Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 03:22 pm GMT

PDB ID	:	6QNW
Title	:	Influenza A Polymerase Heterotrimer Human H3N2 Northern Territory 1968
Authors	:	Keown, J.R.; Fan, H.; Grimes, J.M.
Deposited on	:	2019-02-12
Resolution	:	3.31 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:

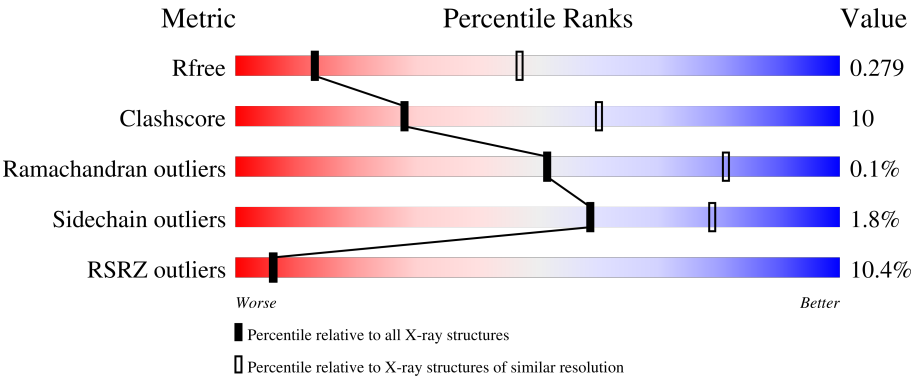
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 <=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	716	3% 72% 25%
1	D	716	17% 73% 21%
1	G	716	2% 72% 25%
1	J	716	10% 75% 22%
2	B	757	4% 70% 20% 10%

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Mol	Chain	Length	Quality of chain
2	E	757	23% 66% 21% 12%
2	H	757	4% 67% 21% 11%
2	K	757	11% 65% 23% 11%
3	C	765	10% 69% 24% 5%
3	F	765	15% 70% 23% 6%
3	I	765	6% 69% 26% 5%
3	L	765	11% 71% 22% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 67232 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	704	Total	C	N	O	S	0	0	0
			5733	3638	969	1084	42			
1	D	686	Total	C	N	O	S	0	0	0
			5604	3556	949	1058	41			
1	G	701	Total	C	N	O	S	0	0	0
			5707	3617	967	1081	42			
1	J	702	Total	C	N	O	S	0	0	0
			5713	3622	966	1083	42			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	679	Total	C	N	O	S	0	0	0
			5426	3417	932	1034	43			
2	E	665	Total	C	N	O	S	0	0	0
			5315	3351	910	1011	43			
2	H	676	Total	C	N	O	S	0	0	0
			5410	3410	929	1028	43			
2	K	673	Total	C	N	O	S	0	0	0
			5382	3390	925	1024	43			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	577	LYS	GLU	conflict	UNP P03432
E	577	LYS	GLU	conflict	UNP P03432
H	577	LYS	GLU	conflict	UNP P03432
K	577	LYS	GLU	conflict	UNP P03432

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	724	Total	C	N	O	S	0	0	0
			5772	3627	1044	1060	41			
3	F	720	Total	C	N	O	S	0	0	0
			5734	3604	1034	1056	40			
3	I	726	Total	C	N	O	S	0	0	0
			5789	3638	1047	1063	41			
3	L	709	Total	C	N	O	S	0	0	0
			5647	3552	1015	1039	41			

There are 24 discrepancies between the modelled and reference sequences:

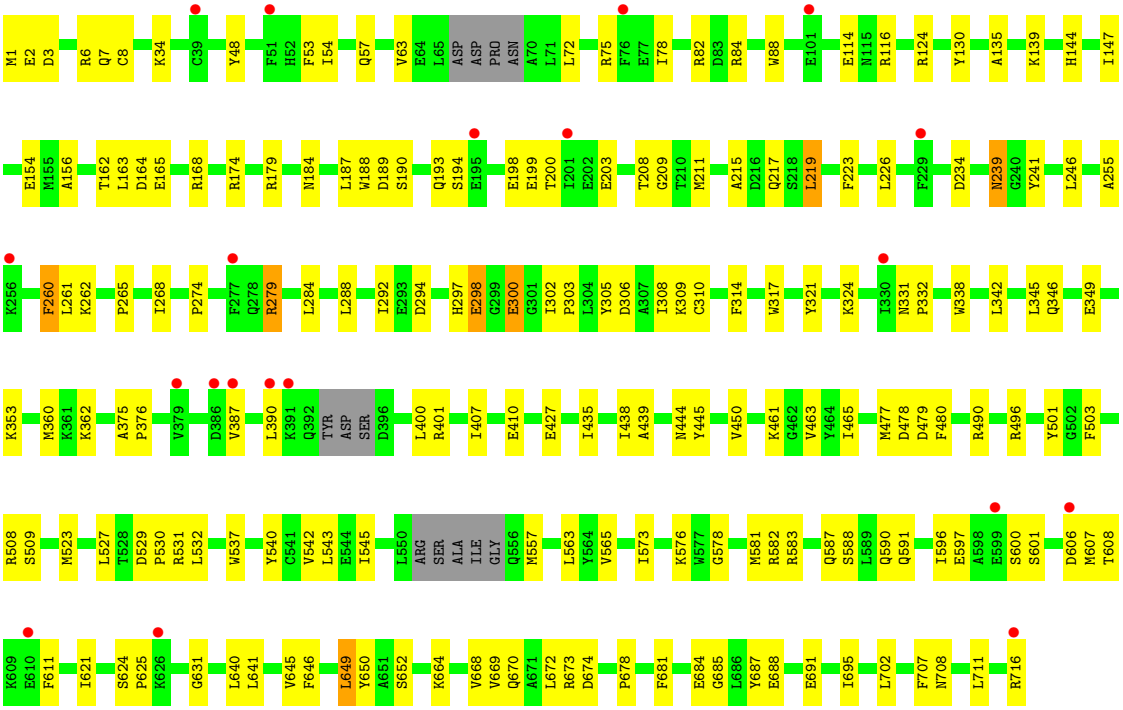
Chain	Residue	Modelled	Actual	Comment	Reference
C	760	GLU	-	expression tag	UNP P03429
C	761	ASN	-	expression tag	UNP P03429
C	762	LEU	-	expression tag	UNP P03429
C	763	TYR	-	expression tag	UNP P03429
C	764	PHE	-	expression tag	UNP P03429
C	765	GLN	-	expression tag	UNP P03429
F	760	GLU	-	expression tag	UNP P03429
F	761	ASN	-	expression tag	UNP P03429
F	762	LEU	-	expression tag	UNP P03429
F	763	TYR	-	expression tag	UNP P03429
F	764	PHE	-	expression tag	UNP P03429
F	765	GLN	-	expression tag	UNP P03429
I	760	GLU	-	expression tag	UNP P03429
I	761	ASN	-	expression tag	UNP P03429
I	762	LEU	-	expression tag	UNP P03429
I	763	TYR	-	expression tag	UNP P03429
I	764	PHE	-	expression tag	UNP P03429
I	765	GLN	-	expression tag	UNP P03429
L	760	GLU	-	expression tag	UNP P03429
L	761	ASN	-	expression tag	UNP P03429
L	762	LEU	-	expression tag	UNP P03429
L	763	TYR	-	expression tag	UNP P03429
L	764	PHE	-	expression tag	UNP P03429
L	765	GLN	-	expression tag	UNP P03429

3 Residue-property plots (i)

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.

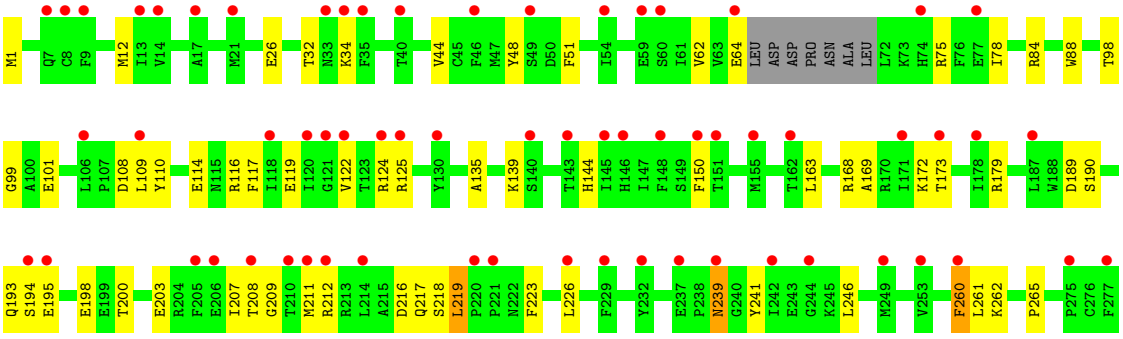
• Molecule 1: Polymerase acidic protein

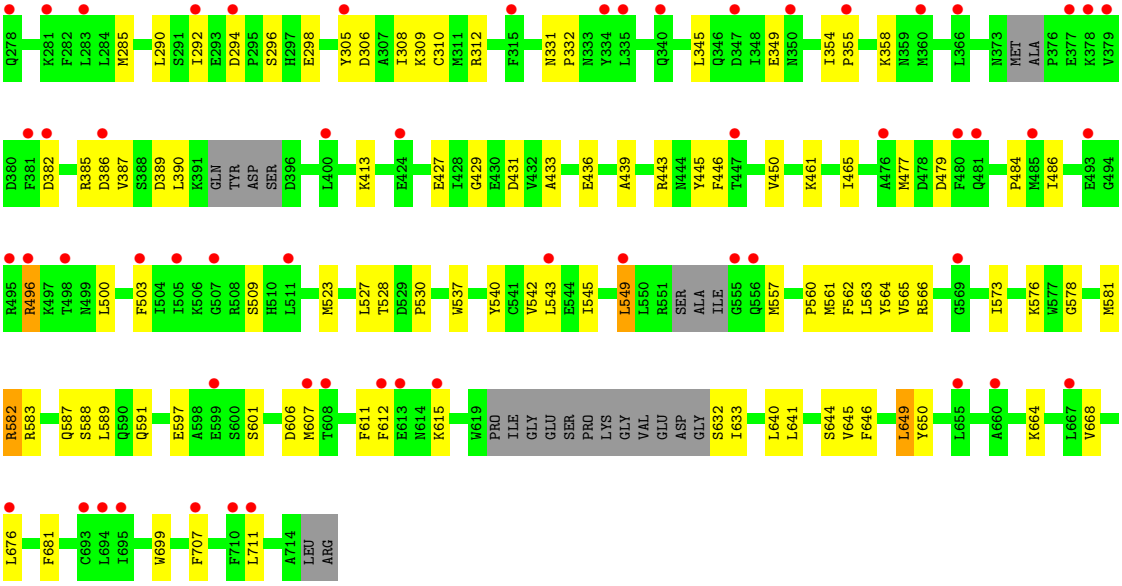
Chain A:



• Molecule 1: Polymerase acidic protein

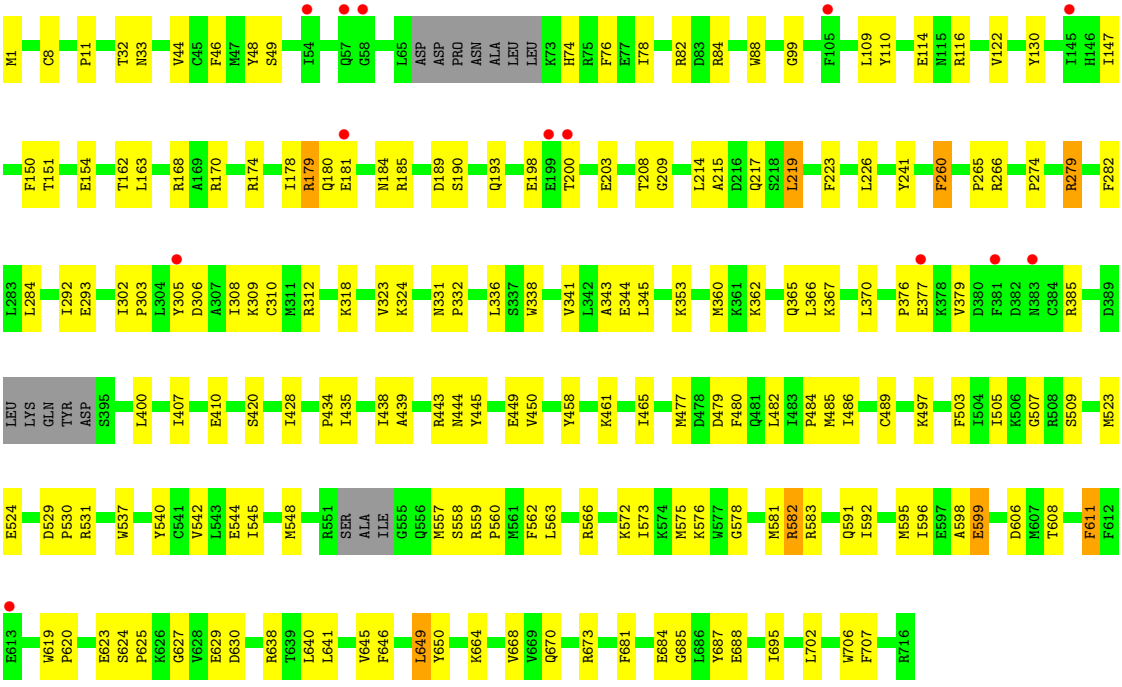
Chain D:





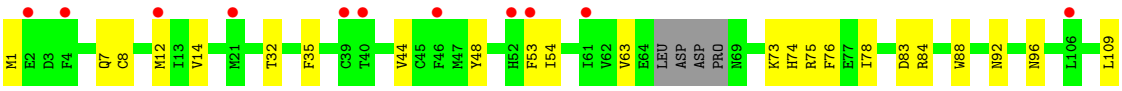
• Molecule 1: Polymerase acidic protein

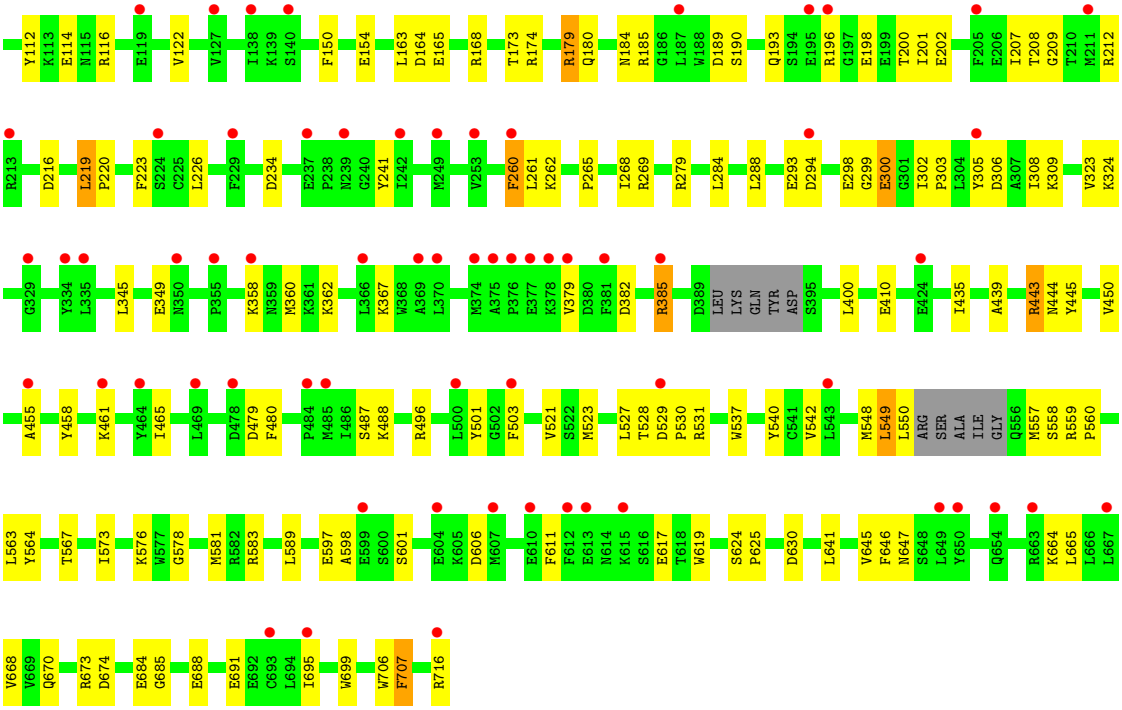
Chain G:



• Molecule 1: Polymerase acidic protein

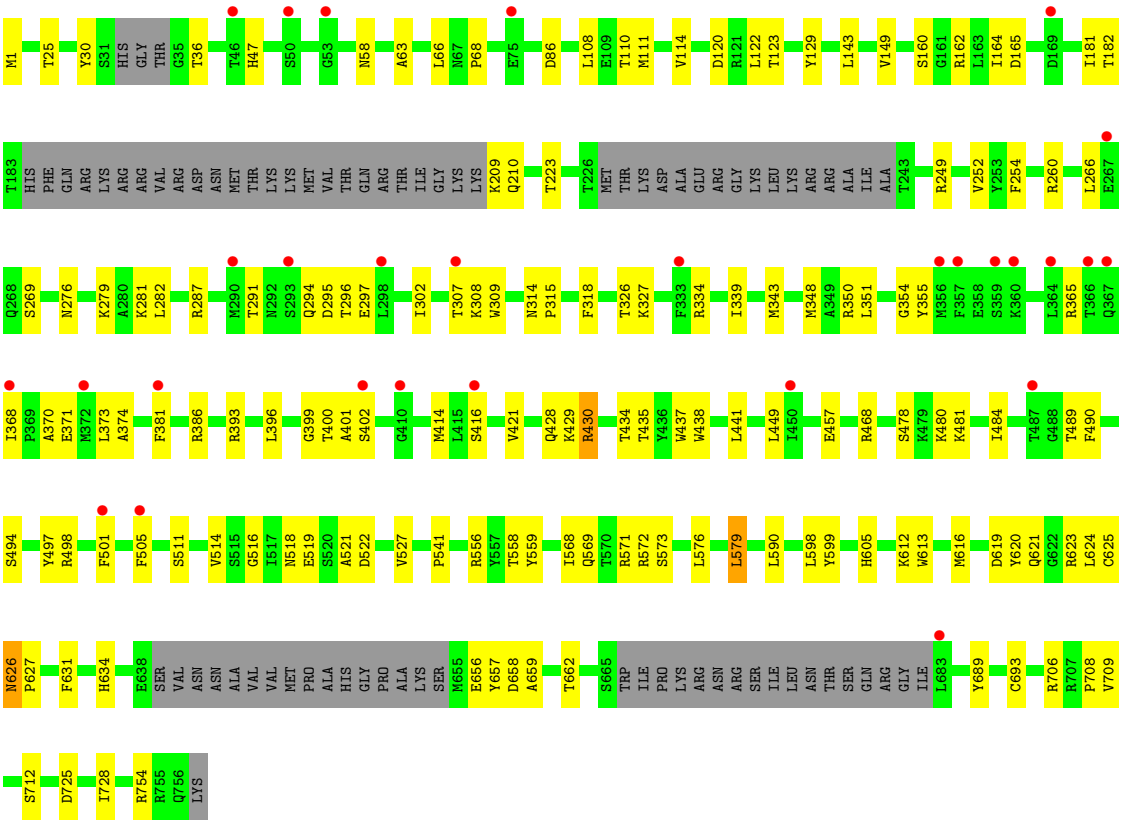
Chain J:





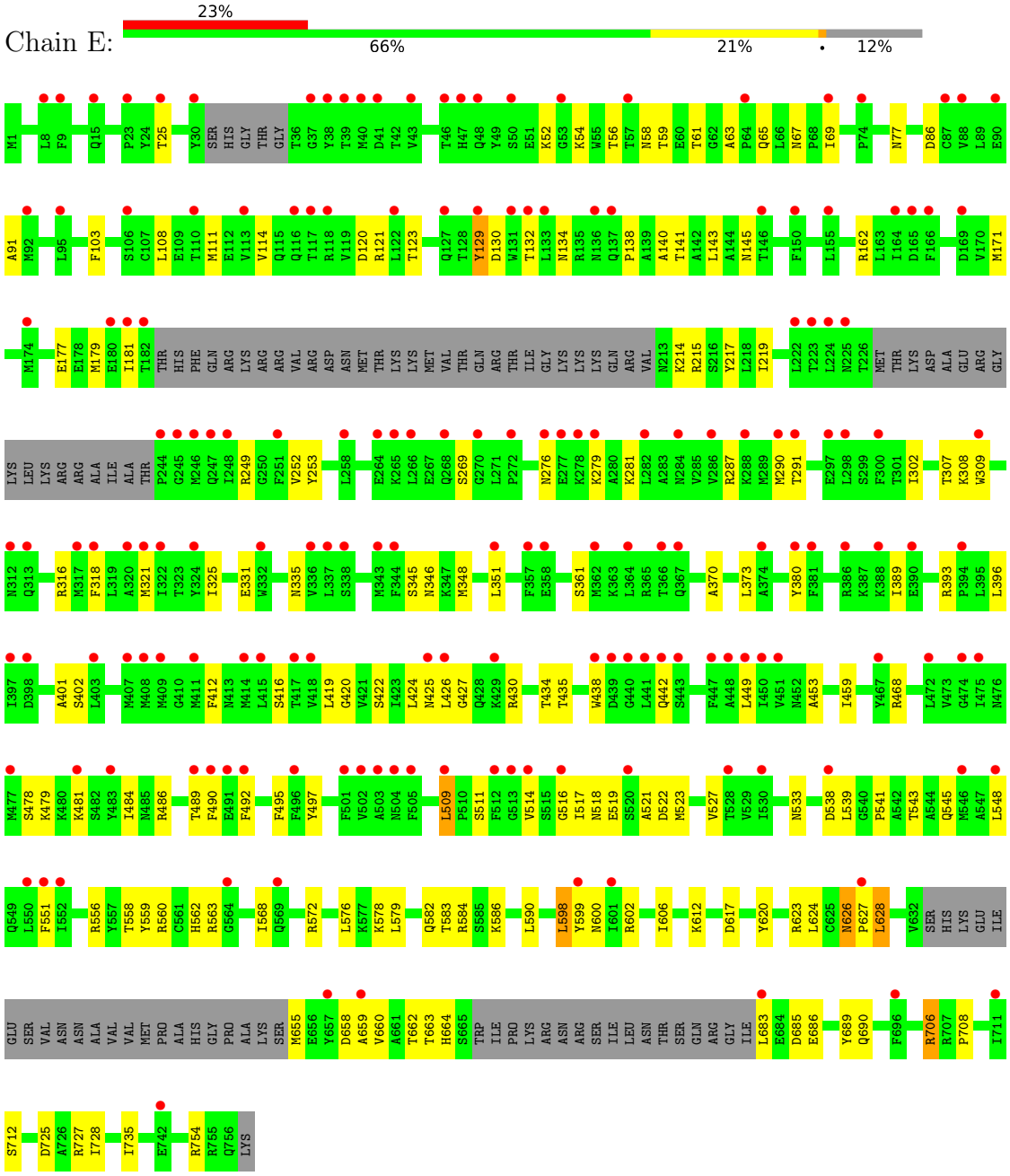
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain B:



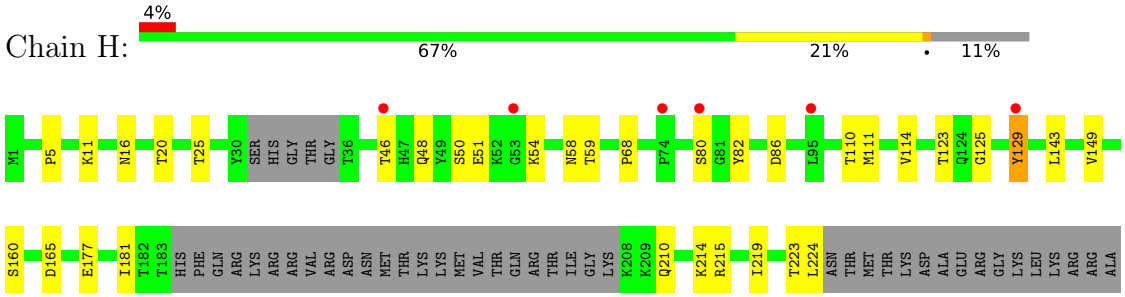
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

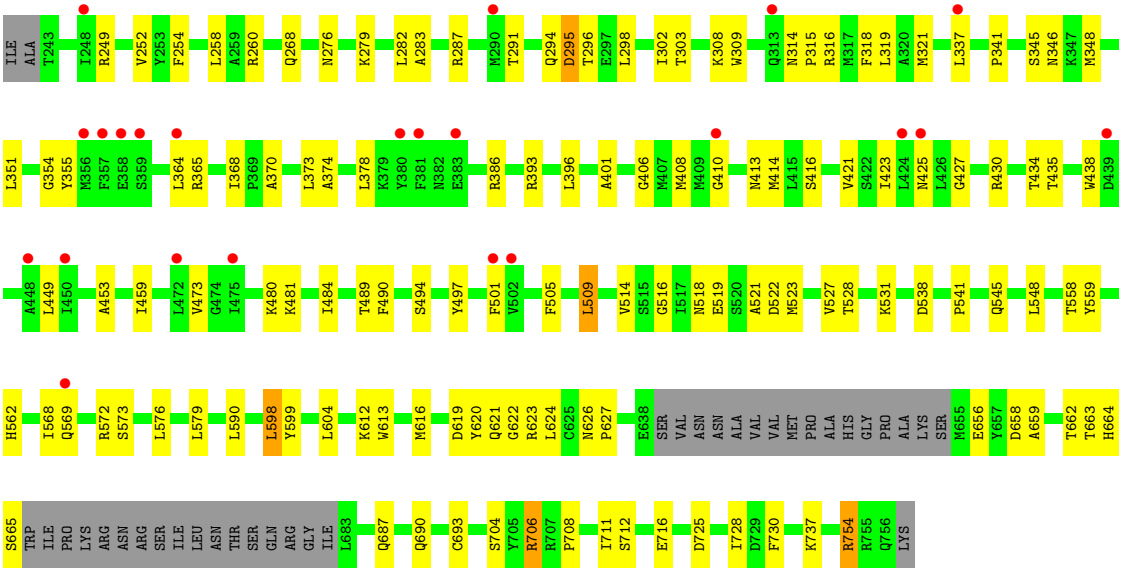
Chain E:



• Molecule 2: RNA-directed RNA polymerase catalytic subunit

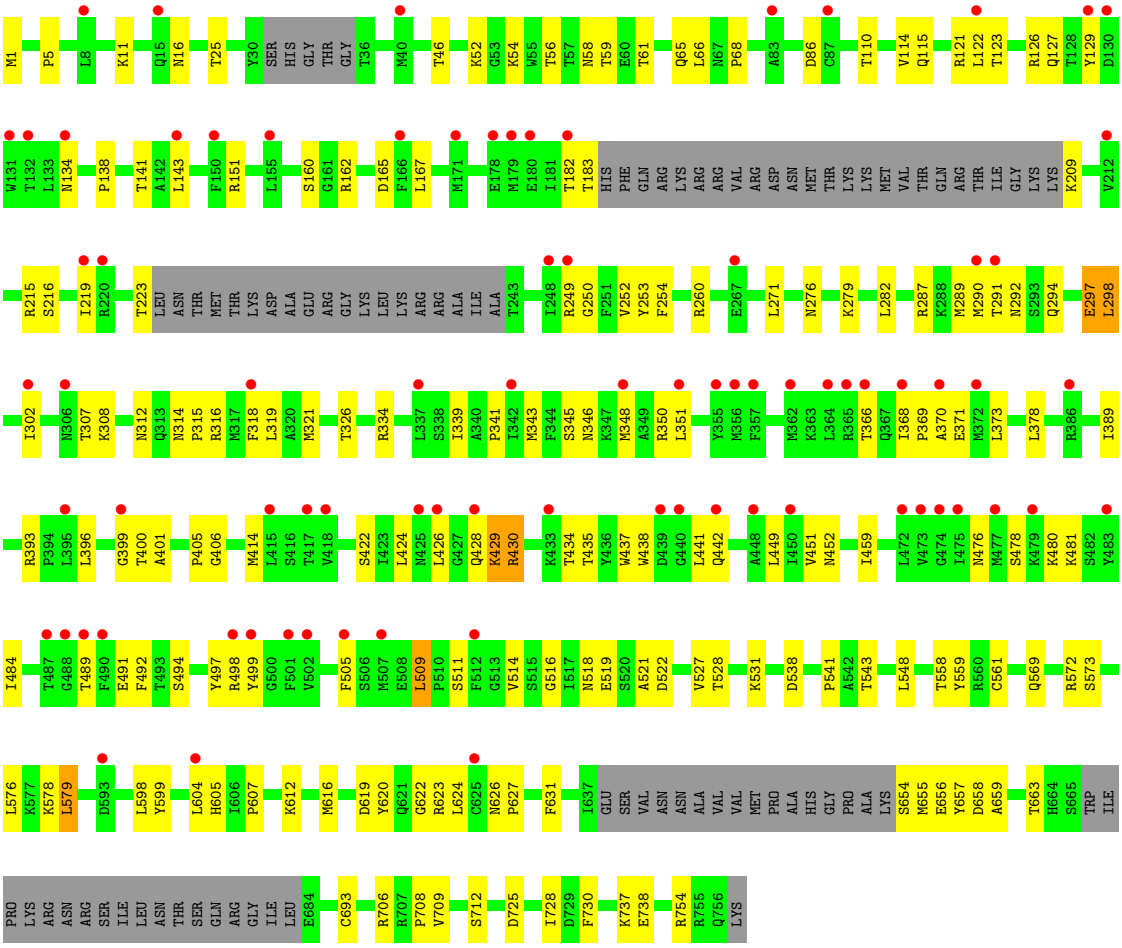
Chain H:





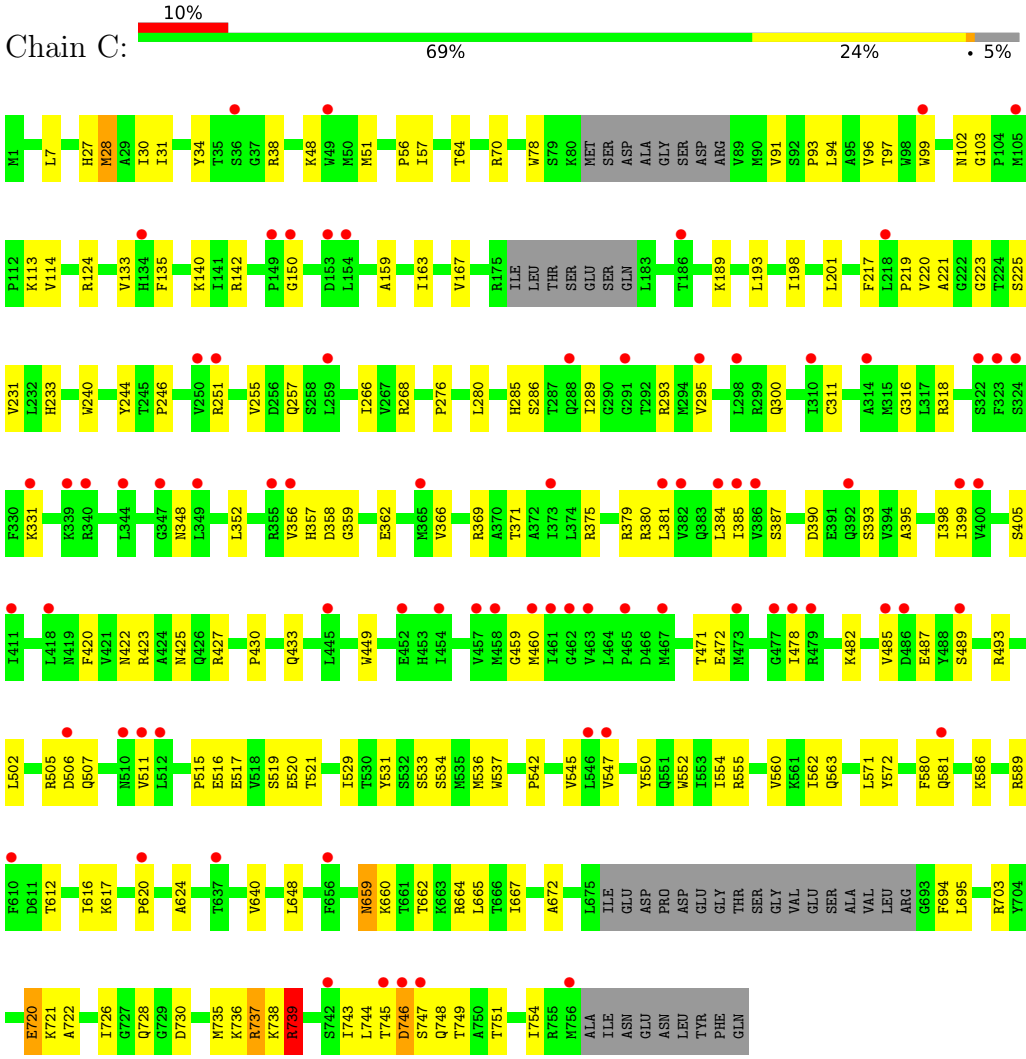
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain K:



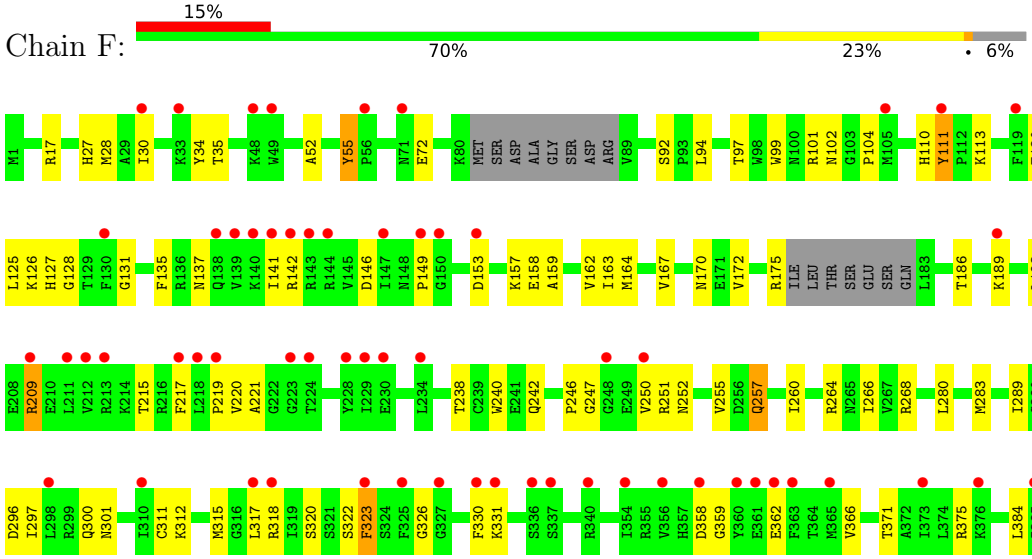
• Molecule 3: Polymerase basic protein 2

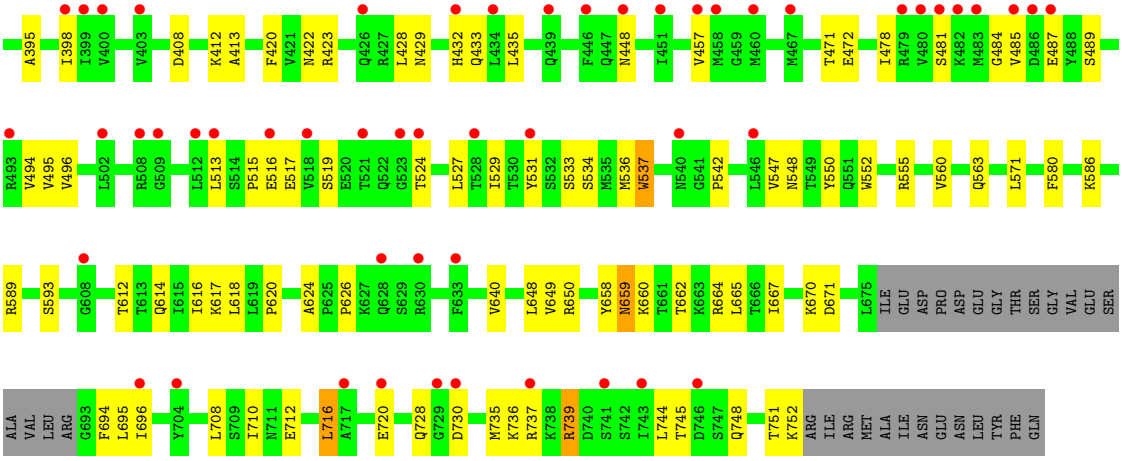
Chain C:



• Molecule 3: Polymerase basic protein 2

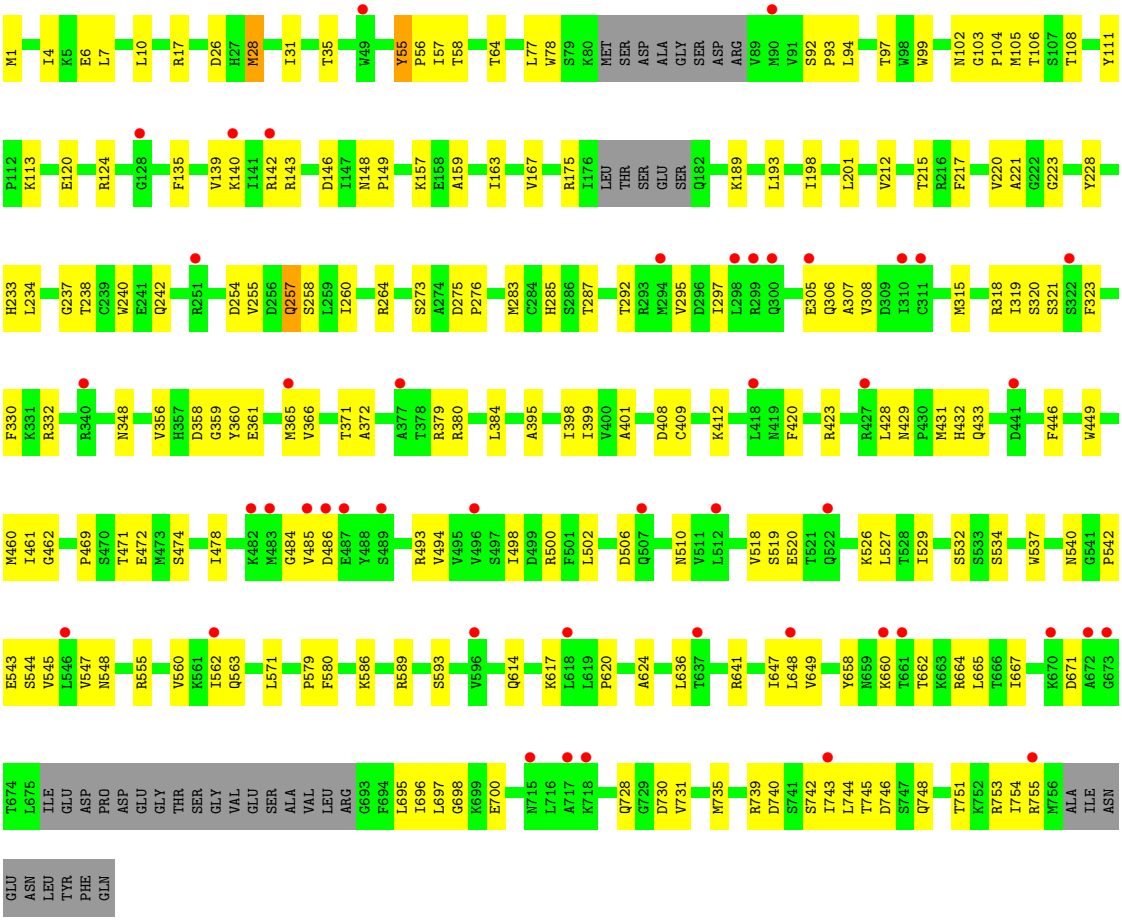
Chain F:





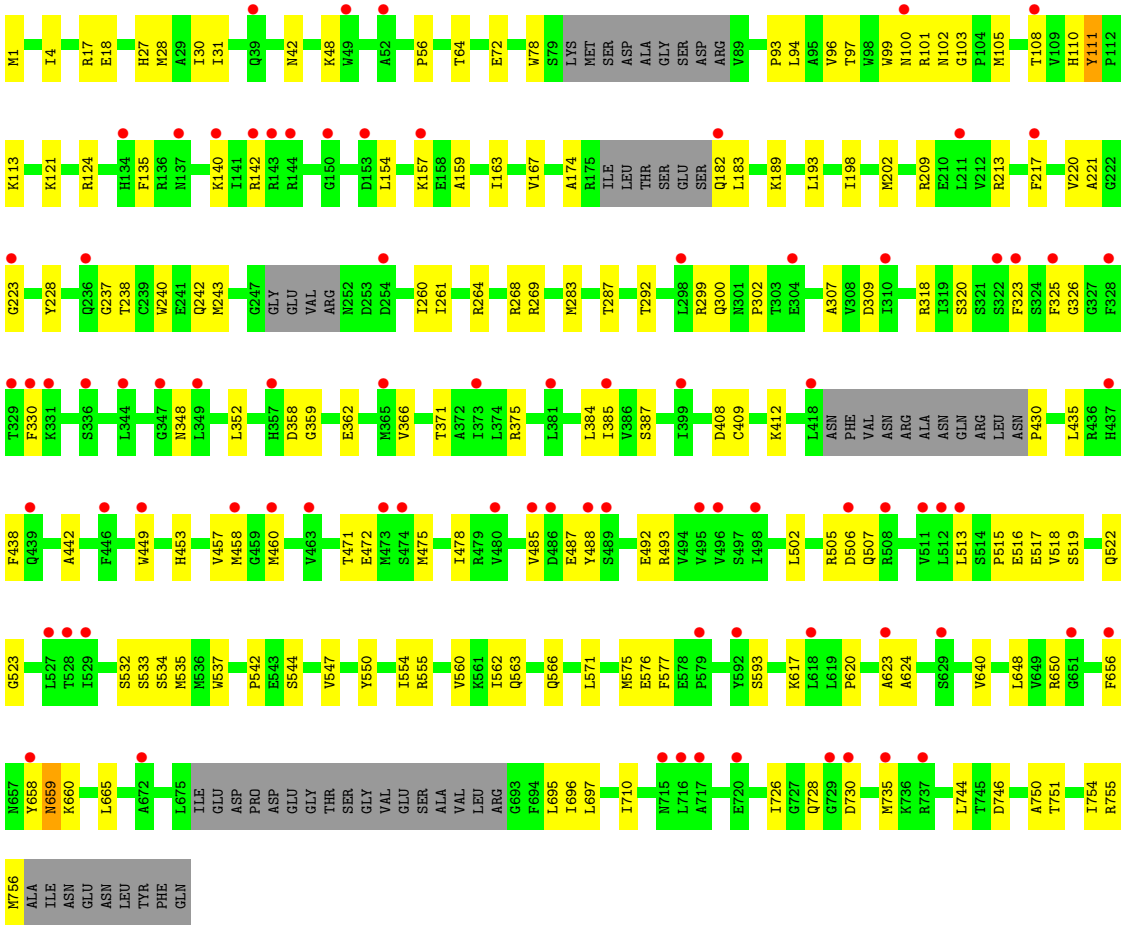
• Molecule 3: Polymerase basic protein 2

Chain I:



• Molecule 3: Polymerase basic protein 2

Chain L:


M1 I4 R17 E18 H27 M28 A29 I30 I31 Q39 N42 K48 W49 A52 P56 T64 E72 W78 S79 LYS MET SER ASP ALA GLY SER ASP ARG V89 P93 L94 A95 V96 T97 W98 W99 N100 R101 N102 G103 P104 M105 T108 V109 H110 Y111 P112
K113 K121 R124 H134 F135 R136 N137 K140 I141 R142 R143 R144 G150 D153 L154 K157 E158 A159 I163 V167 A174 R176 ILE LEU THR SER GLU SER Q182 L183 K189 L193 I198 M202 R209 E210 L211 V212 R213 F217 V220 A221 G222
G223 Y228 Q236 G237 T238 C239 W240 E241 Q242 M243 G247 GLY GLU VAL ARG N252 D253 D254 I260 I261 R264 R268 R269 M283 T287 T292 L298 R299 Q300 N301 P302 T303 E304 A307 V308 D309 I310 R318 I319 S320 S321 S322 F323 S324 F325 G326 G327 F328
T329 F330 K331 S336 L344 G347 N348 L349 L352 H357 D358 G359 E362 M365 V366 T371 A372 I373 L374 R375 L381 L384 I385 V386 S387 I399 D408 C409 K412 L418 ASN PHE VAL ASN ARG ALA ASN GLN ARG LEU ASN P430 L435 R436 H437
F438 Q439 A442 F446 W449 H453 V457 M458 G459 M460 V463 T471 E472 M473 S474 M475 I478 R479 V480 V485 D486 E487 Y488 S489 E492 R493 V494 V495 V496 S497 I498 L502 R505 D506 Q507 R508 V511 L512 L513 S514 P515 E516 E517 V518 S519 Q522
G523 L527 T528 I529 S532 S533 S534 M535 M536 W537 P542 E543 S544 V547 Y550 I554 R555 V560 K561 T562 Q563 Q566 L571 M575 E576 F577 E578 P579 Y592 S593 K617 L618 L619 P620 A623 A624 S629 V640 L648 V649 R650 G651 F656
N657 Y658 N659 K660 L665 A672 L675 ILE GLU ASP PRO ASP GLU GLY THR SER GLY VAL GLU SER ALA VAL LEU ARG G693 F694 L695 I696 L697 I710 W715 L716 A717 E720 I726 G727 Q728 G729 D730 M735 K736 R737 L744 T745 D746 A750 T751 I754 R755
M756 ALA ILE ASN GLU ASN LEU TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	336.48Å 191.90Å 235.74Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	138.62 – 3.31 138.62 – 3.31	Depositor EDS
% Data completeness (in resolution range)	55.1 (138.62-3.31) 55.1 (138.62-3.31)	Depositor EDS
R_{merge}	0.46	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.235 , 0.279 0.235 , 0.279	Depositor DCC
R_{free} test set	6172 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	88.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 76.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.025 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.024 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.027 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.024 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	67232	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/5853	0.46	0/7886
1	D	0.25	0/5720	0.44	0/7701
1	G	0.25	0/5827	0.45	0/7850
1	J	0.25	0/5833	0.45	0/7860
2	B	0.25	0/5529	0.45	1/7456 (0.0%)
2	E	0.25	0/5417	0.43	0/7306
2	H	0.25	0/5513	0.44	0/7433
2	K	0.25	0/5485	0.44	0/7396
3	C	0.24	0/5866	0.47	0/7900
3	F	0.24	0/5828	0.47	1/7851 (0.0%)
3	I	0.24	0/5883	0.46	0/7923
3	L	0.24	0/5738	0.46	0/7725
All	All	0.25	0/68492	0.45	2/92287 (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
3	C	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	579	LEU	CB-CG-CD2	-9.30	95.18	111.00
3	F	716	LEU	CA-CB-CG	6.75	130.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	HIS	Peptide
3	C	739	ARG	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	5733	0	5662	123	0
1	D	5604	0	5527	120	0
1	G	5707	0	5624	134	0
1	J	5713	0	5630	116	0
2	B	5426	0	5374	109	0
2	E	5315	0	5262	129	0
2	H	5410	0	5366	138	0
2	K	5382	0	5330	136	0
3	C	5772	0	5915	141	0
3	F	5734	0	5869	138	0
3	I	5789	0	5934	152	0
3	L	5647	0	5786	120	0
All	All	67232	0	67279	1334	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 10.

All (1334) 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)
3:F:317:LEU:HD12	3:F:496:VAL:H	1.41	0.86
3:F:289:ILE:HG22	3:F:529:ILE:HG13	1.63	0.81
2:E:708:PRO:HA	3:F:728:GLN:HE21	1.46	0.79
3:F:149:PRO:HD2	3:F:209:ARG:HH12	1.49	0.77
2:B:309:TRP:HZ2	2:B:416:SER:HB3	1.49	0.77
3:I:275:ASP:HB3	1:J:96:ASN:HD21	1.47	0.77
2:H:309:TRP:HZ2	2:H:416:SER:HB3	1.50	0.77
2:B:708:PRO:HA	3:C:728:GLN:HE21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:744:LEU:HD12	3:F:745:THR:H	1.49	0.76
2:K:302:ILE:HG22	2:K:484:ILE:HG23	1.69	0.75
3:I:398:ILE:HD11	3:I:478:ILE:HD11	1.68	0.75
2:H:627:PRO:HB3	3:I:198:ILE:HG23	1.67	0.74
2:H:708:PRO:HA	3:I:728:GLN:HE21	1.53	0.74
1:A:450:VAL:HG13	1:A:641:LEU:HD22	1.68	0.74
2:E:572:ARG:HA	3:F:94:LEU:HD12	1.69	0.74
3:I:323:PHE:HB2	3:I:330:PHE:HB2	1.67	0.74
3:F:323:PHE:HB3	3:F:330:PHE:HB2	1.68	0.73
2:K:708:PRO:HA	3:L:728:GLN:HE21	1.53	0.73
2:H:687:GLN:HG3	2:H:690:GLN:HB2	1.70	0.73
1:A:578:GLY:HA2	1:A:581:MET:HG3	1.69	0.73
3:C:352:LEU:HD12	3:C:430:PRO:HB3	1.70	0.73
3:C:505:ARG:HG3	3:C:511:VAL:HA	1.70	0.73
3:F:153:ASP:OD2	3:F:301:ASN:ND2	2.22	0.73
3:C:398:ILE:HD11	3:C:478:ILE:HD11	1.68	0.72
3:F:141:ILE:HB	3:F:220:VAL:O	1.89	0.72
1:J:450:VAL:HG13	1:J:641:LEU:HD22	1.70	0.72
2:E:132:THR:HG23	2:E:181:ILE:HD13	1.70	0.72
2:H:378:LEU:HD23	2:H:386:ARG:HG3	1.72	0.72
3:L:554:ILE:HD11	3:L:665:LEU:HD23	1.72	0.71
2:E:309:TRP:HZ2	2:E:416:SER:HB3	1.56	0.71
2:H:302:ILE:HG22	2:H:484:ILE:HG23	1.73	0.71
1:A:292:ILE:HD13	1:A:309:LYS:HG3	1.73	0.71
2:E:302:ILE:HG12	2:E:449:LEU:HB3	1.72	0.71
1:G:84:ARG:HE	1:G:88:TRP:HE1	1.37	0.71
2:E:302:ILE:HG22	2:E:484:ILE:HG23	1.73	0.71
2:E:626:ASN:ND2	3:F:104:PRO:O	2.23	0.71
3:F:614:GLN:NE2	3:F:649:VAL:O	2.24	0.70
1:D:387:VAL:HG12	1:D:390:LEU:HB2	1.71	0.70
3:F:736:LYS:HG2	3:F:737:ARG:H	1.55	0.70
3:I:306:GLN:HG3	3:I:518:VAL:HA	1.73	0.70
2:B:302:ILE:HG22	2:B:484:ILE:HG23	1.74	0.70
2:E:538:ASP:HB3	3:F:238:THR:HG22	1.73	0.69
1:D:260:PHE:HE1	1:D:265:PRO:HG3	1.58	0.69
2:H:302:ILE:HG12	2:H:449:LEU:HB3	1.73	0.69
3:L:323:PHE:HB2	3:L:330:PHE:HB2	1.75	0.69
2:E:316:ARG:NH2	2:E:345:SER:OG	2.26	0.68
1:J:323:VAL:HG12	1:J:324:LYS:H	1.58	0.68
2:K:182:THR:HG23	2:K:209:LYS:HE2	1.76	0.68
3:C:331:LYS:HE3	3:C:489:SER:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:373:LEU:HD21	2:E:389:ILE:HD13	1.76	0.68
2:K:289:MET:SD	2:K:452:ASN:ND2	2.66	0.68
2:B:429:LYS:HB3	2:B:437:TRP:HB3	1.74	0.68
2:E:287:ARG:NH1	3:F:484:GLY:O	2.26	0.68
1:J:298:GLU:OE1	1:J:488:LYS:NZ	2.25	0.68
2:B:302:ILE:HG12	2:B:449:LEU:HB3	1.74	0.68
1:D:583:ARG:HB3	2:E:25:THR:HG21	1.76	0.68
2:K:538:ASP:HB3	3:L:238:THR:HG22	1.75	0.67
1:G:443:ARG:NH2	2:H:545:GLN:OE1	2.26	0.67
2:H:50:SER:HB3	2:H:68:PRO:HG3	1.77	0.67
1:A:234:ASP:O	2:B:327:LYS:NZ	2.28	0.67
1:D:431:ASP:OD1	2:E:600:ASN:ND2	2.28	0.67
3:I:420:PHE:O	3:I:433:GLN:NE2	2.25	0.67
1:J:48:TYR:HE1	1:J:163:LEU:HG	1.57	0.67
1:A:302:ILE:HD12	1:A:303:PRO:HD2	1.77	0.67
2:E:489:THR:HA	2:E:497:TYR:O	1.94	0.67
1:G:266:ARG:HG2	1:G:687:TYR:HE2	1.60	0.66
1:D:443:ARG:NH2	2:E:545:GLN:OE1	2.28	0.66
1:J:54:ILE:HG12	1:J:75:ARG:HB2	1.76	0.66
1:A:427:GLU:OE2	2:B:556:ARG:NH2	2.29	0.66
3:C:366:VAL:HA	3:C:371:THR:HG22	1.78	0.65
1:D:578:GLY:HA2	1:D:581:MET:HG3	1.76	0.65
1:D:530:PRO:HG3	1:D:542:VAL:HG11	1.77	0.65
3:I:547:VAL:HG12	3:I:667:ILE:HB	1.78	0.65
2:K:438:TRP:HB3	2:K:451:VAL:HG12	1.78	0.65
3:F:432:HIS:NE2	3:F:517:GLU:OE2	2.30	0.65
2:B:428:GLN:O	2:B:430:ARG:NE	2.27	0.65
1:J:435:ILE:HD11	3:L:242:GLN:HB2	1.78	0.65
2:B:627:PRO:HB3	3:C:198:ILE:HG23	1.77	0.65
1:D:296:SER:OG	1:D:496:ARG:NH1	2.30	0.65
3:I:255:VAL:HA	3:I:527:LEU:HD11	1.78	0.65
1:J:302:ILE:HD12	1:J:303:PRO:HD2	1.77	0.65
2:B:266:LEU:HD13	2:B:421:VAL:HG11	1.78	0.64
3:C:318:ARG:HD3	3:C:493:ARG:HB3	1.80	0.64
1:J:185:ARG:HH21	3:L:157:LYS:HE2	1.62	0.64
1:G:578:GLY:HA2	1:G:581:MET:HG3	1.78	0.64
1:A:260:PHE:HE1	1:A:265:PRO:HG3	1.61	0.64
1:A:387:VAL:HG23	1:A:390:LEU:HB2	1.80	0.64
2:H:430:ARG:HH21	3:I:360:TYR:HB2	1.62	0.64
2:H:160:SER:OG	2:H:165:ASP:OD2	2.13	0.64
2:E:686:GLU:N	2:E:686:GLU:OE1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:316:ARG:NH2	2:K:345:SER:OG	2.31	0.64
1:G:450:VAL:HG13	1:G:641:LEU:HD22	1.79	0.64
2:K:302:ILE:HG12	2:K:449:LEU:HB3	1.79	0.64
1:A:400:LEU:HD23	1:A:695:ILE:HG23	1.80	0.63
1:G:557:MET:HG3	1:G:559:ARG:HG3	1.79	0.63
1:J:548:MET:O	1:J:558:SER:HA	1.98	0.63
3:C:736:LYS:HG2	3:C:737:ARG:H	1.63	0.63
2:B:281:LYS:HG3	3:C:142:ARG:HH22	1.64	0.63
1:G:1:MET:HG2	1:G:32:THR:HB	1.81	0.63
1:G:179:ARG:NH2	3:I:26:ASP:OD2	2.30	0.63
1:G:345:LEU:HD11	1:G:503:PHE:HE2	1.63	0.63
3:I:461:ILE:HD12	3:I:469:PRO:HB3	1.80	0.63
3:F:317:LEU:HG	3:F:495:VAL:HG12	1.79	0.63
3:F:593:SER:HB2	3:F:624:ALA:HB3	1.81	0.63
1:G:44:VAL:O	1:G:48:TYR:HB2	1.98	0.63
2:K:276:ASN:HB3	3:L:140:LYS:HG3	1.80	0.63
3:L:223:GLY:HA2	3:L:228:TYR:HD2	1.63	0.63
1:G:302:ILE:HD12	1:G:303:PRO:HD2	1.79	0.62
1:J:670:GLN:OE1	1:J:673:ARG:NH2	2.33	0.62
2:B:123:THR:HG22	2:B:143:LEU:HD13	1.82	0.62
2:H:626:ASN:HB3	3:I:99:TRP:HH2	1.62	0.62
2:K:294:GLN:HG3	3:L:453:HIS:HB2	1.82	0.62
2:E:65:GLN:NE2	2:E:346:ASN:OD1	2.32	0.62
2:E:518:ASN:HB3	2:E:521:ALA:HB3	1.82	0.62
1:J:557:MET:HG2	1:J:559:ARG:HE	1.64	0.62
2:K:708:PRO:HB3	3:L:728:GLN:HG3	1.82	0.62
2:B:620:TYR:CZ	2:B:624:LEU:HD12	2.35	0.62
2:H:572:ARG:HA	3:I:94:LEU:HD12	1.81	0.62
3:I:157:LYS:HD2	3:I:175:ARG:NH1	2.15	0.61
3:I:384:LEU:HD23	3:I:478:ILE:HD11	1.82	0.61
1:J:173:THR:OG1	3:L:696:ILE:N	2.27	0.61
1:J:439:ALA:HB2	2:K:541:PRO:HB2	1.82	0.61
1:G:150:PHE:HB3	1:G:179:ARG:HB2	1.82	0.61
3:C:268:ARG:HE	3:C:519:SER:HB2	1.65	0.61
2:K:123:THR:HG22	2:K:143:LEU:HD13	1.81	0.61
2:H:287:ARG:O	2:H:291:THR:OG1	2.18	0.61
1:G:606:ASP:OD2	1:G:608:THR:OG1	2.19	0.61
3:I:614:GLN:NE2	3:I:649:VAL:O	2.33	0.61
3:F:312:LYS:HD3	3:F:318:ARG:HD2	1.82	0.61
3:I:318:ARG:HB3	3:I:493:ARG:HD2	1.82	0.61
1:J:578:GLY:HA2	1:J:581:MET:HG3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:SER:HB3	2:B:1:MET:HA	1.82	0.61
2:B:576:LEU:HD12	3:C:97:THR:HG21	1.82	0.61
1:J:345:LEU:HD11	1:J:503:PHE:HE2	1.65	0.61
1:A:345:LEU:HD11	1:A:503:PHE:HE2	1.66	0.61
1:D:390:LEU:HB3	2:E:380:TYR:CE1	2.36	0.61
1:J:114:GLU:HB3	1:J:116:ARG:HG2	1.82	0.61
3:L:384:LEU:HD23	3:L:478:ILE:HD11	1.81	0.61
2:H:287:ARG:NH1	3:I:484:GLY:O	2.34	0.61
3:C:425:ASN:ND2	1:D:99:GLY:O	2.34	0.61
2:H:518:ASN:HB3	2:H:521:ALA:HB3	1.83	0.61
3:L:362:GLU:HG2	3:L:375:ARG:HG2	1.83	0.61
3:C:560:VAL:HG13	3:C:571:LEU:HD11	1.82	0.60
3:F:560:VAL:HG13	3:F:571:LEU:HD11	1.83	0.60
3:I:157:LYS:HD2	3:I:175:ARG:HH12	1.66	0.60
1:D:537:TRP:HB3	1:D:540:TYR:HB2	1.82	0.60
1:G:170:ARG:HH12	3:I:739:ARG:HB3	1.67	0.60
2:B:260:ARG:HE	2:B:414:MET:HE1	1.65	0.60
2:B:572:ARG:HA	3:C:94:LEU:HD12	1.82	0.60
1:G:198:GLU:HG2	1:G:200:THR:HG22	1.83	0.60
1:G:606:ASP:HB3	3:I:135:PHE:CG	2.36	0.60
1:A:219:LEU:HD22	1:A:223:PHE:HB2	1.82	0.60
3:C:751:THR:HA	3:C:754:ILE:HG22	1.83	0.60
3:F:362:GLU:HG2	3:F:375:ARG:HG2	1.82	0.60
3:I:139:VAL:HG21	3:I:484:GLY:HA2	1.83	0.60
3:I:254:ASP:HB2	3:I:526:LYS:HD3	1.81	0.60
1:A:268:ILE:N	1:A:708:ASN:OD1	2.34	0.60
2:B:396:LEU:HA	2:B:401:ALA:HA	1.84	0.60
3:F:159:ALA:O	3:F:163:ILE:HG12	2.02	0.60
1:G:435:ILE:HD11	3:I:234:LEU:HD23	1.83	0.60
1:J:583:ARG:HB3	2:K:25:THR:HG21	1.81	0.60
1:A:353:LYS:HB3	1:G:353:LYS:HB3	1.83	0.60
3:C:593:SER:HB2	3:C:624:ALA:HB3	1.83	0.60
2:E:219:ILE:HG23	2:E:348:MET:HG3	1.82	0.60
2:H:309:TRP:CZ2	2:H:416:SER:HB3	2.35	0.60
3:C:289:ILE:HG12	3:C:529:ILE:HD11	1.83	0.60
1:G:162:THR:O	1:G:163:LEU:HD22	2.02	0.60
3:I:135:PHE:CE1	3:I:240:TRP:HB3	2.37	0.60
3:L:697:LEU:HD21	3:L:735:MET:HB2	1.83	0.60
2:B:489:THR:HA	2:B:497:TYR:O	2.02	0.60
2:E:108:LEU:HA	2:E:111:MET:HE2	1.84	0.60
2:K:519:GLU:HA	2:K:559:TYR:HE2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:538:ASP:HB3	3:I:238:THR:HG22	1.82	0.60
1:J:208:THR:HG22	1:J:209:GLY:H	1.67	0.59
2:B:294:GLN:O	2:B:296:THR:N	2.34	0.59
1:J:379:VAL:HG23	2:K:366:THR:HB	1.84	0.59
3:C:384:LEU:HD23	3:C:478:ILE:HD11	1.83	0.59
1:G:379:VAL:HG21	2:H:364:LEU:HD13	1.84	0.59
1:D:193:GLN:HE21	1:D:203:GLU:HG3	1.68	0.59
2:H:712:SER:HB2	3:I:730:ASP:HB3	1.83	0.59
2:K:429:LYS:HB3	2:K:437:TRP:HB3	1.83	0.59
2:B:276:ASN:O	2:B:279:LYS:HB2	2.03	0.59
2:K:287:ARG:O	2:K:291:THR:OG1	2.20	0.59
3:F:317:LEU:HD12	3:F:496:VAL:N	2.16	0.59
2:H:438:TRP:HB2	2:H:449:LEU:HD11	1.83	0.59
3:I:143:ARG:HH12	3:I:366:VAL:HG11	1.68	0.59
2:H:613:TRP:O	2:H:621:GLN:NE2	2.36	0.59
2:K:65:GLN:OE1	2:K:346:ASN:ND2	2.35	0.59
3:C:380:ARG:HA	3:C:407:GLU:HG2	1.85	0.59
2:E:276:ASN:HB2	3:F:219:PRO:HG3	1.85	0.59
3:F:141:ILE:HD13	3:F:221:ALA:HA	1.83	0.59
3:F:255:VAL:HG22	3:F:527:LEU:HD11	1.85	0.59
2:H:664:HIS:HB2	3:I:57:ILE:HG23	1.84	0.59
1:J:260:PHE:HE1	1:J:265:PRO:HG3	1.67	0.59
3:F:366:VAL:HA	3:F:371:THR:HG22	1.85	0.58
2:K:626:ASN:HB3	3:L:99:TRP:HH2	1.66	0.58
2:H:396:LEU:HA	2:H:401:ALA:HA	1.85	0.58
2:K:489:THR:HA	2:K:497:TYR:O	2.02	0.58
3:L:135:PHE:CE1	3:L:240:TRP:HB3	2.38	0.58
1:D:450:VAL:HG13	1:D:641:LEU:HD22	1.84	0.58
2:E:514:VAL:HG22	2:E:516:GLY:H	1.68	0.58
1:G:292:ILE:HD13	1:G:309:LYS:HG3	1.85	0.58
1:J:150:PHE:HB3	1:J:179:ARG:HB2	1.85	0.58
1:A:573:ILE:HA	1:A:576:LYS:HG2	1.84	0.58
2:K:527:VAL:HG21	2:K:599:TYR:HE2	1.69	0.58
3:L:751:THR:HA	3:L:754:ILE:HG22	1.86	0.58
3:C:531:TYR:CD1	3:C:536:MET:HG2	2.39	0.58
3:F:317:LEU:CD1	3:F:496:VAL:H	2.13	0.58
3:C:230:GLU:HG3	3:C:231:VAL:HG13	1.85	0.58
3:I:593:SER:HB2	3:I:624:ALA:HB3	1.86	0.58
1:J:400:LEU:HD23	1:J:695:ILE:HG23	1.86	0.58
2:K:216:SER:HA	2:K:219:ILE:HD12	1.85	0.58
2:E:427:GLY:HA3	2:E:438:TRP:CE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:645:VAL:O	1:G:649:LEU:HD23	2.02	0.58
1:G:685:GLY:HA3	2:H:480:LYS:HG2	1.85	0.58
1:J:198:GLU:HG2	1:J:200:THR:HG22	1.86	0.58
2:H:623:ARG:HD3	3:I:103:GLY:H	1.68	0.58
1:A:479:ASP:N	1:A:479:ASP:OD1	2.36	0.58
3:C:748:GLN:N	3:C:748:GLN:OE1	2.37	0.58
1:G:530:PRO:HG3	1:G:542:VAL:HG11	1.86	0.58
1:J:202:GLU:OE2	2:K:115:GLN:NE2	2.36	0.58
1:D:198:GLU:HG2	1:D:200:THR:HG22	1.86	0.58
2:E:509:LEU:H	2:E:509:LEU:HD23	1.68	0.58
2:H:514:VAL:HG11	2:H:558:THR:HG21	1.85	0.58
2:H:576:LEU:HD12	3:I:97:THR:HG21	1.85	0.58
1:J:647:ASN:OD1	1:J:699:TRP:NE1	2.28	0.58
1:D:219:LEU:HD22	1:D:223:PHE:HB2	1.86	0.57
2:E:582:GLN:NE2	3:F:101:ARG:O	2.36	0.57
3:F:158:GLU:OE1	3:F:300:GLN:NE2	2.37	0.57
2:K:497:TYR:OH	3:L:458:MET:SD	2.53	0.57
2:B:626:ASN:HB3	3:C:99:TRP:HH2	1.68	0.57
1:G:208:THR:HG22	1:G:209:GLY:H	1.70	0.57
2:H:351:LEU:HD12	2:H:370:ALA:HB1	1.86	0.57
3:C:135:PHE:CE1	3:C:240:TRP:HB3	2.38	0.57
2:E:69:ILE:HB	2:E:316:ARG:HD2	1.86	0.57
1:G:114:GLU:HB3	1:G:116:ARG:HG2	1.85	0.57
2:H:129:TYR:HE2	2:H:223:THR:HG23	1.70	0.57
2:H:370:ALA:HA	2:H:373:LEU:HD13	1.86	0.57
1:J:269:ARG:HB2	1:J:691:GLU:HG2	1.86	0.57
1:J:576:LYS:NZ	3:L:42:ASN:OD1	2.32	0.57
1:A:279:ARG:NH1	1:A:652:SER:OG	2.37	0.57
1:A:606:ASP:HB2	3:C:135:PHE:CG	2.39	0.57
1:G:219:LEU:HD22	1:G:223:PHE:HB2	1.85	0.57
2:H:518:ASN:HD21	2:H:663:THR:HG23	1.69	0.57
2:K:712:SER:HB2	3:L:730:ASP:HB3	1.87	0.57
2:B:355:TYR:HB2	2:B:368:ILE:HD11	1.86	0.57
1:D:208:THR:HG22	1:D:209:GLY:H	1.69	0.57
3:F:128:GLY:HA2	3:F:246:PRO:HA	1.87	0.57
3:F:552:TRP:HD1	3:F:555:ARG:HH21	1.52	0.57
2:H:294:GLN:O	2:H:296:THR:N	2.38	0.57
3:I:429:ASN:OD1	3:I:432:HIS:ND1	2.38	0.57
2:K:151:ARG:NH2	3:L:18:GLU:OE1	2.36	0.57
2:B:712:SER:HB2	3:C:730:ASP:HB3	1.87	0.57
2:H:123:THR:HG22	2:H:143:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:241:TYR:HD2	2:K:86:ASP:HB2	1.68	0.57
2:K:438:TRP:CB	2:K:451:VAL:HG12	2.34	0.57
1:G:241:TYR:HD2	2:H:86:ASP:HB2	1.69	0.57
3:I:744:LEU:HD12	3:I:746:ASP:H	1.68	0.57
1:A:48:TYR:HE1	1:A:163:LEU:HG	1.69	0.57
1:D:285:MET:HB2	1:D:413:LYS:HG2	1.87	0.57
3:F:422:ASN:OD1	3:F:423:ARG:N	2.37	0.57
2:H:522:ASP:OD2	2:H:559:TYR:OH	2.23	0.57
1:J:362:LYS:HB3	1:J:367:LYS:HE3	1.87	0.57
1:G:266:ARG:NH2	1:G:684:GLU:OE2	2.38	0.57
1:G:461:LYS:O	1:G:465:ILE:HG12	2.05	0.57
1:A:478:ASP:O	1:A:508:ARG:NE	2.38	0.56
1:A:530:PRO:HG3	1:A:542:VAL:HG11	1.87	0.56
1:J:606:ASP:HB2	3:L:135:PHE:CG	2.40	0.56
2:B:315:PRO:HA	2:B:318:PHE:HD2	1.70	0.56
3:C:552:TRP:HD1	3:C:555:ARG:HH21	1.53	0.56
3:F:744:LEU:HD12	3:F:745:THR:N	2.20	0.56
3:I:320:SER:OG	3:I:321:SER:N	2.39	0.56
1:J:583:ARG:HH22	2:K:511:SER:HA	1.70	0.56
2:K:519:GLU:HA	2:K:559:TYR:CE2	2.40	0.56
2:K:572:ARG:HA	3:L:94:LEU:HD12	1.87	0.56
2:B:309:TRP:CZ2	2:B:416:SER:HB3	2.37	0.56
2:B:438:TRP:HB2	2:B:449:LEU:HD11	1.87	0.56
2:B:522:ASP:OD2	2:B:559:TYR:OH	2.19	0.56
3:C:358:ASP:OD1	3:C:359:GLY:N	2.38	0.56
1:D:84:ARG:HE	1:D:88:TRP:HE1	1.53	0.56
3:F:257:GLN:NE2	3:F:524:THR:O	2.35	0.56
2:H:527:VAL:HG21	2:H:599:TYR:HE2	1.69	0.56
3:C:362:GLU:HG2	3:C:375:ARG:HG2	1.87	0.56
1:G:438:ILE:HG23	1:G:608:THR:HG21	1.86	0.56
1:J:537:TRP:HB3	1:J:540:TYR:HB2	1.88	0.56
2:K:370:ALA:HA	2:K:373:LEU:HD13	1.87	0.56
3:C:56:PRO:HD2	3:C:93:PRO:HD3	1.87	0.56
3:C:266:ILE:HG22	3:C:280:LEU:HD22	1.88	0.56
1:G:82:ARG:HA	3:I:754:ILE:HD13	1.88	0.56
3:I:428:LEU:HB2	3:I:433:GLN:HE21	1.71	0.56
2:K:260:ARG:HE	2:K:414:MET:HE1	1.70	0.56
3:C:710:ILE:HD11	3:C:726:ILE:HA	1.88	0.56
1:J:154:GLU:OE2	1:J:168:ARG:HD2	2.05	0.56
1:A:669:VAL:HG22	1:A:716:ARG:HH11	1.71	0.55
2:B:182:THR:HA	2:B:209:LYS:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:VAL:HG11	2:B:558:THR:HG21	1.88	0.55
3:C:357:HIS:H	3:C:406:GLN:HE22	1.55	0.55
3:L:533:SER:H	3:L:537:TRP:HE1	1.54	0.55
3:I:146:ASP:HA	3:I:215:THR:HA	1.88	0.55
1:D:292:ILE:HD11	1:D:310:CYS:SG	2.47	0.55
2:E:177:GLU:HA	2:E:214:LYS:HB2	1.88	0.55
1:G:154:GLU:OE2	1:G:168:ARG:HD2	2.06	0.55
3:L:242:GLN:NE2	3:L:243:MET:O	2.38	0.55
2:B:269:SER:O	2:B:281:LYS:NZ	2.36	0.55
3:C:747:SER:OG	3:C:748:GLN:OE1	2.20	0.55
1:D:12:MET:HG2	3:F:751:THR:HG22	1.87	0.55
1:A:669:VAL:HG22	1:A:716:ARG:NH1	2.21	0.55
1:D:48:TYR:HE1	1:D:163:LEU:HG	1.71	0.55
2:E:25:THR:HG23	2:E:509:LEU:HD21	1.89	0.55
3:F:471:THR:OG1	3:F:472:GLU:OE1	2.21	0.55
1:G:591:GLN:HE21	1:G:640:LEU:HD22	1.72	0.55
2:H:316:ARG:NH2	2:H:345:SER:OG	2.39	0.55
1:J:573:ILE:HA	1:J:576:LYS:HG2	1.88	0.55
2:E:518:ASN:OD1	2:E:519:GLU:N	2.38	0.55
1:G:44:VAL:HG21	1:G:122:VAL:HG21	1.89	0.55
2:H:514:VAL:HG22	2:H:516:GLY:H	1.71	0.55
2:K:656:GLU:O	3:L:209:ARG:NH2	2.39	0.55
2:B:708:PRO:HB3	3:C:728:GLN:HG3	1.89	0.55
1:D:645:VAL:O	1:D:649:LEU:HD23	2.07	0.55
1:D:676:LEU:HD22	2:E:486:ARG:HB3	1.89	0.55
3:L:471:THR:OG1	3:L:472:GLU:OE1	2.22	0.55
3:L:550:TYR:CE1	3:L:620:PRO:HG3	2.42	0.55
1:A:193:GLN:NE2	1:A:203:GLU:OE2	2.40	0.55
2:B:160:SER:OG	2:B:165:ASP:OD2	2.18	0.55
3:L:577:PHE:HD2	3:L:623:ALA:HB2	1.70	0.55
2:B:514:VAL:HG22	2:B:516:GLY:H	1.72	0.54
3:C:520:GLU:O	3:C:521:THR:HG23	2.07	0.54
3:C:617:LYS:HE3	3:C:648:LEU:O	2.07	0.54
1:D:606:ASP:HB2	3:F:135:PHE:CG	2.42	0.54
1:G:215:ALA:HB1	1:G:226:LEU:HD13	1.88	0.54
3:I:223:GLY:HA2	3:I:228:TYR:HD2	1.72	0.54
1:J:549:LEU:H	1:J:549:LEU:HD23	1.72	0.54
1:A:375:ALA:HB1	1:A:376:PRO:HD2	1.89	0.54
1:A:407:ILE:HG13	1:A:702:LEU:HD22	1.89	0.54
3:C:293:ARG:CZ	3:C:743:ILE:HG21	2.38	0.54
2:E:708:PRO:HB3	3:F:728:GLN:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:408:ASP:O	3:L:412:LYS:HD2	2.08	0.54
2:B:569:GLN:HG3	2:B:573:SER:HB2	1.87	0.54
1:D:549:LEU:HD23	1:D:549:LEU:H	1.73	0.54
1:G:292:ILE:HD11	1:G:310:CYS:SG	2.48	0.54
2:H:283:ALA:HB2	2:H:501:PHE:HE2	1.73	0.54
1:A:463:VAL:HG11	1:A:582:ARG:HH11	1.72	0.54
1:A:645:VAL:O	1:A:649:LEU:HD23	2.07	0.54
1:J:624:SER:OG	1:J:625:PRO:HD3	2.08	0.54
2:K:315:PRO:HA	2:K:318:PHE:HD2	1.72	0.54
1:A:84:ARG:HE	1:A:88:TRP:HE1	1.55	0.54
1:A:208:THR:HG22	1:A:209:GLY:H	1.72	0.54
3:C:381:LEU:HB2	3:C:405:SER:HB2	1.88	0.54
3:L:72:GLU:OE2	3:L:101:ARG:NH1	2.41	0.54
1:A:324:LYS:HE3	1:A:537:TRP:O	2.07	0.54
1:A:674:ASP:OD2	2:B:498:ARG:NH2	2.39	0.54
1:G:407:ILE:HG13	1:G:702:LEU:HD22	1.90	0.54
1:G:583:ARG:HB3	2:H:25:THR:HG21	1.89	0.54
3:I:159:ALA:O	3:I:163:ILE:HG12	2.08	0.54
3:I:366:VAL:HA	3:I:371:THR:HG22	1.88	0.54
2:E:130:ASP:OD2	2:E:145:ASN:ND2	2.40	0.54
3:L:750:ALA:O	3:L:754:ILE:N	2.40	0.54
1:D:573:ILE:HA	1:D:576:LYS:HG2	1.90	0.54
2:H:125:GLY:HA3	2:H:249:ARG:HH21	1.72	0.54
3:I:423:ARG:NH2	3:I:519:SER:OG	2.40	0.54
1:J:48:TYR:CE1	1:J:163:LEU:HG	2.42	0.54
1:J:530:PRO:HG3	1:J:542:VAL:HG11	1.89	0.54
2:K:522:ASP:OD2	2:K:559:TYR:OH	2.26	0.54
3:L:268:ARG:HH12	3:L:522:GLN:HA	1.71	0.54
1:A:124:ARG:HD3	1:A:194:SER:HB3	1.89	0.53
3:I:365:MET:HE3	3:I:372:ALA:HB3	1.90	0.53
1:A:537:TRP:HB3	1:A:540:TYR:HB2	1.89	0.53
3:C:276:PRO:HG2	3:C:501:PHE:HA	1.90	0.53
1:G:479:ASP:OD1	1:G:479:ASP:N	2.40	0.53
2:K:518:ASN:HB3	2:K:521:ALA:HB3	1.89	0.53
3:C:563:GLN:HB3	3:C:571:LEU:HD12	1.89	0.53
1:D:389:ASP:OD2	2:E:361:SER:OG	2.20	0.53
1:D:543:LEU:HD12	1:D:563:LEU:HD23	1.91	0.53
2:H:355:TYR:HB2	2:H:368:ILE:HD11	1.90	0.53
2:H:528:THR:HA	2:H:531:LYS:HG2	1.90	0.53
1:A:292:ILE:HD11	1:A:310:CYS:SG	2.48	0.53
3:C:537:TRP:O	3:C:545:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:74:HIS:CD2	3:I:753:ARG:HD3	2.44	0.53
1:J:479:ASP:OD1	1:J:479:ASP:N	2.40	0.53
3:F:293:ARG:O	3:F:297:ILE:HD12	2.07	0.53
1:G:309:LYS:HA	1:G:312:ARG:HD3	1.90	0.53
3:I:148:ASN:ND2	3:I:212:VAL:O	2.41	0.53
1:J:7:GLN:HG3	3:L:299:ARG:HD3	1.91	0.53
1:J:299:GLY:O	1:J:300:GLU:HG3	2.08	0.53
1:D:479:ASP:N	1:D:479:ASP:OD1	2.42	0.53
1:D:664:LYS:HE2	2:E:481:LYS:HB3	1.91	0.53
2:E:438:TRP:HB2	2:E:449:LEU:HD11	1.90	0.53
3:C:738:LYS:O	3:C:739:ARG:HD2	2.09	0.53
1:D:461:LYS:O	1:D:465:ILE:HG12	2.09	0.53
2:E:389:ILE:O	2:E:393:ARG:HG2	2.09	0.53
1:G:293:GLU:HA	1:G:497:LYS:HA	1.91	0.53
1:G:596:ILE:HG12	1:G:611:PHE:CD2	2.43	0.53
2:B:68:PRO:HD2	2:B:314:ASN:HD21	1.73	0.53
3:F:429:ASN:OD1	3:F:432:HIS:ND1	2.40	0.53
1:J:664:LYS:HE2	2:K:481:LYS:HB3	1.91	0.53
2:K:509:LEU:HD23	2:K:509:LEU:H	1.73	0.53
3:L:532:SER:OG	3:L:555:ARG:NH2	2.42	0.53
1:D:560:PRO:HB2	1:D:562:PHE:HE1	1.73	0.53
3:F:550:TYR:CE1	3:F:620:PRO:HG3	2.44	0.53
1:J:189:ASP:OD1	1:J:190:SER:N	2.42	0.53
1:J:619:TRP:CD1	2:K:11:LYS:HD3	2.44	0.53
2:K:531:LYS:HB3	2:K:604:LEU:HB3	1.90	0.53
3:L:534:SER:HB3	3:L:576:GLU:HG3	1.90	0.53
1:D:345:LEU:HD11	1:D:503:PHE:HE2	1.74	0.53
2:E:63:ALA:HB1	2:E:402:SER:HB3	1.90	0.53
2:E:627:PRO:HB3	3:F:198:ILE:HG23	1.91	0.53
3:F:358:ASP:OD1	3:F:359:GLY:N	2.42	0.53
3:L:283:MET:O	3:L:287:THR:OG1	2.20	0.53
1:A:288:LEU:HG	1:A:527:LEU:HG	1.91	0.52
3:F:320:SER:HB2	3:F:494:VAL:HG23	1.91	0.52
3:I:258:SER:HB3	3:I:529:ILE:HD11	1.91	0.52
3:I:384:LEU:HB3	3:I:478:ILE:HD12	1.91	0.52
1:J:461:LYS:O	1:J:465:ILE:HG12	2.09	0.52
2:K:351:LEU:HD12	2:K:370:ALA:HB1	1.91	0.52
2:H:518:ASN:OD1	2:H:519:GLU:N	2.40	0.52
2:H:622:GLY:HA3	3:I:105:MET:SD	2.50	0.52
2:K:160:SER:OG	2:K:165:ASP:OD2	2.23	0.52
2:K:371:GLU:HG3	2:K:399:GLY:HA3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:358:ASP:OD1	3:L:359:GLY:N	2.42	0.52
1:A:198:GLU:HG2	1:A:200:THR:HG22	1.91	0.52
2:H:509:LEU:H	2:H:509:LEU:HD23	1.73	0.52
2:K:292:ASN:HD22	2:K:297:GLU:HB3	1.73	0.52
3:L:56:PRO:HD2	3:L:93:PRO:HD3	1.91	0.52
1:G:154:GLU:OE2	1:G:168:ARG:NH1	2.34	0.52
2:H:489:THR:HA	2:H:497:TYR:O	2.08	0.52
3:I:358:ASP:OD1	3:I:359:GLY:N	2.42	0.52
1:J:8:CYS:O	1:J:174:ARG:NH2	2.42	0.52
1:A:342:LEU:O	1:A:346:GLN:NE2	2.41	0.52
2:E:396:LEU:HA	2:E:401:ALA:HA	1.92	0.52
3:F:550:TYR:HE1	3:F:620:PRO:HG3	1.75	0.52
1:G:193:GLN:OE1	1:G:193:GLN:N	2.43	0.52
1:G:366:LEU:HD11	1:G:505:ILE:HG21	1.92	0.52
2:K:389:ILE:O	2:K:393:ARG:HG2	2.10	0.52
3:L:560:VAL:HG13	3:L:571:LEU:HD11	1.91	0.52
3:C:268:ARG:HH21	3:C:519:SER:HA	1.75	0.52
1:D:125:ARG:HB3	1:D:195:GLU:HG3	1.92	0.52
1:D:212:ARG:HG3	1:D:226:LEU:HD21	1.92	0.52
1:D:241:TYR:HD2	2:E:86:ASP:HB2	1.74	0.52
1:G:189:ASP:OD1	1:G:190:SER:N	2.42	0.52
2:H:519:GLU:HA	2:H:559:TYR:HE2	1.75	0.52
2:K:514:VAL:HG22	2:K:516:GLY:H	1.74	0.52
3:C:379:ARG:HG2	3:C:406:GLN:HB3	1.91	0.52
3:C:737:ARG:O	3:C:737:ARG:NH2	2.37	0.52
3:I:56:PRO:HD2	3:I:93:PRO:HD3	1.91	0.52
1:A:461:LYS:O	1:A:465:ILE:HG12	2.10	0.52
3:C:286:SER:OG	3:C:533:SER:HB3	2.10	0.52
1:D:114:GLU:HB3	1:D:116:ARG:HG2	1.92	0.52
1:G:591:GLN:NE2	1:G:640:LEU:HD22	2.25	0.52
1:J:219:LEU:HD22	1:J:223:PHE:HB2	1.91	0.52
1:J:284:LEU:HB2	1:J:410:GLU:OE2	2.09	0.52
1:A:583:ARG:HH22	2:B:511:SER:HA	1.74	0.52
1:A:606:ASP:OD1	1:A:607:MET:N	2.43	0.52
2:B:527:VAL:HG21	2:B:599:TYR:HE2	1.74	0.52
1:D:26:GLU:HG3	1:D:34:LYS:NZ	2.25	0.52
2:E:287:ARG:O	2:E:291:THR:OG1	2.26	0.52
1:G:306:ASP:HA	1:G:309:LYS:HG2	1.92	0.52
2:H:114:VAL:HG12	2:H:254:PHE:CD1	2.45	0.52
1:G:284:LEU:HB2	1:G:410:GLU:OE2	2.09	0.52
2:K:576:LEU:HD12	3:L:97:THR:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:385:ILE:HG23	3:L:460:MET:HE1	1.92	0.52
1:A:189:ASP:OD1	1:A:190:SER:N	2.43	0.51
2:E:56:THR:HG23	2:E:65:GLN:HB2	1.92	0.51
3:I:124:ARG:NH2	3:I:149:PRO:HB2	2.25	0.51
3:I:163:ILE:O	3:I:167:VAL:HG12	2.10	0.51
3:I:276:PRO:HB2	3:I:502:LEU:HG	1.92	0.51
1:J:44:VAL:HG21	1:J:122:VAL:HG21	1.92	0.51
1:J:84:ARG:HE	1:J:88:TRP:HE1	1.58	0.51
3:I:543:GLU:OE2	3:I:641:ARG:NE	2.43	0.51
1:J:75:ARG:HA	1:J:112:TYR:HB2	1.93	0.51
1:A:260:PHE:CE1	1:A:265:PRO:HG3	2.43	0.51
1:A:664:LYS:HE2	2:B:481:LYS:HB3	1.93	0.51
3:C:542:PRO:HB2	3:C:640:VAL:HG12	1.92	0.51
1:G:664:LYS:O	1:G:668:VAL:HG23	2.11	0.51
2:H:598:LEU:HD21	2:H:612:LYS:HE2	1.93	0.51
1:J:382:ASP:HA	1:J:385:ARG:NH2	2.25	0.51
1:J:435:ILE:H	1:J:435:ILE:HD12	1.74	0.51
1:D:382:ASP:O	1:D:385:ARG:NH1	2.43	0.51
2:H:374:ALA:O	2:H:393:ARG:NH2	2.33	0.51
3:L:260:ILE:O	3:L:264:ARG:HG2	2.10	0.51
1:A:1:MET:HB2	1:A:187:LEU:HD22	1.91	0.51
2:B:693:CYS:SG	3:C:31:ILE:HG23	2.50	0.51
3:F:146:ASP:HA	3:F:215:THR:HA	1.91	0.51
3:F:153:ASP:N	3:F:252:ASN:HD21	2.09	0.51
2:H:434:THR:HG22	2:H:435:THR:H	1.76	0.51
3:L:182:GLN:OE1	3:L:292:THR:OG1	2.29	0.51
1:A:194:SER:HA	1:A:199:GLU:HA	1.91	0.51
2:E:351:LEU:HD12	2:E:370:ALA:HB1	1.91	0.51
2:K:579:LEU:HD21	3:L:101:ARG:HA	1.91	0.51
3:L:154:LEU:HD21	3:L:182:GLN:HG2	1.92	0.51
3:L:213:ARG:CZ	3:L:302:PRO:HD3	2.41	0.51
1:A:114:GLU:HB3	1:A:116:ARG:HG2	1.93	0.51
1:D:218:SER:O	2:E:316:ARG:NH1	2.43	0.51
1:D:246:LEU:O	2:E:468:ARG:NH2	2.44	0.51
2:E:58:ASN:ND2	2:E:61:THR:OG1	2.44	0.51
2:E:77:ASN:ND2	2:E:479:LYS:HD2	2.26	0.51
2:E:527:VAL:HG11	2:E:599:TYR:CD2	2.46	0.51
1:G:591:GLN:HE21	2:H:20:THR:HG22	1.75	0.51
3:I:532:SER:OG	3:I:555:ARG:NH2	2.44	0.51
3:L:387:SER:OG	3:L:485:VAL:N	2.44	0.51
3:C:471:THR:OG1	3:C:472:GLU:OE1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:268:ARG:HH21	3:L:519:SER:HA	1.75	0.51
3:L:387:SER:HB3	3:L:485:VAL:HG23	1.92	0.51
3:L:593:SER:HB2	3:L:624:ALA:HB3	1.93	0.51
1:A:439:ALA:HB2	2:B:541:PRO:HB2	1.92	0.51
1:D:108:ASP:HB2	1:D:119:GLU:HA	1.93	0.51
3:F:408:ASP:O	3:F:412:LYS:HD2	2.10	0.51
1:G:76:PHE:HA	1:G:110:TYR:O	2.10	0.51
3:I:189:LYS:O	3:I:193:LEU:HG	2.10	0.51
2:K:620:TYR:CZ	2:K:624:LEU:HD12	2.45	0.51
2:K:737:LYS:H	2:K:737:LYS:HD3	1.76	0.51
3:C:427:ARG:NE	1:D:101:GLU:OE1	2.38	0.51
2:E:548:LEU:HD11	2:E:599:TYR:HB3	1.92	0.51
3:F:428:LEU:HB2	3:F:433:GLN:HE21	1.76	0.51
2:H:572:ARG:HG2	2:H:576:LEU:HD13	1.93	0.51
3:I:285:HIS:ND1	3:I:295:VAL:HG11	2.26	0.51
3:I:319:ILE:HA	3:I:493:ARG:HD3	1.93	0.51
2:K:528:THR:HA	2:K:531:LYS:HG2	1.93	0.51
2:K:622:GLY:HA3	3:L:105:MET:SD	2.50	0.51
1:D:390:LEU:HB3	2:E:380:TYR:HE1	1.75	0.50
2:E:590:LEU:HD23	2:E:612:LYS:HD2	1.93	0.50
3:F:384:LEU:HB3	3:F:478:ILE:HD12	1.94	0.50
1:J:589:LEU:HD23	2:K:543:THR:HA	1.94	0.50
2:K:631:PHE:CE2	3:L:96:VAL:HA	2.46	0.50
2:B:619:ASP:HB3	2:B:623:ARG:NH1	2.26	0.50
3:F:398:ILE:HD11	3:F:478:ILE:HD11	1.92	0.50
3:I:55:TYR:HD1	3:I:92:SER:HB2	1.76	0.50
3:L:159:ALA:O	3:L:163:ILE:HG12	2.11	0.50
3:L:213:ARG:NH1	3:L:300:GLN:O	2.25	0.50
1:D:433:ALA:HB3	1:D:436:GLU:HB2	1.94	0.50
2:E:91:ALA:HA	2:E:426:LEU:HD21	1.93	0.50
3:F:547:VAL:HG12	3:F:667:ILE:HB	1.92	0.50
1:J:193:GLN:N	1:J:193:GLN:OE1	2.44	0.50
2:K:434:THR:HG22	2:K:435:THR:H	1.76	0.50
1:A:7:GLN:NE2	3:C:300:GLN:OE1	2.44	0.50
2:B:658:ASP:OD1	2:B:659:ALA:N	2.44	0.50
3:C:159:ALA:O	3:C:163:ILE:HG12	2.11	0.50
3:C:223:GLY:HA2	3:C:228:TYR:HD2	1.75	0.50
1:D:189:ASP:OD1	1:D:190:SER:N	2.44	0.50
3:F:260:ILE:O	3:F:264:ARG:HG2	2.11	0.50
1:A:8:CYS:O	1:A:174:ARG:NH2	2.43	0.50
1:A:624:SER:OG	1:A:625:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:322:SER:HB3	3:F:513:LEU:HD11	1.94	0.50
3:F:748:GLN:O	3:F:751:THR:OG1	2.22	0.50
2:B:434:THR:HG22	2:B:435:THR:H	1.77	0.50
3:C:140:LYS:HB3	3:C:219:PRO:HB2	1.94	0.50
3:I:755:ARG:NH1	3:L:756:MET:O	2.45	0.50
2:B:494:SER:HB2	2:B:505:PHE:HA	1.94	0.50
3:C:744:LEU:HD12	3:C:746:ASP:H	1.77	0.50
2:H:519:GLU:HB2	2:H:662:THR:O	2.12	0.50
1:A:685:GLY:HA3	2:B:480:LYS:HG2	1.93	0.50
3:C:459:GLY:O	3:C:482:LYS:HG2	2.12	0.50
1:D:588:SER:O	1:D:591:GLN:HG2	2.11	0.50
2:E:276:ASN:O	2:E:279:LYS:HB2	2.11	0.50
2:H:68:PRO:HD2	2:H:314:ASN:HD21	1.76	0.50
2:E:434:THR:HG22	2:E:435:THR:H	1.76	0.49
3:I:55:TYR:CD1	3:I:92:SER:HB2	2.47	0.49
2:K:654:SER:OG	2:K:655:MET:N	2.44	0.49
1:A:687:TYR:O	1:A:691:GLU:HG2	2.12	0.49
2:B:63:ALA:HB1	2:B:402:SER:HB3	1.93	0.49
3:F:72:GLU:OE2	3:F:101:ARG:NH1	2.44	0.49
3:F:162:VAL:HG13	3:F:186:THR:HG23	1.94	0.49
1:G:400:LEU:HD23	1:G:695:ILE:HG23	1.93	0.49
2:H:626:ASN:ND2	3:I:106:THR:OG1	2.45	0.49
2:H:664:HIS:CG	3:I:57:ILE:HD12	2.48	0.49
2:K:658:ASP:OD1	2:K:659:ALA:N	2.45	0.49
1:A:664:LYS:O	1:A:668:VAL:HG23	2.12	0.49
3:C:547:VAL:HG12	3:C:667:ILE:HB	1.93	0.49
2:E:518:ASN:OD1	2:E:663:THR:HA	2.12	0.49
2:E:690:GLN:HG3	3:F:35:THR:HG23	1.93	0.49
3:F:111:TYR:O	3:F:113:LYS:N	2.43	0.49
1:J:597:GLU:O	1:J:601:SER:N	2.46	0.49
3:L:754:ILE:HG23	3:L:755:ARG:HG2	1.93	0.49
1:A:360:MET:N	1:A:480:PHE:O	2.43	0.49
3:C:550:TYR:HE1	3:C:620:PRO:HG3	1.77	0.49
3:F:617:LYS:HE3	3:F:648:LEU:O	2.13	0.49
1:G:684:GLU:O	1:G:688:GLU:HG2	2.12	0.49
2:K:25:THR:HG23	2:K:509:LEU:HD21	1.93	0.49
2:K:215:ARG:O	2:K:219:ILE:HG13	2.13	0.49
1:A:338:TRP:HE1	1:A:545:ILE:HD11	1.78	0.49
3:C:422:ASN:OD1	3:C:423:ARG:N	2.45	0.49
1:D:305:TYR:O	1:D:308:ILE:HG13	2.11	0.49
2:E:689:TYR:HD2	3:F:34:TYR:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:324:LYS:NZ	1:J:537:TRP:O	2.33	0.49
1:A:529:ASP:HB2	1:A:532:LEU:HG	1.95	0.49
3:F:251:ARG:O	3:F:255:VAL:HG23	2.12	0.49
3:F:542:PRO:HB2	3:F:640:VAL:HG12	1.95	0.49
1:G:99:GLY:HA3	3:L:575:MET:HG3	1.94	0.49
1:G:241:TYR:CD2	2:H:86:ASP:HB2	2.48	0.49
1:G:548:MET:O	1:G:558:SER:HA	2.12	0.49
1:J:305:TYR:O	1:J:308:ILE:HG13	2.12	0.49
3:F:618:LEU:HD21	3:F:649:VAL:HG12	1.94	0.49
1:G:670:GLN:OE1	1:G:673:ARG:NH2	2.46	0.49
1:A:209:GLY:C	1:A:211:MET:H	2.16	0.49
1:A:529:ASP:HB3	1:A:531:ARG:HG2	1.94	0.49
2:B:326:THR:HB	2:B:334:ARG:HG2	1.93	0.49
1:D:125:ARG:HD3	1:D:195:GLU:HG3	1.95	0.49
1:D:445:TYR:HD2	1:D:612:PHE:HD2	1.58	0.49
2:E:712:SER:OG	3:F:730:ASP:HB3	2.13	0.49
2:H:658:ASP:OD1	2:H:659:ALA:N	2.46	0.49
3:I:28:MET:HA	3:I:31:ILE:HG22	1.95	0.49
3:I:500:ARG:NH2	1:J:92:ASN:OD1	2.45	0.49
2:K:68:PRO:HD2	2:K:314:ASN:HD21	1.77	0.49
1:D:189:ASP:HB2	2:E:162:ARG:HH12	1.78	0.49
2:E:519:GLU:HA	2:E:559:TYR:HE2	1.77	0.49
1:G:336:LEU:HB3	1:G:365:GLN:HG2	1.94	0.49
1:J:685:GLY:HA3	2:K:480:LYS:HG2	1.93	0.49
2:B:120:ASP:OD1	3:C:30:ILE:HA	2.13	0.49
3:F:131:GLY:H	3:F:242:GLN:NE2	2.10	0.49
1:G:260:PHE:CE1	1:G:265:PRO:HG3	2.48	0.49
2:H:287:ARG:HH12	3:I:485:VAL:HA	1.78	0.49
1:J:180:GLN:HE22	3:L:174:ALA:H	1.61	0.49
2:B:374:ALA:O	2:B:393:ARG:NH2	2.46	0.48
3:C:533:SER:OG	3:C:534:SER:N	2.45	0.48
1:D:239:ASN:O	1:D:239:ASN:ND2	2.41	0.48
1:D:582:ARG:H	1:D:582:ARG:HD2	1.77	0.48
2:E:290:MET:HG3	3:F:457:VAL:HG21	1.95	0.48
1:G:193:GLN:NE2	1:G:203:GLU:OE2	2.46	0.48
1:G:537:TRP:HB3	1:G:540:TYR:HB2	1.95	0.48
2:H:223:THR:HA	2:H:348:MET:O	2.13	0.48
1:A:588:SER:O	1:A:591:GLN:HG2	2.14	0.48
3:C:721:LYS:HG2	3:C:735:MET:HG3	1.94	0.48
1:D:664:LYS:O	1:D:668:VAL:HG23	2.12	0.48
2:E:560:ARG:HH21	3:F:52:ALA:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:530:PRO:HB3	1:G:542:VAL:HG21	1.95	0.48
1:G:598:ALA:HB1	2:H:16:ASN:HD22	1.78	0.48
2:H:494:SER:HB2	2:H:505:PHE:HA	1.95	0.48
1:J:288:LEU:HG	1:J:527:LEU:HG	1.95	0.48
2:B:114:VAL:HG12	2:B:254:PHE:CD1	2.48	0.48
2:B:708:PRO:HG2	3:C:28:MET:SD	2.54	0.48
3:F:131:GLY:H	3:F:242:GLN:HE22	1.61	0.48
2:H:129:TYR:CE2	2:H:223:THR:HG23	2.48	0.48
1:J:284:LEU:HB3	1:J:458:TYR:CZ	2.48	0.48
1:A:239:ASN:O	1:A:239:ASN:ND2	2.40	0.48
2:E:620:TYR:CZ	2:E:624:LEU:HD12	2.48	0.48
1:G:78:ILE:HA	1:G:109:LEU:HD12	1.94	0.48
3:I:283:MET:O	3:I:287:THR:OG1	2.23	0.48
2:K:514:VAL:HG11	2:K:558:THR:HG21	1.96	0.48
2:H:258:LEU:HD22	2:H:337:LEU:HD13	1.96	0.48
3:C:531:TYR:CG	3:C:536:MET:HG2	2.49	0.48
3:F:534:SER:H	3:F:537:TRP:HE1	1.60	0.48
3:L:318:ARG:HB3	3:L:493:ARG:HB3	1.95	0.48
2:B:370:ALA:HA	2:B:373:LEU:HD13	1.96	0.48
2:E:576:LEU:HD12	3:F:97:THR:HG21	1.95	0.48
1:G:362:LYS:HG3	1:G:480:PHE:CE2	2.49	0.48
1:G:624:SER:OG	1:G:625:PRO:HD3	2.12	0.48
2:H:110:THR:O	2:H:114:VAL:HG13	2.14	0.48
3:I:408:ASP:HB3	3:I:412:LYS:NZ	2.28	0.48
1:A:241:TYR:HD2	2:B:86:ASP:HB2	1.78	0.48
1:A:305:TYR:O	1:A:308:ILE:HG13	2.14	0.48
2:B:558:THR:HG23	3:C:48:LYS:HG2	1.95	0.48
3:C:142:ARG:HB3	3:C:217:PHE:CE1	2.49	0.48
3:C:227:VAL:HB	3:C:246:PRO:HG2	1.96	0.48
3:F:312:LYS:HD3	3:F:318:ARG:HH11	1.77	0.48
1:J:382:ASP:HA	1:J:385:ARG:HH21	1.78	0.48
1:J:624:SER:HB3	2:K:1:MET:HA	1.96	0.48
3:C:398:ILE:HD11	3:C:478:ILE:CD1	2.42	0.48
1:G:664:LYS:HE2	2:H:481:LYS:HB3	1.96	0.48
1:J:299:GLY:HA2	2:K:569:GLN:O	2.13	0.48
2:E:287:ARG:HH12	3:F:485:VAL:HA	1.78	0.48
3:F:739:ARG:HA	3:F:739:ARG:HD2	1.56	0.48
1:G:305:TYR:O	1:G:308:ILE:HG13	2.14	0.48
1:G:318:LYS:NZ	1:G:544:GLU:OE2	2.47	0.48
1:J:684:GLU:O	1:J:688:GLU:HG2	2.14	0.48
1:A:438:ILE:HG23	1:A:608:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:LEU:HD23	1:A:678:PRO:HD2	1.96	0.47
3:C:384:LEU:HB3	3:C:478:ILE:HD12	1.96	0.47
1:J:360:MET:N	1:J:480:PHE:O	2.43	0.47
1:A:444:ASN:OD1	1:A:445:TYR:N	2.46	0.47
1:D:135:ALA:O	1:D:139:LYS:HB2	2.14	0.47
3:F:317:LEU:HD12	3:F:495:VAL:HA	1.96	0.47
1:G:439:ALA:HB2	2:H:541:PRO:HB2	1.96	0.47
3:I:315:MET:SD	3:I:315:MET:N	2.87	0.47
3:I:562:ILE:HD12	3:I:563:GLN:N	2.29	0.47
1:J:349:GLU:N	1:J:349:GLU:OE1	2.47	0.47
2:K:612:LYS:O	2:K:616:MET:HG3	2.13	0.47
3:L:366:VAL:HA	3:L:371:THR:HG22	1.95	0.47
1:D:597:GLU:O	1:D:601:SER:N	2.47	0.47
1:D:612:PHE:CD1	1:D:633:ILE:HG21	2.49	0.47
3:F:163:ILE:O	3:F:167:VAL:HG12	2.13	0.47
1:G:606:ASP:HB3	3:I:135:PHE:CD1	2.49	0.47
3:I:586:LYS:HG2	3:I:589:ARG:NH2	2.29	0.47
1:A:583:ARG:HD3	2:B:25:THR:HG21	1.95	0.47
1:D:523:MET:HB3	1:D:563:LEU:HD11	1.97	0.47
1:G:180:GLN:NE2	3:I:175:ARG:HG3	2.28	0.47
2:H:569:GLN:HG3	2:H:573:SER:HB2	1.97	0.47
3:L:326:GLY:HA2	3:L:435:LEU:HD21	1.96	0.47
1:A:6:ARG:HD3	3:C:316:GLY:O	2.13	0.47
1:D:150:PHE:HB3	1:D:179:ARG:HB2	1.96	0.47
3:F:563:GLN:HB3	3:F:571:LEU:HD12	1.97	0.47
3:C:409:CYS:SG	3:C:449:TRP:HA	2.55	0.47
2:E:121:ARG:HG2	2:E:253:TYR:CZ	2.50	0.47
1:G:681:PHE:CZ	2:H:484:ILE:HD11	2.49	0.47
2:K:548:LEU:HD11	2:K:599:TYR:HB3	1.95	0.47
1:A:130:TYR:HD2	1:A:147:ILE:HD13	1.80	0.47
1:A:193:GLN:N	1:A:193:GLN:OE1	2.47	0.47
1:A:306:ASP:HA	1:A:309:LYS:HG2	1.97	0.47
1:A:681:PHE:CZ	2:B:484:ILE:HD11	2.49	0.47
1:D:12:MET:HG2	3:F:751:THR:CG2	2.45	0.47
1:D:261:LEU:O	1:D:265:PRO:HD3	2.14	0.47
1:G:420:SER:HB3	1:G:489:CYS:HB2	1.97	0.47
1:G:573:ILE:HA	1:G:576:LYS:HG2	1.95	0.47
3:I:409:CYS:SG	3:I:449:TRP:HA	2.54	0.47
3:I:662:THR:HG22	3:I:664:ARG:HG2	1.96	0.47
1:J:207:ILE:HG22	1:J:212:ARG:HB2	1.96	0.47
1:J:630:ASP:N	1:J:630:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:542:PRO:HB2	3:L:640:VAL:HG12	1.95	0.47
3:L:617:LYS:HE3	3:L:648:LEU:O	2.13	0.47
3:C:280:LEU:HD11	3:C:311:CYS:HA	1.97	0.47
1:D:124:ARG:HD3	1:D:194:SER:HB3	1.97	0.47
1:D:589:LEU:HD23	2:E:543:THR:HA	1.95	0.47
1:G:49:SER:HB3	1:G:109:LEU:HD11	1.97	0.47
1:G:217:GLN:NE2	2:H:58:ASN:HA	2.30	0.47
3:I:111:TYR:O	3:I:113:LYS:N	2.42	0.47
3:C:276:PRO:HB2	3:C:502:LEU:HG	1.96	0.47
2:E:453:ALA:HB3	2:E:459:ILE:HG12	1.97	0.47
3:F:331:LYS:HE3	3:F:489:SER:HA	1.97	0.47
3:I:1:MET:HA	3:I:4:ILE:HG22	1.96	0.47
1:J:78:ILE:HA	1:J:109:LEU:HD12	1.97	0.47
1:J:189:ASP:HB2	2:K:162:ARG:HH12	1.80	0.47
1:J:216:ASP:OD1	1:J:226:LEU:N	2.45	0.47
2:K:627:PRO:HB3	3:L:198:ILE:HG23	1.96	0.47
1:A:543:LEU:HD12	1:A:563:LEU:HD23	1.97	0.47
2:B:572:ARG:HG2	2:B:576:LEU:HD13	1.96	0.47
3:C:371:THR:HG21	3:C:487:GLU:HG2	1.96	0.47
3:C:395:ALA:O	3:C:398:ILE:HG22	2.15	0.47
2:H:319:LEU:HB2	2:H:341:PRO:HB2	1.96	0.47
2:H:619:ASP:HB3	2:H:623:ARG:NH1	2.30	0.47
3:I:471:THR:OG1	3:I:472:GLU:OE1	2.26	0.47
2:K:54:LYS:HG3	2:K:68:PRO:HA	1.97	0.47
2:B:108:LEU:HA	2:B:111:MET:HE2	1.98	0.46
2:E:123:THR:HG22	2:E:143:LEU:HD13	1.97	0.46
2:H:308:LYS:HD3	2:H:308:LYS:HA	1.64	0.46
2:H:518:ASN:OD1	2:H:663:THR:HA	2.14	0.46
3:I:306:GLN:HG2	3:I:307:ALA:N	2.30	0.46
1:J:664:LYS:O	1:J:668:VAL:HG23	2.15	0.46
2:K:223:THR:HA	2:K:348:MET:O	2.15	0.46
3:L:562:ILE:HD12	3:L:563:GLN:N	2.30	0.46
2:B:518:ASN:HB3	2:B:521:ALA:HB3	1.96	0.46
3:C:189:LYS:O	3:C:193:LEU:HG	2.14	0.46
1:D:44:VAL:HG21	1:D:122:VAL:HG21	1.97	0.46
3:F:135:PHE:CE1	3:F:240:TRP:HB3	2.50	0.46
2:H:527:VAL:HG11	2:H:599:TYR:CD2	2.51	0.46
2:K:627:PRO:HG2	3:L:108:THR:HG21	1.98	0.46
1:A:349:GLU:OE1	1:A:349:GLU:N	2.48	0.46
2:B:351:LEU:HD12	2:B:370:ALA:HB1	1.96	0.46
3:C:163:ILE:O	3:C:167:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:369:ARG:HD2	3:C:393:SER:OG	2.15	0.46
3:C:581:GLN:HG2	3:C:589:ARG:HD3	1.96	0.46
1:D:64:GLU:HG3	3:F:739:ARG:HD3	1.97	0.46
3:F:531:TYR:CD1	3:F:536:MET:HG2	2.50	0.46
2:H:690:GLN:NE2	3:I:35:THR:HG22	2.30	0.46
3:I:462:GLY:HA3	3:I:474:SER:HB3	1.96	0.46
3:I:537:TRP:HE3	3:I:579:PRO:HG3	1.79	0.46
3:I:540:ASN:HB2	3:I:544:SER:HB3	1.96	0.46
1:J:455:ALA:HB1	1:J:645:VAL:HG21	1.97	0.46
3:L:659:ASN:HD22	3:L:660:LYS:N	2.14	0.46
1:A:670:GLN:OE1	1:A:673:ARG:NH2	2.49	0.46
2:B:623:ARG:HD3	3:C:103:GLY:H	1.79	0.46
1:D:26:GLU:HG3	1:D:34:LYS:HZ3	1.81	0.46
1:D:429:GLY:HA3	2:E:598:LEU:HA	1.97	0.46
3:F:586:LYS:HG2	3:F:589:ARG:NH2	2.30	0.46
1:G:11:PRO:HG3	3:I:285:HIS:CE1	2.51	0.46
2:H:291:THR:HG21	3:I:460:MET:HG3	1.98	0.46
2:H:716:GLU:HB2	2:H:754:ARG:HH12	1.80	0.46
1:A:179:ARG:HG3	1:A:188:TRP:CH2	2.50	0.46
1:A:591:GLN:HE21	1:A:640:LEU:HB3	1.81	0.46
2:H:276:ASN:O	2:H:279:LYS:HB2	2.15	0.46
3:I:589:ARG:HG2	3:I:624:ALA:HB1	1.98	0.46
1:A:274:PRO:HG2	1:A:401:ARG:HG2	1.96	0.46
2:B:122:LEU:HD11	2:B:249:ARG:HB3	1.97	0.46
2:B:725:ASP:HA	2:B:728:ILE:HG12	1.98	0.46
3:C:251:ARG:O	3:C:255:VAL:HG23	2.15	0.46
3:F:124:ARG:NH2	3:F:149:PRO:HB2	2.30	0.46
1:G:523:MET:HB3	1:G:563:LEU:HD11	1.98	0.46
2:H:149:VAL:HG21	2:H:181:ILE:HG12	1.98	0.46
3:L:189:LYS:O	3:L:193:LEU:HG	2.15	0.46
1:A:597:GLU:O	1:A:601:SER:N	2.49	0.46
1:D:308:ILE:O	1:D:312:ARG:HG2	2.16	0.46
1:D:591:GLN:HG3	1:D:640:LEU:HD13	1.97	0.46
2:E:492:PHE:O	2:E:495:PHE:HB2	2.15	0.46
2:E:578:LYS:HE2	3:F:72:GLU:OE2	2.16	0.46
1:G:434:PRO:HD2	3:I:242:GLN:OE1	2.16	0.46
1:J:14:VAL:HG13	1:J:35:PHE:HZ	1.81	0.46
2:B:36:THR:HG21	2:B:354:GLY:H	1.81	0.46
2:B:287:ARG:O	2:B:291:THR:OG1	2.28	0.46
2:B:689:TYR:CG	3:C:34:TYR:HD2	2.34	0.46
2:E:519:GLU:HG3	2:E:664:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:584:ARG:HH21	2:E:617:ASP:HB3	1.80	0.46
3:F:296:ASP:O	3:F:300:GLN:HG3	2.16	0.46
3:F:752:LYS:HB2	3:F:752:LYS:HE3	1.70	0.46
3:I:220:VAL:HG12	3:I:221:ALA:H	1.81	0.46
1:J:674:ASP:OD2	2:K:498:ARG:NH2	2.47	0.46
2:K:219:ILE:HG23	2:K:348:MET:HG3	1.97	0.46
2:B:381:PHE:HB2	2:B:386:ARG:HG3	1.97	0.46
2:B:605:HIS:HD2	3:C:233:HIS:CE1	2.34	0.46
1:D:439:ALA:HB2	2:E:541:PRO:HB2	1.97	0.46
2:E:420:GLY:HA3	2:E:442:GLN:HG2	1.97	0.46
1:G:341:VAL:HA	1:G:360:MET:HE1	1.97	0.46
1:G:376:PRO:HG2	2:H:365:ARG:HH21	1.81	0.46
2:H:80:SER:HB2	2:H:82:TYR:CD2	2.50	0.46
2:H:590:LEU:HD23	2:H:612:LYS:HD2	1.96	0.46
1:J:220:PRO:HG2	1:J:223:PHE:HE2	1.81	0.46
2:K:182:THR:HG22	2:K:183:THR:H	1.80	0.46
3:L:27:HIS:O	3:L:30:ILE:HG12	2.16	0.46
1:D:545:ILE:HD12	1:D:545:ILE:HA	1.78	0.46
2:E:490:PHE:HE1	2:E:497:TYR:HD2	1.62	0.46
2:E:602:ARG:O	3:F:125:LEU:HD21	2.15	0.46
2:E:658:ASP:OD1	2:E:659:ALA:N	2.49	0.46
3:F:659:ASN:HD22	3:F:660:LYS:N	2.14	0.46
2:K:138:PRO:HG2	2:K:141:THR:HB	1.98	0.46
2:K:271:LEU:HD13	2:K:414:MET:HG2	1.97	0.46
2:K:730:PHE:CE1	2:K:737:LYS:HG3	2.50	0.46
2:K:738:GLU:CD	2:K:738:GLU:H	2.19	0.46
3:L:163:ILE:O	3:L:167:VAL:HG12	2.15	0.46
3:C:612:THR:O	3:C:616:ILE:HG12	2.15	0.45
1:D:427:GLU:OE1	2:E:563:ARG:NH1	2.49	0.45
2:E:424:LEU:HD12	2:E:442:GLN:HB2	1.98	0.45
2:K:276:ASN:O	2:K:279:LYS:HB2	2.15	0.45
3:L:550:TYR:HE1	3:L:620:PRO:HG3	1.79	0.45
2:B:350:ARG:HA	2:B:400:THR:HG22	1.97	0.45
1:G:279:ARG:HA	1:G:566:ARG:HH22	1.81	0.45
2:H:708:PRO:HB3	3:I:728:GLN:HG3	1.99	0.45
3:I:260:ILE:O	3:I:264:ARG:HG3	2.16	0.45
3:I:395:ALA:O	3:I:398:ILE:HG22	2.16	0.45
1:J:261:LEU:HG	1:J:262:LYS:H	1.81	0.45
1:J:444:ASN:OD1	1:J:445:TYR:N	2.49	0.45
1:J:529:ASP:HB3	1:J:531:ARG:HG2	1.98	0.45
1:A:284:LEU:HB2	1:A:410:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:157:LYS:NZ	3:F:175:ARG:HH12	2.14	0.45
3:F:170:ASN:HA	3:F:710:ILE:HB	1.99	0.45
2:H:177:GLU:HA	2:H:214:LYS:HB2	1.97	0.45
2:H:260:ARG:HE	2:H:414:MET:HE1	1.80	0.45
3:I:264:ARG:NH1	3:I:520:GLU:HB3	2.30	0.45
1:J:523:MET:HB3	1:J:563:LEU:HD11	1.97	0.45
2:K:319:LEU:HB2	2:K:341:PRO:HB2	1.98	0.45
3:L:475:MET:HB2	3:L:478:ILE:HB	1.98	0.45
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.75	0.45
2:B:590:LEU:HD23	2:B:612:LYS:HD2	1.98	0.45
1:D:193:GLN:N	1:D:193:GLN:OE1	2.48	0.45
1:D:207:ILE:HG22	1:D:212:ARG:HB2	1.98	0.45
1:D:217:GLN:NE2	2:E:58:ASN:HA	2.31	0.45
1:D:606:ASP:OD1	1:D:607:MET:N	2.49	0.45
3:F:280:LEU:HD21	3:F:311:CYS:HA	1.97	0.45
3:F:658:TYR:HB2	3:F:665:LEU:HD13	1.99	0.45
2:H:531:LYS:HB3	2:H:604:LEU:HB3	1.99	0.45
2:H:620:TYR:CZ	2:H:624:LEU:HD12	2.52	0.45
1:J:53:PHE:CE2	1:J:63:VAL:HG11	2.51	0.45
3:L:111:TYR:O	3:L:113:LYS:N	2.42	0.45
3:L:142:ARG:HB3	3:L:217:PHE:CE1	2.50	0.45
2:B:634:HIS:HB2	3:C:201:LEU:HD12	1.98	0.45
3:C:57:ILE:HB	3:C:91:VAL:HB	1.97	0.45
1:D:298:GLU:O	1:D:298:GLU:HG3	2.16	0.45
2:E:307:THR:H	2:E:478:SER:HB2	1.81	0.45
3:F:531:TYR:HB3	3:F:536:MET:HB3	1.98	0.45
1:G:428:ILE:HD12	1:G:443:ARG:CZ	2.47	0.45
1:J:550:LEU:HD13	1:J:559:ARG:HD2	1.98	0.45
2:K:607:PRO:HB3	2:K:657:TYR:HB3	1.99	0.45
1:A:34:LYS:HD2	1:A:200:THR:OG1	2.17	0.45
2:B:625:CYS:HB3	3:C:111:TYR:CE2	2.52	0.45
3:C:220:VAL:HG12	3:C:221:ALA:H	1.82	0.45
1:D:173:THR:OG1	3:F:696:ILE:N	2.39	0.45
1:D:560:PRO:HB2	1:D:562:PHE:CE1	2.52	0.45
2:E:52:LYS:HA	2:E:52:LYS:HD3	1.84	0.45
2:E:533:ASN:HB3	2:E:539:LEU:HD21	1.98	0.45
2:H:54:LYS:HG3	2:H:68:PRO:HA	1.99	0.45
2:K:428:GLN:O	2:K:430:ARG:NE	2.50	0.45
2:B:527:VAL:HG11	2:B:599:TYR:CD2	2.51	0.45
3:C:580:PHE:CD2	3:C:620:PRO:HB2	2.52	0.45
2:H:58:ASN:OD1	2:H:59:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:423:ILE:HD11	2:H:473:VAL:HG21	1.97	0.45
3:I:739:ARG:NH2	3:I:740:ASP:OD2	2.47	0.45
2:K:307:THR:H	2:K:478:SER:HB2	1.81	0.45
3:L:371:THR:HG21	3:L:487:GLU:HG2	1.99	0.45
3:L:544:SER:HA	3:L:547:VAL:HG22	1.99	0.45
1:A:135:ALA:O	1:A:139:LYS:HB2	2.17	0.45
1:A:154:GLU:OE2	1:A:168:ARG:HD2	2.16	0.45
1:A:362:LYS:HG3	1:A:480:PHE:CE2	2.52	0.45
1:A:435:ILE:HD11	3:C:133:VAL:HG11	1.99	0.45
3:C:111:TYR:O	3:C:113:LYS:N	2.43	0.45
3:C:720:GLU:OE2	3:C:722:ALA:HB2	2.17	0.45
2:H:612:LYS:O	2:H:616:MET:HG3	2.17	0.45
2:K:623:ARG:HD3	3:L:103:GLY:H	1.81	0.45
3:L:563:GLN:HB3	3:L:571:LEU:HD12	1.98	0.45
2:B:223:THR:HA	2:B:348:MET:O	2.17	0.45
2:B:457:GLU:OE1	2:B:457:GLU:N	2.50	0.45
2:B:579:LEU:HA	2:B:579:LEU:HD23	1.64	0.45
3:C:356:VAL:HG13	3:C:379:ARG:HG3	1.99	0.45
3:C:562:ILE:HD12	3:C:563:GLN:N	2.32	0.45
1:D:583:ARG:HH22	2:E:511:SER:HA	1.82	0.45
1:G:572:LYS:HA	1:G:575:MET:HE3	1.99	0.45
2:H:215:ARG:O	2:H:219:ILE:HG12	2.15	0.45
2:K:378:LEU:HD11	2:K:393:ARG:HH12	1.82	0.45
1:A:314:PHE:HD2	1:A:317:TRP:CE2	2.34	0.45
2:E:706:ARG:HH11	3:F:164:MET:HG3	1.82	0.45
1:G:217:GLN:HE22	2:H:58:ASN:HA	1.82	0.45
2:H:315:PRO:HA	2:H:318:PHE:HD2	1.82	0.45
2:H:318:PHE:HA	2:H:321:MET:HG2	1.98	0.45
2:H:519:GLU:HA	2:H:559:TYR:CE2	2.52	0.45
2:K:58:ASN:ND2	2:K:61:THR:OG1	2.49	0.45
2:B:519:GLU:HB2	2:B:662:THR:HB	1.98	0.44
3:C:716:LEU:HD12	3:C:720:GLU:CD	2.38	0.44
2:E:120:ASP:OD1	3:F:30:ILE:HA	2.17	0.44
2:E:129:TYR:OH	2:E:134:ASN:OD1	2.13	0.44
2:E:215:ARG:O	2:E:219:ILE:HG13	2.17	0.44
3:I:617:LYS:HE3	3:I:648:LEU:O	2.17	0.44
2:K:121:ARG:HG2	2:K:253:TYR:CZ	2.52	0.44
2:K:298:LEU:HD12	2:K:459:ILE:HD11	1.99	0.44
3:C:390:ASP:HB2	3:C:393:SER:OG	2.17	0.44
3:C:420:PHE:O	3:C:433:GLN:NE2	2.46	0.44
3:C:554:ILE:HD11	3:C:665:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ALA:HA	1:D:172:LYS:HE2	1.99	0.44
2:E:562:HIS:CG	2:E:568:ILE:HD11	2.53	0.44
2:H:268:GLN:HB2	2:H:421:VAL:HG13	1.98	0.44
3:I:332:ARG:NH2	3:I:361:GLU:OE2	2.48	0.44
1:J:521:VAL:HG22	1:J:567:THR:HG22	2.00	0.44
3:L:506:ASP:OD1	3:L:507:GLN:N	2.48	0.44
3:L:710:ILE:HD11	3:L:726:ILE:HA	2.00	0.44
1:A:82:ARG:HH12	3:C:754:ILE:HA	1.82	0.44
1:A:523:MET:HG2	1:A:565:VAL:HG13	1.99	0.44
1:J:234:ASP:OD1	2:K:334:ARG:NH2	2.41	0.44
1:J:306:ASP:HA	1:J:309:LYS:HG2	1.99	0.44
1:A:684:GLU:O	1:A:688:GLU:HG2	2.18	0.44
3:C:387:SER:HB3	3:C:485:VAL:HG23	1.99	0.44
2:E:269:SER:O	2:E:281:LYS:NZ	2.35	0.44
1:G:582:ARG:H	1:G:582:ARG:HD2	1.81	0.44
3:I:142:ARG:HB3	3:I:217:PHE:CE1	2.52	0.44
1:D:168:ARG:HG2	1:D:172:LYS:NZ	2.33	0.44
1:G:595:MET:O	1:G:599:GLU:HB2	2.18	0.44
1:G:646:PHE:O	1:G:650:TYR:HB2	2.18	0.44
1:J:598:ALA:HB1	2:K:16:ASN:HD22	1.83	0.44
2:K:56:THR:HG23	2:K:65:GLN:HB2	1.98	0.44
1:A:490:ARG:HH21	1:A:496:ARG:HE	1.64	0.44
1:G:592:ILE:O	1:G:596:ILE:HG13	2.18	0.44
1:G:630:ASP:OD1	1:G:630:ASP:N	2.47	0.44
2:H:181:ILE:O	2:H:210:GLN:HA	2.18	0.44
2:H:287:ARG:HH22	3:I:486:ASP:H	1.65	0.44
3:I:498:ILE:HD11	3:I:502:LEU:HA	1.99	0.44
3:I:540:ASN:HB2	3:I:544:SER:CB	2.48	0.44
3:I:563:GLN:HB3	3:I:571:LEU:HD12	1.98	0.44
3:I:580:PHE:CE2	3:I:620:PRO:HB2	2.53	0.44
2:H:626:ASN:HB3	3:I:99:TRP:CH2	2.49	0.44
2:B:36:THR:HG21	2:B:354:GLY:N	2.32	0.44
1:D:217:GLN:HE22	2:E:58:ASN:HA	1.82	0.44
3:F:124:ARG:HH21	3:F:250:VAL:HG11	1.83	0.44
1:G:484:PRO:HB2	1:G:486:ILE:HG13	2.00	0.44
2:H:725:ASP:HA	2:H:728:ILE:HG12	1.98	0.44
3:L:502:LEU:O	3:L:515:PRO:HD3	2.18	0.44
1:A:54:ILE:HG12	1:A:75:ARG:HB2	1.99	0.44
1:A:530:PRO:HG3	1:A:542:VAL:HG21	2.00	0.44
3:C:665:LEU:HB3	3:C:672:ALA:O	2.17	0.44
2:E:517:ILE:H	2:E:522:ASP:CG	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:522:ASP:OD2	2:E:559:TYR:OH	2.35	0.44
2:E:606:ILE:HD13	3:F:122:VAL:HG22	2.00	0.44
3:F:172:VAL:HG12	3:F:710:ILE:HG21	2.00	0.44
1:G:529:ASP:HB3	1:G:531:ARG:HG2	1.99	0.44
2:H:453:ALA:HB3	2:H:459:ILE:HG12	1.99	0.44
3:I:664:ARG:NH2	3:I:671:ASP:OD2	2.37	0.44
3:L:307:ALA:HB2	3:L:518:VAL:HG23	1.98	0.44
3:L:325:PHE:HA	3:L:517:GLU:OE1	2.18	0.44
1:A:261:LEU:HG	1:A:262:LYS:H	1.83	0.43
1:A:274:PRO:HD2	1:A:400:LEU:O	2.18	0.43
3:C:659:ASN:HD22	3:C:660:LYS:N	2.15	0.43
1:D:48:TYR:CE1	1:D:163:LEU:HG	2.50	0.43
1:D:211:MET:HG2	2:E:171:MET:SD	2.58	0.43
1:D:615:LYS:HD2	1:D:632:SER:HB2	1.99	0.43
2:H:224:LEU:HD22	2:H:408:MET:HG3	2.00	0.43
3:I:506:ASP:OD1	3:I:510:ASN:N	2.36	0.43
1:J:293:GLU:HA	1:J:496:ARG:O	2.17	0.43
3:L:64:THR:HA	3:L:78:TRP:CZ2	2.53	0.43
3:F:122:VAL:HG12	3:F:126:LYS:HE3	2.00	0.43
1:G:178:ILE:O	1:G:181:GLU:HB2	2.18	0.43
1:J:358:LYS:HA	1:J:358:LYS:HD2	1.81	0.43
2:K:531:LYS:HE3	2:K:605:HIS:HB3	2.00	0.43
3:L:183:LEU:HD23	3:L:183:LEU:H	1.83	0.43
3:L:352:LEU:HD11	3:L:430:PRO:HB3	2.01	0.43
1:A:184:ASN:HB3	2:B:709:VAL:HG11	2.00	0.43
3:C:326:GLY:N	3:C:517:GLU:OE1	2.45	0.43
2:E:519:GLU:HB2	2:E:662:THR:O	2.18	0.43
2:E:628:LEU:HD23	2:E:628:LEU:H	1.83	0.43
1:G:449:GLU:O	1:G:638:ARG:NH2	2.50	0.43
2:H:665:SER:OG	3:I:58:THR:HG22	2.19	0.43
3:I:306:GLN:HG2	3:I:307:ALA:H	1.83	0.43
3:I:534:SER:HA	3:I:537:TRP:CH2	2.54	0.43
1:J:528:THR:O	1:J:564:TYR:OH	2.24	0.43
1:A:217:GLN:NE2	2:B:58:ASN:HA	2.34	0.43
3:F:220:VAL:HG12	3:F:221:ALA:H	1.82	0.43
2:H:50:SER:HA	2:H:82:TYR:CE1	2.53	0.43
2:H:427:GLY:HA3	2:H:438:TRP:CE2	2.54	0.43
2:K:350:ARG:HG3	2:K:400:THR:HG22	2.00	0.43
1:A:3:ASP:OD1	3:C:318:ARG:HD2	2.18	0.43
2:B:110:THR:O	2:B:114:VAL:HG13	2.19	0.43
2:B:291:THR:HG21	3:C:460:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:VAL:HG11	3:C:198:ILE:HD12	2.00	0.43
3:C:586:LYS:HG2	3:C:589:ARG:NH2	2.33	0.43
2:E:249:ARG:O	2:E:252:VAL:HG12	2.18	0.43
1:J:180:GLN:NE2	3:L:174:ALA:H	2.17	0.43
2:K:126:ARG:HG2	2:K:127:GLN:H	1.83	0.43
2:K:396:LEU:HA	2:K:401:ALA:HA	2.01	0.43
1:A:646:PHE:O	1:A:650:TYR:HB2	2.17	0.43
2:B:276:ASN:HB2	3:C:219:PRO:HG3	2.01	0.43
3:C:102:ASN:OD1	3:C:102:ASN:N	2.49	0.43
3:C:498:ILE:HD11	3:C:502:LEU:HA	1.99	0.43
3:F:395:ALA:O	3:F:398:ILE:HG22	2.19	0.43
2:H:410:GLY:HA2	2:H:413:ASN:HD21	1.84	0.43
3:I:7:LEU:HD23	3:I:7:LEU:HA	1.86	0.43
2:K:249:ARG:O	2:K:252:VAL:HG12	2.18	0.43
2:K:318:PHE:HA	2:K:321:MET:HG2	2.01	0.43
3:L:102:ASN:OD1	3:L:102:ASN:N	2.52	0.43
1:A:596:ILE:O	1:A:600:SER:HB2	2.18	0.43
2:B:281:LYS:HB3	2:B:441:LEU:HD21	2.00	0.43
3:C:399:ILE:HD13	3:C:399:ILE:HA	1.84	0.43
3:F:127:HIS:HB2	3:F:247:GLY:HA3	2.00	0.43
3:I:120:GLU:HB3	3:I:124:ARG:NH2	2.34	0.43
3:I:742:SER:OG	3:I:743:ILE:N	2.52	0.43
2:K:527:VAL:HG11	2:K:599:TYR:CD2	2.54	0.43
1:D:591:GLN:HE21	1:D:640:LEU:HB3	1.84	0.43
3:F:255:VAL:HA	3:F:527:LEU:HD11	1.99	0.43
3:F:515:PRO:O	3:F:516:GLU:HB2	2.19	0.43
3:I:77:LEU:HD12	3:I:78:TRP:CD1	2.54	0.43
3:I:542:PRO:HA	3:I:545:VAL:HG23	2.01	0.43
3:I:544:SER:HA	3:I:547:VAL:HG22	2.01	0.43
2:K:46:THR:HG21	2:K:406:GLY:HA2	1.99	0.43
3:C:385:ILE:HG23	3:C:460:MET:HE1	2.00	0.43
1:G:444:ASN:OD1	1:G:445:TYR:N	2.52	0.43
1:G:619:TRP:CD1	2:H:11:LYS:HD3	2.54	0.43
3:I:6:GLU:O	3:I:10:LEU:CB	2.67	0.43
3:I:408:ASP:O	3:I:412:LYS:HG2	2.18	0.43
3:I:537:TRP:HD1	3:I:548:ASN:CG	2.22	0.43
1:J:606:ASP:HB2	3:L:135:PHE:CD1	2.53	0.43
1:J:716:ARG:HD2	1:J:716:ARG:HA	1.75	0.43
2:B:249:ARG:O	2:B:252:VAL:HG12	2.19	0.43
1:D:261:LEU:HG	1:D:262:LYS:H	1.84	0.43
2:E:145:ASN:HA	2:E:683:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:252:VAL:HG23	2:E:412:PHE:CE1	2.53	0.43
1:G:362:LYS:HB3	1:G:367:LYS:HE3	2.01	0.43
2:E:179:MET:HE3	2:E:217:TYR:CZ	2.54	0.42
3:F:27:HIS:O	3:F:30:ILE:HG12	2.19	0.42
3:F:189:LYS:O	3:F:193:LEU:HG	2.18	0.42
1:G:130:TYR:HD2	1:G:147:ILE:HD13	1.84	0.42
3:I:700:GLU:HB2	3:I:731:VAL:HB	2.01	0.42
1:J:646:PHE:HD2	1:J:699:TRP:CZ3	2.36	0.42
2:K:569:GLN:HG3	2:K:573:SER:HB2	2.01	0.42
2:K:578:LYS:HE2	3:L:72:GLU:OE2	2.19	0.42
3:L:101:ARG:HH21	3:L:102:ASN:HD21	1.65	0.42
2:B:209:LYS:O	2:B:210:GLN:HG2	2.19	0.42
3:F:268:ARG:HH21	3:F:519:SER:HA	1.84	0.42
1:G:331:ASN:N	1:G:332:PRO:HD2	2.34	0.42
3:I:257:GLN:OE1	3:I:526:LYS:HG2	2.19	0.42
1:J:1:MET:HG2	1:J:32:THR:HB	2.01	0.42
2:K:52:LYS:HA	2:K:52:LYS:HD3	1.82	0.42
2:K:312:ASN:OD1	2:K:476:ASN:ND2	2.52	0.42
2:K:339:ILE:O	2:K:343:MET:HG3	2.20	0.42
2:K:518:ASN:HD21	2:K:663:THR:C	2.23	0.42
2:K:619:ASP:HB3	2:K:623:ARG:NH1	2.34	0.42
1:A:164:ASP:OD1	1:A:165:GLU:N	2.46	0.42
1:D:189:ASP:HB2	2:E:162:ARG:NH1	2.35	0.42
1:D:484:PRO:HB2	1:D:486:ILE:HG13	2.01	0.42
2:E:140:ALA:HB1	3:F:34:TYR:HA	2.01	0.42
2:E:623:ARG:NE	3:F:102:ASN:HA	2.34	0.42
3:F:266:ILE:HG23	3:F:283:MET:HE3	2.00	0.42
2:H:276:ASN:HB3	3:I:140:LYS:HG3	2.00	0.42
3:I:408:ASP:HB3	3:I:412:LYS:HZ3	1.83	0.42
2:K:561:CYS:HA	2:K:576:LEU:HD21	2.01	0.42
3:L:121:LYS:HA	3:L:124:ARG:HG2	2.00	0.42
3:L:318:ARG:HD3	3:L:493:ARG:HB3	2.00	0.42
3:L:409:CYS:SG	3:L:449:TRP:HA	2.59	0.42
3:L:659:ASN:HD22	3:L:660:LYS:H	1.67	0.42
1:A:298:GLU:O	1:A:300:GLU:N	2.53	0.42
1:A:376:PRO:HB2	2:B:365:ARG:HG2	2.02	0.42
2:B:307:THR:HB	2:B:478:SER:HB2	2.02	0.42
1:D:446:PHE:CG	1:D:589:LEU:HD13	2.54	0.42
1:D:528:THR:O	1:D:564:TYR:OH	2.29	0.42
3:F:102:ASN:N	3:F:102:ASN:OD1	2.52	0.42
3:F:664:ARG:HH21	3:F:671:ASP:CG	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ASP:HB3	1:A:531:ARG:CG	2.50	0.42
2:B:339:ILE:O	2:B:343:MET:HG3	2.19	0.42
1:D:310:CYS:SG	1:D:500:LEU:HB2	2.60	0.42
3:F:413:ALA:HB2	3:F:448:ASN:HD22	1.85	0.42
1:G:284:LEU:HB3	1:G:458:TYR:CZ	2.55	0.42
1:G:560:PRO:HB2	1:G:562:PHE:CE1	2.55	0.42
2:H:298:LEU:HB2	2:H:459:ILE:HD11	2.01	0.42
3:I:744:LEU:O	3:I:746:ASP:N	2.53	0.42
1:J:73:LYS:HD2	1:J:73:LYS:N	2.35	0.42
1:J:268:ILE:HD11	1:J:707:PHE:HD2	1.83	0.42
1:J:706:TRP:CD2	2:K:5:PRO:HD2	2.55	0.42
2:K:290:MET:HG3	3:L:457:VAL:HG11	2.00	0.42
2:K:499:TYR:HD1	3:L:458:MET:HE1	1.84	0.42
2:K:725:ASP:HA	2:K:728:ILE:HG12	2.01	0.42
1:A:2:GLU:HG2	3:C:318:ARG:HH12	1.85	0.42
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.85	0.42
1:A:331:ASN:N	1:A:332:PRO:HD2	2.35	0.42
2:B:47:HIS:ND1	2:B:66:LEU:HD12	2.34	0.42
2:B:612:LYS:O	2:B:616:MET:HG3	2.18	0.42
2:E:318:PHE:HA	2:E:321:MET:HG2	2.01	0.42
3:F:283:MET:HG2	3:F:533:SER:HB3	2.02	0.42
3:F:662:THR:HG22	3:F:664:ARG:HG2	2.00	0.42
1:G:184:ASN:HD22	2:H:706:ARG:NH2	2.18	0.42
2:K:122:LEU:HD11	2:K:249:ARG:HB3	2.02	0.42
3:L:261:ILE:HG12	3:L:523:GLY:HA3	2.00	0.42
1:A:116:ARG:NH1	1:A:162:THR:OG1	2.52	0.42
1:A:144:HIS:HE2	1:A:156:ALA:HB1	1.85	0.42
1:A:255:ALA:HB1	1:A:681:PHE:CE2	2.55	0.42
2:B:519:GLU:HA	2:B:559:TYR:HE2	1.84	0.42
3:C:108:THR:C	3:C:110:HIS:N	2.73	0.42
2:E:58:ASN:OD1	2:E:59:THR:N	2.53	0.42
3:F:580:PHE:CD2	3:F:620:PRO:HB2	2.55	0.42
1:G:185:ARG:NH2	3:I:157:LYS:HE2	2.35	0.42
3:I:6:GLU:O	3:I:10:LEU:HB2	2.20	0.42
3:I:365:MET:HE1	3:I:401:ALA:HB2	2.01	0.42
3:I:730:ASP:OD1	3:I:730:ASP:N	2.44	0.42
1:D:117:PHE:O	1:D:144:HIS:N	2.49	0.42
1:D:331:ASN:N	1:D:332:PRO:HD2	2.34	0.42
1:D:681:PHE:CZ	2:E:484:ILE:HD11	2.54	0.42
2:E:556:ARG:HB3	2:E:562:HIS:HA	2.01	0.42
3:F:317:LEU:N	3:F:317:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:547:VAL:HG11	3:F:670:LYS:HD2	2.00	0.42
1:J:487:SER:HG	1:J:501:TYR:HE2	1.66	0.42
2:K:114:VAL:HG12	2:K:254:PHE:CD1	2.54	0.42
3:L:237:GLY:HA3	3:L:240:TRP:CZ2	2.55	0.42
3:L:438:PHE:O	3:L:442:ALA:HB2	2.20	0.42
1:A:57:GLN:HA	3:F:626:PRO:HB2	2.02	0.42
1:A:587:GLN:O	1:A:590:GLN:HG2	2.20	0.42
1:D:78:ILE:HA	1:D:109:LEU:HD12	2.00	0.42
2:E:103:PHE:HB3	2:E:325:ILE:HG23	2.01	0.42
2:E:138:PRO:HG2	2:E:141:THR:HB	2.01	0.42
1:G:360:MET:HE2	1:G:482:LEU:HB2	2.02	0.42
2:H:249:ARG:O	2:H:252:VAL:HG12	2.19	0.42
1:J:443:ARG:HG3	1:J:444:ASN:N	2.34	0.42
1:A:496:ARG:HH22	2:B:568:ILE:HG22	1.84	0.42
2:B:613:TRP:O	2:B:621:GLN:NE2	2.53	0.42
3:C:7:LEU:HD23	3:C:7:LEU:HA	1.93	0.42
2:E:523:MET:HA	2:E:551:PHE:HZ	1.84	0.42
2:E:527:VAL:HG11	2:E:599:TYR:CE2	2.55	0.42
2:H:48:GLN:O	2:H:51:GLU:HG2	2.19	0.42
2:H:627:PRO:HG2	3:I:108:THR:HG21	2.01	0.42
1:J:164:ASP:OD1	1:J:165:GLU:N	2.47	0.42
1:J:207:ILE:HB	1:J:212:ARG:HH21	1.85	0.42
3:L:320:SER:HA	3:L:492:GLU:O	2.20	0.42
3:L:457:VAL:HG22	3:L:458:MET:HG2	2.02	0.42
2:B:631:PHE:HE2	3:C:96:VAL:HA	1.85	0.41
3:C:150:GLY:HA2	3:C:251:ARG:HG3	2.02	0.41
1:D:98:THR:HG21	1:D:110:TYR:OH	2.20	0.41
1:D:203:GLU:HG2	2:E:162:ARG:NH2	2.35	0.41
1:D:641:LEU:O	1:D:645:VAL:HG23	2.20	0.41
1:D:676:LEU:HB3	2:E:486:ARG:H	1.84	0.41
2:E:111:MET:HA	2:E:114:VAL:HG22	2.01	0.41
2:E:514:VAL:HG11	2:E:558:THR:HG21	2.01	0.41
2:E:523:MET:HA	2:E:551:PHE:CZ	2.54	0.41
1:G:274:PRO:HD2	1:G:400:LEU:O	2.20	0.41
1:G:624:SER:OG	1:G:629:GLU:HG3	2.19	0.41
2:H:282:LEU:HD12	2:H:501:PHE:HE1	1.85	0.41
1:J:617:GLU:OE1	2:K:11:LYS:NZ	2.31	0.41
2:K:378:LEU:HD11	2:K:393:ARG:NH1	2.35	0.41
2:K:428:GLN:O	2:K:430:ARG:N	2.53	0.41
3:L:269:ARG:NE	3:L:535:MET:O	2.53	0.41
3:C:27:HIS:O	3:C:30:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:703:ARG:O	3:C:705:GLY:N	2.49	0.41
2:H:548:LEU:HD11	2:H:599:TYR:HB3	2.01	0.41
3:I:589:ARG:HG2	3:I:624:ALA:CB	2.50	0.41
3:I:636:LEU:HB2	3:I:647:ILE:HG23	2.02	0.41
2:K:491:GLU:HG2	2:K:492:PHE:N	2.36	0.41
3:L:64:THR:HA	3:L:78:TRP:CH2	2.55	0.41
1:A:711:LEU:O	1:A:716:ARG:HG3	2.21	0.41
2:B:354:GLY:HA3	2:B:368:ILE:O	2.20	0.41
3:C:506:ASP:OD1	3:C:507:GLN:N	2.47	0.41
3:F:589:ARG:HG2	3:F:624:ALA:HB2	2.01	0.41
3:F:659:ASN:HD22	3:F:660:LYS:H	1.66	0.41
1:G:184:ASN:HD21	3:I:175:ARG:HH11	1.68	0.41
1:G:641:LEU:O	1:G:645:VAL:HG23	2.20	0.41
2:H:303:THR:OG1	2:H:490:PHE:HB2	2.20	0.41
3:I:428:LEU:HB2	3:I:433:GLN:NE2	2.34	0.41
3:I:697:LEU:HD21	3:I:735:MET:HB2	2.01	0.41
1:J:73:LYS:HD2	1:J:73:LYS:H	1.85	0.41
1:J:83:ASP:HB2	3:L:755:ARG:NH1	2.35	0.41
1:J:184:ASN:HB3	2:K:709:VAL:HG11	2.01	0.41
2:K:66:LEU:HB2	2:K:405:PRO:HD3	2.02	0.41
3:C:694:PHE:HB3	3:C:735:MET:O	2.21	0.41
1:D:349:GLU:OE1	1:D:349:GLU:N	2.53	0.41
1:D:523:MET:HG2	1:D:565:VAL:HG13	2.02	0.41
1:G:33:ASN:ND2	1:G:190:SER:HB3	2.35	0.41
1:G:46:PHE:HE1	1:G:78:ILE:HG21	1.86	0.41
1:G:282:PHE:HA	1:G:524:GLU:OE2	2.20	0.41
2:H:374:ALA:HA	2:H:393:ARG:HE	1.85	0.41
3:I:305:GLU:HB3	3:I:308:VAL:HG23	2.01	0.41
2:K:368:ILE:HA	2:K:369:PRO:HD3	1.91	0.41
2:K:494:SER:HB2	2:K:505:PHE:HA	2.02	0.41
3:L:142:ARG:HH22	3:L:488:TYR:HB2	1.85	0.41
3:L:237:GLY:HA3	3:L:240:TRP:CE2	2.55	0.41
1:A:215:ALA:HB1	1:A:226:LEU:HD13	2.01	0.41
2:B:623:ARG:CD	3:C:103:GLY:H	2.32	0.41
3:C:285:HIS:CE1	3:C:295:VAL:HG11	2.55	0.41
1:D:646:PHE:HD2	1:D:699:TRP:CZ3	2.38	0.41
3:F:55:TYR:CD1	3:F:92:SER:HB2	2.56	0.41
3:F:55:TYR:HD1	3:F:92:SER:HB2	1.85	0.41
3:F:420:PHE:O	3:F:433:GLN:NE2	2.42	0.41
1:G:324:LYS:HE3	1:G:537:TRP:O	2.20	0.41
2:H:111:MET:HA	2:H:114:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:562:HIS:CG	2:H:568:ILE:HD11	2.56	0.41
3:I:292:THR:OG1	3:I:297:ILE:HD11	2.20	0.41
1:J:345:LEU:HD11	1:J:503:PHE:CE2	2.51	0.41
2:K:58:ASN:OD1	2:K:59:THR:N	2.53	0.41
2:K:572:ARG:HG2	2:K:576:LEU:HD13	2.02	0.41
2:K:656:GLU:HG2	2:K:657:TYR:H	1.84	0.41
3:L:562:ILE:O	3:L:566:GLN:HG2	2.21	0.41
3:L:658:TYR:HB2	3:L:665:LEU:HD13	2.02	0.41
1:A:246:LEU:O	2:B:468:ARG:NH2	2.53	0.41
1:A:641:LEU:O	1:A:645:VAL:HG23	2.19	0.41
2:B:149:VAL:HG21	2:B:181:ILE:HG12	2.02	0.41
2:B:281:LYS:HG3	3:C:142:ARG:NH2	2.31	0.41
3:C:64:THR:HA	3:C:78:TRP:CZ2	2.55	0.41
3:C:70:ARG:HH21	1:G:343:ALA:HB1	1.85	0.41
2:E:583:THR:O	2:E:586:LYS:NZ	2.51	0.41
2:E:725:ASP:HA	2:E:728:ILE:HG12	2.03	0.41
3:F:387:SER:HB3	3:F:481:SER:HB3	2.02	0.41
1:G:338:TRP:NE1	1:G:545:ILE:HD11	2.36	0.41
1:G:477:MET:HA	1:G:509:SER:OG	2.20	0.41
3:I:748:GLN:O	3:I:751:THR:OG1	2.19	0.41
1:J:74:HIS:C	1:J:76:PHE:H	2.24	0.41
2:K:129:TYR:OH	2:K:134:ASN:OD1	2.27	0.41
2:K:424:LEU:HD12	2:K:442:GLN:HB2	2.01	0.41
2:K:693:CYS:SG	3:L:31:ILE:HG23	2.61	0.41
1:A:621:ILE:HD11	1:A:631:GLY:HA3	2.03	0.41
3:C:502:LEU:O	3:C:515:PRO:HD3	2.20	0.41
1:D:358:LYS:HD2	1:D:358:LYS:HA	1.86	0.41
3:F:142:ARG:HB2	3:F:487:GLU:O	2.21	0.41
1:G:377:GLU:N	2:H:364:LEU:HA	2.36	0.41
1:G:623:GLU:HA	1:G:627:GLY:O	2.21	0.41
2:H:704:SER:HB2	3:I:201:LEU:HD21	2.03	0.41
3:I:64:THR:HA	3:I:78:TRP:CH2	2.56	0.41
3:I:102:ASN:N	3:I:102:ASN:OD1	2.54	0.41
2:K:110:THR:O	2:K:114:VAL:HG13	2.21	0.41
2:K:558:THR:HG23	3:L:48:LYS:HG2	2.03	0.41
3:L:220:VAL:HG12	3:L:221:ALA:H	1.84	0.41
3:L:384:LEU:HB3	3:L:478:ILE:HD12	2.02	0.41
3:L:744:LEU:HD12	3:L:744:LEU:O	2.19	0.41
2:B:282:LEU:HD12	2:B:501:PHE:HE1	1.85	0.41
3:C:662:THR:HG22	3:C:664:ARG:HG3	2.03	0.41
1:D:216:ASP:OD1	1:D:226:LEU:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:MET:HA	1:D:509:SER:OG	2.21	0.41
3:F:120:GLU:O	3:F:124:ARG:HG3	2.20	0.41
3:F:326:GLY:HA2	3:F:435:LEU:HD21	2.03	0.41
1:G:214:LEU:HB3	2:H:346:ASN:HD22	1.86	0.41
2:H:46:THR:HG21	2:H:406:GLY:HA2	2.03	0.41
2:H:354:GLY:HA3	2:H:368:ILE:O	2.21	0.41
2:H:531:LYS:HE2	3:I:233:HIS:CD2	2.56	0.41
3:I:399:ILE:HD11	3:I:446:PHE:CE2	2.56	0.41
3:I:431:MET:HA	3:I:431:MET:HE2	2.01	0.41
2:K:167:LEU:HD21	2:K:250:GLY:HA3	2.03	0.41
2:K:282:LEU:HD23	2:K:441:LEU:HD22	2.03	0.41
1:A:78:ILE:O	1:A:82:ARG:NE	2.44	0.41
1:A:362:LYS:HA	1:A:480:PHE:HE2	1.86	0.41
1:A:461:LYS:HE3	1:A:501:TYR:CG	2.56	0.41
3:C:231:VAL:HG21	3:C:244:TYR:CE2	2.56	0.41
3:C:736:LYS:HG2	3:C:737:ARG:N	2.33	0.41
3:C:745:THR:HG22	3:C:749:THR:HG23	2.03	0.41
1:D:1:MET:HG2	1:D:32:THR:HB	2.03	0.41
1:D:265:PRO:HB3	1:D:711:LEU:HD21	2.03	0.41
1:D:354:ILE:HA	1:D:355:PRO:HD3	1.85	0.41
1:D:540:TYR:CZ	1:D:566:ARG:HD2	2.56	0.41
1:D:646:PHE:O	1:D:650:TYR:HB2	2.21	0.41
1:G:8:CYS:O	1:G:174:ARG:NH2	2.54	0.41
1:G:151:THR:HG22	2:H:711:ILE:HD13	2.03	0.41
1:G:344:GLU:HG3	1:G:360:MET:SD	2.61	0.41
1:G:385:ARG:HA	1:G:385:ARG:HD2	1.91	0.41
1:G:443:ARG:HG3	1:G:444:ASN:N	2.36	0.41
1:G:465:ILE:HD12	1:G:485:MET:HA	2.03	0.41
1:G:545:ILE:HD12	1:G:545:ILE:HA	1.77	0.41
2:H:626:ASN:ND2	3:I:104:PRO:O	2.54	0.41
3:I:237:GLY:HA3	3:I:240:TRP:CZ2	2.56	0.41
3:I:537:TRP:CE3	3:I:579:PRO:HG3	2.55	0.41
1:J:54:ILE:HD11	1:J:75:ARG:HD3	2.03	0.41
1:J:196:ARG:HG3	1:J:201:ILE:HD11	2.03	0.41
3:L:550:TYR:HE2	3:L:656:PHE:HD1	1.68	0.41
1:A:477:MET:HA	1:A:509:SER:OG	2.21	0.41
3:C:28:MET:O	3:C:31:ILE:HG22	2.20	0.41
3:C:659:ASN:HD22	3:C:660:LYS:H	1.69	0.41
3:C:737:ARG:C	3:C:738:LYS:HD3	2.41	0.41
1:D:260:PHE:CE1	1:D:265:PRO:HG3	2.47	0.41
2:E:331:GLU:HG2	2:E:335:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:619:TRP:HA	1:G:620:PRO:HD3	1.95	0.41
2:H:283:ALA:HB2	2:H:501:PHE:CE2	2.55	0.41
3:I:560:VAL:HG13	3:I:571:LEU:HD11	2.01	0.41
3:I:696:ILE:HG22	3:I:698:GLY:H	1.86	0.41
1:J:665:LEU:HD23	1:J:707:PHE:CE2	2.56	0.41
3:L:108:THR:C	3:L:110:HIS:H	2.24	0.41
3:L:309:ASP:HB2	3:L:513:LEU:HD22	2.02	0.41
2:B:571:ARG:NH2	3:C:51:MET:O	2.54	0.40
3:C:550:TYR:CE1	3:C:620:PRO:HG3	2.55	0.40
3:C:572:TYR:OH	3:C:604:ARG:NH2	2.41	0.40
1:D:75:ARG:O	1:D:75:ARG:HG3	2.20	0.40
1:D:306:ASP:HA	1:D:309:LYS:HG2	2.04	0.40
1:D:587:GLN:OE1	1:D:644:SER:OG	2.24	0.40
3:F:142:ARG:HB3	3:F:217:PHE:CE1	2.56	0.40
3:F:612:THR:O	3:F:616:ILE:HG12	2.21	0.40
1:G:706:TRP:CD2	2:H:5:PRO:HD2	2.56	0.40
2:H:730:PHE:CZ	2:H:737:LYS:HG2	2.56	0.40
3:I:273:SER:OG	1:J:96:ASN:OD1	2.38	0.40
3:I:320:SER:CB	3:I:494:VAL:HG12	2.51	0.40
1:J:559:ARG:HA	1:J:560:PRO:HD3	1.96	0.40
2:B:111:MET:HA	2:B:114:VAL:HG22	2.03	0.40
3:C:225:SER:O	3:C:229:ILE:HG12	2.20	0.40
1:D:290:LEU:HD12	1:D:290:LEU:HA	1.95	0.40
1:D:591:GLN:NE2	1:D:640:LEU:HB3	2.36	0.40
2:E:735:ILE:HD12	2:E:735:ILE:HA	1.95	0.40
3:I:658:TYR:HB2	3:I:665:LEU:HD13	2.03	0.40
2:K:518:ASN:OD1	2:K:519:GLU:N	2.49	0.40
3:L:1:MET:HA	3:L:4:ILE:HG22	2.03	0.40
2:E:54:LYS:HB3	2:E:67:ASN:H	1.86	0.40
2:E:626:ASN:HB3	3:F:99:TRP:HH2	1.85	0.40
2:E:660:VAL:O	2:E:663:THR:OG1	2.19	0.40
2:E:727:ARG:NH2	3:F:708:LEU:HA	2.37	0.40
3:F:736:LYS:HG2	3:F:737:ARG:N	2.28	0.40
2:H:531:LYS:HE2	3:I:233:HIS:HD2	1.87	0.40
2:K:326:THR:HB	2:K:334:ARG:HG2	2.03	0.40
3:L:515:PRO:O	3:L:517:GLU:N	2.54	0.40
1:A:53:PHE:CE2	1:A:63:VAL:HG21	2.56	0.40
2:B:371:GLU:HG3	2:B:399:GLY:HA3	2.03	0.40
3:C:124:ARG:HD3	3:C:227:VAL:HG12	2.04	0.40
1:D:527:LEU:HD23	1:D:561:MET:HA	2.04	0.40
2:E:419:LEU:O	2:E:422:SER:OG	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:384:LEU:HD23	3:F:478:ILE:HD11	2.02	0.40
1:G:557:MET:H	1:G:557:MET:HG2	1.75	0.40
2:K:422:SER:O	2:K:426:LEU:HD13	2.21	0.40
2:B:162:ARG:HH21	2:B:164:ILE:HG21	1.87	0.40
2:B:490:PHE:CE1	2:B:497:TYR:HD2	2.39	0.40
2:B:656:GLU:HG2	2:B:657:TYR:H	1.86	0.40
1:D:51:PHE:O	1:D:62:VAL:HA	2.22	0.40
3:F:694:PHE:HB3	3:F:735:MET:O	2.22	0.40
3:F:720:GLU:O	3:F:735:MET:HA	2.22	0.40
1:G:323:VAL:HG23	1:G:544:GLU:H	1.87	0.40
1:G:370:LEU:HD13	1:G:507:GLY:HA2	2.03	0.40
2:H:490:PHE:CE1	2:H:497:TYR:HD2	2.40	0.40
2:H:693:CYS:SG	3:I:31:ILE:HG23	2.61	0.40
3:I:356:VAL:HG13	3:I:379:ARG:HG3	2.03	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	696/716 (97%)	646 (93%)	49 (7%)	1 (0%)	51 81
1	D	674/716 (94%)	632 (94%)	42 (6%)	0	100 100
1	G	693/716 (97%)	644 (93%)	49 (7%)	0	100 100
1	J	694/716 (97%)	646 (93%)	48 (7%)	0	100 100
2	B	667/757 (88%)	628 (94%)	38 (6%)	1 (0%)	51 81
2	E	653/757 (86%)	621 (95%)	32 (5%)	0	100 100
2	H	664/757 (88%)	629 (95%)	34 (5%)	1 (0%)	47 76
2	K	661/757 (87%)	623 (94%)	37 (6%)	1 (0%)	47 76
3	C	716/765 (94%)	658 (92%)	56 (8%)	2 (0%)	41 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	712/765 (93%)	660 (93%)	52 (7%)	0	100	100
3	I	718/765 (94%)	658 (92%)	59 (8%)	1 (0%)	51	81
3	L	697/765 (91%)	647 (93%)	49 (7%)	1 (0%)	51	81
All	All	8245/8952 (92%)	7692 (93%)	545 (7%)	8 (0%)	51	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
2	B	295	ASP
2	K	429	LYS
3	I	745	THR
3	L	516	GLU
3	C	516	GLU
3	C	720	GLU
2	H	295	ASP

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	634/644 (98%)	623 (98%)	11 (2%)	60	79
1	D	620/644 (96%)	608 (98%)	12 (2%)	57	78
1	G	631/644 (98%)	622 (99%)	9 (1%)	67	82
1	J	632/644 (98%)	620 (98%)	12 (2%)	57	78
2	B	602/669 (90%)	593 (98%)	9 (2%)	65	81
2	E	589/669 (88%)	576 (98%)	13 (2%)	52	76
2	H	600/669 (90%)	590 (98%)	10 (2%)	60	79
2	K	597/669 (89%)	588 (98%)	9 (2%)	65	81
3	C	641/676 (95%)	631 (98%)	10 (2%)	62	80
3	F	637/676 (94%)	619 (97%)	18 (3%)	43	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	643/676 (95%)	635 (99%)	8 (1%)	71 84
3	L	628/676 (93%)	617 (98%)	11 (2%)	59 79
All	All	7454/7956 (94%)	7322 (98%)	132 (2%)	59 79

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	LEU
1	A	239	ASN
1	A	260	PHE
1	A	279	ARG
1	A	294	ASP
1	A	300	GLU
1	A	321	TYR
1	A	557	MET
1	A	611	PHE
1	A	649	LEU
1	A	707	PHE
2	B	30	TYR
2	B	129	TYR
2	B	297	GLU
2	B	308	LYS
2	B	430	ARG
2	B	598	LEU
2	B	626	ASN
2	B	706	ARG
2	B	754	ARG
3	C	28	MET
3	C	38	ARG
3	C	111	TYR
3	C	257	GLN
3	C	348	ASN
3	C	659	ASN
3	C	695	LEU
3	C	737	ARG
3	C	739	ARG
3	C	746	ASP
1	D	219	LEU
1	D	239	ASN
1	D	260	PHE
1	D	294	ASP

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Mol	Chain	Res	Type
1	D	386	ASP
1	D	496	ARG
1	D	549	LEU
1	D	557	MET
1	D	582	ARG
1	D	611	PHE
1	D	649	LEU
1	D	707	PHE
2	E	129	TYR
2	E	308	LYS
2	E	425	ASN
2	E	430	ARG
2	E	509	LEU
2	E	579	LEU
2	E	598	LEU
2	E	626	ASN
2	E	628	LEU
2	E	655	MET
2	E	685	ASP
2	E	706	ARG
2	E	754	ARG
3	F	17	ARG
3	F	28	MET
3	F	55	TYR
3	F	110	HIS
3	F	111	TYR
3	F	137	ASN
3	F	209	ARG
3	F	257	GLN
3	F	315	MET
3	F	323	PHE
3	F	537	TRP
3	F	548	ASN
3	F	650	ARG
3	F	659	ASN
3	F	695	LEU
3	F	712	GLU
3	F	716	LEU
3	F	739	ARG
1	G	179	ARG
1	G	219	LEU
1	G	260	PHE

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Mol	Chain	Res	Type
1	G	279	ARG
1	G	582	ARG
1	G	599	GLU
1	G	611	PHE
1	G	649	LEU
1	G	707	PHE
2	H	129	TYR
2	H	295	ASP
2	H	425	ASN
2	H	509	LEU
2	H	523	MET
2	H	579	LEU
2	H	598	LEU
2	H	656	GLU
2	H	706	ARG
2	H	754	ARG
3	I	17	ARG
3	I	28	MET
3	I	55	TYR
3	I	257	GLN
3	I	348	ASN
3	I	380	ARG
3	I	660	LYS
3	I	695	LEU
1	J	12	MET
1	J	179	ARG
1	J	219	LEU
1	J	260	PHE
1	J	279	ARG
1	J	294	ASP
1	J	300	GLU
1	J	385	ARG
1	J	443	ARG
1	J	549	LEU
1	J	611	PHE
1	J	707	PHE
2	K	297	GLU
2	K	298	LEU
2	K	308	LYS
2	K	430	ARG
2	K	509	LEU
2	K	579	LEU

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Mol	Chain	Res	Type
2	K	598	LEU
2	K	706	ARG
2	K	754	ARG
3	L	17	ARG
3	L	28	MET
3	L	100	ASN
3	L	111	TYR
3	L	202	MET
3	L	348	ASN
3	L	505	ARG
3	L	650	ARG
3	L	659	ASN
3	L	695	LEU
3	L	746	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	605	HIS
3	C	406	GLN
3	C	728	GLN
1	D	146	HIS
1	D	591	GLN
3	F	137	ASN
3	F	429	ASN
3	F	728	GLN
1	G	146	HIS
1	G	217	GLN
1	G	591	GLN
2	H	65	GLN
2	H	346	ASN
3	I	285	HIS
3	I	614	GLN
3	I	728	GLN
1	J	146	HIS
1	J	217	GLN
2	K	292	ASN
3	L	453	HIS
3	L	728	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 monosaccharides 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	704/716 (98%)	0.71	20 (2%) 53 51	36, 86, 152, 183	0
1	D	686/716 (95%)	1.11	121 (17%) 1 1	89, 142, 214, 261	0
1	G	701/716 (97%)	0.59	13 (1%) 66 65	39, 86, 147, 214	0
1	J	702/716 (98%)	0.87	75 (10%) 6 5	67, 121, 184, 240	0
2	B	679/757 (89%)	0.77	29 (4%) 35 35	35, 82, 137, 210	0
2	E	665/757 (87%)	1.40	177 (26%) 0 0	93, 164, 215, 239	0
2	H	676/757 (89%)	0.73	29 (4%) 35 35	35, 89, 157, 214	0
2	K	673/757 (88%)	0.92	81 (12%) 4 3	65, 124, 184, 221	0
3	C	724/765 (94%)	0.89	80 (11%) 5 5	46, 110, 167, 217	0
3	F	720/765 (94%)	0.98	116 (16%) 1 1	55, 134, 185, 220	0
3	I	726/765 (94%)	0.70	46 (6%) 20 21	42, 107, 163, 200	0
3	L	709/765 (92%)	0.89	83 (11%) 4 3	70, 123, 173, 215	0
All	All	8365/8952 (93%)	0.88	870 (10%) 6 6	35, 114, 186, 261	0

All (870) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	440	GLY	12.8
3	L	717	ALA	11.4
3	C	250	VAL	9.8
3	F	140	LYS	9.7
2	E	439	ASP	8.3
1	D	205	PHE	8.0
2	E	246	MET	7.8
1	D	221	PRO	7.7
3	L	323	PHE	7.4
2	E	448	ALA	7.1
2	E	407	MET	7.1

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Mol	Chain	Res	Type	RSRZ
2	E	224	LEU	6.9
1	D	667	LEU	6.7
2	K	356	MET	6.6
1	D	378	LYS	6.6
3	L	458	MET	6.6
1	J	599	GLU	6.3
1	D	206	GLU	6.3
3	F	250	VAL	6.1
2	E	408	MET	6.0
2	K	129	TYR	6.0
2	E	505	PHE	5.9
2	E	300	PHE	5.8
1	D	195	GLU	5.7
2	E	390	GLU	5.6
2	K	364	LEU	5.6
1	D	493	GLU	5.6
2	E	298	LEU	5.6
3	C	746	ASP	5.5
2	E	449	LEU	5.4
2	E	131	TRP	5.4
1	D	599	GLU	5.3
1	D	220	PRO	5.3
1	D	382	ASP	5.2
3	F	30	ILE	5.2
2	E	501	PHE	5.1
3	L	716	LEU	5.1
2	E	418	VAL	5.1
3	F	105	MET	5.1
1	D	694	LEU	5.1
2	E	129	TYR	5.0
3	C	347	GLY	4.9
2	E	88	VAL	4.8
2	E	442	GLN	4.8
2	E	397	ILE	4.8
2	E	272	PRO	4.8
3	C	489	SER	4.7
3	F	138	GLN	4.7
3	C	477	GLY	4.7
1	D	21	MET	4.7
3	L	486	ASP	4.7
3	I	489	SER	4.7
3	F	142	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	381	PHE	4.6
2	H	357	PHE	4.6
3	I	487	GLU	4.6
2	E	182	THR	4.6
2	B	53	GLY	4.6
3	F	149	PRO	4.6
1	A	716	ARG	4.6
2	E	324	TYR	4.6
2	K	357	PHE	4.5
3	F	248	GLY	4.5
3	F	330	PHE	4.5
3	C	463	VAL	4.5
2	K	472	LEU	4.5
2	E	409	MET	4.5
3	F	130	PHE	4.5
3	F	218	LEU	4.5
3	L	418	LEU	4.5
1	J	140	SER	4.5
1	A	379	VAL	4.5
2	E	367	GLN	4.5
2	K	131	TRP	4.5
3	C	458	MET	4.5
3	F	139	VAL	4.4
2	E	317	MET	4.4
2	B	357	PHE	4.4
3	C	149	PRO	4.4
2	E	245	GLY	4.4
3	I	715	ASN	4.4
3	I	486	ASP	4.4
2	E	180	GLU	4.3
2	K	440	GLY	4.3
2	E	174	MET	4.3
2	B	381	PHE	4.3
1	D	9	PHE	4.3
2	E	492	PHE	4.3
3	F	217	PHE	4.3
2	E	504	ASN	4.3
2	E	336	VAL	4.2
2	B	293	SER	4.2
3	F	213	ARG	4.2
1	D	239	ASN	4.2
2	E	268	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	E	475	ILE	4.1
3	L	140	LYS	4.1
1	J	695	ILE	4.1
2	E	338	SER	4.1
2	K	178	GLU	4.1
3	I	718	LYS	4.1
1	A	195	GLU	4.1
1	D	210	THR	4.1
1	D	150	PHE	4.0
1	D	608	THR	4.0
2	K	501	PHE	4.0
1	J	381	PHE	4.0
1	J	249	MET	4.0
2	E	282	LEU	4.0
2	E	513	GLY	4.0
2	E	286	VAL	3.9
2	E	441	LEU	3.9
3	F	458	MET	3.9
2	E	64	PRO	3.9
1	D	277	PHE	3.9
1	J	375	ALA	3.9
2	E	223	THR	3.9
2	E	425	ASN	3.9
3	L	511	VAL	3.9
2	K	291	THR	3.9
2	E	92	MET	3.9
2	K	40	MET	3.9
1	D	612	PHE	3.9
1	J	239	ASN	3.9
3	F	212	VAL	3.9
3	F	485	VAL	3.9
2	E	47	HIS	3.8
2	H	381	PHE	3.8
3	L	489	SER	3.8
1	J	604	GLU	3.8
3	F	291	GLY	3.8
2	E	364	LEU	3.8
2	B	356	MET	3.8
2	K	479	LYS	3.8
1	D	607	MET	3.8
2	E	43	VAL	3.8
2	B	501	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	695	ILE	3.8
1	D	381	PHE	3.8
2	E	380	TYR	3.7
3	C	479	ARG	3.7
3	F	144	ARG	3.7
1	D	377	GLU	3.7
3	F	325	PHE	3.7
3	F	361	GLU	3.7
1	A	330	ILE	3.7
3	F	360	TYR	3.7
2	E	538	ASP	3.7
1	D	34	LYS	3.7
2	E	472	LEU	3.7
2	E	509	LEU	3.6
2	E	512	PHE	3.6
3	F	363	PHE	3.6
3	F	521	THR	3.6
3	C	467	MET	3.6
3	F	209	ARG	3.6
1	D	707	PHE	3.6
2	E	40	MET	3.6
3	I	672	ALA	3.6
2	E	659	ALA	3.6
3	L	496	VAL	3.6
1	A	390	LEU	3.6
1	D	253	VAL	3.6
2	E	39	THR	3.6
3	C	747	SER	3.6
2	K	473	VAL	3.6
2	E	23	PRO	3.6
3	F	717	ALA	3.6
1	G	57	GLN	3.6
2	E	244	PRO	3.5
3	C	418	LEU	3.5
3	L	328	PHE	3.5
1	D	187	LEU	3.5
3	L	508	ARG	3.5
2	E	166	PHE	3.5
2	E	514	VAL	3.5
1	D	350	ASN	3.5
2	K	290	MET	3.5
2	E	9	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
3	I	717	ALA	3.5
1	D	424	GLU	3.5
3	I	441	ASP	3.5
2	E	351	LEU	3.5
3	I	418	LEU	3.5
3	F	516	GLU	3.5
1	D	151	THR	3.5
3	F	211	LEU	3.5
3	C	581	GLN	3.4
3	F	746	ASP	3.4
2	E	502	VAL	3.4
2	K	351	LEU	3.4
2	E	496	PHE	3.4
2	K	15	GLN	3.4
3	C	742	SER	3.4
2	E	117	THR	3.4
2	E	132	THR	3.4
3	C	329	THR	3.4
2	E	450	ILE	3.4
1	D	237	GLU	3.4
2	K	372	MET	3.4
1	D	178	ILE	3.4
1	D	242	ILE	3.4
2	B	364	LEU	3.4
3	F	403	VAL	3.4
2	K	87	CYS	3.4
3	L	498	ILE	3.4
1	J	485	MET	3.4
3	L	143	ARG	3.4
1	D	54	ILE	3.4
1	J	385	ARG	3.4
1	D	496	ARG	3.3
3	L	485	VAL	3.3
2	H	358	GLU	3.3
3	L	474	SER	3.3
2	H	501	PHE	3.3
2	K	483	TYR	3.3
1	D	211	MET	3.3
1	D	8	CYS	3.3
2	E	322	ILE	3.3
2	B	410	GLY	3.3
2	E	169	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	358	GLU	3.3
2	E	136	ASN	3.3
3	L	150	GLY	3.3
1	D	162	THR	3.3
2	K	489	THR	3.3
3	C	454	ILE	3.3
3	F	207	LEU	3.3
1	A	626	LYS	3.3
2	E	265	LYS	3.3
3	C	512	LEU	3.2
3	L	142	ARG	3.2
3	F	365	MET	3.2
1	D	208	THR	3.2
3	L	153	ASP	3.2
3	L	512	LEU	3.2
3	F	327	GLY	3.2
2	K	267	GLU	3.2
2	E	415	LEU	3.2
2	K	475	ILE	3.2
3	F	317	LEU	3.2
1	J	667	LEU	3.2
2	E	337	LEU	3.2
2	E	277	GLU	3.2
2	E	483	TYR	3.2
2	B	450	ILE	3.2
3	C	339	LYS	3.2
3	C	153	ASP	3.1
3	I	755	ARG	3.1
2	E	490	PHE	3.1
2	K	182	THR	3.1
3	L	347	GLY	3.1
1	D	379	VAL	3.1
2	K	180	GLU	3.1
3	C	251	ARG	3.1
3	F	513	LEU	3.1
3	C	486	ASP	3.1
3	F	467	MET	3.1
1	J	53	PHE	3.1
1	J	612	PHE	3.1
1	J	613	GLU	3.1
1	J	106	LEU	3.1
2	H	129	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
3	L	513	LEU	3.1
1	J	378	LYS	3.1
3	I	305	GLU	3.1
2	E	146	THR	3.1
2	H	472	LEU	3.1
2	E	150	PHE	3.1
2	E	290	MET	3.1
1	D	140	SER	3.1
1	D	214	LEU	3.1
2	E	110	THR	3.1
2	E	222	LEU	3.1
3	L	349	LEU	3.1
2	E	357	PHE	3.1
2	E	443	SER	3.0
3	C	324	SER	3.0
1	A	101	GLU	3.0
1	J	374	MET	3.0
2	E	711	ILE	3.0
1	D	355	PRO	3.0
2	K	130	ASP	3.0
3	F	49	TRP	3.0
2	B	368	ILE	3.0
3	F	386	VAL	3.0
3	L	623	ALA	3.0
2	E	118	ARG	3.0
2	K	365	ARG	3.0
2	E	552	ILE	3.0
1	D	59	GLU	3.0
2	K	368	ILE	3.0
2	K	179	MET	3.0
3	C	365	MET	3.0
3	L	365	MET	3.0
2	K	134	ASN	3.0
3	F	523	GLY	3.0
3	L	579	PRO	3.0
3	L	329	THR	3.0
1	J	663	ARG	3.0
2	K	498	ARG	3.0
3	F	224	THR	3.0
2	E	106	SER	2.9
1	D	121	GLY	2.9
3	F	48	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	460	MET	2.9
1	J	242	ILE	2.9
3	F	460	MET	2.9
1	J	237	GLU	2.9
1	J	543	LEU	2.9
3	C	399	ILE	2.9
3	L	528	THR	2.9
1	D	118	ILE	2.9
2	H	359	SER	2.9
2	E	403	LEU	2.9
2	E	74	PRO	2.9
1	D	400	LEU	2.9
2	E	46	THR	2.9
2	E	57	THR	2.9
3	C	496	VAL	2.9
2	B	367	GLN	2.9
3	F	486	ASP	2.9
1	D	77	GLU	2.9
3	C	745	THR	2.9
2	E	165	ASP	2.9
2	K	249	ARG	2.9
2	E	321	MET	2.9
2	E	362	MET	2.9
2	K	502	VAL	2.9
3	F	483	MET	2.9
1	D	106	LEU	2.9
2	K	337	LEU	2.9
2	E	181	ILE	2.8
3	F	457	VAL	2.8
2	K	366	THR	2.8
2	E	37	GLY	2.8
2	B	359	SER	2.8
2	K	439	ASP	2.8
3	C	154	LEU	2.8
3	C	382	VAL	2.8
3	F	373	ILE	2.8
2	E	50	SER	2.8
3	C	392	GLN	2.8
1	D	334	TYR	2.8
1	J	224	SER	2.8
2	E	38	TYR	2.8
1	D	447	THR	2.8

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Mol	Chain	Res	Type	RSRZ
3	I	142	ARG	2.8
1	D	294	ASP	2.8
3	F	119	PHE	2.8
1	D	64	GLU	2.8
2	E	297	GLU	2.8
1	D	305	TYR	2.8
2	E	599	TYR	2.8
3	L	488	TYR	2.8
2	K	399	GLY	2.8
2	K	474	GLY	2.8
3	F	33	LYS	2.8
3	C	511	VAL	2.8
3	I	49	TRP	2.8
1	D	480	PHE	2.8
3	F	147	ILE	2.8
2	K	418	VAL	2.8
3	C	36	SER	2.8
2	E	366	THR	2.8
2	K	487	THR	2.8
2	E	164	ILE	2.8
2	K	348	MET	2.8
3	L	223	GLY	2.8
1	J	253	VAL	2.8
3	F	219	PRO	2.8
3	F	743	ILE	2.7
3	L	529	ILE	2.7
1	G	377	GLU	2.7
3	C	756	MET	2.7
1	D	229	PHE	2.7
2	H	448	ALA	2.7
2	E	530	ILE	2.7
2	E	53	GLY	2.7
3	C	411	ILE	2.7
3	C	465	PRO	2.7
3	F	439	GLN	2.7
3	I	660	LYS	2.7
3	L	144	ARG	2.7
3	C	105	MET	2.7
1	A	51	PHE	2.7
1	D	555	GLY	2.7
1	J	649	LEU	2.7
3	L	735	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	130	TYR	2.7
1	J	716	ARG	2.7
3	F	502	LEU	2.7
1	D	347	ASP	2.7
2	E	564	GLY	2.7
3	F	323	PHE	2.7
1	D	122	VAL	2.7
3	C	461	ILE	2.7
2	E	127	GLN	2.7
3	F	608	GLY	2.7
1	J	334	TYR	2.7
2	K	448	ALA	2.7
3	L	108	THR	2.7
1	J	21	MET	2.7
1	D	212	ARG	2.7
1	J	213	ARG	2.7
2	E	278	LYS	2.7
2	K	512	PHE	2.7
2	H	383	GLU	2.7
3	C	381	LEU	2.7
3	F	318	ARG	2.7
1	D	386	ASP	2.7
2	K	220	ARG	2.7
2	E	627	PRO	2.7
1	D	693	CYS	2.7
3	F	479	ARG	2.7
2	K	490	PHE	2.7
3	F	356	VAL	2.7
1	D	74	HIS	2.7
3	F	331	LYS	2.6
3	F	493	ARG	2.6
1	A	386	ASP	2.6
3	L	460	MET	2.6
3	F	385	ILE	2.6
1	D	660	ALA	2.6
3	L	217	PHE	2.6
2	E	284	ASN	2.6
3	L	211	LEU	2.6
3	I	311	CYS	2.6
3	L	357	HIS	2.6
3	L	322	SER	2.6
3	F	153	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	254	ASP	2.6
1	D	335	LEU	2.6
1	J	366	LEU	2.6
3	I	298	LEU	2.6
2	E	30	TYR	2.6
3	L	592	TYR	2.6
2	B	505	PHE	2.6
1	J	329	GLY	2.6
2	E	276	ASN	2.6
3	F	508	ARG	2.6
3	F	729	GLY	2.6
1	D	260	PHE	2.6
2	K	426	LEU	2.6
3	F	531	TYR	2.6
2	E	429	LYS	2.6
2	K	477	MET	2.6
2	K	342	ILE	2.6
2	K	166	PHE	2.6
2	K	442	GLN	2.6
1	A	391	LYS	2.6
3	C	356	VAL	2.6
3	I	637	THR	2.6
3	I	648	LEU	2.6
2	H	450	ILE	2.6
1	J	615	LYS	2.6
2	E	491	GLU	2.6
1	J	187	LEU	2.6
3	L	715	ASN	2.6
3	C	385	ILE	2.6
2	E	113	VAL	2.5
2	E	386	ARG	2.5
3	F	223	GLY	2.5
3	F	298	LEU	2.5
1	J	376	PRO	2.5
2	B	487	THR	2.5
3	F	480	VAL	2.5
2	K	171	MET	2.5
2	K	507	MET	2.5
2	K	83	ALA	2.5
3	C	49	TRP	2.5
1	G	58	GLY	2.5
1	D	120	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	K	450	ILE	2.5
3	L	629	SER	2.5
1	D	556	GLN	2.5
3	L	182	GLN	2.5
3	C	546	LEU	2.5
1	D	249	MET	2.5
3	L	336	SER	2.5
2	E	467	TYR	2.5
1	D	549	LEU	2.5
1	D	275	PRO	2.5
2	E	264	GLU	2.5
3	C	322	SER	2.5
3	L	730	ASP	2.5
1	J	464	TYR	2.5
3	L	157	LYS	2.5
2	K	428	GLN	2.5
2	K	318	PHE	2.5
3	F	229	ILE	2.5
1	D	146	HIS	2.5
1	J	370	LEU	2.5
2	K	143	LEU	2.5
3	L	618	LEU	2.5
3	F	696	ILE	2.5
1	D	226	LEU	2.5
1	J	305	TYR	2.5
2	K	625	CYS	2.5
2	E	374	ALA	2.5
3	L	672	ALA	2.5
1	J	294	ASP	2.5
2	E	251	PHE	2.5
3	C	656	PHE	2.5
1	D	613	GLU	2.5
2	E	447	PHE	2.5
2	H	439	ASP	2.5
1	G	145	ILE	2.5
2	E	90	GLU	2.5
2	K	362	MET	2.5
3	I	310	ILE	2.5
2	E	122	LEU	2.4
2	E	133	LEU	2.4
3	F	400	VAL	2.4
1	D	143	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	610	PHE	2.4
2	H	248	ILE	2.4
1	D	655	LEU	2.4
3	I	546	LEU	2.4
3	I	673	GLY	2.4
3	F	540	ASN	2.4
2	E	155	LEU	2.4
3	L	480	VAL	2.4
2	E	318	PHE	2.4
2	K	355	TYR	2.4
2	E	312	ASN	2.4
1	J	119	GLU	2.4
2	E	248	ILE	2.4
2	K	433	LYS	2.4
1	D	14	VAL	2.4
2	E	258	LEU	2.4
3	C	400	VAL	2.4
1	A	277	PHE	2.4
3	F	230	GLU	2.4
3	L	304	GLU	2.4
1	A	39	CYS	2.4
3	C	473	MET	2.4
3	I	512	LEU	2.4
2	E	270	GLY	2.4
2	K	488	GLY	2.4
3	L	473	MET	2.4
1	G	305	TYR	2.4
3	F	481	SER	2.4
1	D	569	GLY	2.4
2	E	225	ASN	2.4
2	K	155	LEU	2.4
3	C	150	GLY	2.4
3	C	547	VAL	2.4
3	I	618	LEU	2.4
3	L	463	VAL	2.4
3	F	546	LEU	2.4
1	G	383	ASN	2.4
2	E	474	GLY	2.4
1	D	49	SER	2.4
2	K	604	LEU	2.4
1	D	481	GLN	2.4
1	D	498	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	332	TRP	2.4
3	L	310	ILE	2.4
1	J	350	ASN	2.4
2	E	25	THR	2.4
2	H	410	GLY	2.4
3	I	294	MET	2.4
3	I	522	GLN	2.4
3	L	729	GLY	2.4
1	J	650	TYR	2.4
2	E	279	LYS	2.4
2	E	69	ILE	2.4
3	L	373	ILE	2.4
2	E	8	LEU	2.4
2	K	122	LEU	2.4
3	F	512	LEU	2.4
3	L	381	LEU	2.4
1	D	35	PHE	2.3
2	H	53	GLY	2.3
2	E	343	MET	2.3
3	L	39	GLN	2.3
2	E	696	PHE	2.3
3	F	434	LEU	2.3
2	B	402	SER	2.3
3	C	478	ILE	2.3
3	F	143	ARG	2.3
3	I	377	ALA	2.3
3	I	562	ILE	2.3
3	L	385	ILE	2.3
3	F	487	GLU	2.3
3	F	524	THR	2.3
2	H	380	TYR	2.3
3	C	457	VAL	2.3
3	I	251	ARG	2.3
1	D	283	LEU	2.3
2	E	95	LEU	2.3
2	E	320	ALA	2.3
2	K	302	ILE	2.3
1	J	196	ARG	2.3
3	F	630	ARG	2.3
1	D	33	ASN	2.3
2	B	360	LYS	2.3
3	C	349	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	527	LEU	2.3
1	A	599	GLU	2.3
2	E	683	LEU	2.3
3	F	310	ILE	2.3
3	F	398	ILE	2.3
2	E	451	VAL	2.3
3	I	128	GLY	2.3
2	H	424	LEU	2.3
1	D	17	ALA	2.3
1	D	710	PHE	2.3
2	K	417	THR	2.3
3	F	389	ARG	2.3
2	H	290	MET	2.3
1	D	711	LEU	2.3
1	D	278	GLN	2.3
3	F	432	HIS	2.3
1	D	315	PHE	2.3
3	F	111	TYR	2.3
3	L	495	VAL	2.3
2	H	425	ASN	2.3
3	F	189	LYS	2.3
2	E	116	GLN	2.3
2	E	344	PHE	2.3
3	F	336	SER	2.3
3	C	295	VAL	2.3
3	C	452	GLU	2.3
1	J	40	THR	2.3
2	K	425	ASN	2.3
1	J	205	PHE	2.3
2	B	50	SER	2.3
2	E	15	GLN	2.3
3	F	426	GLN	2.3
2	B	267	GLU	2.2
2	E	438	TRP	2.2
3	C	99	TRP	2.2
1	D	485	MET	2.2
2	E	41	ASP	2.2
1	D	505	ILE	2.2
1	J	461	LYS	2.2
3	F	354	ILE	2.2
2	H	502	VAL	2.2
3	I	485	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	741	SER	2.2
1	D	360	MET	2.2
1	A	201	ILE	2.2
1	D	503	PHE	2.2
2	E	489	THR	2.2
3	F	141	ILE	2.2
1	D	244	GLY	2.2
1	D	507	GLY	2.2
3	L	737	ARG	2.2
2	E	288	LYS	2.2
3	C	344	LEU	2.2
3	F	234	LEU	2.2
1	J	211	MET	2.2
1	J	503	PHE	2.2
1	A	387	VAL	2.2
1	D	173	THR	2.2
2	E	87	CYS	2.2
2	E	601	ILE	2.2
3	C	310	ILE	2.2
3	F	446	PHE	2.2
3	F	730	ASP	2.2
2	E	247	GLN	2.2
3	I	299	ARG	2.2
2	E	548	LEU	2.2
3	F	399	ILE	2.2
3	L	330	PHE	2.2
3	C	314	ALA	2.2
3	F	56	PRO	2.2
1	D	46	PHE	2.2
1	D	148	PHE	2.2
1	J	607	MET	2.2
3	I	365	MET	2.2
3	L	325	PHE	2.2
1	J	424	GLU	2.2
1	J	478	ASP	2.2
3	C	506	ASP	2.2
3	F	720	GLU	2.2
3	F	376	LYS	2.2
1	A	610	GLU	2.2
1	G	613	GLU	2.2
1	J	355	PRO	2.2
3	F	228	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	366	THR	2.2
3	F	528	THR	2.2
2	H	356	MET	2.2
3	C	328	PHE	2.2
3	I	482	LYS	2.2
3	I	483	MET	2.2
3	L	437	HIS	2.2
1	D	60	SER	2.2
1	G	199	GLU	2.2
2	B	169	ASP	2.2
2	K	370	ALA	2.2
2	E	137	GLN	2.2
3	C	298	LEU	2.2
3	C	620	PRO	2.2
2	B	46	THR	2.2
2	E	528	THR	2.2
3	F	71	ASN	2.2
1	J	138	ILE	2.2
1	D	109	LEU	2.2
1	D	366	LEU	2.2
1	J	369	ALA	2.2
2	E	313	GLN	2.2
2	H	569	GLN	2.2
3	F	482	LYS	2.2
1	D	40	THR	2.2
1	D	145	ILE	2.2
1	G	54	ILE	2.2
2	B	307	THR	2.2
3	I	596	VAL	2.2
3	L	49	TRP	2.2
3	L	331	LYS	2.2
3	L	658	TYR	2.2
1	G	105	PHE	2.2
1	J	229	PHE	2.2
2	E	398	ASP	2.2
2	E	551	PHE	2.2
2	K	593	ASP	2.2
2	B	75	GLU	2.2
2	E	291	THR	2.2
3	C	510	ASN	2.2
3	I	743	ILE	2.2
1	D	281	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	499	TYR	2.2
3	L	344	LEU	2.2
1	D	340	GLN	2.2
2	H	313	GLN	2.2
3	I	300	GLN	2.2
2	B	290	MET	2.2
2	H	475	ILE	2.2
2	K	306	ASN	2.2
2	E	266	LEU	2.1
2	K	415	LEU	2.1
1	J	260	PHE	2.1
1	D	615	LYS	2.1
1	D	676	LEU	2.1
3	L	137	ASN	2.1
2	E	657	TYR	2.1
1	J	46	PHE	2.1
1	D	7	GLN	2.1
1	D	292	ILE	2.1
1	D	155	MET	2.1
1	J	529	ASP	2.1
3	C	384	LEU	2.1
1	J	610	GLU	2.1
2	E	48	GLN	2.1
3	C	355	ARG	2.1
3	F	340	ARG	2.1
3	I	340	ARG	2.1
2	K	219	ILE	2.1
3	C	386	VAL	2.1
3	F	451	ILE	2.1
2	E	411	MET	2.1
3	C	218	LEU	2.1
1	G	200	THR	2.1
2	E	309	TRP	2.1
2	E	381	PHE	2.1
2	K	505	PHE	2.1
3	C	134	HIS	2.1
3	C	186	THR	2.1
3	I	661	THR	2.1
1	J	2	GLU	2.1
3	I	507	GLN	2.1
1	J	12	MET	2.1
2	E	520	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	364	LEU	2.1
3	C	291	GLY	2.1
1	D	124	ARG	2.1
1	J	455	ALA	2.1
2	K	386	ARG	2.1
3	L	52	ALA	2.1
3	L	134	HIS	2.1
3	C	637	THR	2.1
3	F	362	GLU	2.1
3	L	100	ASN	2.1
3	L	720	GLU	2.1
1	J	693	CYS	2.1
2	E	477	MET	2.1
2	K	8	LEU	2.1
3	C	462	GLY	2.1
3	F	150	GLY	2.1
3	L	651	GLY	2.1
1	D	495	ARG	2.1
2	E	388	LYS	2.1
3	L	439	GLN	2.1
2	B	683	LEU	2.1
1	A	229	PHE	2.1
2	K	150	PHE	2.1
2	E	503	ALA	2.1
3	L	449	TRP	2.1
1	D	125	ARG	2.1
1	J	654	GLN	2.1
2	B	372	MET	2.1
2	E	546	MET	2.1
3	F	509	GLY	2.1
3	I	670	LYS	2.1
1	J	39	CYS	2.1
1	A	256	LYS	2.1
1	J	358	LYS	2.1
1	J	379	VAL	2.1
3	C	485	VAL	2.1
3	I	496	VAL	2.1
1	D	543	LEU	2.1
1	J	335	LEU	2.1
3	C	259	LEU	2.1
3	F	628	GLN	2.1
2	K	132	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	416	SER	2.1
2	E	481	LYS	2.1
1	A	606	ASP	2.1
1	J	61	ILE	2.1
1	D	511	LEU	2.1
1	J	52	HIS	2.1
3	C	288	GLN	2.1
3	C	323	PHE	2.1
2	H	46	THR	2.1
2	E	394	PRO	2.1
1	J	500	LEU	2.1
2	B	298	LEU	2.1
2	E	569	GLN	2.1
3	C	340	ARG	2.1
3	I	140	LYS	2.1
1	J	484	PRO	2.1
2	H	337	LEU	2.1
2	K	395	LEU	2.1
3	F	633	PHE	2.0
3	L	236	GLN	2.0
3	L	446	PHE	2.0
1	G	181	GLU	2.0
3	F	737	ARG	2.0
1	D	194	SER	2.0
3	L	506	ASP	2.0
1	D	476	ALA	2.0
2	E	516	GLY	2.0
2	H	74	PRO	2.0
2	K	248	ILE	2.0
3	C	445	LEU	2.0
1	J	4	PHE	2.0
2	B	333	PHE	2.0
3	I	322	SER	2.0
1	J	127	VAL	2.0
2	K	212	VAL	2.0
3	F	704	TYR	2.0
1	D	171	ILE	2.0
3	I	427	ARG	2.0
3	I	90	MET	2.0
1	J	377	GLU	2.0
2	E	742	GLU	2.0
3	F	358	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	331	LYS	2.0
3	F	518	VAL	2.0
2	E	550	LEU	2.0
3	L	298	LEU	2.0
3	L	399	ILE	2.0
1	A	76	PHE	2.0
3	L	656	PHE	2.0
2	E	414	MET	2.0
3	F	448	ASN	2.0
2	E	426	LEU	2.0
2	H	80	SER	2.0
3	F	337	SER	2.0
1	D	13	ILE	2.0
3	C	373	ILE	2.0
1	J	195	GLU	2.0
2	E	417	THR	2.0
1	D	232	TYR	2.0
1	J	469	LEU	2.0
2	H	95	LEU	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 monosaccharides 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.