Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:53 pm BST

PDB ID	:	5YH0
Title	:	The structure of DrFam20C1
Authors	:	Zhang, H.; Xiao, J.
Deposited on	:	2017-09-27
Resolution	:	3.45 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

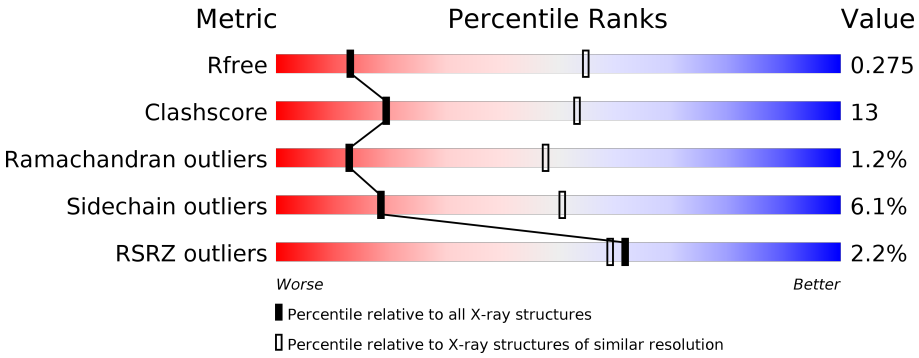
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	560	% 47% 19% • 31%
1	B	560	% 44% 19% • 32%
1	C	560	% 48% 19% • 30%
1	D	560	% 47% 18% • 32%
1	E	560	% 44% 23% • 31%
1	F	560	2% 44% 21% • 33%

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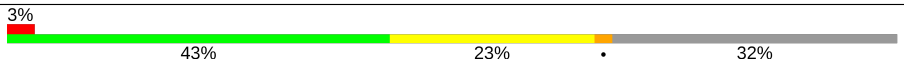
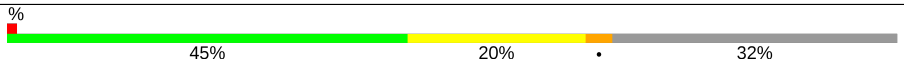
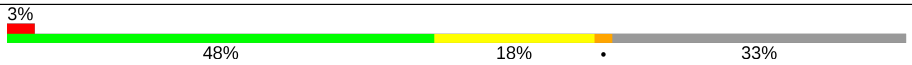
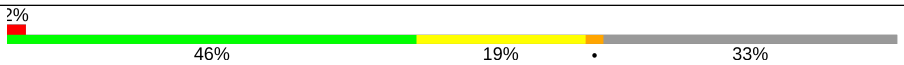
Mol	Chain	Length	Quality of chain
1	G	560	
1	H	560	
1	I	560	
1	J	560	
1	K	560	
1	L	560	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 37919 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 DrFam20C1.

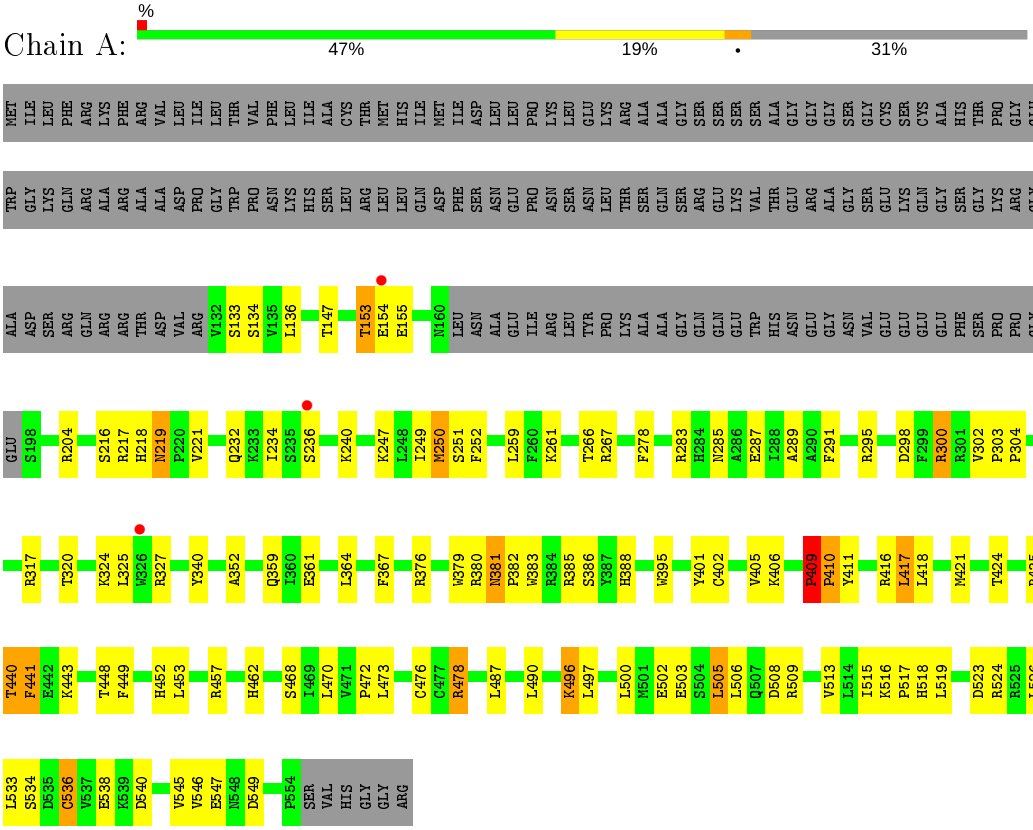
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3181	2028	559	576	18			
1	B	380	Total	C	N	O	S	0	0	0
			3141	2005	551	567	18			
1	C	390	Total	C	N	O	S	0	0	0
			3213	2048	566	581	18			
1	D	382	Total	C	N	O	S	0	0	0
			3157	2013	554	572	18			
1	E	385	Total	C	N	O	S	0	0	0
			3173	2024	557	574	18			
1	F	377	Total	C	N	O	S	0	0	0
			3118	1991	548	561	18			
1	G	386	Total	C	N	O	S	0	0	0
			3181	2028	559	576	18			
1	H	380	Total	C	N	O	S	0	0	0
			3140	2004	551	567	18			
1	I	383	Total	C	N	O	S	0	0	0
			3162	2017	556	571	18			
1	J	378	Total	C	N	O	S	0	0	0
			3124	1994	549	563	18			
1	K	389	Total	C	N	O	S	0	0	0
			3205	2042	565	580	18			
1	L	378	Total	C	N	O	S	0	0	0
			3124	1994	549	563	18			

3 Residue-property plots

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

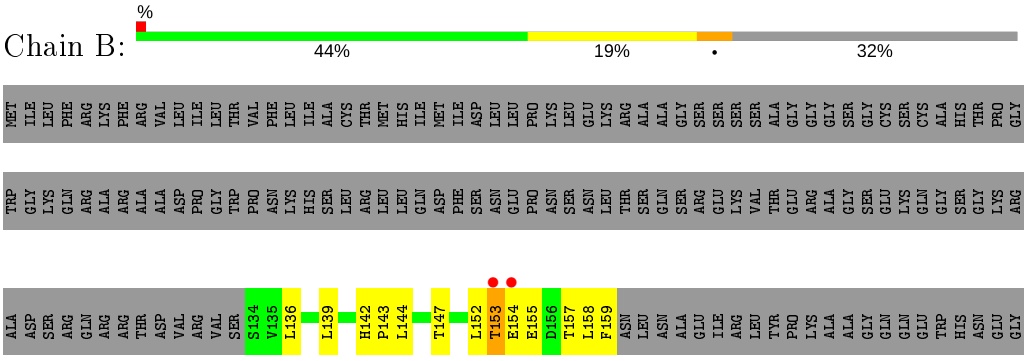
- Molecule 1: DrFam20C1

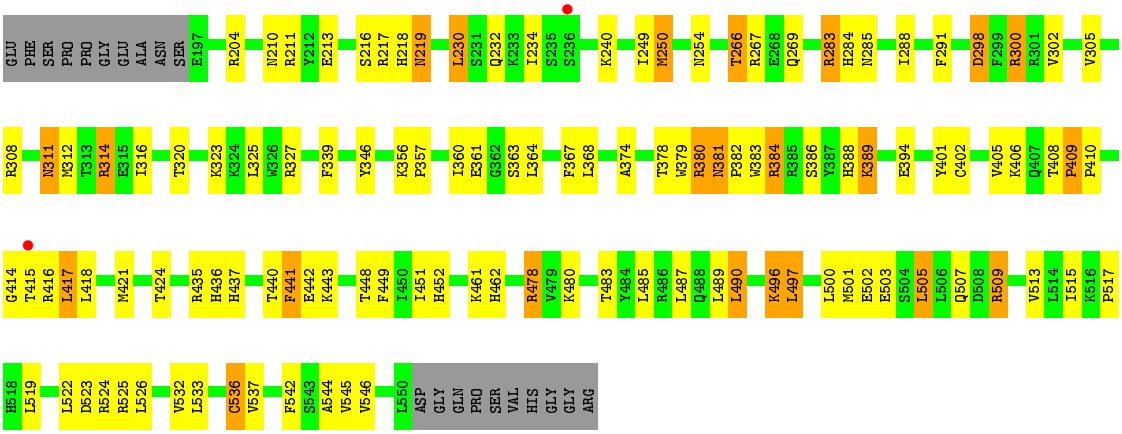
Chain A:



- Molecule 1: DrFam20C1

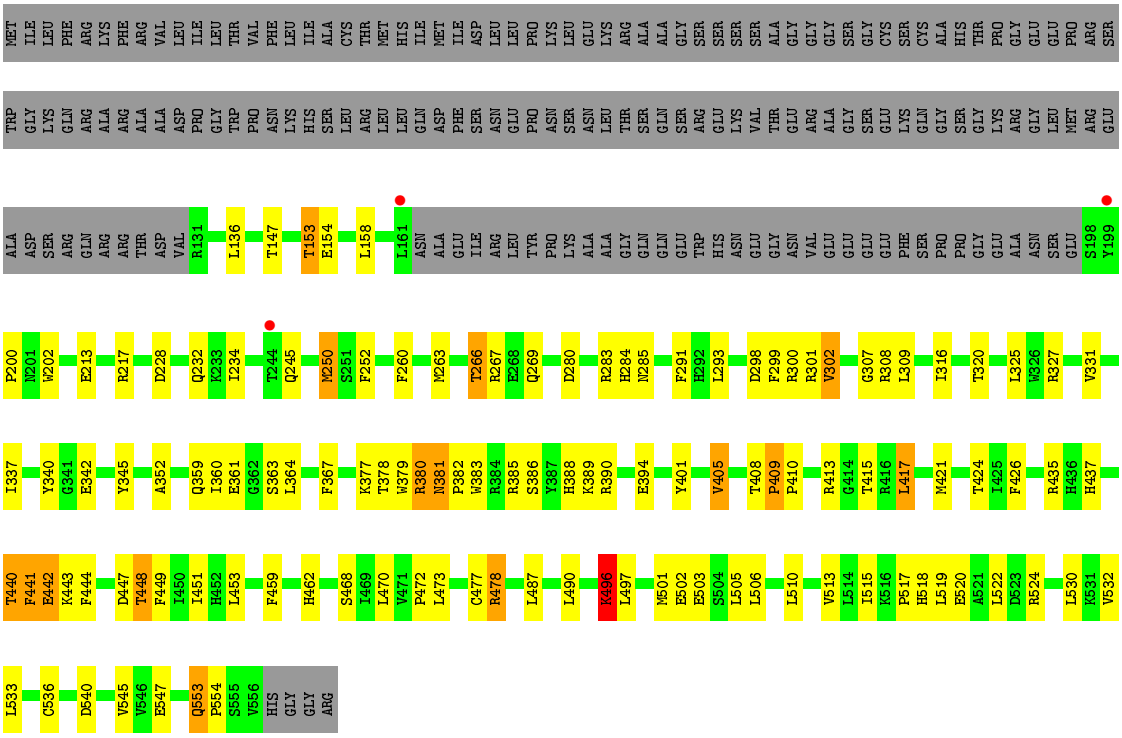
Chain B:





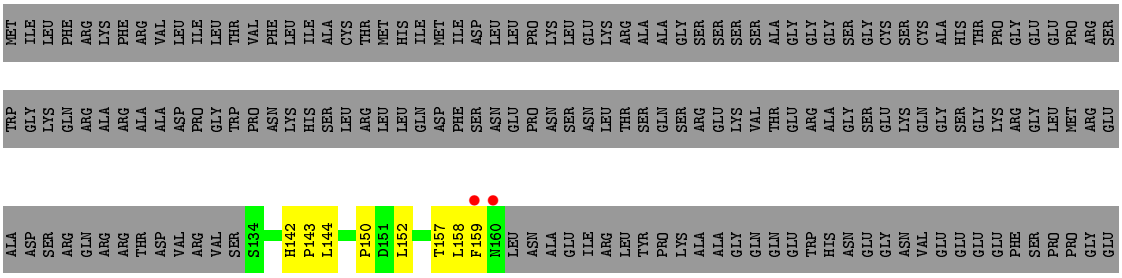
• Molecule 1: DrFam20C1

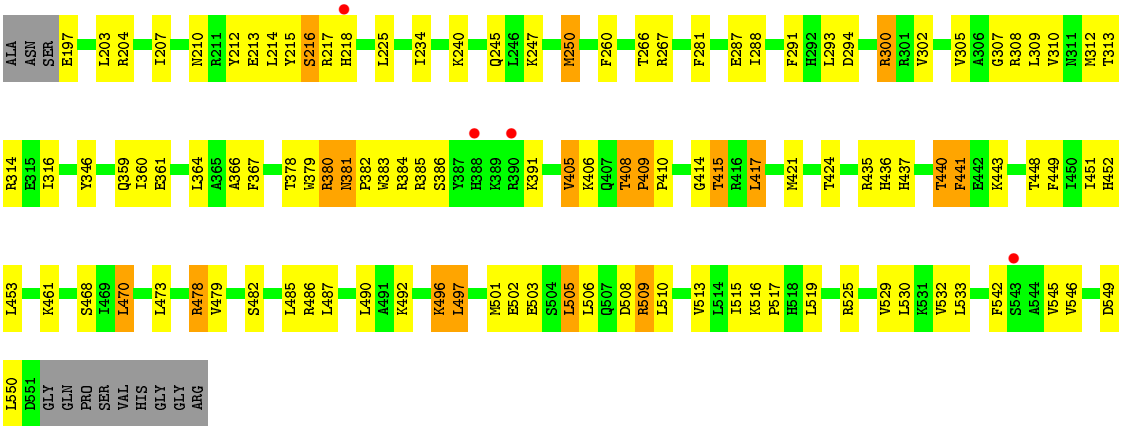
Chain C:



• Molecule 1: DrFam20C1

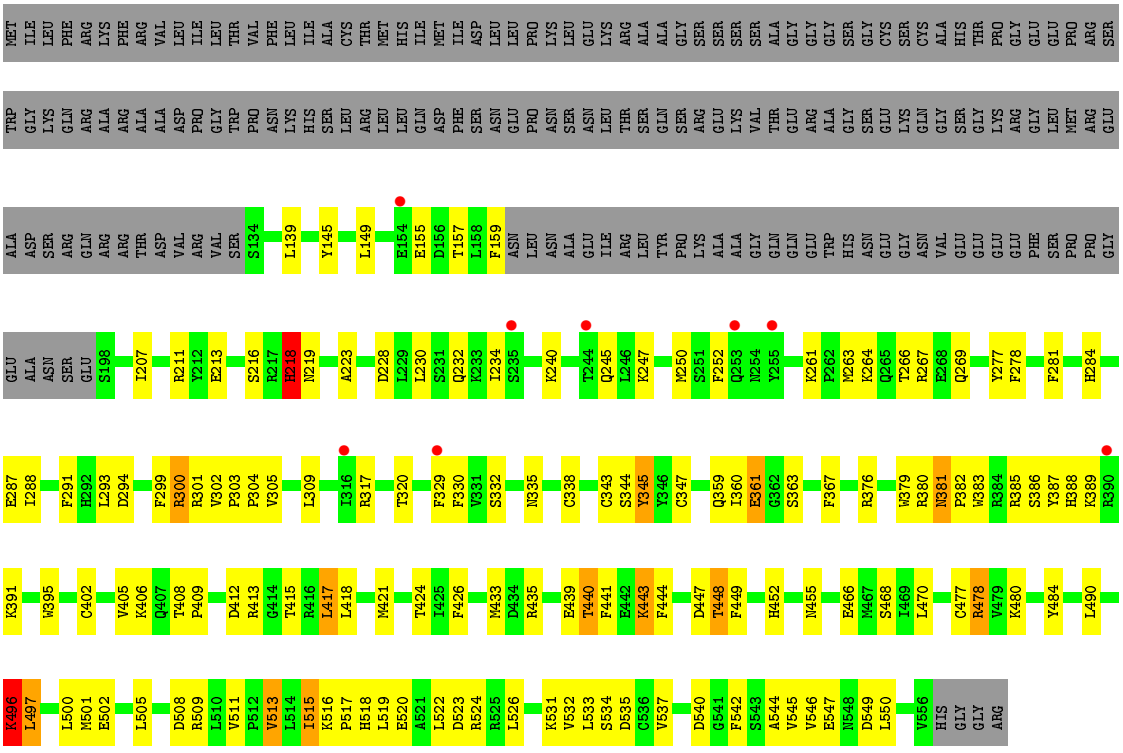
Chain D:





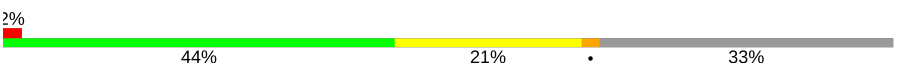
• Molecule 1: DrFam20C1

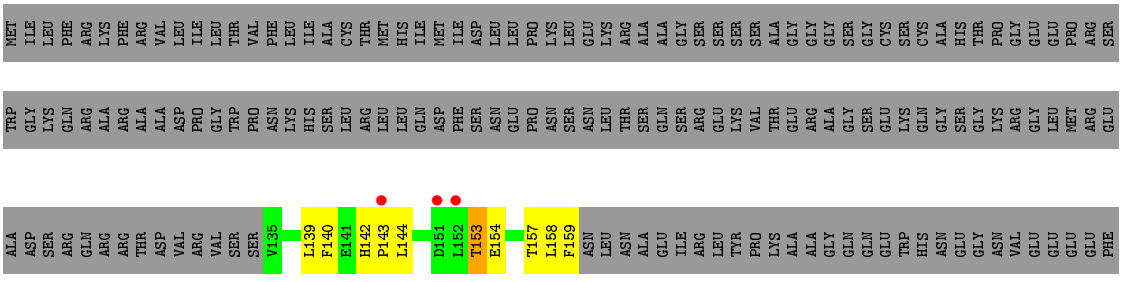
Chain E:

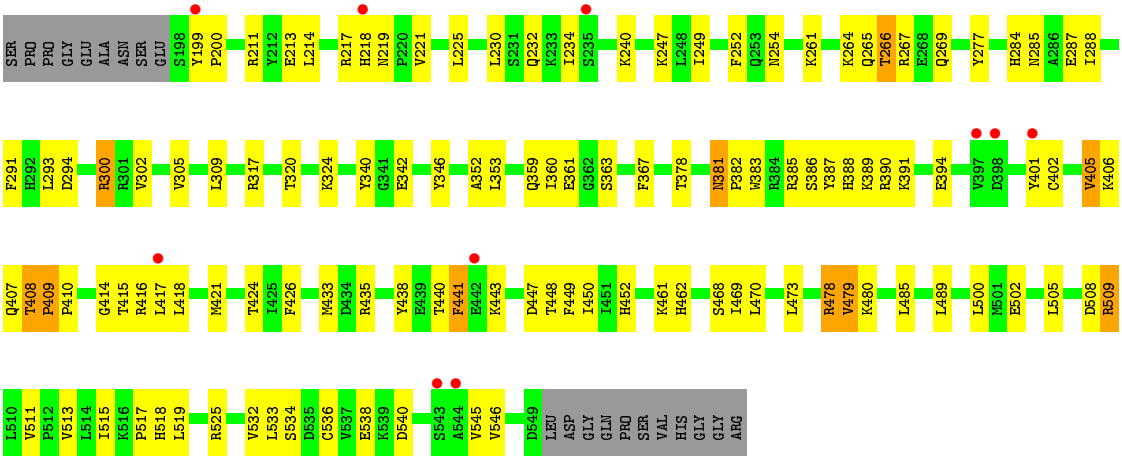


• Molecule 1: DrFam20C1

Chain F:

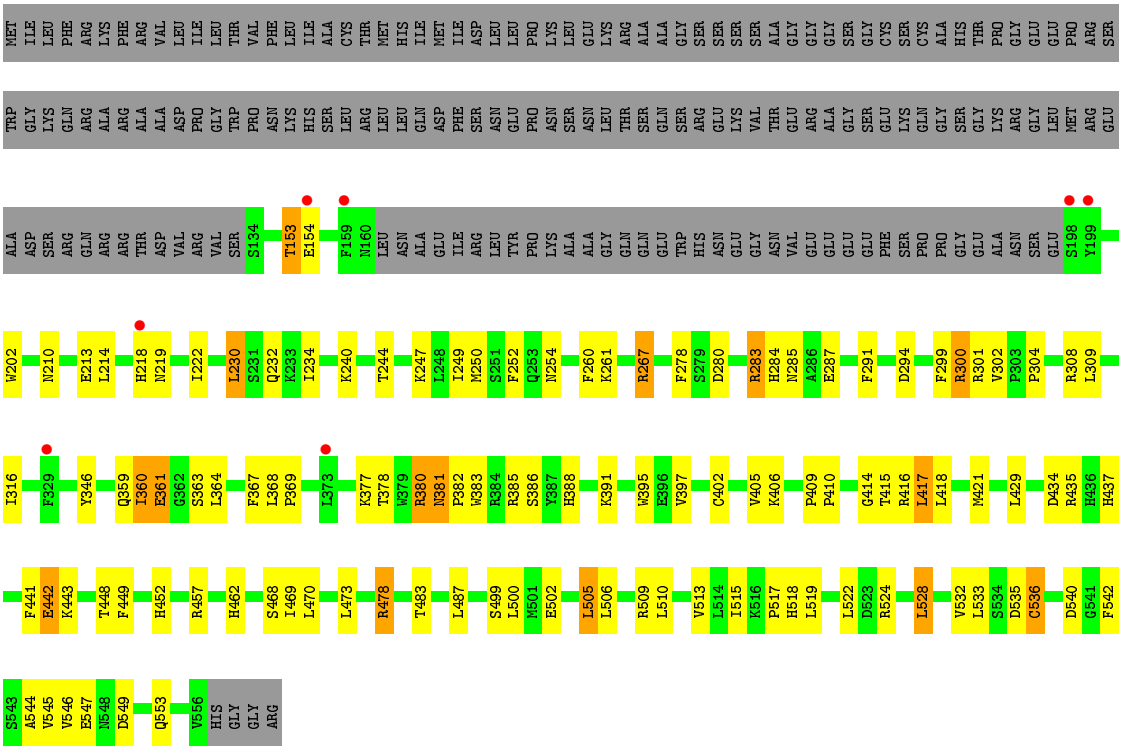






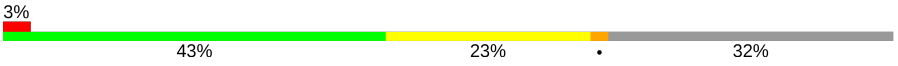
- Molecule 1: DrFam20C1

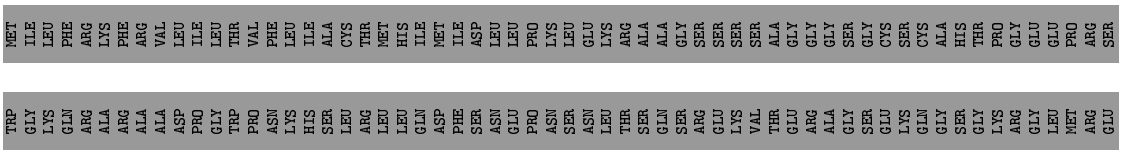
Chain G:

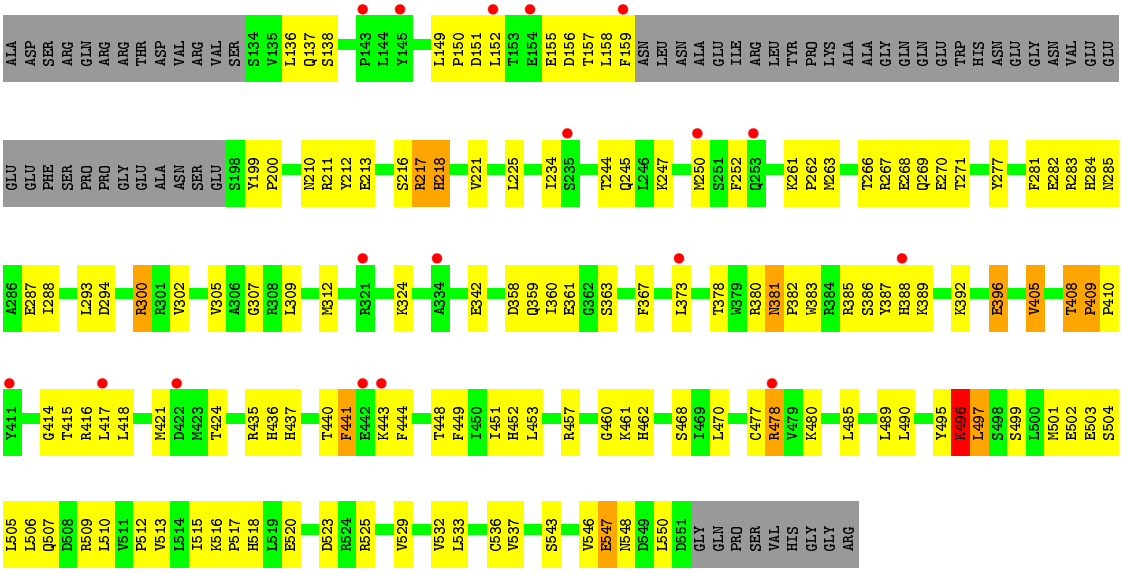


- Molecule 1: DrFam20C1

Chain H:

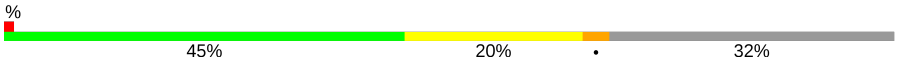


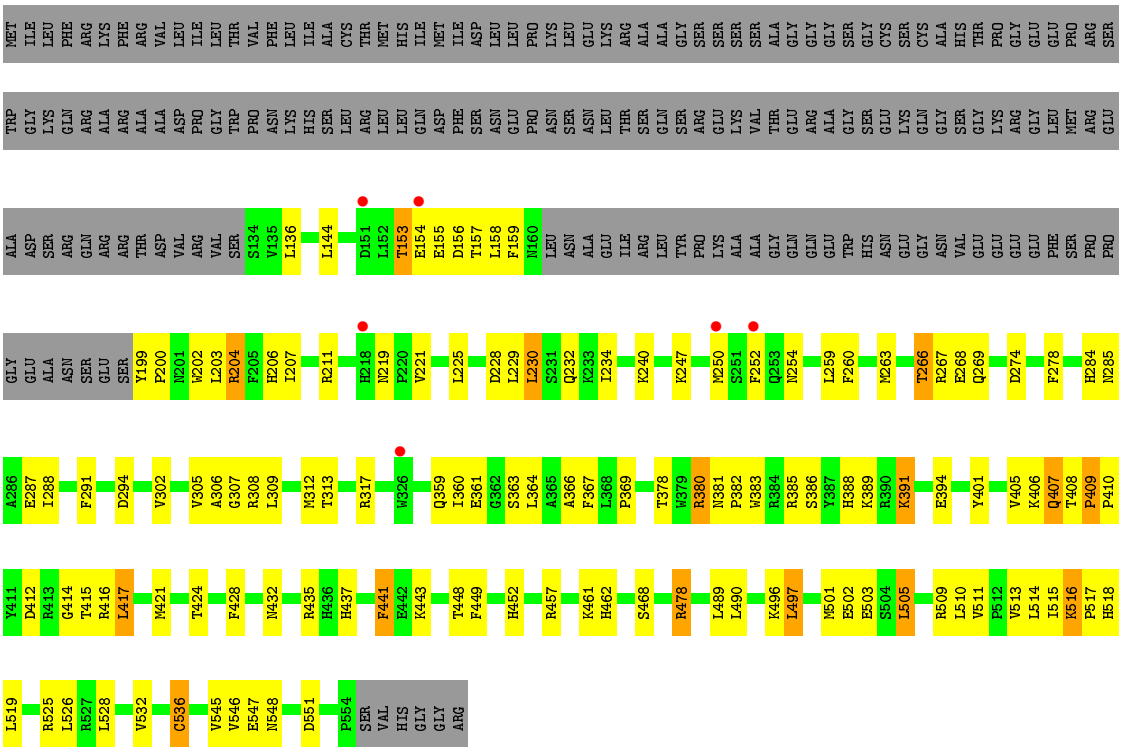




• Molecule 1: DrFam20C1

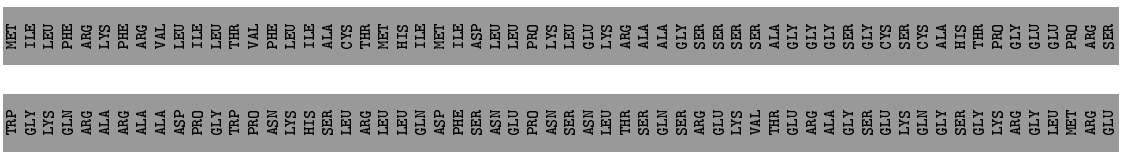
Chain I:

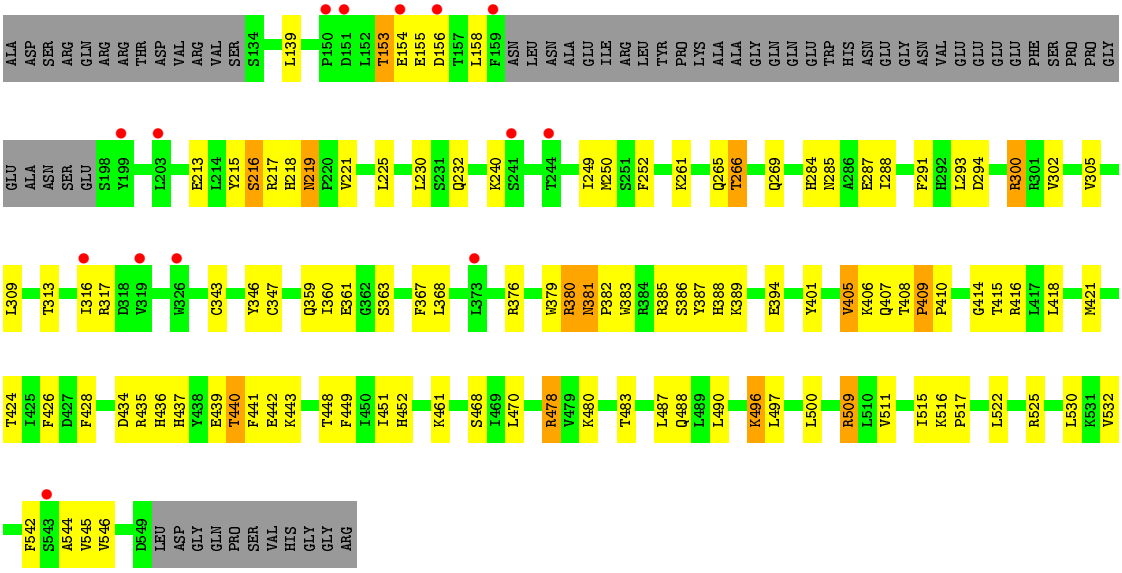




• Molecule 1: DrFam20C1

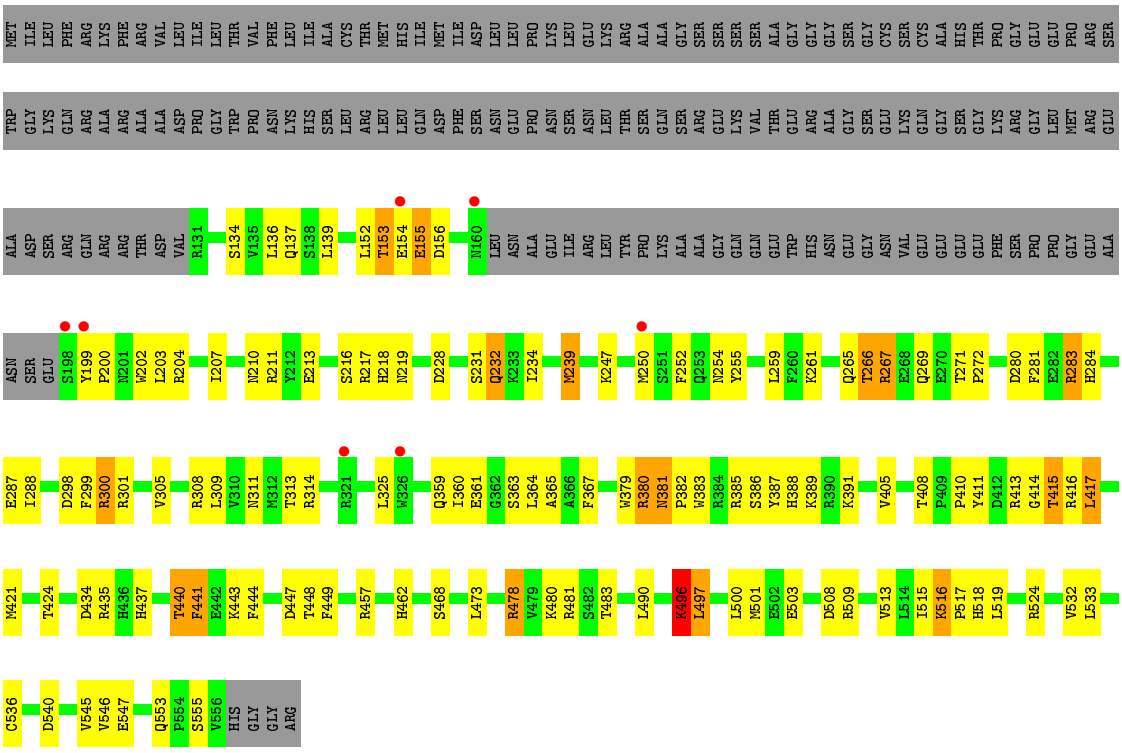
Chain J:





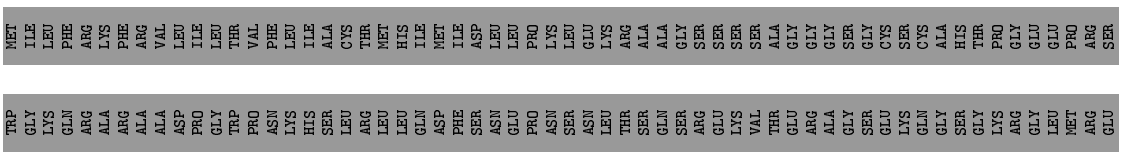
• Molecule 1: DrFam20C1

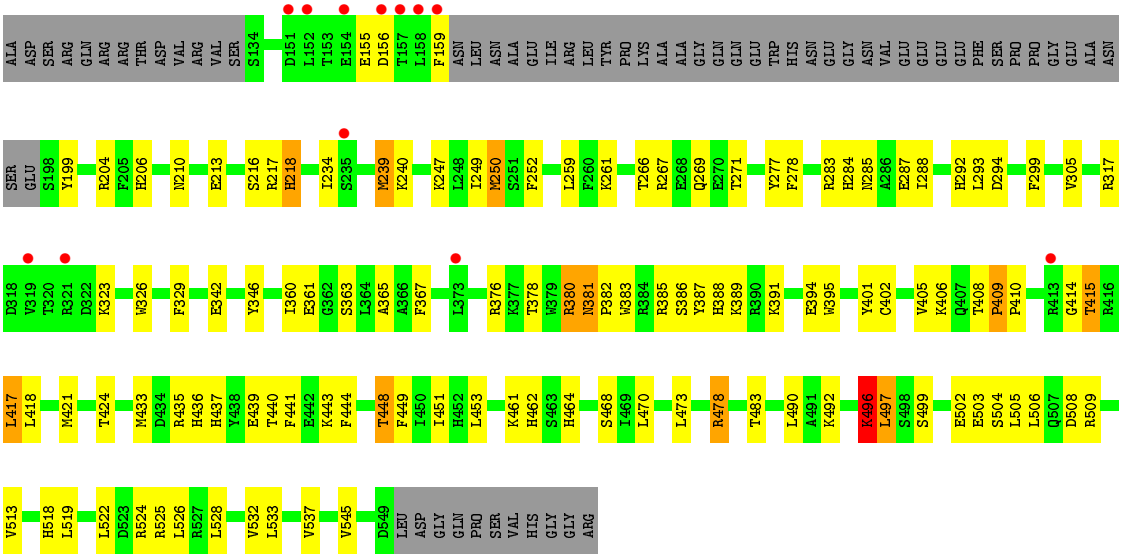
Chain K:



• Molecule 1: DrFam20C1

Chain L:




ALA ASP SER ARG GLN ARG ARG THR ASP VAL ARG VAL SER S134 D151 L152 T153 E154 E155 D156 T157 L158 F159 ASN LEU ASN ALA GLU ILE ARG LEU TYR PRO LYS ALA ALA GLY GLN GLN GLU TRP HIS ASN GLU GLY ASN VAL GLU GLU GLU GLU PHE SER PRO PRO GLY GLU ALA ASN
SER GLU S198 Y199 R204 F205 H206 N210 E213 S216 R217 H218 I234 S235 M239 K240 K247 L248 I249 M250 S251 F252 L259 P260 K261 T266 R267 E268 Q269 E270 T271 Y277 F278 R283 H284 N285 A286 E287 I288 H292 L293 D294 F299 V305 R317
D318 V319 T320 R321 D322 K323 W326 F329 E342 Y346 I360 E361 G362 S363 L364 A365 A366 F367 L373 R376 K377 T378 W379 R380 N381 P382 W383 R384 R385 S386 Y387 H388 K389 R390 K391 E394 W395 Y401 C402 V405 K406 Q407 T408 P409 P410 R413 G414 T415 R416
L417 L418 M421 T424 M433 D434 R435 H436 H437 Y438 E439 T440 F441 E442 K443 F444 T448 F449 I450 I451 H452 L453 K461 H462 S463 H464 S468 I469 L470 L473 R478 T483 L490 A491 K492 K496 L497 S498 S499 E502 E503 S504 L505 L506 Q507 D508 R509
V513 H518 L519 L522 D523 R524 R525 L526 R527 L528 V532 L533 V537 V545 D549 LEU ASP GLY GLN PRO SER VAL HIS GLY GLY ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	114.92Å 135.99Å 219.97Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	47.84 – 3.45 47.84 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.84-3.45) 91.3 (47.84-3.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.225 , 0.279 0.225 , 0.275	Depositor DCC
R_{free} test set	2005 reflections (2.26%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 14.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	37919	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8756e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/3259	0.57	1/4403 (0.0%)
1	B	0.30	0/3218	0.58	2/4346 (0.0%)
1	C	0.32	0/3291	0.59	1/4446 (0.0%)
1	D	0.30	0/3234	0.56	1/4368 (0.0%)
1	E	0.30	0/3251	0.57	1/4392 (0.0%)
1	F	0.29	0/3195	0.57	1/4315 (0.0%)
1	G	0.29	0/3259	0.58	3/4403 (0.1%)
1	H	0.29	0/3217	0.57	1/4345 (0.0%)
1	I	0.29	0/3240	0.56	2/4377 (0.0%)
1	J	0.28	0/3201	0.57	2/4323 (0.0%)
1	K	0.29	0/3283	0.58	1/4435 (0.0%)
1	L	0.29	0/3201	0.56	1/4323 (0.0%)
All	All	0.30	0/38849	0.57	17/52476 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	380	ARG	C-N-CA	-9.59	97.73	121.70
1	D	380	ARG	C-N-CA	-8.24	101.11	121.70
1	A	380	ARG	C-N-CA	-7.79	102.22	121.70
1	I	380	ARG	C-N-CA	-7.70	102.45	121.70
1	J	380	ARG	C-N-CA	-7.20	103.71	121.70
1	B	380	ARG	C-N-CA	-7.07	104.02	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	380	ARG	C-N-CA	-6.91	104.44	121.70
1	G	500	LEU	CA-CB-CG	6.71	130.72	115.30
1	E	380	ARG	C-N-CA	-6.61	105.19	121.70
1	H	380	ARG	C-N-CA	-6.25	106.08	121.70
1	F	407	GLN	C-N-CA	5.73	136.02	121.70
1	L	380	ARG	C-N-CA	-5.64	107.60	121.70
1	K	380	ARG	C-N-CA	-5.59	107.72	121.70
1	G	528	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	490	LEU	CA-CB-CG	5.18	127.22	115.30
1	I	407	GLN	C-N-CA	5.10	134.45	121.70
1	J	407	GLN	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3181	0	3139	80	0
1	B	3141	0	3101	84	0
1	C	3213	0	3175	79	0
1	D	3157	0	3111	73	0
1	E	3173	0	3131	92	0
1	F	3118	0	3079	84	0
1	G	3181	0	3137	80	0
1	H	3140	0	3099	89	0
1	I	3162	0	3118	88	0
1	J	3124	0	3084	73	0
1	K	3205	0	3164	76	0
1	L	3124	0	3084	73	0
All	All	37919	0	37422	962	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 13.

All (962) 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:A:515:ILE:HG13	1:A:517:PRO:HD2	1.44	0.98
1:B:240:LYS:HG3	1:B:249:ILE:HD11	1.54	0.89
1:L:385:ARG:HH22	1:L:468:SER:HB2	1.38	0.86
1:I:291:PHE:HA	1:I:302:VAL:HG21	1.55	0.86
1:K:515:ILE:HG13	1:K:517:PRO:HD2	1.58	0.85
1:G:291:PHE:HA	1:G:302:VAL:HG21	1.56	0.84
1:E:291:PHE:HA	1:E:302:VAL:HG21	1.58	0.84
1:H:478:ARG:HH12	1:H:547:GLU:HG2	1.43	0.83
1:B:291:PHE:HA	1:B:302:VAL:HG21	1.62	0.81
1:D:291:PHE:HA	1:D:302:VAL:HG21	1.60	0.81
1:G:244:THR:HG21	1:G:457:ARG:HH22	1.45	0.81
1:J:408:THR:HG22	1:J:409:PRO:HD2	1.62	0.81
1:J:291:PHE:HA	1:J:302:VAL:HG21	1.61	0.81
1:C:515:ILE:HG13	1:C:517:PRO:HD2	1.62	0.81
1:H:158:LEU:HD12	1:H:443:LYS:HD2	1.62	0.80
1:G:515:ILE:HG13	1:G:517:PRO:HD2	1.62	0.80
1:A:147:THR:O	1:A:217:ARG:NH2	2.15	0.79
1:C:291:PHE:HA	1:C:302:VAL:HG21	1.62	0.79
1:A:385:ARG:HH22	1:A:468:SER:HB2	1.47	0.79
1:A:291:PHE:HA	1:A:302:VAL:HG21	1.63	0.78
1:C:147:THR:O	1:C:217:ARG:NH2	2.17	0.78
1:K:381:ASN:ND2	1:K:435:ARG:O	2.17	0.78
1:H:505:LEU:HD22	1:H:513:VAL:HG21	1.65	0.78
1:A:247:LYS:HE2	1:A:259:LEU:HD21	1.65	0.78
1:H:381:ASN:ND2	1:H:435:ARG:O	2.17	0.77
1:I:136:LEU:HB2	1:I:503:GLU:HG2	1.65	0.77
1:K:311:ASN:HD21	1:K:314:ARG:HH21	1.33	0.77
1:K:388:HIS:ND1	1:K:389:LYS:O	2.18	0.76
1:E:385:ARG:HH22	1:E:468:SER:HB2	1.51	0.75
1:H:266:THR:HG22	1:H:269:GLN:HG3	1.68	0.74
1:H:515:ILE:HG23	1:H:517:PRO:HD2	1.67	0.74
1:K:217:ARG:NH2	1:K:298:ASP:OD2	2.20	0.74
1:D:152:LEU:HD21	1:D:210:ASN:HD22	1.53	0.74
1:F:291:PHE:HA	1:F:302:VAL:HG21	1.70	0.74
1:F:139:LEU:HD22	1:F:500:LEU:HD21	1.70	0.73
1:C:385:ARG:HH22	1:C:468:SER:HB2	1.54	0.73
1:D:385:ARG:HH22	1:D:468:SER:HB2	1.51	0.73
1:K:247:LYS:HE2	1:K:259:LEU:HD21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:461:LYS:O	1:I:525:ARG:NH2	2.20	0.73
1:H:385:ARG:HH22	1:H:468:SER:HB2	1.53	0.73
1:I:386:SER:OG	1:I:391:LYS:O	2.07	0.73
1:K:540:ASP:HB2	1:K:545:VAL:HG23	1.70	0.72
1:K:265:GLN:OE1	1:K:269:GLN:NE2	2.22	0.72
1:G:502:GLU:HB3	1:G:519:LEU:HD13	1.70	0.72
1:I:381:ASN:ND2	1:I:435:ARG:O	2.22	0.72
1:C:413:ARG:NH1	1:C:447:ASP:OD2	2.23	0.72
1:F:213:GLU:OE1	1:F:300:ARG:NH2	2.22	0.72
1:G:414:GLY:HA2	1:G:415:THR:HG22	1.69	0.72
1:K:385:ARG:HH22	1:K:468:SER:HB2	1.53	0.71
1:B:136:LEU:HB2	1:B:503:GLU:HG2	1.71	0.71
1:D:435:ARG:NH1	1:D:453:LEU:O	2.23	0.71
1:D:414:GLY:HA2	1:D:415:THR:HG22	1.72	0.71
1:C:213:GLU:OE1	1:C:300:ARG:NH2	2.23	0.70
1:E:213:GLU:OE1	1:E:300:ARG:NH2	2.23	0.70
1:C:490:LEU:O	1:C:496:LYS:HA	1.92	0.70
1:D:215:TYR:O	1:D:216:SER:OG	2.06	0.69
1:I:266:THR:HG23	1:I:269:GLN:HE21	1.58	0.69
1:J:487:LEU:HB3	1:J:530:LEU:HD11	1.75	0.69
1:F:381:ASN:ND2	1:F:435:ARG:O	2.26	0.69
1:E:490:LEU:O	1:E:496:LYS:HA	1.93	0.69
1:B:388:HIS:ND1	1:B:389:LYS:O	2.26	0.68
1:B:213:GLU:OE1	1:B:300:ARG:NH2	2.27	0.68
1:G:213:GLU:OE1	1:G:300:ARG:NH2	2.26	0.68
1:L:537:VAL:HG23	1:L:545:VAL:HG11	1.76	0.68
1:D:213:GLU:OE1	1:D:300:ARG:NH2	2.27	0.68
1:B:232:GLN:NE2	1:B:254:ASN:OD1	2.26	0.67
1:E:515:ILE:H	1:E:515:ILE:HD12	1.58	0.67
1:A:502:GLU:HB3	1:A:519:LEU:HD13	1.76	0.67
1:B:216:SER:HB2	1:B:219:ASN:H	1.61	0.66
1:C:505:LEU:HD22	1:C:513:VAL:HG21	1.76	0.66
1:F:247:LYS:HD3	1:F:261:LYS:HE3	1.76	0.66
1:K:441:PHE:O	1:K:443:LYS:N	2.27	0.66
1:I:247:LYS:HE2	1:I:259:LEU:HD21	1.78	0.66
1:D:487:LEU:HB3	1:D:530:LEU:HD11	1.78	0.66
1:F:240:LYS:HB2	1:F:249:ILE:HD11	1.78	0.66
1:L:499:SER:O	1:L:503:GLU:HG2	1.96	0.66
1:A:421:MET:HA	1:A:424:THR:HG22	1.78	0.65
1:K:478:ARG:HH12	1:K:547:GLU:HG3	1.62	0.65
1:A:409:PRO:HB2	1:A:410:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:LYS:HB2	1:C:442:GLU:HG2	1.79	0.65
1:K:490:LEU:O	1:K:496:LYS:HA	1.96	0.65
1:L:376:ARG:NH1	1:L:439:GLU:OE1	2.30	0.65
1:G:309:LEU:HD22	1:G:359:GLN:HB3	1.77	0.65
1:C:459:PHE:HE1	1:C:522:LEU:HD11	1.62	0.65
1:H:213:GLU:OE1	1:H:300:ARG:NH2	2.30	0.65
1:L:394:GLU:HB3	1:L:401:TYR:HE2	1.61	0.65
1:A:436:HIS:CD2	1:A:437:HIS:HD2	2.14	0.64
1:K:213:GLU:OE1	1:K:300:ARG:NH2	2.30	0.64
1:A:418:LEU:HD11	1:A:547:GLU:HG3	1.79	0.64
1:B:421:MET:HA	1:B:424:THR:HG22	1.79	0.64
1:B:152:LEU:HD21	1:B:210:ASN:HD22	1.62	0.64
1:J:385:ARG:HH22	1:J:468:SER:HB2	1.62	0.64
1:E:421:MET:HG3	1:E:478:ARG:O	1.97	0.64
1:G:418:LEU:HD11	1:G:547:GLU:HG3	1.79	0.64
1:A:386:SER:O	1:A:388:HIS:N	2.26	0.63
1:C:136:LEU:HB2	1:C:503:GLU:HG2	1.78	0.63
1:I:505:LEU:HD22	1:I:513:VAL:HG21	1.80	0.63
1:J:213:GLU:OE1	1:J:300:ARG:NH2	2.31	0.63
1:I:441:PHE:O	1:I:443:LYS:N	2.30	0.63
1:J:515:ILE:HG13	1:J:517:PRO:HD2	1.81	0.63
1:H:504:SER:C	1:H:506:LEU:H	2.01	0.63
1:H:244:THR:HG21	1:H:457:ARG:HH22	1.63	0.63
1:D:142:HIS:HD2	1:D:144:LEU:H	1.46	0.62
1:D:309:LEU:HD22	1:D:359:GLN:HB3	1.80	0.62
1:L:381:ASN:ND2	1:L:435:ARG:O	2.32	0.62
1:H:267:ARG:NH2	1:H:361:GLU:OE1	2.26	0.62
1:B:147:THR:O	1:B:217:ARG:NH1	2.32	0.62
1:E:381:ASN:ND2	1:E:435:ARG:O	2.33	0.62
1:B:515:ILE:HG23	1:B:517:PRO:HD2	1.81	0.62
1:E:406:LYS:O	1:E:412:ASP:HB3	2.00	0.62
1:F:421:MET:HA	1:F:424:THR:HG22	1.80	0.62
1:H:245:GLN:OE1	1:H:282:GLU:N	2.32	0.62
1:G:545:VAL:HG12	1:G:546:VAL:HG13	1.81	0.62
1:A:379:TRP:HZ3	1:A:410:PRO:HG3	1.65	0.62
1:G:532:VAL:O	1:G:536:CYS:HB3	1.99	0.62
1:D:441:PHE:O	1:D:443:LYS:N	2.32	0.62
1:F:291:PHE:HD1	1:F:302:VAL:HG23	1.64	0.61
1:D:381:ASN:ND2	1:D:435:ARG:O	2.33	0.61
1:C:553:GLN:HG3	1:C:554:PRO:HD2	1.81	0.61
1:E:386:SER:OG	1:E:391:LYS:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:153:THR:OG1	1:J:154:GLU:N	2.33	0.61
1:B:381:ASN:ND2	1:B:435:ARG:O	2.33	0.61
1:D:379:TRP:NE1	1:D:440:THR:OG1	2.33	0.61
1:F:505:LEU:HD22	1:F:513:VAL:HG21	1.82	0.61
1:L:441:PHE:O	1:L:443:LYS:N	2.34	0.61
1:L:505:LEU:HD22	1:L:513:VAL:HG21	1.82	0.61
1:I:502:GLU:HB3	1:I:519:LEU:HD13	1.83	0.61
1:A:505:LEU:HD22	1:A:513:VAL:HG21	1.83	0.61
1:G:502:GLU:O	1:G:506:LEU:HD13	2.01	0.61
1:K:271:THR:HG21	1:K:280:ASP:OD1	2.01	0.61
1:B:153:THR:OG1	1:B:154:GLU:N	2.33	0.60
1:K:311:ASN:HD21	1:K:314:ARG:NH2	1.99	0.60
1:E:531:LYS:NZ	1:E:535:ASP:OD2	2.33	0.60
1:J:216:SER:HB3	1:J:219:ASN:HB2	1.82	0.60
1:K:136:LEU:HB2	1:K:503:GLU:HG2	1.81	0.60
1:C:153:THR:OG1	1:C:154:GLU:N	2.35	0.60
1:K:232:GLN:NE2	1:K:254:ASN:OD1	2.34	0.60
1:B:441:PHE:O	1:B:443:LYS:N	2.31	0.60
1:D:421:MET:HA	1:D:424:THR:HG22	1.83	0.60
1:D:490:LEU:HB3	1:D:497:LEU:HD22	1.83	0.60
1:E:502:GLU:HB3	1:E:519:LEU:HD13	1.84	0.60
1:G:478:ARG:HH22	1:G:547:GLU:HG2	1.65	0.60
1:E:515:ILE:HG21	1:J:511:VAL:HG21	1.84	0.60
1:K:261:LYS:HD2	1:K:287:GLU:HG3	1.84	0.60
1:H:461:LYS:O	1:H:525:ARG:NH2	2.34	0.60
1:I:421:MET:HA	1:I:424:THR:HG22	1.84	0.60
1:L:389:LYS:O	1:L:391:LYS:HD2	2.02	0.60
1:A:409:PRO:O	1:A:411:TYR:N	2.28	0.59
1:K:153:THR:OG1	1:K:154:GLU:N	2.34	0.59
1:B:490:LEU:O	1:B:496:LYS:HA	2.02	0.59
1:E:216:SER:HB2	1:E:219:ASN:HB2	1.83	0.59
1:D:515:ILE:HG13	1:D:517:PRO:HD2	1.85	0.59
1:F:230:LEU:HD11	1:F:509:ARG:HB2	1.85	0.59
1:J:381:ASN:ND2	1:J:435:ARG:O	2.35	0.59
1:J:545:VAL:HG12	1:J:546:VAL:HG23	1.84	0.59
1:L:261:LYS:HD2	1:L:287:GLU:HG3	1.84	0.59
1:L:490:LEU:O	1:L:496:LYS:HA	2.01	0.59
1:I:478:ARG:HH12	1:I:547:GLU:HG3	1.66	0.59
1:F:266:THR:HG23	1:F:269:GLN:OE1	2.03	0.59
1:D:545:VAL:HG12	1:D:546:VAL:HG13	1.83	0.59
1:E:309:LEU:HD22	1:E:359:GLN:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:LYS:HD3	1:G:261:LYS:HE2	1.85	0.59
1:B:230:LEU:HD11	1:B:509:ARG:HB2	1.85	0.59
1:G:386:SER:O	1:G:388:HIS:N	2.33	0.59
1:G:385:ARG:HH22	1:G:468:SER:HB2	1.67	0.59
1:L:317:ARG:HB2	1:L:329:PHE:CE2	2.38	0.59
1:A:153:THR:OG1	1:A:154:GLU:N	2.35	0.58
1:I:497:LEU:HD23	1:I:526:LEU:HD22	1.84	0.58
1:K:386:SER:OG	1:K:391:LYS:O	2.17	0.58
1:L:284:HIS:HB2	1:L:363:SER:HB3	1.85	0.58
1:E:155:GLU:OE2	1:E:211:ARG:NH2	2.36	0.58
1:J:261:LYS:HD2	1:J:287:GLU:HG3	1.83	0.58
1:E:540:ASP:HB2	1:E:545:VAL:HG23	1.85	0.58
1:J:155:GLU:HG2	1:J:156:ASP:H	1.68	0.58
1:K:232:GLN:HB3	1:K:252:PHE:CD2	2.39	0.58
1:A:217:ARG:HB2	1:A:300:ARG:NH1	2.18	0.58
1:I:153:THR:OG1	1:I:154:GLU:N	2.36	0.58
1:I:309:LEU:HD22	1:I:359:GLN:HB3	1.85	0.58
1:B:502:GLU:HB3	1:B:519:LEU:HD13	1.86	0.58
1:B:505:LEU:HD22	1:B:513:VAL:HG21	1.84	0.58
1:H:136:LEU:HB2	1:H:503:GLU:HG2	1.86	0.58
1:C:386:SER:O	1:C:388:HIS:N	2.33	0.58
1:D:386:SER:OG	1:D:391:LYS:O	2.13	0.57
1:K:152:LEU:HD21	1:K:210:ASN:HD22	1.68	0.57
1:F:232:GLN:NE2	1:F:254:ASN:OD1	2.37	0.57
1:E:218:HIS:CE1	1:E:223:ALA:HB2	2.39	0.57
1:K:421:MET:HA	1:K:424:THR:HG22	1.85	0.57
1:E:284:HIS:HB2	1:E:363:SER:HB3	1.86	0.57
1:C:284:HIS:HB2	1:C:363:SER:HB3	1.86	0.57
1:F:385:ARG:HH22	1:F:468:SER:HB2	1.70	0.57
1:E:329:PHE:O	1:F:390:ARG:NH2	2.37	0.57
1:H:490:LEU:O	1:H:496:LYS:HA	2.03	0.57
1:I:308:ARG:HB3	1:I:364:LEU:HD23	1.87	0.57
1:I:385:ARG:HH22	1:I:468:SER:HB2	1.68	0.57
1:J:215:TYR:O	1:J:216:SER:HB2	2.03	0.57
1:A:381:ASN:ND2	1:A:435:ARG:O	2.38	0.57
1:H:478:ARG:NH1	1:H:547:GLU:HG2	2.18	0.57
1:L:461:LYS:O	1:L:525:ARG:NH2	2.32	0.57
1:F:405:VAL:O	1:F:408:THR:OG1	2.23	0.57
1:H:152:LEU:HD21	1:H:210:ASN:HD22	1.70	0.57
1:D:250:MET:HE3	1:D:260:PHE:CG	2.40	0.56
1:J:388:HIS:ND1	1:J:389:LYS:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:ARG:HB2	1:F:300:ARG:HH12	1.69	0.56
1:C:382:PRO:HG2	1:C:383:TRP:CZ3	2.41	0.56
1:D:379:TRP:HE1	1:D:440:THR:HG1	1.51	0.56
1:E:441:PHE:O	1:E:443:LYS:N	2.38	0.56
1:C:266:THR:HG23	1:C:269:GLN:OE1	2.06	0.56
1:D:384:ARG:HG3	1:D:436:HIS:HB2	1.88	0.56
1:I:515:ILE:HG22	1:I:518:HIS:HD2	1.70	0.56
1:J:368:LEU:HD11	1:J:451:ILE:HG21	1.88	0.56
1:A:532:VAL:O	1:A:536:CYS:HB3	2.06	0.56
1:E:261:LYS:HD2	1:E:287:GLU:HG3	1.88	0.56
1:G:499:SER:HA	1:G:502:GLU:HG2	1.85	0.56
1:A:309:LEU:HD22	1:A:359:GLN:HB3	1.87	0.56
1:A:441:PHE:O	1:A:443:LYS:N	2.37	0.56
1:B:144:LEU:HD12	1:B:489:LEU:HD22	1.86	0.56
1:C:308:ARG:HB3	1:C:364:LEU:HD23	1.87	0.56
1:C:478:ARG:HH12	1:C:547:GLU:HG3	1.70	0.56
1:F:309:LEU:HD13	1:F:361:GLU:HB2	1.86	0.56
1:F:158:LEU:HD12	1:F:443:LYS:HD2	1.88	0.56
1:G:210:ASN:OD1	1:G:213:GLU:HG2	2.06	0.56
1:J:376:ARG:NH1	1:J:439:GLU:OE1	2.37	0.56
1:L:240:LYS:HG2	1:L:249:ILE:HD11	1.88	0.56
1:L:394:GLU:HB3	1:L:401:TYR:CE2	2.41	0.56
1:C:413:ARG:HG2	1:C:413:ARG:NH2	2.21	0.56
1:F:545:VAL:HG12	1:F:546:VAL:HG13	1.88	0.56
1:A:417:LEU:O	1:A:421:MET:HG2	2.06	0.55
1:B:380:ARG:HA	1:B:437:HIS:ND1	2.21	0.55
1:I:516:LYS:HD3	1:I:519:LEU:HD12	1.86	0.55
1:G:153:THR:OG1	1:G:154:GLU:N	2.37	0.55
1:I:230:LEU:HD21	1:I:509:ARG:HB2	1.89	0.55
1:J:309:LEU:HD22	1:J:359:GLN:HB3	1.88	0.55
1:G:473:LEU:HD21	1:G:533:LEU:HD21	1.87	0.55
1:K:497:LEU:O	1:K:501:MET:N	2.39	0.55
1:B:217:ARG:NH2	1:B:298:ASP:OD2	2.34	0.55
1:G:441:PHE:O	1:G:443:LYS:N	2.37	0.55
1:F:221:VAL:O	1:F:225:LEU:N	2.35	0.55
1:C:478:ARG:HH12	1:C:547:GLU:CG	2.19	0.55
1:I:501:MET:HE2	1:I:501:MET:HA	1.89	0.55
1:F:153:THR:OG1	1:F:154:GLU:N	2.39	0.55
1:F:418:LEU:HD13	1:F:480:LYS:HG3	1.89	0.55
1:C:381:ASN:ND2	1:C:435:ARG:O	2.39	0.55
1:H:267:ARG:NH1	1:H:512:PRO:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:392:LYS:HB3	1:H:396:GLU:HB3	1.89	0.54
1:I:266:THR:HG23	1:I:269:GLN:NE2	2.20	0.54
1:A:382:PRO:HG2	1:A:383:TRP:CZ3	2.43	0.54
1:G:261:LYS:HD2	1:G:287:GLU:HG3	1.89	0.54
1:J:421:MET:HA	1:J:424:THR:HG22	1.89	0.54
1:A:435:ARG:NH1	1:A:453:LEU:O	2.40	0.54
1:I:448:THR:OG1	1:I:449:PHE:N	2.41	0.54
1:J:158:LEU:HA	1:J:443:LYS:HD3	1.90	0.54
1:I:490:LEU:HB3	1:I:497:LEU:HD22	1.88	0.54
1:J:380:ARG:HA	1:J:437:HIS:ND1	2.22	0.54
1:K:210:ASN:OD1	1:K:213:GLU:HG2	2.08	0.54
1:L:288:ILE:HG21	1:L:508:ASP:OD2	2.08	0.54
1:A:320:THR:HG21	1:A:325:LEU:HD12	1.90	0.54
1:F:140:PHE:CD1	1:F:217:ARG:HD2	2.42	0.54
1:F:211:ARG:NH1	1:F:447:ASP:O	2.40	0.54
1:F:470:LEU:HD11	1:F:532:VAL:HG11	1.89	0.54
1:H:496:LYS:HE2	1:H:523:ASP:OD2	2.08	0.54
1:L:478:ARG:HA	1:L:545:VAL:HG23	1.90	0.54
1:B:158:LEU:HD12	1:B:443:LYS:HD2	1.89	0.54
1:B:384:ARG:HG3	1:B:436:HIS:HB2	1.90	0.54
1:C:232:GLN:HB3	1:C:252:PHE:CD2	2.42	0.54
1:G:524:ARG:O	1:G:528:LEU:HD13	2.08	0.54
1:H:284:HIS:HB2	1:H:363:SER:HB3	1.90	0.53
1:L:490:LEU:HB3	1:L:497:LEU:HD22	1.89	0.53
1:A:204:ARG:HG2	1:A:221:VAL:HG21	1.90	0.53
1:H:287:GLU:O	1:H:305:VAL:HG11	2.08	0.53
1:I:428:PHE:HZ	1:I:528:LEU:HD12	1.74	0.53
1:K:413:ARG:NH1	1:K:447:ASP:OD2	2.40	0.53
1:B:311:ASN:ND2	1:B:314:ARG:H	2.07	0.53
1:C:379:TRP:NE1	1:C:440:THR:OG1	2.41	0.53
1:K:308:ARG:HB3	1:K:364:LEU:HD23	1.89	0.53
1:G:202:TRP:HD1	1:G:254:ASN:HD22	1.56	0.53
1:J:441:PHE:O	1:J:443:LYS:N	2.42	0.53
1:F:317:ARG:O	1:F:320:THR:HG22	2.08	0.53
1:G:448:THR:OG1	1:G:449:PHE:N	2.41	0.53
1:H:448:THR:OG1	1:H:449:PHE:N	2.42	0.53
1:A:421:MET:HG3	1:A:478:ARG:O	2.09	0.53
1:E:382:PRO:HG2	1:E:383:TRP:CZ3	2.43	0.53
1:G:232:GLN:HB3	1:G:252:PHE:HD2	1.74	0.53
1:H:470:LEU:HD11	1:H:532:VAL:HG11	1.91	0.53
1:A:261:LYS:HD2	1:A:287:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HD21	1:A:533:LEU:HD21	1.90	0.53
1:B:284:HIS:HB2	1:B:363:SER:HB3	1.90	0.53
1:F:389:LYS:C	1:F:391:LYS:H	2.12	0.53
1:G:261:LYS:NZ	1:G:287:GLU:OE2	2.33	0.53
1:B:234:ILE:HD13	1:B:250:MET:SD	2.48	0.53
1:D:382:PRO:HG2	1:D:383:TRP:CZ3	2.44	0.53
1:G:402:CYS:HA	1:G:405:VAL:HG12	1.90	0.53
1:I:155:GLU:HG3	1:I:156:ASP:OD1	2.08	0.53
1:I:532:VAL:O	1:I:536:CYS:HB3	2.08	0.53
1:E:515:ILE:CG2	1:J:511:VAL:HG21	2.39	0.53
1:H:157:THR:O	1:H:159:PHE:N	2.40	0.53
1:I:204:ARG:HG2	1:I:221:VAL:HG21	1.90	0.53
1:J:483:THR:O	1:J:487:LEU:HD13	2.09	0.53
1:A:478:ARG:HH12	1:A:547:GLU:CG	2.21	0.53
1:C:217:ARG:NH1	1:C:298:ASP:OD2	2.42	0.53
1:C:417:LEU:O	1:C:421:MET:HG2	2.08	0.53
1:G:230:LEU:HD11	1:G:509:ARG:HB2	1.91	0.53
1:K:448:THR:OG1	1:K:449:PHE:N	2.42	0.53
1:J:490:LEU:O	1:J:496:LYS:HA	2.09	0.52
1:G:382:PRO:HG2	1:G:383:TRP:CZ3	2.44	0.52
1:C:379:TRP:HE1	1:C:440:THR:HG1	1.55	0.52
1:L:159:PHE:HE2	1:L:206:HIS:HB3	1.74	0.52
1:B:320:THR:HG21	1:B:325:LEU:HD12	1.90	0.52
1:C:382:PRO:HG2	1:C:383:TRP:CE3	2.44	0.52
1:G:417:LEU:O	1:G:421:MET:HG2	2.10	0.52
1:H:293:LEU:HA	1:H:501:MET:HE1	1.90	0.52
1:C:440:THR:HG22	1:C:448:THR:HG23	1.91	0.52
1:I:417:LEU:O	1:I:421:MET:HG2	2.09	0.52
1:J:240:LYS:HB2	1:J:249:ILE:HD11	1.92	0.52
1:K:232:GLN:HB3	1:K:252:PHE:HD2	1.75	0.52
1:D:150:PRO:HG2	1:D:212:TYR:CZ	2.45	0.52
1:E:490:LEU:HB3	1:E:497:LEU:HD22	1.92	0.52
1:H:414:GLY:HA3	1:H:415:THR:C	2.30	0.52
1:I:232:GLN:NE2	1:I:254:ASN:OD1	2.42	0.52
1:I:394:GLU:HB3	1:I:401:TYR:CE2	2.45	0.52
1:B:406:LYS:HG2	1:B:417:LEU:HD11	1.91	0.52
1:E:139:LEU:HD22	1:E:500:LEU:HD23	1.92	0.52
1:E:545:VAL:HG12	1:E:546:VAL:HG13	1.90	0.52
1:H:234:ILE:HD12	1:H:250:MET:SD	2.50	0.52
1:H:497:LEU:O	1:H:501:MET:N	2.42	0.52
1:E:293:LEU:HD12	1:E:426:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:GLN:HB3	1:G:252:PHE:CD2	2.45	0.52
1:L:266:THR:HG23	1:L:269:GLN:HE21	1.74	0.52
1:I:405:VAL:O	1:I:408:THR:OG1	2.28	0.52
1:K:311:ASN:ND2	1:K:314:ARG:HH21	2.06	0.52
1:A:515:ILE:HD12	1:A:516:LYS:H	1.75	0.51
1:A:524:ARG:O	1:A:528:LEU:HD13	2.11	0.51
1:B:386:SER:O	1:B:388:HIS:N	2.36	0.51
1:E:291:PHE:HD1	1:E:302:VAL:HG23	1.75	0.51
1:G:414:GLY:HA3	1:G:416:ARG:N	2.25	0.51
1:I:307:GLY:HA3	1:I:510:LEU:HD23	1.90	0.51
1:K:239:MET:HE2	1:K:325:LEU:HB2	1.92	0.51
1:B:448:THR:OG1	1:B:449:PHE:N	2.43	0.51
1:D:288:ILE:HA	1:D:305:VAL:HG13	1.92	0.51
1:F:265:GLN:HE21	1:F:269:GLN:NE2	2.07	0.51
1:A:240:LYS:HB2	1:A:249:ILE:HD11	1.93	0.51
1:E:218:HIS:HA	1:E:219:ASN:C	2.30	0.51
1:F:309:LEU:HG	1:F:359:GLN:OE1	2.10	0.51
1:B:414:GLY:HA3	1:B:416:ARG:N	2.25	0.51
1:L:277:TYR:HE1	1:L:387:TYR:HD1	1.58	0.51
1:L:382:PRO:HG2	1:L:383:TRP:CE3	2.46	0.51
1:A:217:ARG:HG3	1:A:218:HIS:CD2	2.46	0.51
1:B:311:ASN:HD22	1:B:314:ARG:H	1.57	0.51
1:D:417:LEU:O	1:D:421:MET:HG2	2.10	0.51
1:D:448:THR:OG1	1:D:449:PHE:N	2.43	0.51
1:E:379:TRP:HE1	1:E:440:THR:HG1	1.59	0.51
1:B:216:SER:HB2	1:B:219:ASN:HB2	1.93	0.51
1:A:379:TRP:HE1	1:A:440:THR:HG1	1.58	0.51
1:A:379:TRP:CZ3	1:A:410:PRO:HG3	2.44	0.51
1:D:502:GLU:HB2	1:D:519:LEU:HD13	1.92	0.51
1:G:232:GLN:HG2	1:G:254:ASN:OD1	2.11	0.51
1:J:265:GLN:NE2	1:J:269:GLN:OE1	2.43	0.51
1:B:497:LEU:HD23	1:B:526:LEU:HD22	1.93	0.51
1:K:155:GLU:HG3	1:K:156:ASP:H	1.76	0.51
1:K:200:PRO:HB2	1:K:202:TRP:CD1	2.46	0.51
1:E:413:ARG:NH1	1:E:447:ASP:OD2	2.44	0.51
1:I:225:LEU:HD11	1:I:366:ALA:HB2	1.93	0.51
1:A:217:ARG:HB2	1:A:300:ARG:HH12	1.76	0.50
1:I:421:MET:HG3	1:I:478:ARG:O	2.11	0.50
1:L:436:HIS:CD2	1:L:437:HIS:CD2	2.99	0.50
1:A:302:VAL:HG12	1:A:452:HIS:O	2.12	0.50
1:H:157:THR:C	1:H:159:PHE:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HD13	1:B:480:LYS:HG3	1.94	0.50
1:F:389:LYS:O	1:F:391:LYS:N	2.39	0.50
1:F:511:VAL:HG21	1:I:515:ILE:HD11	1.94	0.50
1:K:228:ASP:O	1:K:232:GLN:HB2	2.12	0.50
1:K:414:GLY:HA3	1:K:416:ARG:N	2.26	0.50
1:H:388:HIS:ND1	1:H:389:LYS:O	2.43	0.50
1:B:483:THR:O	1:B:487:LEU:HD13	2.11	0.50
1:D:461:LYS:O	1:D:525:ARG:NH2	2.45	0.50
1:E:343:CYS:H	1:E:347:CYS:CB	2.23	0.50
1:G:381:ASN:ND2	1:G:435:ARG:O	2.44	0.50
1:H:217:ARG:NH2	1:H:218:HIS:HA	2.26	0.50
1:B:155:GLU:OE2	1:B:211:ARG:NH2	2.45	0.50
1:B:266:THR:HG23	1:B:269:GLN:OE1	2.12	0.50
1:H:421:MET:HA	1:H:424:THR:HG22	1.94	0.50
1:I:382:PRO:HG2	1:I:383:TRP:CZ3	2.47	0.50
1:A:418:LEU:HD21	1:A:478:ARG:HH11	1.77	0.50
1:C:293:LEU:HD22	1:C:426:PHE:CE1	2.46	0.50
1:D:505:LEU:HD22	1:D:513:VAL:HG21	1.93	0.50
1:E:263:MET:HE2	1:E:266:THR:HA	1.92	0.50
1:F:340:TYR:HB3	1:F:352:ALA:HA	1.94	0.50
1:J:461:LYS:O	1:J:525:ARG:NH2	2.42	0.50
1:D:288:ILE:HA	1:D:305:VAL:CG1	2.42	0.50
1:I:313:THR:HG23	1:I:317:ARG:HH21	1.76	0.50
1:J:421:MET:HG3	1:J:478:ARG:O	2.12	0.50
1:K:234:ILE:HD13	1:K:250:MET:SD	2.52	0.50
1:L:259:LEU:HB3	1:L:365:ALA:HB3	1.94	0.50
1:K:508:ASP:OD1	1:K:509:ARG:N	2.45	0.49
1:H:485:LEU:HD12	1:H:550:LEU:HD11	1.94	0.49
1:H:387:TYR:OH	1:H:436:HIS:HB3	2.11	0.49
1:E:149:LEU:HD11	1:E:213:GLU:OE2	2.13	0.49
1:E:386:SER:O	1:E:388:HIS:N	2.37	0.49
1:F:284:HIS:HB2	1:F:363:SER:HB3	1.94	0.49
1:A:134:SER:HB2	1:A:503:GLU:OE2	2.12	0.49
1:J:287:GLU:O	1:J:305:VAL:HG11	2.12	0.49
1:K:417:LEU:O	1:K:421:MET:HG2	2.12	0.49
1:L:239:MET:HE3	1:L:342:GLU:H	1.77	0.49
1:B:323:LYS:HE2	1:B:327:ARG:NH2	2.27	0.49
1:D:421:MET:HG3	1:D:478:ARG:O	2.13	0.49
1:D:482:SER:OG	1:D:486:ARG:NH2	2.46	0.49
1:G:380:ARG:HA	1:G:437:HIS:ND1	2.27	0.49
1:B:217:ARG:HG3	1:B:218:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:PHE:O	1:C:443:LYS:N	2.45	0.49
1:F:462:HIS:HB3	1:F:518:HIS:CD2	2.47	0.49
1:I:380:ARG:HA	1:I:437:HIS:ND1	2.28	0.49
1:C:380:ARG:HA	1:C:437:HIS:HD1	1.77	0.49
1:C:421:MET:HG3	1:C:478:ARG:O	2.13	0.49
1:G:267:ARG:HH21	1:G:513:VAL:HA	1.77	0.49
1:A:409:PRO:C	1:A:411:TYR:H	2.13	0.49
1:B:532:VAL:O	1:B:536:CYS:HB3	2.13	0.49
1:A:261:LYS:NZ	1:A:287:GLU:OE2	2.44	0.49
1:C:340:TYR:HB3	1:C:352:ALA:HA	1.95	0.49
1:H:418:LEU:HB3	1:H:480:LYS:HG3	1.94	0.49
1:H:504:SER:C	1:H:506:LEU:N	2.67	0.49
1:J:266:THR:HG23	1:J:269:GLN:NE2	2.28	0.49
1:L:317:ARG:HG3	1:L:326:TRP:CD1	2.48	0.49
1:F:473:LEU:HD21	1:F:533:LEU:HD21	1.94	0.48
1:H:309:LEU:HD22	1:H:359:GLN:HB3	1.94	0.48
1:J:386:SER:O	1:J:388:HIS:N	2.37	0.48
1:C:440:THR:CG2	1:C:448:THR:HG23	2.43	0.48
1:E:505:LEU:HD22	1:E:513:VAL:HG21	1.94	0.48
1:J:288:ILE:HA	1:J:305:VAL:HG13	1.95	0.48
1:K:532:VAL:O	1:K:536:CYS:HB3	2.14	0.48
1:B:157:THR:C	1:B:159:PHE:H	2.16	0.48
1:C:421:MET:HA	1:C:424:THR:HG22	1.94	0.48
1:H:462:HIS:HB3	1:H:518:HIS:CD2	2.48	0.48
1:H:532:VAL:O	1:H:536:CYS:HB3	2.13	0.48
1:A:462:HIS:HB3	1:A:518:HIS:CD2	2.49	0.48
1:K:545:VAL:HG12	1:K:546:VAL:HG23	1.95	0.48
1:B:417:LEU:O	1:B:421:MET:HG2	2.12	0.48
1:E:240:LYS:HB3	1:E:247:LYS:HG3	1.96	0.48
1:E:277:TYR:HE1	1:E:387:TYR:CD1	2.31	0.48
1:F:508:ASP:O	1:F:511:VAL:HG23	2.13	0.48
1:C:360:ILE:O	1:C:361:GLU:HB3	2.14	0.48
1:E:383:TRP:HA	1:E:395:TRP:CD1	2.47	0.48
1:F:414:GLY:HA3	1:F:415:THR:C	2.34	0.48
1:H:217:ARG:HH21	1:H:218:HIS:HA	1.78	0.48
1:I:204:ARG:HB3	1:I:221:VAL:HG11	1.94	0.48
1:I:232:GLN:HB3	1:I:252:PHE:CD1	2.49	0.48
1:J:394:GLU:HB3	1:J:401:TYR:HE2	1.78	0.48
1:J:139:LEU:HD22	1:J:500:LEU:HD23	1.95	0.48
1:G:382:PRO:HG2	1:G:383:TRP:CE3	2.48	0.48
1:G:462:HIS:HB3	1:G:518:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:436:HIS:CD2	1:J:437:HIS:CD2	3.01	0.48
1:K:266:THR:HG23	1:K:269:GLN:CD	2.34	0.48
1:B:414:GLY:HA3	1:B:415:THR:C	2.34	0.48
1:H:155:GLU:HG2	1:H:156:ASP:H	1.78	0.48
1:L:462:HIS:HB3	1:L:518:HIS:CD2	2.49	0.48
1:A:216:SER:HB2	1:A:219:ASN:HB2	1.95	0.48
1:D:549:ASP:OD1	1:D:549:ASP:N	2.44	0.48
1:F:261:LYS:HD2	1:F:287:GLU:HG3	1.95	0.48
1:G:402:CYS:SG	1:G:406:LYS:HE3	2.54	0.48
1:H:533:LEU:O	1:H:537:VAL:N	2.46	0.48
1:J:387:TYR:OH	1:J:434:ASP:OD1	2.18	0.48
1:D:293:LEU:HA	1:D:501:MET:HE1	1.95	0.48
1:F:509:ARG:HA	1:I:516:LYS:HB3	1.95	0.48
1:K:288:ILE:HA	1:K:305:VAL:HG13	1.95	0.48
1:L:409:PRO:HB2	1:L:410:PRO:HD3	1.96	0.48
1:L:524:ARG:O	1:L:528:LEU:HG	2.13	0.48
1:G:434:ASP:HB3	1:G:457:ARG:HG3	1.96	0.47
1:A:411:TYR:CD1	1:A:416:ARG:HG3	2.50	0.47
1:F:382:PRO:HG2	1:F:383:TRP:CE3	2.49	0.47
1:F:402:CYS:HA	1:F:405:VAL:HG12	1.97	0.47
1:A:308:ARG:HB3	1:A:364:LEU:HD23	1.96	0.47
1:E:288:ILE:HA	1:E:305:VAL:CG1	2.44	0.47
1:K:203:LEU:O	1:K:207:ILE:HG12	2.14	0.47
1:A:379:TRP:NE1	1:A:440:THR:OG1	2.46	0.47
1:B:490:LEU:HB3	1:B:497:LEU:HD22	1.95	0.47
1:D:158:LEU:HD12	1:D:443:LYS:HD2	1.95	0.47
1:H:414:GLY:HA3	1:H:416:ARG:N	2.29	0.47
1:I:302:VAL:HG12	1:I:452:HIS:O	2.14	0.47
1:L:418:LEU:HD21	1:L:478:ARG:HH11	1.78	0.47
1:B:394:GLU:HB3	1:B:401:TYR:CE2	2.49	0.47
1:E:218:HIS:HA	1:E:219:ASN:O	2.14	0.47
1:L:288:ILE:HA	1:L:305:VAL:HG13	1.95	0.47
1:B:545:VAL:HG12	1:B:546:VAL:HG13	1.96	0.47
1:D:516:LYS:HB3	1:D:517:PRO:HD3	1.95	0.47
1:E:293:LEU:HA	1:E:501:MET:HE1	1.96	0.47
1:H:360:ILE:O	1:H:361:GLU:HB3	2.15	0.47
1:I:234:ILE:HD13	1:I:252:PHE:CE1	2.50	0.47
1:J:360:ILE:O	1:J:361:GLU:HB3	2.13	0.47
1:K:288:ILE:HA	1:K:305:VAL:CG1	2.44	0.47
1:K:473:LEU:HD21	1:K:533:LEU:HD21	1.96	0.47
1:L:382:PRO:HG2	1:L:383:TRP:CZ3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:497:LEU:HD23	1:L:526:LEU:HD22	1.96	0.47
1:C:158:LEU:HA	1:C:443:LYS:HD3	1.96	0.47
1:D:240:LYS:HD2	1:D:247:LYS:HE2	1.96	0.47
1:D:302:VAL:HG12	1:D:452:HIS:O	2.15	0.47
1:E:444:PHE:HB2	1:E:448:THR:HG21	1.96	0.47
1:E:448:THR:OG1	1:E:449:PHE:N	2.44	0.47
1:E:478:ARG:HH12	1:E:547:GLU:HB2	1.79	0.47
1:J:250:MET:HE1	1:J:316:ILE:CD1	2.45	0.47
1:A:234:ILE:HD13	1:A:252:PHE:CE2	2.49	0.47
1:G:250:MET:HE1	1:G:316:ILE:HD11	1.95	0.47
1:H:234:ILE:HD13	1:H:252:PHE:CE1	2.50	0.47
1:H:441:PHE:O	1:H:443:LYS:N	2.47	0.47
1:I:288:ILE:HA	1:I:305:VAL:CG1	2.45	0.47
1:E:542:PHE:O	1:E:544:ALA:N	2.42	0.47
1:F:234:ILE:HD13	1:F:252:PHE:CE2	2.50	0.47
1:G:234:ILE:HD12	1:G:250:MET:SD	2.55	0.47
1:G:542:PHE:O	1:G:544:ALA:N	2.41	0.47
1:K:284:HIS:HB2	1:K:363:SER:HB3	1.97	0.47
1:K:411:TYR:CD1	1:K:416:ARG:HG3	2.49	0.47
1:D:142:HIS:CD2	1:D:144:LEU:H	2.31	0.47
1:D:380:ARG:CZ	1:D:384:ARG:HD3	2.44	0.47
1:E:157:THR:C	1:E:159:PHE:H	2.18	0.47
1:E:533:LEU:O	1:E:537:VAL:N	2.45	0.47
1:L:277:TYR:HE1	1:L:387:TYR:CD1	2.33	0.47
1:A:418:LEU:HD21	1:A:478:ARG:NH1	2.29	0.47
1:B:250:MET:HE1	1:B:316:ILE:HD11	1.96	0.47
1:C:228:ASP:O	1:C:232:GLN:HB2	2.15	0.47
1:G:409:PRO:HG2	1:G:410:PRO:HD3	1.97	0.47
1:L:492:LYS:N	1:L:492:LYS:HD2	2.30	0.47
1:C:260:PHE:HD1	1:C:364:LEU:HD22	1.80	0.46
1:H:451:ILE:HG22	1:H:453:LEU:HG	1.97	0.46
1:A:218:HIS:CE1	1:A:295:ARG:HG3	2.50	0.46
1:B:402:CYS:SG	1:B:406:LYS:HE3	2.55	0.46
1:C:250:MET:HE1	1:C:316:ILE:CD1	2.45	0.46
1:F:515:ILE:HG13	1:F:517:PRO:HD2	1.98	0.46
1:G:470:LEU:HD11	1:G:532:VAL:HG11	1.96	0.46
1:J:408:THR:CG2	1:J:409:PRO:HD2	2.39	0.46
1:B:291:PHE:HD1	1:B:302:VAL:HG23	1.80	0.46
1:B:302:VAL:HG12	1:B:452:HIS:O	2.15	0.46
1:C:293:LEU:HA	1:C:501:MET:HE1	1.97	0.46
1:D:382:PRO:HG2	1:D:383:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:PRO:HG2	1:E:383:TRP:CE3	2.49	0.46
1:K:217:ARG:HG3	1:K:218:HIS:ND1	2.31	0.46
1:B:217:ARG:HB3	1:B:300:ARG:NH1	2.30	0.46
1:C:487:LEU:HB3	1:C:530:LEU:HD11	1.97	0.46
1:F:360:ILE:O	1:F:361:GLU:HB3	2.16	0.46
1:I:360:ILE:O	1:I:361:GLU:HB3	2.14	0.46
1:A:478:ARG:HH12	1:A:547:GLU:HG3	1.80	0.46
1:B:288:ILE:HA	1:B:305:VAL:HG13	1.97	0.46
1:A:470:LEU:HD13	1:A:532:VAL:HG21	1.97	0.46
1:B:382:PRO:HG2	1:B:383:TRP:CE3	2.50	0.46
1:C:413:ARG:HG2	1:C:413:ARG:HH21	1.80	0.46
1:G:505:LEU:HD22	1:G:513:VAL:HG21	1.97	0.46
1:H:470:LEU:O	1:H:470:LEU:HD13	2.16	0.46
1:A:448:THR:OG1	1:A:449:PHE:N	2.49	0.46
1:F:199:TYR:HB3	1:F:200:PRO:HD2	1.97	0.46
1:F:448:THR:OG1	1:F:449:PHE:N	2.49	0.46
1:H:386:SER:C	1:H:388:HIS:H	2.19	0.46
1:I:199:TYR:HD1	1:I:200:PRO:HD2	1.80	0.46
1:C:409:PRO:HG2	1:C:410:PRO:HD3	1.98	0.46
1:E:417:LEU:O	1:E:421:MET:HG2	2.15	0.46
1:E:302:VAL:HG12	1:E:452:HIS:O	2.16	0.46
1:H:138:SER:HB3	1:H:495:TYR:HE1	1.81	0.46
1:H:221:VAL:O	1:H:225:LEU:N	2.43	0.46
1:E:344:SER:O	1:E:345:TYR:HB2	2.15	0.46
1:H:418:LEU:HD21	1:H:547:GLU:HG3	1.97	0.46
1:D:409:PRO:HG2	1:D:410:PRO:HD3	1.97	0.46
1:G:402:CYS:O	1:G:406:LYS:HG2	2.16	0.46
1:H:302:VAL:HG22	1:H:452:HIS:HB2	1.97	0.46
1:I:409:PRO:HG2	1:I:410:PRO:HD3	1.98	0.46
1:K:134:SER:HB3	1:K:137:GLN:HB2	1.97	0.46
1:L:502:GLU:HB3	1:L:519:LEU:HD13	1.98	0.46
1:A:291:PHE:HD1	1:A:302:VAL:HG23	1.82	0.45
1:C:320:THR:HG21	1:C:325:LEU:HD12	1.98	0.45
1:D:360:ILE:O	1:D:361:GLU:HB3	2.15	0.45
1:E:288:ILE:HA	1:E:305:VAL:HG13	1.96	0.45
1:E:376:ARG:HD2	1:E:439:GLU:OE1	2.17	0.45
1:E:421:MET:HA	1:E:424:THR:HG22	1.96	0.45
1:G:285:ASN:HB2	1:G:513:VAL:O	2.15	0.45
1:H:409:PRO:HG2	1:H:410:PRO:HD3	1.98	0.45
1:I:382:PRO:HG2	1:I:383:TRP:CE3	2.51	0.45
1:K:360:ILE:O	1:K:361:GLU:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:293:LEU:HD12	1:L:522:LEU:HD21	1.99	0.45
1:A:236:SER:HB3	1:A:251:SER:OG	2.16	0.45
1:K:309:LEU:HD22	1:K:359:GLN:HB3	1.98	0.45
1:L:360:ILE:O	1:L:361:GLU:HB3	2.16	0.45
1:B:462:HIS:O	1:B:524:ARG:NH2	2.47	0.45
1:C:424:THR:OG1	1:C:472:PRO:HG2	2.17	0.45
1:D:470:LEU:HD12	1:D:532:VAL:HG11	1.98	0.45
1:E:497:LEU:HD23	1:E:526:LEU:HD22	1.99	0.45
1:H:392:LYS:HD2	1:H:396:GLU:HG2	1.99	0.45
1:E:516:LYS:HB3	1:J:509:ARG:HA	1.98	0.45
1:K:379:TRP:CZ3	1:K:410:PRO:HG3	2.51	0.45
1:F:264:LYS:HD2	1:F:353:LEU:HD21	1.99	0.45
1:H:270:GLU:HA	1:H:460:GLY:O	2.17	0.45
1:J:448:THR:OG1	1:J:449:PHE:N	2.50	0.45
1:L:234:ILE:HD12	1:L:250:MET:SD	2.56	0.45
1:F:144:LEU:HD12	1:F:489:LEU:HD22	1.98	0.45
1:F:438:TYR:HB2	1:F:450:ILE:CG2	2.46	0.45
1:G:478:ARG:HH12	1:G:547:GLU:HG3	1.81	0.45
1:H:504:SER:O	1:H:506:LEU:N	2.46	0.45
1:B:308:ARG:HB3	1:B:364:LEU:HD23	1.99	0.45
1:D:542:PHE:CE2	1:D:546:VAL:HG21	2.51	0.45
1:I:260:PHE:HD1	1:I:364:LEU:HD22	1.81	0.45
1:J:394:GLU:HB3	1:J:401:TYR:CE2	2.51	0.45
1:L:444:PHE:HB2	1:L:448:THR:HG21	1.99	0.45
1:E:501:MET:HB3	1:E:519:LEU:HD22	1.99	0.45
1:F:540:ASP:HB2	1:F:545:VAL:HG23	1.98	0.45
1:J:428:PHE:CG	1:J:470:LEU:HG	2.52	0.45
1:J:542:PHE:O	1:J:544:ALA:N	2.44	0.45
1:K:199:TYR:HB2	1:K:204:ARG:HG3	1.99	0.45
1:L:502:GLU:O	1:L:506:LEU:HD13	2.17	0.45
1:C:234:ILE:HD12	1:C:250:MET:SD	2.57	0.45
1:C:263:MET:HE2	1:C:266:THR:HA	1.98	0.45
1:C:331:VAL:HG22	1:C:337:ILE:HD13	1.98	0.45
1:C:448:THR:OG1	1:C:449:PHE:N	2.50	0.45
1:F:389:LYS:H	1:F:389:LYS:HG2	1.52	0.45
1:F:532:VAL:O	1:F:536:CYS:HB3	2.16	0.45
1:G:280:ASP:OD1	1:G:283:ARG:NH2	2.50	0.45
1:B:360:ILE:O	1:B:361:GLU:HB3	2.15	0.45
1:D:210:ASN:OD1	1:D:213:GLU:HG2	2.17	0.45
1:E:216:SER:O	1:E:218:HIS:N	2.47	0.45
1:G:302:VAL:HG12	1:G:452:HIS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:232:GLN:HG2	1:I:252:PHE:HB3	1.99	0.45
1:I:389:LYS:O	1:I:391:LYS:HD2	2.16	0.45
1:J:382:PRO:HG2	1:J:383:TRP:CE3	2.52	0.45
1:L:213:GLU:OE2	1:L:216:SER:HB2	2.17	0.45
1:L:266:THR:HG23	1:L:269:GLN:NE2	2.32	0.45
1:B:409:PRO:HG2	1:B:410:PRO:HD3	1.99	0.45
1:E:360:ILE:O	1:E:361:GLU:HB3	2.17	0.45
1:G:291:PHE:HD1	1:G:302:VAL:HG23	1.82	0.45
1:G:542:PHE:CZ	1:G:546:VAL:HG21	2.51	0.45
1:A:549:ASP:OD1	1:A:549:ASP:N	2.50	0.44
1:B:356:LYS:HA	1:B:357:PRO:HA	1.67	0.44
1:B:542:PHE:O	1:B:544:ALA:N	2.45	0.44
1:E:470:LEU:HD13	1:E:532:VAL:HG21	1.99	0.44
1:I:234:ILE:HD12	1:I:250:MET:SD	2.57	0.44
1:I:414:GLY:HA3	1:I:416:ARG:N	2.32	0.44
1:J:386:SER:C	1:J:388:HIS:H	2.19	0.44
1:K:478:ARG:HH12	1:K:547:GLU:CG	2.28	0.44
1:A:545:VAL:HG12	1:A:546:VAL:HG23	1.98	0.44
1:D:473:LEU:HD21	1:D:533:LEU:HD21	1.98	0.44
1:E:277:TYR:CE1	1:E:278:PHE:HD2	2.35	0.44
1:F:288:ILE:HA	1:F:305:VAL:HG13	1.99	0.44
1:F:394:GLU:HB3	1:F:401:TYR:HE2	1.83	0.44
1:G:250:MET:HE1	1:G:316:ILE:CD1	2.46	0.44
1:H:499:SER:HA	1:H:502:GLU:HG2	2.00	0.44
1:H:547:GLU:HB3	1:H:548:ASN:H	1.66	0.44
1:J:266:THR:HG23	1:J:269:GLN:HE21	1.83	0.44
1:K:434:ASP:HB3	1:K:457:ARG:HG3	1.99	0.44
1:D:234:ILE:HD12	1:D:250:MET:SD	2.57	0.44
1:D:308:ARG:O	1:D:361:GLU:HA	2.17	0.44
1:E:317:ARG:O	1:E:320:THR:HG22	2.17	0.44
1:G:299:PHE:HB3	1:G:301:ARG:CG	2.47	0.44
1:H:137:GLN:N	1:H:137:GLN:OE1	2.50	0.44
1:H:199:TYR:HB3	1:H:200:PRO:HD2	1.98	0.44
1:K:380:ARG:HA	1:K:437:HIS:ND1	2.32	0.44
1:L:389:LYS:H	1:L:389:LYS:HG2	1.54	0.44
1:A:313:THR:HG23	1:A:317:ARG:HH21	1.83	0.44
1:A:382:PRO:HG2	1:A:383:TRP:CE3	2.53	0.44
1:B:379:TRP:HZ3	1:B:410:PRO:HG3	1.82	0.44
1:C:501:MET:HB3	1:C:519:LEU:HD22	2.00	0.44
1:F:302:VAL:HG12	1:F:452:HIS:O	2.18	0.44
1:C:405:VAL:O	1:C:408:THR:OG1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:NH2	1:C:447:ASP:OD1	2.48	0.44
1:F:511:VAL:HG12	1:I:268:GLU:HG2	1.99	0.44
1:I:156:ASP:CG	1:I:211:ARG:HE	2.19	0.44
1:I:515:ILE:HG23	1:I:517:PRO:HG2	1.99	0.44
1:K:266:THR:HG23	1:K:269:GLN:NE2	2.33	0.44
1:K:382:PRO:HG2	1:K:383:TRP:CZ3	2.52	0.44
1:K:501:MET:HB3	1:K:519:LEU:HD22	1.99	0.44
1:L:323:LYS:HB2	1:L:323:LYS:HE2	1.81	0.44
1:E:534:SER:HA	1:E:537:VAL:HG12	2.00	0.44
1:J:409:PRO:HG2	1:J:410:PRO:HD3	2.00	0.44
1:K:382:PRO:HG2	1:K:383:TRP:CE3	2.52	0.44
1:K:516:LYS:HB3	1:K:516:LYS:HE3	1.61	0.44
1:L:417:LEU:O	1:L:421:MET:HG2	2.18	0.44
1:L:461:LYS:HE3	1:L:464:HIS:HB3	1.99	0.44
1:B:368:LEU:HD11	1:B:451:ILE:HG21	1.99	0.44
1:E:299:PHE:HB3	1:E:301:ARG:HG2	2.00	0.44
1:G:360:ILE:O	1:G:361:GLU:HB3	2.18	0.44
1:L:421:MET:HG3	1:L:478:ARG:O	2.17	0.44
1:F:441:PHE:O	1:F:443:LYS:N	2.49	0.44
1:I:386:SER:O	1:I:388:HIS:N	2.45	0.44
1:L:317:ARG:HB2	1:L:329:PHE:CD2	2.53	0.44
1:L:421:MET:HA	1:L:424:THR:HG22	2.00	0.44
1:B:142:HIS:CG	1:B:143:PRO:HD2	2.53	0.44
1:B:210:ASN:OD1	1:B:213:GLU:HG2	2.17	0.44
1:B:312:MET:HE3	1:B:339:PHE:CD1	2.53	0.44
1:C:540:ASP:HB2	1:C:545:VAL:HG23	2.00	0.44
1:G:284:HIS:HB2	1:G:363:SER:HB3	1.99	0.44
1:H:277:TYR:OH	1:H:386:SER:O	2.36	0.44
1:H:489:LEU:HG	1:H:495:TYR:CD2	2.53	0.44
1:I:515:ILE:HA	1:I:515:ILE:HD12	1.86	0.44
1:L:155:GLU:HG2	1:L:156:ASP:H	1.83	0.44
1:B:382:PRO:HG2	1:B:383:TRP:CZ3	2.53	0.43
1:C:299:PHE:HB3	1:C:301:ARG:CG	2.48	0.43
1:D:307:GLY:HA3	1:D:510:LEU:HG	2.00	0.43
1:D:313:THR:OG1	1:D:314:ARG:N	2.51	0.43
1:E:330:PHE:CB	1:F:389:LYS:HD2	2.48	0.43
1:G:386:SER:C	1:G:388:HIS:H	2.21	0.43
1:G:540:ASP:HB2	1:G:545:VAL:HG23	1.99	0.43
1:H:307:GLY:HA3	1:H:510:LEU:HG	1.99	0.43
1:I:432:ASN:OD1	1:I:457:ARG:HB2	2.18	0.43
1:J:217:ARG:NH2	1:J:218:HIS:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:451:ILE:HG22	1:L:453:LEU:HG	2.00	0.43
1:A:289:ALA:HA	1:A:505:LEU:HD21	1.99	0.43
1:B:496:LYS:HE2	1:B:523:ASP:OD2	2.18	0.43
1:B:515:ILE:HD12	1:B:515:ILE:HA	1.86	0.43
1:C:417:LEU:HD23	1:C:417:LEU:HA	1.81	0.43
1:D:312:MET:O	1:D:316:ILE:HB	2.17	0.43
1:F:388:HIS:HB3	1:F:391:LYS:HB3	1.99	0.43
1:F:409:PRO:HG2	1:F:410:PRO:HD3	2.00	0.43
1:F:473:LEU:HD11	1:F:479:VAL:HG12	2.00	0.43
1:I:153:THR:HG23	1:I:155:GLU:HG2	2.01	0.43
1:I:157:THR:C	1:I:159:PHE:H	2.21	0.43
1:I:144:LEU:HD12	1:I:489:LEU:HD13	1.99	0.43
1:E:417:LEU:HD23	1:E:417:LEU:HA	1.92	0.43
1:H:288:ILE:HD11	1:H:510:LEU:HD12	2.00	0.43
1:J:139:LEU:HD13	1:J:500:LEU:HD21	2.00	0.43
1:K:481:ARG:HB2	1:K:547:GLU:O	2.18	0.43
1:B:240:LYS:HG3	1:B:249:ILE:CD1	2.37	0.43
1:F:217:ARG:NH2	1:F:218:HIS:HA	2.34	0.43
1:F:277:TYR:HE1	1:F:387:TYR:HD1	1.66	0.43
1:F:534:SER:O	1:F:538:GLU:HG2	2.18	0.43
1:G:240:LYS:HB2	1:G:249:ILE:HD11	1.98	0.43
1:H:489:LEU:HD11	1:H:495:TYR:HE2	1.83	0.43
1:H:516:LYS:NZ	1:H:520:GLU:OE1	2.47	0.43
1:I:229:LEU:O	1:I:308:ARG:HD2	2.18	0.43
1:J:313:THR:HG23	1:J:317:ARG:HH21	1.83	0.43
1:J:405:VAL:HA	1:J:408:THR:OG1	2.18	0.43
1:L:217:ARG:NH2	1:L:218:HIS:HA	2.34	0.43
1:A:540:ASP:HB2	1:A:545:VAL:HG23	2.01	0.43
1:C:280:ASP:OD1	1:C:283:ARG:NH2	2.51	0.43
1:C:462:HIS:HB3	1:C:518:HIS:CD2	2.53	0.43
1:D:436:HIS:CD2	1:D:437:HIS:CD2	3.06	0.43
1:D:508:ASP:OD1	1:D:509:ARG:N	2.51	0.43
1:H:149:LEU:HD13	1:H:212:TYR:HB2	2.01	0.43
1:D:305:VAL:HA	1:D:364:LEU:O	2.19	0.43
1:E:266:THR:HG23	1:E:269:GLN:HE21	1.83	0.43
1:E:402:CYS:O	1:E:406:LYS:HG2	2.17	0.43
1:F:414:GLY:HA3	1:F:416:ARG:N	2.34	0.43
1:G:421:MET:HG3	1:G:478:ARG:O	2.18	0.43
1:H:436:HIS:CD2	1:H:437:HIS:CD2	3.06	0.43
1:K:299:PHE:HB3	1:K:301:ARG:CG	2.48	0.43
1:A:386:SER:C	1:A:388:HIS:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:TYR:CE1	1:E:387:TYR:CD1	3.07	0.43
1:G:299:PHE:HB3	1:G:301:ARG:HG2	2.01	0.43
1:H:405:VAL:O	1:H:408:THR:OG1	2.36	0.43
1:I:545:VAL:HG12	1:I:546:VAL:HG23	2.01	0.43
1:L:448:THR:OG1	1:L:449:PHE:N	2.49	0.43
1:A:508:ASP:OD1	1:A:509:ARG:N	2.49	0.43
1:G:549:ASP:OD1	1:G:549:ASP:N	2.52	0.43
1:H:382:PRO:HG2	1:H:383:TRP:CE3	2.54	0.43
1:H:543:SER:H	1:H:546:VAL:HG12	1.84	0.43
1:L:470:LEU:HD13	1:L:532:VAL:HG21	2.01	0.43
1:A:376:ARG:NH1	1:A:439:GLU:OE1	2.52	0.43
1:B:497:LEU:O	1:B:501:MET:N	2.51	0.43
1:C:307:GLY:HA3	1:C:510:LEU:HD23	2.01	0.43
1:D:157:THR:C	1:D:159:PHE:H	2.21	0.43
1:D:203:LEU:O	1:D:207:ILE:HG12	2.19	0.43
1:E:496:LYS:HE2	1:E:523:ASP:OD2	2.19	0.43
1:G:202:TRP:HD1	1:G:254:ASN:ND2	2.16	0.43
1:H:245:GLN:HE22	1:H:281:PHE:HA	1.83	0.43
1:I:263:MET:HG3	1:I:284:HIS:CE1	2.54	0.43
1:I:291:PHE:HD1	1:I:302:VAL:HG23	1.84	0.43
1:I:515:ILE:HG22	1:I:518:HIS:CD2	2.51	0.43
1:J:516:LYS:HB3	1:J:517:PRO:HD3	2.01	0.43
1:K:267:ARG:HH21	1:K:513:VAL:HA	1.84	0.43
1:K:379:TRP:HE1	1:K:440:THR:HG1	1.64	0.43
1:K:524:ARG:HE	1:K:524:ARG:HB3	1.57	0.43
1:A:503:GLU:O	1:A:506:LEU:HB2	2.19	0.43
1:C:444:PHE:HB2	1:C:448:THR:HG21	2.00	0.43
1:C:473:LEU:HD21	1:C:533:LEU:HD21	2.01	0.43
1:E:433:MET:SD	1:E:466:GLU:HG2	2.58	0.43
1:F:293:LEU:HD12	1:F:426:PHE:CE1	2.54	0.43
1:G:222:ILE:HD12	1:G:304:PRO:HG2	2.00	0.43
1:I:156:ASP:OD1	1:I:211:ARG:NE	2.39	0.43
1:I:202:TRP:CD1	1:I:254:ASN:ND2	2.87	0.43
1:C:477:CYS:O	1:C:545:VAL:HG22	2.19	0.42
1:K:414:GLY:HA3	1:K:415:THR:C	2.39	0.42
1:L:402:CYS:SG	1:L:406:LYS:HE3	2.59	0.42
1:B:461:LYS:O	1:B:525:ARG:NH2	2.49	0.42
1:C:309:LEU:HD22	1:C:359:GLN:HB3	2.01	0.42
1:G:483:THR:O	1:G:487:LEU:HG	2.18	0.42
1:F:461:LYS:O	1:F:525:ARG:NH2	2.50	0.42
1:I:514:LEU:HD23	1:I:514:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:379:TRP:HE1	1:J:440:THR:HG1	1.67	0.42
1:B:157:THR:O	1:B:159:PHE:N	2.49	0.42
1:E:413:ARG:HH12	1:E:447:ASP:CG	2.22	0.42
1:E:418:LEU:HD13	1:E:480:LYS:HG3	2.02	0.42
1:F:287:GLU:O	1:F:305:VAL:HG11	2.20	0.42
1:G:478:ARG:HH12	1:G:547:GLU:CG	2.32	0.42
1:I:284:HIS:HB2	1:I:363:SER:HB3	2.00	0.42
1:L:417:LEU:HA	1:L:417:LEU:HD23	1.77	0.42
1:A:490:LEU:O	1:A:496:LYS:HA	2.20	0.42
1:B:383:TRP:HZ2	1:B:402:CYS:HB2	1.85	0.42
1:D:310:VAL:O	1:D:359:GLN:HA	2.20	0.42
1:D:542:PHE:CZ	1:D:546:VAL:HG21	2.55	0.42
1:G:414:GLY:HA3	1:G:415:THR:C	2.39	0.42
1:H:151:ASP:N	1:H:151:ASP:OD1	2.52	0.42
1:I:414:GLY:HA3	1:I:415:THR:C	2.40	0.42
1:J:139:LEU:HD22	1:J:500:LEU:CD2	2.50	0.42
1:J:414:GLY:HA3	1:J:416:ARG:N	2.34	0.42
1:K:386:SER:C	1:K:388:HIS:H	2.22	0.42
1:K:462:HIS:HB3	1:K:518:HIS:CE1	2.55	0.42
1:B:533:LEU:O	1:B:537:VAL:N	2.51	0.42
1:H:324:LYS:HD3	1:I:407:GLN:HE21	1.85	0.42
1:I:228:ASP:O	1:I:232:GLN:HB2	2.20	0.42
1:J:302:VAL:HG12	1:J:452:HIS:O	2.18	0.42
1:L:473:LEU:HD21	1:L:533:LEU:HD21	2.02	0.42
1:A:487:LEU:HD22	1:A:526:LEU:HD13	2.01	0.42
1:B:421:MET:HG3	1:B:478:ARG:O	2.19	0.42
1:D:213:GLU:OE2	1:D:216:SER:OG	2.37	0.42
1:E:332:SER:HB3	1:E:338:CYS:SG	2.60	0.42
1:G:383:TRP:HA	1:G:395:TRP:CD1	2.55	0.42
1:G:385:ARG:HH21	1:G:469:ILE:HG12	1.85	0.42
1:H:324:LYS:HB3	1:H:342:GLU:OE1	2.19	0.42
1:I:288:ILE:HA	1:I:305:VAL:HG13	2.01	0.42
1:L:156:ASP:O	1:L:210:ASN:HB2	2.19	0.42
1:B:440:THR:HG22	1:B:442:GLU:H	1.85	0.42
1:H:312:MET:HG2	1:H:358:ASP:O	2.20	0.42
1:I:158:LEU:HD12	1:I:443:LYS:HD2	2.02	0.42
1:C:245:GLN:HE21	1:C:345:TYR:HB3	1.85	0.42
1:C:327:ARG:NH1	1:C:342:GLU:OE2	2.52	0.42
1:F:402:CYS:O	1:F:406:LYS:HG2	2.20	0.42
1:F:433:MET:HB3	1:F:469:ILE:HG12	2.02	0.42
1:H:213:GLU:OE2	1:H:216:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:406:LYS:O	1:I:412:ASP:HB3	2.20	0.42
1:J:293:LEU:HD22	1:J:426:PHE:CE1	2.55	0.42
1:L:234:ILE:HD13	1:L:252:PHE:CE1	2.54	0.42
1:L:292:HIS:ND1	1:L:504:SER:OG	2.34	0.42
1:A:285:ASN:HB2	1:A:513:VAL:O	2.20	0.42
1:B:496:LYS:O	1:B:500:LEU:HB2	2.20	0.42
1:D:405:VAL:O	1:D:408:THR:OG1	2.38	0.42
1:D:451:ILE:HG22	1:D:453:LEU:HG	2.02	0.42
1:E:228:ASP:O	1:E:232:GLN:HB2	2.20	0.42
1:I:229:LEU:HB2	1:I:306:ALA:HB3	2.02	0.42
1:L:385:ARG:NE	1:L:433:MET:HB2	2.35	0.42
1:A:324:LYS:HA	1:A:327:ARG:NH1	2.35	0.41
1:C:389:LYS:O	1:C:390:ARG:HG2	2.20	0.41
1:D:144:LEU:HD11	1:D:485:LEU:HB3	2.01	0.41
1:H:529:VAL:O	1:H:533:LEU:HG	2.20	0.41
1:I:206:HIS:CE1	1:I:369:PRO:HA	2.54	0.41
1:I:203:LEU:O	1:I:207:ILE:HG12	2.20	0.41
1:A:402:CYS:O	1:A:406:LYS:HG2	2.20	0.41
1:D:503:GLU:O	1:D:506:LEU:HB2	2.19	0.41
1:E:245:GLN:OE1	1:E:281:PHE:HA	2.20	0.41
1:E:389:LYS:H	1:E:389:LYS:HG2	1.62	0.41
1:E:522:LEU:HD12	1:E:522:LEU:HA	1.86	0.41
1:F:157:THR:C	1:F:159:PHE:H	2.23	0.41
1:G:377:LYS:HB2	1:G:442:GLU:HG3	2.01	0.41
1:I:287:GLU:O	1:I:305:VAL:HG11	2.21	0.41
1:J:414:GLY:HA3	1:J:415:THR:C	2.41	0.41
1:J:436:HIS:CD2	1:J:437:HIS:HD2	2.38	0.41
1:J:470:LEU:HD13	1:J:532:VAL:HG21	2.02	0.41
1:K:281:PHE:O	1:K:283:ARG:NH1	2.53	0.41
1:A:234:ILE:HD12	1:A:250:MET:SD	2.61	0.41
1:A:472:PRO:O	1:A:476:CYS:HB2	2.20	0.41
1:B:139:LEU:HD22	1:B:500:LEU:HD13	2.02	0.41
1:B:485:LEU:HA	1:B:485:LEU:HD23	1.81	0.41
1:G:391:LYS:H	1:G:391:LYS:HG3	1.70	0.41
1:H:150:PRO:HG2	1:H:212:TYR:CZ	2.55	0.41
1:J:232:GLN:HB3	1:J:252:PHE:CD2	2.54	0.41
1:J:522:LEU:HD23	1:J:522:LEU:HA	1.86	0.41
1:K:139:LEU:HD22	1:K:500:LEU:HD13	2.00	0.41
1:K:271:THR:HA	1:K:272:PRO:HD3	1.97	0.41
1:L:299:PHE:HE1	1:L:483:THR:CG2	2.33	0.41
1:A:217:ARG:NH1	1:A:298:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ARG:HA	1:C:437:HIS:ND1	2.35	0.41
1:C:459:PHE:CE1	1:C:522:LEU:HD11	2.49	0.41
1:C:470:LEU:HD13	1:C:532:VAL:HG21	2.01	0.41
1:E:549:ASP:OD1	1:E:549:ASP:N	2.53	0.41
1:F:217:ARG:HB2	1:F:300:ARG:NH1	2.34	0.41
1:I:221:VAL:O	1:I:225:LEU:N	2.47	0.41
1:J:382:PRO:HG2	1:J:383:TRP:CZ3	2.55	0.41
1:J:406:LYS:HB3	1:J:406:LYS:HE2	1.92	0.41
1:J:488:GLN:HA	1:J:530:LEU:HD21	2.02	0.41
1:L:199:TYR:HB2	1:L:204:ARG:HG3	2.02	0.41
1:B:374:ALA:HA	1:B:443:LYS:HE3	2.03	0.41
1:C:200:PRO:HB2	1:C:202:TRP:CD1	2.55	0.41
1:C:451:ILE:HG22	1:C:453:LEU:HG	2.02	0.41
1:C:524:ARG:HB3	1:C:524:ARG:HE	1.63	0.41
1:D:142:HIS:CG	1:D:143:PRO:HD2	2.55	0.41
1:E:234:ILE:HD13	1:E:252:PHE:CE1	2.56	0.41
1:E:299:PHE:HB3	1:E:301:ARG:CG	2.51	0.41
1:E:277:TYR:HE1	1:E:387:TYR:HD1	1.67	0.41
1:E:484:TYR:HD2	1:E:546:VAL:HG11	1.85	0.41
1:E:516:LYS:N	1:E:517:PRO:HD2	2.35	0.41
1:F:421:MET:HG3	1:F:478:ARG:O	2.20	0.41
1:G:361:GLU:HG3	1:G:510:LEU:CD1	2.50	0.41
1:H:261:LYS:HA	1:H:262:PRO:HD3	1.94	0.41
1:J:497:LEU:HA	1:J:497:LEU:HD23	1.86	0.41
1:K:211:ARG:HA	1:K:444:PHE:CE2	2.56	0.41
1:D:287:GLU:O	1:D:305:VAL:HG11	2.21	0.41
1:D:529:VAL:O	1:D:533:LEU:HG	2.21	0.41
1:F:470:LEU:HD13	1:F:473:LEU:HB3	2.03	0.41
1:F:502:GLU:HB3	1:F:519:LEU:HD13	2.02	0.41
1:G:260:PHE:HD1	1:G:364:LEU:HD22	1.85	0.41
1:G:368:LEU:HB3	1:G:369:PRO:HD2	2.03	0.41
1:G:522:LEU:HD12	1:G:522:LEU:HA	1.93	0.41
1:L:217:ARG:HH21	1:L:218:HIS:HA	1.85	0.41
1:A:136:LEU:HA	1:A:500:LEU:CD2	2.51	0.41
1:B:283:ARG:H	1:B:283:ARG:HG2	1.74	0.41
1:B:522:LEU:HA	1:B:522:LEU:HD12	1.74	0.41
1:E:515:ILE:HD13	1:E:518:HIS:HD2	1.86	0.41
1:F:479:VAL:HG23	1:F:480:LYS:O	2.21	0.41
1:J:418:LEU:HD13	1:J:480:LYS:HG3	2.02	0.41
1:K:515:ILE:HD12	1:K:516:LYS:H	1.86	0.41
1:A:395:TRP:HB3	1:A:401:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:MET:HG3	1:C:364:LEU:HD11	2.02	0.41
1:C:532:VAL:O	1:C:536:CYS:HB3	2.21	0.41
1:A:303:PRO:HA	1:A:304:PRO:HD3	1.96	0.41
1:B:545:VAL:HG12	1:B:546:VAL:CG1	2.51	0.41
1:C:394:GLU:HB3	1:C:401:TYR:CE2	2.56	0.41
1:D:225:LEU:HD11	1:D:366:ALA:HB2	2.03	0.41
1:E:303:PRO:HA	1:E:304:PRO:HD3	1.95	0.41
1:E:145:TYR:OH	1:E:490:LEU:HD21	2.21	0.41
1:F:240:LYS:HB2	1:F:249:ILE:CD1	2.47	0.41
1:F:386:SER:C	1:F:388:HIS:H	2.23	0.41
1:G:533:LEU:HD23	1:G:533:LEU:HA	1.81	0.41
1:J:343:CYS:H	1:J:347:CYS:CB	2.33	0.41
1:L:383:TRP:HA	1:L:395:TRP:CD1	2.55	0.41
1:A:324:LYS:HE2	1:A:324:LYS:HB2	1.83	0.41
1:B:250:MET:HE1	1:B:316:ILE:CD1	2.51	0.41
1:F:214:LEU:HD13	1:F:449:PHE:HZ	1.86	0.41
1:F:508:ASP:OD1	1:F:509:ARG:N	2.54	0.41
1:H:324:LYS:HE3	1:H:324:LYS:HB2	1.86	0.41
1:H:490:LEU:HB3	1:H:497:LEU:HD22	2.03	0.41
1:L:386:SER:O	1:L:388:HIS:N	2.42	0.41
1:L:387:TYR:OH	1:L:436:HIS:HB3	2.20	0.41
1:C:435:ARG:NH1	1:C:453:LEU:O	2.54	0.40
1:I:548:ASN:ND2	1:I:551:ASP:OD1	2.54	0.40
1:L:414:GLY:HA2	1:L:415:THR:OG1	2.21	0.40
1:E:159:PHE:HD2	1:E:207:ILE:HA	1.86	0.40
1:E:508:ASP:O	1:E:511:VAL:HG23	2.20	0.40
1:G:240:LYS:HD2	1:G:247:LYS:HE2	2.03	0.40
1:H:216:SER:HA	1:H:300:ARG:CZ	2.51	0.40
1:H:489:LEU:HG	1:H:495:TYR:HD2	1.87	0.40
1:I:510:LEU:HA	1:I:510:LEU:HD13	1.76	0.40
1:J:284:HIS:HB2	1:J:363:SER:HB3	2.03	0.40
1:K:480:LYS:HB2	1:K:483:THR:OG1	2.21	0.40
1:A:340:TYR:HB3	1:A:352:ALA:HA	2.03	0.40
1:C:478:ARG:HH11	1:C:478:ARG:HD3	1.72	0.40
1:D:245:GLN:HE22	1:D:281:PHE:HA	1.86	0.40
1:D:406:LYS:HB3	1:D:406:LYS:HE2	1.86	0.40
1:D:490:LEU:O	1:D:496:LYS:HA	2.21	0.40
1:E:264:LYS:HA	1:E:264:LYS:HD2	1.82	0.40
1:I:240:LYS:HE3	1:I:247:LYS:NZ	2.37	0.40
1:J:221:VAL:O	1:J:225:LEU:N	2.43	0.40
1:J:250:MET:HE1	1:J:316:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HB3	1:A:513:VAL:HG22	2.02	0.40
1:A:534:SER:O	1:A:538:GLU:HG2	2.21	0.40
1:E:524:ARG:HE	1:E:524:ARG:HB3	1.78	0.40
1:F:142:HIS:CG	1:F:143:PRO:HD2	2.57	0.40
1:G:308:ARG:HB3	1:G:364:LEU:HD23	2.04	0.40
1:G:524:ARG:HB3	1:G:524:ARG:HE	1.56	0.40
1:H:263:MET:HE2	1:H:266:THR:HA	2.03	0.40
1:I:312:MET:H	1:I:312:MET:HG2	1.70	0.40
1:I:462:HIS:HB3	1:I:518:HIS:CE1	2.56	0.40
1:A:217:ARG:HA	1:A:218:HIS:HA	1.70	0.40
1:C:502:GLU:O	1:C:506:LEU:HD13	2.21	0.40
1:D:414:GLY:HA3	1:D:415:THR:C	2.42	0.40
1:D:492:LYS:HD3	1:D:492:LYS:HA	1.93	0.40
1:F:324:LYS:HB3	1:F:342:GLU:OE1	2.21	0.40
1:F:382:PRO:HG2	1:F:383:TRP:CZ3	2.56	0.40
1:F:485:LEU:HD23	1:F:485:LEU:HA	1.89	0.40
1:H:382:PRO:HG2	1:H:383:TRP:CZ3	2.56	0.40
1:H:211:ARG:HA	1:H:444:PHE:CE2	2.57	0.40
1:K:259:LEU:HB3	1:K:365:ALA:HB3	2.03	0.40
1:L:380:ARG:HA	1:L:437:HIS:ND1	2.36	0.40
1:L:470:LEU:HD23	1:L:470:LEU:HA	1.85	0.40
1:L:418:LEU:HD21	1:L:478:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	382/560 (68%)	338 (88%)	38 (10%)	6 (2%)	9 42
1	B	376/560 (67%)	334 (89%)	38 (10%)	4 (1%)	14 50
1	C	386/560 (69%)	341 (88%)	43 (11%)	2 (0%)	29 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	378/560 (68%)	334 (88%)	38 (10%)	6 (2%)	9	42
1	E	381/560 (68%)	338 (89%)	37 (10%)	6 (2%)	9	42
1	F	373/560 (67%)	331 (89%)	39 (10%)	3 (1%)	19	57
1	G	382/560 (68%)	342 (90%)	35 (9%)	5 (1%)	12	46
1	H	376/560 (67%)	330 (88%)	42 (11%)	4 (1%)	14	50
1	I	379/560 (68%)	334 (88%)	41 (11%)	4 (1%)	14	50
1	J	374/560 (67%)	328 (88%)	41 (11%)	5 (1%)	12	46
1	K	385/560 (69%)	337 (88%)	42 (11%)	6 (2%)	9	42
1	L	374/560 (67%)	331 (88%)	39 (10%)	4 (1%)	14	50
All	All	4546/6720 (68%)	4018 (88%)	473 (10%)	55 (1%)	13	48

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	PRO
1	A	496	LYS
1	D	216	SER
1	D	218	HIS
1	H	218	HIS
1	H	496	LYS
1	I	496	LYS
1	K	216	SER
1	L	218	HIS
1	A	409	PRO
1	B	409	PRO
1	D	346	TYR
1	D	496	LYS
1	F	409	PRO
1	G	218	HIS
1	G	346	TYR
1	H	547	GLU
1	I	505	LEU
1	J	216	SER
1	J	496	LYS
1	K	155	GLU
1	B	505	LEU
1	H	409	PRO
1	J	409	PRO
1	L	409	PRO

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Mol	Chain	Res	Type
1	B	346	TYR
1	C	409	PRO
1	D	505	LEU
1	E	218	HIS
1	E	345	TYR
1	E	496	LYS
1	G	505	LEU
1	I	409	PRO
1	J	219	ASN
1	J	346	TYR
1	K	496	LYS
1	L	496	LYS
1	A	219	ASN
1	B	219	ASN
1	C	496	LYS
1	I	219	ASN
1	K	219	ASN
1	K	555	SER
1	L	346	TYR
1	A	361	GLU
1	A	505	LEU
1	E	361	GLU
1	E	409	PRO
1	E	443	LYS
1	F	219	ASN
1	F	346	TYR
1	G	361	GLU
1	K	387	TYR
1	D	409	PRO
1	G	219	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	352/495 (71%)	330 (94%)	22 (6%)	18 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	347/495 (70%)	320 (92%)	27 (8%)	12 41
1	C	356/495 (72%)	335 (94%)	21 (6%)	19 52
1	D	349/495 (70%)	325 (93%)	24 (7%)	15 47
1	E	351/495 (71%)	326 (93%)	25 (7%)	14 46
1	F	344/495 (70%)	327 (95%)	17 (5%)	25 57
1	G	352/495 (71%)	332 (94%)	20 (6%)	20 52
1	H	347/495 (70%)	323 (93%)	24 (7%)	15 47
1	I	349/495 (70%)	330 (95%)	19 (5%)	22 54
1	J	345/495 (70%)	332 (96%)	13 (4%)	33 64
1	K	355/495 (72%)	332 (94%)	23 (6%)	17 49
1	L	345/495 (70%)	323 (94%)	22 (6%)	17 49
All	All	4192/5940 (71%)	3935 (94%)	257 (6%)	18 51

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	153	THR
1	A	155	GLU
1	A	232	GLN
1	A	250	MET
1	A	266	THR
1	A	267	ARG
1	A	278	PHE
1	A	283	ARG
1	A	300	ARG
1	A	313	THR
1	A	367	PHE
1	A	381	ASN
1	A	405	VAL
1	A	417	LEU
1	A	440	THR
1	A	441	PHE
1	A	457	ARG
1	A	478	ARG
1	A	497	LEU
1	A	523	ASP
1	A	536	CYS

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Mol	Chain	Res	Type
1	B	153	THR
1	B	204	ARG
1	B	230	LEU
1	B	250	MET
1	B	266	THR
1	B	267	ARG
1	B	283	ARG
1	B	285	ASN
1	B	298	ASP
1	B	300	ARG
1	B	311	ASN
1	B	314	ARG
1	B	367	PHE
1	B	378	THR
1	B	381	ASN
1	B	384	ARG
1	B	389	LYS
1	B	405	VAL
1	B	408	THR
1	B	417	LEU
1	B	441	PHE
1	B	478	ARG
1	B	496	LYS
1	B	497	LEU
1	B	507	GLN
1	B	509	ARG
1	B	536	CYS
1	C	153	THR
1	C	250	MET
1	C	266	THR
1	C	267	ARG
1	C	285	ASN
1	C	302	VAL
1	C	367	PHE
1	C	378	THR
1	C	381	ASN
1	C	405	VAL
1	C	415	THR
1	C	417	LEU
1	C	440	THR
1	C	441	PHE
1	C	442	GLU

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Mol	Chain	Res	Type
1	C	448	THR
1	C	478	ARG
1	C	496	LYS
1	C	497	LEU
1	C	520	GLU
1	C	553	GLN
1	D	197	GLU
1	D	204	ARG
1	D	214	LEU
1	D	217	ARG
1	D	250	MET
1	D	266	THR
1	D	267	ARG
1	D	294	ASP
1	D	300	ARG
1	D	367	PHE
1	D	378	THR
1	D	381	ASN
1	D	405	VAL
1	D	408	THR
1	D	415	THR
1	D	417	LEU
1	D	440	THR
1	D	441	PHE
1	D	470	LEU
1	D	478	ARG
1	D	479	VAL
1	D	497	LEU
1	D	509	ARG
1	D	550	LEU
1	E	218	HIS
1	E	230	LEU
1	E	250	MET
1	E	267	ARG
1	E	294	ASP
1	E	300	ARG
1	E	335	ASN
1	E	367	PHE
1	E	381	ASN
1	E	405	VAL
1	E	408	THR
1	E	415	THR

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Mol	Chain	Res	Type
1	E	417	LEU
1	E	440	THR
1	E	448	THR
1	E	455	ASN
1	E	477	CYS
1	E	478	ARG
1	E	496	LYS
1	E	497	LEU
1	E	509	ARG
1	E	513	VAL
1	E	515	ILE
1	E	520	GLU
1	E	550	LEU
1	F	153	THR
1	F	266	THR
1	F	267	ARG
1	F	285	ASN
1	F	294	ASP
1	F	300	ARG
1	F	367	PHE
1	F	378	THR
1	F	381	ASN
1	F	405	VAL
1	F	408	THR
1	F	417	LEU
1	F	440	THR
1	F	441	PHE
1	F	478	ARG
1	F	479	VAL
1	F	509	ARG
1	G	153	THR
1	G	214	LEU
1	G	230	LEU
1	G	267	ARG
1	G	278	PHE
1	G	283	ARG
1	G	294	ASP
1	G	300	ARG
1	G	360	ILE
1	G	367	PHE
1	G	378	THR
1	G	381	ASN

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Mol	Chain	Res	Type
1	G	397	VAL
1	G	417	LEU
1	G	429	LEU
1	G	442	GLU
1	G	478	ARG
1	G	535	ASP
1	G	536	CYS
1	G	553	GLN
1	H	217	ARG
1	H	247	LYS
1	H	268	GLU
1	H	271	THR
1	H	283	ARG
1	H	285	ASN
1	H	294	ASP
1	H	300	ARG
1	H	367	PHE
1	H	373	LEU
1	H	378	THR
1	H	381	ASN
1	H	396	GLU
1	H	405	VAL
1	H	408	THR
1	H	417	LEU
1	H	440	THR
1	H	441	PHE
1	H	477	CYS
1	H	478	ARG
1	H	496	LYS
1	H	497	LEU
1	H	507	GLN
1	H	509	ARG
1	I	153	THR
1	I	204	ARG
1	I	230	LEU
1	I	266	THR
1	I	267	ARG
1	I	274	ASP
1	I	278	PHE
1	I	285	ASN
1	I	294	ASP
1	I	367	PHE

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Mol	Chain	Res	Type
1	I	378	THR
1	I	391	LYS
1	I	417	LEU
1	I	441	PHE
1	I	478	ARG
1	I	497	LEU
1	I	511	VAL
1	I	516	LYS
1	I	536	CYS
1	J	153	THR
1	J	230	LEU
1	J	266	THR
1	J	285	ASN
1	J	294	ASP
1	J	300	ARG
1	J	367	PHE
1	J	381	ASN
1	J	405	VAL
1	J	440	THR
1	J	442	GLU
1	J	478	ARG
1	J	509	ARG
1	K	153	THR
1	K	231	SER
1	K	232	GLN
1	K	239	MET
1	K	255	TYR
1	K	266	THR
1	K	267	ARG
1	K	283	ARG
1	K	300	ARG
1	K	313	THR
1	K	367	PHE
1	K	381	ASN
1	K	405	VAL
1	K	408	THR
1	K	415	THR
1	K	417	LEU
1	K	440	THR
1	K	441	PHE
1	K	478	ARG
1	K	496	LYS

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Mol	Chain	Res	Type
1	K	497	LEU
1	K	516	LYS
1	K	553	GLN
1	L	239	MET
1	L	247	LYS
1	L	250	MET
1	L	267	ARG
1	L	271	THR
1	L	278	PHE
1	L	283	ARG
1	L	285	ASN
1	L	294	ASP
1	L	367	PHE
1	L	378	THR
1	L	381	ASN
1	L	405	VAL
1	L	408	THR
1	L	415	THR
1	L	417	LEU
1	L	440	THR
1	L	448	THR
1	L	478	ARG
1	L	496	LYS
1	L	497	LEU
1	L	509	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	437	HIS
1	B	311	ASN
1	D	142	HIS
1	E	218	HIS
1	E	269	GLN
1	E	518	HIS
1	F	265	GLN
1	I	232	GLN
1	I	269	GLN
1	I	285	ASN
1	I	407	GLN
1	I	518	HIS

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Mol	Chain	Res	Type
1	J	265	GLN
1	K	232	GLN
1	K	269	GLN
1	K	311	ASN
1	L	269	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	386/560 (68%)	-0.05	3 (0%)	86	82	24, 42, 65, 90	0
1	B	380/560 (67%)	0.03	4 (1%)	80	77	22, 44, 75, 99	0
1	C	390/560 (69%)	-0.13	3 (0%)	86	82	19, 34, 58, 82	0
1	D	382/560 (68%)	0.07	6 (1%)	72	69	28, 51, 78, 104	0
1	E	385/560 (68%)	0.06	8 (2%)	63	61	23, 43, 67, 90	0
1	F	377/560 (67%)	0.31	13 (3%)	45	43	34, 71, 104, 120	0
1	G	386/560 (68%)	0.03	7 (1%)	68	65	30, 50, 72, 92	0
1	H	380/560 (67%)	0.36	18 (4%)	31	31	38, 72, 107, 131	0
1	I	383/560 (68%)	0.05	6 (1%)	72	69	38, 56, 79, 100	0
1	J	378/560 (67%)	0.26	14 (3%)	41	40	32, 55, 87, 118	0
1	K	389/560 (69%)	-0.04	7 (1%)	68	65	29, 46, 68, 92	0
1	L	378/560 (67%)	0.18	12 (3%)	47	46	33, 58, 88, 114	0
All	All	4594/6720 (68%)	0.09	101 (2%)	62	59	19, 51, 88, 131	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	LEU	4.5
1	G	154	GLU	4.3
1	L	373	LEU	4.0
1	E	154	GLU	3.5
1	L	159	PHE	3.3
1	L	152	LEU	3.2
1	I	154	GLU	3.2
1	L	151	ASP	3.2
1	J	151	ASP	3.1
1	J	154	GLU	3.1
1	F	544	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	151	ASP	3.0
1	H	417	LEU	3.0
1	B	154	GLU	3.0
1	H	373	LEU	2.9
1	H	159	PHE	2.9
1	H	478	ARG	2.9
1	K	154	GLU	2.9
1	F	235	SER	2.9
1	L	321	ARG	2.9
1	H	152	LEU	2.8
1	C	199	TYR	2.8
1	F	442	GLU	2.8
1	J	199	TYR	2.8
1	H	154	GLU	2.7
1	L	158	LEU	2.7
1	E	316	ILE	2.6
1	F	417	LEU	2.6
1	F	218	HIS	2.6
1	L	413	ARG	2.6
1	F	199	TYR	2.6
1	F	398	ASP	2.6
1	G	218	HIS	2.6
1	F	543	SER	2.6
1	A	154	GLU	2.5
1	E	255	TYR	2.5
1	H	143	PRO	2.5
1	L	235	SER	2.5
1	I	326	TRP	2.5
1	D	543	SER	2.5
1	F	152	LEU	2.5
1	J	159	PHE	2.5
1	L	154	GLU	2.5
1	I	218	HIS	2.5
1	K	250	MET	2.4
1	C	244	THR	2.4
1	I	151	ASP	2.4
1	L	156	ASP	2.4
1	G	329	PHE	2.4
1	H	388	HIS	2.4
1	G	199	TYR	2.4
1	D	218	HIS	2.4
1	E	253	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	329	PHE	2.4
1	F	143	PRO	2.4
1	I	250	MET	2.3
1	J	543	SER	2.3
1	J	156	ASP	2.3
1	J	316	ILE	2.3
1	F	397	VAL	2.3
1	H	442	GLU	2.3
1	D	388	HIS	2.3
1	D	390	ARG	2.3
1	I	252	PHE	2.3
1	A	236	SER	2.2
1	B	236	SER	2.2
1	G	198	SER	2.2
1	K	321	ARG	2.2
1	H	411	TYR	2.2
1	K	198	SER	2.2
1	J	319	VAL	2.2
1	E	235	SER	2.2
1	J	150	PRO	2.2
1	G	159	PHE	2.2
1	K	160	ASN	2.2
1	A	326	TRP	2.2
1	F	401	TYR	2.2
1	H	443	LYS	2.2
1	G	373	LEU	2.2
1	H	235	SER	2.2
1	J	241	SER	2.1
1	J	203	LEU	2.1
1	D	159	PHE	2.1
1	E	244	THR	2.1
1	H	145	TYR	2.1
1	H	253	GLN	2.1
1	L	319	VAL	2.1
1	K	326	TRP	2.1
1	L	157	THR	2.1
1	J	373	LEU	2.1
1	H	422	ASP	2.1
1	E	390	ARG	2.0
1	H	250	MET	2.0
1	H	321	ARG	2.0
1	H	334	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	415	THR	2.0
1	J	244	THR	2.0
1	B	153	THR	2.0
1	J	326	TRP	2.0
1	D	160	ASN	2.0
1	K	199	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.