Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 08:11 AM EDT

PDB ID	:	5UAJ
Title	:	Escherichia coli RNA polymerase RpoB S531L mutant
Authors	:	Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on	:	2016-12-19
Resolution	:	3.92 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 (i) 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 (1)) were used in the production of this report:

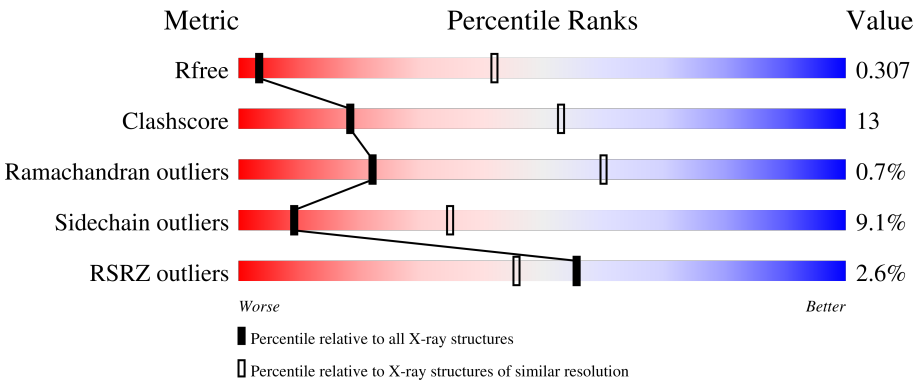
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.92 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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	329	41% 25% • 31%
1	B	329	3% 36% 27% • 35%
1	G	329	2% 43% 21% • 32%
1	H	329	2% 36% 27% • 35%
2	C	1342	3% 63% 33% •

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Mol	Chain	Length	Quality of chain
2	I	1342	3% 67% 30%
3	D	1407	% 54% 25% 17%
3	J	1407	2% 53% 25% 18%
4	E	91	75% 20%
4	K	91	13% 56% 29% 13%
5	F	613	2% 50% 24% 24%
5	L	613	2% 51% 23% 23%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 54994 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1753	1091	311	345	6	0	0	0
1	B	214	1649	1029	290	324	6	0	0	0
1	G	224	1730	1076	308	340	6	0	0	0
1	H	215	1659	1037	291	325	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1342	10587	6644	1843	2056	44	0	0	0
2	I	1340	10568	6632	1840	2053	43	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	531	LEU	SER	engineered mutation	UNP P0A8V2
I	531	LEU	SER	engineered mutation	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1166	9089	5714	1627	1702	46	0	0	0
3	J	1155	9001	5659	1612	1684	46	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	89	691	421	129	140	1	0	0	0
4	K	79	627	382	118	126	1	0	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	468	3813	2389	678	723	23	0	0	0
5	L	469	3821	2393	679	726	23	0	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	D	1	1	1	0	0
6	J	1	1	1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

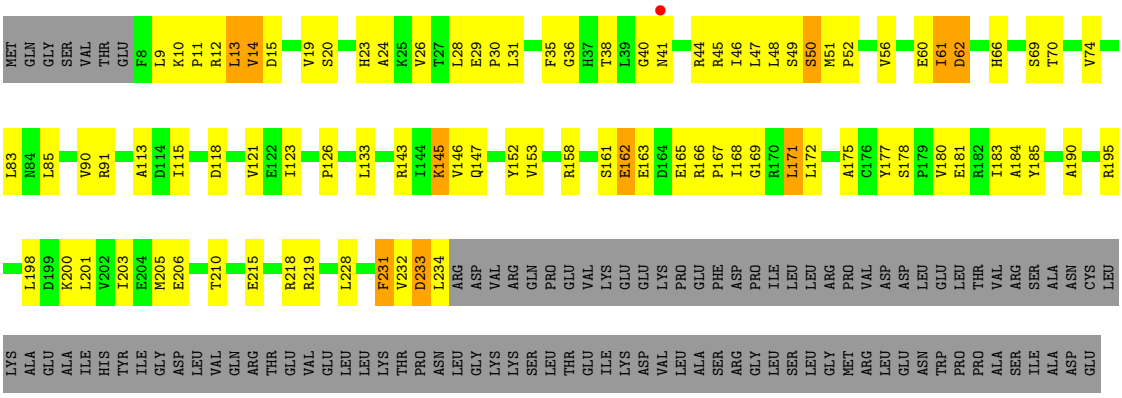
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	D	2	2	2	0	0
7	J	2	2	2	0	0

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.

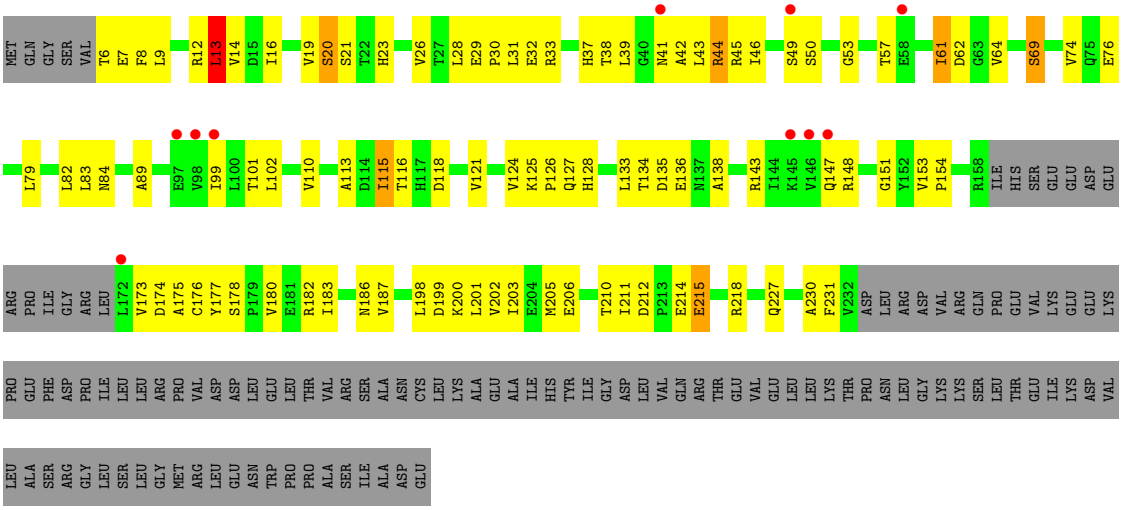
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 41% 25% • 31%



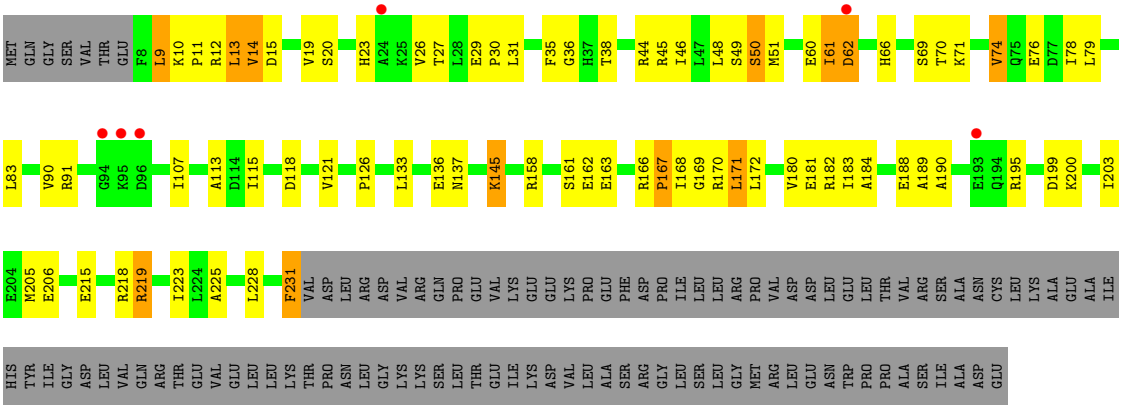
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B: 3% 36% 27% • 35%



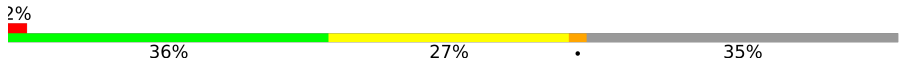
• Molecule 1: DNA-directed RNA polymerase subunit alpha

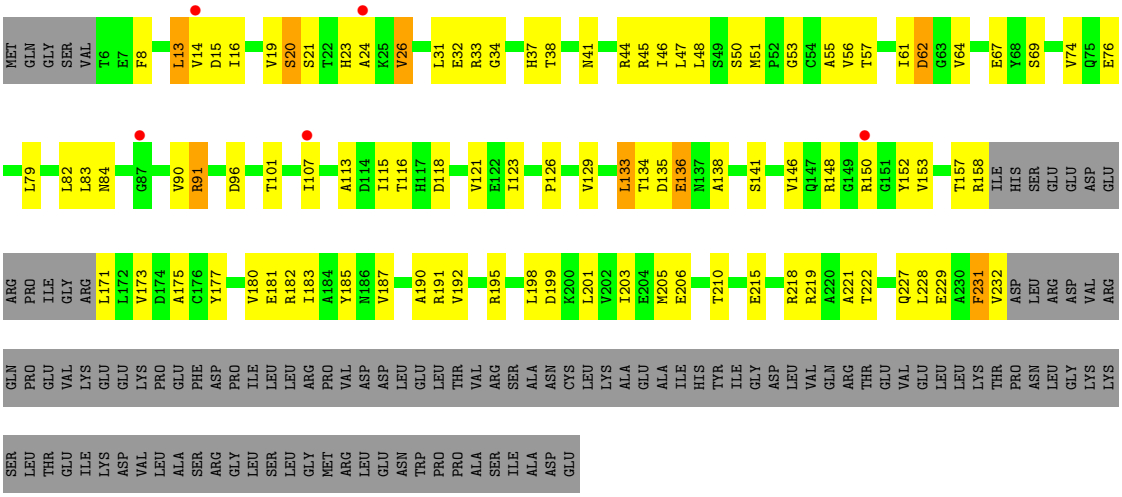
Chain G: 2% 43% 21% • 32%



- Molecule 1: DNA-directed RNA polymerase subunit alpha

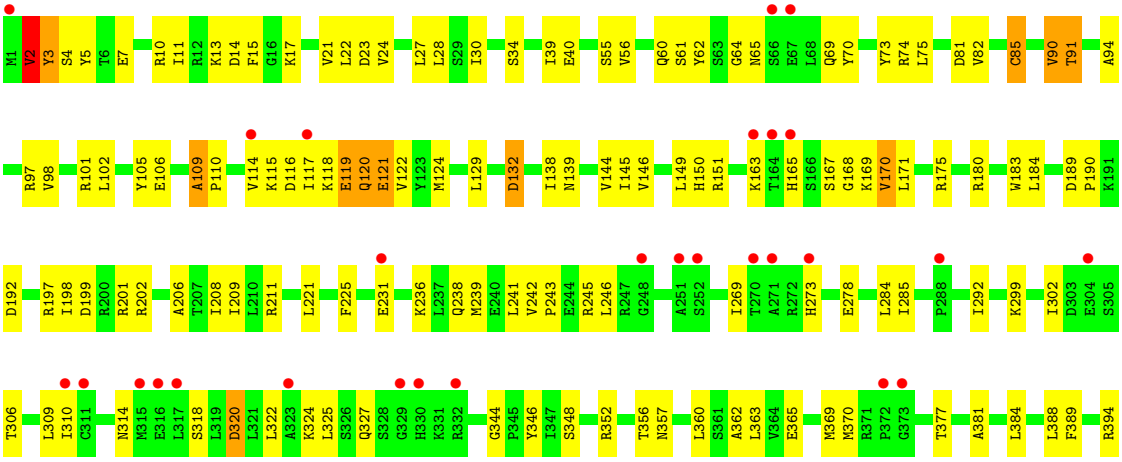
Chain H:

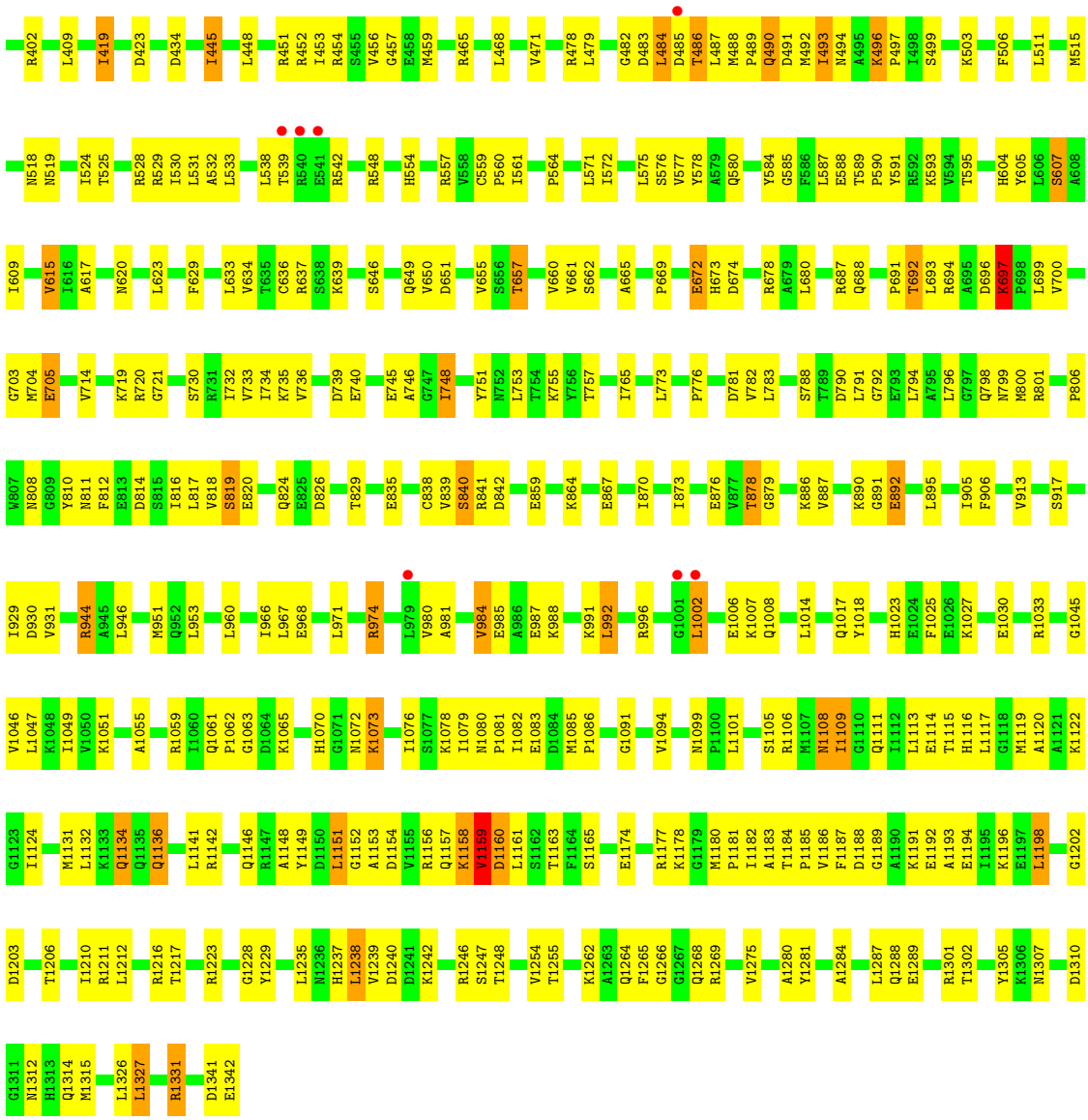




- Molecule 2: DNA-directed RNA polymerase subunit beta

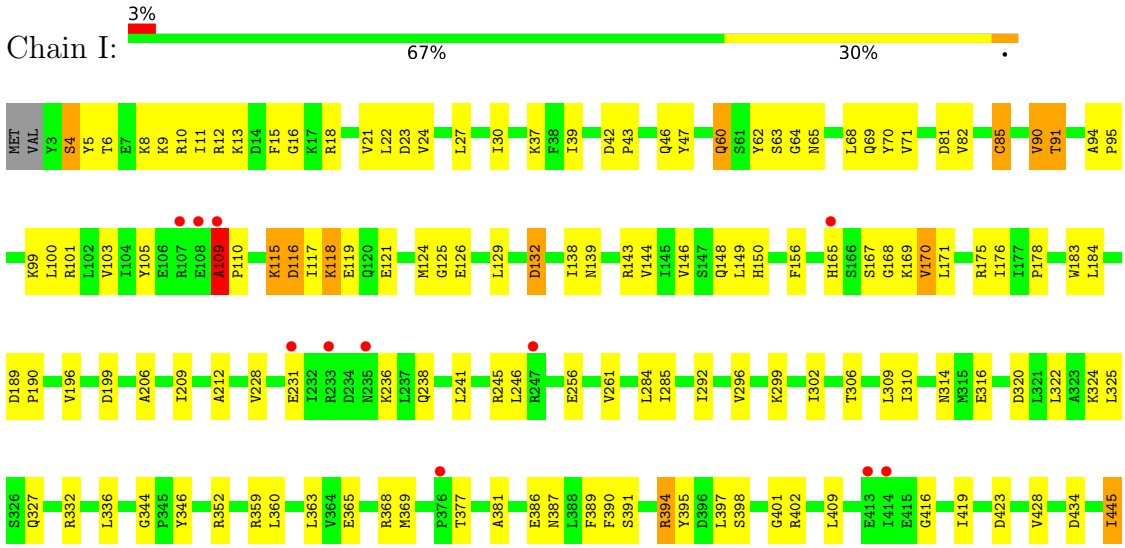
Chain C:

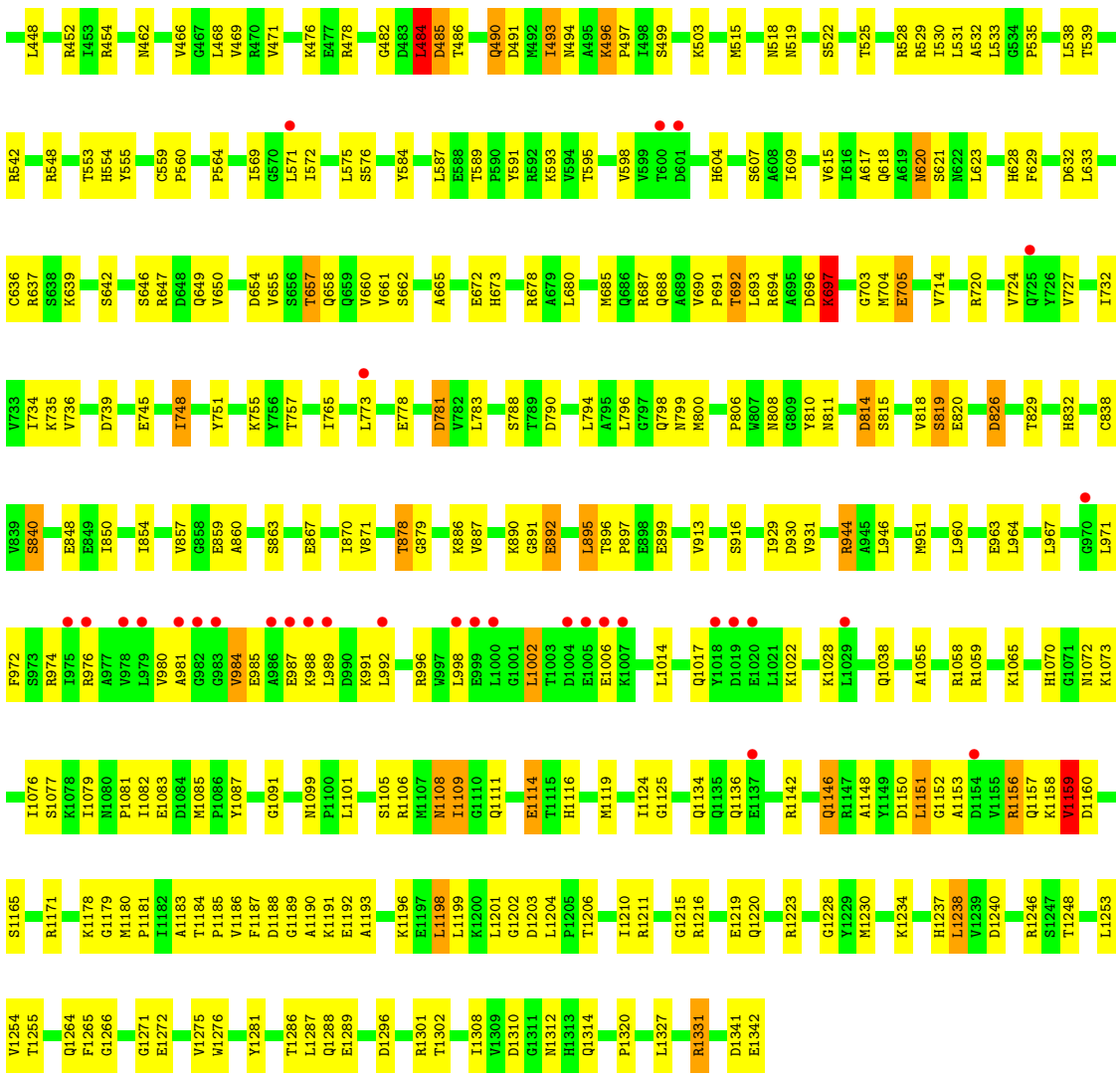




• Molecule 2: DNA-directed RNA polymerase subunit beta

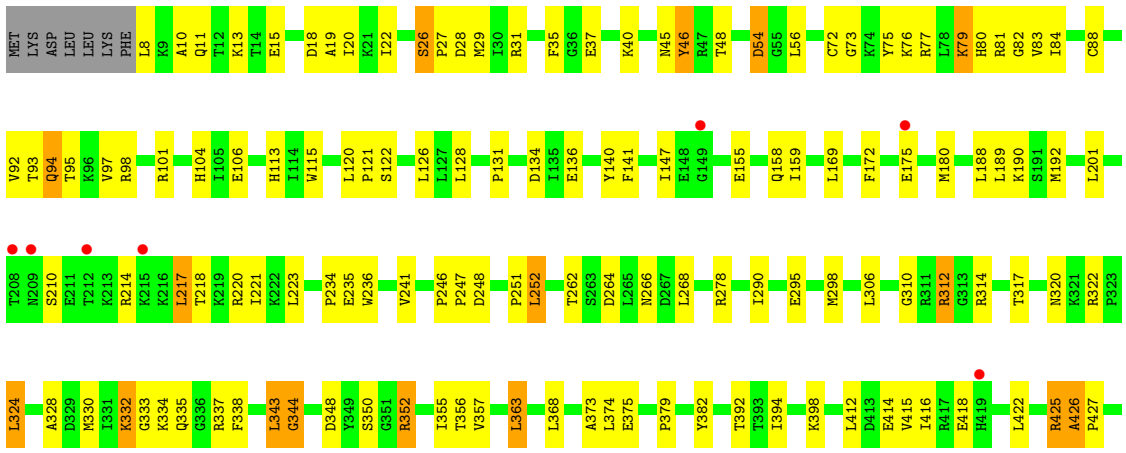
Chain I:

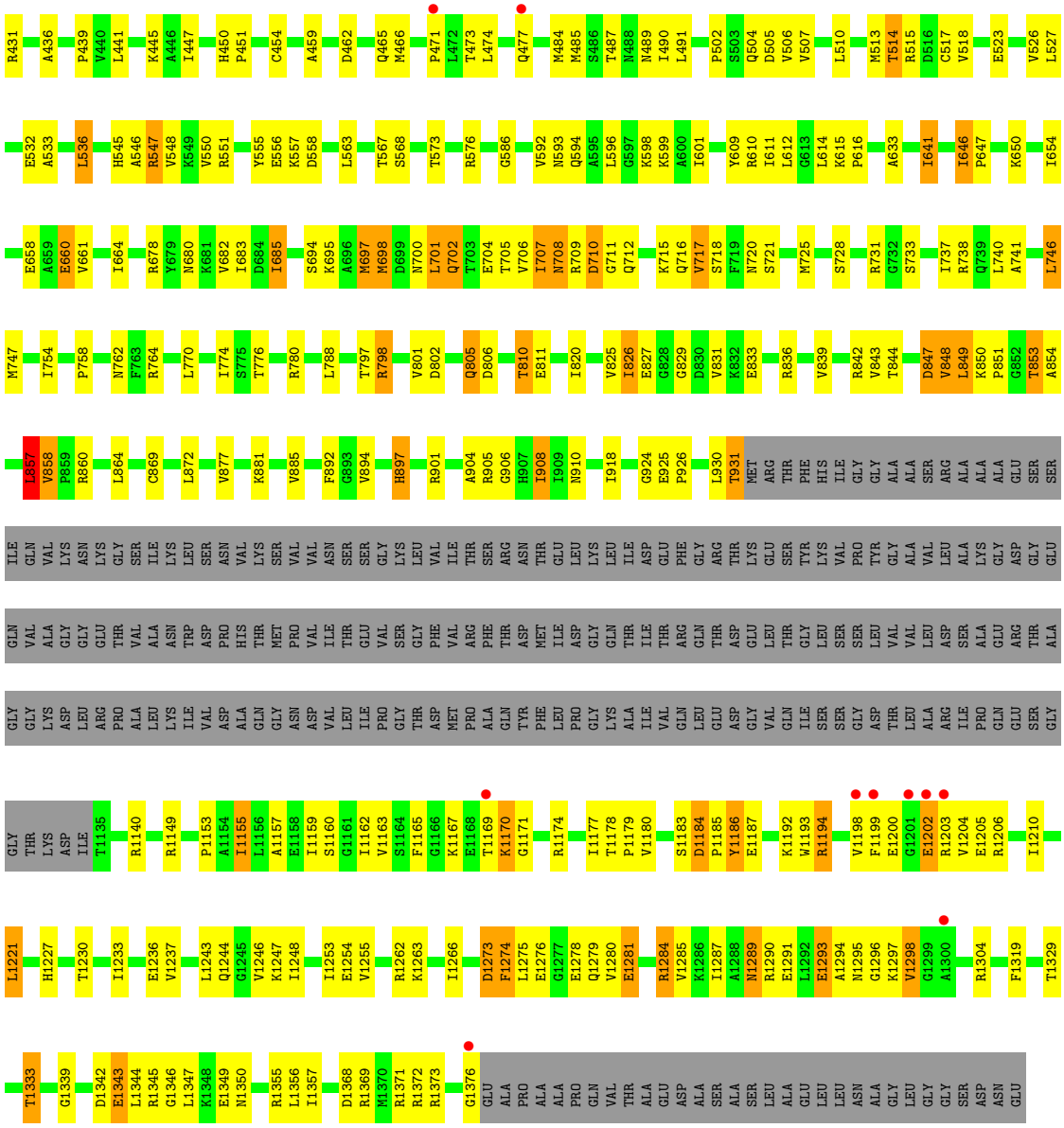




- Molecule 3: DNA-directed RNA polymerase subunit beta'

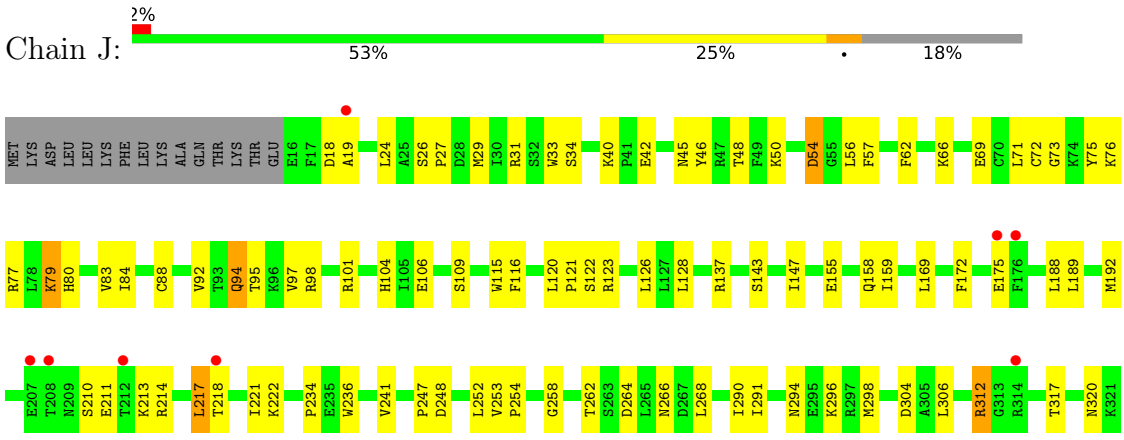
Chain D:

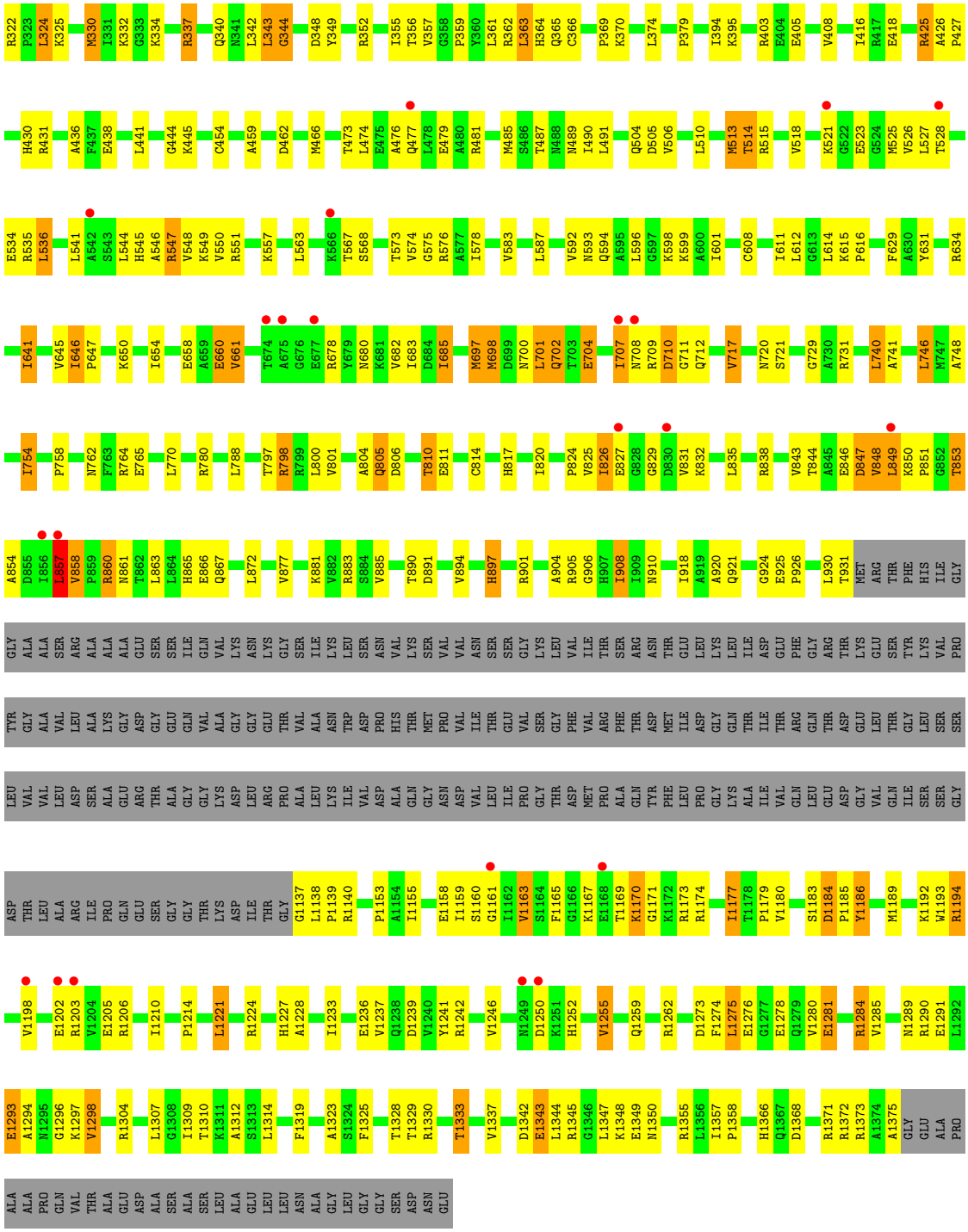




- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:



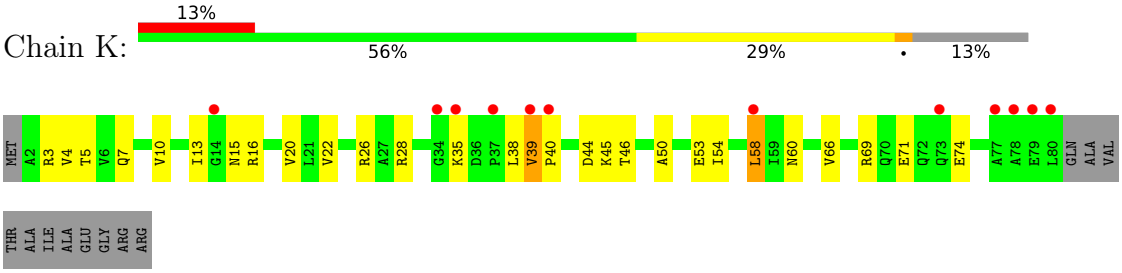


- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

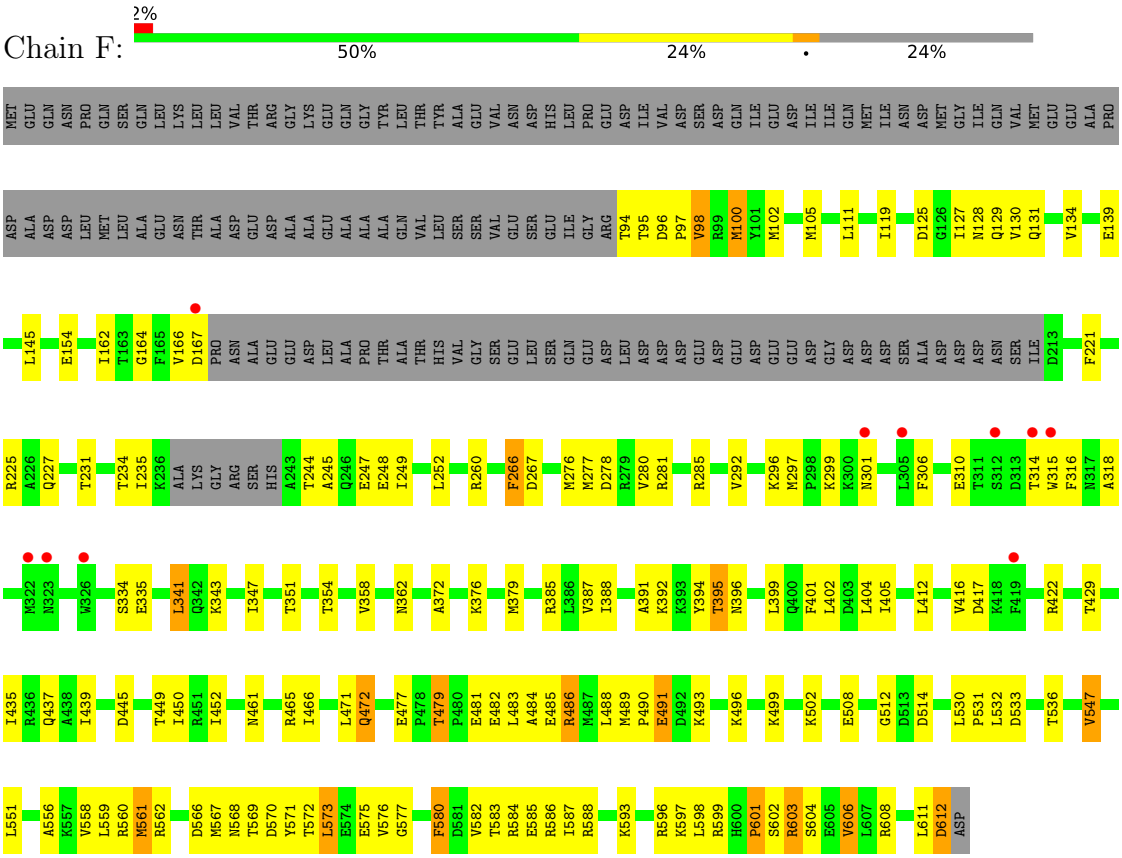
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



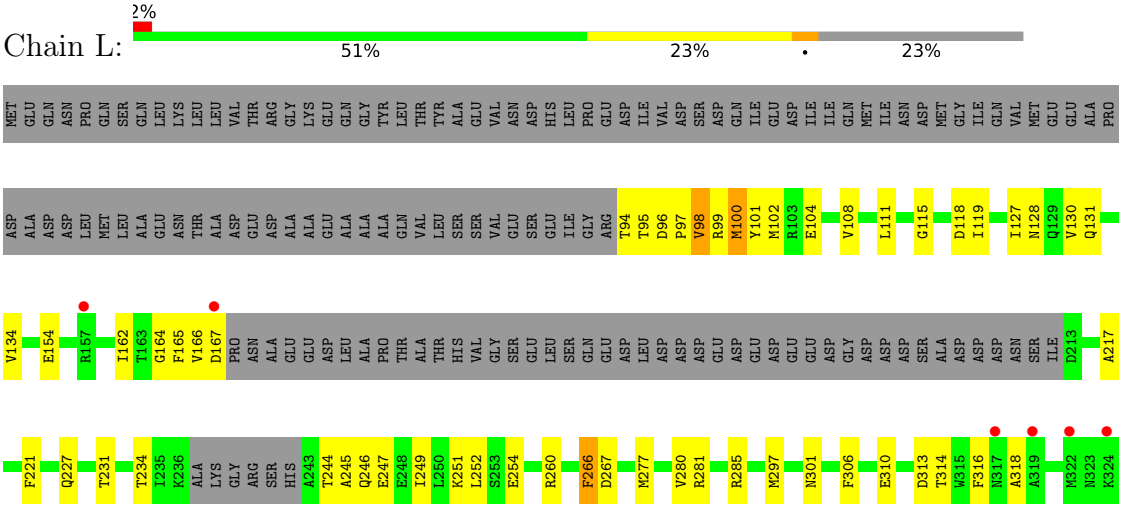
• Molecule 5: RNA polymerase sigma factor RpoD

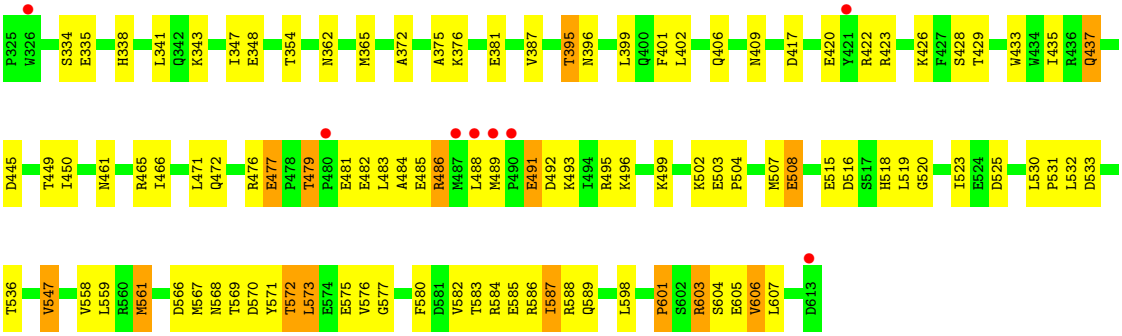
Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:




P325 W326 S334 E335 H338 L341 Q342 K343 I347 E348 T354 N362 M365 A372 A375 K376 E381 V387 T395 N396 L399 Q400 F401 L402 Q406 N409 D417 E420 Y421 R422 R423 K426 F427 S428 T429 W433 W434 I435 R436 Q437
D445 T449 I450 N461 R465 I466 L471 Q472 R476 E477 P478 T479 P480 E481 E482 L483 A484 E485 R486 M487 L488 M489 P490 E491 D492 K493 I494 R495 K496 K499 K502 E503 P504 M507 E508 E515 D516 S517 H518 L519 G520 I523 E524 D525 L530 P531 L532 D533
T536 V547 V558 L559 R560 M561 D566 M567 N568 T569 D570 Y571 T572 L573 E574 E575 V576 G577 F580 D581 V582 T583 R584 E585 R586 I587 R588 Q589 L598 P601 S602 R603 S604 E605 V606 L607 D613

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	187.22Å 204.43Å 310.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.92 29.96 – 3.91	Depositor EDS
% Data completeness (in resolution range)	79.1 (29.96-3.92) 79.1 (29.96-3.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.86Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.260 , 0.307 0.260 , 0.307	Depositor DCC
R_{free} test set	1978 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å^2)	167.5	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 113.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	54994	wwPDB-VP
Average B, all atoms (Å^2)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0.40	1/1774 (0.1%)	0.54	0/2405
1	B	0.32	0/1668	0.70	2/2260 (0.1%)
1	G	0.33	1/1751 (0.1%)	0.54	0/2373
1	H	0.28	0/1678	0.62	0/2274
2	C	0.30	0/10756	0.54	1/14512 (0.0%)
2	I	0.27	0/10737	0.52	1/14487 (0.0%)
3	D	0.32	1/9229 (0.0%)	0.56	2/12459 (0.0%)
3	J	0.29	0/9140	0.54	1/12341 (0.0%)
4	E	0.25	0/693	0.48	0/935
4	K	0.24	0/629	0.47	0/847
5	F	0.26	0/3864	0.51	1/5194 (0.0%)
5	L	0.26	0/3872	0.48	0/5205
All	All	0.30	3/55791 (0.0%)	0.54	8/75292 (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
2	C	0	3
2	I	0	2
3	D	0	2
3	J	0	2
5	F	0	1
5	L	0	1
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	C-N	11.10	1.55	1.34
3	D	426	ALA	C-N	9.32	1.51	1.34
1	G	29	GLU	C-N	7.73	1.49	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	9	LEU	C-N-CA	9.97	146.62	121.70
2	I	109	ALA	C-N-CD	-5.66	108.15	120.60
1	B	13	LEU	CA-CB-CG	5.43	127.80	115.30
3	D	857	LEU	CA-CB-CG	5.22	127.30	115.30
3	J	857	LEU	CA-CB-CG	5.20	127.26	115.30
3	D	344	GLY	N-CA-C	-5.15	100.22	113.10
5	F	602	SER	N-CA-C	-5.06	97.35	111.00
2	C	1160	ASP	C-N-CA	5.05	134.33	121.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	2	VAL	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
5	L	601	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1780	72	0
1	B	1649	0	1673	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1730	0	1756	61	0
1	H	1659	0	1692	72	0
2	C	10587	0	10609	319	0
2	I	10568	0	10582	269	0
3	D	9089	0	9263	265	0
3	J	9001	0	9167	278	0
4	E	691	0	695	13	0
4	K	627	0	634	21	0
5	F	3813	0	3880	96	0
5	L	3821	0	3884	96	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	54994	0	55615	1475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1272:GLU:H	3:J:343:LEU:HD12	1.37	0.90
1:H:32:GLU:HA	1:H:198:LEU:HD22	1.51	0.89
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.54	0.89
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.55	0.88
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.57	0.87
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.54	0.87
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.56	0.85
2:I:18:ARG:NH1	2:I:621:SER:O	2.10	0.84
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.58	0.84
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.59	0.83
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.59	0.83
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.61	0.83
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.61	0.83
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.60	0.82
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.59	0.82
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.62	0.81
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.44	0.80
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.64	0.80
1:B:23:HIS:HB2	1:B:205:MET:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.15	0.79
1:G:45:ARG:HG2	1:H:38:THR:OG1	1.82	0.79
1:A:46:ILE:HD11	1:B:38:THR:HG21	1.65	0.78
2:I:1223:ARG:NH1	3:J:721:SER:OG	2.13	0.78
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.46	0.78
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.66	0.78
5:L:97:PRO:HA	5:L:100:MET:HG3	1.64	0.78
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.66	0.78
5:F:97:PRO:HA	5:F:100:MET:HG3	1.65	0.77
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.16	0.77
1:A:45:ARG:HG2	1:B:38:THR:OG1	1.85	0.77
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.66	0.77
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.50	0.77
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.67	0.76
3:J:337:ARG:HH22	3:J:1323:ALA:HB1	1.50	0.76
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.68	0.76
2:C:490:GLN:HG3	5:F:472:GLN:NE2	2.01	0.76
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.66	0.76
1:H:23:HIS:HB2	1:H:205:MET:O	1.86	0.76
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.67	0.75
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.19	0.75
1:B:29:GLU:OE1	1:B:200:LYS:HE2	1.87	0.75
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.68	0.74
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.20	0.74
2:I:314:ASN:O	2:I:352:ARG:NH1	2.20	0.74
1:H:182:ARG:H	1:H:206:GLU:HB2	1.52	0.74
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.20	0.74
1:B:53:GLY:HA3	1:B:177:TYR:O	1.87	0.74
2:I:560:PRO:O	3:J:780:ARG:NH2	2.19	0.74
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.69	0.74
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.71	0.73
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.51	0.73
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.21	0.73
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.70	0.73
3:J:418:GLU:HG3	4:K:45:LYS:H	1.53	0.73
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.70	0.73
2:C:528:ARG:NH2	2:C:576:SER:O	2.21	0.73
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.54	0.72
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.71	0.72
3:J:700:ASN:O	3:J:704:GLU:HB2	1.89	0.72
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:452:ARG:NH1	2:I:584:TYR:O	2.23	0.72
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.72	0.71
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.70	0.71
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.70	0.71
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.72	0.71
5:F:598:LEU:O	5:F:604:SER:OG	2.09	0.71
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.72	0.71
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.73	0.70
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.73	0.70
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.57	0.70
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.72	0.70
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.72	0.70
3:J:436:ALA:HB3	3:J:485:MET:HA	1.74	0.70
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.25	0.70
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.74	0.70
3:D:901:ARG:HA	3:D:908:ILE:HA	1.74	0.69
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.56	0.69
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.74	0.69
3:D:210:SER:O	3:D:214:ARG:HG2	1.92	0.69
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.58	0.69
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	1.74	0.69
2:C:721:GLY:N	2:C:740:GLU:OE1	2.21	0.69
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.75	0.69
1:G:14:VAL:HG22	1:G:15:ASP:H	1.58	0.69
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.74	0.68
1:H:67:GLU:OE1	1:H:67:GLU:N	2.27	0.68
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.57	0.68
3:J:576:ARG:NH1	3:J:593:ASN:O	2.27	0.68
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.58	0.68
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.25	0.68
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.74	0.67
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.74	0.67
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.42	0.67
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.76	0.67
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.75	0.67
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.76	0.67
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.75	0.67
2:C:1246:ARG:HH11	2:C:1266:GLY:HA2	1.59	0.67
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.59	0.67
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.76	0.67
5:L:598:LEU:O	5:L:604:SER:OG	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.59	0.67
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.77	0.67
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.59	0.67
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.76	0.67
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.77	0.67
3:D:418:GLU:HG3	4:E:45:LYS:H	1.59	0.67
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.77	0.67
3:J:218:THR:HG21	3:J:1275:LEU:HD11	1.77	0.67
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.59	0.67
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.26	0.67
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.77	0.67
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.59	0.67
1:A:233:ASP:OD2	1:A:233:ASP:N	2.27	0.66
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.76	0.66
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.75	0.66
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.59	0.66
2:I:324:LYS:O	2:I:327:GLN:NE2	2.29	0.66
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.95	0.66
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.61	0.66
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.26	0.66
5:F:316:PHE:HZ	5:F:334:SER:HA	1.61	0.66
1:G:38:THR:OG1	1:H:45:ARG:HG2	1.95	0.66
1:G:231:PHE:CZ	1:H:221:ALA:HB3	2.30	0.66
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.78	0.66
2:C:40:GLU:O	2:C:73:TYR:OH	2.15	0.65
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.78	0.65
2:I:499:SER:O	2:I:503:LYS:HB2	1.96	0.65
1:B:214:GLU:O	1:B:218:ARG:HG3	1.96	0.65
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.96	0.65
1:A:23:HIS:HB2	1:A:205:MET:O	1.97	0.65
3:D:436:ALA:HB3	3:D:485:MET:HA	1.78	0.65
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.77	0.65
2:C:1061:GLN:NE2	2:C:1240:ASP:OD2	2.29	0.65
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.79	0.65
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.77	0.65
5:F:573:LEU:H	5:F:573:LEU:HD23	1.61	0.65
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.78	0.65
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.79	0.65
1:G:12:ARG:H	1:G:30:PRO:HD2	1.62	0.65
1:B:118:ASP:H	1:B:121:VAL:HB	1.60	0.65
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.78	0.64
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.79	0.64
5:F:235:ILE:HA	5:F:245:ALA:HB2	1.79	0.64
1:H:79:LEU:HD11	3:J:526:VAL:HG21	1.79	0.64
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	1.80	0.64
2:C:703:GLY:N	2:C:705:GLU:OE2	2.27	0.64
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.79	0.64
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.78	0.64
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.63	0.64
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.80	0.64
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.80	0.64
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.78	0.64
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.31	0.64
3:D:343:LEU:HD13	3:D:344:GLY:HA3	1.79	0.63
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.64	0.63
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.63	0.63
2:C:829:THR:HA	2:C:1059:ARG:HA	1.80	0.63
4:E:80:LEU:O	4:E:84:THR:OG1	2.13	0.63
1:G:45:ARG:NH1	1:H:38:THR:OG1	2.32	0.62
1:H:53:GLY:HA3	1:H:177:TYR:O	1.99	0.62
3:J:514:THR:HB	3:J:576:ARG:HG2	1.81	0.62
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.64	0.62
3:D:741:ALA:O	3:D:762:ASN:ND2	2.32	0.62
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.80	0.62
1:H:195:ARG:HH21	1:H:198:LEU:HD21	1.65	0.62
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.32	0.62
3:J:337:ARG:NH2	3:J:1323:ALA:HB1	2.14	0.62
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.82	0.62
2:C:109:ALA:HB1	2:C:110:PRO:C	2.19	0.62
1:A:14:VAL:HG22	1:A:15:ASP:H	1.65	0.62
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.82	0.62
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.82	0.61
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.81	0.61
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.82	0.61
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.81	0.61
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.82	0.61
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.82	0.61
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.82	0.61
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.15	0.61
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.16	0.61
1:B:79:LEU:HD11	3:D:526:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.35	0.61
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.65	0.61
1:B:182:ARG:H	1:B:206:GLU:HB2	1.65	0.61
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.83	0.61
3:D:576:ARG:NH1	3:D:593:ASN:O	2.34	0.61
3:D:700:ASN:O	3:D:704:GLU:HB2	1.99	0.61
2:I:30:ILE:HD12	2:I:30:ILE:H	1.66	0.61
2:C:1247:SER:HB3	3:D:375:GLU:O	1.99	0.61
3:D:392:THR:HG21	5:F:606:VAL:HA	1.81	0.61
3:D:45:ASN:HB3	3:D:48:THR:O	2.00	0.61
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.83	0.60
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.83	0.60
1:H:190:ALA:N	1:H:198:LEU:O	2.29	0.60
3:J:1159:ILE:HD12	3:J:1206:ARG:HD2	1.83	0.60
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.64	0.60
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.83	0.60
2:C:518:ASN:O	2:C:691:PRO:HD3	2.01	0.60
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.81	0.60
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.65	0.60
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.82	0.60
2:C:30:ILE:HD12	2:C:30:ILE:H	1.64	0.60
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.84	0.60
1:H:153:VAL:H	1:H:175:ALA:HB3	1.67	0.60
1:A:38:THR:OG1	1:B:45:ARG:HG2	2.01	0.60
1:A:161:SER:O	1:A:163:GLU:N	2.35	0.60
1:H:74:VAL:HG12	1:H:76:GLU:H	1.66	0.60
2:I:296:VAL:HB	2:I:336:LEU:HD12	1.83	0.60
2:I:109:ALA:HB1	2:I:110:PRO:C	2.22	0.60
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.32	0.60
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.66	0.60
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.66	0.60
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.67	0.60
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.84	0.60
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.83	0.60
1:G:181:GLU:HB3	1:G:206:GLU:HG3	1.84	0.59
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.84	0.59
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.84	0.59
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.37	0.59
1:G:46:ILE:HD11	1:H:38:THR:HG21	1.83	0.59
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.19	0.59
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ARG:H	1:B:30:PRO:HD2	1.66	0.59
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.84	0.59
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.84	0.59
1:G:9:LEU:HD21	1:G:195:ARG:HH21	1.68	0.59
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.84	0.59
2:I:528:ARG:NH2	2:I:576:SER:O	2.34	0.59
2:C:490:GLN:HG3	5:F:472:GLN:HE21	1.67	0.59
5:F:343:LYS:HD2	5:F:343:LYS:H	1.66	0.59
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.84	0.59
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.36	0.59
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.85	0.59
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.85	0.59
1:B:49:SER:O	1:B:151:GLY:HA2	2.02	0.59
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.85	0.59
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.85	0.59
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.37	0.59
2:C:864:LYS:NZ	2:C:876:GLU:O	2.31	0.59
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.18	0.59
2:C:1223:ARG:NH1	3:D:721:SER:OG	2.24	0.58
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.85	0.58
1:G:231:PHE:HZ	1:H:221:ALA:HB3	1.67	0.58
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.85	0.58
2:C:356:THR:HG21	2:C:362:ALA:HA	1.84	0.58
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.36	0.58
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.85	0.58
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.86	0.58
3:J:211:GLU:OE2	3:J:214:ARG:NH2	2.37	0.58
2:C:1248:THR:HB	5:F:532:LEU:HD11	1.85	0.58
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.32	0.58
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.85	0.58
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.85	0.58
1:G:13:LEU:H	1:G:13:LEU:HD23	1.69	0.58
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.86	0.58
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.67	0.58
1:B:61:ILE:HG22	1:B:62:ASP:H	1.68	0.58
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.37	0.58
1:H:64:VAL:HG11	1:H:69:SER:OG	2.03	0.58
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.85	0.58
3:J:1160:SER:HB2	3:J:1206:ARG:HG2	1.86	0.57
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.05	0.57
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.69	0.57
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.86	0.57
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.85	0.57
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.04	0.57
5:L:164:GLY:O	5:L:260:ARG:HB2	2.04	0.57
3:D:1174:ARG:NH2	3:D:1187:GLU:OE2	2.37	0.57
5:F:388:ILE:O	5:F:392:LYS:HG3	2.05	0.57
3:J:210:SER:O	3:J:214:ARG:HG2	2.05	0.57
1:A:45:ARG:NH1	1:B:38:THR:OG1	2.37	0.57
1:B:113:ALA:HB2	1:B:126:PRO:HB3	1.87	0.57
1:B:212:ASP:CG	1:B:215:GLU:HB2	2.25	0.57
5:F:479:THR:HG23	5:F:481:GLU:H	1.70	0.57
5:F:547:VAL:HG23	5:F:603:ARG:HH11	1.69	0.57
1:G:71:LYS:HB2	1:G:78:ILE:HD11	1.86	0.57
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.87	0.57
3:D:847:ASP:OD1	3:D:847:ASP:N	2.31	0.57
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.68	0.57
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.69	0.56
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.87	0.56
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.70	0.56
3:D:317:THR:HB	3:D:324:LEU:HB3	1.86	0.56
1:A:13:LEU:HD23	1:A:13:LEU:H	1.71	0.56
1:B:82:LEU:HD13	1:B:173:VAL:HG12	1.87	0.56
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.40	0.56
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.86	0.56
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.87	0.56
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.87	0.56
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.86	0.56
3:J:504:GLN:OE1	3:J:731:ARG:NH1	2.39	0.56
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.71	0.56
2:C:197:ARG:NH1	2:C:201:ARG:O	2.38	0.56
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.88	0.56
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.39	0.56
3:J:901:ARG:HD2	3:J:906:GLY:O	2.06	0.56
5:L:508:GLU:HG3	5:L:518:HIS:ND1	2.21	0.56
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.04	0.56
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.39	0.56
5:L:244:THR:O	5:L:247:GLU:HG2	2.06	0.56
1:A:166:ARG:O	1:A:168:ILE:N	2.38	0.56
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.88	0.56
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.87	0.56
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.87	0.56
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.86	0.56
2:C:688:GLN:HB2	2:C:1235:LEU:HD22	1.88	0.56
3:J:45:ASN:HB3	3:J:48:THR:O	2.05	0.56
5:L:585:GLU:OE2	5:L:588:ARG:NH1	2.39	0.56
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.53	0.56
2:I:870:ILE:HB	2:I:944:ARG:HD3	1.87	0.56
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.70	0.56
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.88	0.56
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.87	0.56
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.53	0.56
2:C:615:VAL:HG22	2:C:650:VAL:HA	1.88	0.55
1:H:31:LEU:HB2	1:H:199:ASP:O	2.07	0.55
5:F:461:ASN:O	5:F:465:ARG:HG2	2.06	0.55
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.42	0.55
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.87	0.55
2:C:511:LEU:HD23	2:C:531:LEU:HD12	1.89	0.55
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.72	0.55
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.41	0.55
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.88	0.55
3:D:422:LEU:HD13	3:D:471:PRO:HG3	1.88	0.55
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.87	0.55
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.89	0.55
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.41	0.55
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.88	0.55
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.07	0.55
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.87	0.55
3:D:35:PHE:HD1	3:D:101:ARG:HB3	1.71	0.55
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.70	0.55
5:L:461:ASN:O	5:L:465:ARG:HG2	2.07	0.55
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.88	0.55
1:G:218:ARG:HH11	1:H:232:VAL:HG22	1.71	0.55
2:I:530:ILE:O	2:I:531:LEU:HD23	2.07	0.55
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.38	0.55
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.89	0.55
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.88	0.55
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.42	0.55
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.88	0.55
4:E:50:ALA:O	4:E:54:ILE:HG12	2.07	0.55
1:H:91:ARG:NH2	1:H:210:THR:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:705:GLU:HB2	2:I:794:LEU:H	1.72	0.55
3:J:709:ARG:O	3:J:711:GLY:N	2.40	0.55
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.89	0.55
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.07	0.55
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.87	0.55
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.39	0.55
3:J:905:ARG:NH1	3:J:910:ASN:HD21	2.05	0.55
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.22	0.55
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.89	0.55
2:I:148:GLN:NE2	2:I:535:PRO:O	2.40	0.55
3:J:709:ARG:C	3:J:711:GLY:H	2.10	0.55
5:L:573:LEU:HD23	5:L:573:LEU:H	1.72	0.55
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.89	0.55
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.88	0.55
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.88	0.55
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.72	0.55
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.89	0.54
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.72	0.54
4:E:15:ASN:O	4:E:16:ARG:HB3	2.07	0.54
3:J:1329:THR:O	3:J:1333:THR:OG1	2.23	0.54
5:L:561:MET:HA	5:L:567:MET:HE1	1.89	0.54
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.73	0.54
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.88	0.54
5:L:483:LEU:HD12	5:L:483:LEU:H	1.72	0.54
5:L:582:VAL:CG1	5:L:586:ARG:HG2	2.38	0.54
3:D:515:ARG:NH2	3:D:717:VAL:O	2.40	0.54
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.88	0.54
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.89	0.54
3:D:214:ARG:HA	3:D:217:LEU:HB2	1.90	0.54
3:D:333:GLY:HA3	3:D:338:PHE:CZ	2.42	0.54
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.21	0.54
1:H:67:GLU:OE2	1:H:171:LEU:N	2.39	0.54
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.42	0.54
2:I:228:VAL:HG22	2:I:245:ARG:HH21	1.70	0.54
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.88	0.54
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.90	0.54
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.89	0.54
1:A:83:LEU:HD23	2:C:694:ARG:NE	2.22	0.54
2:C:705:GLU:HB2	2:C:794:LEU:H	1.73	0.54
5:F:314:THR:O	5:F:318:ALA:HB3	2.08	0.54
5:F:395:THR:OG1	5:F:396:ASN:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.89	0.54
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.23	0.54
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.89	0.54
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.08	0.54
2:I:206:ALA:O	2:I:209:ILE:HG22	2.06	0.54
2:I:829:THR:HA	2:I:1059:ARG:HA	1.89	0.54
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.89	0.54
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.90	0.54
2:I:4:SER:OG	2:I:5:TYR:N	2.41	0.54
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.90	0.54
3:J:1307:LEU:HB3	3:J:1312:ALA:HB2	1.90	0.54
5:L:395:THR:OG1	5:L:396:ASN:N	2.38	0.54
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.23	0.54
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.90	0.54
1:G:23:HIS:HB2	1:G:205:MET:O	2.08	0.54
2:C:669:PRO:O	2:C:1070:HIS:HE1	1.90	0.54
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.48	0.54
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.72	0.54
1:B:12:ARG:H	1:B:30:PRO:CD	2.21	0.53
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.90	0.53
2:C:980:VAL:O	2:C:984:VAL:HB	2.08	0.53
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.06	0.53
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.89	0.53
3:J:838:ARG:NH1	3:J:1250:ASP:OD1	2.41	0.53
2:C:617:ALA:HA	2:C:636:CYS:SG	2.48	0.53
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.90	0.53
2:C:170:VAL:HG23	2:C:171:LEU:N	2.24	0.53
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.89	0.53
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.90	0.53
2:C:692:THR:OG1	2:C:693:LEU:N	2.42	0.53
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.90	0.53
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.89	0.53
2:I:47:TYR:OH	2:I:398:SER:HB2	2.08	0.53
2:I:963:GLU:O	2:I:967:LEU:HB2	2.08	0.53
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.90	0.53
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.91	0.53
5:F:166:VAL:O	5:F:167:ASP:HB2	2.08	0.53
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.44	0.53
5:L:601:PRO:HA	5:L:604:SER:HB2	1.90	0.53
5:F:162:ILE:HD13	5:F:221:PHE:HE2	1.73	0.53
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:ARG:O	1:G:168:ILE:N	2.41	0.53
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.89	0.53
2:I:980:VAL:O	2:I:984:VAL:HB	2.08	0.53
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.23	0.53
3:D:514:THR:OG1	3:D:594:GLN:O	2.25	0.53
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.91	0.53
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.23	0.53
3:J:515:ARG:NH2	3:J:717:VAL:O	2.42	0.53
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.89	0.53
1:B:74:VAL:HG12	1:B:76:GLU:H	1.74	0.53
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.91	0.53
2:C:960:LEU:HB3	2:C:1025:PHE:HE2	1.74	0.53
3:D:514:THR:HB	3:D:576:ARG:HG2	1.89	0.53
1:H:205:MET:HG2	1:H:206:GLU:H	1.74	0.53
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.91	0.53
3:J:34:SER:HG	3:J:104:HIS:HD1	1.51	0.53
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.89	0.53
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.90	0.53
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.90	0.53
2:C:102:LEU:HD22	2:C:492:MET:HE1	1.91	0.53
2:C:452:ARG:NH1	2:C:584:TYR:O	2.42	0.53
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.74	0.53
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.09	0.53
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.91	0.52
3:D:854:ALA:HB2	3:J:1372:ARG:HE	1.74	0.52
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.44	0.52
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.39	0.52
3:D:598:LYS:N	3:D:728:SER:O	2.38	0.52
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.09	0.52
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.09	0.52
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.92	0.52
2:C:905:ILE:O	5:F:599:ARG:NH1	2.35	0.52
1:H:48:LEU:HD22	3:J:535:ARG:HD3	1.91	0.52
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.90	0.52
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.45	0.52
5:L:166:VAL:O	5:L:167:ASP:HB2	2.09	0.52
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.75	0.52
3:D:527:LEU:HD22	3:D:533:ALA:HA	1.90	0.52
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.92	0.52
3:D:1376:GLY:O	3:J:853:THR:OG1	2.28	0.52
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.10	0.52
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.91	0.52
2:I:930:ASP:OD2	2:I:931:VAL:N	2.42	0.52
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.92	0.52
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.45	0.52
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.90	0.52
1:H:96:ASP:OD2	1:H:148:ARG:NH1	2.43	0.52
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.90	0.52
3:D:73:GLY:O	3:D:76:LYS:NZ	2.31	0.52
2:I:490:GLN:HG2	2:I:491:ASP:N	2.25	0.52
3:J:901:ARG:HA	3:J:908:ILE:HA	1.91	0.52
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.25	0.52
2:C:1124:ILE:HB	2:C:1180:MET:HB2	1.90	0.52
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.92	0.52
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.92	0.52
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.92	0.52
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.25	0.52
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.25	0.52
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.10	0.52
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.75	0.52
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.43	0.52
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.42	0.51
3:D:709:ARG:C	3:D:711:GLY:H	2.14	0.51
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.91	0.51
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.92	0.51
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.92	0.51
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.92	0.51
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.46	0.51
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.13	0.51
2:C:132:ASP:OD1	2:C:132:ASP:N	2.37	0.51
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.92	0.51
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.45	0.51
3:J:682:VAL:O	3:J:685:ILE:HG12	2.10	0.51
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.93	0.51
3:D:416:ILE:HG23	3:D:439:PRO:HB2	1.91	0.51
5:F:483:LEU:HD12	5:F:483:LEU:H	1.75	0.51
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.92	0.51
3:J:1290:ARG:CG	3:J:1298:VAL:HG12	2.40	0.51
3:D:56:LEU:HD12	3:D:56:LEU:H	1.75	0.51
3:J:337:ARG:HH21	3:J:1328:THR:HG23	1.74	0.51
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:930:ASP:OD2	2:C:931:VAL:N	2.43	0.51
5:F:134:VAL:HG21	5:F:266:PHE:CE1	2.42	0.51
1:H:19:VAL:HG23	1:H:24:ALA:HA	1.91	0.51
2:I:826:ASP:OD1	2:I:829:THR:OG1	2.27	0.51
5:L:227:GLN:HG2	5:L:252:LEU:HA	1.91	0.51
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.93	0.51
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.10	0.51
2:I:170:VAL:HG23	2:I:171:LEU:N	2.25	0.51
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.93	0.51
3:J:356:THR:OG1	3:J:357:VAL:N	2.43	0.51
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.92	0.51
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.93	0.51
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.91	0.51
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.92	0.51
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.43	0.51
2:I:90:VAL:HG12	2:I:91:THR:H	1.75	0.51
2:I:168:GLY:C	2:I:170:VAL:H	2.12	0.51
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.45	0.51
3:J:798:ARG:HH12	3:J:1325:PHE:HB3	1.75	0.51
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.41	0.51
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.74	0.51
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	2.11	0.51
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.46	0.51
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.93	0.51
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.93	0.51
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.44	0.51
3:D:298:MET:SD	5:F:402:LEU:HB3	2.51	0.51
1:G:161:SER:O	1:G:163:GLU:N	2.44	0.51
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.91	0.51
3:J:1184:ASP:O	3:J:1186:TYR:N	2.44	0.51
1:A:228:LEU:HD23	1:A:231:PHE:HD2	1.75	0.50
2:C:27:LEU:O	2:C:528:ARG:NH1	2.42	0.50
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.26	0.50
2:C:1117:LEU:HD11	2:C:1182:ILE:HG21	1.93	0.50
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.93	0.50
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.26	0.50
2:I:12:ARG:HG2	2:I:1183:ALA:HB2	1.92	0.50
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.92	0.50
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.27	0.50
2:C:324:LYS:O	2:C:327:GLN:NE2	2.41	0.50
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.93	0.50
3:D:843:VAL:HG11	3:D:897:HIS:O	2.11	0.50
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.93	0.50
3:J:518:VAL:O	3:J:547:ARG:NH1	2.44	0.50
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.93	0.50
2:C:730:SER:O	2:C:753:LEU:HB2	2.11	0.50
3:D:414:GLU:O	4:E:45:LYS:NZ	2.28	0.50
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.44	0.50
5:F:94:THR:O	5:F:95:THR:OG1	2.27	0.50
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.47	0.50
3:J:34:SER:OG	3:J:104:HIS:ND1	2.40	0.50
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.47	0.50
5:F:582:VAL:CG1	5:F:586:ARG:HG2	2.40	0.50
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.11	0.50
1:B:176:CYS:O	1:B:178:SER:N	2.45	0.50
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.94	0.50
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.12	0.50
1:H:55:ALA:O	1:H:146:VAL:HG13	2.11	0.50
2:I:632:ASP:O	2:I:647:ARG:HB2	2.12	0.50
3:J:213:LYS:O	3:J:217:LEU:HB2	2.11	0.50
4:K:10:VAL:HG13	4:K:16:ARG:HB2	1.93	0.50
5:L:479:THR:HG23	5:L:481:GLU:H	1.76	0.50
2:C:1149:TYR:HE2	2:C:1180:MET:SD	2.35	0.50
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.94	0.50
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.43	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.93	0.50
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.42	0.50
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	1.92	0.50
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.27	0.50
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.94	0.50
5:L:343:LYS:H	5:L:343:LYS:HD2	1.76	0.50
2:C:530:ILE:O	2:C:531:LEU:HD23	2.12	0.50
3:D:122:SER:O	3:D:126:LEU:HG	2.12	0.50
3:D:290:ILE:HD12	3:D:290:ILE:H	1.77	0.50
5:F:585:GLU:HA	5:F:588:ARG:HD3	1.94	0.50
2:I:68:LEU:HD21	2:I:100:LEU:HD13	1.94	0.50
3:J:290:ILE:H	3:J:290:ILE:HD12	1.77	0.50
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.50
5:L:314:THR:O	5:L:318:ALA:HB3	2.12	0.50
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.94	0.50
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.94	0.50
2:I:132:ASP:OD1	2:I:132:ASP:N	2.36	0.50
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.11	0.50
2:I:1114:GLU:OE1	2:I:1230:MET:HA	2.12	0.50
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.77	0.50
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.93	0.50
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.44	0.50
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.12	0.49
2:I:878:THR:OG1	2:I:879:GLY:N	2.43	0.49
3:J:527:LEU:HD21	3:J:536:LEU:HG	1.94	0.49
2:C:13:LYS:O	2:C:1183:ALA:N	2.38	0.49
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.42	0.49
3:D:654:ILE:O	3:D:658:GLU:HB2	2.12	0.49
3:D:842:ARG:NH2	3:D:1254:GLU:OE1	2.39	0.49
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.93	0.49
3:J:801:VAL:O	3:J:805:GLN:HB2	2.12	0.49
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.11	0.49
5:L:245:ALA:O	5:L:249:ILE:HG13	2.12	0.49
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.93	0.49
2:C:886:LYS:H	2:C:917:SER:HB3	1.77	0.49
3:D:709:ARG:O	3:D:711:GLY:N	2.45	0.49
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.78	0.49
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.44	0.49
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.93	0.49
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.93	0.49
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.52	0.49
3:D:77:ARG:HG3	3:D:79:LYS:H	1.77	0.49
3:D:797:THR:O	3:D:801:VAL:HG13	2.12	0.49
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.47	0.49
2:C:878:THR:OG1	2:C:879:GLY:N	2.45	0.49
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.94	0.49
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.16	0.49
2:C:519:ASN:ND2	2:C:796:LEU:HD23	2.25	0.49
3:D:1329:THR:O	3:D:1333:THR:OG1	2.29	0.49
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.12	0.49
2:I:13:LYS:O	2:I:1183:ALA:N	2.27	0.49
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.94	0.49
5:L:507:MET:HG2	5:L:520:GLY:HA3	1.95	0.49
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.94	0.49
3:D:356:THR:OG1	3:D:357:VAL:N	2.46	0.49
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.92	0.49
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.94	0.49
2:C:499:SER:O	2:C:503:LYS:HB2	2.13	0.49
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.95	0.49
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.94	0.49
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.78	0.49
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.27	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.46	0.49
2:I:703:GLY:N	2:I:705:GLU:OE2	2.43	0.49
1:A:169:GLY:O	1:A:171:LEU:HD22	2.13	0.48
2:C:459:MET:SD	2:C:511:LEU:HD13	2.53	0.48
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.94	0.48
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.42	0.48
5:L:507:MET:HG2	5:L:520:GLY:CA	2.43	0.48
3:D:126:LEU:HD13	3:D:223:LEU:HD22	1.95	0.48
3:D:705:THR:OG1	3:D:718:SER:HA	2.13	0.48
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.94	0.48
1:H:192:VAL:HB	1:H:195:ARG:HB2	1.95	0.48
2:I:231:GLU:HG2	2:I:332:ARG:HD3	1.94	0.48
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.53	0.48
2:I:964:LEU:HD11	2:I:1022:LYS:HD2	1.95	0.48
3:J:817:HIS:CD2	3:J:860:ARG:HH21	2.31	0.48
3:J:930:LEU:HD11	3:J:1241:TYR:CZ	2.48	0.48
5:L:246:GLN:HE21	5:L:249:ILE:HD12	1.77	0.48
5:L:532:LEU:HD12	5:L:532:LEU:H	1.77	0.48
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.95	0.48
2:C:402:ARG:NH2	2:C:419:ILE:O	2.47	0.48
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.94	0.48
2:I:818:VAL:HB	2:I:1076:ILE:HD13	1.95	0.48
2:I:1124:ILE:HB	2:I:1180:MET:HB2	1.95	0.48
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.95	0.48
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.94	0.48
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.77	0.48
1:A:44:ARG:HA	1:A:183:ILE:HG21	1.95	0.48
1:B:39:LEU:O	1:B:43:LEU:HD13	2.14	0.48
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.14	0.48
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.48	0.48
5:F:127:ILE:O	5:F:130:VAL:HG22	2.13	0.48
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.94	0.48
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.28	0.48
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.95	0.48
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.95	0.48
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.95	0.48
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.49	0.48
1:H:90:VAL:HG23	1:H:123:ILE:HD13	1.96	0.48
2:I:617:ALA:HA	2:I:636:CYS:SG	2.53	0.48
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.96	0.48
1:B:84:ASN:OD1	3:D:551:ARG:NH2	2.36	0.48
1:B:147:GLN:NE2	1:B:177:TYR:OH	2.45	0.48
2:C:370:MET:HG3	2:C:384:LEU:HD21	1.96	0.48
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.96	0.48
3:D:201:LEU:HD11	3:D:220:ARG:HH11	1.79	0.48
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.95	0.48
1:H:37:HIS:NE2	2:I:1216:ARG:HD2	2.28	0.48
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.96	0.48
3:J:557:LYS:HA	3:J:563:LEU:HA	1.94	0.48
5:L:316:PHE:HZ	5:L:334:SER:HA	1.79	0.48
5:L:372:ALA:O	5:L:376:LYS:HG3	2.12	0.48
1:B:125:LYS:HE2	1:B:128:HIS:CD2	2.49	0.48
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.96	0.48
1:H:82:LEU:HD13	1:H:173:VAL:HG12	1.96	0.48
3:J:19:ALA:HB2	3:J:1373:ARG:NH2	2.29	0.48
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.49	0.48
2:C:2:VAL:O	2:C:3:TYR:HB2	2.14	0.48
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.95	0.48
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.46	0.48
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.77	0.48
2:I:685:MET:HA	2:I:688:GLN:HE21	1.79	0.48
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.78	0.48
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.14	0.48
3:D:825:VAL:C	3:D:826:ILE:HG13	2.33	0.48
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.48	0.48
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.28	0.48
1:G:182:ARG:H	1:G:206:GLU:HB3	1.78	0.48
1:H:152:TYR:CZ	3:J:536:LEU:HD21	2.49	0.48
2:I:778:GLU:O	2:I:781:ASP:HB2	2.14	0.48
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.78	0.48
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.44	0.47
3:D:218:THR:HA	3:D:221:ILE:HG22	1.96	0.47
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.96	0.47
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.13	0.47
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.49	0.47
2:I:819:SER:HB2	2:I:1085:MET:SD	2.54	0.47
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.96	0.47
3:J:800:LEU:HB3	3:J:920:ALA:CB	2.44	0.47
3:J:1174:ARG:HG2	3:J:1189:MET:SD	2.54	0.47
1:G:10:LYS:HA	1:H:227:GLN:NE2	2.29	0.47
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.23	0.47
2:I:637:ARG:HA	2:I:642:SER:HA	1.95	0.47
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.49	0.47
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.96	0.47
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.96	0.47
1:A:61:ILE:HG22	1:A:62:ASP:H	1.80	0.47
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.45	0.47
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.97	0.47
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.96	0.47
5:F:276:MET:O	5:F:280:VAL:HG23	2.13	0.47
2:I:860:ALA:O	2:I:863:SER:OG	2.26	0.47
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.29	0.47
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.14	0.47
2:C:468:LEU:O	2:C:471:VAL:HG12	2.14	0.47
3:D:518:VAL:O	3:D:547:ARG:NH1	2.46	0.47
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.72	0.47
5:F:145:LEU:HB3	5:F:225:ARG:HH21	1.80	0.47
5:F:561:MET:HA	5:F:567:MET:HE1	1.96	0.47
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.96	0.47
1:A:56:VAL:HA	1:A:146:VAL:HG22	1.95	0.47
2:C:184:LEU:HB2	2:C:389:PHE:CE1	2.50	0.47
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.49	0.47
3:D:849:LEU:HB3	3:D:853:THR:HG23	1.97	0.47
4:E:13:ILE:HD12	4:E:19:LEU:HA	1.97	0.47
5:F:227:GLN:HG2	5:F:252:LEU:HA	1.97	0.47
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.45	0.47
1:G:45:ARG:NH1	1:H:34:GLY:O	2.48	0.47
1:H:83:LEU:HD11	3:J:526:VAL:CG2	2.45	0.47
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.14	0.47
2:I:1286:THR:N	3:J:479:GLU:OE2	2.46	0.47
3:J:325:LYS:HE2	3:J:330:MET:HA	1.97	0.47
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.96	0.47
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.14	0.47
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:564:PRO:HG3	2:I:572:ILE:HG13	1.96	0.47
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.96	0.47
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.50	0.47
1:B:134:THR:OG1	1:B:135:ASP:N	2.46	0.47
2:C:580:GLN:HB2	2:C:605:TYR:HE1	1.79	0.47
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.78	0.47
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.15	0.47
3:D:546:ALA:O	3:D:573:THR:HA	2.15	0.47
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.97	0.47
3:D:1184:ASP:O	3:D:1186:TYR:N	2.48	0.47
3:D:1227:HIS:CB	3:J:1293:GLU:HG2	2.44	0.47
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.50	0.47
3:D:1347:LEU:HG	3:D:1357:ILE:HG23	1.97	0.47
5:F:139:GLU:HG2	5:F:351:THR:HA	1.97	0.47
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.96	0.47
2:I:387:ASN:HA	2:I:391:SER:HB2	1.97	0.47
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.95	0.47
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.15	0.47
3:J:592:VAL:HA	3:J:596:LEU:HD21	1.96	0.47
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.96	0.47
3:J:843:VAL:HG11	3:J:897:HIS:O	2.14	0.47
5:L:127:ILE:O	5:L:130:VAL:HG22	2.15	0.47
1:B:89:ALA:O	1:B:124:VAL:HG12	2.15	0.47
2:C:488:MET:O	2:C:490:GLN:N	2.40	0.47
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.46	0.47
3:D:694:SER:OG	3:D:738:ARG:NE	2.48	0.47
5:F:94:THR:HG23	5:F:96:ASP:OD1	2.15	0.47
1:H:183:ILE:HG13	1:H:205:MET:HG3	1.97	0.47
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.96	0.47
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.97	0.47
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.45	0.47
5:L:515:GLU:HG2	5:L:516:ASP:N	2.30	0.47
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.55	0.47
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.80	0.47
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.97	0.47
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.42	0.47
1:A:12:ARG:H	1:A:30:PRO:HD2	1.79	0.47
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.97	0.47
2:C:1109:ILE:HG23	2:C:1113:LEU:HD13	1.96	0.47
3:D:901:ARG:HD2	3:D:906:GLY:O	2.15	0.47
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:GLN:O	3:J:97:VAL:HG23	2.15	0.47
3:J:846:GLU:HA	3:J:860:ARG:HD3	1.97	0.47
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.15	0.47
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.30	0.47
1:B:201:LEU:HG	1:B:203:ILE:HG13	1.96	0.46
2:C:1268:GLN:N	3:D:350:SER:OG	2.38	0.46
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.18	0.46
2:C:1124:ILE:HG21	2:C:1180:MET:HG3	1.97	0.46
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	1.96	0.46
1:H:16:ILE:HG23	1:H:26:VAL:HG13	1.97	0.46
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.30	0.46
3:J:298:MET:SD	5:L:402:LEU:HB3	2.55	0.46
3:J:741:ALA:O	3:J:762:ASN:ND2	2.48	0.46
1:B:19:VAL:O	1:B:20:SER:HB3	2.15	0.46
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.98	0.46
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.50	0.46
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.80	0.46
1:G:188:GLU:O	1:G:200:LYS:N	2.38	0.46
1:G:219:ARG:O	1:G:223:ILE:HG13	2.15	0.46
3:J:1291:GLU:HG2	3:J:1297:LYS:HD3	1.97	0.46
2:C:23:ASP:OD1	2:C:23:ASP:N	2.47	0.46
2:C:314:ASN:O	2:C:352:ARG:NH1	2.41	0.46
2:C:588:GLU:HG3	2:C:605:TYR:HD1	1.79	0.46
2:C:1326:LEU:HD22	3:D:337:ARG:HD3	1.96	0.46
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.97	0.46
3:D:810:THR:HG23	3:D:811:GLU:H	1.80	0.46
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.98	0.46
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.98	0.46
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.47	0.46
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.50	0.46
1:B:57:THR:O	1:B:173:VAL:HG22	2.15	0.46
2:C:169:LYS:O	2:C:169:LYS:HG2	2.14	0.46
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.50	0.46
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.51	0.46
2:C:739:ASP:OD1	2:C:739:ASP:N	2.48	0.46
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.16	0.46
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.30	0.46
1:H:20:SER:OG	1:H:21:SER:N	2.48	0.46
2:I:310:ILE:HD13	2:I:325:LEU:HA	1.98	0.46
3:J:473:THR:HG23	3:J:476:ALA:H	1.81	0.46
2:C:801:ARG:HD3	2:C:1094:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.97	0.46
3:J:846:GLU:HA	3:J:860:ARG:CD	2.46	0.46
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.15	0.46
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.80	0.46
1:A:172:LEU:HD12	1:A:172:LEU:H	1.80	0.46
2:C:81:ASP:O	2:C:85:CYS:HB2	2.15	0.46
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.45	0.46
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	2.16	0.46
3:D:1263:LYS:HE2	3:D:1279:GLN:HE21	1.80	0.46
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	1.98	0.46
5:F:245:ALA:O	5:F:249:ILE:HG13	2.16	0.46
2:I:212:ALA:HA	2:I:359:ARG:HG3	1.96	0.46
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.27	0.46
3:J:810:THR:HG23	3:J:811:GLU:H	1.81	0.46
3:J:825:VAL:C	3:J:826:ILE:HG13	2.36	0.46
2:C:90:VAL:HG12	2:C:91:THR:H	1.81	0.46
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.98	0.46
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.81	0.46
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.51	0.46
5:L:585:GLU:O	5:L:589:GLN:HG3	2.15	0.46
1:A:49:SER:OG	1:A:50:SER:N	2.47	0.46
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.96	0.46
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	1.96	0.46
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.80	0.46
1:G:10:LYS:HE2	1:H:229:GLU:OE1	2.16	0.46
1:H:55:ALA:HB3	1:H:177:TYR:CD1	2.51	0.46
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.98	0.46
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.98	0.46
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.97	0.46
2:C:891:GLY:O	2:C:892:GLU:HG3	2.16	0.46
2:C:1248:THR:HG21	5:F:531:PRO:CG	2.46	0.46
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.97	0.46
3:D:1165:PHE:CE1	3:D:1200:GLU:HB3	2.50	0.46
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.46	0.46
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.98	0.46
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.98	0.46
2:C:119:GLU:HB2	2:C:489:PRO:HB2	1.99	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.15	0.45
2:C:548:ARG:O	3:D:780:ARG:NH1	2.49	0.45
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.98	0.45
3:D:557:LYS:HA	3:D:563:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:125:ASP:O	5:F:129:GLN:HG3	2.16	0.45
5:F:164:GLY:O	5:F:260:ARG:HB2	2.16	0.45
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.98	0.45
1:H:84:ASN:ND2	1:H:129:VAL:O	2.49	0.45
1:H:201:LEU:HG	1:H:203:ILE:HG13	1.98	0.45
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.19	0.45
3:J:122:SER:O	3:J:126:LEU:HG	2.16	0.45
3:J:698:MET:O	3:J:702:GLN:HB3	2.15	0.45
2:C:168:GLY:C	2:C:170:VAL:H	2.19	0.45
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.98	0.45
3:D:328:ALA:O	3:D:332:LYS:HB2	2.16	0.45
5:F:601:PRO:HA	5:F:604:SER:HB2	1.99	0.45
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	1.98	0.45
3:J:222:LYS:HE2	3:J:1276:GLU:OE1	2.17	0.45
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.99	0.45
2:C:122:VAL:HG21	2:C:493:ILE:HG23	1.98	0.45
2:C:169:LYS:HE2	2:C:190:PRO:O	2.16	0.45
2:C:225:PHE:HZ	2:C:348:SER:H	1.63	0.45
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.98	0.45
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.42	0.45
5:F:499:LYS:HA	5:F:502:LYS:HE2	1.98	0.45
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.99	0.45
3:J:79:LYS:HB2	5:L:569:THR:H	1.82	0.45
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.81	0.45
5:L:584:ARG:HH11	5:L:584:ARG:HA	1.80	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.16	0.45
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.98	0.45
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.50	0.45
4:E:10:VAL:HG13	4:E:16:ARG:HB2	1.98	0.45
1:G:49:SER:OG	1:G:50:SER:N	2.48	0.45
1:G:172:LEU:HD12	1:G:172:LEU:H	1.81	0.45
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.96	0.45
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.80	0.45
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.81	0.45
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.98	0.45
3:J:614:LEU:HB3	4:K:7:GLN:HG2	1.99	0.45
3:J:827:GLU:O	3:J:829:GLY:N	2.39	0.45
3:J:1183:SER:OG	3:J:1185:PRO:HD3	2.16	0.45
5:L:94:THR:OG1	5:L:95:THR:N	2.49	0.45
5:L:234:THR:O	5:L:245:ALA:HB2	2.16	0.45
1:A:181:GLU:HB3	1:A:206:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD23	1:B:214:GLU:HG3	1.98	0.45
2:C:1099:ASN:HD21	3:D:505:ASP:CG	2.19	0.45
2:I:735:LYS:HA	2:I:748:ILE:HG22	1.99	0.45
3:J:137:ARG:HD3	3:J:143:SER:OG	2.16	0.45
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.98	0.45
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.83	0.45
3:D:555:TYR:HB2	3:D:586:GLY:HA2	1.99	0.45
2:I:1070:HIS:CD2	2:I:1111:GLN:HA	2.51	0.45
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.98	0.45
1:G:107:ILE:HG13	1:G:136:GLU:HA	1.98	0.45
1:G:189:ALA:HA	1:G:199:ASP:HA	1.98	0.45
1:H:181:GLU:HA	3:J:535:ARG:HH21	1.81	0.45
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.97	0.45
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.99	0.45
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.16	0.45
5:L:433:TRP:O	5:L:437:GLN:HB3	2.16	0.45
1:A:162:GLU:HG3	1:A:165:GLU:HG2	1.99	0.45
1:B:186:ASN:HD22	1:B:202:VAL:HB	1.81	0.45
2:C:55:SER:OG	2:C:56:VAL:N	2.49	0.45
2:C:453:ILE:HD13	2:C:530:ILE:HD12	1.99	0.45
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.98	0.45
3:D:252:LEU:HD23	3:D:262:THR:HB	1.99	0.45
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	1.99	0.45
5:F:466:ILE:HB	5:F:483:LEU:HD23	1.98	0.45
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.67	0.45
2:I:871:VAL:O	2:I:944:ARG:NH1	2.50	0.45
3:J:365:GLN:HA	3:J:438:GLU:H	1.81	0.45
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.31	0.45
5:L:601:PRO:HB2	5:L:605:GLU:HG2	1.98	0.45
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.47	0.45
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.98	0.45
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.49	0.45
2:C:138:ILE:HG22	2:C:139:ASN:N	2.32	0.45
2:C:996:ARG:HA	2:C:996:ARG:HD3	1.58	0.45
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.30	0.45
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.99	0.45
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.99	0.45
2:I:409:LEU:HD21	2:I:428:VAL:HA	1.97	0.45
2:I:896:THR:HB	2:I:897:PRO:HD2	1.99	0.45
3:J:525:MET:O	3:J:548:VAL:HG13	2.16	0.45
5:L:101:TYR:O	5:L:104:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG22	1:A:91:ARG:H	1.82	0.45
1:B:125:LYS:HE2	1:B:128:HIS:HD2	1.82	0.45
1:B:153:VAL:H	1:B:175:ALA:HB3	1.82	0.45
3:D:40:LYS:HB2	3:D:54:ASP:O	2.17	0.45
5:F:296:LYS:HD3	5:F:296:LYS:HA	1.81	0.45
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.99	0.45
1:G:19:VAL:HG13	1:G:20:SER:H	1.81	0.45
2:I:1296:ASP:HB3	2:I:1320:PRO:HB3	1.98	0.45
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.98	0.45
3:J:847:ASP:OD1	3:J:847:ASP:N	2.31	0.45
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.37	0.45
3:D:827:GLU:O	3:D:829:GLY:N	2.38	0.44
1:G:90:VAL:HG22	1:G:91:ARG:H	1.81	0.44
2:I:466:VAL:O	2:I:469:VAL:HG22	2.16	0.44
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.69	0.44
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.98	0.44
5:L:251:LYS:HA	5:L:254:GLU:HG2	1.99	0.44
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.99	0.44
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.98	0.44
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.48	0.44
5:F:96:ASP:O	5:F:98:VAL:N	2.50	0.44
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.44
3:J:362:ARG:H	3:J:365:GLN:HE21	1.64	0.44
3:J:546:ALA:O	3:J:573:THR:HA	2.17	0.44
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.99	0.44
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.67	0.44
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.82	0.44
3:D:19:ALA:O	3:D:20:ILE:HG13	2.18	0.44
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.81	0.44
5:F:145:LEU:HB3	5:F:225:ARG:NH2	2.31	0.44
5:F:571:TYR:CD1	5:F:575:GLU:HG2	2.53	0.44
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.98	0.44
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.17	0.44
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.32	0.44
2:I:739:ASP:OD1	2:I:739:ASP:N	2.49	0.44
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.98	0.44
4:K:15:ASN:O	4:K:16:ARG:HB3	2.17	0.44
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.99	0.44
2:C:149:LEU:HD12	2:C:452:ARG:O	2.17	0.44
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	2.00	0.44
3:D:26:SER:HA	3:D:236:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.98	0.44
2:I:389:PHE:HD1	2:I:395:TYR:CE1	2.36	0.44
5:L:108:VAL:HG11	5:L:381:GLU:C	2.37	0.44
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.99	0.44
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.52	0.44
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.32	0.44
2:C:835:GLU:OE2	2:C:1051:LYS:HD3	2.18	0.44
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.82	0.44
3:J:123:ARG:HD2	3:J:1337:VAL:HG11	1.99	0.44
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.46	0.44
1:B:12:ARG:O	1:B:30:PRO:HD3	2.18	0.44
1:B:16:ILE:HG23	1:B:26:VAL:HG22	2.00	0.44
1:B:20:SER:OG	1:B:21:SER:N	2.50	0.44
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.99	0.44
3:D:885:VAL:HG12	3:D:894:VAL:HG11	2.00	0.44
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.77	0.44
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.99	0.44
3:J:805:GLN:OE1	3:J:1348:LYS:HD3	2.18	0.44
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.47	0.44
5:L:281:ARG:O	5:L:285:ARG:HG3	2.18	0.44
5:L:585:GLU:HA	5:L:588:ARG:HD3	1.98	0.44
5:L:603:ARG:H	5:L:603:ARG:HG2	1.60	0.44
1:B:101:THR:O	1:B:116:THR:HG22	2.18	0.44
1:B:154:PRO:HA	1:B:174:ASP:HB3	1.99	0.44
1:B:211:ILE:HD13	1:B:211:ILE:HA	1.88	0.44
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.83	0.44
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.98	0.44
3:D:682:VAL:O	3:D:685:ILE:HG12	2.18	0.44
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.53	0.44
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.18	0.44
3:J:544:LEU:O	3:J:574:VAL:HB	2.18	0.44
3:J:804:ALA:HA	3:J:1259:GLN:HE21	1.83	0.44
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.99	0.44
5:L:479:THR:HG22	5:L:482:GLU:HB2	2.00	0.44
1:A:218:ARG:HG3	1:B:231:PHE:O	2.18	0.44
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.83	0.44
1:B:187:VAL:HG13	1:B:199:ASP:HB3	1.99	0.44
2:C:4:SER:HB2	2:C:7:GLU:HG3	1.99	0.44
2:C:15:PHE:CE1	2:C:1151:LEU:HD13	2.53	0.44
2:C:615:VAL:HG13	2:C:651:ASP:H	1.83	0.44
3:D:334:LYS:HA	3:D:335:GLN:HA	1.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.99	0.44
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.85	0.44
2:C:577:VAL:HG23	2:C:661:VAL:O	2.18	0.44
2:C:1178:LYS:HA	2:C:1178:LYS:HD3	1.78	0.44
5:F:612:ASP:OD1	5:F:612:ASP:N	2.47	0.44
1:H:107:ILE:HG12	1:H:134:THR:O	2.18	0.44
2:I:24:VAL:HG21	2:I:704:MET:SD	2.58	0.44
2:I:27:LEU:O	2:I:528:ARG:NH1	2.47	0.44
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.16	0.44
5:L:247:GLU:O	5:L:251:LYS:HG3	2.18	0.44
5:L:572:THR:HG23	5:L:575:GLU:HB2	2.00	0.44
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.99	0.43
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.33	0.43
2:I:976:ARG:HD2	2:I:989:LEU:HD23	2.00	0.43
3:J:218:THR:HA	3:J:221:ILE:HG22	2.00	0.43
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.18	0.43
1:A:28:LEU:HB2	1:A:201:LEU:HB3	1.99	0.43
2:C:980:VAL:HA	2:C:984:VAL:HA	2.00	0.43
2:C:1086:PRO:HB2	2:C:1212:LEU:HD23	1.99	0.43
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.82	0.43
3:D:320:ASN:OD1	3:D:322:ARG:HB3	2.18	0.43
1:G:145:LYS:HE3	1:G:145:LYS:HB3	1.88	0.43
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.58	0.43
3:J:748:ALA:HA	3:J:754:ILE:HA	2.00	0.43
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.99	0.43
5:L:96:ASP:O	5:L:98:VAL:N	2.51	0.43
1:A:56:VAL:HG11	1:A:85:LEU:HB3	1.99	0.43
2:C:1132:LEU:HD11	2:C:1174:GLU:HG2	2.00	0.43
3:D:189:LEU:HD22	3:D:234:PRO:HB3	2.01	0.43
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.68	0.43
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.75	0.43
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.83	0.43
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.33	0.43
2:I:138:ILE:HG22	2:I:139:ASN:N	2.33	0.43
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	2.00	0.43
3:J:583:VAL:HG21	3:J:592:VAL:HG11	2.00	0.43
5:L:348:GLU:HG2	5:L:354:THR:HA	1.99	0.43
5:L:533:ASP:O	5:L:536:THR:N	2.48	0.43
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.52	0.43
2:C:867:GLU:H	2:C:867:GLU:HG3	1.53	0.43
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.81	0.43
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.43
5:F:499:LYS:HB2	5:F:499:LYS:HE3	1.84	0.43
1:H:13:LEU:HD23	1:H:13:LEU:H	1.82	0.43
2:I:91:THR:HG21	2:I:503:LYS:NZ	2.33	0.43
2:I:548:ARG:HB3	2:I:569:ILE:O	2.18	0.43
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.18	0.43
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.18	0.43
3:J:291:ILE:HG12	5:L:409:ASN:HD22	1.83	0.43
5:L:582:VAL:O	5:L:587:ILE:HD12	2.18	0.43
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.00	0.43
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.66	0.43
5:F:391:ALA:HB3	5:F:405:ILE:HG22	2.00	0.43
5:F:394:TYR:HB2	5:F:404:LEU:HD13	2.00	0.43
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.34	0.43
3:J:740:LEU:HD12	3:J:740:LEU:HA	1.74	0.43
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.16	0.43
1:B:212:ASP:OD2	1:B:215:GLU:HB2	2.18	0.43
2:C:629:PHE:HE2	2:C:650:VAL:HG21	1.80	0.43
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	2.01	0.43
3:J:56:LEU:HD12	3:J:56:LEU:H	1.82	0.43
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.33	0.43
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.01	0.43
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.53	0.43
2:C:992:LEU:H	2:C:992:LEU:HD23	1.84	0.43
5:F:354:THR:O	5:F:358:VAL:HG23	2.18	0.43
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.53	0.43
2:I:115:LYS:HG3	2:I:485:ASP:OD2	2.17	0.43
3:J:317:THR:HG22	3:J:322:ARG:O	2.19	0.43
1:A:19:VAL:HG13	1:A:20:SER:H	1.83	0.43
1:B:31:LEU:HB2	1:B:199:ASP:O	2.19	0.43
2:C:318:SER:OG	2:C:320:ASP:OD2	2.32	0.43
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.54	0.43
2:C:1160:ASP:HB2	2:C:1163:THR:OG1	2.18	0.43
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.01	0.43
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.87	0.43
5:F:244:THR:O	5:F:247:GLU:HG2	2.18	0.43
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.84	0.43
2:I:15:PHE:CG	2:I:1190:ALA:HB2	2.54	0.43
2:I:150:HIS:CD2	2:I:454:ARG:HE	2.36	0.43
2:I:618:GLN:HG3	2:I:620:ASN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.54	0.43
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.75	0.43
2:I:1077:SER:HA	3:J:356:THR:OG1	2.18	0.43
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.48	0.43
3:J:521:LYS:HE3	3:J:541:LEU:O	2.19	0.43
1:A:40:GLY:HA3	1:A:185:TYR:CD2	2.54	0.43
1:A:47:LEU:O	1:A:180:VAL:HG21	2.18	0.43
1:A:48:LEU:HA	1:A:180:VAL:HG21	2.01	0.43
1:B:28:LEU:HD23	1:B:31:LEU:HD11	2.00	0.43
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.84	0.43
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.99	0.43
1:G:225:ALA:HB2	1:H:228:LEU:HD12	2.01	0.43
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.00	0.43
3:J:646:ILE:H	3:J:646:ILE:HG12	1.64	0.43
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.53	0.43
5:L:519:LEU:HD23	5:L:523:ILE:HD11	2.01	0.43
2:C:840:SER:O	2:C:1047:LEU:N	2.49	0.43
1:G:35:PHE:HE1	1:H:46:ILE:HG23	1.84	0.43
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.54	0.43
1:G:74:VAL:HG22	1:G:76:GLU:H	1.84	0.43
2:I:165:HIS:CD2	2:I:190:PRO:HG2	2.54	0.43
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.54	0.43
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.32	0.43
2:I:484:LEU:CD1	2:I:485:ASP:H	2.32	0.43
2:I:811:ASN:HB2	2:I:1099:ASN:HB2	2.01	0.43
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.49	0.43
3:J:264:ASP:HB3	3:J:324:LEU:HB2	2.01	0.43
1:A:201:LEU:HG	1:A:203:ILE:HG13	2.01	0.42
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.99	0.42
5:F:231:THR:HG23	5:F:249:ILE:HG12	2.00	0.42
5:F:580:PHE:HD1	5:F:580:PHE:HA	1.66	0.42
1:H:14:VAL:HG13	1:H:15:ASP:N	2.34	0.42
1:H:51:MET:O	1:H:150:ARG:HA	2.19	0.42
2:I:1038:GLN:O	2:I:1038:GLN:HG3	2.19	0.42
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.39	0.42
3:J:925:GLU:HB3	3:J:926:PRO:HD3	2.01	0.42
3:J:1241:TYR:HD2	3:J:1246:VAL:HG11	1.83	0.42
2:C:15:PHE:CE1	2:C:1194:GLU:HB3	2.54	0.42
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.19	0.42
2:C:719:LYS:N	2:C:751:TYR:OH	2.35	0.42
2:C:782:VAL:HG11	2:C:792:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:HD3	2:C:1161:LEU:CD1	2.49	0.42
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.54	0.42
3:D:425:ARG:HD2	3:D:459:ALA:HB2	2.00	0.42
5:F:532:LEU:HD12	5:F:532:LEU:H	1.84	0.42
5:F:562:ARG:HH21	5:F:573:LEU:HD22	1.83	0.42
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.91	0.42
1:G:166:ARG:N	1:G:167:PRO:HD2	2.34	0.42
2:I:292:ILE:HD12	2:I:322:LEU:HD11	2.01	0.42
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	2.00	0.42
2:C:165:HIS:CD2	2:C:190:PRO:HG2	2.55	0.42
2:C:490:GLN:HG2	2:C:491:ASP:N	2.33	0.42
2:C:906:PHE:CZ	5:F:608:ARG:HG3	2.54	0.42
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.54	0.42
3:D:1198:VAL:HG11	3:D:1210:ILE:HG23	2.00	0.42
4:E:8:ASP:HB2	4:E:55:GLU:HG2	2.01	0.42
2:I:402:ARG:HG2	2:I:416:GLY:H	1.84	0.42
2:I:891:GLY:O	2:I:892:GLU:HG3	2.19	0.42
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.91	0.42
1:A:153:VAL:HB	1:A:175:ALA:HB3	2.00	0.42
1:B:89:ALA:HB1	1:B:210:THR:CG2	2.47	0.42
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.01	0.42
3:D:931:THR:O	3:D:931:THR:OG1	2.34	0.42
1:G:44:ARG:HG3	1:G:183:ILE:HG22	2.01	0.42
1:G:79:LEU:HD11	2:I:693:LEU:HD21	2.01	0.42
2:I:494:ASN:HB3	2:I:497:PRO:HD2	2.00	0.42
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	2.00	0.42
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.83	0.42
3:J:746:LEU:HB2	3:J:754:ILE:HD11	2.01	0.42
3:J:850:LYS:HB3	3:J:851:PRO:HD2	2.01	0.42
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.54	0.42
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.84	0.42
2:C:24:VAL:HG21	2:C:704:MET:SD	2.59	0.42
2:C:557:ARG:HH21	2:C:607:SER:C	2.23	0.42
3:D:11:GLN:CG	3:D:15:GLU:HG3	2.48	0.42
3:D:592:VAL:HA	3:D:596:LEU:HD21	2.01	0.42
5:F:593:LYS:HA	5:F:596:ARG:HB3	2.02	0.42
1:G:137:ASN:OD1	1:G:137:ASN:N	2.51	0.42
1:H:56:VAL:HG22	1:H:146:VAL:HG22	2.01	0.42
2:I:101:ARG:HE	2:I:118:LYS:HD2	1.83	0.42
2:I:981:ALA:O	2:I:1002:LEU:HD11	2.19	0.42
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:42:GLU:OE1	3:J:42:GLU:N	2.52	0.42
3:J:405:GLU:O	3:J:408:VAL:HG22	2.20	0.42
2:C:211:ARG:NH1	2:C:357:ASN:O	2.52	0.42
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.02	0.42
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.32	0.42
1:H:90:VAL:HG22	1:H:91:ARG:H	1.84	0.42
2:I:169:LYS:O	2:I:170:VAL:HG22	2.19	0.42
2:I:522:SER:O	2:I:525:THR:HG22	2.20	0.42
2:I:1178:LYS:HA	2:I:1178:LYS:HD3	1.81	0.42
3:J:364:HIS:CD2	4:K:4:VAL:HG23	2.55	0.42
3:J:514:THR:OG1	3:J:594:GLN:O	2.35	0.42
3:J:849:LEU:HD13	3:J:849:LEU:H	1.84	0.42
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	2.02	0.42
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.55	0.42
5:L:130:VAL:HB	5:L:365:MET:HG3	2.01	0.42
2:C:175:ARG:HD3	2:C:183:TRP:CE3	2.55	0.42
2:C:496:LYS:HB3	2:C:496:LYS:HE3	1.80	0.42
2:C:1269:ARG:CG	3:D:343:LEU:HD12	2.50	0.42
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.83	0.42
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	2.02	0.42
5:F:292:VAL:HG21	5:F:299:LYS:HG2	2.02	0.42
1:H:74:VAL:HG22	1:H:133:LEU:HD12	2.02	0.42
2:I:176:ILE:HB	2:I:184:LEU:HB3	2.02	0.42
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.84	0.42
3:J:77:ARG:HG3	3:J:79:LYS:H	1.85	0.42
5:L:476:ARG:HG3	5:L:477:GLU:N	2.34	0.42
1:A:10:LYS:HA	1:B:227:GLN:NE2	2.35	0.42
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.53	0.42
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.20	0.42
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.50	0.42
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.85	0.42
2:I:448:LEU:HG	2:I:553:THR:OG1	2.20	0.42
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.84	0.42
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	2.01	0.42
3:J:824:PRO:HD3	3:J:835:LEU:HD13	2.02	0.42
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	2.01	0.42
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.20	0.42
1:A:177:TYR:O	1:A:178:SER:HB2	2.20	0.42
1:A:232:VAL:O	1:B:218:ARG:HG2	2.20	0.42
1:B:180:VAL:HB	1:B:183:ILE:CD1	2.49	0.42
2:C:75:LEU:HD13	2:C:75:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.86	0.42
2:C:184:LEU:HD13	2:C:389:PHE:CZ	2.55	0.42
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.87	0.42
2:C:842:ASP:N	2:C:1045:GLY:O	2.53	0.42
2:C:1023:HIS:O	2:C:1027:LYS:HG2	2.20	0.42
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	2.02	0.42
5:F:493:LYS:HA	5:F:496:LYS:HE2	2.02	0.42
1:G:13:LEU:HD22	1:H:231:PHE:CE1	2.55	0.42
3:J:416:ILE:HG12	3:J:441:LEU:HD21	2.01	0.42
3:J:425:ARG:HG2	3:J:426:ALA:H	1.84	0.42
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.61	0.42
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.35	0.42
4:K:22:VAL:HG11	4:K:60:ASN:HA	2.02	0.42
2:C:292:ILE:HB	2:C:322:LEU:HD11	2.02	0.42
3:D:75:TYR:CE2	3:D:83:VAL:HG21	2.54	0.42
3:D:733:SER:O	3:D:737:ILE:HG12	2.20	0.42
5:F:412:LEU:HB2	5:F:435:ILE:HD11	2.01	0.42
2:I:256:GLU:HB3	2:I:261:VAL:HG22	2.02	0.42
2:I:757:THR:HG23	2:I:765:ILE:HG23	2.02	0.42
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.01	0.42
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.51	0.42
2:C:10:ARG:NH2	2:C:791:LEU:HB2	2.33	0.41
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.35	0.41
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.41
2:I:867:GLU:H	2:I:867:GLU:HG3	1.70	0.41
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.35	0.41
3:J:27:PRO:HB3	3:J:241:VAL:HG23	2.00	0.41
3:J:528:THR:O	3:J:551:ARG:HB3	2.20	0.41
2:C:1131:MET:HE2	2:C:1141:LEU:HA	2.01	0.41
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.77	0.41
3:D:646:ILE:H	3:D:646:ILE:HG12	1.62	0.41
3:D:1183:SER:OG	3:D:1185:PRO:HD3	2.20	0.41
1:G:14:VAL:HG12	1:G:27:THR:O	2.19	0.41
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.18	0.41
1:A:91:ARG:HD3	1:A:210:THR:O	2.20	0.41
2:C:198:ILE:HD13	2:C:388:LEU:HD13	2.01	0.41
2:C:820:GLU:HA	2:C:1079:ILE:HD11	2.01	0.41
3:D:487:THR:HG21	4:E:4:VAL:HG23	2.03	0.41
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.20	0.41
3:D:650:LYS:HE2	3:D:654:ILE:HD11	2.03	0.41
3:D:708:ASN:OD1	3:D:708:ASN:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:801:VAL:O	3:D:805:GLN:HB2	2.19	0.41
3:D:926:PRO:HG2	3:D:1248:ILE:HD11	2.02	0.41
5:F:569:THR:OG1	5:F:570:ASP:N	2.52	0.41
1:H:101:THR:H	1:H:116:THR:CG2	2.33	0.41
2:I:870:ILE:HG21	2:I:931:VAL:HG11	2.03	0.41
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.54	0.41
3:J:54:ASP:N	3:J:54:ASP:OD1	2.53	0.41
3:J:596:LEU:HD12	3:J:601:ILE:HG13	2.02	0.41
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.32	0.41
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.36	0.41
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.55	0.41
5:L:499:LYS:HA	5:L:502:LYS:HE2	2.01	0.41
2:C:5:TYR:CE2	2:C:776:PRO:HB2	2.54	0.41
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	2.02	0.41
2:C:1063:GLY:HA3	2:C:1239:VAL:HB	2.02	0.41
3:D:264:ASP:HB3	3:D:324:LEU:HB2	2.02	0.41
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.53	0.41
1:G:51:MET:HE3	1:G:51:MET:HB3	1.90	0.41
1:G:169:GLY:O	1:G:171:LEU:HD22	2.20	0.41
2:I:462:ASN:O	2:I:466:VAL:HG23	2.21	0.41
2:I:811:ASN:C	2:I:815:SER:HB2	2.41	0.41
2:I:1219:GLU:OE2	3:J:634:ARG:NE	2.53	0.41
2:I:1271:GLY:HA2	3:J:344:GLY:HA3	2.02	0.41
2:I:1281:TYR:OH	3:J:431:ARG:O	2.35	0.41
1:A:51:MET:HE3	1:A:52:PRO:HD2	2.03	0.41
1:A:145:LYS:HB3	1:A:145:LYS:HE3	1.90	0.41
2:C:145:ILE:HA	2:C:511:LEU:O	2.21	0.41
2:C:180:ARG:NH2	2:C:465:ARG:HH22	2.18	0.41
3:D:609:TYR:HD1	3:D:610:ARG:HH11	1.68	0.41
3:D:698:MET:O	3:D:702:GLN:HB3	2.20	0.41
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	2.20	0.41
2:I:62:TYR:C	2:I:64:GLY:H	2.24	0.41
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.20	0.41
3:J:1224:ARG:HB3	3:J:1228:ALA:CB	2.50	0.41
5:L:111:LEU:HA	5:L:111:LEU:HD23	1.78	0.41
1:A:118:ASP:H	1:A:121:VAL:HB	1.86	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
2:C:808:ASN:H	3:D:633:ALA:HB2	1.86	0.41
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.35	0.41
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.21	0.41
3:D:278:ARG:HD2	3:D:295:GLU:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:310:GLY:HA2	3:D:314:ARG:HG2	2.03	0.41
1:H:37:HIS:NE2	1:H:187:VAL:HG21	2.35	0.41
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.34	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.03	0.41
3:J:474:LEU:HA	3:J:477:GLN:HG3	2.03	0.41
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.75	0.41
1:B:64:VAL:HG11	1:B:69:SER:HB2	2.03	0.41
2:C:97:ARG:HB3	2:C:121:GLU:HB2	2.02	0.41
2:C:981:ALA:O	2:C:1002:LEU:HD11	2.21	0.41
3:D:646:ILE:HD11	3:D:764:ARG:HD2	2.02	0.41
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.19	0.41
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.75	0.41
1:H:107:ILE:HG13	1:H:136:GLU:O	2.20	0.41
2:I:21:VAL:HG13	2:I:655:VAL:HG13	2.02	0.41
2:I:60:GLN:O	2:I:476:LYS:HE2	2.20	0.41
2:I:62:TYR:O	2:I:64:GLY:N	2.53	0.41
2:I:81:ASP:O	2:I:85:CYS:HB2	2.20	0.41
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.86	0.41
2:I:387:ASN:O	2:I:394:ARG:HB2	2.20	0.41
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.91	0.41
2:I:468:LEU:O	2:I:471:VAL:HG12	2.21	0.41
2:I:732:ILE:O	2:I:751:TYR:N	2.41	0.41
3:J:510:LEU:HA	3:J:513:MET:HB2	2.03	0.41
3:J:594:GLN:HG3	3:J:596:LEU:HD22	2.03	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.71	0.41
5:L:606:VAL:HG13	5:L:607:LEU:HD12	2.02	0.41
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.55	0.41
2:C:61:SER:HB3	2:C:479:LEU:CB	2.50	0.41
2:C:409:LEU:HD23	2:C:409:LEU:HA	1.92	0.41
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.56	0.41
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.96	0.41
5:F:281:ARG:O	5:F:285:ARG:HG3	2.21	0.41
5:F:556:ALA:O	5:F:560:ARG:HG3	2.21	0.41
1:G:113:ALA:HB2	1:G:126:PRO:HB3	2.03	0.41
2:I:316:GLU:H	2:I:316:GLU:CD	2.24	0.41
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.02	0.41
3:J:578:ILE:HG21	3:J:631:TYR:OH	2.21	0.41
4:K:35:LYS:NZ	4:K:71:GLU:OE2	2.47	0.41
5:L:227:GLN:CG	5:L:252:LEU:HA	2.50	0.41
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.76	0.41
5:L:569:THR:OG1	5:L:570:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG11	1:A:23:HIS:CE1	2.56	0.41
1:B:42:ALA:O	1:B:46:ILE:HG13	2.21	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.02	0.41
2:C:202:ARG:H	2:C:202:ARG:HG3	1.65	0.41
2:C:231:GLU:O	2:C:238:GLN:N	2.54	0.41
2:C:494:ASN:HB3	2:C:497:PRO:HD2	2.02	0.41
2:C:560:PRO:HB3	3:D:776:THR:HG21	2.03	0.41
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.56	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.90	0.41
3:D:697:MET:O	3:D:701:LEU:HB2	2.20	0.41
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	2.03	0.41
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.21	0.41
5:F:394:TYR:CD2	5:F:439:ILE:HG21	2.56	0.41
1:H:47:LEU:HA	1:H:47:LEU:HD23	1.87	0.41
1:H:57:THR:HG21	1:H:158:ARG:HH21	1.85	0.41
1:H:113:ALA:HB2	1:H:126:PRO:HB3	2.02	0.41
2:I:23:ASP:OD1	2:I:23:ASP:N	2.49	0.41
2:I:658:GLN:O	2:I:661:VAL:HG22	2.21	0.41
2:I:854:ILE:HB	2:I:857:VAL:HG21	2.02	0.41
3:J:403:ARG:HB3	3:J:405:GLU:HG3	2.03	0.41
3:J:481:ARG:NH1	4:K:3:ARG:O	2.54	0.41
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.36	0.41
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.86	0.41
2:C:696:ASP:HB3	2:C:697:LYS:H	1.67	0.41
3:D:93:THR:HG22	3:D:94:GLN:H	1.85	0.41
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.56	0.41
3:D:925:GLU:HB3	3:D:926:PRO:HD3	2.03	0.41
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.20	0.41
4:E:15:ASN:OD1	4:E:17:PHE:HB2	2.21	0.41
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.02	0.41
5:F:512:GLY:C	5:F:514:ASP:H	2.25	0.41
5:F:533:ASP:O	5:F:536:THR:N	2.54	0.41
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.50	0.41
2:I:724:VAL:HG13	2:I:734:ILE:HD13	2.02	0.41
3:J:849:LEU:HB3	3:J:853:THR:HG23	2.03	0.41
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.54	0.41
1:A:45:ARG:HH11	1:B:38:THR:HG1	1.69	0.40
1:B:127:GLN:O	1:B:127:GLN:HG2	2.21	0.40
2:C:149:LEU:O	2:C:532:ALA:HA	2.20	0.40
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.56	0.40
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:850:LYS:HG2	3:D:857:LEU:HD23	2.03	0.40
5:F:372:ALA:O	5:F:376:LYS:HG3	2.20	0.40
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.94	0.40
2:I:591:TYR:CA	2:I:655:VAL:HG23	2.51	0.40
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.35	0.40
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.88	0.40
5:L:426:LYS:HE2	5:L:428:SER:OG	2.21	0.40
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.84	0.40
2:C:34:SER:OG	2:C:457:GLY:N	2.52	0.40
2:C:62:TYR:O	2:C:64:GLY:N	2.53	0.40
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.92	0.40
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	2.02	0.40
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.56	0.40
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.03	0.40
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.20	0.40
1:G:61:ILE:HG22	1:G:62:ASP:H	1.86	0.40
2:I:138:ILE:HB	2:I:143:ARG:HD3	2.03	0.40
2:I:518:ASN:O	2:I:691:PRO:HD3	2.21	0.40
2:I:819:SER:HB2	2:I:1085:MET:CG	2.51	0.40
3:J:73:GLY:O	3:J:76:LYS:NZ	2.37	0.40
3:J:369:PRO:HB3	3:J:444:GLY:O	2.21	0.40
4:K:50:ALA:O	4:K:54:ILE:HG12	2.21	0.40
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.84	0.40
2:C:953:LEU:HD12	2:C:953:LEU:HA	1.84	0.40
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.51	0.40
3:D:660:GLU:O	3:D:664:ILE:HG12	2.20	0.40
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.02	0.40
1:H:219:ARG:O	1:H:222:THR:HB	2.22	0.40
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.85	0.40
3:J:79:LYS:HG3	3:J:80:HIS:N	2.36	0.40
1:B:83:LEU:HD11	3:D:526:VAL:HG23	2.04	0.40
2:C:149:LEU:HD13	2:C:453:ILE:HG12	2.03	0.40
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.20	0.40
2:C:1305:TYR:HE1	3:D:379:PRO:HG3	1.86	0.40
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.03	0.40
3:D:1160:SER:HA	3:D:1204:VAL:O	2.22	0.40
5:F:105:MET:HE3	5:F:385:ARG:HG2	2.03	0.40
1:H:118:ASP:H	1:H:121:VAL:HB	1.87	0.40
2:I:69:GLN:HG3	2:I:101:ARG:HB3	2.03	0.40
2:I:149:LEU:O	2:I:532:ALA:HA	2.22	0.40
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.56	0.40
3:J:342:LEU:HA	3:J:343:LEU:HA	1.63	0.40
3:J:513:MET:O	3:J:575:GLY:HA3	2.22	0.40
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.47	0.40
1:B:102:LEU:HD23	1:B:115:ILE:HG12	2.03	0.40
1:B:102:LEU:HD11	1:B:110:VAL:HG11	2.03	0.40
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.40	0.40
2:C:239:MET:O	2:C:284:LEU:HD12	2.21	0.40
2:C:564:PRO:HG3	2:C:572:ILE:HG13	2.02	0.40
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.69	0.40
3:D:11:GLN:HG3	3:D:13:LYS:H	1.87	0.40
3:D:248:ASP:O	3:D:251:PRO:HG3	2.21	0.40
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.04	0.40
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.93	0.40
5:F:486:ARG:CZ	5:F:486:ARG:HB2	2.52	0.40
1:H:62:ASP:HB2	1:H:141:SER:O	2.22	0.40
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.86	0.40
3:J:557:LYS:HE3	3:J:557:LYS:HB2	1.86	0.40
3:J:598:LYS:HD2	3:J:729:GLY:O	2.21	0.40
3:J:658:GLU:O	3:J:661:VAL:HG13	2.22	0.40
3:J:891:ASP:HB3	3:J:1281:GLU: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	225/329 (68%)	193 (86%)	28 (12%)	4 (2%)	8 41
1	B	210/329 (64%)	182 (87%)	23 (11%)	5 (2%)	6 36
1	G	222/329 (68%)	191 (86%)	27 (12%)	4 (2%)	8 41
1	H	211/329 (64%)	183 (87%)	22 (10%)	6 (3%)	5 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1340/1342 (100%)	1230 (92%)	102 (8%)	8 (1%)	25	63
2	I	1338/1342 (100%)	1234 (92%)	98 (7%)	6 (0%)	34	71
3	D	1162/1407 (83%)	1069 (92%)	86 (7%)	7 (1%)	25	63
3	J	1151/1407 (82%)	1058 (92%)	84 (7%)	9 (1%)	19	57
4	E	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	425 (92%)	36 (8%)	1 (0%)	47	79
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	47	79
All	All	6948/8222 (84%)	6343 (91%)	554 (8%)	51 (1%)	22	60

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	LEU
2	C	1159	VAL
3	D	332	LYS
1	H	20	SER
2	I	1159	VAL
3	J	332	LYS
3	J	334	LYS
1	A	162	GLU
1	A	167	PRO
1	B	20	SER
2	C	3	TYR
2	C	170	VAL
3	D	10	ALA
1	G	167	PRO
2	I	170	VAL
3	J	340	GLN
1	B	136	GLU
2	C	697	LYS
3	J	337	ARG
1	A	62	ASP
1	G	14	VAL
1	G	162	GLU
1	H	135	ASP
1	H	136	GLU
1	H	138	ALA
1	H	157	THR

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Mol	Chain	Res	Type
2	I	484	LEU
2	I	697	LYS
3	J	710	ASP
1	A	14	VAL
1	B	138	ALA
2	C	484	LEU
3	D	710	ASP
1	G	62	ASP
1	H	62	ASP
3	J	344	GLY
1	B	14	VAL
2	C	1158	LYS
3	D	806	ASP
2	I	63	SER
3	D	831	VAL
5	F	477	GLU
3	J	831	VAL
2	C	1186	VAL
3	D	826	ILE
2	I	1186	VAL
3	J	826	ILE
5	L	477	GLU
3	D	1180	VAL
3	J	1180	VAL
2	C	2	VAL

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	194/286 (68%)	181 (93%)	13 (7%)	16 45
1	B	182/286 (64%)	170 (93%)	12 (7%)	16 46
1	G	191/286 (67%)	179 (94%)	12 (6%)	18 47
1	H	184/286 (64%)	174 (95%)	10 (5%)	22 51
2	C	1157/1157 (100%)	1054 (91%)	103 (9%)	9 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1154/1157 (100%)	1051 (91%)	103 (9%)	9	36
3	D	970/1168 (83%)	873 (90%)	97 (10%)	7	30
3	J	960/1168 (82%)	863 (90%)	97 (10%)	7	30
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	27
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	48
5	F	417/540 (77%)	374 (90%)	43 (10%)	7	29
5	L	418/540 (77%)	376 (90%)	42 (10%)	7	30
All	All	5966/7024 (85%)	5422 (91%)	544 (9%)	9	35

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	50	SER
1	A	61	ILE
1	A	74	VAL
1	A	115	ILE
1	A	133	LEU
1	A	145	LYS
1	A	171	LEU
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	A	233	ASP
1	B	6	THR
1	B	7	GLU
1	B	8	PHE
1	B	13	LEU
1	B	44	ARG
1	B	50	SER
1	B	61	ILE
1	B	69	SER
1	B	115	ILE
1	B	133	LEU
1	B	148	ARG
1	B	215	GLU
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE

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Mol	Chain	Res	Type
2	C	60	GLN
2	C	70	TYR
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	132	ASP
2	C	167	SER
2	C	189	ASP
2	C	285	ILE
2	C	299	LYS
2	C	306	THR
2	C	320	ASP
2	C	360	LEU
2	C	369	MET
2	C	377	THR
2	C	394	ARG
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	496	LYS
2	C	538	LEU
2	C	539	THR
2	C	542	ARG
2	C	554	HIS
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE

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Mol	Chain	Res	Type
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	799	ASN
2	C	800	MET
2	C	814	ASP
2	C	819	SER
2	C	826	ASP
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	944	ARG
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1073	LYS
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN

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Mol	Chain	Res	Type
2	C	1136	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1198	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1238	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	18	ASP
3	D	26	SER
3	D	29	MET
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	159	ILE
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	217	LEU
3	D	252	LEU
3	D	312	ARG
3	D	324	LEU
3	D	330	MET
3	D	343	LEU
3	D	352	ARG
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	425	ARG

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Mol	Chain	Res	Type
3	D	454	CYS
3	D	490	ILE
3	D	506	VAL
3	D	513	MET
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	805	GLN
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR

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Mol	Chain	Res	Type
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
3	D	1278	GLU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1333	THR
3	D	1343	GLU
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	154	GLU
5	F	266	PHE

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Mol	Chain	Res	Type
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
5	F	395	THR
5	F	401	PHE
5	F	417	ASP
5	F	422	ARG
5	F	429	THR
5	F	437	GLN
5	F	445	ASP
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	485	GLU
5	F	486	ARG
5	F	488	LEU
5	F	489	MET
5	F	491	GLU
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	587	ILE
5	F	603	ARG
5	F	606	VAL
5	F	612	ASP
1	G	9	LEU
1	G	13	LEU
1	G	50	SER
1	G	61	ILE

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Mol	Chain	Res	Type
1	G	74	VAL
1	G	115	ILE
1	G	133	LEU
1	G	145	LYS
1	G	171	LEU
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	13	LEU
1	H	26	VAL
1	H	50	SER
1	H	61	ILE
1	H	91	ARG
1	H	115	ILE
1	H	133	LEU
1	H	191	ARG
1	H	215	GLU
1	H	231	PHE
2	I	4	SER
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	60	GLN
2	I	70	TYR
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	132	ASP
2	I	167	SER
2	I	189	ASP
2	I	285	ILE
2	I	299	LYS
2	I	306	THR
2	I	320	ASP
2	I	360	LEU

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Mol	Chain	Res	Type
2	I	369	MET
2	I	377	THR
2	I	394	ARG
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	496	LYS
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
2	I	554	HIS
2	I	589	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	819	SER
2	I	826	ASP

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Mol	Chain	Res	Type
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	944	ARG
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	984	VAL
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1073	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1198	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1238	LEU
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	26	SER
3	J	29	MET
3	J	46	TYR
3	J	54	ASP

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Mol	Chain	Res	Type
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	159	ILE
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	217	LEU
3	J	252	LEU
3	J	312	ARG
3	J	324	LEU
3	J	330	MET
3	J	343	LEU
3	J	352	ARG
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	425	ARG
3	J	454	CYS
3	J	490	ILE
3	J	506	VAL
3	J	513	MET
3	J	514	THR
3	J	523	GLU
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU

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Mol	Chain	Res	Type
3	J	702	GLN
3	J	704	GLU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	770	LEU
3	J	788	LEU
3	J	798	ARG
3	J	805	GLN
3	J	810	THR
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	931	THR
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU

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Mol	Chain	Res	Type
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	154	GLU
5	L	266	PHE
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	306	PHE
5	L	310	GLU
5	L	335	GLU
5	L	341	LEU
5	L	395	THR
5	L	401	PHE
5	L	417	ASP
5	L	422	ARG
5	L	429	THR
5	L	437	GLN
5	L	445	ASP
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	508	GLU

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Mol	Chain	Res	Type
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	587	ILE
5	L	603	ARG
5	L	606	VAL

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

Mol	Chain	Res	Type
1	B	147	GLN
1	B	186	ASN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	628	HIS
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1313	HIS
2	C	1314	GLN
3	D	94	GLN
3	D	200	GLN
3	D	419	HIS
3	D	450	HIS
3	D	594	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1218	HIS
3	D	1268	ASN
5	F	131	GLN
5	F	227	GLN

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Mol	Chain	Res	Type
5	F	301	ASN
5	F	362	ASN
5	F	446	GLN
5	F	455	HIS
5	F	472	GLN
1	H	186	ASN
2	I	69	GLN
2	I	139	ASN
2	I	494	ASN
2	I	568	ASN
2	I	628	HIS
2	I	688	GLN
2	I	1116	HIS
2	I	1136	GLN
2	I	1146	GLN
2	I	1220	GLN
2	I	1288	GLN
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	365	GLN
3	J	477	GLN
3	J	594	GLN
3	J	665	GLN
3	J	702	GLN
3	J	716	GLN
3	J	817	HIS
3	J	861	ASN
3	J	910	ASN
3	J	929	GLN
3	J	1259	GLN
3	J	1366	HIS
5	L	131	GLN
5	L	246	GLN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	227/329 (68%)	-0.25	1 (0%)	92	87	133, 170, 230, 390	0
1	B	214/329 (65%)	0.15	10 (4%)	31	26	146, 213, 308, 463	0
1	G	224/329 (68%)	-0.08	6 (2%)	54	44	171, 216, 299, 368	0
1	H	215/329 (65%)	0.09	5 (2%)	60	51	173, 222, 293, 418	0
2	C	1342/1342 (100%)	-0.15	35 (2%)	56	46	107, 161, 300, 496	0
2	I	1340/1342 (99%)	-0.00	42 (3%)	49	38	146, 194, 325, 509	0
3	D	1166/1407 (82%)	-0.17	17 (1%)	73	64	108, 149, 239, 419	0
3	J	1155/1407 (82%)	-0.07	30 (2%)	56	46	127, 170, 264, 409	0
4	E	89/91 (97%)	-0.02	0	100	100	186, 210, 243, 257	0
4	K	79/91 (86%)	0.69	12 (15%)	2	2	242, 288, 354, 398	0
5	F	468/613 (76%)	-0.08	10 (2%)	63	54	151, 209, 338, 459	0
5	L	469/613 (76%)	-0.10	14 (2%)	50	39	162, 215, 360, 527	0
All	All	6988/8222 (84%)	-0.08	182 (2%)	56	46	107, 184, 306, 527	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	167	ASP	9.1
2	C	373	GLY	8.1
2	I	982	GLY	7.0
2	C	252	SER	6.2
2	C	251	ALA	5.9
1	H	14	VAL	5.7
2	I	999	GLU	5.7
2	C	485	ASP	5.6
1	B	172	LEU	5.5
2	C	330	HIS	5.4
2	I	1006	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	G	95	LYS	4.8
2	I	1000	LEU	4.7
3	J	1161	GLY	4.6
5	L	490	PRO	4.3
2	I	978	VAL	4.2
2	I	998	LEU	4.1
2	I	247	ARG	4.1
5	L	326	TRP	4.1
3	D	1202	GLU	4.0
2	C	1	MET	4.0
5	F	305	LEU	4.0
1	B	145	LYS	3.9
3	J	521	LYS	3.9
5	L	167	ASP	3.9
2	I	1154	ASP	3.9
5	F	326	TRP	3.8
5	L	480	PRO	3.8
3	J	542	ALA	3.8
1	B	146	VAL	3.7
2	I	108	GLU	3.7
3	D	1198	VAL	3.7
2	C	1002	LEU	3.6
5	L	322	MET	3.6
2	I	1007	LYS	3.6
3	J	674	THR	3.6
2	C	248	GLY	3.5
2	I	981	ALA	3.5
3	J	707	ILE	3.4
3	J	19	ALA	3.4
2	I	1005	GLU	3.4
3	J	1198	VAL	3.3
2	C	539	THR	3.3
3	D	1201	GLY	3.2
5	F	323	ASN	3.2
3	J	207	GLU	3.2
2	C	288	PRO	3.2
2	I	975	ILE	3.1
3	J	830	ASP	3.1
1	B	99	ILE	3.1
2	I	979	LEU	3.1
2	I	1020	GLU	3.0
2	C	273	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	I	988	LYS	3.0
2	I	231	GLU	3.0
2	C	541	GLU	3.0
5	L	489	MET	3.0
2	I	107	ARG	3.0
2	C	311	CYS	3.0
2	C	231	GLU	2.9
3	D	1203	ARG	2.9
3	J	708	ASN	2.9
5	F	301	ASN	2.9
2	I	983	GLY	2.9
3	J	1249	ASN	2.9
5	F	314	THR	2.9
3	D	471	PRO	2.9
5	L	613	ASP	2.9
3	D	1300	ALA	2.9
5	L	319	ALA	2.9
2	I	233	ARG	2.8
5	F	315	TRP	2.8
2	C	271	ALA	2.8
2	C	270	THR	2.8
3	D	1169	THR	2.8
2	C	66	SER	2.8
2	C	114	VAL	2.8
4	K	34	GLY	2.8
2	C	540	ARG	2.8
3	D	1376	GLY	2.8
2	I	987	GLU	2.7
3	J	477	GLN	2.7
2	I	414	ILE	2.7
5	L	488	LEU	2.7
3	J	212	THR	2.7
2	C	310	ILE	2.7
4	K	37	PRO	2.7
3	J	566	LYS	2.7
2	C	1001	GLY	2.7
4	K	40	PRO	2.7
1	H	24	ALA	2.6
1	G	96	ASP	2.6
1	B	97	GLU	2.6
2	C	315	MET	2.6
3	J	314	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	1029	LEU	2.6
2	I	235	ASN	2.6
2	C	332	ARG	2.6
3	J	856	ILE	2.6
5	L	157	ARG	2.5
1	G	193	GLU	2.5
5	F	322	MET	2.5
1	H	87	GLY	2.5
3	J	208	THR	2.5
2	I	773	LEU	2.5
2	I	601	ASP	2.5
2	C	323	ALA	2.5
3	J	175	GLU	2.5
5	L	421	TYR	2.5
2	I	571	LEU	2.5
2	I	976	ARG	2.5
3	D	477	GLN	2.5
2	I	970	GLY	2.4
2	I	992	LEU	2.4
3	J	1250	ASP	2.4
4	K	58	LEU	2.4
1	A	41	ASN	2.4
1	B	147	GLN	2.4
2	C	165	HIS	2.4
2	C	164	THR	2.4
3	J	677	GLU	2.4
3	D	149	GLY	2.4
2	I	165	HIS	2.4
3	D	1199	PHE	2.4
2	C	372	PRO	2.4
1	G	62	ASP	2.4
2	I	986	ALA	2.3
5	L	324	LYS	2.3
3	J	849	LEU	2.3
4	K	77	ALA	2.3
2	I	376	PRO	2.3
5	F	312	SER	2.3
2	I	1018	TYR	2.3
1	H	150	ARG	2.2
1	G	94	GLY	2.2
3	J	857	LEU	2.2
3	D	215	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
4	K	80	LEU	2.2
3	J	1202	GLU	2.2
1	B	98	VAL	2.2
2	C	329	GLY	2.2
2	C	317	LEU	2.2
4	K	78	ALA	2.2
5	F	419	PHE	2.2
3	D	212	THR	2.2
2	C	117	ILE	2.2
4	K	73	GLN	2.2
1	B	58	GLU	2.2
5	L	487	MET	2.2
2	I	109	ALA	2.2
2	C	67	GLU	2.2
2	I	1004	ASP	2.2
3	J	218	THR	2.2
3	J	176	PHE	2.2
2	I	725	GLN	2.1
2	I	1137	GLU	2.1
1	G	24	ALA	2.1
2	I	600	THR	2.1
3	D	419	HIS	2.1
3	J	1203	ARG	2.1
2	I	413	GLU	2.1
2	I	989	LEU	2.1
4	K	14	GLY	2.1
1	B	41	ASN	2.1
3	J	1168	GLU	2.1
2	C	316	GLU	2.1
3	D	175	GLU	2.1
3	D	209	ASN	2.1
4	K	35	LYS	2.1
2	C	304	GLU	2.1
3	J	528	THR	2.1
2	C	163	LYS	2.1
5	L	317	ASN	2.1
2	C	979	LEU	2.1
1	B	49	SER	2.0
1	H	107	ILE	2.0
4	K	39	VAL	2.0
3	J	827	GLU	2.0
3	J	675	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
4	K	79	GLU	2.0
2	I	1019	ASP	2.0
3	D	208	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	J	1501	1/1	0.93	0.39	130,130,130,130	0
7	ZN	J	1502	1/1	0.94	0.06	213,213,213,213	0
6	MG	D	1501	1/1	0.95	0.27	104,104,104,104	0
7	ZN	J	1503	1/1	0.98	0.17	135,135,135,135	0
7	ZN	D	1502	1/1	0.99	0.09	177,177,177,177	0
7	ZN	D	1503	1/1	0.99	0.17	117,117,117,117	0

6.5 Other polymers (i)

There are no such residues in this entry.