



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:34 PM UTC

PDB ID : 4H02 / pdb_00004h02
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

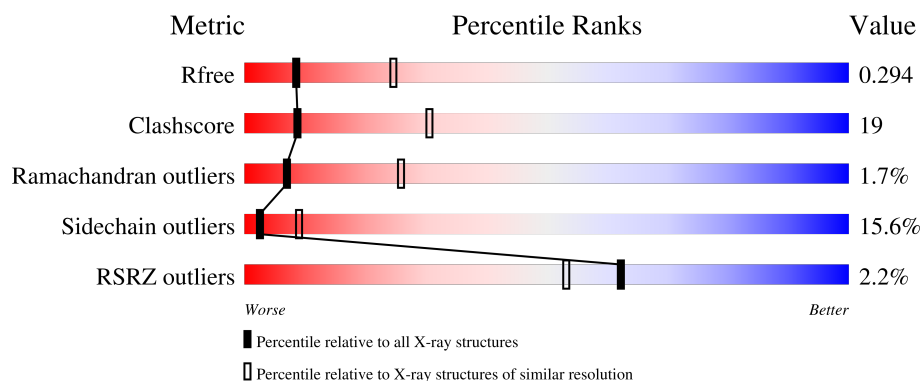
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	507	
1	C	507	
1	D	507	
1	E	507	

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Mol	Chain	Length	Quality of chain				
1	F	507	2%	48%	35%	9%	7%
1	G	507	%	52%	34%	7%	7%
1	H	507	2%	48%	36%	8%	7%

2 Entry composition [i](#)

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			

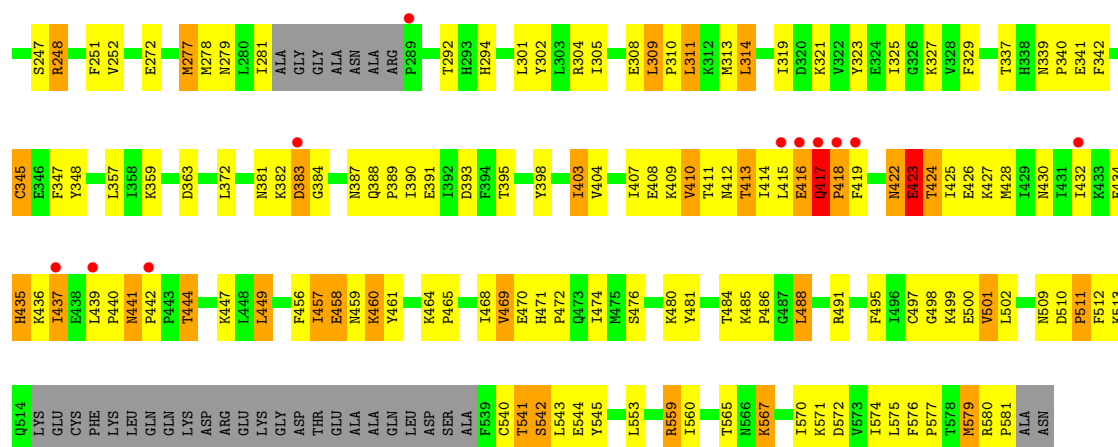
- Molecule 2 is water.

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		

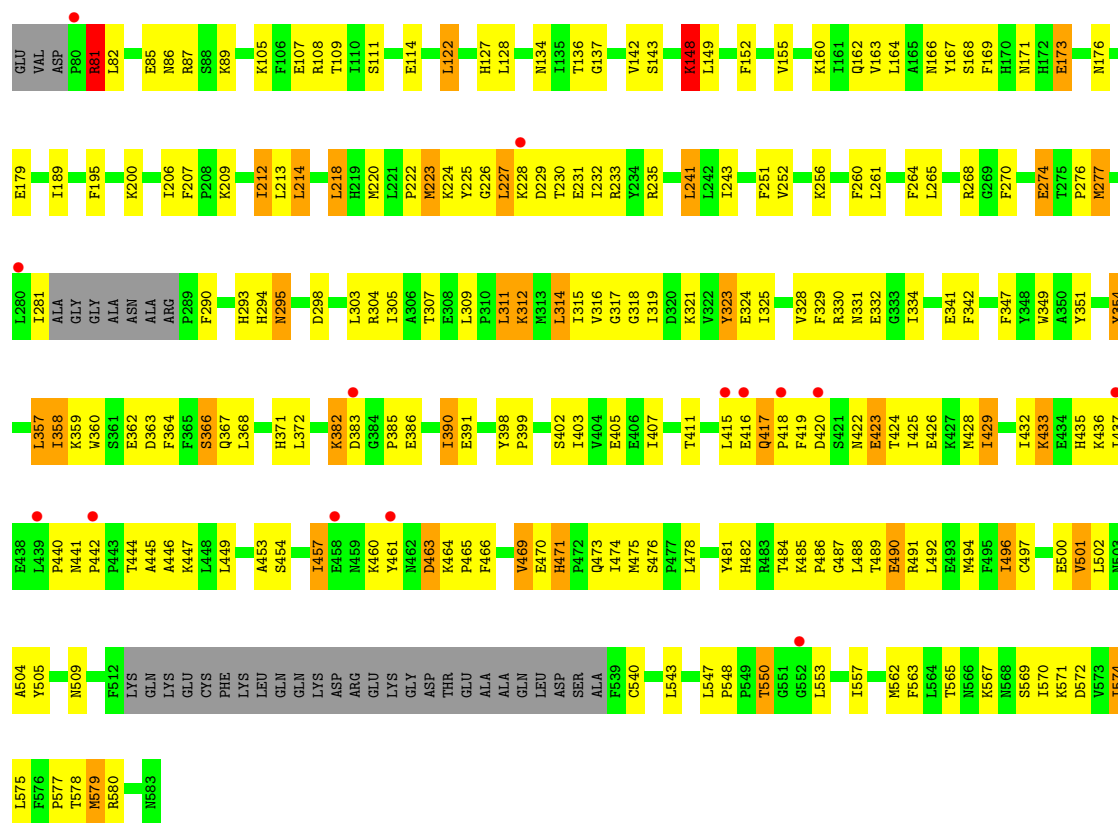
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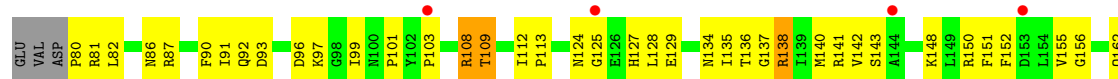
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	9	Total	O	0	0
			9	9		
2	H	18	Total	O	0	0
			18	18		

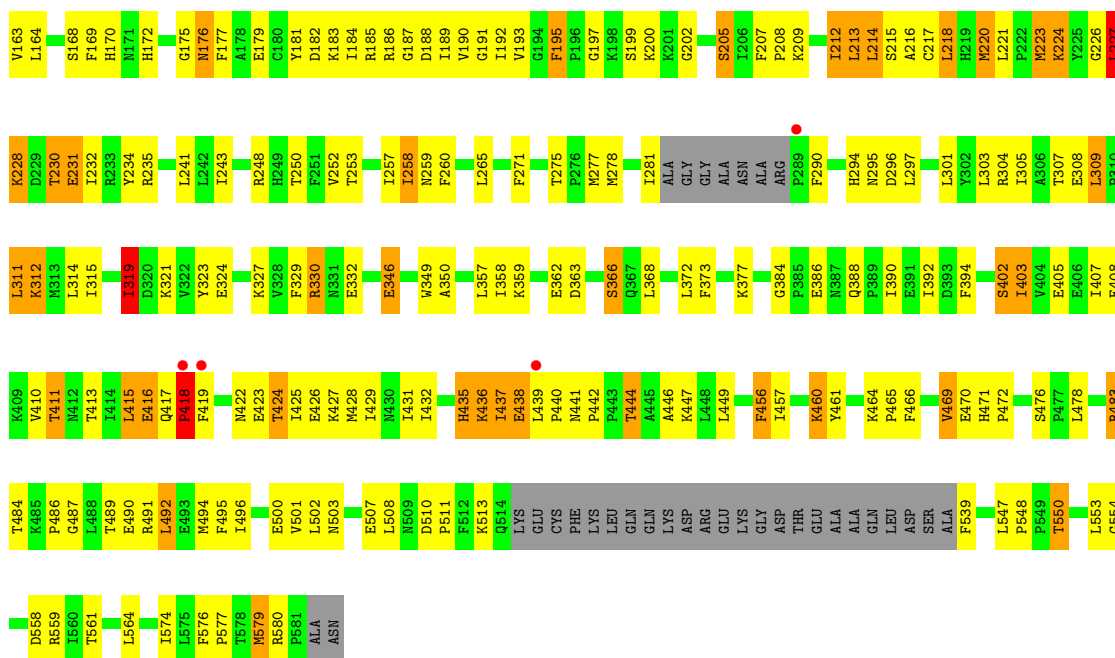


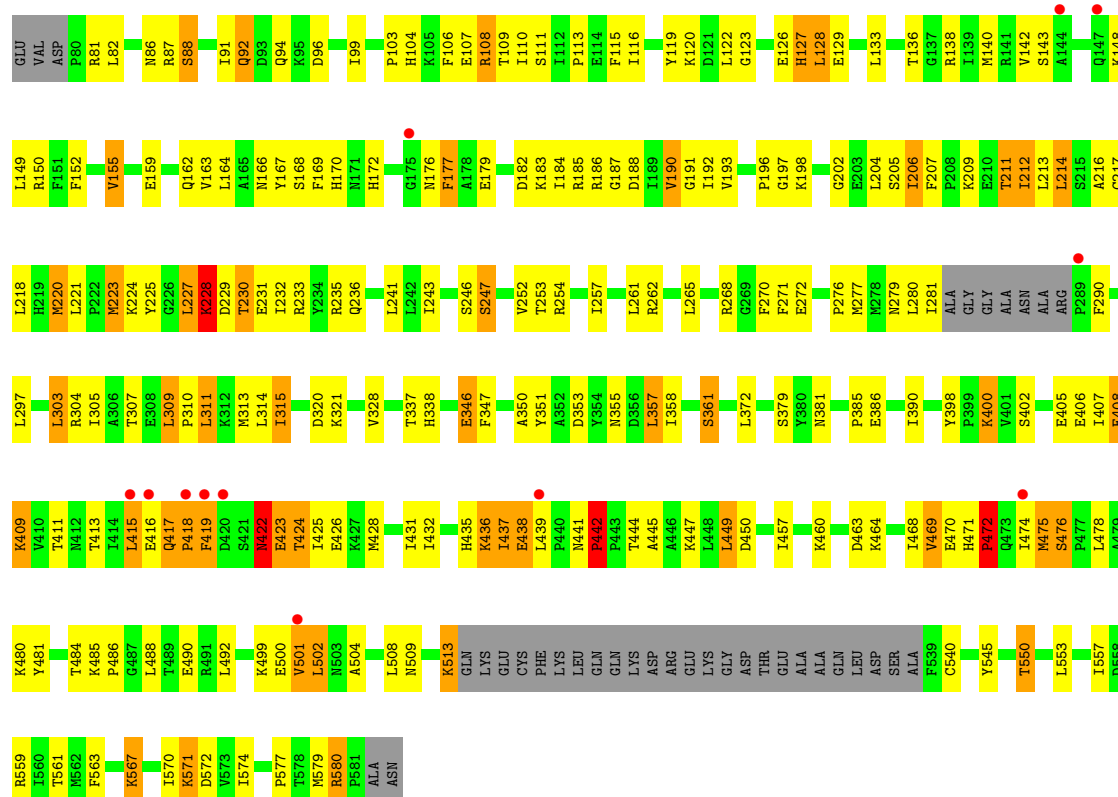
• Molecule 1: Lysyl-tRNA synthetase

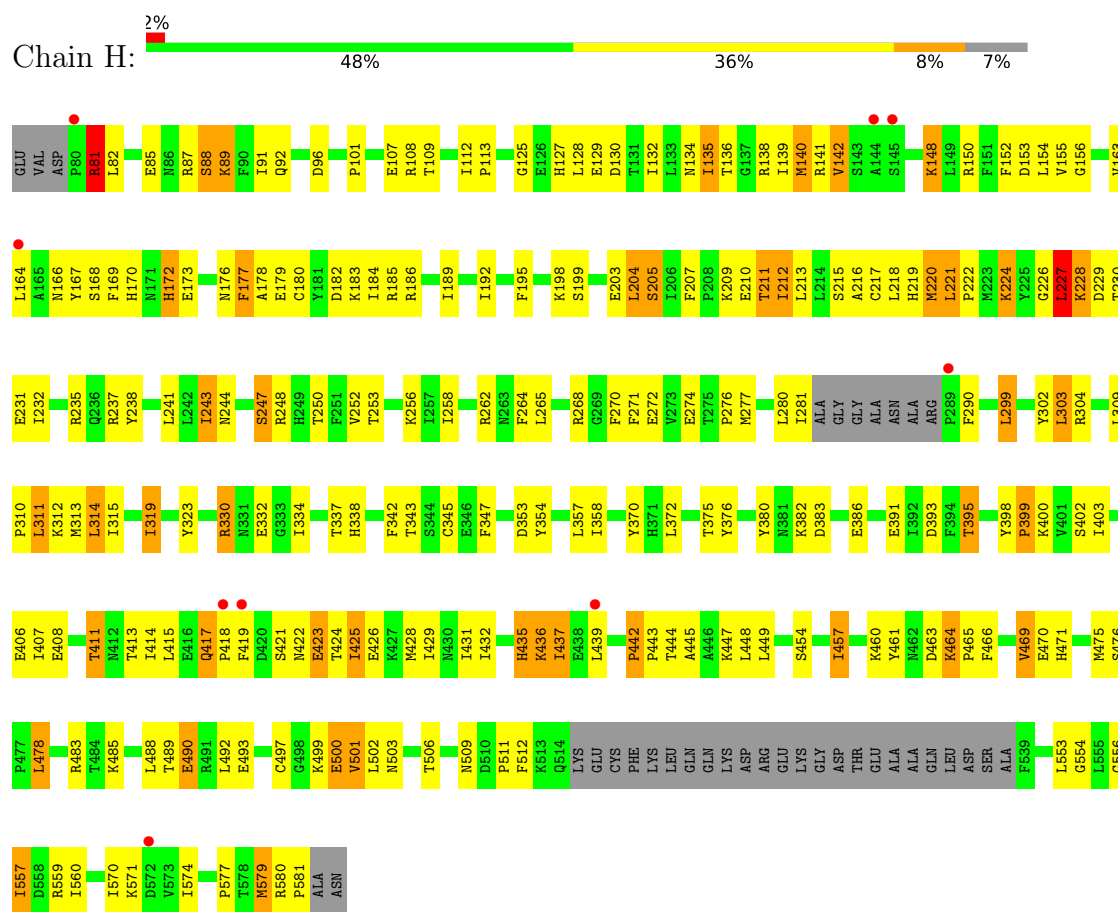


• Molecule 1: Lysyl-tRNA synthetase









4 Data and refinement statistics

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) 93.3 (48.70-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7.1_743, REFMAC	Depositor
R, R_{free}	0.226 , 0.298 0.221 , 0.294	Depositor DCC
R_{free} test set	3110 reflections (2.85%)	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 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.57	0/3954	0.96	8/5342 (0.1%)
1	B	0.58	0/3952	1.01	9/5339 (0.2%)
1	C	0.63	1/3941 (0.0%)	1.01	9/5326 (0.2%)
1	D	0.61	0/3946	0.96	11/5331 (0.2%)
1	E	0.62	2/3929 (0.1%)	0.96	8/5308 (0.2%)
1	F	0.59	0/3943	0.94	5/5327 (0.1%)
1	G	0.60	0/3937	0.98	12/5319 (0.2%)
1	H	0.61	0/3935	0.96	8/5316 (0.2%)
All	All	0.60	3/31537 (0.0%)	0.97	70/42608 (0.2%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	360	TRP	NE1-CE2	-6.25	1.30	1.37
1	E	127	HIS	CG-ND1	-6.24	1.31	1.38
1	E	127	HIS	ND1-CE1	5.36	1.38	1.32

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	GLU	N-CA-C	-8.36	103.67	114.04
1	A	148	LYS	N-CA-C	-8.06	103.24	113.72
1	B	148	LYS	N-CA-C	-8.04	103.48	113.38
1	G	209	LYS	N-CA-C	-7.98	103.67	113.41
1	F	148	LYS	N-CA-C	-7.78	103.39	113.12
1	B	403	ILE	N-CA-C	7.13	117.65	110.23
1	C	209	LYS	N-CA-C	-7.12	104.75	113.50
1	H	457	ILE	N-CA-C	7.00	117.58	111.56
1	H	148	LYS	N-CA-C	-6.95	104.95	113.50
1	F	190	VAL	N-CA-C	6.93	118.46	108.48
1	B	384	GLY	CA-C-N	6.78	126.37	119.19
1	B	384	GLY	C-N-CA	6.78	126.37	119.19
1	B	209	LYS	N-CA-C	-6.74	105.35	113.97
1	C	148	LYS	N-CA-C	-6.63	104.78	114.39
1	G	548	PRO	CA-C-N	-6.62	113.15	119.90
1	G	548	PRO	C-N-CA	-6.62	113.15	119.90
1	A	209	LYS	N-CA-C	-6.57	105.41	113.50
1	H	81	ARG	N-CA-C	-6.33	104.82	112.54
1	A	384	GLY	CA-C-N	6.29	125.99	119.64
1	A	384	GLY	C-N-CA	6.29	125.99	119.64
1	B	417	GLN	CA-C-N	6.29	127.70	119.84
1	B	417	GLN	C-N-CA	6.29	127.70	119.84
1	E	148	LYS	N-CA-C	-6.24	104.04	113.89
1	A	279	ASN	N-CA-C	6.23	116.23	108.19
1	G	81	ARG	N-CA-C	-6.23	105.64	113.18
1	C	81	ARG	N-CA-C	-6.22	105.55	113.01
1	E	155	VAL	N-CA-C	6.15	116.72	108.11
1	D	148	LYS	N-CA-C	-6.01	103.39	112.04
1	G	403	ILE	N-CA-C	5.99	116.65	110.36
1	G	155	VAL	N-CA-C	5.95	116.50	108.17
1	C	295	ASN	N-CA-C	5.93	117.75	111.28
1	C	323	TYR	N-CA-C	5.92	118.69	109.52
1	C	277	MET	N-CA-C	-5.91	105.90	113.23
1	H	172	HIS	N-CA-C	5.89	119.73	112.54
1	G	484	THR	N-CA-C	5.82	117.31	110.97
1	D	195	PHE	CA-C-N	5.72	125.69	120.03
1	D	195	PHE	C-N-CA	5.72	125.69	120.03
1	E	384	GLY	CA-C-N	5.69	126.19	120.04
1	E	384	GLY	C-N-CA	5.69	126.19	120.04
1	E	476	SER	CA-C-N	5.66	125.36	119.82
1	E	476	SER	C-N-CA	5.66	125.36	119.82
1	C	360	TRP	CD2-CE2-CZ2	-5.58	116.82	122.40
1	H	403	ILE	N-CA-C	5.56	115.76	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	456	PHE	CA-C-N	-5.52	116.97	122.77
1	D	456	PHE	C-N-CA	-5.52	116.97	122.77
1	D	457	ILE	N-CA-C	5.48	116.72	112.12
1	G	442	PRO	CA-C-N	5.46	129.28	121.91
1	G	442	PRO	C-N-CA	5.46	129.28	121.91
1	F	442	PRO	CA-C-N	5.40	126.59	119.84
1	F	442	PRO	C-N-CA	5.40	126.59	119.84
1	C	550	THR	N-CA-C	5.36	117.11	108.32
1	D	319	ILE	CB-CA-C	-5.35	106.13	111.80
1	D	155	VAL	N-CA-C	5.28	115.56	108.17
1	D	384	GLY	CA-C-N	5.23	124.92	119.64
1	D	384	GLY	C-N-CA	5.23	124.92	119.64
1	F	155	VAL	N-CA-C	5.23	115.43	108.11
1	B	106	PHE	N-CA-C	-5.19	102.09	110.14
1	E	462	ASN	N-CA-C	-5.19	106.91	114.12
1	G	104	HIS	N-CA-C	5.17	116.73	111.14
1	H	442	PRO	CA-C-N	5.17	126.30	119.84
1	H	442	PRO	C-N-CA	5.17	126.30	119.84
1	H	142	VAL	N-CA-C	5.16	115.56	108.12
1	A	339	ASN	CA-C-N	5.16	124.95	119.28
1	A	339	ASN	C-N-CA	5.16	124.95	119.28
1	B	81	ARG	N-CA-C	-5.15	106.78	113.16
1	D	403	ILE	N-CA-C	5.14	115.87	110.62
1	G	384	GLY	CA-C-N	5.11	125.56	120.04
1	G	384	GLY	C-N-CA	5.11	125.56	120.04
1	C	540	CYS	N-CA-C	-5.08	105.18	111.33
1	E	81	ARG	N-CA-C	-5.00	107.22	113.72

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 ⓘ

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	152	0
1	B	3852	0	3819	155	1
1	C	3844	0	3804	148	0
1	D	3849	0	3814	161	0
1	E	3833	0	3799	143	0
1	F	3843	0	3811	144	0
1	G	3840	0	3806	130	1
1	H	3839	0	3803	161	0
2	A	10	0	0	1	0
2	B	14	0	0	2	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	1143	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 19.

All (1143) 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:C:578:THR:O	1:C:579:MET:HE3	1.64	0.96
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:HG3	1:A:268:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:277:MET:HE2	1:D:304:ARG:NH2	1.89	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:HG3	1:A:268:ARG:NH1	1.91	0.82
1:G:502:LEU:C	1:G:502:LEU:HD23	2.05	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:228:LYS:HG3	1:B:233:ARG:HD3	1.62	0.80
1:B:231:GLU:O	1:B:235:ARG:HG3	1.80	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:D:465:PRO:HB2	1:D:494:MET:HE3	1.64	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
1:D:187:GLY:O	1:D:217:CYS:HB2	1.84	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:B:444:THR:HG22	1:B:447:LYS:H	1.51	0.76
1:A:365:PHE:CD2	1:A:494:MET:HE1	2.21	0.75
1:F:408:GLU:OE2	1:F:415:LEU:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:329:PHE:C	1:C:330:ARG:HG2	2.13	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:B:187:GLY:C	1:B:217:CYS:HB2	2.15	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
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:C:562:MET:HE3	1:C:569:SER:C	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:277:MET:HE2	1:G:304:ARG:NH2	2.06	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: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:F:435:HIS:O	1:F:436:LYS:C	2.35	0.68
1:D:417:GLN:C	1:D:419:PHE:H	2.01	0.68
1:G:428:MET:HE1	1:G:449:LEU:HD22	1.75	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:B:277:MET:HE2	1:B:304:ARG:NH2	2.09	0.67
1:F:152:PHE:HB2	1:F:163:VAL:HB	1.74	0.67
1:G:358:ILE:CD1	1:G:492:LEU:HD13	2.24	0.67
1:G:484:THR:OG1	1:G:485:LYS:HG3	1.95	0.67
1:G:435:HIS:O	1:G:436:LYS:C	2.37	0.67
1:G:149:LEU:HD23	1:G:151:PHE:HZ	1.58	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:B:485:LYS:HB3	1:B:488:LEU:HD22	1.78	0.66
1:G:473:GLN:HG3	1:G:487:GLY:C	2.21	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:H:417:GLN:C	1:H:419:PHE:H	2.00	0.66
1:A:440:PRO:O	1:A:441:ASN:HB2	1.96	0.66
1:E:398:TYR:O	1:E:400:LYS:NZ	2.23	0.65
1:C:277:MET:HE2	1:C:304:ARG:HH21	1.60	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:LYS:HG2	1:D:349:TRP:CD1	2.32	0.65
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:E:571:LYS:HD3	1:E: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: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: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:D:435:HIS:O	1:D:436:LYS:C	2.41	0.63
1:E:151:PHE:HD1	1:E:162:GLN:HE21	1.46	0.63
1:A:365:PHE:CE2	1:A:494:MET:HE1	2.33	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:C:277:MET:HE2	1:C:304:ARG:NH2	2.13	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: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:D:359:LYS:NZ	1:D:363:ASP:OD2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:103:PRO:HG3	1:D:212:ILE:HD11	1.81	0.62
1:D:141:ARG:O	1:D:152:PHE:HA	1.99	0.62
1:H:81:ARG:O	1:H:85:GLU:HG3	1.99	0.62
1:A:502:LEU:C	1:A:502:LEU:HD23	2.25	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:H:347:PHE:CD1	1:H:347:PHE:C	2.77	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:C:471:HIS:HB3	1:C:475:MET:HE2	1.82	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:140:MET:HE1	1:E:221:LEU:HD23	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: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: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:C:316:VAL:C	1:C:318:GLY:H	2.09	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:E:571:LYS:NZ	1:E:579:MET:HE2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:80:PRO:HA	1:D:220:MET:HE1	1.83	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: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:D:417:GLN:C	1:D:419:PHE:N	2.60	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: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:E:105:LYS:NZ	1:F:351:TYR:O	2.37	0.58
1:E:363:ASP:O	1:E:367:GLN:HG3	2.04	0.58
1:G:394:PHE:CZ	1:G:496:ILE:HD13	2.39	0.58
1:A:313:MET:HE1	1:B:576:PHE:HE1	1.67	0.58
1:B:435:HIS:O	1:B:436:LYS:C	2.45	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:C:562:MET:HE3	1:C:570:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:H:501:VAL:HG22	1:H:560:ILE:HG12	1.85	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:C:224:LYS:O	1:C:225:TYR:HB3	2.04	0.57
1:D:90:PHE:CE1	1:D:183:LYS:HB3	2.40	0.57
1:D:416:GLU:O	1:D:417:GLN:CG	2.51	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:G:88:SER:HB3	1:H:512:PHE:CZ	2.40	0.56
1:H:173:GLU:OE1	1:H:173:GLU:N	2.28	0.56
1:H:330:ARG:HG3	1:H:342:PHE:HE2	1.70	0.56
1:A:410:VAL:O	1:A:412:ASN:ND2	2.38	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:309:LEU:O	1:A:313:MET:HG3	2.06	0.56
1:A:313:MET:CE	1:B:576:PHE:CE1	2.89	0.56
1:A:472:PRO:HD2	1:A:475:MET:SD	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:277:MET:HE2	1:E:304:ARG:NH2	2.21	0.56
1:F:186:ARG:NH1	1:F:221:LEU:O	2.39	0.56
1:D:465:PRO:CB	1:D:494:MET:HE3	2.35	0.56
1:E:290:PHE:HB2	1:E:303:LEU:HB2	1.87	0.56
1:B:416:GLU:O	1:B:417:GLN:C	2.47	0.55
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:G:502:LEU:C	1:G:502:LEU:CD2	2.78	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:81:ARG:O	1:B:85:GLU:HG3	2.07	0.55
1:B:308:GLU:HG3	1:B:309:LEU:HD13	1.87	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:H:502:LEU:C	1:H:502:LEU:HD23	2.32	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: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:F:402[B]:SER:OG	1:F:405:GLU:OE1	2.19	0.54
1:A:577:PRO:HG2	1:A:579:MET:HE1	1.88	0.54
1:E:138:ARG:O	1:E:154:LEU:HA	2.07	0.54
1:E:406:GLU:O	1:E:406:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:347:PHE:CD1	1:A:347:PHE:C	2.86	0.54
1:A:567:LYS:HD2	1:A:572:ASP:HB3	1.88	0.54
1:C:435:HIS:O	1:C:436:LYS:C	2.50	0.54
1:B:179:GLU:OE1	1:B:183:LYS:NZ	2.38	0.54
1:C:235:ARG:NH2	1:C:580:ARG:O	2.39	0.54
1:C:570:ILE:HG12	1:C:574:ILE:CD1	2.38	0.54
1:E:213:LEU:HD21	1:E:216:ALA:HB2	1.89	0.54
1:C:347:PHE:CD1	1:C:347:PHE:C	2.85	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: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:B:321:LYS:NZ	2:B:606:HOH:O	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:GLY:C	1:D:217:CYS:HB2	2.34	0.53
1:F:176:ASN:HB3	1:F:179:GLU:CB	2.35	0.53
1:B:281:ILE:HG23	1:B:281:ILE:O	2.09	0.53
1:E:145:SER:HA	1:H:391:GLU:OE2	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: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
1:F:265:LEU:HB3	1:F:270:PHE:HB2	1.91	0.53
1:H:435:HIS:O	1:H:436:LYS:C	2.51	0.53
1:E:84:PHE:O	1:E:88:SER:OG	2.27	0.52
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:316:VAL:C	1:C:318:GLY:N	2.67	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: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:HD23	1:C:492:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:304:ARG:HH12	1:C:324:GLU:CD	2.18	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: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
1:F:277:MET:HE2	1:F:304:ARG:NH2	2.25	0.51
1:B:468:ILE:HD12	1:B:495:PHE:CE2	2.44	0.51
1:C:416:GLU:O	1:C:417:GLN:C	2.53	0.51
1:D:184:ILE:HG22	1:D:184:ILE:O	2.08	0.51
1:D:277:MET:HE2	1:D:304:ARG:HH21	1.73	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:B:140:MET:HE1	1:B:221:LEU:HD21	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:H:471:HIS:HB3	1:H:475:MET:HE2	1.93	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:B:425:ILE:HA	1:B:428:MET:HE2	1.91	0.51
1:F:417:GLN:C	1:F:419:PHE:H	2.18	0.51
1:A:264:PHE:CE1	1:A:268:ARG:NH2	2.79	0.51
1:C:316:VAL:O	1:C:318:GLY:N	2.43	0.51
1:C:417:GLN:C	1:C:419:PHE:H	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:F:439:LEU:H	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:F:337:THR:C	1:F:338:HIS:ND1	2.70	0.50
1:C:171:ASN:OD1	1:C:173:GLU:HG2	2.12	0.50
1:E:247:SER:O	1:E:248:ARG:C	2.52	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
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: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:G:347:PHE:CD1	1:G:347:PHE:C	2.90	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:224:LYS:C	1:H:226:GLY:H	2.20	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:D:190:VAL:C	1:D:214:LEU:HD22	2.37	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:347:PHE:C	1:H:347:PHE:HD1	2.20	0.49
1:H:358:ILE:HD13	1:H:492:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:THR:HB	1:H:447:LYS:HG3	1.93	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:H:406:GLU:O	1:H:406:GLU:HG3	2.11	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:E:571:LYS:HZ2	1:E:579:MET:HE2	1.77	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: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:G:277:MET:HE2	1:G:304:ARG:HH21	1.75	0.49
1:A:119:TYR:O	1:A:122:LEU:HB2	2.12	0.49
1:A:564:LEU:N	1:A:564:LEU:HD23	2.26	0.49
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:O	1:G:304:ARG:HG3	2.13	0.49
1:F:87:ARG:NH2	1:F:188:ASP:OD2	2.46	0.49
1:F:422:ASN:H	1:F:425:ILE:HD12	1.78	0.49
1:G:466:PHE:CD2	1:G:466:PHE:N	2.81	0.49
1:C:261:LEU:HD23	1:C:325:ILE:HD11	1.93	0.49
1:D:439:LEU:H	1:D:439:LEU:CD1	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:88:SER:O	1:H:89:LYS:C	2.56	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:H:476:SER:C	1:H:478:LEU:H	2.21	0.48
1:C:329:PHE:CD1	1:D:278:MET:HE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:G:237:ARG:HG3	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:HD12	1:D:311:LEU:HA	1.65	0.48
1:D:386:GLU:CD	1:D:386:GLU:H	2.21	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: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: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
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:112:ILE:HD12	1:H:156:GLY:CA	2.44	0.48
1:H:130:ASP:O	1:H:132:ILE:HG12	2.14	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:E:128:LEU:C	1:E:130:ASP:H	2.21	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:HE3	1:E:209:LYS:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:GLY:N	1:D:214:LEU:CD1	2.77	0.47
1:E:435:HIS:O	1:E:436:LYS:C	2.56	0.47
1:H:271:PHE:HA	2:H:601:HOH:O	2.13	0.47
1:A:365:PHE:CE2	1:A:494:MET:CE	2.96	0.47
1:B:571:LYS:HD3	1:B:579:MET:HE1	1.96	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:347:PHE:CD1	1:F:347:PHE:C	2.92	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
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:H:471:HIS:HD2	1:H:475:MET:HE1	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:GLN:NE2	1:F:96:ASP:OD1	2.48	0.47
1:F:128:LEU:HD12	1:F:196:PRO:HG2	1.96	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:B:422:ASN:O	1:B:423:GLU:C	2.57	0.47
1:C:264:PHE:CE1	1:C:268:ARG:CZ	2.98	0.47
1:D:108:ARG:HD2	1:D:136:THR:OG1	2.15	0.47
1:D:138:ARG:HG3	1:D:189:ILE:HG13	1.96	0.47
1:D:151:PHE:O	1:D:152:PHE:CG	2.68	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:C:224:LYS:C	1:C:226:GLY:H	2.23	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: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: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: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:E:407:ILE:HG13	1:E:457:ILE:HD11	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:317:GLY:CA	1:H:238:TYR:HB2	2.46	0.46
1:G:324:GLU:O	1:G:345:CYS:HA	2.14	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:O	1:D:92:GLN:NE2	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:HD12	1:C:214:LEU:HA	1.73	0.46
1:E:339:ASN:CG	1:E:340:PRO:HD2	2.40	0.46
1:D:502:LEU:HD23	1:D:502:LEU:C	2.41	0.46
1:E:416:GLU:O	1:E:417:GLN:C	2.58	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: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
1:A:239:LEU:HD21	1:B:545:TYR:CD1	2.51	0.45
1:B:124:ASN:OD1	1:B:202:GLY:HA3	2.16	0.45
1:D:437:ILE:O	1:D:438:GLU:CB	2.64	0.45
1:E:422:ASN:HB3	1:E:423:GLU:H	1.60	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:A:363:ASP:O	1:A:364:PHE:C	2.59	0.45
1:C:127:HIS:O	1:C:128:LEU:HD23	2.16	0.45
1:D:234:TYR:HB2	1:D:579:MET:SD	2.56	0.45
1:D:547:LEU:HD12	1:D:548:PRO:HD2	1.97	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:H:176:ASN:O	1:H:177:PHE:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:579:MET:HB2	1:A:579:MET:HE3	1.75	0.45
1:B:347:PHE:CD1	1:B:347:PHE:C	2.95	0.45
1:E:347:PHE:CD1	1:E:347:PHE:C	2.95	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:264:PHE:HE2	1:G:360:TRP:CE2	2.35	0.45
1:G:308:GLU:HG3	1:G:309:LEU:HD13	1.99	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: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:C:504:ALA:HB2	1:C:553:LEU:HG	1.98	0.45
1:D:140:MET:HE1	1:D:221:LEU:HD21	1.99	0.45
1:D:212:ILE:O	1:D:214:LEU:HD13	2.16	0.45
1:A:94:GLN:HE22	1:A:183:LYS:NZ	2.15	0.45
1:D:82:LEU:O	1:D:86:ASN:ND2	2.50	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: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:F:246:SER:OG	1:F:247:SER:N	2.49	0.45
1:F:416:GLU:O	1:F:417:GLN:C	2.59	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:HE	1:B:108:ARG:HB2	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:A:411:THR:OG1	1:A:431:ILE:HD13	2.17	0.45
1:A:423:GLU:HG3	1:A:424:THR:N	2.30	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:386:GLU:CD	1:E:386:GLU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:386:GLU:H	1:C:386:GLU:CD	2.23	0.45
1:E:277:MET:HE2	1:E:304:ARG:HH21	1.81	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:87:ARG:O	1:E:90:PHE:HB3	2.17	0.44
1:E:311:LEU:HA	1:E:311:LEU:HD12	1.77	0.44
1:F:227:LEU:HA	1:F:230:THR:OG1	2.17	0.44
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:E:417:GLN:C	1:E:419:PHE:H	2.25	0.44
1:F:82:LEU:HG	1:F:86:ASN:HD21	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:MET:HE2	1:H:220:MET:HB2	1.84	0.44
1:H:402:SER:HA	1:H:469:VAL:HG12	1.99	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:B:223:MET:HE3	1:B:223:MET:HB3	1.82	0.44
1:B:510:ASP:C	1:B:512:PHE:H	2.24	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:A:279:ASN:C	1:A:280:LEU:HG	2.42	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: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:HA	1:G:559:ARG:HD3	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
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: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:H:217:CYS:C	1:H:219:HIS:H	2.26	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: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:A:328:VAL:C	1:A:329:PHE:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:223:MET:HE3	1:D:223:MET:HB3	1.77	0.43
1:D:441:ASN:O	1:D:442:PRO:C	2.58	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:ND1	1:C:471:HIS:N	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:C:471:HIS:HB3	1:C:475:MET:CE	2.48	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:HD23	1:H:303:LEU:HA	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: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:A:141:ARG:HG2	1:A:142:VAL:N	2.33	0.43
1:A:316:VAL:C	1:A:318:GLY:N	2.77	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
1:D:358:ILE:HD13	1:D:492:LEU:HD13	2.01	0.43
1:E:261:LEU:O	1:E:262:ARG:C	2.60	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:HD1	1:F:419:PHE:HA	1.77	0.43
1:G:346:GLU:HA	1:G:553:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:140:MET:HE1	1:G:221:LEU:CD2	2.49	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:190:VAL:C	1:F:214:LEU:HD22	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:176:ASN:O	1:G:177:PHE:C	2.60	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:428:MET:HE3	1:H:448:LEU:HD12	2.01	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:223:MET:HE3	1:C:223:MET:HB3	1.62	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:123:GLY:O	1:B:124:ASN:C	2.61	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
1:E:100:ASN:O	1:E:103:PRO:HD3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:365:PHE:CE2	1:E:494:MET:HE2	2.54	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:A:510:ASP:OD1	1:A:510:ASP:C	2.62	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:H:277:MET:HE2	1:H:304:ARG:NH2	2.34	0.42
1:B:137:GLY:HA3	1:B:154:LEU:CD1	2.50	0.42
1:B:137:GLY:C	1:B:154:LEU:HD11	2.44	0.42
1:B:471:HIS:CG	1:B:491:ARG:HD3	2.55	0.42
1:B:574:ILE:O	1:B:575:LEU:C	2.61	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:441:ASN:O	1:E:442:PRO:C	2.62	0.42
1:E:496:ILE:HG13	1:E:501:VAL:HG21	2.01	0.42
1:H:309:LEU:O	1:H:310:PRO:C	2.62	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:OD1	1:C:509:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:SER:C	1:F:478:LEU:H	2.27	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
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:C:358:ILE:O	1:C:359:LYS:C	2.63	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:87:ARG:NH2	1:D:188:ASP:OD1	2.52	0.42
1:D:135:ILE:HG23	1:D:192:ILE:HB	2.02	0.42
1:D:510:ASP:O	1:D:511:PRO:C	2.62	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:E:224:LYS:C	1:E:226:GLY:H	2.28	0.42
1:E:239:LEU:O	1:E:240:ASP:C	2.63	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:220:MET:HE2	1:B:220:MET:HB2	1.78	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:89:LYS:HE3	1:A:89:LYS:HB2	1.87	0.41
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: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:220:MET:HE2	1:F:220:MET:HB2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:H:302:TYR:CD2	2.88	0.41
1:H:419:PHE:C	1:H:421:SER:H	2.28	0.41
1:A:93:ASP:O	1:A:97:LYS:HB2	2.21	0.41
1:C:105:LYS:HA	1:C:105:LYS:HD2	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:G:220:MET:HE2	1:G:220:MET:HB2	1.89	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:177:PHE:C	1:H:177:PHE:CD2	2.98	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:128:LEU:C	1:E:130:ASP:N	2.78	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:HD12	1:A:221:LEU:HA	1.93	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:416:GLU:O	1:E:418:PRO:N	2.54	0.41
1:G:579:MET:HE3	1:G:579:MET:HB2	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LEU:HD12	1:B:311:LEU:HA	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:C:562:MET:HE3	1:C:570:ILE:CA	2.51	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
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:D:329:PHE:C	1:D:330:ARG:HG2	2.45	0.41
1:E:241:LEU:HA	1:E:241:LEU:HD12	1.82	0.41
1:H:571:LYS:HD3	1:H:579:MET:HE1	2.02	0.41
1:A:227:LEU:HA	1:A:230:THR:OG1	2.21	0.41
1:A:312:LYS:HD2	1:A:507:GLU:CD	2.46	0.41
1:A:399:PRO:C	1:A:400:LYS:HD2	2.45	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:C:562:MET:HE3	1:C:570:ILE:HA	2.03	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: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:92:GLN:NE2	1:F:92:GLN:O	2.54	0.41
1:F:315:ILE:HD12	1:F:550:THR:CG2	2.51	0.41
1:F:480:LYS:HA	1:F:508:LEU:HD13	2.03	0.41
1:F:567:LYS:HD2	1:F:572:ASP:HB3	2.02	0.41
1:G:251:PHE:O	1:G:252:VAL:C	2.64	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:170:HIS:CB	1:H:177:PHE:HD1	2.34	0.41
1:H:204:LEU:HD12	1:H:205:SER:N	2.35	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:312:LYS:O	1:H:313:MET:C	2.64	0.41
1:H:463:ASP:OD2	1:H:464:LYS:HE2	2.21	0.41
1:H:469:VAL:HG13	1:H:470:GLU:CG	2.50	0.41
1:H:509:ASN:O	1:H:511:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:350:ALA:HA	1:D:550:THR:HG23	2.03	0.41
1:D:394:PHE:HZ	1:D:496:ILE:HD13	1.85	0.41
1:E:140:MET:HG2	1:E:155:VAL:HG22	2.03	0.41
1:E:365:PHE:CD2	1:E:494:MET:HE1	2.55	0.41
1:E:411:THR:O	1:E:413:THR:HG23	2.21	0.41
1:E:417:GLN:C	1:E:419:PHE:N	2.79	0.41
1:E:570:ILE:HA	1:E:573:VAL:HG22	2.02	0.41
1:F:223:MET:HB3	1:F:223:MET:HE3	1.87	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
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:541:THR:O	1:B:542:SER:C	2.63	0.40
1:C:232:ILE:O	1:C:233:ARG:C	2.64	0.40
1:C:484:THR:OG1	1:C:485:LYS:N	2.55	0.40
1:D:224:LYS:C	1:D:226:GLY:H	2.29	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:171:ASN:C	1:G:173:GLU:H	2.30	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:HD12	1:G:415:LEU:O	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:H:398:TYR:O	1:H:399:PRO:C	2.65	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:CD2	1:D:172:HIS:H	2.39	0.40
1:D:258:ILE:O	1:D:259:ASN:C	2.62	0.40
1:D:510:ASP:OD1	1:D:510:ASP:C	2.64	0.40
1:H:198:LYS:HA	1:H:203:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLU:OE1	1:A:386:GLU:N	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:317:GLY:HA2	1:H:238:TYR:HB2	2.04	0.40
1:G:510:ASP:O	1:G:512:PHE:N	2.55	0.40
1:A:192:ILE:HG23	1:A:208:PRO:HB3	2.03	0.40
1:C:328:VAL:C	1:C:329:PHE:CD2	3.00	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: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:557:ILE:HD13	1:F:557:ILE:HA	1.96	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
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:F:502:LEU:C	1:F:502:LEU:HD23	2.47	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	466/507 (92%)	425 (91%)	35 (8%)	6 (1%)	9	32
1	B	466/507 (92%)	414 (89%)	44 (9%)	8 (2%)	7	26
1	C	465/507 (92%)	408 (88%)	51 (11%)	6 (1%)	9	32
1	D	465/507 (92%)	410 (88%)	49 (10%)	6 (1%)	9	32
1	E	464/507 (92%)	417 (90%)	40 (9%)	7 (2%)	8	28
1	F	465/507 (92%)	420 (90%)	33 (7%)	12 (3%)	4	17
1	G	464/507 (92%)	419 (90%)	33 (7%)	12 (3%)	4	17
1	H	465/507 (92%)	419 (90%)	38 (8%)	8 (2%)	7	26
All	All	3720/4056 (92%)	3332 (90%)	323 (9%)	65 (2%)	7	26

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	371 (87%)	56 (13%)	4	13
1	B	427/457 (93%)	356 (83%)	71 (17%)	2	7
1	C	425/457 (93%)	361 (85%)	64 (15%)	3	10
1	D	426/457 (93%)	355 (83%)	71 (17%)	2	7
1	E	424/457 (93%)	361 (85%)	63 (15%)	3	10
1	F	426/457 (93%)	348 (82%)	78 (18%)	2	6
1	G	425/457 (93%)	364 (86%)	61 (14%)	3	11
1	H	424/457 (93%)	357 (84%)	67 (16%)	2	8
All	All	3404/3656 (93%)	2873 (84%)	531 (16%)	2	9

All (531) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	99	ILE
1	A	110	ILE
1	A	117[A]	GLU
1	A	117[B]	GLU
1	A	122	LEU
1	A	142	VAL
1	A	149	LEU
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	230	THR
1	A	232	ILE
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	250	THR
1	A	274	GLU
1	A	299	LEU
1	A	305	ILE
1	A	308	GLU
1	A	309	LEU
1	A	311	LEU
1	A	312	LYS
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	403	ILE
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
1	A	464	LYS
1	A	469	VAL
1	A	476	SER
1	A	478	LEU
1	A	490	GLU
1	A	540	CYS
1	A	550	THR
1	A	557	ILE
1	A	579	MET
1	A	580	ARG
1	B	81	ARG
1	B	89	LYS
1	B	91	ILE
1	B	96	ASP
1	B	99	ILE

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Mol	Chain	Res	Type
1	B	108	ARG
1	B	109	THR
1	B	122	LEU
1	B	129	GLU
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	224	LYS
1	B	227	LEU
1	B	228	LYS
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	305	ILE
1	B	309	LEU
1	B	311	LEU
1	B	314	LEU
1	B	337	THR
1	B	345	CYS
1	B	357	LEU
1	B	372	LEU
1	B	383	ASP
1	B	390	ILE
1	B	391	GLU
1	B	404	VAL
1	B	410	VAL

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Mol	Chain	Res	Type
1	B	413	THR
1	B	417	GLN
1	B	422	ASN
1	B	423	GLU
1	B	424	THR
1	B	426	GLU
1	B	435	HIS
1	B	444	THR
1	B	449	LEU
1	B	457	ILE
1	B	460	LYS
1	B	469	VAL
1	B	476	SER
1	B	484	THR
1	B	488	LEU
1	B	500	GLU
1	B	501	VAL
1	B	540	CYS
1	B	542	SER
1	B	543	LEU
1	B	559	ARG
1	B	567	LYS
1	B	570	ILE
1	B	579	MET
1	C	81	ARG
1	C	89	LYS
1	C	107	GLU
1	C	122	LEU
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	173	GLU
1	C	200	LYS
1	C	212	ILE
1	C	214	LEU
1	C	218	LEU
1	C	220	MET
1	C	223	MET
1	C	227	LEU

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Mol	Chain	Res	Type
1	C	230	THR
1	C	241	LEU
1	C	256	LYS
1	C	274	GLU
1	C	281	ILE
1	C	298	ASP
1	C	305	ILE
1	C	309	LEU
1	C	311	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	382	LYS
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	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	469	VAL
1	C	471	HIS
1	C	476	SER
1	C	478	LEU
1	C	490	GLU
1	C	496	ILE
1	C	500	GLU
1	C	501	VAL

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Mol	Chain	Res	Type
1	C	543	LEU
1	C	571	LYS
1	C	574	ILE
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	142	VAL
1	D	143	SER
1	D	168	SER
1	D	176	ASN
1	D	193	VAL
1	D	200	LYS
1	D	205	SER
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	258	ILE
1	D	281	ILE
1	D	296	ASP
1	D	305	ILE
1	D	309	LEU
1	D	311	LEU
1	D	312	LYS
1	D	314	LEU
1	D	319	ILE
1	D	330	ARG
1	D	346	GLU
1	D	357	LEU

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Mol	Chain	Res	Type
1	D	366	SER
1	D	372	LEU
1	D	377	LYS
1	D	388	GLN
1	D	390	ILE
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	429	ILE
1	D	432	ILE
1	D	435	HIS
1	D	444	THR
1	D	449	LEU
1	D	460	LYS
1	D	464	LYS
1	D	469	VAL
1	D	476	SER
1	D	478	LEU
1	D	483	ARG
1	D	490	GLU
1	D	492	LEU
1	D	500	GLU
1	D	501	VAL
1	D	550	THR
1	D	558	ASP
1	D	559	ARG
1	D	579	MET
1	E	82	LEU
1	E	88	SER
1	E	92	GLN
1	E	99	ILE
1	E	122	LEU
1	E	140	MET
1	E	142	VAL
1	E	149	LEU
1	E	150	ARG

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Mol	Chain	Res	Type
1	E	160	LYS
1	E	168	SER
1	E	193	VAL
1	E	198	LYS
1	E	201	LYS
1	E	206	ILE
1	E	209	LYS
1	E	211	THR
1	E	212	ILE
1	E	218	LEU
1	E	220	MET
1	E	221	LEU
1	E	223	MET
1	E	224	LYS
1	E	227	LEU
1	E	228	LYS
1	E	230	THR
1	E	232	ILE
1	E	235	ARG
1	E	241	LEU
1	E	247	SER
1	E	267	GLU
1	E	311	LEU
1	E	314	LEU
1	E	319	ILE
1	E	335	ASP
1	E	351	TYR
1	E	357	LEU
1	E	372	LEU
1	E	390	ILE
1	E	395	THR
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	452	LEU
1	E	454	SER
1	E	457	ILE

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Mol	Chain	Res	Type
1	E	460	LYS
1	E	463	ASP
1	E	464	LYS
1	E	469	VAL
1	E	478	LEU
1	E	490	GLU
1	E	492	LEU
1	E	499	LYS
1	E	509	ASN
1	E	540	CYS
1	E	579	MET
1	E	580	ARG
1	F	81	ARG
1	F	88	SER
1	F	92	GLN
1	F	99	ILE
1	F	107	GLU
1	F	108	ARG
1	F	120	LYS
1	F	122	LEU
1	F	127	HIS
1	F	128	LEU
1	F	129	GLU
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	209	LYS
1	F	211	THR
1	F	212	ILE
1	F	214	LEU
1	F	218	LEU
1	F	220	MET
1	F	223	MET
1	F	227	LEU
1	F	228	LYS
1	F	230	THR
1	F	241	LEU
1	F	243	ILE

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Mol	Chain	Res	Type
1	F	247	SER
1	F	253	THR
1	F	281	ILE
1	F	297	LEU
1	F	303	LEU
1	F	305	ILE
1	F	309	LEU
1	F	311	LEU
1	F	314	LEU
1	F	315	ILE
1	F	328	VAL
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	390	ILE
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
1	F	432	ILE
1	F	444	THR
1	F	449	LEU
1	F	457	ILE
1	F	464	LYS
1	F	469	VAL
1	F	472	PRO
1	F	475	MET
1	F	476	SER
1	F	484	THR
1	F	490	GLU
1	F	500	GLU
1	F	501	VAL
1	F	502	LEU
1	F	513	LYS
1	F	540	CYS

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Mol	Chain	Res	Type
1	F	550	THR
1	F	567	LYS
1	F	570	ILE
1	F	571	LYS
1	F	579	MET
1	F	580	ARG
1	G	88	SER
1	G	89	LYS
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	214	LEU
1	G	220	MET
1	G	227	LEU
1	G	228	LYS
1	G	230	THR
1	G	241	LEU
1	G	258	ILE
1	G	277	MET
1	G	305	ILE
1	G	309	LEU
1	G	311	LEU
1	G	314	LEU
1	G	319	ILE
1	G	337	THR
1	G	338	HIS
1	G	341	GLU
1	G	357	LEU
1	G	372	LEU
1	G	383	ASP
1	G	390	ILE
1	G	403	ILE
1	G	407	ILE

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Mol	Chain	Res	Type
1	G	415	LEU
1	G	423	GLU
1	G	424	THR
1	G	426	GLU
1	G	427	LYS
1	G	432	ILE
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	484	THR
1	G	490	GLU
1	G	501	VAL
1	G	502	LEU
1	G	505	TYR
1	G	513	LYS
1	G	543	LEU
1	G	550	THR
1	G	557	ILE
1	G	559	ARG
1	G	562	MET
1	G	579	MET
1	H	81	ARG
1	H	82	LEU
1	H	92	GLN
1	H	96	ASP
1	H	127	HIS
1	H	129	GLU
1	H	135	ILE
1	H	140	MET
1	H	142	VAL
1	H	148	LYS
1	H	168	SER
1	H	184	ILE
1	H	204	LEU
1	H	205	SER
1	H	209	LYS
1	H	210	GLU
1	H	211	THR

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Mol	Chain	Res	Type
1	H	212	ILE
1	H	218	LEU
1	H	220	MET
1	H	221	LEU
1	H	224	LYS
1	H	227	LEU
1	H	228	LYS
1	H	230	THR
1	H	232	ILE
1	H	243	ILE
1	H	247	SER
1	H	256	LYS
1	H	258	ILE
1	H	280	LEU
1	H	281	ILE
1	H	299	LEU
1	H	303	LEU
1	H	311	LEU
1	H	314	LEU
1	H	319	ILE
1	H	330	ARG
1	H	337	THR
1	H	357	LEU
1	H	372	LEU
1	H	383	ASP
1	H	386	GLU
1	H	395	THR
1	H	411	THR
1	H	415	LEU
1	H	417	GLN
1	H	422	ASN
1	H	423	GLU
1	H	424	THR
1	H	425	ILE
1	H	429	ILE
1	H	435	HIS
1	H	439	LEU
1	H	449	LEU
1	H	454	SER
1	H	460	LYS
1	H	464	LYS
1	H	469	VAL

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Mol	Chain	Res	Type
1	H	478	LEU
1	H	490	GLU
1	H	500	GLU
1	H	501	VAL
1	H	506	THR
1	H	557	ILE
1	H	570	ILE
1	H	579	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	176	ASN
1	A	455	HIS
1	A	473	GLN
1	A	482	HIS
1	B	162	GLN
1	B	172	HIS
1	B	244	ASN
1	B	336	ASN
1	B	339	ASN
1	B	371	HIS
1	B	387	ASN
1	B	412	ASN
1	B	417	GLN
1	B	441	ASN
1	B	459	ASN
1	C	236	GLN
1	C	293	HIS
1	D	92	GLN
1	D	219	HIS
1	D	279	ASN
1	D	371	HIS
1	D	417	GLN
1	D	451	GLN
1	E	94	GLN
1	E	170	HIS
1	E	176	ASN
1	E	295	ASN
1	E	339	ASN
1	E	388	GLN

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Mol	Chain	Res	Type
1	E	417	GLN
1	E	455	HIS
1	E	459	ASN
1	F	86	ASN
1	F	92	GLN
1	F	94	GLN
1	F	104	HIS
1	F	162	GLN
1	F	170	HIS
1	F	381	ASN
1	F	441	ASN
1	F	471	HIS
1	F	503	ASN
1	G	86	ASN
1	G	94	GLN
1	G	170	HIS
1	G	176	ASN
1	G	294	HIS
1	G	371	HIS
1	H	94	GLN
1	H	162	GLN
1	H	170	HIS
1	H	172	HIS
1	H	279	ASN
1	H	293	HIS
1	H	294	HIS
1	H	295	ASN
1	H	422	ASN
1	H	455	HIS
1	H	503	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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%)	0.07	9 (1%) 66 58	22, 45, 91, 122	3 (0%)
1	B	471/507 (92%)	0.05	12 (2%) 58 48	22, 47, 88, 118	1 (0%)
1	C	471/507 (92%)	0.17	14 (2%) 52 43	22, 48, 93, 129	0
1	D	471/507 (92%)	0.19	8 (1%) 69 61	22, 49, 91, 121	0
1	E	470/507 (92%)	0.07	10 (2%) 63 54	26, 49, 92, 126	0
1	F	470/507 (92%)	0.12	12 (2%) 57 48	26, 51, 92, 118	1 (0%)
1	G	470/507 (92%)	0.06	7 (1%) 72 64	27, 49, 90, 123	0
1	H	471/507 (92%)	0.08	9 (1%) 66 58	26, 50, 91, 125	0
All	All	3763/4056 (92%)	0.10	81 (2%) 62 53	22, 49, 92, 129	5 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	418	PRO	4.0
1	E	144	ALA	3.9
1	H	144	ALA	3.9
1	G	439	LEU	3.4
1	C	442	PRO	3.3
1	E	80	PRO	3.3
1	E	439	LEU	3.3
1	B	416	GLU	3.3
1	F	439	LEU	3.2
1	A	415	LEU	3.1
1	B	419	PHE	3.1
1	C	80	PRO	3.1
1	G	80	PRO	3.1
1	D	144	ALA	3.0
1	H	418	PRO	3.0
1	B	432	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	289	PRO	2.9
1	H	145	SER	2.9
1	D	289	PRO	2.9
1	G	418	PRO	2.9
1	C	420	ASP	2.9
1	F	175	GLY	2.9
1	C	416	GLU	2.9
1	F	416	GLU	2.8
1	B	415	LEU	2.8
1	G	416	GLU	2.7
1	B	289	PRO	2.7
1	B	418	PRO	2.7
1	H	80	PRO	2.7
1	C	552	GLY	2.7
1	E	415	LEU	2.7
1	C	439	LEU	2.7
1	G	436	LYS	2.7
1	H	164	LEU	2.7
1	D	419	PHE	2.6
1	G	419	PHE	2.6
1	H	419	PHE	2.6
1	G	442	PRO	2.6
1	E	230	THR	2.6
1	C	415	LEU	2.6
1	H	439	LEU	2.6
1	B	442	PRO	2.6
1	E	418	PRO	2.6
1	F	144	ALA	2.6
1	B	439	LEU	2.6
1	B	163	VAL	2.6
1	E	281	ILE	2.5
1	C	418	PRO	2.5
1	E	416	GLU	2.5
1	B	383	ASP	2.5
1	A	439	LEU	2.4
1	C	280	LEU	2.4
1	F	501	VAL	2.4
1	F	289	PRO	2.4
1	A	419	PHE	2.4
1	A	225	TYR	2.4
1	H	572	ASP	2.3
1	C	228	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	289	PRO	2.3
1	C	461	TYR	2.3
1	B	417	GLN	2.2
1	A	281	ILE	2.2
1	F	418	PRO	2.2
1	D	153	ASP	2.2
1	E	202	GLY	2.1
1	F	415	LEU	2.1
1	D	125	GLY	2.1
1	A	418	PRO	2.1
1	A	539	PHE	2.1
1	F	419	PHE	2.1
1	A	414	ILE	2.1
1	D	103	PRO	2.1
1	B	437	ILE	2.1
1	F	147	GLN	2.0
1	C	383	ASP	2.0
1	F	420	ASP	2.0
1	C	458	GLU	2.0
1	A	289	PRO	2.0
1	D	439	LEU	2.0
1	C	437	ILE	2.0
1	F	474	ILE	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 oligosaccharides 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.