48
1:E:230:THR:HG22	1:E:231:GLU:H	1.79	0.48
1:F:261:LEU:HD22	1:F:557:ILE:HD11	1.95	0.48
1:C:496:ILE:HB	1:C:563:PHE:CE2	2.49	0.48
1:D:187:GLY:C	1:D:217:CYS:HB2	2.34	0.48
1:H:112:ILE:HB	1:H:113:PRO:HD3	1.95	0.48
1:H:152:PHE:HB2	1:H:163:VAL:HG21	1.94	0.48
1:A:265:LEU:HB3	1:A:270:PHE:HB2	1.95	0.48
1:A:365:PHE:CE2	1:A:494:MET:CE	2.96	0.48
1:C:251:PHE:CD1	1:C:575:LEU:CD2	2.97	0.48
1:D:227:LEU:HD11	1:D:243:ILE:HD13	1.95	0.48
1:D:435:HIS:O	1:D:437:ILE:N	2.47	0.48
1:E:422:ASN:O	1:E:425:ILE:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:ILE:HD12	1:F:159:GLU:OE1	2.13	0.48
1:F:469:VAL:HG13	1:F:470:GLU:HG3	1.94	0.48
1:H:130:ASP:O	1:H:132:ILE:HG12	2.14	0.48
1:H:112:ILE:HD12	1:H:156:GLY:CA	2.44	0.48
1:D:128:LEU:O	1:D:195:PHE:HB2	2.14	0.48
1:E:385:PRO:HD2	1:E:386:GLU:OE1	2.14	0.48
1:G:152:PHE:HB2	1:G:163:VAL:HB	1.96	0.48
1:G:252:VAL:HA	1:H:271:PHE:HZ	1.78	0.48
1:H:370:TYR:HB2	1:H:376:TYR:CE1	2.48	0.48
1:H:435:HIS:O	1:H:436:LYS:C	2.51	0.48
1:E:128:LEU:HD12	1:E:196:PRO:HG2	1.95	0.48
1:E:198:LYS:HG2	1:E:202:GLY:HA2	1.96	0.48
1:E:209:LYS:HB3	1:E:209:LYS:HE3	1.44	0.48
1:E:501:VAL:HG12	1:E:502:LEU:HB2	1.96	0.48
1:F:111:SER:OG	1:F:113:PRO:HD2	2.14	0.48
1:H:213:LEU:HD11	1:H:216:ALA:HB2	1.94	0.48
1:E:457:ILE:O	1:E:460:LYS:HB2	2.13	0.48
1:F:224:LYS:O	1:F:225:TYR:CB	2.62	0.48
1:H:227:LEU:O	1:H:228:LYS:HB2	2.13	0.48
1:C:316:VAL:C	1:C:318:GLY:N	2.67	0.47
1:D:191:GLY:N	1:D:214:LEU:CD1	2.77	0.47
1:H:271:PHE:HA	2:H:601:HOH:O	2.13	0.47
1:C:111:SER:OG	1:C:114:GLU:HG3	2.15	0.47
1:E:138:ARG:NH1	1:F:545:TYR:O	2.35	0.47
1:G:138:ARG:NH1	1:G:187:GLY:O	2.46	0.47
1:A:351:TYR:CD2	1:B:108:ARG:NH1	2.81	0.47
1:A:453:ALA:O	1:A:458:GLU:HG3	2.14	0.47
1:F:119:TYR:CZ	1:F:196:PRO:HG3	2.50	0.47
1:H:290:PHE:HB2	1:H:303:LEU:HB2	1.94	0.47
1:H:501:VAL:HG22	1:H:560:ILE:CG1	2.43	0.47
1:B:251:PHE:CG	1:B:575:LEU:HD23	2.49	0.47
1:C:105:LYS:HB2	1:D:483:ARG:NH2	2.28	0.47
1:B:183:LYS:O	1:B:185:ARG:HG2	2.15	0.47
1:C:494:MET:HB3	1:C:502:LEU:HB3	1.96	0.47
1:D:191:GLY:H	1:D:214:LEU:CD1	2.27	0.47
1:F:499:LYS:HG3	1:F:559:ARG:NH1	2.30	0.47
1:H:135:ILE:HG22	1:H:192:ILE:HB	1.96	0.47
1:H:213:LEU:HD21	1:H:216:ALA:HB2	1.96	0.47
1:A:272:GLU:HB2	1:A:323:TYR:CZ	2.48	0.47
1:B:108:ARG:NH2	2:B:608:HOH:O	2.48	0.47
1:C:264:PHE:CE1	1:C:268:ARG:NH2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:HD13	1:D:576:PHE:CZ	2.49	0.47
1:E:446:ALA:O	1:E:450:ASP:N	2.44	0.47
1:G:354:TYR:HD1	1:G:490:GLU:O	1.98	0.47
1:A:166:ASN:HB3	1:A:169:PHE:CD2	2.50	0.47
1:C:261:LEU:HD23	1:C:325:ILE:CD1	2.44	0.47
1:D:312:LYS:HE3	1:D:539:PHE:CZ	2.50	0.47
1:H:354:TYR:HD1	1:H:490:GLU:O	1.97	0.47
1:A:502:LEU:HD23	1:A:503:ASN:N	2.30	0.47
1:B:499:LYS:HB3	1:B:559:ARG:HD2	1.97	0.47
1:C:137:GLY:O	1:C:189:ILE:HA	2.14	0.47
1:A:151:PHE:HD1	1:A:162:GLN:NE2	2.13	0.47
1:A:268:ARG:NH1	1:A:268:ARG:CG	2.68	0.47
1:A:279:ASN:N	1:A:302:TYR:O	2.45	0.47
1:A:429:ILE:CG2	1:A:433:LYS:HE3	2.44	0.47
1:C:398:TYR:HB3	1:C:465:PRO:O	2.14	0.47
1:F:128:LEU:HD12	1:F:196:PRO:HG2	1.96	0.47
1:F:92:GLN:NE2	1:F:96:ASP:OD1	2.48	0.47
1:G:146:GLY:O	1:G:147:GLN:HB2	2.14	0.47
1:H:393:ASP:OD1	1:H:395:THR:OG1	2.22	0.47
1:A:484:THR:OG1	1:A:485:LYS:HG3	2.14	0.47
1:C:264:PHE:CE1	1:C:268:ARG:CZ	2.98	0.47
1:C:416:GLU:O	1:C:417:GLN:C	2.53	0.47
1:D:108:ARG:HD2	1:D:136:THR:OG1	2.15	0.47
1:D:151:PHE:O	1:D:152:PHE:CG	2.68	0.47
1:D:138:ARG:HG3	1:D:189:ILE:HG13	1.96	0.47
1:E:292:THR:O	1:E:301:LEU:N	2.48	0.47
1:B:231:GLU:OE1	1:B:235:ARG:NH1	2.48	0.46
1:B:251:PHE:CD2	1:B:575:LEU:HD23	2.50	0.46
1:E:392:ILE:HD11	1:E:497:CYS:SG	2.55	0.46
1:F:447:LYS:HA	1:F:450:ASP:HB2	1.96	0.46
1:G:265:LEU:HD13	1:G:323:TYR:CG	2.50	0.46
1:G:449:LEU:HD13	1:G:449:LEU:HA	1.63	0.46
1:A:197:GLY:HA3	1:A:207:PHE:HE2	1.80	0.46
1:C:228:LYS:HA	1:C:229:ASP:HA	1.65	0.46
1:C:304:ARG:HH12	1:C:324:GLU:CD	2.18	0.46
1:C:331:ASN:HD21	1:D:295:ASN:H	1.61	0.46
1:D:170:HIS:CB	1:D:177:PHE:HD1	2.28	0.46
1:F:228:LYS:HG3	1:F:229:ASP:OD1	2.15	0.46
1:D:90:PHE:CZ	1:D:183:LYS:HB3	2.49	0.46
1:E:294:HIS:HB2	1:E:301:LEU:HD12	1.96	0.46
1:E:577:PRO:HB2	1:E:579:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:SER:O	1:F:91:ILE:HB	2.15	0.46
1:H:167:TYR:CE1	1:H:172:HIS:HE1	2.34	0.46
1:A:329:PHE:O	1:A:330:ARG:HD3	2.15	0.46
1:D:235:ARG:NH1	1:D:579:MET:HG2	2.31	0.46
1:D:394:PHE:CZ	1:D:496:ILE:HD13	2.51	0.46
1:E:228:LYS:HA	1:E:229:ASP:HA	1.47	0.46
1:E:407:ILE:HG13	1:E:457:ILE:HD11	1.96	0.46
1:E:235:ARG:NH2	1:E:580:ARG:O	2.41	0.46
1:E:252:VAL:HA	1:F:271:PHE:CZ	2.50	0.46
1:G:427:LYS:O	1:G:431:ILE:HG13	2.15	0.46
1:C:164:LEU:HD22	1:C:207:PHE:HE1	1.79	0.46
1:C:241:LEU:HD12	1:C:241:LEU:HA	1.68	0.46
1:F:417:GLN:C	1:F:419:PHE:H	2.18	0.46
1:G:108:ARG:HD2	1:G:136:THR:OG1	2.15	0.46
1:H:231:GLU:O	1:H:235:ARG:HG3	2.14	0.46
1:A:228:LYS:HA	1:A:229:ASP:HA	1.48	0.46
1:C:166:ASN:HB3	1:C:169:PHE:CD2	2.51	0.46
1:C:417:GLN:C	1:C:419:PHE:H	2.17	0.46
1:F:398:TYR:O	1:F:400:LYS:HE3	2.15	0.46
1:F:423:GLU:O	1:F:426:GLU:HB2	2.15	0.46
1:F:463:ASP:OD1	1:F:463:ASP:N	2.41	0.46
1:G:122:LEU:O	1:G:198:LYS:NZ	2.38	0.46
1:G:193:VAL:O	1:G:208:PRO:HA	2.16	0.46
1:G:324:GLU:O	1:G:345:CYS:HA	2.14	0.46
1:G:317:GLY:CA	1:H:238:TYR:HB2	2.46	0.46
1:A:428:MET:SD	1:A:449:LEU:HD13	2.56	0.46
1:C:274:GLU:OE2	1:D:327:LYS:HE3	2.16	0.46
1:D:92:GLN:NE2	1:D:92:GLN:O	2.49	0.46
1:G:228:LYS:HA	1:G:229:ASP:HA	1.67	0.46
1:G:327:LYS:HE3	1:H:274:GLU:OE2	2.15	0.46
1:C:214:LEU:HA	1:C:214:LEU:HD12	1.73	0.46
1:F:246:SER:OG	1:F:247:SER:N	2.49	0.46
1:G:580:ARG:HG2	1:G:581:PRO:HD2	1.98	0.46
1:H:167:TYR:HA	1:H:177:PHE:CD1	2.51	0.46
1:A:184:ILE:HD11	1:A:211:THR:HG21	1.98	0.46
1:C:155:VAL:HG12	1:C:160:LYS:HG3	1.98	0.46
1:F:186:ARG:NH1	1:F:221:LEU:HB3	2.30	0.46
1:F:337:THR:C	1:F:338:HIS:ND1	2.70	0.46
1:G:264:PHE:HE2	1:G:360:TRP:NE1	2.14	0.46
1:A:219:HIS:ND1	2:A:603:HOH:O	2.24	0.45
1:A:235:ARG:NH2	1:A:581:PRO:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:OD1	1:B:202:GLY:HA3	2.16	0.45
1:A:239:LEU:HD21	1:B:545:TYR:CD1	2.51	0.45
1:D:437:ILE:O	1:D:438:GLU:CB	2.64	0.45
1:E:247:SER:O	1:E:248:ARG:C	2.52	0.45
1:E:422:ASN:HB3	1:E:423:GLU:H	1.60	0.45
1:H:224:LYS:C	1:H:226:GLY:H	2.20	0.45
1:H:228:LYS:HA	1:H:229:ASP:HA	1.62	0.45
1:H:241:LEU:HD12	1:H:247:SER:OG	2.16	0.45
1:H:461:TYR:HB2	1:H:466:PHE:CD2	2.52	0.45
1:C:127:HIS:O	1:C:128:LEU:HD23	2.16	0.45
1:D:547:LEU:HD12	1:D:548:PRO:HD2	1.97	0.45
1:D:234:TYR:HB2	1:D:579:MET:SD	2.56	0.45
1:E:237:ARG:NH2	1:E:571:LYS:O	2.45	0.45
1:F:480:LYS:NZ	1:F:509:ASN:OD1	2.49	0.45
1:A:307:THR:O	1:A:311:LEU:HB2	2.16	0.45
1:D:191:GLY:H	1:D:214:LEU:HD13	1.81	0.45
1:E:382:LYS:HB2	1:E:390:ILE:HD13	1.98	0.45
1:F:228:LYS:HA	1:F:229:ASP:HA	1.48	0.45
1:G:483:ARG:HB2	1:G:484:THR:H	1.55	0.45
1:H:176:ASN:HB3	1:H:179:GLU:CB	2.46	0.45
1:E:84:PHE:O	1:E:88:SER:OG	2.27	0.45
1:A:415:LEU:HB3	1:A:424:THR:HG22	1.97	0.45
1:A:429:ILE:HG13	1:A:448:LEU:HD11	1.99	0.45
1:D:469:VAL:CG1	1:D:470:GLU:HG3	2.46	0.45
1:E:184:ILE:HD11	1:E:211:THR:HG21	1.99	0.45
1:F:235:ARG:O	1:F:236:GLN:HG3	2.16	0.45
1:G:308:GLU:HG3	1:G:309:LEU:HD13	1.99	0.45
1:G:347:PHE:CD1	1:G:347:PHE:C	2.90	0.45
1:G:264:PHE:HE2	1:G:360:TRP:CE2	2.35	0.45
1:G:575:LEU:HD13	1:H:314:LEU:HD21	1.98	0.45
1:H:408:GLU:HG2	1:H:414:ILE:HA	1.98	0.45
1:A:398:TYR:O	1:A:400:LYS:HD2	2.17	0.45
1:C:504:ALA:HB2	1:C:553:LEU:HG	1.98	0.45
1:D:212:ILE:O	1:D:214:LEU:HD13	2.16	0.45
1:C:105:LYS:HB2	1:D:483:ARG:HH22	1.82	0.45
1:C:314:LEU:HD11	1:D:576:PHE:CE2	2.51	0.45
1:A:94:GLN:HE22	1:A:183:LYS:NZ	2.15	0.45
1:D:190:VAL:C	1:D:214:LEU:HD22	2.37	0.45
1:D:411:THR:OG1	1:D:431:ILE:HD13	2.17	0.45
1:D:553:LEU:HD23	1:D:554:GLY:N	2.32	0.45
1:D:82:LEU:O	1:D:86:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:GLY:CA	1:E:207:PHE:HE2	2.25	0.45
1:F:115:PHE:HE2	1:F:204:LEU:HG	1.82	0.45
1:H:471:HIS:HD2	1:H:475:MET:HE1	1.81	0.45
1:H:485:LYS:CB	1:H:488:LEU:HD22	2.47	0.45
1:A:120:LYS:HG3	1:A:121:ASP:H	1.78	0.45
1:A:570:ILE:HG12	1:A:574:ILE:HD12	1.98	0.45
1:B:108:ARG:HB2	1:B:108:ARG:HE	1.66	0.45
1:B:294:HIS:HB2	1:B:301:LEU:HD12	1.99	0.45
1:F:197:GLY:HA3	1:F:207:PHE:HE2	1.81	0.45
1:H:347:PHE:HD1	1:H:347:PHE:C	2.20	0.45
1:A:423:GLU:HG3	1:A:424:THR:N	2.30	0.45
1:A:411:THR:OG1	1:A:431:ILE:HD13	2.17	0.45
1:B:327:LYS:HD3	1:B:342:PHE:O	2.17	0.45
1:D:214:LEU:CD1	1:D:214:LEU:N	2.79	0.45
1:D:308:GLU:HG3	1:D:309:LEU:CD1	2.29	0.45
1:E:407:ILE:O	1:E:411:THR:HG22	2.17	0.45
1:F:445:ALA:O	1:F:449:LEU:HB2	2.17	0.45
1:H:311:LEU:HD12	1:H:311:LEU:HA	1.66	0.45
1:H:556:GLY:O	1:H:560:ILE:HG13	2.17	0.45
1:A:248:ARG:O	1:A:252:VAL:HG23	2.17	0.45
1:B:227:LEU:O	1:B:228:LYS:CB	2.64	0.45
1:B:457:ILE:O	1:B:460:LYS:N	2.45	0.45
1:E:428:MET:SD	1:E:449:LEU:HD13	2.56	0.45
1:F:472:PRO:CB	1:F:474:ILE:HG22	2.48	0.45
1:H:164:LEU:HD13	1:H:207:PHE:CE1	2.39	0.45
1:H:176:ASN:HB3	1:H:179:GLU:HB3	1.98	0.45
1:A:260:PHE:CE2	1:A:368:LEU:HA	2.52	0.44
1:A:482:HIS:HD2	1:A:489:THR:O	2.00	0.44
1:B:138:ARG:NH1	1:B:187:GLY:O	2.49	0.44
1:B:460:LYS:HE3	1:B:461:TYR:CE2	2.53	0.44
1:E:87:ARG:CZ	1:E:185:ARG:HG3	2.46	0.44
1:G:392:ILE:HD11	1:G:497:CYS:SG	2.57	0.44
1:H:170:HIS:HB2	1:H:177:PHE:HD1	1.82	0.44
1:H:212:ILE:HD12	1:H:213:LEU:H	1.80	0.44
1:A:381:ASN:HB3	1:A:384:GLY:O	2.17	0.44
1:B:228:LYS:HA	1:B:229:ASP:HA	1.51	0.44
1:B:233:ARG:HE	1:B:233:ARG:HB2	1.55	0.44
1:B:248:ARG:O	1:B:252:VAL:HG23	2.17	0.44
1:E:311:LEU:HA	1:E:311:LEU:HD12	1.77	0.44
1:E:87:ARG:O	1:E:90:PHE:HB3	2.17	0.44
1:F:227:LEU:HA	1:F:230:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:402[A]:SER:HB2	1:F:405:GLU:HB3	1.98	0.44
1:H:501:VAL:CG2	1:H:560:ILE:HG12	2.47	0.44
1:F:350:ALA:HA	1:F:550:THR:HG23	1.98	0.44
1:G:199:SER:OG	1:G:203:GLU:HB3	2.18	0.44
1:G:335:ASP:O	1:G:571:LYS:HE3	2.18	0.44
1:H:299:LEU:HD23	1:H:299:LEU:HA	1.77	0.44
1:B:224:LYS:O	1:B:225:TYR:HB3	2.17	0.44
1:F:82:LEU:HG	1:F:86:ASN:HD21	1.82	0.44
1:A:141:ARG:HG2	1:A:142:VAL:N	2.33	0.44
1:A:335:ASP:OD2	1:A:338:HIS:CD2	2.71	0.44
1:C:444:THR:HG22	1:C:446:ALA:N	2.32	0.44
1:D:192:ILE:HG23	1:D:208:PRO:HB3	2.00	0.44
1:F:358:ILE:HG12	1:F:492:LEU:HD13	2.00	0.44
1:H:402:SER:HA	1:H:469:VAL:HG12	1.99	0.44
1:A:365:PHE:CD2	1:A:494:MET:HE1	2.53	0.44
1:B:510:ASP:O	1:B:512:PHE:N	2.50	0.44
1:D:250:THR:O	1:D:253:THR:HB	2.17	0.44
1:E:87:ARG:HA	1:E:87:ARG:HD2	1.76	0.44
1:D:112:ILE:N	1:D:113:PRO:CD	2.81	0.44
1:F:290:PHE:HB2	1:F:303:LEU:HB2	1.99	0.44
1:G:485:LYS:O	1:G:488:LEU:HB2	2.17	0.44
1:G:574:ILE:O	1:G:577:PRO:HD3	2.17	0.44
1:B:323:TYR:HB3	1:B:347:PHE:HB3	2.00	0.44
1:B:432:ILE:O	1:B:437:ILE:HA	2.18	0.44
1:B:501:VAL:HG13	1:B:560:ILE:HD11	2.00	0.44
1:C:152:PHE:HB2	1:C:163:VAL:HB	2.00	0.44
1:C:491:ARG:HB2	1:C:505:TYR:HB3	2.00	0.44
1:G:228:LYS:HG3	1:G:229:ASP:OD1	2.18	0.44
1:H:476:SER:C	1:H:478:LEU:H	2.21	0.44
1:H:88:SER:O	1:H:89:LYS:C	2.56	0.44
1:B:235:ARG:NH1	1:B:579:MET:HG2	2.33	0.44
1:B:310:PRO:HA	1:B:313:MET:HG3	1.99	0.44
1:D:315:ILE:HD13	1:D:319:ILE:O	2.18	0.44
1:E:481:TYR:O	1:F:104:HIS:HE1	2.01	0.44
1:E:509:ASN:OD1	1:E:509:ASN:N	2.43	0.44
1:G:363:ASP:O	1:G:367:GLN:HG3	2.18	0.44
1:G:559:ARG:HD3	1:G:559:ARG:HA	1.84	0.44
1:H:177:PHE:HD2	1:H:178:ALA:N	2.15	0.44
1:H:343:THR:HG22	1:H:557:ILE:HD12	1.99	0.44
1:A:260:PHE:HD2	1:A:368:LEU:HD13	1.82	0.43
1:B:251:PHE:CD1	1:B:575:LEU:HD23	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PHE:O	1:C:206:ILE:HD12	2.18	0.43
1:E:112:ILE:O	1:E:116:ILE:HG13	2.18	0.43
1:E:411:THR:OG1	1:E:431:ILE:HD13	2.17	0.43
1:E:365:PHE:CE2	1:E:494:MET:HE2	2.53	0.43
1:F:268:ARG:NH1	1:F:268:ARG:HG3	2.33	0.43
1:F:358:ILE:HD13	1:F:492:LEU:CD1	2.47	0.43
1:F:574:ILE:O	1:F:577:PRO:HD3	2.18	0.43
1:A:231:GLU:O	1:A:235:ARG:HG3	2.18	0.43
1:B:191:GLY:H	1:B:214:LEU:HD13	1.84	0.43
1:D:386:GLU:CD	1:D:386:GLU:H	2.21	0.43
1:G:297:LEU:HD21	1:H:334:ILE:HD12	2.00	0.43
1:A:308:GLU:HG3	1:A:309:LEU:HD13	1.99	0.43
1:B:116:ILE:O	1:B:120:LYS:HB3	2.18	0.43
1:B:234:TYR:HB3	1:B:577:PRO:HG2	1.99	0.43
1:C:227:LEU:HD23	1:C:232:ILE:HD11	2.01	0.43
1:D:212:ILE:HD12	1:D:213:LEU:N	2.33	0.43
1:E:329:PHE:CD2	1:E:329:PHE:N	2.86	0.43
1:G:309:LEU:HD13	1:G:309:LEU:N	2.33	0.43
1:H:140:MET:O	1:H:186:ARG:HG3	2.18	0.43
1:H:152:PHE:HB2	1:H:163:VAL:CB	2.49	0.43
1:B:383:ASP:HB2	1:B:387:ASN:HD22	1.82	0.43
1:C:87:ARG:HB3	1:C:218:LEU:HD12	2.01	0.43
1:C:471:HIS:N	1:C:471:HIS:ND1	2.65	0.43
1:D:260:PHE:CD2	1:D:368:LEU:HD13	2.53	0.43
1:E:139:ILE:O	1:E:187:GLY:N	2.33	0.43
1:E:359:LYS:NZ	1:E:363:ASP:OD2	2.48	0.43
1:A:234:TYR:HD1	1:A:237:ARG:NH2	2.17	0.43
1:B:162:GLN:O	1:B:205:SER:HA	2.18	0.43
1:B:170:HIS:CD2	1:B:177:PHE:HB2	2.53	0.43
1:D:407:ILE:O	1:D:411:THR:HG22	2.18	0.43
1:D:471:HIS:O	1:D:489:THR:HG23	2.18	0.43
1:G:309:LEU:HB2	1:G:310:PRO:HD3	2.01	0.43
1:H:303:LEU:HA	1:H:303:LEU:HD23	1.80	0.43
1:H:476:SER:HB2	1:H:489:THR:HG21	2.00	0.43
1:A:437:ILE:O	1:A:438:GLU:CB	2.66	0.43
1:E:128:LEU:C	1:E:130:ASP:H	2.21	0.43
1:E:252:VAL:HA	1:F:271:PHE:HZ	1.83	0.43
1:F:415:LEU:HD22	1:F:424:THR:HG22	1.99	0.43
1:H:264:PHE:O	1:H:268:ARG:HD2	2.18	0.43
1:C:148:LYS:HG3	1:C:167:TYR:HB3	2.00	0.43
1:C:228:LYS:HD2	1:C:233:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ILE:HD13	1:D:492:LEU:HD13	2.01	0.43
1:E:353:ASP:OD1	1:E:355:ASN:HB2	2.19	0.43
1:F:167:TYR:HA	1:F:177:PHE:CE1	2.53	0.43
1:F:170:HIS:CB	1:F:177:PHE:HD1	2.32	0.43
1:F:413:THR:HG21	1:F:431:ILE:HD11	2.00	0.43
1:F:419:PHE:HA	1:F:419:PHE:HD1	1.77	0.43
1:G:346:GLU:HA	1:G:553:LEU:O	2.19	0.43
1:H:109:THR:HB	1:H:134:ASN:H	1.83	0.43
1:H:312:LYS:O	1:H:315:ILE:N	2.50	0.43
1:B:541:THR:O	1:B:544:GLU:N	2.38	0.43
1:C:354:TYR:HD1	1:C:490:GLU:O	2.01	0.43
1:C:398:TYR:HB3	1:C:399:PRO:HD2	2.00	0.43
1:D:444:THR:HG22	1:D:446:ALA:N	2.34	0.43
1:D:471:HIS:CG	1:D:491:ARG:HD3	2.54	0.43
1:E:160:LYS:HB2	1:E:160:LYS:HE2	1.81	0.43
1:E:435:HIS:O	1:E:436:LYS:C	2.56	0.43
1:E:571:LYS:NZ	1:E:579:MET:HE2	2.33	0.43
1:A:351:TYR:HD2	1:B:108:ARG:NH1	2.16	0.43
1:B:149:LEU:O	1:B:150:ARG:HD2	2.18	0.43
1:C:251:PHE:CZ	1:C:575:LEU:HD23	2.54	0.43
1:D:218:LEU:HD12	1:D:218:LEU:HA	1.80	0.43
1:E:480:LYS:NZ	1:E:509:ASN:OD1	2.44	0.43
1:F:211:THR:O	1:F:211:THR:HG22	2.18	0.43
1:F:262:ARG:NH1	1:F:272:GLU:OE1	2.52	0.43
1:F:357:LEU:HG	1:F:504:ALA:HB1	1.99	0.43
1:G:440:PRO:O	1:G:441:ASN:HB2	2.19	0.43
1:H:108:ARG:CD	1:H:136:THR:OG1	2.66	0.43
1:H:413:THR:HG21	1:H:431:ILE:HD11	2.00	0.43
1:A:155:VAL:HG12	1:A:160:LYS:HG3	2.01	0.43
1:A:271:PHE:CZ	1:B:252:VAL:HA	2.54	0.43
1:C:496:ILE:HG13	1:C:501:VAL:HG21	2.01	0.43
1:E:403:ILE:HG22	1:E:469:VAL:O	2.18	0.43
1:F:405:GLU:O	1:F:409:LYS:HB3	2.19	0.43
1:H:398:TYR:HB3	1:H:465:PRO:O	2.19	0.43
1:H:499:LYS:HE3	1:H:559:ARG:NH1	2.29	0.43
1:A:125:GLY:N	1:A:199:SER:O	2.52	0.42
1:B:227:LEU:HA	1:B:230:THR:OG1	2.19	0.42
1:C:277:MET:HA	1:C:304:ARG:HG2	2.00	0.42
1:A:427:LYS:O	1:A:431:ILE:HG13	2.19	0.42
1:B:502:LEU:HD11	1:B:553:LEU:HD11	2.01	0.42
1:C:557:ILE:HD13	1:C:557:ILE:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ASN:O	1:E:103:PRO:HD3	2.19	0.42
1:F:347:PHE:CD1	1:F:347:PHE:C	2.92	0.42
1:G:358:ILE:HD13	1:G:492:LEU:CD1	2.39	0.42
1:G:403:ILE:HG21	1:G:471:HIS:HA	2.01	0.42
1:H:217:CYS:SG	1:H:221:LEU:HD13	2.58	0.42
1:B:146:GLY:O	1:B:147:GLN:HB2	2.20	0.42
1:C:314:LEU:CD1	1:D:576:PHE:CZ	3.01	0.42
1:D:92:GLN:NE2	1:D:96:ASP:OD1	2.52	0.42
1:H:180:CYS:HA	1:H:183:LYS:HD2	2.01	0.42
1:H:189:ILE:HD12	1:H:215:SER:HB3	2.01	0.42
1:A:171:ASN:OD1	1:A:173:GLU:HB2	2.20	0.42
1:A:224:LYS:O	1:A:225:TYR:CB	2.67	0.42
1:A:351:TYR:CD2	1:B:108:ARG:HD3	2.55	0.42
1:C:402:SER:HB3	1:C:405:GLU:HB3	2.00	0.42
1:D:231:GLU:O	1:D:235:ARG:HG3	2.20	0.42
1:E:353:ASP:O	1:E:356:ASP:N	2.52	0.42
1:E:411:THR:HG23	1:E:413:THR:HG23	2.01	0.42
1:F:191:GLY:H	1:F:214:LEU:HD13	1.84	0.42
1:F:468:ILE:O	1:F:471:HIS:HE1	2.03	0.42
1:G:128:LEU:HD12	1:G:196:PRO:HG2	2.01	0.42
1:G:353:ASP:O	1:G:356:ASP:N	2.40	0.42
1:G:502:LEU:HD23	1:G:503:ASN:N	2.33	0.42
1:H:167:TYR:HA	1:H:177:PHE:CE1	2.54	0.42
1:B:137:GLY:HA3	1:B:154:LEU:CD1	2.50	0.42
1:B:471:HIS:CG	1:B:491:ARG:HD3	2.55	0.42
1:C:222:PRO:HG2	1:C:243:ILE:CD1	2.49	0.42
1:D:169:PHE:CE2	1:D:195:PHE:CZ	3.00	0.42
1:E:496:ILE:HG13	1:E:501:VAL:HG21	2.01	0.42
1:H:345:CYS:O	1:H:554:GLY:HA2	2.20	0.42
1:A:435:HIS:O	1:A:437:ILE:N	2.53	0.42
1:B:278:MET:HA	1:B:302:TYR:O	2.20	0.42
1:B:339:ASN:ND2	1:B:340:PRO:CD	2.80	0.42
1:B:481:TYR:CE2	1:B:513:LYS:HD3	2.54	0.42
1:C:122:LEU:HD12	1:C:122:LEU:HA	1.80	0.42
1:C:484:THR:O	1:C:486:PRO:HD3	2.20	0.42
1:C:509:ASN:N	1:C:509:ASN:OD1	2.52	0.42
1:D:197:GLY:HA3	1:D:207:PHE:HE2	1.83	0.42
1:D:410:VAL:HG11	1:D:456:PHE:HD1	1.85	0.42
1:F:499:LYS:HD2	1:F:559:ARG:NH2	2.35	0.42
1:H:380:TYR:CE2	1:H:382:LYS:HA	2.54	0.42
1:B:237:ARG:O	1:B:241:LEU:HD22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:ARG:NH1	1:F:187:GLY:O	2.51	0.42
1:A:139:ILE:HD12	1:A:152:PHE:HB3	2.01	0.42
1:B:422:ASN:O	1:B:423:GLU:C	2.57	0.42
1:C:224:LYS:C	1:C:226:GLY:H	2.23	0.42
1:B:408:GLU:OE2	1:B:415:LEU:N	2.53	0.42
1:B:410:VAL:O	1:B:412:ASN:ND2	2.53	0.42
1:C:351:TYR:CD2	1:D:108:ARG:HD3	2.55	0.42
1:D:135:ILE:HG23	1:D:192:ILE:HB	2.02	0.42
1:D:87:ARG:NH2	1:D:188:ASP:OD1	2.52	0.42
1:E:128:LEU:O	1:E:130:ASP:N	2.53	0.42
1:E:137:GLY:HA3	1:E:154:LEU:HG	2.01	0.42
1:F:449:LEU:HD13	1:F:449:LEU:HA	1.79	0.42
1:G:432:ILE:HG23	1:G:438:GLU:CB	2.49	0.42
1:G:460:LYS:HG2	1:G:461:TYR:CD2	2.54	0.42
1:A:469:VAL:CG1	1:A:470:GLU:HG3	2.38	0.42
1:B:464:LYS:HB2	1:B:465:PRO:HD2	2.02	0.42
1:B:472:PRO:CB	1:B:474:ILE:HG22	2.50	0.42
1:F:353:ASP:OD1	1:F:355:ASN:ND2	2.37	0.42
1:F:481:TYR:CE2	1:F:513:LYS:HE3	2.55	0.42
1:A:254:ARG:HB2	1:A:561:THR:HG21	2.00	0.41
1:A:463:ASP:OD1	1:A:463:ASP:N	2.53	0.41
1:A:504:ALA:HB1	1:A:552:GLY:O	2.19	0.41
1:A:89:LYS:HB2	1:A:89:LYS:HE3	1.87	0.41
1:B:442:PRO:O	1:B:447:LYS:HD3	2.20	0.41
1:D:417:GLN:NE2	1:D:424:THR:HG23	2.34	0.41
1:E:164:LEU:HD13	1:E:207:PHE:HE1	1.85	0.41
1:F:579:MET:HE3	1:F:579:MET:HB2	1.94	0.41
1:H:493:GLU:OE2	1:H:500:GLU:HG3	2.20	0.41
1:B:217:CYS:SG	1:B:221:LEU:HD13	2.60	0.41
1:B:398:TYR:HB3	1:B:465:PRO:O	2.20	0.41
1:C:270:PHE:CG	1:C:321:LYS:HB3	2.55	0.41
1:D:248:ARG:O	1:D:252:VAL:HG23	2.20	0.41
1:E:354:TYR:HD1	1:E:490:GLU:O	2.03	0.41
1:E:576:PHE:HB2	1:F:276:PRO:HG3	2.02	0.41
1:A:383:ASP:HB2	1:A:387:ASN:HB2	2.02	0.41
1:B:87:ARG:NE	1:B:185:ARG:HG3	2.35	0.41
1:B:403:ILE:HG22	1:B:469:VAL:O	2.19	0.41
1:B:509:ASN:O	1:B:511:PRO:HD3	2.19	0.41
1:C:176:ASN:HB3	1:C:179:GLU:HB3	2.02	0.41
1:C:307:THR:O	1:C:311:LEU:HB2	2.21	0.41
1:E:384:GLY:HA3	1:E:386:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:415:LEU:HD21	1:G:428:MET:HG2	2.01	0.41
1:G:576:PHE:HB2	1:H:276:PRO:CG	2.50	0.41
1:H:302:TYR:CD2	1:H:302:TYR:N	2.88	0.41
1:A:93:ASP:O	1:A:97:LYS:HB2	2.21	0.41
1:C:105:LYS:HD2	1:C:105:LYS:HA	1.78	0.41
1:C:312:LYS:O	1:C:315:ILE:N	2.51	0.41
1:D:176:ASN:HB3	1:D:179:GLU:HB3	2.01	0.41
1:D:307:THR:OG1	1:D:346:GLU:HG3	2.20	0.41
1:D:415:LEU:CD2	1:D:428:MET:HG2	2.49	0.41
1:E:293:HIS:CE1	1:E:298:ASP:HA	2.55	0.41
1:E:510:ASP:HA	1:E:511:PRO:HD3	1.88	0.41
1:F:571:LYS:HB3	1:F:577:PRO:HG3	2.03	0.41
1:G:187:GLY:O	1:G:217:CYS:HB2	2.20	0.41
1:H:108:ARG:HA	1:H:134:ASN:HB3	2.02	0.41
1:H:166:ASN:HB3	1:H:169:PHE:CD2	2.55	0.41
1:H:483:ARG:H	1:H:483:ARG:HG3	1.57	0.41
1:A:87:ARG:NH2	1:A:188:ASP:OD1	2.54	0.41
1:C:425:ILE:HD11	1:C:445:ALA:HB2	2.01	0.41
1:D:177:PHE:O	1:D:181:TYR:HD2	2.03	0.41
1:D:444:THR:HG22	1:D:446:ALA:H	1.86	0.41
1:E:343:THR:O	1:E:557:ILE:HB	2.20	0.41
1:F:358:ILE:CG1	1:F:492:LEU:HD13	2.50	0.41
1:H:107:GLU:O	1:H:134:ASN:ND2	2.39	0.41
1:A:221:LEU:HA	1:A:221:LEU:HD12	1.93	0.41
1:A:313:MET:HE1	1:B:576:PHE:CE1	2.50	0.41
1:B:251:PHE:CE2	1:B:575:LEU:HD23	2.55	0.41
1:D:191:GLY:N	1:D:214:LEU:HD13	2.35	0.41
1:E:339:ASN:CG	1:E:340:PRO:HD2	2.40	0.41
1:E:416:GLU:O	1:E:418:PRO:N	2.54	0.41
1:A:543:LEU:HD12	1:A:543:LEU:HA	1.83	0.41
1:B:251:PHE:CG	1:B:575:LEU:HD21	2.56	0.41
1:B:311:LEU:HA	1:B:311:LEU:HD12	1.65	0.41
1:B:417:GLN:HE21	1:B:417:GLN:HB3	1.76	0.41
1:B:439:LEU:H	1:B:439:LEU:HD12	1.86	0.41
1:D:502:LEU:C	1:D:502:LEU:HD23	2.41	0.41
1:D:373:PHE:HE2	1:D:564:LEU:HD22	1.85	0.41
1:F:580:ARG:HE	1:F:580:ARG:HB2	1.56	0.41
1:G:138:ARG:HA	1:G:188:ASP:O	2.21	0.41
1:G:368:LEU:O	1:G:371:HIS:HB3	2.20	0.41
1:G:411:THR:HG21	1:G:431:ILE:HD13	2.02	0.41
1:H:140:MET:HG2	1:H:155:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:LEU:HB3	1:H:207:PHE:HD1	1.85	0.41
1:A:312:LYS:O	1:A:315:ILE:HB	2.21	0.41
1:E:241:LEU:HD12	1:E:241:LEU:HA	1.82	0.41
1:E:416:GLU:O	1:E:417:GLN:C	2.58	0.41
1:A:436:LYS:O	1:A:437:ILE:CB	2.69	0.41
1:B:409:LYS:O	1:B:409:LYS:HG2	2.19	0.41
1:B:571:LYS:HB3	1:B:577:PRO:HG3	2.03	0.41
1:E:417:GLN:O	1:E:419:PHE:N	2.54	0.41
1:E:482:HIS:HB3	1:E:485:LYS:O	2.21	0.41
1:F:315:ILE:HD12	1:F:550:THR:CG2	2.51	0.41
1:F:567:LYS:HD2	1:F:572:ASP:HB3	2.02	0.41
1:G:388:GLN:HG2	1:G:389:PRO:HD2	2.03	0.41
1:G:460:LYS:CE	1:G:461:TYR:HE2	2.33	0.41
1:H:204:LEU:HD12	1:H:205:SER:N	2.35	0.41
1:H:469:VAL:HG13	1:H:470:GLU:CG	2.50	0.41
1:A:227:LEU:HA	1:A:230:THR:OG1	2.21	0.41
1:D:234:TYR:CB	1:D:579:MET:SD	3.09	0.41
1:D:312:LYS:NZ	1:D:507:GLU:OE1	2.47	0.41
1:F:480:LYS:HA	1:F:508:LEU:HD13	2.03	0.41
1:F:92:GLN:NE2	1:F:92:GLN:O	2.54	0.41
1:H:170:HIS:CB	1:H:177:PHE:HD1	2.34	0.41
1:H:176:ASN:O	1:H:177:PHE:C	2.59	0.41
1:H:265:LEU:HB3	1:H:270:PHE:HB2	2.01	0.41
1:H:265:LEU:HD13	1:H:323:TYR:CG	2.56	0.41
1:H:463:ASP:OD2	1:H:464:LYS:HE2	2.21	0.41
1:H:509:ASN:O	1:H:511:PRO:HD3	2.20	0.41
1:A:108:ARG:HG2	1:A:136:THR:HG23	2.02	0.41
1:A:151:PHE:HD1	1:A:162:GLN:HE22	1.69	0.41
1:A:363:ASP:O	1:A:364:PHE:C	2.59	0.41
1:B:381:ASN:ND2	1:B:389:PRO:HB3	2.36	0.41
1:B:393:ASP:OD1	1:B:395:THR:OG1	2.31	0.41
1:C:422:ASN:HB3	1:C:423:GLU:H	1.69	0.41
1:C:428:MET:O	1:C:432:ILE:HG12	2.21	0.41
1:D:394:PHE:HZ	1:D:496:ILE:HD13	1.85	0.41
1:D:350:ALA:HA	1:D:550:THR:HG23	2.03	0.41
1:E:140:MET:HG2	1:E:155:VAL:HG22	2.03	0.41
1:E:411:THR:O	1:E:413:THR:HG23	2.21	0.41
1:E:570:ILE:HA	1:E:573:VAL:HG22	2.02	0.41
1:F:320:ASP:HB3	1:F:350:ALA:HB3	2.03	0.41
1:F:492:LEU:HD23	1:F:492:LEU:N	2.36	0.41
1:G:213:LEU:HD21	1:G:216:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:332:GLU:OE1	1:H:338:HIS:HD2	2.03	0.41
1:H:442:PRO:O	1:H:444:THR:N	2.45	0.41
1:A:294:HIS:HB2	1:A:301:LEU:HD12	2.03	0.40
1:B:347:PHE:C	1:B:347:PHE:CD1	2.95	0.40
1:C:484:THR:OG1	1:C:485:LYS:N	2.55	0.40
1:E:392:ILE:HA	1:E:463:ASP:O	2.21	0.40
1:G:112:ILE:N	1:G:113:PRO:CD	2.84	0.40
1:G:228:LYS:HA	1:G:229:ASP:OD1	2.21	0.40
1:G:270:PHE:CD1	1:G:321:LYS:HB3	2.56	0.40
1:G:273:VAL:HG13	1:G:322:VAL:HG23	2.04	0.40
1:G:415:LEU:O	1:G:415:LEU:HD12	2.21	0.40
1:G:485:LYS:HA	1:G:486:PRO:HD2	1.98	0.40
1:H:250:THR:O	1:H:253:THR:HB	2.21	0.40
1:A:265:LEU:HD13	1:A:323:TYR:CD1	2.55	0.40
1:B:151:PHE:HD1	1:B:162:GLN:NE2	2.18	0.40
1:C:109:THR:HB	1:C:134:ASN:H	1.86	0.40
1:D:172:HIS:H	1:D:172:HIS:CD2	2.39	0.40
1:E:347:PHE:C	1:E:347:PHE:CD1	2.95	0.40
1:H:198:LYS:HA	1:H:203:GLU:O	2.21	0.40
1:A:386:GLU:N	1:A:386:GLU:OE1	2.40	0.40
1:A:393:ASP:OD1	1:A:395:THR:OG1	2.40	0.40
1:B:428:MET:SD	1:B:449:LEU:HD22	2.61	0.40
1:E:162:GLN:O	1:E:205:SER:HA	2.21	0.40
1:F:428:MET:SD	1:F:449:LEU:HD22	2.62	0.40
1:G:510:ASP:O	1:G:512:PHE:N	2.55	0.40
1:G:317:GLY:HA2	1:H:238:TYR:HB2	2.04	0.40
1:A:192:ILE:HG23	1:A:208:PRO:HB3	2.03	0.40
1:C:341:GLU:HG2	1:D:278:MET:HE2	2.03	0.40
1:C:357:LEU:HA	1:C:357:LEU:HD12	1.81	0.40
1:C:482:HIS:HB2	1:C:488:LEU:O	2.20	0.40
1:D:176:ASN:HB3	1:D:179:GLU:CB	2.51	0.40
1:D:574:ILE:O	1:D:577:PRO:HD3	2.21	0.40
1:E:386:GLU:H	1:E:386:GLU:CD	2.24	0.40
1:E:431:ILE:O	1:E:435:HIS:HB3	2.21	0.40
1:F:311:LEU:HD12	1:F:311:LEU:HA	1.83	0.40
1:F:416:GLU:O	1:F:417:GLN:C	2.59	0.40
1:F:557:ILE:HD13	1:F:557:ILE:HA	1.96	0.40
1:H:428:MET:HE1	1:H:448:LEU:HB2	2.02	0.40
1:B:94:GLN:OE1	1:B:99:ILE:HD12	2.22	0.40
1:C:293:HIS:HD2	1:C:295:ASN:OD1	2.04	0.40
1:D:137:GLY:O	1:D:189:ILE:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ASN:HB3	1:E:179:GLU:HB3	2.03	0.40
1:E:359:LYS:HD2	1:E:363:ASP:OD1	2.22	0.40
1:E:485:LYS:HA	1:E:486:PRO:HD2	1.95	0.40
1:H:398:TYR:O	1:H:400:LYS:HD2	2.22	0.40
1:H:580:ARG:HA	1:H:581:PRO:HD3	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:TYR:OH	1:G:434:GLU:OE2[1_465]	1.96	0.24

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	466/507 (92%)	425 (91%)	35 (8%)	6 (1%)	12	37
1	B	466/507 (92%)	414 (89%)	44 (9%)	8 (2%)	9	31
1	C	465/507 (92%)	408 (88%)	51 (11%)	6 (1%)	12	37
1	D	465/507 (92%)	410 (88%)	49 (10%)	6 (1%)	12	37
1	E	464/507 (92%)	417 (90%)	40 (9%)	7 (2%)	10	34
1	F	465/507 (92%)	420 (90%)	33 (7%)	12 (3%)	5	20
1	G	464/507 (92%)	419 (90%)	33 (7%)	12 (3%)	5	20
1	H	465/507 (92%)	419 (90%)	38 (8%)	8 (2%)	9	31
All	All	3720/4056 (92%)	3332 (90%)	323 (9%)	65 (2%)	9	31

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	ILE
1	B	416	GLU
1	B	418	PRO
1	B	423	GLU
1	B	458	GLU
1	C	418	PRO
1	D	436	LYS
1	E	414	ILE
1	E	438	GLU
1	F	437	ILE
1	F	438	GLU
1	G	354	TYR
1	G	422	ASN
1	G	483	ARG
1	H	418	PRO
1	A	438	GLU
1	B	437	ILE
1	C	317	GLY
1	D	422	ASN
1	D	437	ILE
1	D	438	GLU
1	E	354	TYR
1	G	172	HIS
1	G	414	ILE
1	G	417	GLN
1	G	436	LYS
1	G	437	ILE
1	H	437	ILE
1	A	436	LYS
1	B	541	THR
1	C	437	ILE
1	C	442	PRO
1	D	418	PRO
1	D	472	PRO
1	E	295	ASN
1	F	177	PHE
1	F	418	PRO
1	F	422	ASN
1	G	225	TYR
1	G	409	LYS
1	A	296	ASP
1	A	417	GLN
1	C	332	GLU

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Mol	Chain	Res	Type
1	F	228	LYS
1	F	436	LYS
1	H	88	SER
1	H	177	PHE
1	H	436	LYS
1	E	177	PHE
1	E	417	GLN
1	F	309	LEU
1	F	408	GLU
1	F	442	PRO
1	G	442	PRO
1	C	354	TYR
1	E	437	ILE
1	F	472	PRO
1	H	89	LYS
1	F	441	ASN
1	H	443	PRO
1	G	358	ILE
1	B	441	ASN
1	B	511	PRO
1	A	317	GLY
1	H	399	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	427/457 (93%)	382 (90%)	45 (10%)	7 21
1	B	427/457 (93%)	365 (86%)	62 (14%)	3 9
1	C	425/457 (93%)	366 (86%)	59 (14%)	3 10
1	D	426/457 (93%)	363 (85%)	63 (15%)	3 9
1	E	424/457 (93%)	370 (87%)	54 (13%)	4 13
1	F	426/457 (93%)	364 (85%)	62 (15%)	3 9
1	G	425/457 (93%)	372 (88%)	53 (12%)	4 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	424/457 (93%)	370 (87%)	54 (13%)	4 13
All	All	3404/3656 (93%)	2952 (87%)	452 (13%)	4 11

All (452) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	142	VAL
1	A	164	LEU
1	A	179	GLU
1	A	212	ILE
1	A	214	LEU
1	A	218	LEU
1	A	220	MET
1	A	227	LEU
1	A	228	LYS
1	A	232	ILE
1	A	241	LEU
1	A	256	LYS
1	A	274	GLU
1	A	299	LEU
1	A	308	GLU
1	A	309	LEU
1	A	311	LEU
1	A	314	LEU
1	A	319	ILE
1	A	341	GLU
1	A	357	LEU
1	A	372	LEU
1	A	379	SER
1	A	404	VAL
1	A	413	THR
1	A	415	LEU
1	A	421	SER
1	A	422	ASN
1	A	423	GLU
1	A	424	THR
1	A	425	ILE
1	A	449	LEU
1	A	454	SER
1	A	457	ILE
1	A	460	LYS

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Mol	Chain	Res	Type
1	A	464	LYS
1	A	476	SER
1	A	478	LEU
1	A	492	LEU
1	A	500	GLU
1	A	540	CYS
1	A	550	THR
1	A	557	ILE
1	A	579	MET
1	B	81	ARG
1	B	89	LYS
1	B	91	ILE
1	B	96	ASP
1	B	99	ILE
1	B	108	ARG
1	B	127	HIS
1	B	138	ARG
1	B	141	ARG
1	B	142	VAL
1	B	143	SER
1	B	149	LEU
1	B	162	GLN
1	B	168	SER
1	B	173	GLU
1	B	176	ASN
1	B	209	LYS
1	B	212	ILE
1	B	214	LEU
1	B	217	CYS
1	B	220	MET
1	B	223	MET
1	B	227	LEU
1	B	230	THR
1	B	235	ARG
1	B	238	TYR
1	B	241	LEU
1	B	247	SER
1	B	248	ARG
1	B	277	MET
1	B	292	THR
1	B	304	ARG
1	B	305	ILE

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Mol	Chain	Res	Type
1	B	309	LEU
1	B	311	LEU
1	B	314	LEU
1	B	337	THR
1	B	339	ASN
1	B	345	CYS
1	B	357	LEU
1	B	363	ASP
1	B	372	LEU
1	B	391	GLU
1	B	404	VAL
1	B	415	LEU
1	B	417	GLN
1	B	422	ASN
1	B	423	GLU
1	B	424	THR
1	B	435	HIS
1	B	444	THR
1	B	449	LEU
1	B	469	VAL
1	B	476	SER
1	B	484	THR
1	B	492	LEU
1	B	500	GLU
1	B	540	CYS
1	B	542	SER
1	B	559	ARG
1	B	579	MET
1	B	580	ARG
1	C	81	ARG
1	C	87	ARG
1	C	89	LYS
1	C	107	GLU
1	C	122	LEU
1	C	127	HIS
1	C	142	VAL
1	C	143	SER
1	C	148	LYS
1	C	149	LEU
1	C	162	GLN
1	C	168	SER
1	C	212	ILE

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Mol	Chain	Res	Type
1	C	214	LEU
1	C	218	LEU
1	C	220	MET
1	C	223	MET
1	C	227	LEU
1	C	229	ASP
1	C	230	THR
1	C	241	LEU
1	C	274	GLU
1	C	298	ASP
1	C	305	ILE
1	C	309	LEU
1	C	312	LYS
1	C	314	LEU
1	C	341	GLU
1	C	357	LEU
1	C	358	ILE
1	C	366	SER
1	C	372	LEU
1	C	383	ASP
1	C	390	ILE
1	C	391	GLU
1	C	403	ILE
1	C	415	LEU
1	C	417	GLN
1	C	419	PHE
1	C	420	ASP
1	C	423	GLU
1	C	424	THR
1	C	426	GLU
1	C	429	ILE
1	C	433	LYS
1	C	449	LEU
1	C	454	SER
1	C	457	ILE
1	C	463	ASP
1	C	464	LYS
1	C	471	HIS
1	C	476	SER
1	C	478	LEU
1	C	490	GLU
1	C	492	LEU

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Mol	Chain	Res	Type
1	C	496	ILE
1	C	500	GLU
1	C	543	LEU
1	C	579	MET
1	D	81	ARG
1	D	99	ILE
1	D	108	ARG
1	D	109	THR
1	D	127	HIS
1	D	138	ARG
1	D	143	SER
1	D	150	ARG
1	D	168	SER
1	D	176	ASN
1	D	200	LYS
1	D	209	LYS
1	D	212	ILE
1	D	213	LEU
1	D	214	LEU
1	D	218	LEU
1	D	220	MET
1	D	223	MET
1	D	224	LYS
1	D	227	LEU
1	D	228	LYS
1	D	230	THR
1	D	231	GLU
1	D	241	LEU
1	D	247	SER
1	D	281	ILE
1	D	290	PHE
1	D	296	ASP
1	D	304	ARG
1	D	305	ILE
1	D	309	LEU
1	D	311	LEU
1	D	314	LEU
1	D	319	ILE
1	D	330	ARG
1	D	345	CYS
1	D	357	LEU
1	D	366	SER

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Mol	Chain	Res	Type
1	D	372	LEU
1	D	377	LYS
1	D	388	GLN
1	D	392	ILE
1	D	402	SER
1	D	411	THR
1	D	415	LEU
1	D	423	GLU
1	D	424	THR
1	D	425	ILE
1	D	426	GLU
1	D	427	LYS
1	D	432	ILE
1	D	435	HIS
1	D	449	LEU
1	D	460	LYS
1	D	464	LYS
1	D	476	SER
1	D	478	LEU
1	D	490	GLU
1	D	492	LEU
1	D	500	GLU
1	D	550	THR
1	D	558	ASP
1	D	579	MET
1	E	81	ARG
1	E	82	LEU
1	E	87	ARG
1	E	88	SER
1	E	92	GLN
1	E	99	ILE
1	E	118	LYS
1	E	122	LEU
1	E	127	HIS
1	E	142	VAL
1	E	150	ARG
1	E	160	LYS
1	E	168	SER
1	E	185	ARG
1	E	198	LYS
1	E	201	LYS
1	E	206	ILE

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Mol	Chain	Res	Type
1	E	209	LYS
1	E	212	ILE
1	E	218	LEU
1	E	220	MET
1	E	227	LEU
1	E	228	LYS
1	E	230	THR
1	E	232	ILE
1	E	241	LEU
1	E	247	SER
1	E	311	LEU
1	E	314	LEU
1	E	335	ASP
1	E	351	TYR
1	E	357	LEU
1	E	372	LEU
1	E	386	GLU
1	E	390	ILE
1	E	400	LYS
1	E	403	ILE
1	E	408	GLU
1	E	409	LYS
1	E	415	LEU
1	E	422	ASN
1	E	423	GLU
1	E	424	THR
1	E	425	ILE
1	E	454	SER
1	E	457	ILE
1	E	460	LYS
1	E	463	ASP
1	E	478	LEU
1	E	492	LEU
1	E	499	LYS
1	E	540	CYS
1	E	579	MET
1	E	580	ARG
1	F	81	ARG
1	F	87	ARG
1	F	88	SER
1	F	92	GLN
1	F	99	ILE

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Mol	Chain	Res	Type
1	F	107	GLU
1	F	108	ARG
1	F	120	LYS
1	F	122	LEU
1	F	127	HIS
1	F	129	GLU
1	F	138	ARG
1	F	142	VAL
1	F	143	SER
1	F	149	LEU
1	F	164	LEU
1	F	168	SER
1	F	193	VAL
1	F	206	ILE
1	F	212	ILE
1	F	214	LEU
1	F	218	LEU
1	F	220	MET
1	F	227	LEU
1	F	228	LYS
1	F	230	THR
1	F	247	SER
1	F	281	ILE
1	F	297	LEU
1	F	311	LEU
1	F	314	LEU
1	F	328	VAL
1	F	338	HIS
1	F	346	GLU
1	F	357	LEU
1	F	361	SER
1	F	372	LEU
1	F	379	SER
1	F	386	GLU
1	F	400	LYS
1	F	409	LYS
1	F	415	LEU
1	F	417	GLN
1	F	419	PHE
1	F	422	ASN
1	F	423	GLU
1	F	424	THR

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Mol	Chain	Res	Type
1	F	444	THR
1	F	449	LEU
1	F	464	LYS
1	F	471	HIS
1	F	476	SER
1	F	484	THR
1	F	490	GLU
1	F	500	GLU
1	F	501	VAL
1	F	513	LYS
1	F	540	CYS
1	F	550	THR
1	F	567	LYS
1	F	571	LYS
1	F	579	MET
1	G	81	ARG
1	G	88	SER
1	G	99	ILE
1	G	108	ARG
1	G	122	LEU
1	G	142	VAL
1	G	149	LEU
1	G	162	GLN
1	G	164	LEU
1	G	168	SER
1	G	173	GLU
1	G	198	LYS
1	G	205	SER
1	G	212	ILE
1	G	220	MET
1	G	227	LEU
1	G	228	LYS
1	G	230	THR
1	G	241	LEU
1	G	305	ILE
1	G	309	LEU
1	G	314	LEU
1	G	335	ASP
1	G	337	THR
1	G	338	HIS
1	G	341	GLU
1	G	357	LEU

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Mol	Chain	Res	Type
1	G	363	ASP
1	G	372	LEU
1	G	383	ASP
1	G	403	ILE
1	G	415	LEU
1	G	423	GLU
1	G	424	THR
1	G	426	GLU
1	G	433	LYS
1	G	449	LEU
1	G	454	SER
1	G	457	ILE
1	G	464	LYS
1	G	469	VAL
1	G	474	ILE
1	G	490	GLU
1	G	492	LEU
1	G	500	GLU
1	G	502	LEU
1	G	505	TYR
1	G	513	LYS
1	G	543	LEU
1	G	559	ARG
1	G	562	MET
1	G	579	MET
1	G	580	ARG
1	H	81	ARG
1	H	82	LEU
1	H	87	ARG
1	H	127	HIS
1	H	129	GLU
1	H	138	ARG
1	H	140	MET
1	H	142	VAL
1	H	168	SER
1	H	204	LEU
1	H	205	SER
1	H	209	LYS
1	H	210	GLU
1	H	211	THR
1	H	212	ILE
1	H	218	LEU

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Mol	Chain	Res	Type
1	H	220	MET
1	H	224	LYS
1	H	227	LEU
1	H	228	LYS
1	H	230	THR
1	H	243	ILE
1	H	247	SER
1	H	256	LYS
1	H	280	LEU
1	H	281	ILE
1	H	311	LEU
1	H	314	LEU
1	H	330	ARG
1	H	337	THR
1	H	347	PHE
1	H	357	LEU
1	H	372	LEU
1	H	383	ASP
1	H	386	GLU
1	H	395	THR
1	H	415	LEU
1	H	417	GLN
1	H	422	ASN
1	H	423	GLU
1	H	424	THR
1	H	435	HIS
1	H	449	LEU
1	H	454	SER
1	H	464	LYS
1	H	469	VAL
1	H	478	LEU
1	H	490	GLU
1	H	492	LEU
1	H	500	GLU
1	H	501	VAL
1	H	506	THR
1	H	540	CYS
1	H	579	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	412	ASN
1	B	92	GLN
1	B	162	GLN
1	B	166	ASN
1	B	172	HIS
1	B	336	ASN
1	B	339	ASN
1	B	387	ASN
1	B	412	ASN
1	B	417	GLN
1	B	441	ASN
1	C	86	ASN
1	C	293	HIS
1	D	219	HIS
1	D	279	ASN
1	D	417	GLN
1	E	94	GLN
1	E	172	HIS
1	E	295	ASN
1	E	339	ASN
1	E	388	GLN
1	E	417	GLN
1	F	86	ASN
1	F	92	GLN
1	F	94	GLN
1	F	104	HIS
1	F	170	HIS
1	F	417	GLN
1	F	441	ASN
1	F	471	HIS
1	G	86	ASN
1	G	94	GLN
1	G	170	HIS
1	G	387	ASN
1	H	94	GLN
1	H	162	GLN
1	H	170	HIS
1	H	172	HIS
1	H	422	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	469/507 (92%)	-0.09	6 (1%)	77	77	22, 46, 91, 122	0
1	B	471/507 (92%)	-0.05	9 (1%)	66	65	22, 47, 88, 118	0
1	C	471/507 (92%)	-0.01	9 (1%)	66	65	22, 48, 93, 129	0
1	D	471/507 (92%)	0.12	18 (3%)	40	36	22, 49, 91, 121	0
1	E	470/507 (92%)	-0.04	13 (2%)	53	49	26, 49, 92, 126	0
1	F	470/507 (92%)	0.09	22 (4%)	31	28	27, 51, 92, 118	0
1	G	470/507 (92%)	-0.07	5 (1%)	80	80	27, 49, 90, 123	0
1	H	471/507 (92%)	0.08	24 (5%)	28	24	26, 50, 91, 125	0
All	All	3763/4056 (92%)	0.00	106 (2%)	53	49	22, 49, 92, 129	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	145	SER	5.6
1	H	164	LEU	5.1
1	C	448	LEU	4.6
1	D	125	GLY	4.4
1	B	432	ILE	4.4
1	D	164	LEU	4.4
1	E	439	LEU	4.2
1	E	443	PRO	3.8
1	E	425	ILE	3.8
1	D	201	LYS	3.8
1	D	204	LEU	3.5
1	G	432	ILE	3.5
1	F	456	PHE	3.5
1	F	201	LYS	3.5
1	H	474	ILE	3.4
1	C	434	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	124	ASN	3.3
1	F	440	PRO	3.3
1	D	418	PRO	3.3
1	F	429	ILE	3.3
1	E	444	THR	3.2
1	F	425	ILE	3.2
1	D	434	GLU	3.2
1	H	144	ALA	3.2
1	D	415	LEU	3.2
1	H	418	PRO	3.2
1	D	123	GLY	3.1
1	F	147	GLN	3.1
1	E	452	LEU	3.1
1	F	439	LEU	3.1
1	H	201	LYS	3.1
1	F	144	ALA	3.1
1	E	432	ILE	3.0
1	D	122	LEU	3.0
1	E	202	GLY	3.0
1	E	433	LYS	3.0
1	C	415	LEU	2.9
1	G	439	LEU	2.9
1	A	430	ASN	2.9
1	E	440	PRO	2.8
1	F	452	LEU	2.8
1	F	432	ILE	2.7
1	A	434	GLU	2.7
1	H	429	ILE	2.7
1	F	121	ASP	2.7
1	D	419	PHE	2.7
1	F	204	LEU	2.7
1	A	443	PRO	2.6
1	C	444	THR	2.6
1	D	431	ILE	2.6
1	B	163	VAL	2.6
1	C	416	GLU	2.5
1	H	456	PHE	2.5
1	H	122	LEU	2.5
1	D	145	SER	2.5
1	D	429	ILE	2.5
1	A	445	ALA	2.5
1	F	173	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	123	GLY	2.4
1	D	196	PRO	2.4
1	B	89	LYS	2.4
1	H	434	GLU	2.4
1	E	422	ASN	2.4
1	B	449	LEU	2.4
1	H	203	GLU	2.4
1	C	447	LYS	2.4
1	H	202	GLY	2.4
1	H	581	PRO	2.3
1	E	145	SER	2.3
1	H	149	LEU	2.3
1	E	84	PHE	2.3
1	F	146	GLY	2.3
1	F	175	GLY	2.3
1	H	199	SER	2.3
1	E	442	PRO	2.3
1	H	440	PRO	2.3
1	G	440	PRO	2.3
1	F	176	ASN	2.3
1	H	198	LYS	2.2
1	G	418	PRO	2.2
1	H	431	ILE	2.2
1	C	445	ALA	2.2
1	G	443	PRO	2.2
1	H	443	PRO	2.2
1	D	144	ALA	2.1
1	D	198	LYS	2.1
1	F	81	ARG	2.1
1	H	476	SER	2.1
1	F	197	GLY	2.1
1	H	146	GLY	2.1
1	F	149	LEU	2.1
1	B	448	LEU	2.1
1	C	446	ALA	2.1
1	A	429	ILE	2.1
1	B	443	PRO	2.1
1	A	439	LEU	2.1
1	B	81	ARG	2.1
1	F	200	LYS	2.1
1	F	441	ASN	2.1
1	H	419	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	165	ALA	2.0
1	H	165	ALA	2.0
1	C	435	HIS	2.0
1	B	429	ILE	2.0
1	H	446	ALA	2.0
1	B	86	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.