



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:34 AM UTC

PDB ID : 5IKN / pdb_00005ikn
Title : Crystal Structure of the T7 Replisome in the Absence of DNA
Authors : Wallen, J.R.; Ellenberger, T.
Deposited on : 2016-03-03
Resolution : 4.80 Å(reported)

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

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

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

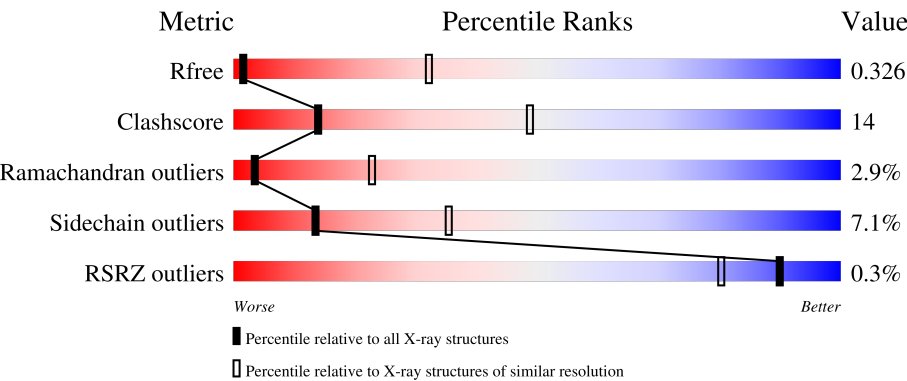
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
Sidechain outliers	187428	1085 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

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	704	65%22%9%
1	B	704	65%23%10%
1	C	704	65%23%10%
2	D	486	65%30%
2	E	486	63%31%5%

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Mol	Chain	Length	Quality of chain
2	F	486	% 59% 35% 6%
2	G	486	63% 31% 5%
2	H	486	% 64% 30% 5%
2	I	486	52% 36% 7%
2	J	486	62% 33%
3	K	105	78% 19%
3	L	105	2% 65% 32%
3	M	105	85% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43846 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 DNA-directed DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5092	3236	888	947	21			
1	B	636	Total	C	N	O	S	0	0	0
			5073	3226	884	942	21			
1	C	633	Total	C	N	O	S	0	0	0
			5041	3201	880	939	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	ASP	engineered mutation	UNP P00581
A	7	ALA	GLU	engineered mutation	UNP P00581
B	5	ALA	ASP	engineered mutation	UNP P00581
B	7	ALA	GLU	engineered mutation	UNP P00581
C	5	ALA	ASP	engineered mutation	UNP P00581
C	7	ALA	GLU	engineered mutation	UNP P00581

- Molecule 2 is a protein called DNA primase/helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	485	Total	C	N	O	S	0	0	0
			3763	2353	660	725	25			
2	E	485	Total	C	N	O	S	0	0	0
			3763	2353	660	725	25			
2	F	486	Total	C	N	O	S	0	0	0
			3768	2355	661	727	25			
2	G	484	Total	C	N	O	S	0	0	0
			3757	2350	659	723	25			
2	H	486	Total	C	N	O	S	0	0	0
			3768	2355	661	727	25			
2	I	472	Total	C	N	O	S	0	0	0
			3670	2295	647	703	25			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	483	Total	C	N	O	S	0	0	0
			3745	2341	658	721	25			

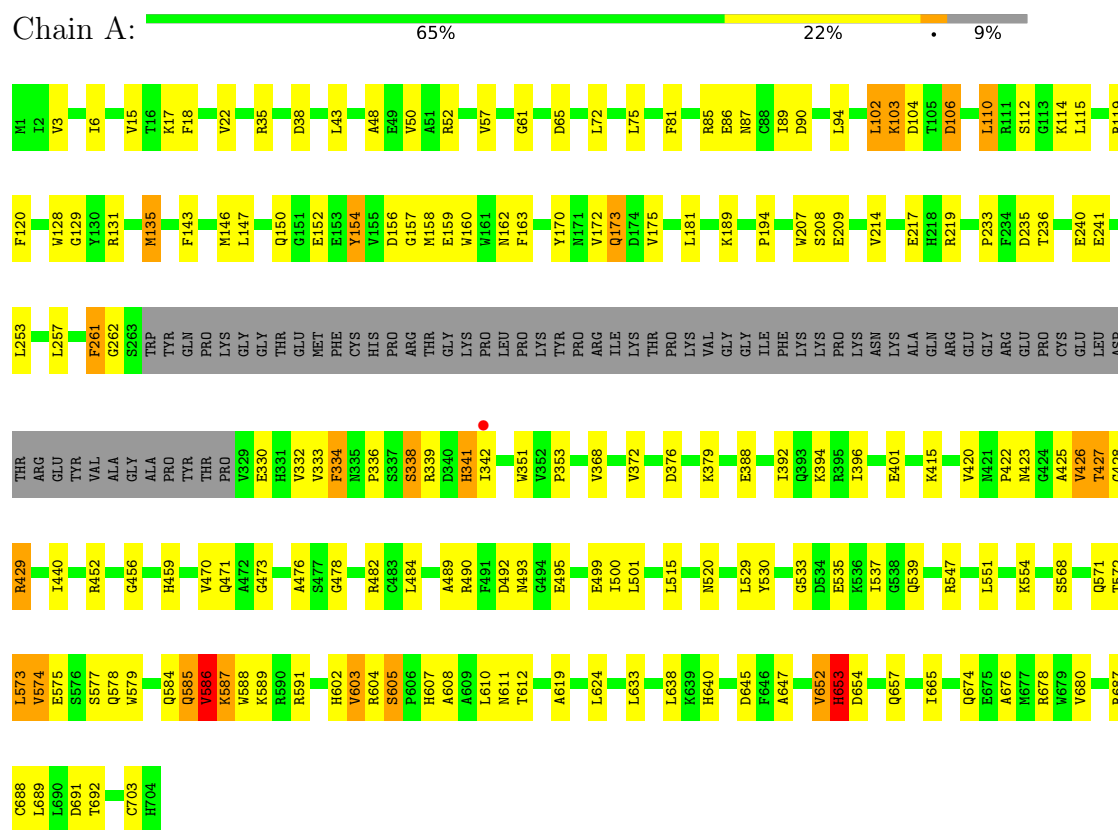
- Molecule 3 is a protein called Thioredoxin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			
3	L	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			
3	M	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			

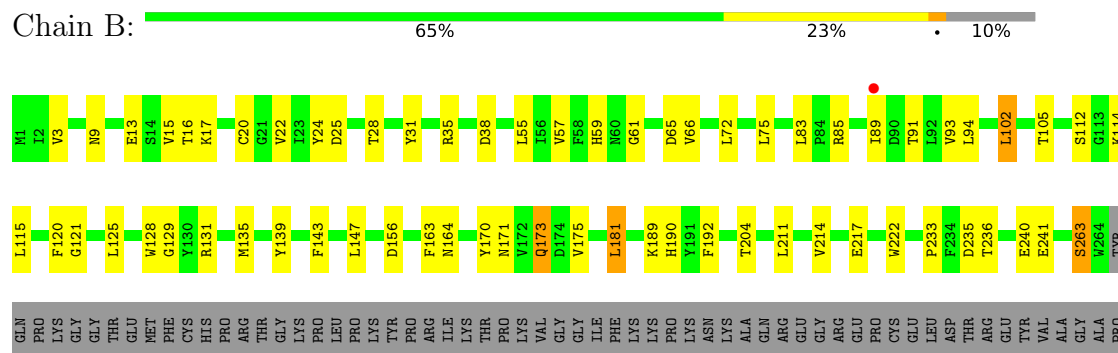
3 Residue-property plots

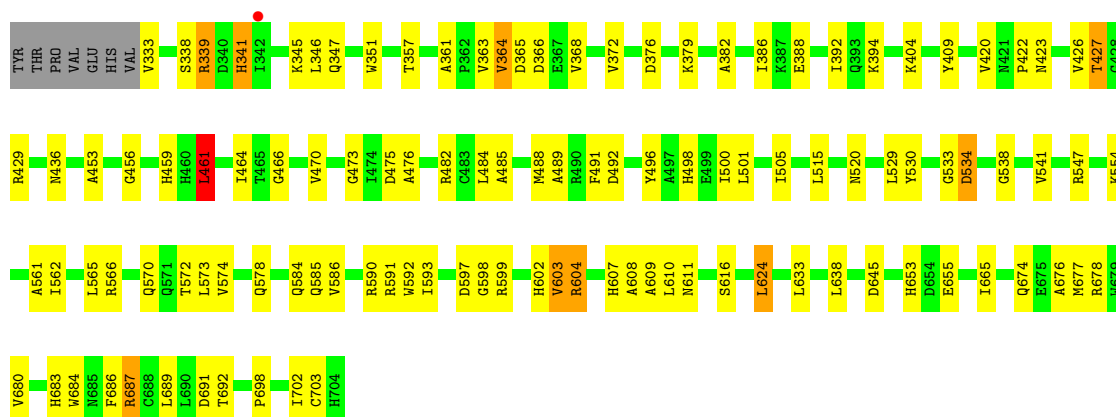
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



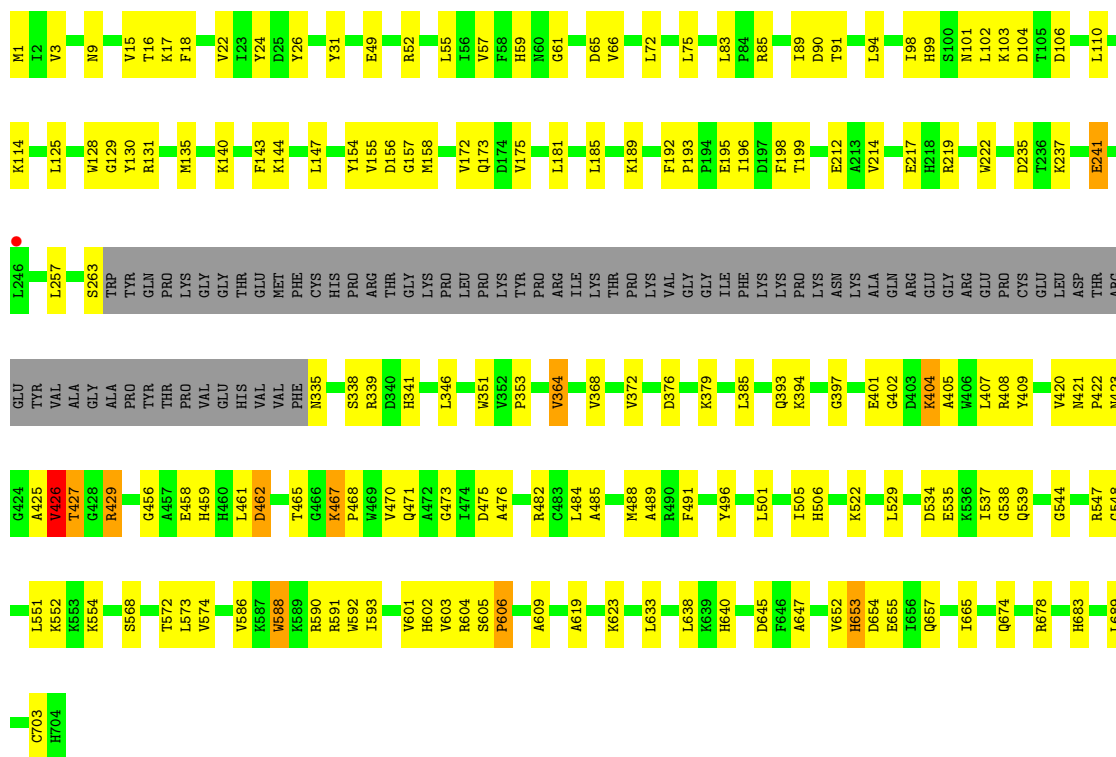
• Molecule 1: DNA-directed DNA polymerase





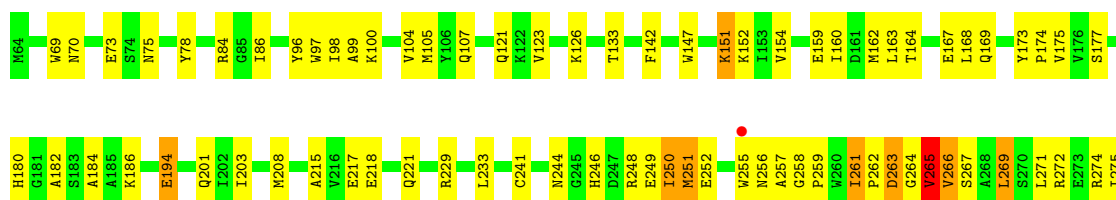
• Molecule 1: DNA-directed DNA polymerase

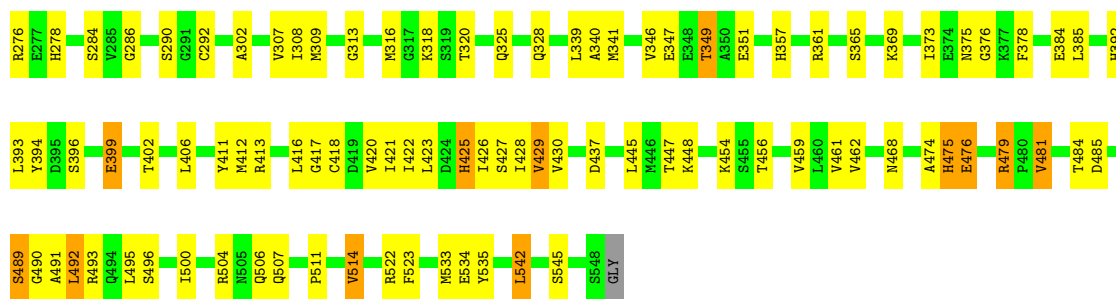
Chain C: 65% 23% 10%



• Molecule 2: DNA primase/helicase

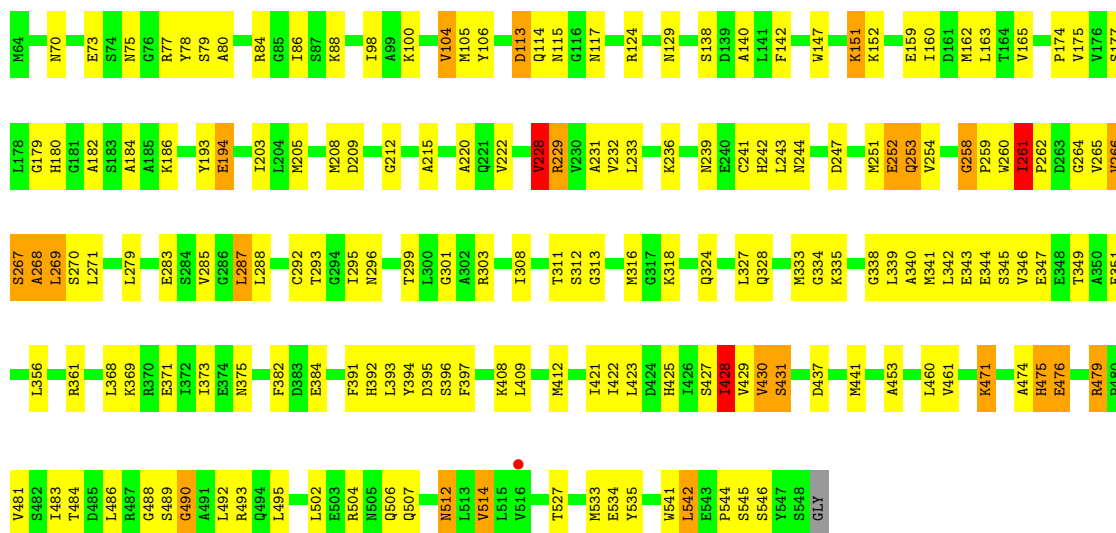
Chain D: 65% 30% 5%





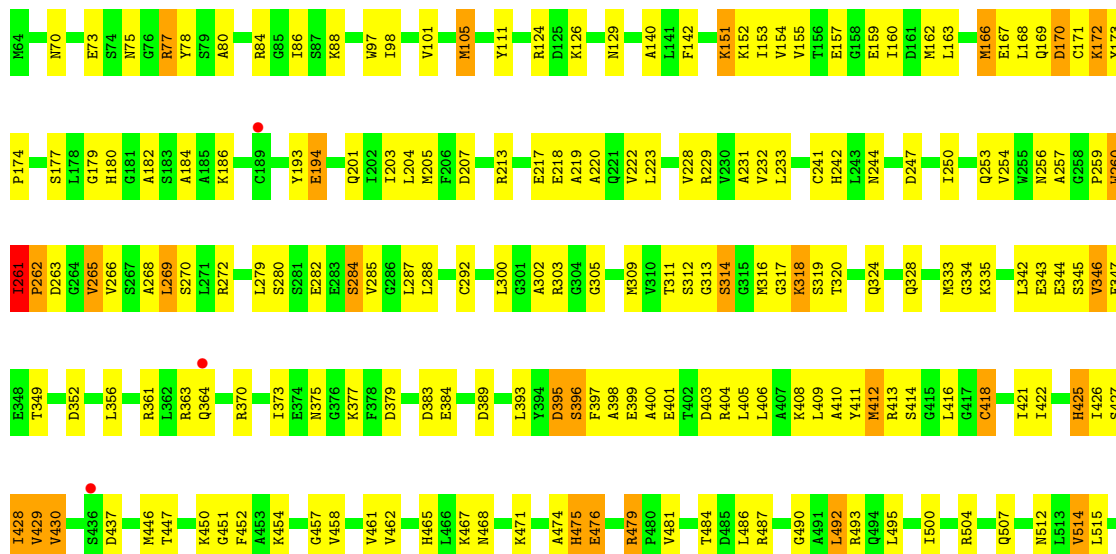
• Molecule 2: DNA primase/helicase

Chain E: 63% 31% 5%



• Molecule 2: DNA primase/helicase

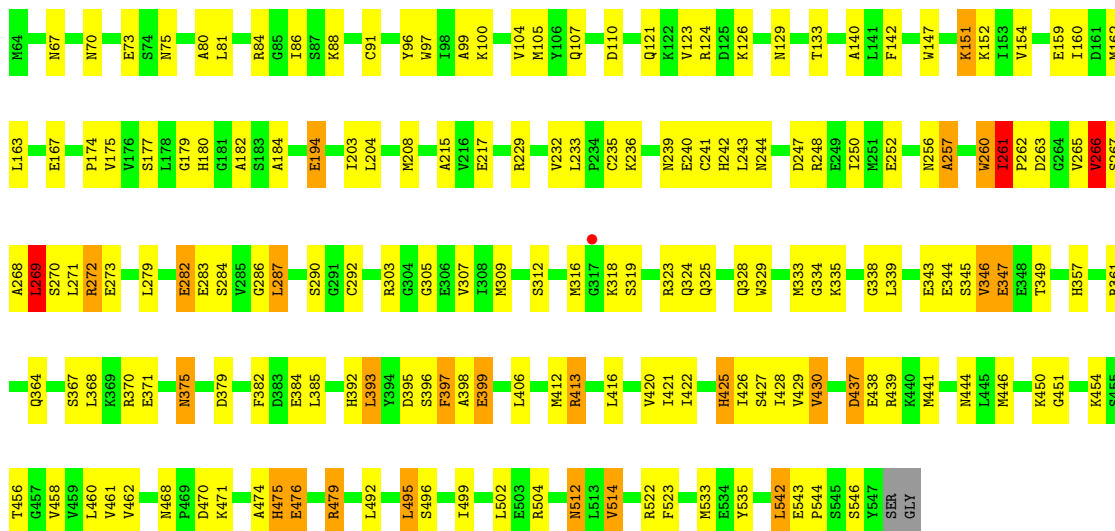
Chain F: 59% 35% 6%





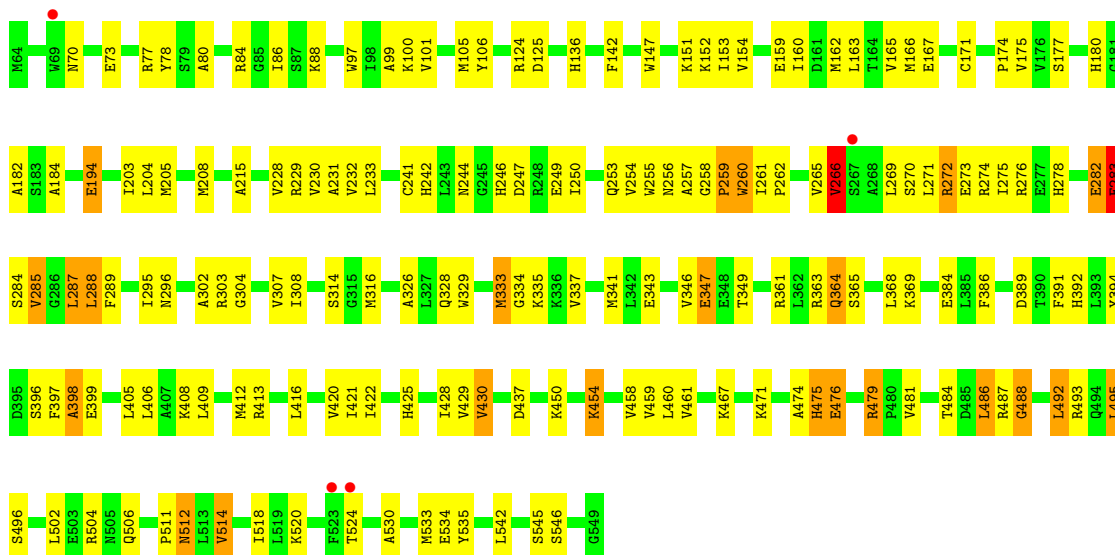
• Molecule 2: DNA primase/helicase

Chain G: 63% 31% 5%



• Molecule 2: DNA primase/helicase

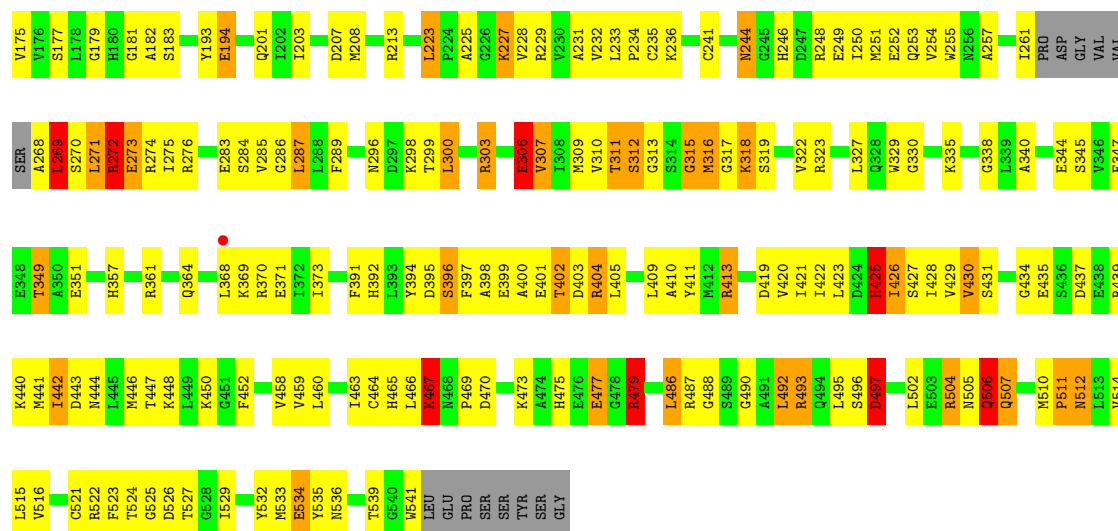
Chain H: 64% 30% 5%



• Molecule 2: DNA primase/helicase

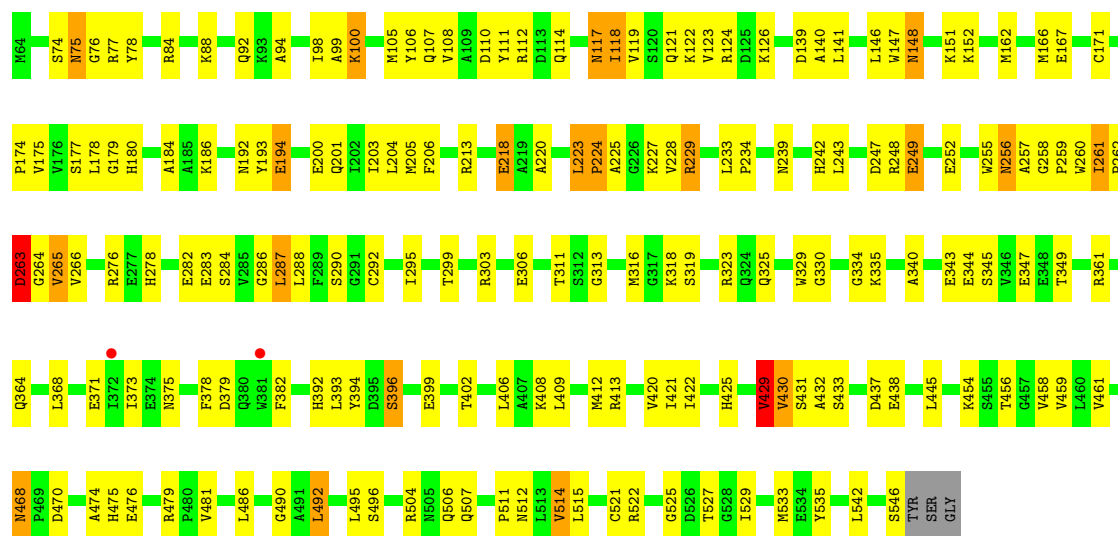
Chain I: 52% 36% 7%





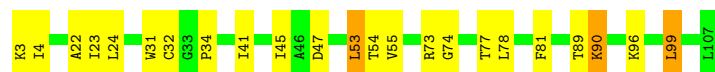
• Molecule 2: DNA primase/helicase

Chain J: 62% 33%



• Molecule 3: Thioredoxin-1

Chain K: 78% 19%



• Molecule 3: Thioredoxin-1

Chain L: 2% 65% 32%



● Molecule 3: Thioredoxin-1

Chain M:  85% 14% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.87Å 238.09Å 243.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 4.80 29.98 – 4.80	Depositor EDS
% Data completeness (in resolution range)	82.2 (29.98-4.80) 82.0 (29.98-4.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 4.86Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.275 , 0.318 0.284 , 0.326	Depositor DCC
R_{free} test set	2113 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	177.0	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 218.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	43846	wwPDB-VP
Average B, all atoms (Å ²)	240.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/5211	0.45	0/7045
1	B	0.16	0/5193	0.44	0/7021
1	C	0.15	0/5158	0.42	0/6972
2	D	0.16	0/3826	0.44	0/5152
2	E	0.19	0/3826	0.50	0/5152
2	F	0.19	0/3831	0.51	0/5157
2	G	0.16	0/3820	0.46	0/5144
2	H	0.18	0/3831	0.52	2/5157 (0.0%)
2	I	0.29	2/3729 (0.1%)	0.56	5/5016 (0.1%)
2	J	0.16	0/3807	0.48	0/5126
3	K	0.13	0/817	0.34	0/1108
3	L	0.17	0/817	0.43	0/1108
3	M	0.14	0/817	0.35	0/1108
All	All	0.18	2/44683 (0.0%)	0.47	7/60266 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	312	SER	CA-CB	6.11	1.64	1.53
2	I	318	LYS	CG-CD	5.17	1.68	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	318	LYS	CD-CE-NZ	9.63	142.71	111.90
2	I	318	LYS	CA-CB-CG	-6.57	100.96	114.10
2	I	312	SER	N-CA-CB	5.95	121.60	111.66
2	I	312	SER	CA-CB-OG	5.73	122.56	111.10
2	I	311	THR	CB-CA-C	-5.57	100.48	109.89
2	H	259	PRO	CA-C-N	5.20	131.05	121.70
2	H	259	PRO	C-N-CA	5.20	131.05	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5092	0	4986	117	0
1	B	5073	0	4965	104	0
1	C	5041	0	4937	99	0
2	D	3763	0	3724	125	0
2	E	3763	0	3724	127	0
2	F	3768	0	3727	150	1
2	G	3757	0	3719	136	0
2	H	3768	0	3727	136	0
2	I	3670	0	3638	193	0
2	J	3745	0	3710	131	0
3	K	802	0	816	15	0
3	L	802	0	816	24	1
3	M	802	0	816	10	0
All	All	43846	0	43305	1254	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 14.

All (1254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:318:LYS:NZ	2:I:502:LEU:H	1.20	1.34
2:I:318:LYS:HZ1	2:I:502:LEU:N	1.34	1.25
2:I:318:LYS:HE3	2:I:502:LEU:HB2	1.47	0.95
2:I:312:SER:HB3	2:I:318:LYS:CE	1.97	0.94
2:I:318:LYS:NZ	2:I:502:LEU:N	2.03	0.93
2:F:166:MET:HE3	2:F:166:MET:H	1.35	0.92
2:E:252:GLU:CD	2:E:252:GLU:H	1.79	0.87
2:I:311:THR:O	2:I:318:LYS:NZ	2.06	0.86
2:E:261:ILE:HB	2:E:262:PRO:HD3	1.58	0.83
2:G:105:MET:HB2	2:G:126:LYS:HD3	1.60	0.81
3:L:74:GLY:O	3:L:77:THR:OG1	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:GLU:HA	2:E:544:PRO:HG2	1.64	0.79
2:I:312:SER:N	2:I:318:LYS:HD2	1.97	0.79
2:J:283:GLU:HB3	2:J:286:GLY:HA3	1.64	0.79
2:I:425:HIS:H	2:I:463:ILE:HB	1.47	0.79
2:I:318:LYS:HE2	2:I:502:LEU:HD13	1.65	0.78
2:E:220:ALA:HB1	2:E:260:TRP:CD1	2.18	0.78
2:G:283:GLU:HB3	2:G:286:GLY:HA2	1.66	0.78
2:F:344:GLU:HA	2:G:454:LYS:HE2	1.66	0.78
2:J:223:LEU:HD13	2:J:228:VAL:HG21	1.66	0.78
2:E:344:GLU:HA	2:F:454:LYS:HE2	1.66	0.77
1:C:501:LEU:HD11	2:G:370:ARG:HD3	1.65	0.76
2:E:220:ALA:HB1	2:E:260:TRP:HD1	1.49	0.76
2:G:271:LEU:O	2:G:273:GLU:N	2.19	0.76
1:A:603:VAL:HG22	1:A:604:ARG:H	1.52	0.75
2:G:261:ILE:HG23	2:G:262:PRO:HD3	1.69	0.74
2:E:342:LEU:HB2	2:E:428:ILE:HD12	1.68	0.74
1:C:212:GLU:OE2	1:C:683:HIS:NE2	2.20	0.74
2:H:77:ARG:HH12	2:H:100:LYS:HD2	1.51	0.74
2:H:534:GLU:HG3	2:H:545:SER:HB2	1.70	0.74
2:G:379:ASP:OD1	2:H:276:ARG:NH2	2.21	0.73
2:F:124:ARG:HH22	2:F:159:GLU:HB2	1.53	0.73
2:H:328:GLN:HG3	2:H:333:MET:HE1	1.70	0.73
1:B:22:VAL:HB	1:B:175:VAL:HG21	1.71	0.73
2:E:324:GLN:HE22	2:E:542:LEU:HB2	1.54	0.73
1:C:55:LEU:HD13	1:C:89:ILE:HD11	1.72	0.72
2:E:259:PRO:HA	2:E:260:TRP:HB3	1.72	0.72
1:A:604:ARG:HG3	1:A:605:SER:H	1.55	0.72
3:L:77:THR:HG23	3:L:91:VAL:HG22	1.72	0.71
2:J:98:ILE:HG13	2:J:107:GLN:HG2	1.71	0.71
2:I:492:LEU:H	2:I:492:LEU:HD12	1.55	0.71
2:D:201:GLN:OE1	2:D:229:ARG:NH1	2.20	0.71
2:H:142:PHE:HB3	2:H:177:SER:HB3	1.72	0.71
2:E:412:MET:HE3	2:E:421:ILE:HD12	1.73	0.71
2:G:346:VAL:HB	2:G:393:LEU:HD13	1.72	0.71
1:A:484:LEU:HD22	1:A:529:LEU:HD21	1.73	0.71
2:G:412:MET:HE3	2:G:421:ILE:HD12	1.72	0.71
2:I:486:LEU:O	2:I:493:ARG:NH1	2.23	0.71
1:B:22:VAL:HG23	1:B:171:ASN:HD22	1.57	0.70
2:G:437:ASP:HB3	2:G:439:ARG:HG2	1.73	0.70
2:J:223:LEU:O	2:J:225:ALA:N	2.23	0.70
2:H:232:VAL:N	2:H:253:GLN:OE1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:ASN:ND2	2:D:100:LYS:O	2.24	0.70
2:I:515:LEU:HD21	2:I:529:ILE:HD12	1.72	0.70
2:E:408:LYS:HD3	2:F:263:ASP:HB3	1.73	0.70
2:I:208:MET:HE3	2:I:233:LEU:H	1.57	0.70
1:A:114:LYS:HG3	1:A:115:LEU:HG	1.74	0.69
3:L:26:ASP:HB3	3:L:57:LYS:HD2	1.73	0.69
3:L:38:ILE:HA	3:L:41:ILE:HD13	1.74	0.69
2:H:364:GLN:HG3	2:I:300:LEU:HD11	1.74	0.69
2:D:523:PHE:O	2:J:364:GLN:NE2	2.26	0.69
1:B:263:SER:HG	1:B:333:VAL:N	1.89	0.69
1:C:568:SER:O	1:C:572:THR:OG1	2.07	0.69
2:D:251:MET:SD	2:D:252:GLU:N	2.65	0.69
1:A:572:THR:N	1:A:573:LEU:HA	2.08	0.69
1:A:633:LEU:HD22	1:A:638:LEU:HD12	1.74	0.69
2:H:152:LYS:HD2	2:H:255:TRP:HD1	1.56	0.69
2:H:347:GLU:HB3	2:I:275:ILE:HG12	1.73	0.69
2:I:318:LYS:CE	2:I:502:LEU:HD13	2.23	0.69
2:E:471:LYS:O	2:E:479:ARG:NH2	2.25	0.69
1:C:674:GLN:HE21	1:C:678:ARG:HH22	1.38	0.68
2:H:361:ARG:NH1	2:H:535:TYR:OH	2.25	0.68
2:I:86:ILE:HG12	2:I:163:LEU:HB3	1.75	0.68
2:E:84:ARG:HE	2:E:160:ILE:HG21	1.59	0.68
2:F:395:ASP:HB3	2:G:266:VAL:HG21	1.75	0.68
1:B:376:ASP:HB3	1:B:379:LYS:HB2	1.75	0.68
1:C:1:MET:HB3	1:C:199:THR:HG23	1.75	0.68
2:H:307:VAL:HG22	2:H:460:LEU:HB3	1.74	0.68
2:I:312:SER:H	2:I:466:LEU:HD21	1.59	0.68
2:I:272:ARG:HD2	2:I:273:GLU:H	1.58	0.68
2:I:318:LYS:HZ2	2:I:502:LEU:H	1.38	0.68
2:J:361:ARG:NH1	2:J:535:TYR:OH	2.26	0.68
2:G:84:ARG:HE	2:G:160:ILE:HG21	1.59	0.68
2:I:318:LYS:HZ1	2:I:502:LEU:H	0.68	0.68
2:G:204:LEU:N	2:G:229:ARG:O	2.26	0.68
2:J:152:LYS:HG3	2:J:201:GLN:HG3	1.74	0.68
3:M:45:ILE:HG13	3:M:99:LEU:HD13	1.76	0.68
2:D:261:ILE:HG13	2:J:396:SER:HA	1.75	0.68
2:G:70:ASN:HB3	2:G:73:GLU:HB2	1.75	0.68
2:I:322:VAL:HG21	2:I:463:ILE:HD11	1.76	0.67
2:F:287:LEU:HD11	2:F:303:ARG:HD3	1.75	0.67
2:H:204:LEU:N	2:H:229:ARG:O	2.22	0.67
2:J:152:LYS:HD3	2:J:203:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:318:LYS:HE2	2:I:502:LEU:CD1	2.24	0.67
2:F:364:GLN:NE2	2:G:523:PHE:O	2.28	0.67
2:G:124:ARG:HH22	2:G:159:GLU:HB2	1.60	0.67
2:F:219:ALA:HA	2:F:223:LEU:HD13	1.77	0.67
2:F:287:LEU:HA	2:F:302:ALA:H	1.58	0.67
2:G:361:ARG:NH1	2:G:535:TYR:OH	2.27	0.66
2:I:307:VAL:HG22	2:I:460:LEU:HD23	1.75	0.66
2:J:180:HIS:HB2	2:J:184:ALA:HB3	1.76	0.66
1:A:471:GLN:NE2	1:A:657:GLN:OE1	2.26	0.66
2:I:312:SER:HB3	2:I:318:LYS:HE3	1.78	0.66
2:J:402:THR:HG23	2:J:445:LEU:HD13	1.75	0.66
1:B:345:LYS:O	1:B:347:GLN:N	2.24	0.66
2:H:287:LEU:HD21	2:H:302:ALA:HB3	1.78	0.66
2:I:234:PRO:HG3	2:I:249:GLU:HG2	1.78	0.66
2:G:252:GLU:O	2:G:257:ALA:N	2.28	0.66
2:G:154:VAL:HA	2:G:203:ILE:HB	1.77	0.66
2:I:246:HIS:HB3	2:I:249:GLU:HB2	1.78	0.66
2:I:400:ALA:HB1	2:I:404:ARG:HD2	1.77	0.66
1:B:427:THR:HG22	1:B:429:ARG:H	1.61	0.66
2:G:393:LEU:HD21	2:H:271:LEU:HD11	1.78	0.66
2:I:272:ARG:HD2	2:I:273:GLU:N	2.10	0.66
2:J:263:ASP:O	2:J:265:VAL:N	2.29	0.66
1:A:61:GLY:N	1:A:90:ASP:OD1	2.28	0.65
1:C:574:VAL:HG13	1:C:586:VAL:HG13	1.78	0.65
2:G:345:SER:HA	2:H:454:LYS:HE3	1.77	0.65
1:A:575:GLU:HB2	1:A:589:LYS:HG3	1.78	0.65
2:D:186:LYS:HB2	2:D:218:GLU:HB3	1.79	0.65
3:L:45:ILE:HG12	3:L:99:LEU:HD23	1.76	0.65
2:E:313:GLY:O	2:E:318:LYS:NZ	2.30	0.65
2:J:412:MET:HE3	2:J:421:ILE:HD12	1.79	0.65
2:E:475:HIS:H	2:E:479:ARG:HD2	1.62	0.65
2:F:162:MET:HB2	2:F:177:SER:HB2	1.79	0.65
2:F:422:ILE:HD13	2:F:461:VAL:HB	1.78	0.65
1:B:9:ASN:ND2	1:B:16:THR:OG1	2.29	0.64
1:C:15:VAL:HG22	1:C:72:LEU:HD21	1.79	0.64
2:D:454:LYS:HE2	2:J:344:GLU:HA	1.78	0.64
2:E:422:ILE:HD13	2:E:461:VAL:HB	1.79	0.64
1:A:112:SER:HB2	1:A:114:LYS:HG2	1.79	0.64
2:H:506:GLN:NE2	2:I:529:ILE:O	2.31	0.64
2:F:228:VAL:HB	2:F:260:TRP:CD1	2.31	0.64
2:G:397:PHE:HB2	2:H:454:LYS:HD2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:425:HIS:CE1	2:G:427:SER:HB2	2.33	0.64
2:J:330:GLY:HA2	2:J:335:LYS:H	1.61	0.64
2:H:288:LEU:HD21	2:H:333:MET:HG2	1.79	0.64
2:I:318:LYS:CE	2:I:502:LEU:HB2	2.25	0.64
2:J:107:GLN:OE1	2:J:124:ARG:NH1	2.30	0.64
2:F:324:GLN:HG3	2:F:356:LEU:HD21	1.80	0.64
2:J:287:LEU:HD21	2:J:335:LYS:HG3	1.80	0.64
2:I:467:LYS:HA	2:I:487:ARG:HG3	1.79	0.64
2:D:316:MET:HE3	2:D:504:ARG:HG2	1.79	0.63
2:H:486:LEU:HD12	2:H:487:ARG:H	1.64	0.63
2:F:342:LEU:HD12	2:F:428:ILE:HD13	1.80	0.63
2:H:266:VAL:HG11	2:H:271:LEU:HD13	1.79	0.63
3:M:23:ILE:HB	3:M:81:PHE:HB2	1.81	0.63
1:A:22:VAL:HG21	1:A:172:VAL:HG22	1.79	0.63
2:D:229:ARG:HH21	2:D:257:ALA:H	1.47	0.63
2:G:450:LYS:HG2	2:G:495:LEU:HD12	1.80	0.63
1:C:94:LEU:HD21	1:C:214:VAL:HG13	1.79	0.63
2:D:447:THR:HB	2:J:430:VAL:HG22	1.80	0.63
2:J:429:VAL:O	2:J:431:SER:N	2.31	0.63
1:A:103:LYS:N	1:A:104:ASP:HB2	2.14	0.63
1:A:577:SER:HA	1:A:587:LYS:HE2	1.81	0.63
2:J:186:LYS:HD3	2:J:218:GLU:HG3	1.81	0.63
2:E:394:TYR:HA	2:F:265:VAL:HG21	1.79	0.63
3:K:41:ILE:HD12	3:K:96:LYS:HB2	1.80	0.63
1:C:476:ALA:HB3	1:C:654:ASP:HB2	1.80	0.63
1:C:339:ARG:NH1	1:C:364:VAL:O	2.31	0.63
2:F:268:ALA:O	2:F:270:SER:N	2.30	0.63
2:I:521:CYS:O	2:I:525:GLY:N	2.24	0.63
2:D:84:ARG:HE	2:D:160:ILE:HG21	1.63	0.62
1:C:602:HIS:CG	1:C:603:VAL:H	2.18	0.62
2:E:260:TRP:CD1	2:E:261:ILE:HG12	2.33	0.62
1:C:217:GLU:OE2	1:C:623:LYS:NZ	2.30	0.62
2:E:484:THR:HA	2:E:493:ARG:HH22	1.65	0.62
2:E:267:SER:O	2:E:269:LEU:N	2.30	0.62
1:B:501:LEU:HD21	1:B:689:LEU:HB3	1.81	0.62
2:D:412:MET:HE3	2:D:421:ILE:HD12	1.80	0.62
2:I:284:SER:HA	2:I:523:PHE:HZ	1.65	0.62
1:B:94:LEU:HD21	1:B:214:VAL:HG13	1.82	0.61
1:B:645:ASP:HB3	1:B:665:ILE:HD13	1.82	0.61
2:F:163:LEU:C	2:F:166:MET:HE1	2.25	0.61
2:E:340:ALA:HB3	2:E:423:LEU:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:311:THR:O	2:I:311:THR:HG23	1.99	0.61
1:B:530:TYR:HA	1:B:611:ASN:HB2	1.83	0.61
1:C:49:GLU:OE1	1:C:52:ARG:NH2	2.26	0.61
2:E:299:THR:O	2:E:303:ARG:NH1	2.33	0.61
2:H:242:HIS:ND1	2:H:247:ASP:OD1	2.30	0.61
2:E:209:ASP:OD1	2:E:212:GLY:N	2.31	0.61
2:I:490:GLY:HA2	2:I:493:ARG:HE	1.66	0.61
2:G:316:MET:HE3	2:G:504:ARG:HG2	1.83	0.61
1:B:15:VAL:HG22	1:B:72:LEU:HD21	1.83	0.61
1:C:633:LEU:HD22	1:C:638:LEU:HD12	1.81	0.61
2:F:242:HIS:ND1	2:F:247:ASP:OD1	2.26	0.61
1:A:3:VAL:HA	1:A:57:VAL:HB	1.83	0.61
2:D:142:PHE:HB3	2:D:177:SER:HB3	1.82	0.61
2:E:341:MET:HB3	2:E:344:GLU:HG2	1.81	0.61
2:E:474:ALA:O	2:E:476:GLU:N	2.34	0.61
1:A:573:LEU:HD23	1:A:574:VAL:H	1.67	0.60
1:B:61:GLY:HA2	1:B:65:ASP:HB2	1.82	0.60
2:E:261:ILE:HB	2:E:262:PRO:CD	2.30	0.60
2:G:282:GLU:HG3	2:G:284:SER:H	1.65	0.60
1:C:404:LYS:HA	1:C:409:TYR:HE2	1.66	0.60
2:D:402:THR:HG23	2:D:445:LEU:HD13	1.82	0.60
2:J:506:GLN:HA	2:J:511:PRO:HB3	1.81	0.60
2:D:276:ARG:HD3	2:J:373:ILE:HG12	1.82	0.60
1:A:571:GLN:HA	1:A:573:LEU:HG	1.83	0.60
2:I:316:MET:SD	2:I:316:MET:N	2.72	0.60
2:I:395:ASP:H	2:J:265:VAL:HG11	1.66	0.60
1:B:128:TRP:CE3	1:B:131:ARG:HD2	2.37	0.60
2:F:260:TRP:HA	2:F:261:ILE:HB	1.82	0.60
2:F:305:GLY:HA2	2:F:454:LYS:HA	1.84	0.60
2:I:351:GLU:OE1	2:J:278:HIS:ND1	2.34	0.60
2:G:422:ILE:HD13	2:G:461:VAL:HB	1.84	0.60
2:D:105:MET:HB2	2:D:126:LYS:HE3	1.83	0.60
2:D:265:VAL:HG13	2:D:266:VAL:H	1.65	0.60
2:G:86:ILE:HG12	2:G:163:LEU:HB3	1.82	0.60
1:A:429:ARG:HH12	1:A:652:VAL:HG12	1.67	0.59
2:E:86:ILE:HG12	2:E:163:LEU:HB3	1.83	0.59
1:A:129:GLY:HA3	1:A:135:MET:HG2	1.83	0.59
2:E:431:SER:HB3	2:E:441:MET:HE2	1.83	0.59
2:H:316:MET:HE3	2:H:504:ARG:HG2	1.84	0.59
2:F:409:LEU:HA	2:F:412:MET:HE2	1.84	0.59
1:A:476:ALA:HB3	1:A:654:ASP:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:180:HIS:HB2	2:G:184:ALA:HB3	1.85	0.59
1:A:341:HIS:CG	1:A:342:ILE:H	2.21	0.59
2:D:276:ARG:NH2	2:J:379:ASP:OD2	2.34	0.59
2:F:260:TRP:CD2	2:F:261:ILE:HG22	2.38	0.59
2:H:394:TYR:CZ	2:H:396:SER:HB2	2.37	0.59
2:I:312:SER:HB3	2:I:318:LYS:CD	2.32	0.59
2:D:250:ILE:HD12	2:D:251:MET:H	1.67	0.59
2:H:474:ALA:O	2:H:476:GLU:N	2.35	0.59
2:I:312:SER:O	2:I:466:LEU:HG	2.03	0.59
2:E:345:SER:H	2:F:454:LYS:HE3	1.67	0.59
2:H:258:GLY:N	2:H:259:PRO:HD3	2.18	0.59
3:M:23:ILE:O	3:M:81:PHE:N	2.31	0.59
2:D:426:ILE:HD12	2:D:462:VAL:HG11	1.84	0.59
1:A:18:PHE:HB2	1:A:72:LEU:HD13	1.85	0.59
1:B:363:VAL:HG22	1:B:364:VAL:H	1.68	0.59
2:G:346:VAL:HG11	2:G:395:ASP:HB2	1.84	0.59
1:C:590:ARG:HD2	1:C:592:TRP:O	2.02	0.58
2:D:506:GLN:HA	2:D:511:PRO:HB3	1.84	0.58
2:I:505:ASN:O	2:I:507:GLN:N	2.36	0.58
2:H:154:VAL:HA	2:H:203:ILE:HB	1.84	0.58
2:I:207:ASP:O	2:I:213:ARG:NH2	2.32	0.58
2:J:514:VAL:HG13	2:J:533:MET:HB2	1.85	0.58
1:A:515:LEU:HD12	1:A:520:ASN:HB3	1.84	0.58
1:B:633:LEU:HD22	1:B:638:LEU:HD12	1.85	0.58
2:F:352:ASP:OD2	2:F:363:ARG:NH2	2.37	0.58
2:H:271:LEU:HD12	2:H:275:ILE:HD11	1.84	0.58
2:F:166:MET:SD	2:F:167:GLU:N	2.76	0.58
1:A:233:PRO:HA	1:A:415:LYS:HG2	1.85	0.58
1:A:425:ALA:O	1:A:427:THR:N	2.36	0.58
2:D:86:ILE:HG12	2:D:163:LEU:HB3	1.84	0.58
2:I:521:CYS:SG	2:I:524:THR:OG1	2.58	0.58
1:A:61:GLY:HA2	1:A:65:ASP:HB2	1.85	0.58
2:H:256:ASN:O	2:H:258:GLY:N	2.36	0.58
2:H:287:LEU:HD11	2:H:302:ALA:H	1.69	0.58
2:J:84:ARG:NH1	2:J:239:ASN:OD1	2.36	0.58
2:J:201:GLN:HB2	2:J:229:ARG:HD2	1.86	0.58
1:A:376:ASP:HB3	1:A:379:LYS:HB2	1.86	0.58
1:A:473:GLY:HA3	1:A:703:CYS:HB3	1.84	0.58
1:A:585:GLN:O	1:A:587:LYS:HD3	2.04	0.58
2:D:373:ILE:HA	2:D:378:PHE:HB2	1.86	0.58
2:D:399:GLU:HB3	2:D:430:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:LYS:HG3	2:E:105:MET:SD	2.44	0.58
2:F:166:MET:HE3	2:F:166:MET:N	2.13	0.58
2:G:248:ARG:O	2:G:252:GLU:HG3	2.04	0.58
2:G:474:ALA:O	2:G:476:GLU:N	2.37	0.58
1:A:501:LEU:HD21	1:A:689:LEU:HB3	1.85	0.58
2:I:396:SER:O	2:I:398:ALA:N	2.37	0.58
2:J:313:GLY:O	2:J:318:LYS:NZ	2.37	0.58
2:I:312:SER:OG	2:I:315:GLY:O	2.22	0.58
1:B:590:ARG:NH1	1:B:592:TRP:O	2.37	0.57
2:E:142:PHE:HB3	2:E:177:SER:HB3	1.86	0.57
2:I:162:MET:HB2	2:I:177:SER:HB2	1.85	0.57
2:D:393:LEU:O	2:E:265:VAL:HB	2.03	0.57
2:F:186:LYS:HG3	2:F:222:VAL:HG21	1.86	0.57
1:C:263:SER:HB2	3:M:64:PRO:HB2	1.86	0.57
2:G:399:GLU:HB2	2:G:430:VAL:HG11	1.85	0.57
2:H:154:VAL:HG11	2:H:165:VAL:HG11	1.86	0.57
2:I:251:MET:SD	2:I:252:GLU:N	2.77	0.57
2:G:397:PHE:CD2	2:H:454:LYS:HB3	2.39	0.57
2:H:506:GLN:HA	2:H:511:PRO:HB3	1.86	0.57
2:H:162:MET:HG2	2:H:175:VAL:HG12	1.85	0.57
2:J:422:ILE:HD13	2:J:461:VAL:HB	1.85	0.57
2:J:118:ILE:HD13	2:J:118:ILE:H	1.67	0.57
1:A:645:ASP:HB3	1:A:665:ILE:HD13	1.85	0.57
2:D:493:ARG:NH2	2:J:468:ASN:OD1	2.38	0.57
2:H:422:ILE:HD13	2:H:461:VAL:HB	1.86	0.57
2:H:475:HIS:H	2:H:479:ARG:HD2	1.69	0.57
2:I:241:CYS:HB3	2:I:246:HIS:HB2	1.87	0.57
2:J:228:VAL:O	2:J:259:PRO:HA	2.04	0.57
1:B:404:LYS:HA	1:B:409:TYR:HE2	1.70	0.57
2:E:361:ARG:NH1	2:E:535:TYR:OH	2.38	0.57
2:F:70:ASN:HB3	2:F:73:GLU:HB2	1.86	0.57
2:F:416:LEU:HG	2:G:262:PRO:HG2	1.85	0.57
2:F:474:ALA:O	2:F:476:GLU:N	2.38	0.57
2:I:147:TRP:CE2	2:I:174:PRO:HA	2.39	0.57
1:B:473:GLY:HA3	1:B:703:CYS:HB3	1.87	0.57
2:D:425:HIS:CE1	2:D:427:SER:HB2	2.40	0.57
1:C:26:TYR:CG	1:C:199:THR:HG21	2.40	0.56
2:H:389:ASP:HA	2:I:268:ALA:HB2	1.85	0.56
3:L:82:LYS:NZ	3:L:106:ASN:O	2.38	0.56
1:C:212:GLU:CD	1:C:683:HIS:HE2	2.12	0.56
2:G:252:GLU:HG2	2:G:256:ASN:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:405:LEU:O	2:I:409:LEU:HD12	2.06	0.56
2:J:229:ARG:HH21	2:J:259:PRO:HD3	1.71	0.56
1:B:482:ARG:HG2	1:B:500:ILE:HG21	1.86	0.56
2:E:488:GLY:O	2:E:490:GLY:N	2.39	0.56
2:H:282:GLU:HG2	2:H:283:GLU:HG2	1.87	0.56
2:H:283:GLU:OE1	2:H:304:GLY:N	2.33	0.56
2:H:484:THR:HA	2:H:493:ARG:HH22	1.70	0.56
2:I:306:GLU:N	2:I:497:ASP:HB2	2.20	0.56
1:B:674:GLN:HG2	1:B:692:THR:OG1	2.05	0.56
2:F:426:ILE:HD12	2:F:462:VAL:HG11	1.86	0.56
2:H:412:MET:HE3	2:H:421:ILE:HD12	1.88	0.56
2:H:496:SER:O	2:H:520:LYS:NZ	2.38	0.56
2:J:234:PRO:HG2	2:J:249:GLU:HG2	1.86	0.56
2:D:229:ARG:HE	2:D:257:ALA:HB3	1.70	0.56
2:D:365:SER:O	2:D:369:LYS:HG3	2.06	0.56
2:D:475:HIS:H	2:D:479:ARG:HB3	1.71	0.56
2:E:338:GLY:O	2:E:422:ILE:N	2.38	0.56
2:D:476:GLU:HG3	2:E:483:ILE:HD12	1.88	0.56
2:F:413:ARG:HD3	2:F:458:VAL:HB	1.87	0.56
2:G:96:TYR:OH	2:G:107:GLN:NE2	2.34	0.56
2:I:327:LEU:HD21	2:I:357:HIS:CD2	2.41	0.56
2:J:239:ASN:HA	2:J:242:HIS:CD2	2.41	0.56
3:K:74:GLY:O	3:K:77:THR:OG1	2.24	0.56
1:B:603:VAL:HG13	1:B:604:ARG:H	1.70	0.56
2:F:400:ALA:HB1	2:F:405:LEU:HD22	1.87	0.56
1:A:674:GLN:HG2	1:A:692:THR:OG1	2.06	0.55
2:F:410:ALA:HA	2:F:452:PHE:CE1	2.41	0.55
1:A:170:TYR:HA	1:A:173:GLN:HB2	1.89	0.55
2:D:484:THR:HG21	2:J:474:ALA:HB3	1.89	0.55
2:D:489:SER:O	2:D:491:ALA:N	2.40	0.55
2:F:166:MET:HG2	2:F:171:CYS:HA	1.89	0.55
2:H:283:GLU:HA	2:H:285:VAL:HG12	1.88	0.55
2:I:229:ARG:HA	2:I:257:ALA:HA	1.88	0.55
2:J:278:HIS:CE1	2:J:282:GLU:HG3	2.41	0.55
2:F:425:HIS:CE1	2:F:427:SER:HB2	2.41	0.55
2:J:193:TYR:OH	2:J:224:PRO:O	2.23	0.55
1:B:591:ARG:O	1:B:602:HIS:ND1	2.39	0.55
2:D:221:GLN:O	2:D:274:ARG:NH2	2.39	0.55
2:F:180:HIS:HB2	2:F:184:ALA:HB3	1.89	0.55
3:L:45:ILE:HD11	3:L:96:LYS:HG3	1.89	0.55
1:C:61:GLY:HA2	1:C:65:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:ILE:H	2:D:261:ILE:HD13	1.72	0.55
2:I:403:ASP:OD1	2:I:448:LYS:NZ	2.27	0.55
2:D:70:ASN:HB3	2:D:73:GLU:HB2	1.88	0.55
2:H:386:PHE:HB3	2:I:268:ALA:N	2.22	0.55
1:A:189:LYS:HG2	1:A:194:PRO:HG3	1.89	0.55
1:B:129:GLY:HA3	1:B:135:MET:HG2	1.89	0.55
2:F:142:PHE:HB3	2:F:177:SER:HB3	1.89	0.55
2:F:412:MET:O	2:F:414:SER:N	2.34	0.55
1:B:20:CYS:HB3	1:B:163:PHE:HE1	1.71	0.55
2:D:180:HIS:HB2	2:D:184:ALA:HB3	1.88	0.55
2:F:203:ILE:HA	2:F:229:ARG:HB2	1.88	0.55
2:H:408:LYS:HE2	2:I:261:ILE:HD12	1.89	0.55
2:D:339:LEU:N	2:D:392:HIS:O	2.36	0.55
2:F:282:GLU:CD	2:F:285:VAL:HG22	2.31	0.55
3:M:74:GLY:O	3:M:77:THR:OG1	2.24	0.55
1:A:106:ASP:O	1:A:110:LEU:N	2.36	0.54
1:B:170:TYR:HA	1:B:173:GLN:HB2	1.89	0.54
2:E:162:MET:HG2	2:E:175:VAL:HG12	1.88	0.54
2:E:194:GLU:H	2:E:194:GLU:CD	2.14	0.54
2:I:272:ARG:HB3	2:I:275:ILE:HD12	1.89	0.54
2:I:467:LYS:HG3	2:I:487:ARG:HA	1.87	0.54
1:A:591:ARG:HG2	1:A:602:HIS:O	2.07	0.54
2:E:205:MET:HA	2:E:231:ALA:HB3	1.87	0.54
2:H:271:LEU:HB3	2:H:275:ILE:HD12	1.88	0.54
3:K:23:ILE:HB	3:K:81:PHE:HB2	1.88	0.54
3:K:45:ILE:HG13	3:K:99:LEU:HD13	1.88	0.54
2:H:289:PHE:HB2	2:H:296:ASN:OD1	2.07	0.54
2:I:446:MET:HG3	2:I:492:LEU:HG	1.89	0.54
1:A:22:VAL:HB	1:A:175:VAL:HG21	1.89	0.54
2:E:180:HIS:HB2	2:E:184:ALA:HB3	1.90	0.54
2:F:343:GLU:OE1	2:G:522:ARG:NH2	2.41	0.54
2:H:260:TRP:C	2:H:262:PRO:HD3	2.33	0.54
1:C:501:LEU:HD21	1:C:689:LEU:HB3	1.89	0.54
2:D:276:ARG:HH21	2:J:378:PHE:HD2	1.54	0.54
2:G:343:GLU:HA	2:G:397:PHE:HE1	1.73	0.54
2:H:397:PHE:O	2:H:399:GLU:N	2.39	0.54
2:J:242:HIS:HB2	2:J:247:ASP:OD1	2.07	0.54
2:D:392:HIS:CD2	2:D:416:LEU:HD13	2.43	0.54
2:F:425:HIS:HE1	2:F:427:SER:HB2	1.73	0.54
2:H:314:SER:HG	2:I:527:THR:HG1	1.55	0.54
2:J:340:ALA:HA	2:J:394:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:MET:HE2	1:A:150:GLN:HE22	1.72	0.54
1:C:9:ASN:ND2	1:C:16:THR:OG1	2.41	0.54
2:E:514:VAL:HG13	2:E:533:MET:HB2	1.90	0.54
2:G:81:LEU:HD21	2:G:96:TYR:HE2	1.72	0.54
2:G:100:LYS:HG3	2:G:105:MET:SD	2.48	0.54
2:H:333:MET:SD	2:H:333:MET:N	2.81	0.54
2:I:232:VAL:HG21	2:I:270:SER:HB3	1.89	0.54
1:A:102:LEU:HD11	1:A:131:ARG:NH2	2.23	0.54
1:C:461:LEU:HD22	1:C:468:PRO:HA	1.90	0.54
2:F:151:LYS:HD2	2:F:152:LYS:HG3	1.89	0.54
2:F:383:ASP:OD1	2:G:272:ARG:NH2	2.40	0.54
2:D:290:SER:N	2:D:325:GLN:OE1	2.41	0.54
2:G:339:LEU:HB2	2:G:393:LEU:HB3	1.89	0.54
2:J:261:ILE:O	2:J:263:ASP:N	2.40	0.54
1:B:204:THR:O	2:F:375:ASN:ND2	2.42	0.53
1:B:608:ALA:C	1:B:610:LEU:H	2.15	0.53
1:B:683:HIS:CE1	2:F:370:ARG:HH12	2.26	0.53
2:F:232:VAL:N	2:F:253:GLN:OE1	2.23	0.53
2:H:86:ILE:HG12	2:H:163:LEU:HB3	1.90	0.53
2:J:74:SER:O	2:J:76:GLY:N	2.35	0.53
2:E:70:ASN:HB3	2:E:73:GLU:HB2	1.90	0.53
2:F:259:PRO:HA	2:F:260:TRP:HB3	1.90	0.53
3:L:90:LYS:HD3	3:L:91:VAL:N	2.23	0.53
2:G:268:ALA:O	2:G:270:SER:N	2.39	0.53
2:I:401:GLU:H	2:I:431:SER:HB3	1.74	0.53
1:A:86:GLU:O	1:A:207:TRP:NE1	2.35	0.53
1:B:102:LEU:HD23	1:B:105:THR:HB	1.90	0.53
2:H:272:ARG:HH21	2:H:276:ARG:HB3	1.73	0.53
2:I:318:LYS:CE	2:I:502:LEU:CD1	2.85	0.53
1:C:22:VAL:HB	1:C:175:VAL:HG21	1.90	0.53
1:C:423:ASN:HB2	1:C:623:LYS:NZ	2.24	0.53
2:D:272:ARG:HB2	2:J:382:PHE:CZ	2.44	0.53
2:I:442:ILE:HD12	2:I:492:LEU:HD11	1.91	0.53
2:I:477:GLU:HG3	2:I:507:GLN:HE22	1.73	0.53
2:J:162:MET:HB2	2:J:177:SER:HB2	1.91	0.53
1:A:493:ASN:ND2	2:E:292:CYS:SG	2.82	0.53
2:I:70:ASN:HB3	2:I:73:GLU:HB2	1.90	0.53
2:I:124:ARG:HH22	2:I:159:GLU:HB2	1.73	0.53
2:J:110:ASP:OD1	2:J:121:GLN:NE2	2.39	0.53
1:C:573:LEU:HD11	1:C:593:ILE:HG12	1.91	0.53
2:E:409:LEU:HA	2:E:412:MET:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:201:GLN:HA	2:I:227:LYS:HG2	1.91	0.53
2:H:399:GLU:HB3	2:H:430:VAL:HG11	1.91	0.53
2:F:395:ASP:HB3	2:G:266:VAL:CG2	2.39	0.53
2:G:438:GLU:HA	2:G:441:MET:HG2	1.91	0.53
2:I:231:ALA:HA	2:I:253:GLN:HB3	1.91	0.53
1:C:482:ARG:NH1	1:C:689:LEU:O	2.43	0.52
2:E:79:SER:HB3	2:E:98:ILE:HD13	1.91	0.52
2:E:397:PHE:CE2	2:F:450:LYS:HG3	2.44	0.52
2:F:261:ILE:HG23	2:F:262:PRO:HD3	1.91	0.52
2:J:162:MET:HG2	2:J:175:VAL:HG12	1.90	0.52
1:B:235:ASP:HB2	1:B:459:HIS:CG	2.44	0.52
2:J:166:MET:O	2:J:171:CYS:N	2.36	0.52
1:A:233:PRO:HG3	1:A:415:LYS:HE3	1.91	0.52
2:E:371:GLU:O	2:E:375:ASN:ND2	2.39	0.52
1:A:575:GLU:CB	1:A:589:LYS:HG3	2.40	0.52
1:B:492:ASP:HB3	1:B:561:ALA:HB2	1.90	0.52
2:D:422:ILE:HD13	2:D:461:VAL:HB	1.91	0.52
2:E:316:MET:HA	2:E:504:ARG:HH11	1.75	0.52
2:F:220:ALA:HB2	2:F:261:ILE:HG21	1.90	0.52
2:G:395:ASP:CG	2:H:274:ARG:HH12	2.17	0.52
2:H:194:GLU:CD	2:H:194:GLU:H	2.16	0.52
2:H:450:LYS:NZ	2:H:495:LEU:O	2.34	0.52
2:J:141:LEU:HD23	2:J:192:ASN:HD22	1.74	0.52
2:J:429:VAL:HG13	2:J:430:VAL:H	1.74	0.52
1:B:541:VAL:HG21	1:B:547:ARG:HD3	1.90	0.52
2:D:250:ILE:HD12	2:D:251:MET:N	2.24	0.52
2:D:411:TYR:OH	2:E:260:TRP:O	2.26	0.52
2:F:312:SER:N	2:F:318:LYS:HD3	2.23	0.52
2:F:317:GLY:O	2:F:319:SER:N	2.40	0.52
2:H:333:MET:O	2:H:335:LYS:HG2	2.09	0.52
2:D:351:GLU:HG3	2:E:279:LEU:HD21	1.91	0.52
2:G:392:HIS:CD2	2:G:416:LEU:HD13	2.45	0.52
2:H:502:LEU:HD23	2:H:514:VAL:HG21	1.92	0.52
2:I:248:ARG:HA	2:I:251:MET:HE1	1.90	0.52
2:I:373:ILE:HD12	2:J:276:ARG:HD3	1.91	0.52
2:E:333:MET:O	2:E:335:LYS:N	2.42	0.52
2:G:241:CYS:HB2	2:G:250:ILE:HD11	1.90	0.52
2:G:364:GLN:HE21	2:H:524:THR:HA	1.73	0.52
2:I:84:ARG:HE	2:I:160:ILE:HG21	1.75	0.52
2:I:287:LEU:HD11	2:I:335:LYS:HE2	1.91	0.52
2:I:404:ARG:HB3	2:I:404:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:505:ASN:HB2	2:I:510:MET:HB2	1.91	0.52
2:E:340:ALA:N	2:E:422:ILE:O	2.42	0.52
2:E:343:GLU:OE1	2:F:522:ARG:NH2	2.42	0.52
2:I:533:MET:SD	2:I:534:GLU:N	2.83	0.52
1:C:22:VAL:HG21	1:C:172:VAL:HG22	1.92	0.52
2:D:269:LEU:HD13	2:J:382:PHE:HE1	1.74	0.52
2:F:389:ASP:HA	2:G:269:LEU:HD13	1.91	0.52
2:I:420:VAL:HG22	2:I:459:VAL:HB	1.92	0.52
1:A:608:ALA:O	1:A:610:LEU:N	2.38	0.52
2:D:246:HIS:HB3	2:D:249:GLU:HB2	1.92	0.52
2:E:232:VAL:HB	2:E:253:GLN:HE22	1.75	0.52
2:E:339:LEU:HB2	2:E:393:LEU:HA	1.92	0.52
2:E:512:ASN:OD1	2:E:512:ASN:N	2.43	0.52
2:F:284:SER:HB3	2:F:303:ARG:HG3	1.92	0.52
1:B:55:LEU:HD13	1:B:89:ILE:HD11	1.91	0.51
2:D:392:HIS:HD2	2:D:416:LEU:HD13	1.74	0.51
2:G:514:VAL:HG13	2:G:533:MET:HB2	1.93	0.51
2:H:420:VAL:HG22	2:H:459:VAL:HB	1.92	0.51
1:A:396:ILE:HG22	1:A:401:GLU:HB2	1.92	0.51
2:G:194:GLU:H	2:G:194:GLU:CD	2.17	0.51
2:H:266:VAL:HB	2:H:270:SER:O	2.10	0.51
2:I:181:GLY:O	2:I:183:SER:N	2.36	0.51
2:J:117:ASN:OD1	2:J:117:ASN:N	2.27	0.51
1:B:608:ALA:O	1:B:610:LEU:N	2.39	0.51
3:L:22:ALA:HB1	3:L:80:LEU:HD11	1.90	0.51
1:A:147:LEU:HD13	1:A:154:TYR:HB3	1.92	0.51
1:B:35:ARG:H	1:B:38:ASP:HB2	1.75	0.51
2:F:170:ASP:CG	2:F:170:ASP:O	2.52	0.51
2:I:75:ASN:ND2	2:I:100:LYS:O	2.40	0.51
2:I:80:ALA:HB2	2:I:88:LYS:HG3	1.92	0.51
1:C:235:ASP:HB2	1:C:459:HIS:CE1	2.45	0.51
1:C:456:GLY:HA2	1:C:471:GLN:OE1	2.10	0.51
2:D:484:THR:HA	2:D:493:ARG:HH22	1.74	0.51
2:H:467:LYS:HE3	2:H:487:ARG:HD3	1.92	0.51
2:I:312:SER:N	2:I:466:LEU:HD21	2.23	0.51
1:B:484:LEU:HD22	1:B:529:LEU:HD21	1.92	0.51
1:C:106:ASP:CG	1:C:131:ARG:HH22	2.17	0.51
1:C:484:LEU:HD22	1:C:529:LEU:HD21	1.93	0.51
2:E:324:GLN:HG3	2:E:356:LEU:HD21	1.92	0.51
1:B:496:TYR:CZ	1:B:505:ILE:HD11	2.45	0.51
2:E:308:ILE:HB	2:E:461:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:397:PHE:CD2	2:G:451:GLY:HA2	2.46	0.51
2:H:492:LEU:O	2:H:496:SER:OG	2.25	0.51
2:F:266:VAL:HA	2:F:268:ALA:H	1.75	0.51
2:H:70:ASN:HB3	2:H:73:GLU:HB2	1.93	0.51
2:I:289:PHE:N	2:I:296:ASN:OD1	2.44	0.51
2:D:514:VAL:HG13	2:D:533:MET:HB2	1.92	0.51
2:E:233:LEU:HB3	2:E:241:CYS:SG	2.51	0.51
2:I:152:LYS:HE3	2:I:255:TRP:CH2	2.46	0.51
2:J:147:TRP:CE2	2:J:174:PRO:HA	2.46	0.51
2:J:229:ARG:HB2	2:J:257:ALA:HB1	1.93	0.51
2:G:492:LEU:O	2:G:496:SER:OG	2.27	0.51
2:I:409:LEU:HD23	2:I:421:ILE:HG21	1.92	0.51
2:F:217:GLU:HA	2:F:261:ILE:HD11	1.92	0.50
2:I:338:GLY:O	2:I:422:ILE:N	2.40	0.50
1:B:573:LEU:HD22	1:B:590:ARG:HG3	1.92	0.50
2:E:266:VAL:HG11	2:E:271:LEU:HG	1.92	0.50
2:E:316:MET:HE3	2:E:504:ARG:HG2	1.94	0.50
2:F:346:VAL:HG13	2:F:395:ASP:HB2	1.93	0.50
2:H:283:GLU:HG3	2:H:303:ARG:HG3	1.92	0.50
2:I:447:THR:HG22	2:I:495:LEU:HD21	1.93	0.50
1:C:85:ARG:HD2	1:C:219:ARG:HA	1.94	0.50
2:H:476:GLU:HG3	2:I:529:ILE:HG12	1.92	0.50
2:I:225:ALA:HA	2:I:228:VAL:HG22	1.94	0.50
2:I:473:LYS:HB2	2:I:477:GLU:HB2	1.93	0.50
1:B:85:ARG:HG3	1:B:222:TRP:CG	2.46	0.50
1:C:471:GLN:NE2	1:C:657:GLN:OE1	2.37	0.50
2:I:490:GLY:HA2	2:I:493:ARG:NE	2.26	0.50
1:A:584:GLN:HG2	1:A:586:VAL:HG22	1.92	0.50
1:B:566:ARG:O	1:B:570:GLN:HB3	2.11	0.50
1:C:3:VAL:HA	1:C:57:VAL:HB	1.94	0.50
2:D:208:MET:HE3	2:D:233:LEU:H	1.76	0.50
2:D:221:GLN:NE2	2:D:266:VAL:HA	2.26	0.50
2:F:393:LEU:O	2:G:267:SER:HB2	2.12	0.50
2:G:345:SER:O	2:G:349:THR:HG23	2.12	0.50
2:I:311:THR:C	2:I:318:LYS:CE	2.85	0.50
2:D:425:HIS:ND1	2:D:428:ILE:HG13	2.27	0.50
2:F:515:LEU:HD11	2:F:529:ILE:HD13	1.94	0.50
2:H:421:ILE:HG12	2:H:458:VAL:HG21	1.94	0.50
2:I:84:ARG:HH21	2:I:160:ILE:HG21	1.75	0.50
1:C:588:TRP:CE3	1:C:591:ARG:HG2	2.46	0.50
2:D:147:TRP:CE2	2:D:174:PRO:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:151:LYS:HD2	2:E:152:LYS:HG3	1.94	0.50
2:I:340:ALA:N	2:I:422:ILE:O	2.44	0.50
1:B:66:VAL:HG22	1:B:83:LEU:HD12	1.94	0.50
2:D:413:ARG:NH2	2:D:456:THR:O	2.30	0.50
2:F:86:ILE:HA	2:F:167:GLU:OE2	2.12	0.50
2:H:180:HIS:HB2	2:H:184:ALA:HB3	1.94	0.50
2:H:302:ALA:HB2	2:H:308:ILE:HD11	1.94	0.50
2:I:426:ILE:HG22	2:I:464:CYS:HA	1.94	0.50
2:J:194:GLU:CD	2:J:194:GLU:H	2.20	0.50
2:J:371:GLU:O	2:J:375:ASN:ND2	2.45	0.50
1:C:496:TYR:CZ	1:C:505:ILE:HD11	2.47	0.49
2:F:260:TRP:HA	2:F:261:ILE:CB	2.41	0.49
2:H:78:TYR:CE1	2:H:97:TRP:HB3	2.47	0.49
2:I:411:TYR:HE2	2:J:266:VAL:HG11	1.76	0.49
2:I:446:MET:HE2	2:I:492:LEU:HA	1.94	0.49
2:J:261:ILE:C	2:J:263:ASP:H	2.20	0.49
1:B:363:VAL:HG13	1:B:365:ASP:H	1.76	0.49
1:C:26:TYR:CD1	1:C:199:THR:HG21	2.47	0.49
2:E:84:ARG:HA	2:E:243:LEU:HD11	1.94	0.49
2:E:140:ALA:HB3	2:E:179:GLY:HA3	1.94	0.49
2:E:339:LEU:N	2:E:392:HIS:O	2.43	0.49
2:F:152:LYS:HG2	2:F:201:GLN:HB2	1.94	0.49
2:I:306:GLU:HB3	2:I:450:LYS:HD3	1.93	0.49
1:C:645:ASP:HB3	1:C:665:ILE:HD13	1.95	0.49
2:D:534:GLU:HG3	2:D:545:SER:HB2	1.94	0.49
2:G:151:LYS:HD2	2:G:152:LYS:HG3	1.92	0.49
2:G:292:CYS:HA	2:G:544:PRO:HB3	1.93	0.49
2:G:316:MET:HA	2:G:504:ARG:HH11	1.77	0.49
2:I:316:MET:HE3	2:J:522:ARG:HA	1.93	0.49
2:E:203:ILE:HD12	2:E:229:ARG:HD2	1.94	0.49
2:F:220:ALA:HB2	2:F:261:ILE:CG2	2.43	0.49
2:D:340:ALA:HA	2:D:394:TYR:HB3	1.95	0.49
1:B:357:THR:HG21	1:B:363:VAL:HB	1.93	0.49
1:B:368:VAL:O	1:B:372:VAL:HG23	2.12	0.49
2:G:512:ASN:OD1	2:G:512:ASN:N	2.37	0.49
2:H:282:GLU:C	2:H:284:SER:HB3	2.37	0.49
2:I:272:ARG:O	2:I:274:ARG:N	2.40	0.49
2:I:311:THR:O	2:I:318:LYS:CE	2.60	0.49
3:L:24:LEU:HB2	3:L:53:LEU:HD11	1.93	0.49
1:B:678:ARG:NH1	1:B:691:ASP:OD1	2.46	0.49
2:D:420:VAL:HG22	2:D:459:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:484:THR:HA	2:F:493:ARG:HH22	1.78	0.49
2:I:194:GLU:CD	2:I:194:GLU:H	2.18	0.49
2:I:313:GLY:HA3	2:I:475:HIS:HB3	1.93	0.49
1:A:85:ARG:HD2	1:A:219:ARG:HA	1.94	0.49
1:B:25:ASP:HB3	1:B:28:THR:OG1	2.12	0.49
2:G:80:ALA:HB2	2:G:88:LYS:HG3	1.94	0.49
2:I:299:THR:HA	2:I:521:CYS:SG	2.53	0.49
2:I:311:THR:C	2:I:318:LYS:HD2	2.37	0.49
2:I:318:LYS:NZ	2:I:502:LEU:HB2	2.27	0.49
2:J:75:ASN:HB2	2:J:100:LYS:HG2	1.95	0.49
3:L:37:MET:SD	3:L:37:MET:N	2.85	0.49
1:A:128:TRP:CE3	1:A:131:ARG:HD2	2.48	0.49
1:A:154:TYR:HB2	1:A:158:MET:SD	2.52	0.49
2:D:412:MET:O	2:D:417:GLY:N	2.46	0.49
2:E:80:ALA:HB2	2:E:88:LYS:HG3	1.95	0.49
2:I:311:THR:C	2:I:318:LYS:CD	2.86	0.49
1:B:363:VAL:HG22	1:B:364:VAL:HG12	1.95	0.49
1:B:423:ASN:OD1	1:B:599:ARG:NH2	2.45	0.49
2:F:194:GLU:CD	2:F:194:GLU:H	2.20	0.49
1:A:15:VAL:HG22	1:A:72:LEU:HD21	1.93	0.48
1:A:103:LYS:HD3	1:A:120:PHE:CG	2.48	0.48
2:G:110:ASP:OD1	2:G:121:GLN:NE2	2.38	0.48
2:H:153:ILE:HA	2:H:174:PRO:HB2	1.94	0.48
2:H:314:SER:OG	2:I:527:THR:OG1	2.25	0.48
2:I:344:GLU:HA	2:J:454:LYS:HZ1	1.77	0.48
2:I:444:ASN:O	2:I:447:THR:OG1	2.25	0.48
2:I:510:MET:N	2:I:511:PRO:HD2	2.27	0.48
2:J:204:LEU:N	2:J:229:ARG:O	2.43	0.48
1:A:588:TRP:CZ2	1:A:591:ARG:HD3	2.49	0.48
2:D:286:GLY:O	2:D:302:ALA:N	2.43	0.48
2:G:290:SER:N	2:G:325:GLN:OE1	2.43	0.48
2:H:283:GLU:HA	2:H:285:VAL:N	2.28	0.48
2:G:142:PHE:HB3	2:G:177:SER:HB3	1.94	0.48
1:C:376:ASP:HB3	1:C:379:LYS:HB2	1.96	0.48
2:E:392:HIS:HB3	2:F:266:VAL:HG12	1.95	0.48
2:F:153:ILE:HA	2:F:174:PRO:HB2	1.95	0.48
2:G:147:TRP:CD2	2:G:174:PRO:HA	2.49	0.48
2:G:397:PHE:CE2	2:H:450:LYS:HE2	2.49	0.48
2:I:284:SER:HA	2:I:523:PHE:CZ	2.45	0.48
3:K:24:LEU:HD11	3:K:78:LEU:HB3	1.95	0.48
1:C:59:HIS:CD2	1:C:125:LEU:HG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:412:MET:HB3	2:F:418:CYS:SG	2.54	0.48
2:I:235:CYS:HB2	2:I:241:CYS:SG	2.54	0.48
2:I:340:ALA:HA	2:I:394:TYR:HB3	1.95	0.48
2:D:162:MET:HG2	2:D:175:VAL:HG12	1.95	0.48
2:D:194:GLU:CD	2:D:194:GLU:H	2.22	0.48
2:D:474:ALA:HA	2:D:479:ARG:HD2	1.95	0.48
2:G:333:MET:O	2:G:335:LYS:N	2.46	0.48
2:H:208:MET:HE3	2:H:233:LEU:H	1.77	0.48
2:I:283:GLU:HG3	2:I:303:ARG:HG3	1.96	0.48
2:I:477:GLU:HA	2:I:507:GLN:HE22	1.78	0.48
3:L:13:ASP:O	3:L:18:LYS:HD3	2.14	0.48
1:A:575:GLU:HG3	1:A:589:LYS:HE3	1.96	0.48
1:C:24:TYR:HB2	1:C:31:TYR:CD2	2.49	0.48
2:E:397:PHE:HD2	2:F:451:GLY:HA2	1.79	0.48
2:E:502:LEU:HD23	2:E:514:VAL:HG21	1.94	0.48
2:F:77:ARG:HH21	2:F:98:ILE:HG21	1.79	0.48
2:G:84:ARG:O	2:G:239:ASN:ND2	2.45	0.48
3:K:90:LYS:NZ	3:K:90:LYS:HA	2.29	0.48
2:D:341:MET:HG3	2:D:349:THR:HB	1.96	0.48
1:B:578:GLN:HG3	1:B:585:GLN:HB2	1.95	0.48
1:C:473:GLY:HA3	1:C:703:CYS:HB3	1.96	0.48
2:D:221:GLN:HE21	2:D:266:VAL:HA	1.78	0.48
2:D:506:GLN:HB2	2:E:527:THR:OG1	2.14	0.48
2:G:124:ARG:HA	2:G:129:ASN:O	2.14	0.48
2:I:392:HIS:ND1	2:J:266:VAL:O	2.46	0.48
2:J:292:CYS:HB2	2:J:533:MET:HG2	1.95	0.48
2:E:242:HIS:ND1	2:E:247:ASP:OD1	2.32	0.48
2:E:351:GLU:HG3	2:F:279:LEU:HD21	1.96	0.48
2:E:393:LEU:O	2:F:265:VAL:HB	2.13	0.48
2:I:504:ARG:HH11	2:I:512:ASN:HA	1.79	0.48
1:B:453:ALA:O	1:B:459:HIS:NE2	2.33	0.47
2:G:75:ASN:ND2	2:G:100:LYS:O	2.47	0.47
2:I:223:LEU:HD21	2:I:228:VAL:HG13	1.95	0.47
2:I:286:GLY:O	2:I:303:ARG:NH1	2.47	0.47
1:B:584:GLN:HG2	1:B:586:VAL:HG23	1.95	0.47
2:D:474:ALA:O	2:D:476:GLU:N	2.47	0.47
2:E:312:SER:OG	2:E:318:LYS:HG3	2.15	0.47
2:F:345:SER:O	2:F:349:THR:HG23	2.14	0.47
2:G:425:HIS:ND1	2:G:428:ILE:HG13	2.28	0.47
2:J:295:ILE:HD12	2:J:295:ILE:H	1.79	0.47
1:A:143:PHE:HE2	1:A:158:MET:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:MET:HG2	1:B:692:THR:HG23	1.95	0.47
2:F:207:ASP:O	2:F:213:ARG:NH2	2.37	0.47
2:F:379:ASP:OD1	2:G:272:ARG:NH1	2.47	0.47
2:F:397:PHE:HD2	2:G:451:GLY:HA2	1.79	0.47
2:F:412:MET:C	2:F:414:SER:H	2.20	0.47
2:G:305:GLY:HA2	2:G:454:LYS:HA	1.95	0.47
2:J:409:LEU:HA	2:J:412:MET:HE2	1.97	0.47
3:L:45:ILE:HG23	3:L:49:TYR:HD1	1.78	0.47
1:A:235:ASP:HB2	1:A:459:HIS:CE1	2.49	0.47
2:D:248:ARG:HH21	2:E:138:SER:HB2	1.79	0.47
2:H:100:LYS:HG3	2:H:105:MET:SD	2.54	0.47
2:H:365:SER:HB3	2:H:368:LEU:HB2	1.97	0.47
2:I:318:LYS:NZ	2:I:502:LEU:CA	2.75	0.47
2:J:94:ALA:HA	2:J:146:LEU:HD11	1.96	0.47
1:A:341:HIS:CG	1:A:342:ILE:N	2.82	0.47
1:C:491:PHE:HA	2:H:333:MET:HE3	1.96	0.47
2:F:393:LEU:H	2:G:267:SER:HB2	1.78	0.47
2:G:107:GLN:HB2	2:G:124:ARG:HG3	1.97	0.47
2:G:425:HIS:HE1	2:G:427:SER:HB2	1.77	0.47
1:C:59:HIS:CG	1:C:125:LEU:HG	2.49	0.47
1:C:401:GLU:OE1	1:C:404:LYS:HB3	2.14	0.47
2:D:522:ARG:NH2	2:J:343:GLU:OE1	2.47	0.47
2:G:412:MET:HG2	2:G:416:LEU:HD12	1.96	0.47
2:H:283:GLU:N	2:H:284:SER:HB3	2.30	0.47
1:A:429:ARG:HD3	1:A:653:HIS:CG	2.49	0.47
1:A:588:TRP:CE2	1:A:591:ARG:HD3	2.50	0.47
1:B:143:PHE:O	1:B:147:LEU:HG	2.14	0.47
1:B:515:LEU:HD12	1:B:520:ASN:HB3	1.96	0.47
1:C:99:HIS:HB3	1:C:102:LEU:HG	1.97	0.47
1:C:368:VAL:O	1:C:372:VAL:HG23	2.15	0.47
1:C:604:ARG:HE	1:C:606:PRO:HD3	1.79	0.47
2:F:259:PRO:HA	2:F:260:TRP:CB	2.44	0.47
2:H:326:ALA:HB1	2:H:337:VAL:HG11	1.96	0.47
2:I:151:LYS:HD2	2:I:152:LYS:HG3	1.96	0.47
2:I:272:ARG:CZ	2:I:276:ARG:HE	2.28	0.47
2:J:421:ILE:HG12	2:J:458:VAL:HG21	1.96	0.47
1:B:190:HIS:NE2	1:B:598:GLY:O	2.48	0.47
2:D:96:TYR:CE1	2:D:107:GLN:HB3	2.50	0.47
2:F:169:GLN:NE2	2:F:173:TYR:HB2	2.30	0.47
2:F:309:MET:O	2:F:500:ILE:N	2.42	0.47
2:H:106:TYR:CE2	2:H:125:ASP:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:OE2	1:A:423:ASN:ND2	2.31	0.47
1:B:3:VAL:HA	1:B:57:VAL:HB	1.96	0.47
2:D:267:SER:HB2	2:J:393:LEU:H	1.80	0.47
2:D:475:HIS:H	2:D:479:ARG:HD2	1.79	0.47
2:H:162:MET:HB2	2:H:177:SER:HB2	1.97	0.47
2:H:229:ARG:HA	2:H:259:PRO:HD2	1.97	0.47
1:A:233:PRO:HB2	1:A:456:GLY:O	2.15	0.47
1:C:338:SER:HB3	1:C:341:HIS:CG	2.49	0.47
1:C:485:ALA:HA	1:C:488:MET:HG2	1.97	0.47
2:D:69:TRP:CH2	2:D:123:VAL:HG11	2.50	0.47
2:D:412:MET:HB3	2:D:418:CYS:SG	2.55	0.47
2:E:162:MET:HB2	2:E:177:SER:HB2	1.97	0.47
2:G:84:ARG:HA	2:G:243:LEU:HD11	1.97	0.47
2:I:487:ARG:HG2	2:I:488:GLY:H	1.80	0.47
2:J:287:LEU:HG	2:J:329:TRP:CG	2.50	0.47
1:B:489:ALA:HA	1:B:492:ASP:OD1	2.16	0.46
1:C:18:PHE:HB2	1:C:72:LEU:HD13	1.97	0.46
3:L:3:LYS:NZ	3:L:47:ASP:OD1	2.34	0.46
1:A:35:ARG:H	1:A:38:ASP:HB2	1.80	0.46
1:B:603:VAL:HG13	1:B:604:ARG:N	2.30	0.46
1:C:538:GLY:HA3	1:C:544:GLY:O	2.15	0.46
2:I:401:GLU:HG2	2:I:402:THR:HG22	1.96	0.46
3:L:37:MET:O	3:L:40:PRO:HD2	2.16	0.46
1:B:574:VAL:HG13	1:B:586:VAL:HG13	1.97	0.46
1:C:193:PRO:O	1:C:198:PHE:HZ	1.97	0.46
2:D:276:ARG:HD2	2:J:373:ILE:HG23	1.96	0.46
2:D:492:LEU:O	2:D:496:SER:OG	2.25	0.46
2:G:307:VAL:HG22	2:G:460:LEU:HB3	1.96	0.46
2:H:271:LEU:HB3	2:H:275:ILE:CD1	2.45	0.46
2:I:287:LEU:HD21	2:I:335:LYS:HG3	1.96	0.46
2:D:233:LEU:HB3	2:D:241:CYS:SG	2.55	0.46
2:D:274:ARG:O	2:D:278:HIS:N	2.46	0.46
2:E:147:TRP:CE2	2:E:174:PRO:HA	2.49	0.46
2:F:261:ILE:H	2:F:262:PRO:CD	2.28	0.46
2:G:339:LEU:O	2:G:393:LEU:HA	2.16	0.46
2:J:299:THR:O	2:J:303:ARG:NH1	2.29	0.46
2:G:236:LYS:H	2:G:240:GLU:HG2	1.81	0.46
2:H:77:ARG:HH22	2:H:100:LYS:NZ	2.13	0.46
2:I:505:ASN:C	2:I:507:GLN:H	2.23	0.46
2:J:139:ASP:HB2	2:J:192:ASN:ND2	2.30	0.46
1:A:106:ASP:OD1	1:A:131:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:HG3	3:K:31:TRP:CH2	2.51	0.46
1:A:428:GLY:HA3	1:A:619:ALA:HB3	1.98	0.46
2:F:80:ALA:HB2	2:F:88:LYS:HG3	1.96	0.46
2:F:105:MET:HG2	2:F:126:LYS:NZ	2.31	0.46
2:H:391:PHE:O	2:I:268:ALA:HB3	2.15	0.46
2:I:315:GLY:C	2:I:317:GLY:H	2.24	0.46
2:I:318:LYS:HE3	2:I:502:LEU:CB	2.32	0.46
1:B:139:TYR:OH	1:B:164:ASN:ND2	2.34	0.46
1:C:429:ARG:H	1:C:619:ALA:HB1	1.81	0.46
2:G:269:LEU:C	2:G:271:LEU:H	2.24	0.46
2:H:341:MET:HG3	2:H:349:THR:HG21	1.97	0.46
2:I:287:LEU:HD23	2:I:329:TRP:CD2	2.50	0.46
2:J:345:SER:O	2:J:349:THR:HG23	2.16	0.46
1:A:578:GLN:NE2	1:A:579:TRP:O	2.49	0.46
2:D:313:GLY:O	2:D:318:LYS:NZ	2.49	0.46
2:E:203:ILE:HG13	2:E:254:VAL:HG13	1.97	0.46
2:F:155:VAL:HB	2:F:204:LEU:HD23	1.97	0.46
2:J:319:SER:HB3	2:J:323:ARG:NH2	2.31	0.46
1:C:489:ALA:O	2:H:288:LEU:HD23	2.16	0.46
2:D:292:CYS:HB2	2:D:533:MET:HG2	1.98	0.46
2:D:339:LEU:HB2	2:D:393:LEU:HA	1.98	0.46
2:F:361:ARG:NH1	2:F:535:TYR:OH	2.48	0.46
2:F:514:VAL:HG13	2:F:533:MET:HB2	1.98	0.46
2:H:84:ARG:HH21	2:H:160:ILE:HG21	1.80	0.46
2:H:272:ARG:CZ	2:H:273:GLU:HA	2.45	0.46
2:J:205:MET:HG3	2:J:233:LEU:HD11	1.97	0.46
1:A:209:GLU:OE2	2:D:375:ASN:ND2	2.49	0.46
1:B:139:TYR:HB2	1:B:170:TYR:CB	2.46	0.46
1:C:462:ASP:OD2	1:C:465:THR:OG1	2.28	0.46
2:E:373:ILE:HD11	2:F:280:SER:HA	1.97	0.46
2:F:411:TYR:CE2	2:G:262:PRO:HA	2.51	0.46
2:I:287:LEU:HB2	2:I:303:ARG:HH12	1.81	0.46
2:I:510:MET:O	2:I:512:ASN:N	2.48	0.46
2:J:290:SER:N	2:J:325:GLN:OE1	2.46	0.46
2:J:311:THR:HG21	2:J:486:LEU:HD21	1.97	0.46
3:K:23:ILE:HD13	3:K:54:THR:HB	1.97	0.46
3:M:34:PRO:HB2	3:M:76:PRO:HD3	1.98	0.46
2:D:151:LYS:HD2	2:D:152:LYS:HG3	1.98	0.45
2:D:542:LEU:HD13	2:D:542:LEU:HA	1.75	0.45
2:E:124:ARG:HH22	2:E:159:GLU:HB2	1.80	0.45
2:E:430:VAL:HG11	2:F:447:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:229:ARG:HE	2:H:229:ARG:HB3	1.57	0.45
2:I:497:ASP:OD1	2:I:522:ARG:HB3	2.16	0.45
2:E:382:PHE:HE2	2:F:272:ARG:HG3	1.82	0.45
2:F:333:MET:O	2:F:335:LYS:HG2	2.16	0.45
2:F:421:ILE:HG12	2:F:458:VAL:HG21	1.96	0.45
1:B:22:VAL:HG23	1:B:171:ASN:ND2	2.27	0.45
1:C:237:LYS:O	1:C:241:GLU:HB2	2.16	0.45
1:C:405:ALA:O	1:C:407:LEU:N	2.41	0.45
2:F:413:ARG:NH2	2:F:457:GLY:O	2.49	0.45
2:G:421:ILE:HG12	2:G:458:VAL:HG21	1.98	0.45
2:I:77:ARG:HH12	2:I:100:LYS:HB2	1.81	0.45
2:I:486:LEU:HD22	2:I:487:ARG:H	1.80	0.45
2:J:432:ALA:N	2:J:433:SER:HA	2.32	0.45
1:A:341:HIS:CD2	1:A:342:ILE:HG13	2.50	0.45
1:A:608:ALA:C	1:A:610:LEU:H	2.23	0.45
1:B:143:PHE:CE2	1:B:147:LEU:HD11	2.51	0.45
1:C:257:LEU:HD21	1:C:385:LEU:HB2	1.98	0.45
2:H:246:HIS:HB3	2:H:249:GLU:OE1	2.16	0.45
1:A:57:VAL:HG13	1:A:89:ILE:HD11	1.98	0.45
1:A:103:LYS:HE3	1:A:106:ASP:CG	2.42	0.45
1:A:495:GLU:OE2	2:E:546:SER:HB3	2.17	0.45
1:C:128:TRP:CE3	1:C:131:ARG:HD2	2.51	0.45
1:C:427:THR:HA	1:C:601:VAL:HG13	1.98	0.45
2:E:260:TRP:HA	2:E:261:ILE:HA	1.45	0.45
2:E:301:GLY:O	2:E:303:ARG:NH1	2.50	0.45
2:G:162:MET:HB2	2:G:177:SER:HB2	1.98	0.45
3:M:41:ILE:HD12	3:M:96:LYS:HB2	1.97	0.45
1:C:101:ASN:C	1:C:103:LYS:H	2.24	0.45
2:E:208:MET:HE3	2:E:233:LEU:H	1.81	0.45
2:G:242:HIS:ND1	2:G:247:ASP:OD1	2.38	0.45
2:I:269:LEU:HD22	2:I:270:SER:HA	1.98	0.45
2:J:256:ASN:O	2:J:256:ASN:ND2	2.49	0.45
1:A:50:VAL:HG13	1:A:87:ASN:ND2	2.31	0.45
1:C:140:LYS:HG2	1:C:144:LYS:HE3	1.99	0.45
1:C:397:GLY:HA2	1:C:401:GLU:HB3	1.99	0.45
2:D:75:ASN:HD22	2:D:100:LYS:HB3	1.82	0.45
2:D:481:VAL:HG23	2:D:485:ASP:HB2	1.98	0.45
2:E:232:VAL:O	2:E:253:GLN:NE2	2.50	0.45
2:G:426:ILE:HD12	2:G:462:VAL:HG11	1.99	0.45
2:H:363:ARG:O	2:H:365:SER:N	2.41	0.45
2:J:108:VAL:HG13	2:J:123:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:394:TYR:HE2	2:J:408:LYS:HD2	1.81	0.45
1:A:6:ILE:HG12	1:A:65:ASP:OD2	2.17	0.45
2:D:229:ARG:HB3	2:D:257:ALA:HB3	1.99	0.45
2:D:309:MET:O	2:D:500:ILE:N	2.45	0.45
2:F:396:SER:C	2:F:398:ALA:H	2.25	0.45
2:G:97:TRP:CZ3	2:G:99:ALA:HB2	2.51	0.45
1:A:57:VAL:HG22	1:A:89:ILE:HD11	1.99	0.45
1:A:495:GLU:O	1:A:499:GLU:HG2	2.17	0.45
1:B:102:LEU:HD13	1:B:121:GLY:HA2	1.97	0.45
1:B:678:ARG:NE	1:B:689:LEU:HD11	2.32	0.45
2:E:533:MET:HA	2:E:544:PRO:HA	1.98	0.45
2:F:316:MET:HB2	2:F:504:ARG:HH11	1.82	0.45
2:G:140:ALA:HB3	2:G:179:GLY:HA3	1.98	0.45
2:G:232:VAL:HG23	2:G:260:TRP:CE3	2.51	0.45
2:H:392:HIS:CD2	2:H:416:LEU:HD13	2.52	0.45
2:I:311:THR:O	2:I:311:THR:CG2	2.65	0.45
2:J:515:LEU:HD11	2:J:529:ILE:HD13	1.99	0.45
1:A:236:THR:O	1:A:240:GLU:HG3	2.17	0.45
2:E:397:PHE:CD2	2:F:451:GLY:HA2	2.52	0.45
2:G:502:LEU:HD23	2:G:514:VAL:HG21	1.98	0.45
2:I:244:ASN:HB3	2:I:246:HIS:CE1	2.52	0.45
2:J:147:TRP:CD2	2:J:174:PRO:HA	2.52	0.45
3:M:17:LEU:HA	3:M:84:GLY:HA2	1.99	0.45
1:A:368:VAL:O	1:A:372:VAL:HG23	2.17	0.44
1:A:482:ARG:HG2	1:A:500:ILE:HG21	1.98	0.44
1:B:211:LEU:HD21	1:B:598:GLY:C	2.42	0.44
1:B:235:ASP:HB2	1:B:459:HIS:CD2	2.52	0.44
1:C:491:PHE:O	2:H:333:MET:HG3	2.17	0.44
2:F:403:ASP:HA	2:F:404:ARG:HA	1.61	0.44
2:H:147:TRP:CE2	2:H:174:PRO:HA	2.52	0.44
2:I:535:TYR:CD2	2:I:541:TRP:HB2	2.50	0.44
2:J:486:LEU:HD13	2:J:492:LEU:HD13	1.98	0.44
3:L:28:TRP:HB2	3:L:35:CYS:SG	2.57	0.44
1:A:147:LEU:HD13	1:A:154:TYR:CB	2.46	0.44
1:B:189:LYS:HA	1:B:192:PHE:O	2.17	0.44
2:D:320:THR:HG21	2:D:535:TYR:HE1	1.83	0.44
2:H:278:HIS:O	2:H:282:GLU:N	2.50	0.44
2:H:369:LYS:NZ	2:I:284:SER:HB3	2.31	0.44
3:K:3:LYS:HD2	3:K:47:ASP:OD1	2.18	0.44
3:L:45:ILE:HG23	3:L:49:TYR:CD1	2.51	0.44
2:D:78:TYR:CE1	2:D:97:TRP:HB3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:84:ARG:O	2:E:239:ASN:ND2	2.42	0.44
2:F:124:ARG:NH2	2:F:159:GLU:HB2	2.28	0.44
2:F:314:SER:OG	2:F:465:HIS:ND1	2.41	0.44
2:G:107:GLN:O	2:G:123:VAL:HA	2.17	0.44
2:G:124:ARG:NH2	2:G:159:GLU:HB2	2.31	0.44
2:H:205:MET:HG3	2:H:231:ALA:HB3	1.98	0.44
1:B:339:ARG:H	1:B:339:ARG:HD2	1.82	0.44
2:D:375:ASN:OD1	2:D:376:GLY:N	2.51	0.44
2:F:484:THR:HA	2:F:493:ARG:NH2	2.33	0.44
2:H:347:GLU:H	2:H:347:GLU:HG2	1.42	0.44
2:I:411:TYR:CE1	2:J:260:TRP:HA	2.52	0.44
2:J:114:GLN:OE1	2:J:148:ASN:ND2	2.50	0.44
2:J:139:ASP:HB2	2:J:192:ASN:HD21	1.82	0.44
1:A:338:SER:O	1:A:341:HIS:ND1	2.50	0.44
1:A:640:HIS:CD2	1:A:647:ALA:HA	2.53	0.44
1:B:59:HIS:CG	1:B:125:LEU:HG	2.53	0.44
2:D:252:GLU:O	2:D:256:ASN:HB2	2.18	0.44
2:D:271:LEU:O	2:D:275:ILE:HG13	2.18	0.44
2:E:229:ARG:NH1	2:E:254:VAL:O	2.42	0.44
3:L:38:ILE:HG21	3:L:93:ALA:HA	2.00	0.44
1:A:261:PHE:HA	1:A:262:GLY:HA3	1.76	0.44
1:B:491:PHE:CE2	1:B:565:LEU:HA	2.53	0.44
2:E:138:SER:HA	2:E:180:HIS:NE2	2.32	0.44
2:E:369:LYS:O	2:E:373:ILE:HG13	2.16	0.44
1:A:489:ALA:HA	1:A:492:ASP:OD1	2.18	0.44
1:B:235:ASP:HB2	1:B:459:HIS:CE1	2.52	0.44
2:D:100:LYS:HG3	2:D:105:MET:SD	2.58	0.44
2:D:251:MET:O	2:D:255:TRP:HD1	1.99	0.44
2:F:320:THR:HG21	2:F:535:TYR:HE1	1.83	0.44
2:G:182:ALA:HB1	2:G:215:ALA:HB2	2.00	0.44
2:D:269:LEU:C	2:D:271:LEU:H	2.26	0.44
2:E:113:ASP:HB3	2:E:117:ASN:O	2.18	0.44
2:J:74:SER:HB2	2:J:99:ALA:HB1	1.99	0.44
2:J:278:HIS:O	2:J:282:GLU:HB2	2.18	0.44
1:C:423:ASN:HB2	1:C:623:LYS:HZ1	1.82	0.44
2:F:475:HIS:H	2:F:479:ARG:HD2	1.82	0.44
2:H:250:ILE:O	2:H:254:VAL:HG23	2.18	0.44
2:I:410:ALA:HA	2:I:452:PHE:CE1	2.52	0.44
1:A:535:GLU:O	1:A:539:GLN:HG3	2.18	0.43
1:B:676:ALA:O	1:B:680:VAL:HG23	2.17	0.43
1:C:351:TRP:CZ3	1:C:353:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ASP:HA	1:C:655:GLU:HA	2.00	0.43
2:D:121:GLN:HB2	2:D:133:THR:OG1	2.18	0.43
2:G:147:TRP:CE2	2:G:174:PRO:HA	2.52	0.43
2:G:357:HIS:ND1	2:G:385:LEU:HB2	2.32	0.43
2:I:77:ARG:NH2	2:I:105:MET:HE1	2.33	0.43
2:I:312:SER:HB3	2:I:318:LYS:NZ	2.30	0.43
3:L:23:ILE:HB	3:L:81:PHE:HB2	1.99	0.43
1:A:103:LYS:HD3	1:A:120:PHE:CD1	2.53	0.43
1:A:429:ARG:HH11	1:A:653:HIS:N	2.17	0.43
2:D:154:VAL:HA	2:D:203:ILE:HB	2.00	0.43
2:F:162:MET:CB	2:F:177:SER:HB2	2.48	0.43
2:G:426:ILE:HG12	2:G:426:ILE:O	2.18	0.43
3:K:32:CYS:SG	3:K:34:PRO:HD2	2.58	0.43
1:A:547:ARG:O	1:A:551:LEU:HB2	2.18	0.43
1:B:388:GLU:O	1:B:392:ILE:HG12	2.19	0.43
2:D:250:ILE:H	2:D:250:ILE:HG13	1.44	0.43
2:D:307:VAL:HB	2:D:496:SER:HA	2.01	0.43
2:I:427:SER:HB2	2:I:465:HIS:CE1	2.53	0.43
2:J:78:TYR:CD2	2:J:92:GLN:HG2	2.53	0.43
2:J:258:GLY:HA3	2:J:260:TRP:CH2	2.54	0.43
1:B:603:VAL:HG21	1:B:609:ALA:HA	2.01	0.43
1:A:388:GLU:O	1:A:392:ILE:HG12	2.18	0.43
1:B:13:GLU:OE1	1:B:13:GLU:N	2.51	0.43
2:D:229:ARG:NH2	2:D:257:ALA:H	2.15	0.43
2:D:267:SER:HB2	2:J:392:HIS:HA	1.99	0.43
2:F:84:ARG:HH21	2:F:160:ILE:HG21	1.82	0.43
2:F:311:THR:HG21	2:F:486:LEU:HD21	1.99	0.43
2:G:162:MET:HG2	2:G:175:VAL:HG12	2.01	0.43
2:G:284:SER:O	2:G:303:ARG:HG3	2.19	0.43
2:H:512:ASN:OD1	2:H:512:ASN:N	2.47	0.43
2:I:251:MET:O	2:I:254:VAL:HB	2.18	0.43
2:J:105:MET:HE2	2:J:105:MET:HB3	1.76	0.43
2:J:122:LYS:HE2	2:J:122:LYS:HB3	1.79	0.43
2:J:420:VAL:HG22	2:J:459:VAL:HB	2.01	0.43
3:K:22:ALA:HB1	3:K:53:LEU:HD12	2.01	0.43
3:M:34:PRO:HB3	3:M:93:ALA:HB2	2.00	0.43
1:A:490:ARG:NH1	1:A:568:SER:OG	2.52	0.43
1:A:530:TYR:CD1	1:A:611:ASN:HB2	2.54	0.43
2:D:164:THR:O	2:D:168:LEU:HG	2.17	0.43
2:D:221:GLN:HE21	2:D:266:VAL:HG22	1.82	0.43
2:E:77:ARG:HH12	2:E:100:LYS:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:111:TYR:CZ	2:F:142:PHE:HB2	2.53	0.43
2:H:80:ALA:HB2	2:H:88:LYS:HG3	2.00	0.43
2:I:269:LEU:HA	2:I:270:SER:HA	1.66	0.43
2:I:303:ARG:NE	2:I:303:ARG:HA	2.33	0.43
2:I:443:ASP:O	2:I:447:THR:HG23	2.18	0.43
1:A:533:GLY:O	1:A:537:ILE:HG12	2.19	0.43
2:D:426:ILE:HG12	2:D:426:ILE:O	2.19	0.43
2:E:504:ARG:NH1	2:E:506:GLN:HE21	2.16	0.43
2:E:534:GLU:HG3	2:E:545:SER:HB2	2.00	0.43
2:F:166:MET:HG2	2:F:171:CYS:SG	2.58	0.43
2:F:169:GLN:CD	2:F:173:TYR:HB2	2.44	0.43
2:G:287:LEU:HG	2:G:329:TRP:CE2	2.54	0.43
2:H:329:TRP:CZ3	2:H:420:VAL:HG11	2.54	0.43
2:H:405:LEU:O	2:H:409:LEU:HG	2.19	0.43
2:H:484:THR:HA	2:H:493:ARG:NH2	2.32	0.43
2:J:178:LEU:HD11	2:J:206:PHE:CZ	2.53	0.43
1:C:535:GLU:O	1:C:539:GLN:HG3	2.19	0.43
2:D:169:GLN:HB3	2:D:173:TYR:HD2	1.84	0.43
2:G:208:MET:HE3	2:G:233:LEU:HB2	2.01	0.43
2:G:367:SER:HA	2:G:370:ARG:NH1	2.32	0.43
2:H:166:MET:HE2	2:H:171:CYS:HB3	2.00	0.43
2:I:298:LYS:HG2	2:I:526:ASP:OD2	2.19	0.43
2:I:330:GLY:HA3	2:I:391:PHE:CZ	2.53	0.43
2:I:340:ALA:HB3	2:I:423:LEU:HA	2.01	0.43
2:J:429:VAL:HG23	2:J:438:GLU:OE1	2.19	0.43
3:L:76:PRO:HG2	3:L:92:GLY:O	2.18	0.43
1:A:330:GLU:HG3	3:K:31:TRP:HH2	1.84	0.43
1:C:426:VAL:HB	1:C:602:HIS:HB2	2.00	0.43
2:E:324:GLN:NE2	2:E:542:LEU:HB2	2.27	0.43
2:E:356:LEU:O	2:E:541:TRP:NE1	2.46	0.43
2:F:140:ALA:HB3	2:F:179:GLY:HA3	2.01	0.43
2:F:408:LYS:HE2	2:G:217:GLU:HG3	2.00	0.43
2:G:382:PHE:CE2	2:H:272:ARG:HB2	2.54	0.43
2:G:542:LEU:HD12	2:G:542:LEU:HA	1.83	0.43
2:H:492:LEU:H	2:H:492:LEU:HG	1.63	0.43
2:I:401:GLU:HA	2:I:430:VAL:O	2.19	0.43
1:A:478:GLY:O	1:A:482:ARG:HG3	2.19	0.43
1:A:688:CYS:SG	1:A:689:LEU:N	2.92	0.43
1:B:112:SER:HB2	1:B:114:LYS:HG2	2.01	0.43
1:C:59:HIS:ND1	1:C:91:THR:OG1	2.35	0.43
1:C:129:GLY:HA3	1:C:135:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ALA:O	1:C:427:THR:N	2.52	0.43
2:E:311:THR:HG21	2:E:486:LEU:HD21	2.01	0.43
2:I:142:PHE:HB3	2:I:177:SER:HB3	2.01	0.43
1:A:48:ALA:HB1	1:A:52:ARG:HH12	1.84	0.42
1:A:143:PHE:CD2	1:A:159:GLU:HB3	2.54	0.42
1:A:603:VAL:HG23	1:A:612:THR:HB	2.01	0.42
1:B:351:TRP:NE1	1:B:372:VAL:HG22	2.35	0.42
1:C:66:VAL:HG22	1:C:83:LEU:HD12	2.01	0.42
2:F:313:GLY:O	2:F:316:MET:HG2	2.18	0.42
2:F:397:PHE:CE2	2:G:450:LYS:HG3	2.53	0.42
2:I:91:CYS:HB3	2:I:96:TYR:O	2.19	0.42
2:J:429:VAL:HG22	2:J:430:VAL:N	2.34	0.42
1:B:427:THR:HG23	1:B:616:SER:HA	2.01	0.42
1:B:461:LEU:HD13	1:B:466:GLY:HA2	2.00	0.42
1:C:335:ASN:HB3	1:C:341:HIS:ND1	2.34	0.42
1:C:402:GLY:HA2	1:C:408:ARG:HE	1.83	0.42
2:D:258:GLY:HA2	2:D:259:PRO:HD3	1.91	0.42
2:F:534:GLU:HG3	2:F:545:SER:HB2	2.00	0.42
2:G:67:ASN:C	2:G:133:THR:HB	2.44	0.42
2:H:518:ILE:HD13	2:H:530:ALA:HB2	2.01	0.42
2:I:78:TYR:CE1	2:I:97:TRP:HB3	2.54	0.42
2:I:201:GLN:HE21	2:I:203:ILE:HD11	1.84	0.42
1:A:676:ALA:O	1:A:680:VAL:HG23	2.19	0.42
1:B:233:PRO:HB2	1:B:456:GLY:O	2.19	0.42
2:F:78:TYR:CE1	2:F:97:TRP:HB3	2.54	0.42
2:F:292:CYS:HB2	2:F:533:MET:HG2	2.01	0.42
2:F:425:HIS:HB3	2:F:428:ILE:HD11	2.01	0.42
2:G:81:LEU:HD21	2:G:96:TYR:CE2	2.53	0.42
2:G:333:MET:O	2:G:335:LYS:HG2	2.19	0.42
2:I:413:ARG:HD3	2:I:458:VAL:HB	2.00	0.42
2:I:493:ARG:H	2:I:493:ARG:HG2	1.52	0.42
1:B:485:ALA:HA	1:B:488:MET:HG2	2.01	0.42
1:B:534:ASP:O	1:B:538:GLY:N	2.43	0.42
1:C:573:LEU:HD22	1:C:590:ARG:O	2.19	0.42
2:E:392:HIS:HB3	2:F:266:VAL:CG1	2.49	0.42
2:F:373:ILE:HD11	2:G:279:LEU:HB3	2.02	0.42
2:G:344:GLU:HG3	2:G:349:THR:HG22	2.01	0.42
2:H:233:LEU:HB3	2:H:241:CYS:SG	2.59	0.42
2:I:401:GLU:HG3	2:I:431:SER:O	2.19	0.42
2:J:316:MET:HE3	2:J:504:ARG:HG2	2.00	0.42
2:J:492:LEU:O	2:J:496:SER:OG	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:GLU:HB2	1:A:589:LYS:N	2.35	0.42
1:A:603:VAL:HG23	1:A:612:THR:CB	2.50	0.42
1:C:85:ARG:HG3	1:C:222:TRP:CG	2.54	0.42
1:C:393:GLN:O	1:C:397:GLY:N	2.43	0.42
2:F:250:ILE:O	2:F:254:VAL:HG23	2.19	0.42
2:G:91:CYS:HB3	2:G:96:TYR:O	2.19	0.42
2:G:265:VAL:O	2:G:266:VAL:HG22	2.20	0.42
2:G:309:MET:HB3	2:G:499:ILE:HG12	2.02	0.42
2:I:140:ALA:HB3	2:I:179:GLY:HA3	2.01	0.42
2:I:395:ASP:N	2:J:265:VAL:HG11	2.33	0.42
1:B:351:TRP:CD1	1:B:372:VAL:HG13	2.55	0.42
2:D:263:ASP:HA	2:D:264:GLY:HA2	1.51	0.42
2:E:333:MET:O	2:E:335:LYS:HG2	2.19	0.42
2:H:124:ARG:HH22	2:H:159:GLU:HB2	1.85	0.42
2:H:347:GLU:OE2	2:I:274:ARG:NH2	2.53	0.42
2:I:361:ARG:HB3	2:I:364:GLN:HB2	2.00	0.42
3:K:4:ILE:HG23	3:K:55:VAL:HG12	2.01	0.42
2:F:300:LEU:HD12	2:F:524:THR:HG22	2.01	0.42
2:G:325:GLN:HG3	2:G:329:TRP:CZ2	2.54	0.42
2:H:284:SER:O	2:H:285:VAL:HB	2.20	0.42
2:I:306:GLU:O	2:I:496:SER:HA	2.20	0.42
2:I:465:HIS:HB2	2:I:487:ARG:NH1	2.34	0.42
1:B:624:LEU:HD12	1:B:684:TRP:CH2	2.53	0.42
1:C:98:ILE:HD12	1:C:185:LEU:HD22	2.02	0.42
1:C:674:GLN:NE2	1:C:678:ARG:HH22	2.10	0.42
2:D:402:THR:HG21	2:D:448:LYS:NZ	2.35	0.42
2:E:104:VAL:HB	2:E:106:TYR:CE1	2.54	0.42
2:F:256:ASN:HB3	2:F:257:ALA:H	1.56	0.42
2:F:324:GLN:HE22	2:F:542:LEU:N	2.18	0.42
2:H:77:ARG:HH22	2:H:100:LYS:HZ2	1.66	0.42
2:H:343:GLU:HG3	2:H:428:ILE:HD11	2.01	0.42
2:H:514:VAL:HG13	2:H:533:MET:HB2	2.00	0.42
2:I:124:ARG:HA	2:I:129:ASN:O	2.20	0.42
1:B:24:TYR:HB2	1:B:31:TYR:CD2	2.55	0.42
1:B:687:ARG:HH11	1:B:687:ARG:HB3	1.84	0.42
1:C:534:ASP:O	1:C:548:GLY:HA3	2.20	0.42
2:F:542:LEU:HA	2:F:542:LEU:HD13	1.76	0.42
2:G:347:GLU:HG3	2:H:278:HIS:CG	2.55	0.42
2:H:476:GLU:HG3	2:I:529:ILE:CG1	2.49	0.42
2:J:78:TYR:O	2:J:88:LYS:HG3	2.19	0.42
3:K:22:ALA:HB3	3:K:53:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:23:ILE:O	3:K:81:PHE:N	2.41	0.42
1:A:334:PHE:CE1	1:A:341:HIS:HB3	2.55	0.42
1:C:189:LYS:HA	1:C:192:PHE:O	2.19	0.42
2:D:252:GLU:O	2:D:256:ASN:N	2.52	0.42
2:D:272:ARG:HD3	2:J:382:PHE:CG	2.54	0.42
2:D:308:ILE:HB	2:D:461:VAL:HG22	2.01	0.42
2:E:78:TYR:O	2:E:88:LYS:HE3	2.20	0.42
2:E:295:ILE:HD12	2:E:295:ILE:H	1.84	0.42
2:E:346:VAL:CG1	2:E:395:ASP:HB2	2.50	0.42
2:G:413:ARG:NH2	2:G:456:THR:O	2.34	0.42
2:I:287:LEU:HD13	2:I:303:ARG:HH22	1.84	0.42
2:I:345:SER:O	2:I:349:THR:HG22	2.19	0.42
2:I:437:ASP:OD1	2:I:439:ARG:HG3	2.20	0.42
2:J:248:ARG:O	2:J:252:GLU:HG3	2.20	0.42
1:A:217:GLU:OE1	1:A:423:ASN:HB2	2.19	0.41
1:A:429:ARG:NH1	1:A:653:HIS:HB2	2.35	0.41
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.77	0.41
1:B:475:ASP:HA	1:B:655:GLU:HA	2.01	0.41
1:C:421:ASN:HA	1:C:422:PRO:HD2	1.91	0.41
2:E:288:LEU:HB3	2:E:296:ASN:ND2	2.35	0.41
2:H:78:TYR:O	2:H:88:LYS:HE3	2.20	0.41
2:H:486:LEU:H	2:H:486:LEU:HG	1.73	0.41
2:J:118:ILE:O	2:J:118:ILE:HG12	2.20	0.41
1:A:493:ASN:ND2	2:E:293:THR:O	2.48	0.41
2:D:98:ILE:HG13	2:D:107:GLN:HG2	2.03	0.41
2:E:312:SER:H	2:E:318:LYS:HD3	1.85	0.41
2:E:373:ILE:CD1	2:F:280:SER:HA	2.49	0.41
2:F:233:LEU:HB3	2:F:241:CYS:SG	2.60	0.41
2:J:413:ARG:HE	2:J:456:THR:HB	1.85	0.41
1:B:236:THR:O	1:B:240:GLU:HG3	2.20	0.41
2:E:327:LEU:HA	2:E:391:PHE:CE1	2.55	0.41
2:F:154:VAL:HA	2:F:203:ILE:HB	2.01	0.41
2:G:324:GLN:OE1	2:G:542:LEU:N	2.53	0.41
2:G:392:HIS:HA	2:H:266:VAL:CG2	2.51	0.41
2:J:99:ALA:N	2:J:106:TYR:O	2.44	0.41
2:J:288:LEU:HD12	2:J:288:LEU:H	1.85	0.41
1:B:93:VAL:CG1	1:B:217:GLU:HB3	2.50	0.41
1:B:698:PRO:HD2	1:B:702:ILE:HG13	2.01	0.41
2:D:217:GLU:O	2:D:221:GLN:HG3	2.19	0.41
2:E:75:ASN:HD22	2:E:100:LYS:HB3	1.84	0.41
2:E:124:ARG:HA	2:E:129:ASN:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:260:TRP:CE3	2:F:261:ILE:HG22	2.56	0.41
2:I:272:ARG:NH1	2:I:276:ARG:HB2	2.35	0.41
2:I:272:ARG:NH2	2:I:276:ARG:HH21	2.18	0.41
2:I:469:PRO:HD3	2:I:475:HIS:NE2	2.35	0.41
2:J:140:ALA:HB3	2:J:179:GLY:HA3	2.02	0.41
3:L:62:GLN:C	3:L:64:PRO:HD3	2.46	0.41
3:M:32:CYS:SG	3:M:34:PRO:HD2	2.61	0.41
1:A:253:LEU:O	1:A:257:LEU:N	2.45	0.41
1:C:506:HIS:CG	1:C:522:LYS:HG2	2.56	0.41
1:C:678:ARG:NH2	2:G:371:GLU:OE2	2.47	0.41
2:D:159:GLU:OE1	2:D:159:GLU:N	2.50	0.41
2:D:162:MET:HB2	2:D:177:SER:HB2	2.03	0.41
2:D:182:ALA:HB1	2:D:215:ALA:HB2	2.02	0.41
2:F:78:TYR:O	2:F:88:LYS:HE3	2.21	0.41
2:H:396:SER:C	2:H:398:ALA:H	2.28	0.41
2:I:411:TYR:CZ	2:J:260:TRP:HA	2.55	0.41
2:I:473:LYS:O	2:I:479:ARG:NE	2.51	0.41
2:J:141:LEU:HD23	2:J:192:ASN:ND2	2.35	0.41
3:L:52:LYS:NZ	3:L:107:LEU:HD13	2.35	0.41
1:A:86:GLU:H	1:A:86:GLU:HG2	1.72	0.41
1:B:66:VAL:HG11	1:B:222:TRP:CH2	2.56	0.41
2:E:182:ALA:HB1	2:E:215:ALA:HB2	2.02	0.41
2:F:205:MET:HA	2:F:231:ALA:HB3	2.03	0.41
2:F:492:LEU:H	2:F:492:LEU:HG	1.58	0.41
2:I:154:VAL:HB	2:I:175:VAL:HG22	2.03	0.41
2:I:310:VAL:HB	2:I:463:ILE:HD13	2.02	0.41
2:J:319:SER:O	2:J:323:ARG:HB2	2.20	0.41
3:L:28:TRP:HE1	3:L:57:LYS:HB3	1.86	0.41
1:C:154:TYR:HA	1:C:158:MET:SD	2.61	0.41
2:G:290:SER:OG	2:G:328:GLN:HG2	2.20	0.41
2:H:230:VAL:H	2:H:259:PRO:HG2	1.86	0.41
2:J:112:ARG:HG2	2:J:118:ILE:HG22	2.03	0.41
2:J:166:MET:HE2	2:J:171:CYS:HB3	2.03	0.41
1:B:482:ARG:HD3	1:B:689:LEU:O	2.21	0.41
1:C:143:PHE:CE2	1:C:147:LEU:HD11	2.55	0.41
1:C:467:LYS:HA	1:C:468:PRO:HD2	1.92	0.41
1:C:652:VAL:O	1:C:654:ASP:N	2.53	0.41
2:D:361:ARG:NH1	2:D:535:TYR:OH	2.53	0.41
2:F:446:MET:SD	2:F:492:LEU:HB3	2.61	0.41
2:G:338:GLY:O	2:G:422:ILE:N	2.51	0.41
1:A:43:LEU:HD22	1:A:81:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD21	1:A:214:VAL:HG13	2.03	0.41
1:A:102:LEU:O	1:A:106:ASP:N	2.54	0.41
1:A:159:GLU:HG2	1:A:160:TRP:CD1	2.55	0.41
1:A:440:ILE:HG22	1:A:452:ARG:HE	1.85	0.41
1:B:488:MET:HE1	1:B:562:ILE:HG13	2.03	0.41
1:C:61:GLY:N	1:C:90:ASP:OD2	2.54	0.41
1:C:547:ARG:O	1:C:551:LEU:HB2	2.20	0.41
1:C:602:HIS:CG	1:C:603:VAL:N	2.84	0.41
2:D:97:TRP:CZ3	2:D:99:ALA:HB2	2.56	0.41
2:D:272:ARG:HG3	2:J:378:PHE:CE2	2.56	0.41
2:E:186:LYS:O	2:E:222:VAL:HG21	2.21	0.41
2:E:258:GLY:N	2:E:259:PRO:HD2	2.36	0.41
2:E:338:GLY:HA2	2:E:392:HIS:HB2	2.02	0.41
2:E:453:ALA:HB2	2:E:460:LEU:HD22	2.03	0.41
2:F:124:ARG:HA	2:F:129:ASN:O	2.21	0.41
2:F:157:GLU:CD	2:F:182:ALA:HB2	2.45	0.41
2:F:430:VAL:HG13	2:G:444:ASN:ND2	2.35	0.41
2:G:319:SER:O	2:G:323:ARG:HB2	2.21	0.41
2:G:347:GLU:HG3	2:H:278:HIS:CE1	2.56	0.41
2:G:475:HIS:H	2:G:479:ARG:HD2	1.85	0.41
2:H:97:TRP:CZ3	2:H:99:ALA:HB2	2.55	0.41
2:H:182:ALA:HB1	2:H:215:ALA:HB2	2.03	0.41
2:H:295:ILE:H	2:H:295:ILE:HD12	1.86	0.41
2:H:474:ALA:O	2:H:476:GLU:HG2	2.21	0.41
2:H:488:GLY:O	2:H:493:ARG:NH2	2.54	0.41
2:H:545:SER:OG	2:H:546:SER:N	2.53	0.41
2:I:97:TRP:CZ3	2:I:99:ALA:HB2	2.56	0.41
2:I:173:TYR:HA	2:I:174:PRO:HD3	1.98	0.41
2:I:251:MET:O	2:I:255:TRP:HD1	2.04	0.41
2:I:298:LYS:HB3	2:I:526:ASP:O	2.21	0.41
2:I:446:MET:HE3	2:I:446:MET:HB3	1.83	0.41
2:I:506:GLN:O	2:J:527:THR:OG1	2.31	0.41
1:A:208:SER:HB2	2:D:375:ASN:HB2	2.02	0.41
1:A:351:TRP:CZ3	1:A:353:PRO:HG3	2.56	0.41
1:B:338:SER:OG	1:B:341:HIS:HB2	2.21	0.41
2:D:340:ALA:HB3	2:D:423:LEU:HA	2.01	0.41
2:E:542:LEU:HD12	2:E:542:LEU:HA	1.69	0.41
2:F:172:LYS:HE2	2:F:172:LYS:HB3	1.68	0.41
2:F:426:ILE:HG12	2:F:426:ILE:O	2.20	0.41
2:F:467:LYS:HE3	2:F:487:ARG:HA	2.02	0.41
2:G:329:TRP:CZ3	2:G:420:VAL:HG11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:203:ILE:HD12	2:H:229:ARG:CZ	2.50	0.41
2:J:220:ALA:HA	2:J:223:LEU:HD11	2.03	0.41
2:J:255:TRP:O	2:J:256:ASN:C	2.64	0.41
2:J:521:CYS:O	2:J:525:GLY:N	2.50	0.41
1:B:91:THR:HB	1:B:181:LEU:HD12	2.02	0.40
1:B:573:LEU:HD11	1:B:593:ILE:HG12	2.03	0.40
1:B:591:ARG:HB3	1:B:602:HIS:CE1	2.56	0.40
1:B:597:ASP:OD1	1:B:597:ASP:N	2.51	0.40
2:G:235:CYS:HB3	2:G:240:GLU:CG	2.51	0.40
2:G:312:SER:H	2:G:318:LYS:HD3	1.86	0.40
2:J:229:ARG:HE	2:J:229:ARG:HB3	1.72	0.40
2:J:284:SER:HA	2:J:303:ARG:HG3	2.03	0.40
2:J:303:ARG:HE	2:J:306:GLU:CD	2.30	0.40
1:A:50:VAL:HG13	1:A:87:ASN:HD21	1.86	0.40
1:A:159:GLU:OE1	1:A:159:GLU:N	2.43	0.40
1:C:537:ILE:HG13	1:C:552:LYS:HD2	2.03	0.40
1:C:640:HIS:CD2	1:C:647:ALA:HA	2.56	0.40
2:D:429:VAL:HG23	2:D:430:VAL:H	1.85	0.40
2:E:165:VAL:HB	2:E:175:VAL:HG11	2.02	0.40
2:E:259:PRO:CA	2:E:260:TRP:HB3	2.46	0.40
2:F:166:MET:CG	2:F:171:CYS:HA	2.51	0.40
2:G:203:ILE:HA	2:G:229:ARG:HB2	2.03	0.40
2:I:107:GLN:O	2:I:123:VAL:HA	2.21	0.40
2:I:271:LEU:HD23	2:I:271:LEU:HA	1.86	0.40
1:A:678:ARG:NH1	1:A:691:ASP:OD1	2.55	0.40
1:B:476:ALA:HA	1:B:692:THR:HG22	2.03	0.40
1:C:114:LYS:O	1:C:130:TYR:HB3	2.21	0.40
2:E:228:VAL:HG11	2:E:260:TRP:CD1	2.55	0.40
2:E:395:ASP:H	2:F:265:VAL:HG21	1.87	0.40
2:G:368:LEU:HD23	2:G:368:LEU:HA	1.97	0.40
2:H:272:ARG:NH2	2:H:276:ARG:HB3	2.36	0.40
2:I:318:LYS:NZ	2:I:502:LEU:CB	2.84	0.40
2:I:319:SER:HB3	2:I:323:ARG:NH1	2.36	0.40
2:J:77:ARG:HE	2:J:77:ARG:HB2	1.77	0.40
2:D:357:HIS:ND1	2:D:385:LEU:HD13	2.37	0.40
2:E:262:PRO:O	2:E:264:GLY:N	2.54	0.40
2:F:446:MET:HA	2:F:446:MET:HE2	2.04	0.40
2:G:261:ILE:H	2:G:262:PRO:CD	2.35	0.40
2:H:329:TRP:HZ3	2:H:420:VAL:HG11	1.85	0.40
2:I:311:THR:C	2:I:318:LYS:HZ3	2.10	0.40
2:J:111:TYR:CD2	2:J:140:ALA:HB1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ALA:O	1:B:386:ILE:HG13	2.21	0.40
1:B:498:HIS:NE2	2:G:543:GLU:HG2	2.37	0.40
1:C:155:VAL:O	1:C:157:GLY:N	2.55	0.40
2:E:268:ALA:HA	2:E:271:LEU:HD12	2.04	0.40
2:E:346:VAL:HG11	2:F:265:VAL:CG1	2.51	0.40
2:F:162:MET:O	2:F:166:MET:CE	2.70	0.40
2:G:263:ASP:C	2:G:265:VAL:H	2.30	0.40
2:H:347:GLU:HB3	2:I:275:ILE:CG1	2.48	0.40
2:I:398:ALA:C	2:I:400:ALA:H	2.28	0.40
2:J:258:GLY:HA2	2:J:259:PRO:HD3	1.91	0.40
2:J:287:LEU:HD11	2:J:335:LYS:HG3	2.04	0.40
2:J:316:MET:HA	2:J:504:ARG:HH11	1.85	0.40
3:L:52:LYS:HZ2	3:L:107:LEU:HD13	1.86	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)
2:F:75:ASN:O	3:L:73:ARG:NH2[2_455]	2.17	0.03

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	635/704 (90%)	579 (91%)	44 (7%)	12 (2%)	6	32
1	B	632/704 (90%)	577 (91%)	44 (7%)	11 (2%)	7	35
1	C	629/704 (89%)	568 (90%)	50 (8%)	11 (2%)	7	35
2	D	483/486 (99%)	418 (86%)	52 (11%)	13 (3%)	4	25
2	E	483/486 (99%)	414 (86%)	51 (11%)	18 (4%)	2	19
2	F	484/486 (100%)	403 (83%)	60 (12%)	21 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	482/486 (99%)	411 (85%)	52 (11%)	19 (4%)	2	18
2	H	484/486 (100%)	409 (84%)	56 (12%)	19 (4%)	2	18
2	I	468/486 (96%)	382 (82%)	63 (14%)	23 (5%)	1	16
2	J	481/486 (99%)	413 (86%)	51 (11%)	17 (4%)	3	20
3	K	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
3	L	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
3	M	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
All	All	5570/5829 (96%)	4862 (87%)	544 (10%)	164 (3%)	3	23

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	PRO
1	A	426	VAL
1	A	586	VAL
1	B	346	LEU
1	C	156	ASP
1	C	426	VAL
2	D	490	GLY
2	E	228	VAL
2	E	229	ARG
2	E	261	ILE
2	E	334	GLY
2	E	475	HIS
2	F	261	ILE
2	F	334	GLY
2	F	429	VAL
2	F	475	HIS
2	G	244	ASN
2	G	266	VAL
2	G	334	GLY
2	G	399	GLU
2	G	475	HIS
2	H	257	ALA
2	H	265	VAL
2	H	285	VAL
2	H	334	GLY
2	H	398	ALA
2	H	475	HIS
2	I	430	VAL

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Mol	Chain	Res	Type
2	I	511	PRO
2	J	265	VAL
2	J	430	VAL
1	A	339	ARG
1	A	603	VAL
1	B	422	PRO
1	B	461	LEU
1	C	104	ASP
1	C	404	LYS
1	C	588	TRP
1	C	605	SER
1	C	653	HIS
2	D	244	ASN
2	D	399	GLU
2	D	489	SER
2	E	244	ASN
2	E	425	HIS
2	E	489	SER
2	E	490	GLY
2	F	244	ASN
2	F	412	MET
2	F	490	GLY
2	G	257	ALA
2	G	261	ILE
2	G	396	SER
2	G	398	ALA
2	G	546	SER
2	H	244	ASN
2	H	260	TRP
2	H	266	VAL
2	H	283	GLU
2	H	364	GLN
2	I	244	ASN
2	I	273	GLU
2	I	306	GLU
2	I	396	SER
2	I	397	PHE
2	I	506	GLN
2	I	536	ASN
2	J	75	ASN
2	J	256	ASN
2	J	264	GLY

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Mol	Chain	Res	Type
2	J	334	GLY
2	J	490	GLY
1	A	157	GLY
1	A	338	SER
1	A	653	HIS
1	B	156	ASP
1	B	263	SER
1	B	603	VAL
1	B	604	ARG
1	C	462	ASP
2	D	263	ASP
2	D	265	VAL
2	D	437	ASP
2	D	475	HIS
2	E	437	ASP
2	E	479	ARG
2	F	101	VAL
2	F	262	PRO
2	F	269	LEU
2	F	284	SER
2	F	314	SER
2	F	399	GLU
2	F	425	HIS
2	F	437	ASP
2	F	479	ARG
2	G	260	TRP
2	G	272	ARG
2	G	425	HIS
2	G	437	ASP
2	H	287	LEU
2	H	437	ASP
2	I	227	LYS
2	I	287	LEU
2	I	425	HIS
2	I	434	GLY
2	I	479	ARG
2	J	224	PRO
2	J	425	HIS
2	J	429	VAL
2	J	437	ASP
2	J	475	HIS
2	J	479	ARG

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Mol	Chain	Res	Type
1	A	156	ASP
1	A	333	VAL
1	C	429	ARG
1	C	606	PRO
1	C	609	ALA
2	D	425	HIS
2	E	258	GLY
2	E	287	LEU
2	F	288	LEU
2	F	396	SER
2	G	375	ASN
2	G	413	ARG
2	G	479	ARG
2	H	425	HIS
2	H	479	ARG
2	I	272	ARG
2	I	307	VAL
2	I	315	GLY
2	I	467	LYS
2	J	262	PRO
2	J	396	SER
2	J	399	GLU
1	A	152	GLU
1	B	436	ASN
2	D	262	PRO
2	D	479	ARG
2	E	266	VAL
2	E	267	SER
2	E	268	ALA
2	E	396	SER
2	F	318	LYS
2	G	269	LEU
2	H	101	VAL
2	H	430	VAL
2	I	182	ALA
2	I	269	LEU
2	I	413	ARG
2	I	428	ILE
2	I	497	ASP
2	J	263	ASP
1	B	653	HIS
2	D	396	SER

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Mol	Chain	Res	Type
2	H	413	ARG
2	H	488	GLY
1	A	336	PRO
1	B	533	GLY
2	F	428	ILE
1	B	361	ALA
2	D	266	VAL
2	E	428	ILE
2	F	430	VAL
2	G	430	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	527/582 (90%)	491 (93%)	36 (7%)	14	36
1	B	524/582 (90%)	499 (95%)	25 (5%)	23	45
1	C	521/582 (90%)	502 (96%)	19 (4%)	31	52
2	D	403/403 (100%)	378 (94%)	25 (6%)	16	38
2	E	403/403 (100%)	366 (91%)	37 (9%)	8	27
2	F	403/403 (100%)	369 (92%)	34 (8%)	10	30
2	G	402/403 (100%)	376 (94%)	26 (6%)	15	37
2	H	403/403 (100%)	375 (93%)	28 (7%)	14	36
2	I	391/403 (97%)	339 (87%)	52 (13%)	4	16
2	J	401/403 (100%)	366 (91%)	35 (9%)	9	29
3	K	85/85 (100%)	80 (94%)	5 (6%)	18	40
3	L	85/85 (100%)	81 (95%)	4 (5%)	23	45
3	M	85/85 (100%)	83 (98%)	2 (2%)	43	63
All	All	4633/4822 (96%)	4305 (93%)	328 (7%)	13	35

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	75	LEU
1	A	102	LEU
1	A	103	LYS
1	A	106	ASP
1	A	110	LEU
1	A	119	ARG
1	A	135	MET
1	A	154	TYR
1	A	162	ASN
1	A	163	PHE
1	A	173	GLN
1	A	181	LEU
1	A	241	GLU
1	A	261	PHE
1	A	332	VAL
1	A	334	PHE
1	A	341	HIS
1	A	394	LYS
1	A	420	VAL
1	A	426	VAL
1	A	427	THR
1	A	429	ARG
1	A	470	VAL
1	A	554	LYS
1	A	573	LEU
1	A	574	VAL
1	A	585	GLN
1	A	586	VAL
1	A	587	LYS
1	A	605	SER
1	A	607	HIS
1	A	624	LEU
1	A	652	VAL
1	A	653	HIS
1	A	687	ARG
1	B	17	LYS
1	B	75	LEU
1	B	102	LEU
1	B	120	PHE
1	B	173	GLN
1	B	181	LEU
1	B	241	GLU

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Mol	Chain	Res	Type
1	B	339	ARG
1	B	341	HIS
1	B	364	VAL
1	B	366	ASP
1	B	394	LYS
1	B	420	VAL
1	B	426	VAL
1	B	427	THR
1	B	461	LEU
1	B	464	ILE
1	B	470	VAL
1	B	534	ASP
1	B	554	LYS
1	B	572	THR
1	B	607	HIS
1	B	624	LEU
1	B	686	PHE
1	B	687	ARG
1	C	17	LYS
1	C	75	LEU
1	C	110	LEU
1	C	173	GLN
1	C	181	LEU
1	C	195	GLU
1	C	196	ILE
1	C	241	GLU
1	C	346	LEU
1	C	364	VAL
1	C	394	LYS
1	C	420	VAL
1	C	426	VAL
1	C	427	THR
1	C	458	GLU
1	C	467	LYS
1	C	470	VAL
1	C	554	LYS
1	C	653	HIS
2	D	104	VAL
2	D	151	LYS
2	D	167	GLU
2	D	194	GLU
2	D	250	ILE

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Mol	Chain	Res	Type
2	D	251	MET
2	D	261	ILE
2	D	265	VAL
2	D	269	LEU
2	D	284	SER
2	D	328	GLN
2	D	346	VAL
2	D	347	GLU
2	D	349	THR
2	D	384	GLU
2	D	406	LEU
2	D	429	VAL
2	D	468	ASN
2	D	476	GLU
2	D	481	VAL
2	D	492	LEU
2	D	495	LEU
2	D	507	GLN
2	D	514	VAL
2	D	542	LEU
2	E	104	VAL
2	E	113	ASP
2	E	114	GLN
2	E	115	ASN
2	E	151	LYS
2	E	193	TYR
2	E	194	GLU
2	E	228	VAL
2	E	236	LYS
2	E	251	MET
2	E	252	GLU
2	E	253	GLN
2	E	261	ILE
2	E	269	LEU
2	E	270	SER
2	E	283	GLU
2	E	285	VAL
2	E	287	LEU
2	E	328	GLN
2	E	347	GLU
2	E	349	THR
2	E	368	LEU

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Mol	Chain	Res	Type
2	E	384	GLU
2	E	427	SER
2	E	428	ILE
2	E	429	VAL
2	E	430	VAL
2	E	431	SER
2	E	471	LYS
2	E	476	GLU
2	E	481	VAL
2	E	492	LEU
2	E	495	LEU
2	E	507	GLN
2	E	512	ASN
2	E	514	VAL
2	E	542	LEU
2	F	77	ARG
2	F	105	MET
2	F	151	LYS
2	F	166	MET
2	F	168	LEU
2	F	170	ASP
2	F	172	LYS
2	F	193	TYR
2	F	194	GLU
2	F	218	GLU
2	F	260	TRP
2	F	261	ILE
2	F	265	VAL
2	F	269	LEU
2	F	328	GLN
2	F	346	VAL
2	F	347	GLU
2	F	377	LYS
2	F	384	GLU
2	F	395	ASP
2	F	401	GLU
2	F	406	LEU
2	F	418	CYS
2	F	429	VAL
2	F	468	ASN
2	F	471	LYS
2	F	476	GLU

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Mol	Chain	Res	Type
2	F	481	VAL
2	F	492	LEU
2	F	495	LEU
2	F	507	GLN
2	F	512	ASN
2	F	514	VAL
2	F	542	LEU
2	G	104	VAL
2	G	151	LYS
2	G	167	GLU
2	G	194	GLU
2	G	261	ILE
2	G	266	VAL
2	G	269	LEU
2	G	282	GLU
2	G	287	LEU
2	G	346	VAL
2	G	347	GLU
2	G	375	ASN
2	G	384	GLU
2	G	393	LEU
2	G	397	PHE
2	G	406	LEU
2	G	429	VAL
2	G	446	MET
2	G	468	ASN
2	G	470	ASP
2	G	471	LYS
2	G	476	GLU
2	G	495	LEU
2	G	512	ASN
2	G	514	VAL
2	G	542	LEU
2	H	136	HIS
2	H	151	LYS
2	H	167	GLU
2	H	194	GLU
2	H	228	VAL
2	H	261	ILE
2	H	266	VAL
2	H	269	LEU
2	H	272	ARG

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Mol	Chain	Res	Type
2	H	282	GLU
2	H	283	GLU
2	H	288	LEU
2	H	333	MET
2	H	346	VAL
2	H	347	GLU
2	H	384	GLU
2	H	406	LEU
2	H	429	VAL
2	H	454	LYS
2	H	471	LYS
2	H	476	GLU
2	H	481	VAL
2	H	486	LEU
2	H	492	LEU
2	H	495	LEU
2	H	512	ASN
2	H	514	VAL
2	H	542	LEU
2	I	68	VAL
2	I	104	VAL
2	I	126	LYS
2	I	151	LYS
2	I	193	TYR
2	I	194	GLU
2	I	223	LEU
2	I	236	LYS
2	I	250	ILE
2	I	269	LEU
2	I	271	LEU
2	I	272	ARG
2	I	285	VAL
2	I	300	LEU
2	I	303	ARG
2	I	306	GLU
2	I	309	MET
2	I	316	MET
2	I	347	GLU
2	I	349	THR
2	I	368	LEU
2	I	369	LYS
2	I	370	ARG

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Mol	Chain	Res	Type
2	I	371	GLU
2	I	399	GLU
2	I	402	THR
2	I	404	ARG
2	I	419	ASP
2	I	425	HIS
2	I	426	ILE
2	I	429	VAL
2	I	435	GLU
2	I	440	LYS
2	I	441	MET
2	I	442	ILE
2	I	467	LYS
2	I	470	ASP
2	I	477	GLU
2	I	479	ARG
2	I	486	LEU
2	I	492	LEU
2	I	493	ARG
2	I	497	ASP
2	I	504	ARG
2	I	506	GLN
2	I	507	GLN
2	I	512	ASN
2	I	514	VAL
2	I	516	VAL
2	I	532	TYR
2	I	534	GLU
2	I	539	THR
2	J	100	LYS
2	J	117	ASN
2	J	118	ILE
2	J	119	VAL
2	J	126	LYS
2	J	148	ASN
2	J	151	LYS
2	J	167	GLU
2	J	194	GLU
2	J	200	GLU
2	J	213	ARG
2	J	218	GLU
2	J	223	LEU

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Mol	Chain	Res	Type
2	J	227	LYS
2	J	229	ARG
2	J	243	LEU
2	J	249	GLU
2	J	261	ILE
2	J	263	ASP
2	J	287	LEU
2	J	347	GLU
2	J	368	LEU
2	J	406	LEU
2	J	429	VAL
2	J	468	ASN
2	J	470	ASP
2	J	476	GLU
2	J	481	VAL
2	J	492	LEU
2	J	495	LEU
2	J	507	GLN
2	J	512	ASN
2	J	514	VAL
2	J	542	LEU
2	J	546	SER
3	K	53	LEU
3	K	73	ARG
3	K	89	THR
3	K	90	LYS
3	K	99	LEU
3	L	35	CYS
3	L	37	MET
3	L	73	ARG
3	L	89	THR
3	M	89	THR
3	M	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	78	ASN
1	A	82	HIS
1	A	150	GLN
1	A	162	ASN

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Mol	Chain	Res	Type
1	A	171	ASN
1	A	173	GLN
1	A	227	GLN
1	A	450	GLN
1	A	493	ASN
1	A	498	HIS
1	A	502	ASN
1	A	539	GLN
1	A	578	GLN
1	B	78	ASN
1	B	101	ASN
1	B	171	ASN
1	B	227	GLN
1	C	99	HIS
1	C	227	GLN
1	C	343	GLN
1	C	493	ASN
1	C	539	GLN
1	C	607	HIS
2	D	107	GLN
2	D	129	ASN
2	D	221	GLN
2	D	364	GLN
2	D	425	HIS
2	D	475	HIS
2	E	129	ASN
2	E	136	HIS
2	E	221	GLN
2	E	425	HIS
2	E	506	GLN
2	E	507	GLN
2	F	75	ASN
2	F	129	ASN
2	F	328	GLN
2	F	358	ASN
2	F	475	HIS
2	G	364	GLN
2	G	375	ASN
2	G	388	ASN
2	G	475	HIS
2	G	494	GLN
2	H	75	ASN

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Mol	Chain	Res	Type
2	H	129	ASN
2	H	221	GLN
2	H	380	GLN
2	H	425	HIS
2	I	129	ASN
2	I	246	HIS
2	I	444	ASN
2	I	506	GLN
2	I	507	GLN
2	J	148	ASN
2	J	192	ASN
2	J	198	GLN
2	J	253	GLN
2	J	444	ASN
2	J	465	HIS
3	L	98	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

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	639/704 (90%)	-0.10	1 (0%) 91 83	137, 214, 280, 318	0
1	B	636/704 (90%)	-0.07	2 (0%) 90 80	135, 192, 256, 283	0
1	C	633/704 (89%)	-0.20	1 (0%) 91 83	180, 240, 332, 354	0
2	D	485/486 (99%)	-0.16	1 (0%) 91 83	190, 241, 349, 382	0
2	E	485/486 (99%)	-0.07	1 (0%) 91 83	174, 220, 262, 278	0
2	F	486/486 (100%)	0.02	3 (0%) 85 73	177, 230, 274, 298	0
2	G	484/486 (99%)	-0.09	1 (0%) 91 83	170, 238, 358, 443	0
2	H	486/486 (100%)	-0.01	4 (0%) 82 69	158, 232, 285, 346	0
2	I	472/486 (97%)	-0.04	1 (0%) 91 83	207, 282, 332, 359	0
2	J	483/486 (99%)	-0.17	2 (0%) 88 77	174, 244, 298, 378	0
3	K	105/105 (100%)	0.03	0 100 100	219, 359, 416, 451	0
3	L	105/105 (100%)	0.03	2 (1%) 66 53	225, 255, 277, 292	0
3	M	105/105 (100%)	-0.06	0 100 100	242, 345, 382, 388	0
All	All	5604/5829 (96%)	-0.09	19 (0%) 90 80	135, 233, 335, 451	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	523	PHE	3.5
1	B	342	ILE	3.4
2	J	381	TRP	2.9
3	L	36	LYS	2.9
2	F	364	GLN	2.8
3	L	75	ILE	2.7
1	A	342	ILE	2.5
2	F	189	CYS	2.5
2	D	255	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	368	LEU	2.3
1	B	89	ILE	2.3
2	F	436	SER	2.3
1	C	246	LEU	2.2
2	E	516	VAL	2.2
2	G	317	GLY	2.2
2	J	372	ILE	2.1
2	H	267	SER	2.1
2	H	69	TRP	2.0
2	H	524	THR	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.