Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 08:51 PM EDT

PDB ID	:	5UAL
Title	:	Escherichia coli RNA polymerase and Rifampin complex, RpoB S531L mutant
Authors	:	Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on	:	2016-12-19
Resolution	:	3.89 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 (i)) were used in the production of this report:

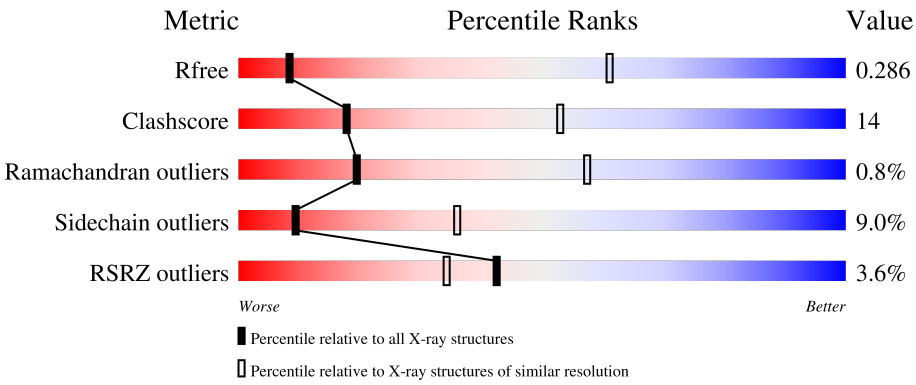
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.89 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	1026 (4.12-3.64)
Clashscore	141614	1045 (4.10-3.66)
Ramachandran outliers	138981	1008 (4.10-3.66)
Sidechain outliers	138945	1001 (4.10-3.66)
RSRZ outliers	127900	1213 (4.16-3.60)

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	% 44% 22% • 31%
1	B	329	2% 39% 24% • 35%
1	G	329	2% 41% 23% • 32%
1	H	329	2% 37% 26% • 35%
2	C	1342	5% 62% 34% • •

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Mol	Chain	Length	Quality of chain
2	I	1342	5% 67% 29%
3	D	1407	% 52% 27% 17%
3	J	1407	3% 53% 25% 18%
4	E	91	% 78% 18%
4	K	91	21% 56% 27% 13%
5	F	613	3% 50% 23% 24%
5	L	613	3% 53% 21% 23%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 54898 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	1332	10514	6600	1827	2043	44	0	0	0
2	I	1328	10486	6583	1822	2038	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

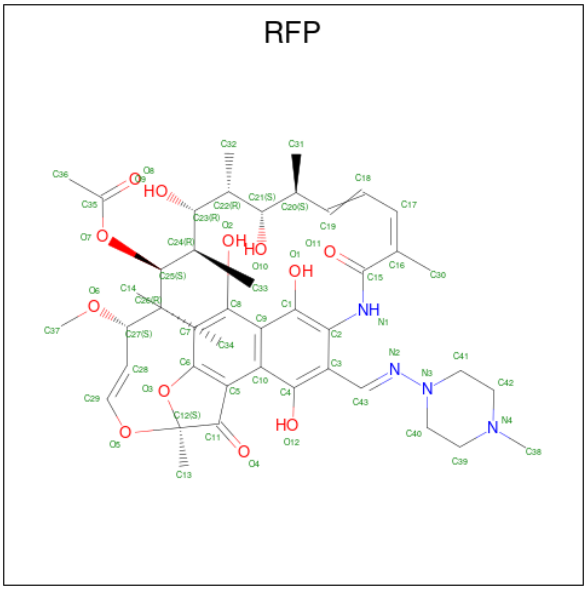
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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 RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	59	43	4	12	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

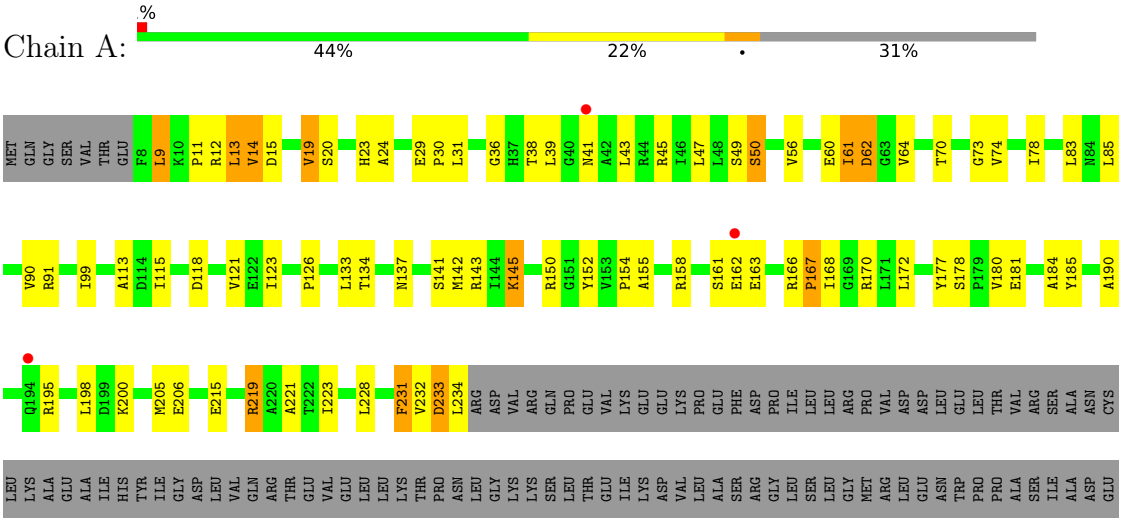
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

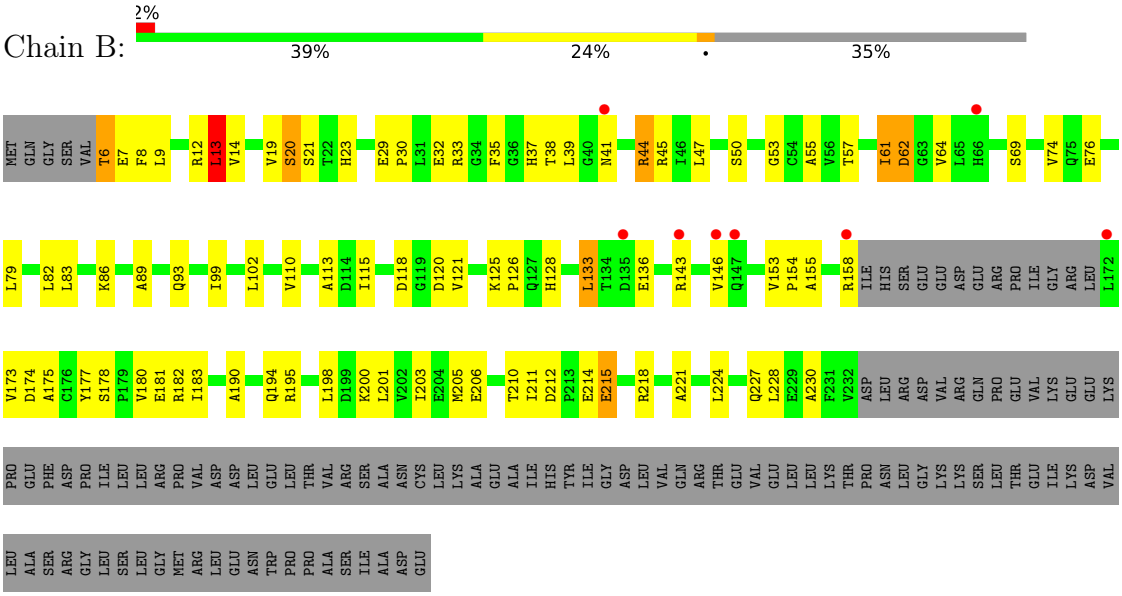
3 Residue-property plots (i)

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

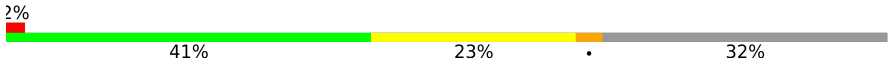


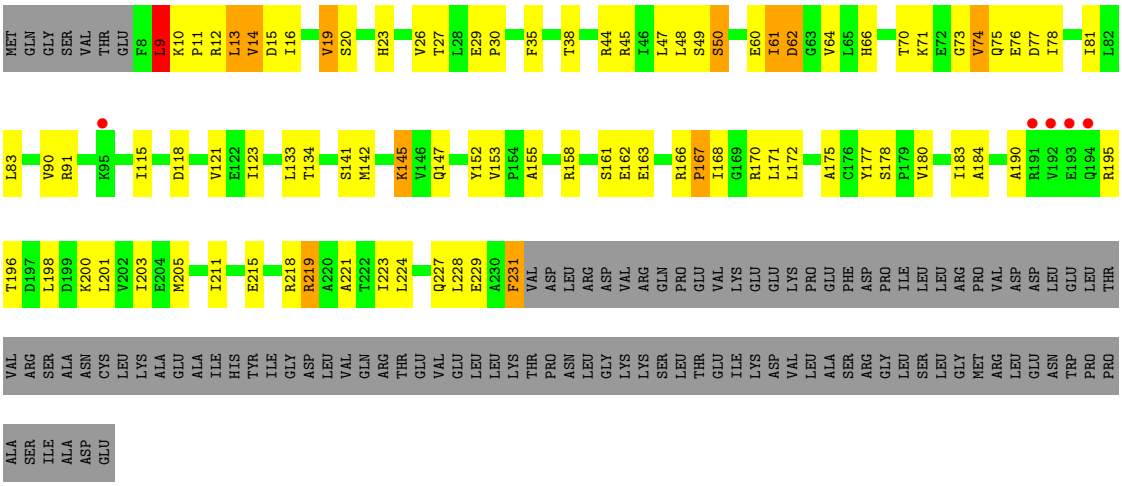
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

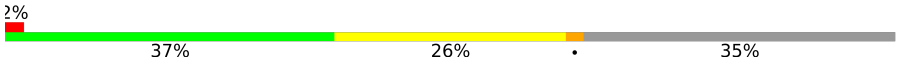
Chain G:

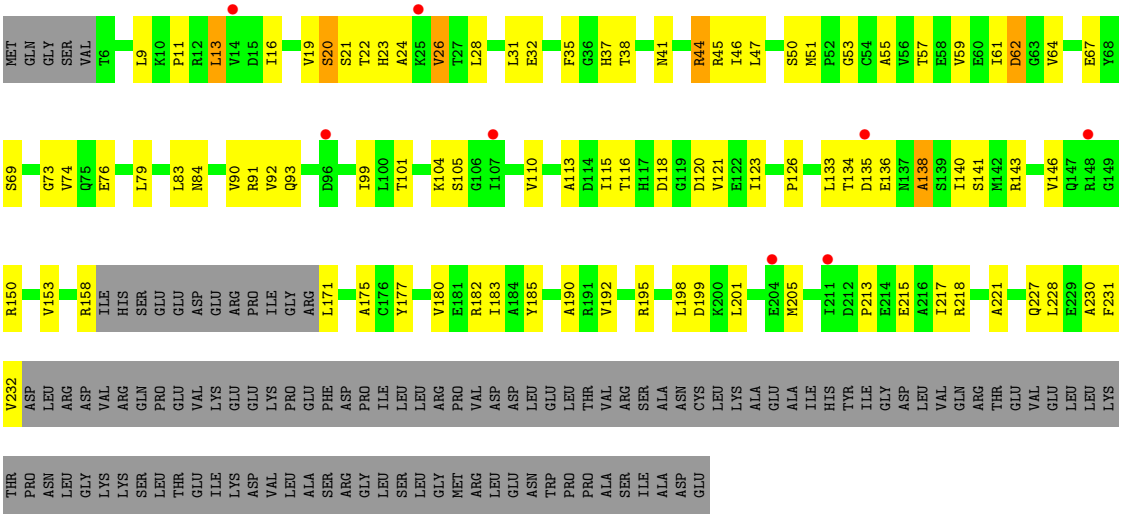




• Molecule 1: DNA-directed RNA polymerase subunit alpha

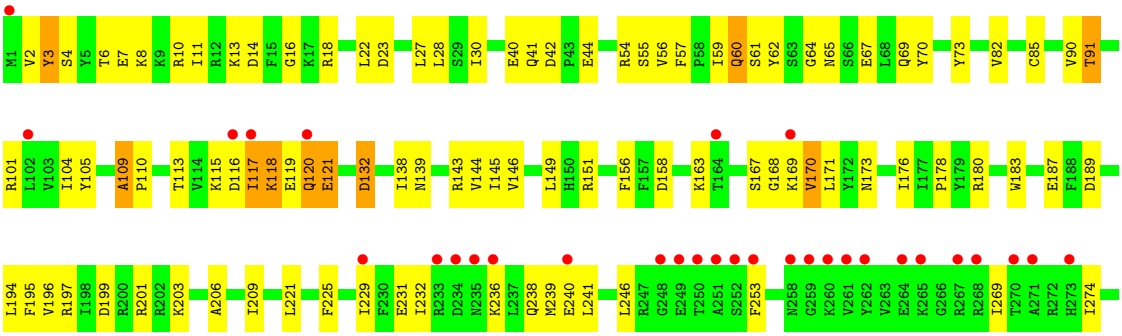
Chain H:

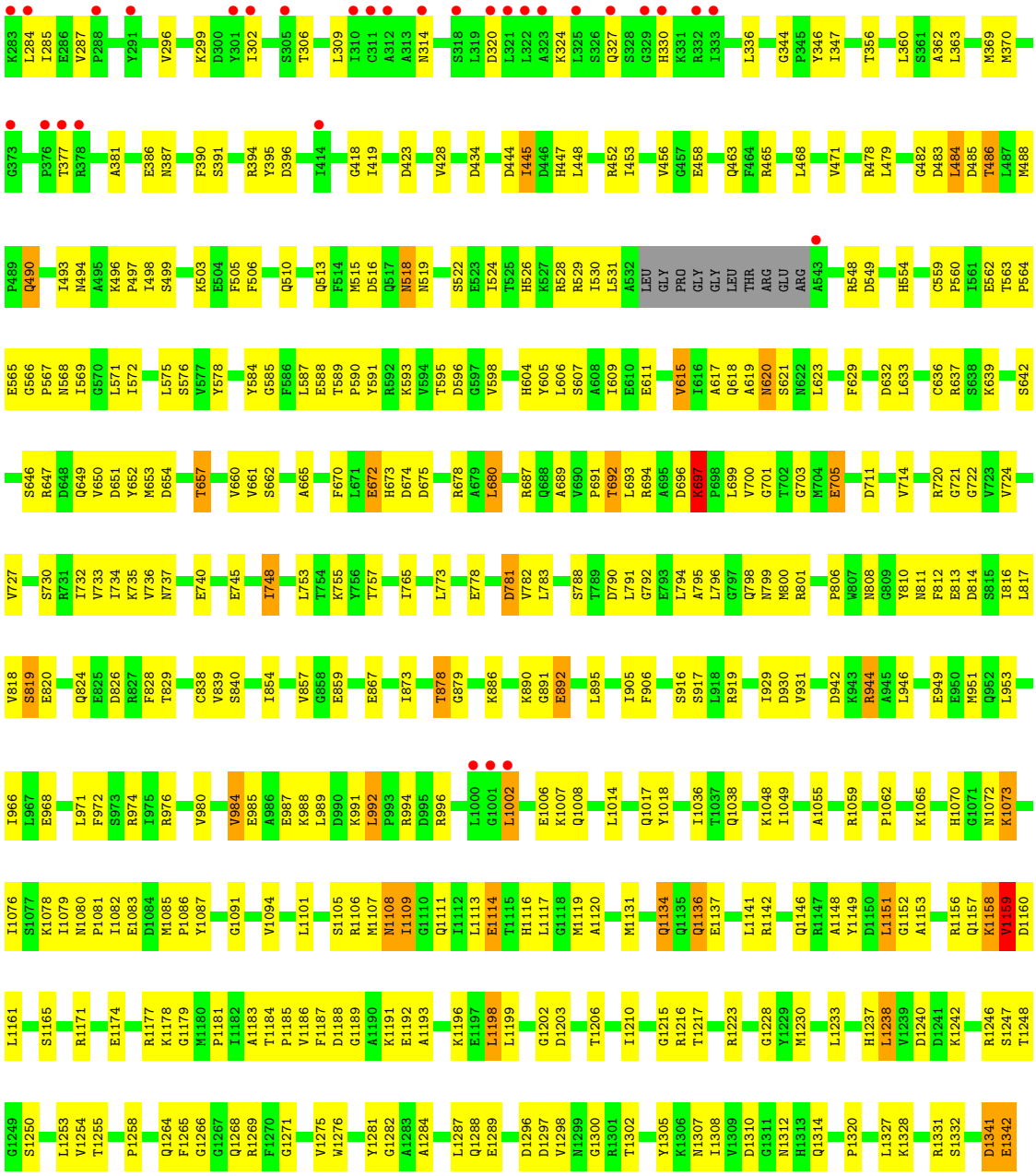




• Molecule 2: DNA-directed RNA polymerase subunit beta

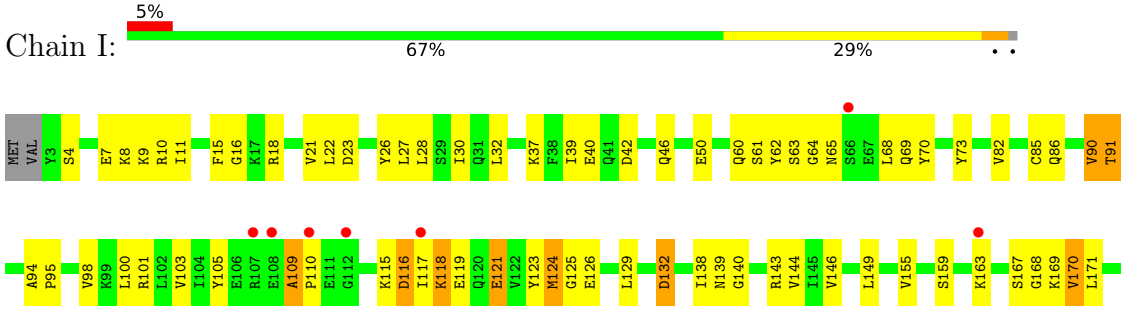
Chain C:

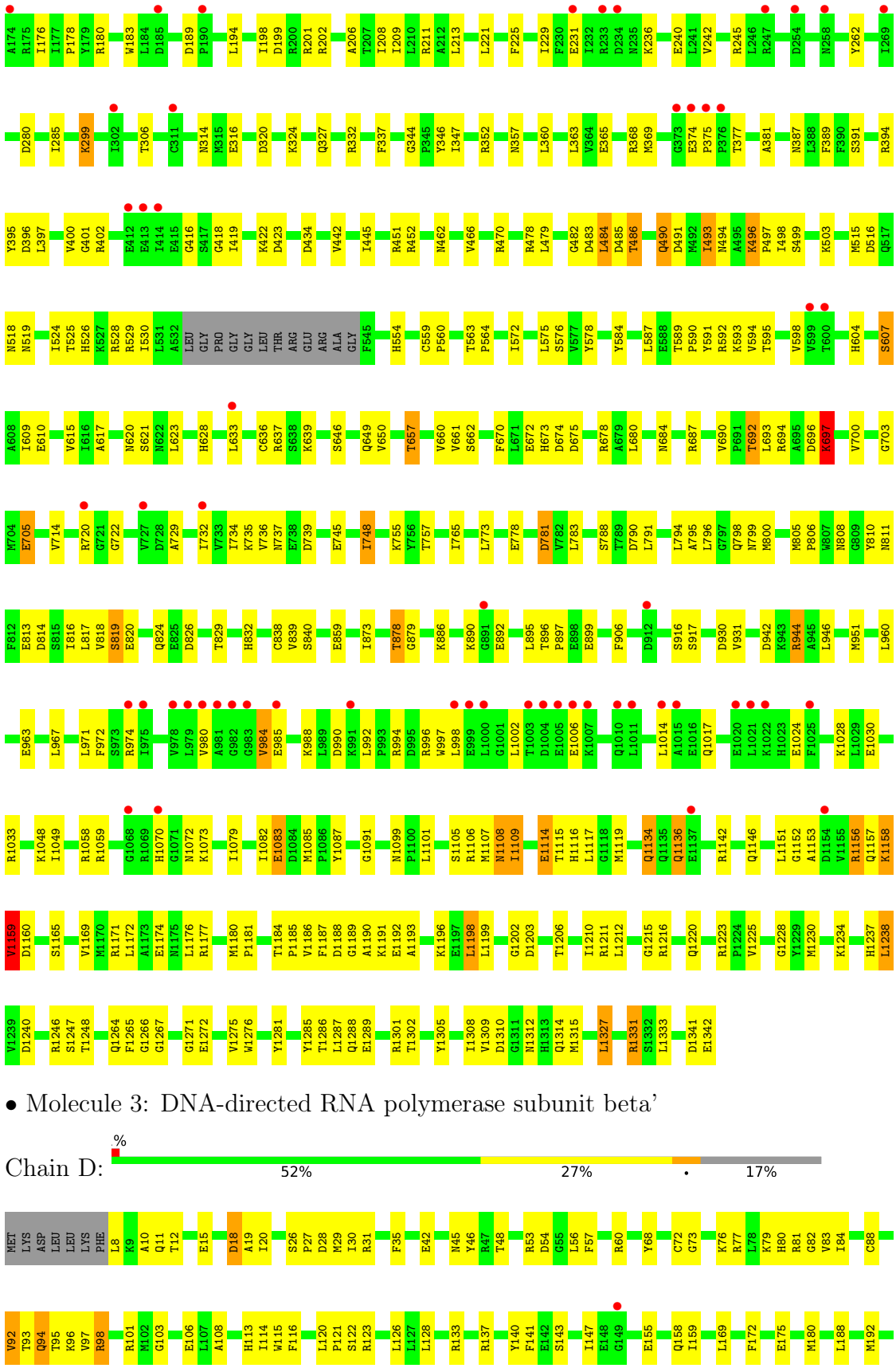




• Molecule 2: DNA-directed RNA polymerase subunit beta

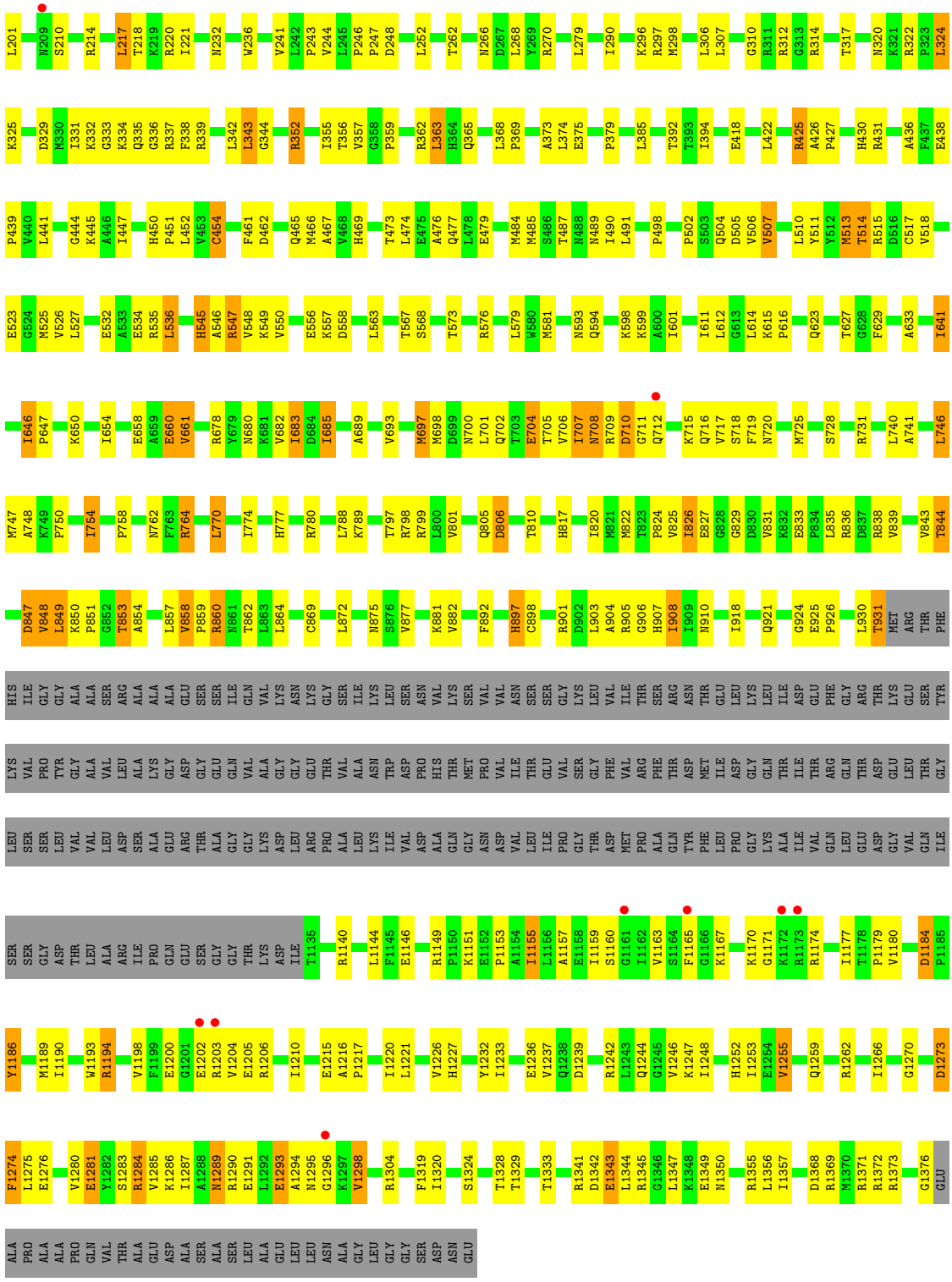
Chain I:





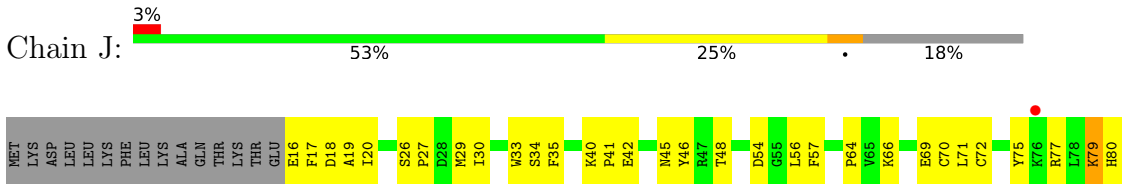
• Molecule 3: DNA-directed RNA polymerase subunit beta'

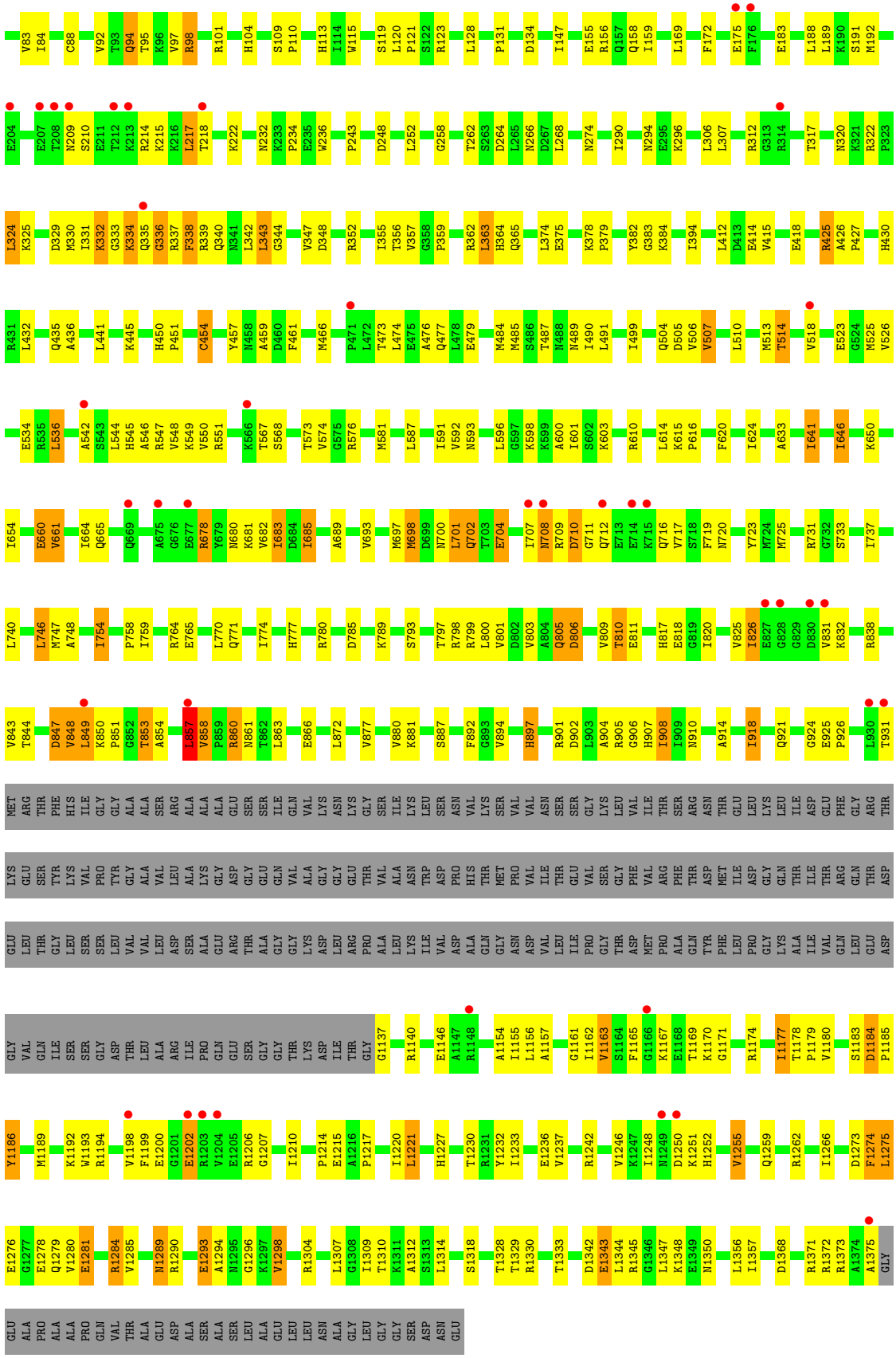
Chain D:



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

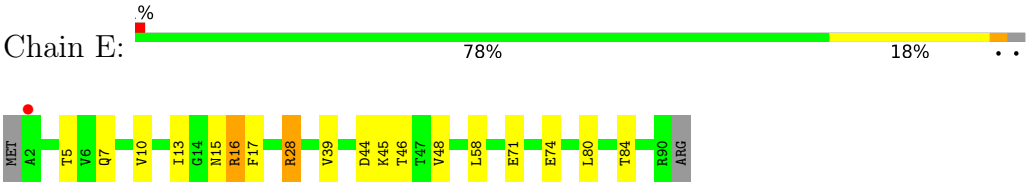
Chain J:





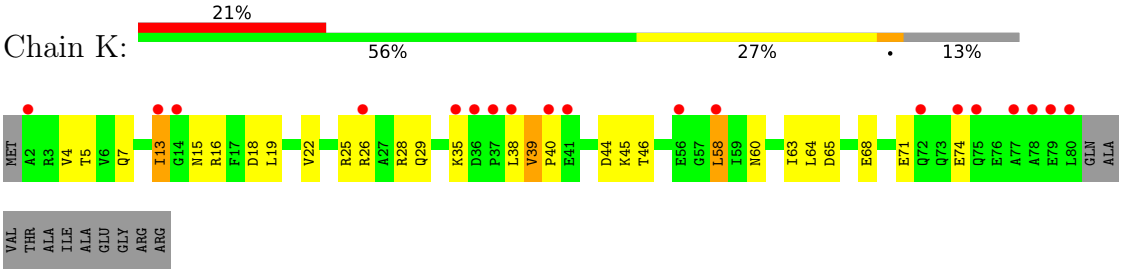
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



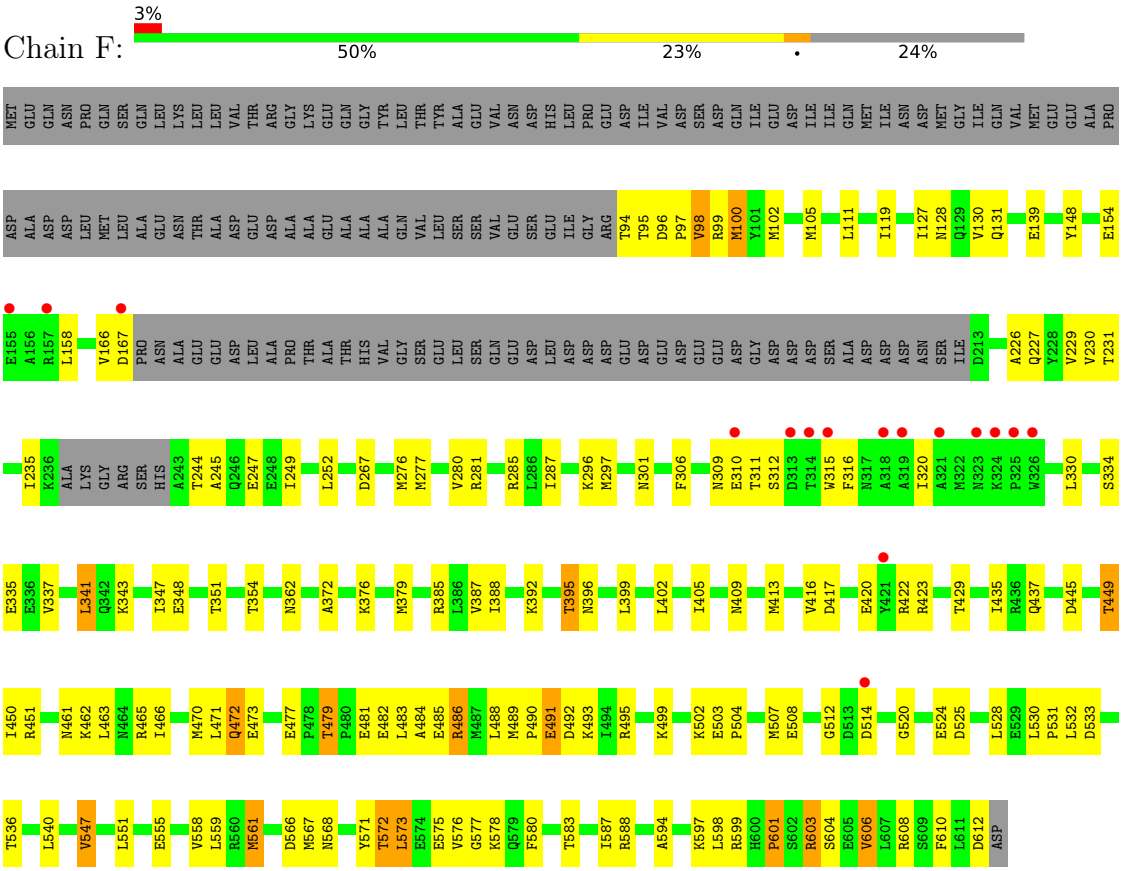
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



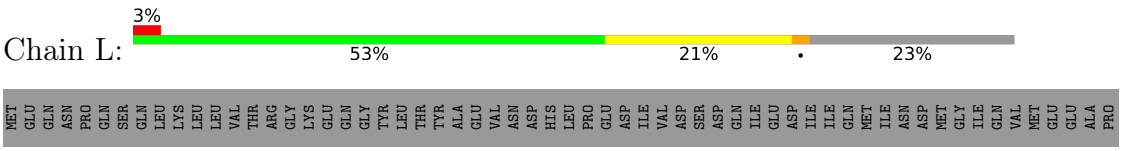
• Molecule 5: RNA polymerase sigma factor RpoD

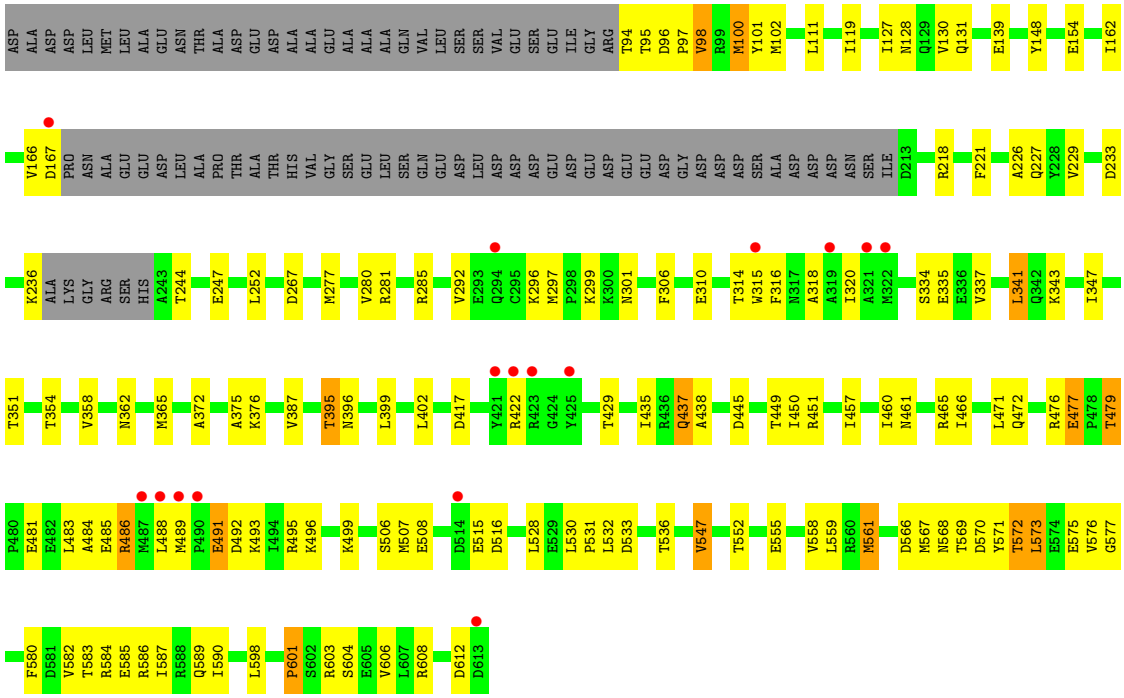
Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:




ASP ALA ASP ASP LEU MET LEU ALA GLU ASN THR ALA ASP GLU ASP ALA ALA GLU ALA ALA ALA GLN VAL LEU SER SER VAL GLU SER GLU ILE GLY ARG T94 T95 D96 P97 V98 R99 M100 Y101 M102 L111 I119 I127 N128 Q129 V130 Q131 E139 Y148 E154 I162
V166 D167 PRO ASN ALA GLU GLU ASP LEU ALA PRO THR ALA THR HIS VAL GLY SER GLU LEU SER GLN GLU ASP LEU ASP ASP GLU ASP ASP GLU GLU ASP GLY ASP ASP ASP SER ALA ASP ASP ASP ASN SER ILE D213 R218 F221 A226 Q227 Y228 V229 D233
K236 ALA LYS GLY ARG SER HIS A243 T244 E247 L252 D267 M277 V280 R281 R285 V292 E293 Q294 C295 K296 ASP M297 P298 K299 K300 N301 F306 E310 T314 W315 F316 N317 A318 A319 I320 A321 M322 S334 E335 E336 V337 L341 Q342 K343 I347
T351 T354 V358 N362 M365 A372 A375 K376 V387 T395 N396 L399 L402 D417 Y421 R422 R423 G424 Y425 T429 I435 R436 Q437 A438 D445 T449 I450 R451 I457 I460 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 S506 M507 E508 D514 E515 D516 L528 E529 L530 P531 L532 D533 T536 V547 T552 E555 V558 L559 R560 M561 D566 M567 N568 T569 D570 Y571 T572 L573 E574 E575 V576 G577
F580 D581 V582 T583 R584 E585 R586 T587 R588 Q589 I590 L598 P601 S602 R603 S604 E605 V606 L607 R608 D612 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	187.37Å 205.95Å 309.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 3.89 29.94 – 3.89	Depositor EDS
% Data completeness (in resolution range)	82.9 (29.94-3.89) 82.9 (29.94-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.86Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.230 , 0.286 0.230 , 0.286	Depositor DCC
R_{free} test set	1979 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å^2)	168.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 134.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	54898	wwPDB-VP
Average B, all atoms (Å^2)	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, RFP

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	0.42	1/1774 (0.1%)	0.57	0/2405
1	B	0.34	0/1668	0.71	2/2260 (0.1%)
1	G	0.36	1/1751 (0.1%)	0.55	1/2373 (0.0%)
1	H	0.29	0/1678	0.62	0/2274
2	C	0.37	0/10681	0.57	0/14410
2	I	0.30	0/10653	0.53	0/14373
3	D	0.39	1/9229 (0.0%)	0.61	0/12459
3	J	0.34	0/9140	0.58	2/12341 (0.0%)
4	E	0.29	0/693	0.51	0/935
4	K	0.26	0/629	0.47	0/847
5	F	0.30	0/3864	0.53	0/5194
5	L	0.28	0/3872	0.50	0/5205
All	All	0.34	3/55632 (0.0%)	0.57	5/75076 (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	2
2	I	0	2
3	D	0	2
3	J	0	2
5	F	0	1
5	L	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	C-N	10.64	1.54	1.34
1	G	29	GLU	C-N	9.19	1.51	1.34
3	D	898	CYS	CB-SG	-5.28	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	343	LEU	CA-CB-CG	12.07	143.06	115.30
1	B	9	LEU	C-N-CA	9.90	146.46	121.70
1	G	9	LEU	C-N-CA	5.58	135.64	121.70
3	J	857	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	13	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	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	64	0
1	B	1649	0	1673	71	0
1	G	1730	0	1756	66	0
1	H	1659	0	1692	72	0
2	C	10514	0	10531	335	0
2	I	10486	0	10496	268	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9089	0	9263	310	0
3	J	9001	0	9167	288	0
4	E	691	0	695	11	0
4	K	627	0	634	22	0
5	F	3813	0	3880	96	0
5	L	3821	0	3884	82	0
6	C	59	0	56	9	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	54898	0	55507	1505	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 14.

All (1505) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.36	1.07
2:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.44	0.99
2:C:1269:ARG:HG3	3:D:343:LEU:HD12	1.49	0.94
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.50	0.91
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.52	0.91
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.54	0.89
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.53	0.89
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.55	0.88
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.40	0.85
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.56	0.85
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.57	0.85
3:D:342:LEU:HA	3:D:343:LEU:HD23	1.59	0.85
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.62	0.81
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.59	0.81
5:L:97:PRO:HA	5:L:100:MET:HG3	1.60	0.81
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.63	0.80
1:G:45:ARG:HG2	1:H:38:THR:HB	1.62	0.80
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.46	0.79
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.63	0.79
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.65	0.79
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.63	0.78
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:ARG:HH11	1:H:232:VAL:HG22	1.48	0.78
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.66	0.78
1:H:32:GLU:HA	1:H:198:LEU:HD22	1.67	0.77
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.67	0.77
1:B:29:GLU:OE1	1:B:200:LYS:HE2	1.84	0.77
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.18	0.77
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.50	0.77
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.66	0.76
2:I:560:PRO:O	3:J:780:ARG:NH2	2.18	0.76
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.67	0.76
2:C:1271:GLY:HA2	3:D:343:LEU:CD2	2.15	0.76
1:H:23:HIS:HB2	1:H:205:MET:O	1.86	0.76
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.19	0.75
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.68	0.75
2:C:1247:SER:HB3	3:D:375:GLU:O	1.87	0.75
2:C:1248:THR:HB	5:F:532:LEU:HD11	1.69	0.74
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.20	0.74
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.68	0.74
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.53	0.74
3:D:576:ARG:NH1	3:D:593:ASN:O	2.20	0.74
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.69	0.74
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.21	0.73
5:F:598:LEU:O	5:F:604:SER:OG	2.06	0.73
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.69	0.73
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.70	0.73
3:J:665:GLN:HE22	3:J:678:ARG:HH21	1.36	0.72
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.54	0.72
3:J:156:ARG:NH2	3:J:191:SER:OG	2.21	0.72
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.71	0.72
2:I:324:LYS:O	2:I:327:GLN:NE2	2.22	0.72
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.23	0.72
3:J:436:ALA:HB3	3:J:485:MET:HA	1.72	0.72
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.22	0.71
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.72	0.71
3:D:700:ASN:O	3:D:704:GLU:HB2	1.89	0.71
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.22	0.71
2:I:18:ARG:NH1	2:I:621:SER:O	2.22	0.71
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.24	0.71
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.72	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.73	0.70
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:NH1	3:D:581:MET:SD	2.64	0.70
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.71	0.70
2:I:452:ARG:NH1	2:I:584:TYR:O	2.23	0.70
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.57	0.70
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.73	0.70
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.57	0.70
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.39	0.69
1:G:12:ARG:H	1:G:30:PRO:HD2	1.56	0.69
1:G:23:HIS:HB2	1:G:205:MET:O	1.92	0.69
3:J:700:ASN:O	3:J:704:GLU:HB2	1.91	0.69
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.92	0.69
5:F:97:PRO:HA	5:F:100:MET:HG3	1.73	0.69
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.75	0.69
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.74	0.69
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.73	0.69
1:A:45:ARG:HG2	1:B:38:THR:HB	1.74	0.69
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.73	0.69
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.74	0.69
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.74	0.69
5:F:316:PHE:HZ	5:F:334:SER:HA	1.56	0.69
1:A:23:HIS:HB2	1:A:205:MET:O	1.92	0.68
2:I:30:ILE:HD12	2:I:30:ILE:H	1.59	0.68
5:L:316:PHE:HZ	5:L:334:SER:HA	1.57	0.68
2:C:197:ARG:NH1	2:C:201:ARG:O	2.25	0.68
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.58	0.68
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.74	0.68
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.58	0.68
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.59	0.68
1:B:23:HIS:HB2	1:B:205:MET:O	1.94	0.67
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.76	0.67
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.76	0.67
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.42	0.67
1:A:12:ARG:H	1:A:30:PRO:HD2	1.58	0.67
3:D:392:THR:HG21	5:F:606:VAL:HA	1.76	0.67
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.76	0.67
1:H:101:THR:H	1:H:116:THR:HG22	1.60	0.67
1:A:14:VAL:HG22	1:A:15:ASP:H	1.60	0.67
1:B:102:LEU:HD11	1:B:110:VAL:HG11	1.75	0.67
2:C:615:VAL:HG13	2:C:651:ASP:H	1.60	0.67
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	1.94	0.67
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.25	0.67
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.09	0.67
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.77	0.66
3:J:848:VAL:HG11	3:J:880:VAL:HG22	1.76	0.66
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.26	0.66
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.76	0.66
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.77	0.66
1:B:32:GLU:OE2	1:B:195:ARG:NH2	2.29	0.66
2:C:30:ILE:HD12	2:C:30:ILE:H	1.61	0.66
3:J:901:ARG:HD2	3:J:906:GLY:O	1.95	0.66
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.26	0.66
1:G:14:VAL:HG22	1:G:15:ASP:H	1.61	0.66
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.61	0.66
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.76	0.66
3:J:576:ARG:NH1	3:J:593:ASN:O	2.28	0.66
2:C:40:GLU:O	2:C:73:TYR:OH	2.13	0.66
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.78	0.66
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.76	0.66
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.29	0.66
3:J:514:THR:HB	3:J:576:ARG:HG2	1.78	0.66
2:C:386:GLU:HA	2:C:390:PHE:HD2	1.61	0.65
3:J:905:ARG:NH1	3:J:910:ASN:HD21	1.94	0.65
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.77	0.65
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.26	0.65
2:C:721:GLY:N	2:C:740:GLU:OE1	2.29	0.65
2:C:531:LEU:HD13	6:C:3001:RFP:H141	1.78	0.65
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.76	0.65
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.28	0.65
6:C:3001:RFP:O11	6:C:3001:RFP:O1	2.14	0.65
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.79	0.65
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.30	0.65
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.11	0.65
1:H:79:LEU:HD11	3:J:526:VAL:HG21	1.79	0.65
2:I:499:SER:O	2:I:503:LYS:HB2	1.98	0.64
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.78	0.64
1:B:181:GLU:HA	3:D:535:ARG:HH21	1.60	0.64
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.62	0.64
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.79	0.64
2:I:27:LEU:O	2:I:528:ARG:NH1	2.30	0.64
2:I:109:ALA:HB1	2:I:110:PRO:C	2.17	0.64
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.80	0.64
3:J:418:GLU:HG3	4:K:45:LYS:H	1.62	0.64
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.62	0.64
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.79	0.64
2:I:155:VAL:HG23	2:I:176:ILE:HG12	1.80	0.64
5:L:601:PRO:HB3	5:L:608:ARG:HH22	1.62	0.64
2:C:109:ALA:HB1	2:C:110:PRO:C	2.19	0.64
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.31	0.64
1:H:67:GLU:OE1	1:H:67:GLU:N	2.31	0.64
2:I:40:GLU:O	2:I:73:TYR:OH	2.16	0.63
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.80	0.63
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.81	0.63
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.30	0.63
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.98	0.63
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.14	0.63
2:C:1142:ARG:HD3	2:C:1161:LEU:HD11	1.80	0.63
3:J:843:VAL:HG11	3:J:897:HIS:O	1.99	0.63
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.63	0.63
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.62	0.63
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.81	0.63
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.80	0.63
1:G:166:ARG:O	1:G:168:ILE:N	2.32	0.62
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.80	0.62
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.81	0.62
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.82	0.62
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.80	0.62
2:C:905:ILE:O	5:F:599:ARG:NH1	2.31	0.62
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.80	0.62
1:A:166:ARG:O	1:A:168:ILE:N	2.32	0.62
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.32	0.62
3:D:343:LEU:CD2	3:D:344:GLY:HA3	2.23	0.62
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.64	0.62
3:D:1155:ILE:HD13	3:D:1190:ILE:HD13	1.81	0.62
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.35	0.62
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.80	0.62
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.80	0.62
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	1.81	0.62
2:C:560:PRO:O	3:D:780:ARG:NH2	2.31	0.62
1:G:62:ASP:OD1	1:G:141:SER:OG	2.15	0.62
1:H:16:ILE:HG23	1:H:26:VAL:HG13	1.81	0.62
3:J:901:ARG:HA	3:J:908:ILE:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.35	0.62
1:H:53:GLY:HA3	1:H:177:TYR:O	2.00	0.62
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.82	0.62
2:C:6:THR:OG1	2:C:781:ASP:OD2	2.13	0.62
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.15	0.62
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.63	0.62
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.31	0.62
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.81	0.62
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.64	0.62
3:D:140:TYR:O	3:D:297:ARG:NH1	2.33	0.62
3:D:901:ARG:HA	3:D:908:ILE:HA	1.80	0.61
2:C:705:GLU:HB2	2:C:794:LEU:H	1.65	0.61
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.81	0.61
2:C:27:LEU:O	2:C:528:ARG:NH1	2.31	0.61
1:G:228:LEU:HD22	1:H:221:ALA:HB1	1.81	0.61
5:F:479:THR:HG23	5:F:481:GLU:H	1.66	0.61
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.81	0.61
5:L:601:PRO:HA	5:L:604:SER:HB2	1.82	0.61
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.82	0.61
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.83	0.61
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.82	0.61
2:I:1271:GLY:HA3	3:J:343:LEU:HD12	1.83	0.61
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.65	0.61
1:B:182:ARG:H	1:B:206:GLU:HB2	1.65	0.61
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.83	0.61
3:J:45:ASN:HB3	3:J:48:THR:O	2.01	0.61
2:C:588:GLU:HG3	2:C:605:TYR:HD1	1.66	0.61
1:G:13:LEU:HD22	1:H:231:PHE:CE1	2.36	0.61
1:H:32:GLU:OE2	1:H:195:ARG:NH2	2.33	0.61
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.66	0.61
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.82	0.60
5:F:573:LEU:H	5:F:573:LEU:HD23	1.64	0.60
3:D:1344:LEU:HB3	3:D:1350:ASN:HD21	1.65	0.60
5:L:533:ASP:O	5:L:536:THR:N	2.32	0.60
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.65	0.60
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.32	0.60
3:D:336:GLY:HA3	3:D:1324:SER:O	2.01	0.60
5:L:316:PHE:CZ	5:L:334:SER:HA	2.36	0.60
2:C:516:ASP:OD2	2:C:522:SER:OG	2.20	0.60
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.83	0.60
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.83	0.60
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.84	0.60
3:D:298:MET:SD	5:F:402:LEU:HB3	2.42	0.60
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.66	0.60
1:H:64:VAL:HG11	1:H:69:SER:OG	2.01	0.60
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.67	0.59
1:H:74:VAL:HG12	1:H:76:GLU:H	1.67	0.59
1:B:53:GLY:HA3	1:B:177:TYR:O	2.02	0.59
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.02	0.59
3:D:342:LEU:HA	3:D:343:LEU:CD2	2.31	0.59
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.36	0.59
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.84	0.59
2:C:528:ARG:NH2	2:C:576:SER:O	2.36	0.59
3:D:317:THR:HB	3:D:324:LEU:HB3	1.84	0.59
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.85	0.59
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	2.03	0.59
3:D:45:ASN:HB3	3:D:48:THR:O	2.02	0.59
3:D:847:ASP:OD1	3:D:847:ASP:N	2.33	0.59
3:J:115:TRP:O	3:J:119:SER:HB3	2.02	0.59
3:D:121:PRO:HG2	3:D:123:ARG:NH2	2.17	0.59
2:I:930:ASP:OD2	2:I:931:VAL:N	2.35	0.59
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.37	0.58
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.29	0.58
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.68	0.58
2:C:387:ASN:HA	2:C:391:SER:HB2	1.86	0.58
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.85	0.58
5:F:343:LYS:HD2	5:F:343:LYS:H	1.68	0.58
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.85	0.58
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.86	0.58
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.03	0.58
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.18	0.58
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.85	0.58
5:F:601:PRO:HA	5:F:604:SER:HB2	1.85	0.58
3:D:210:SER:O	3:D:214:ARG:HG2	2.03	0.58
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.86	0.58
1:G:161:SER:O	1:G:163:GLU:N	2.36	0.58
2:C:692:THR:OG1	2:C:693:LEU:N	2.36	0.58
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.67	0.58
2:C:930:ASP:OD2	2:C:931:VAL:N	2.36	0.58
3:D:436:ALA:HB3	3:D:485:MET:HA	1.85	0.58
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.84	0.58
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.67	0.58
3:J:683:ILE:HD11	3:J:754:ILE:HG23	1.86	0.58
2:C:2:VAL:O	2:C:3:TYR:HB2	2.03	0.58
2:C:529:ARG:NH1	6:C:3001:RFP:O11	2.36	0.58
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.85	0.58
3:D:56:LEU:HD12	3:D:56:LEU:H	1.69	0.58
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.84	0.58
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.69	0.58
3:D:525:MET:O	3:D:548:VAL:HG13	2.03	0.58
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.67	0.58
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.15	0.58
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.37	0.58
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.84	0.58
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.44	0.58
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.85	0.57
2:C:730:SER:O	2:C:753:LEU:HB2	2.04	0.57
3:D:270:ARG:NH2	5:F:449:THR:HG23	2.19	0.57
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.85	0.57
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.66	0.57
3:J:709:ARG:O	3:J:711:GLY:N	2.38	0.57
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.85	0.57
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.85	0.57
1:A:13:LEU:HD23	1:A:13:LEU:H	1.70	0.57
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.87	0.57
3:J:218:THR:HG21	3:J:1275:LEU:HD11	1.86	0.57
2:C:617:ALA:HA	2:C:636:CYS:SG	2.43	0.57
3:D:425:ARG:HG2	3:D:426:ALA:H	1.68	0.57
2:I:607:SER:N	2:I:610:GLU:OE1	2.36	0.57
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.38	0.57
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.87	0.57
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.22	0.57
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.86	0.57
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.70	0.57
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.36	0.57
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.70	0.57
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.35	0.57
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.69	0.57
5:F:561:MET:HA	5:F:567:MET:HE1	1.87	0.57
3:J:1198:VAL:HB	3:J:1210:ILE:HA	1.87	0.57
5:L:479:THR:HG23	5:L:481:GLU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.85	0.57
3:D:1376:GLY:O	3:J:853:THR:OG1	2.21	0.57
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.70	0.57
1:A:161:SER:O	1:A:163:GLU:N	2.38	0.56
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.87	0.56
3:J:356:THR:OG1	3:J:357:VAL:N	2.38	0.56
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.85	0.56
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.87	0.56
1:H:190:ALA:N	1:H:198:LEU:O	2.33	0.56
2:I:208:ILE:HD11	2:I:365:GLU:HB3	1.85	0.56
1:B:6:THR:O	1:B:6:THR:OG1	2.16	0.56
1:B:55:ALA:O	1:B:146:VAL:HG13	2.04	0.56
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.38	0.56
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.85	0.56
5:F:461:ASN:O	5:F:465:ARG:HG2	2.04	0.56
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.87	0.56
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.86	0.56
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.87	0.56
5:F:540:LEU:HD12	5:F:610:PHE:CD1	2.39	0.56
3:D:1259:GLN:NE2	3:D:1262:ARG:HH12	2.03	0.56
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.88	0.56
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.86	0.56
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.87	0.56
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.52	0.56
1:G:49:SER:HB3	2:I:1083:GLU:HG2	1.88	0.56
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.87	0.56
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.88	0.56
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.87	0.56
2:I:684:ASN:OD1	2:I:687:ARG:NH1	2.39	0.56
2:C:201:ARG:NH2	2:C:370:MET:O	2.32	0.56
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.87	0.56
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.71	0.56
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.41	0.56
5:L:395:THR:OG1	5:L:396:ASN:N	2.36	0.56
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.88	0.56
5:F:348:GLU:HG2	5:F:354:THR:HA	1.86	0.56
5:L:601:PRO:HB3	5:L:608:ARG:NH2	2.21	0.56
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.87	0.56
5:L:244:THR:O	5:L:247:GLU:HG2	2.06	0.56
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.88	0.55
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.88	0.55
3:J:362:ARG:H	3:J:365:GLN:NE2	2.04	0.55
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.89	0.55
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.89	0.55
3:D:843:VAL:HG11	3:D:897:HIS:O	2.06	0.55
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.86	0.55
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.07	0.55
5:F:533:ASP:O	5:F:536:THR:N	2.39	0.55
1:G:13:LEU:H	1:G:13:LEU:HD23	1.71	0.55
2:I:1271:GLY:CA	3:J:343:LEU:HD12	2.36	0.55
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.89	0.55
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.21	0.55
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.87	0.55
2:I:829:THR:HA	2:I:1059:ARG:HA	1.89	0.55
5:L:598:LEU:O	5:L:604:SER:OG	2.21	0.55
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.88	0.55
1:B:61:ILE:HG22	1:B:62:ASP:H	1.71	0.55
3:D:518:VAL:O	3:D:547:ARG:NH1	2.39	0.55
2:I:528:ARG:NH2	2:I:576:SER:O	2.40	0.55
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.87	0.55
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.89	0.55
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.89	0.55
2:I:692:THR:OG1	2:I:693:LEU:N	2.40	0.55
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.41	0.55
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.88	0.55
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.07	0.55
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.42	0.55
3:D:709:ARG:O	3:D:711:GLY:N	2.36	0.55
2:I:206:ALA:O	2:I:209:ILE:HG22	2.06	0.55
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.07	0.55
5:L:94:THR:OG1	5:L:95:THR:N	2.40	0.55
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.89	0.55
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.89	0.55
2:I:231:GLU:HG2	2:I:332:ARG:HD3	1.89	0.55
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.87	0.55
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.89	0.55
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.87	0.55
5:L:573:LEU:HD23	5:L:573:LEU:H	1.71	0.55
2:C:829:THR:HA	2:C:1059:ARG:HA	1.89	0.55
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.88	0.55
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.89	0.55
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.40	0.55
2:C:518:ASN:O	2:C:691:PRO:HD3	2.07	0.54
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.89	0.54
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.72	0.54
1:B:214:GLU:O	1:B:218:ARG:HG3	2.07	0.54
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.72	0.54
2:C:703:GLY:N	2:C:705:GLU:OE2	2.39	0.54
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.08	0.54
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.88	0.54
2:C:1296:ASP:HB3	2:C:1320:PRO:HB3	1.90	0.54
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.88	0.54
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.89	0.54
2:C:91:THR:HG21	2:C:503:LYS:NZ	2.23	0.54
2:C:1131:MET:HE1	2:C:1141:LEU:HD12	1.89	0.54
5:F:547:VAL:HG23	5:F:603:ARG:HH11	1.72	0.54
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.90	0.54
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.90	0.54
3:J:210:SER:O	3:J:214:ARG:HG2	2.08	0.54
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.73	0.54
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.90	0.54
4:E:80:LEU:O	4:E:84:THR:OG1	2.19	0.54
3:J:264:ASP:OD2	5:L:506:SER:OG	2.22	0.54
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.89	0.54
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.90	0.54
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.72	0.54
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.88	0.54
1:B:212:ASP:CG	1:B:215:GLU:HB2	2.28	0.54
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.90	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.88	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.43	0.54
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.54
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.89	0.54
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.90	0.53
2:C:562:GLU:OE2	2:C:662:SER:OG	2.17	0.53
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.48	0.53
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.43	0.53
3:J:338:PHE:HA	3:J:342:LEU:O	2.08	0.53
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.90	0.53
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:ALA:HB2	1:H:126:PRO:HB3	1.91	0.53
2:I:213:LEU:HB3	2:I:422:LYS:HD2	1.90	0.53
2:I:314:ASN:O	2:I:352:ARG:NH1	2.34	0.53
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.74	0.53
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.39	0.53
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.43	0.53
3:D:53:ARG:NH2	3:D:60:ARG:HD2	2.24	0.53
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.43	0.53
5:F:166:VAL:O	5:F:167:ASP:HB2	2.09	0.53
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.89	0.53
1:H:110:VAL:HG21	1:H:140:ILE:HD11	1.89	0.53
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.23	0.53
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.24	0.53
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.39	0.53
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.90	0.53
5:F:395:THR:OG1	5:F:396:ASN:N	2.40	0.53
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.90	0.53
2:I:819:SER:HB2	2:I:1085:MET:SD	2.49	0.53
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.89	0.53
2:C:819:SER:HB2	2:C:1085:MET:SD	2.47	0.53
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.73	0.53
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.91	0.53
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.49	0.53
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.91	0.53
1:H:182:ARG:HG3	3:J:534:GLU:OE1	2.09	0.53
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.73	0.53
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.08	0.53
2:C:471:VAL:HG21	2:C:498:ILE:HD11	1.90	0.53
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.91	0.53
2:I:598:VAL:HG22	2:I:628:HIS:HE1	1.74	0.53
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.08	0.53
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.90	0.53
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.90	0.53
1:B:195:ARG:HB2	1:B:198:LEU:HD21	1.91	0.53
2:C:548:ARG:NH2	2:C:567:PRO:O	2.42	0.53
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.73	0.53
1:H:59:VAL:O	1:H:171:LEU:N	2.41	0.53
3:J:1262:ARG:HD2	3:J:1279:GLN:OE1	2.09	0.53
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.90	0.53
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.09	0.53
5:L:130:VAL:HB	5:L:365:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.92	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.90	0.52
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.09	0.52
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.73	0.52
2:I:211:ARG:NH1	2:I:357:ASN:O	2.41	0.52
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.91	0.52
1:B:12:ARG:H	1:B:30:PRO:CD	2.22	0.52
2:C:886:LYS:H	2:C:917:SER:HB3	1.74	0.52
3:D:709:ARG:C	3:D:711:GLY:H	2.13	0.52
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.74	0.52
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.09	0.52
1:G:49:SER:OG	1:G:50:SER:N	2.40	0.52
1:H:55:ALA:O	1:H:146:VAL:HG13	2.08	0.52
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.92	0.52
1:A:45:ARG:HG2	1:B:38:THR:CB	2.38	0.52
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.92	0.52
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.73	0.52
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.91	0.52
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.91	0.52
3:D:654:ILE:O	3:D:658:GLU:HB2	2.10	0.52
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.90	0.52
2:C:490:GLN:HE21	5:F:472:GLN:NE2	2.07	0.52
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.92	0.52
5:F:483:LEU:HD12	5:F:483:LEU:H	1.74	0.52
1:H:35:PHE:HA	1:H:38:THR:HG22	1.92	0.52
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.92	0.52
3:J:847:ASP:OD1	3:J:847:ASP:N	2.35	0.52
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.09	0.52
1:H:59:VAL:N	1:H:171:LEU:O	2.32	0.52
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.74	0.52
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.91	0.52
2:I:878:THR:OG1	2:I:879:GLY:N	2.40	0.52
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.23	0.52
3:D:73:GLY:O	3:D:76:LYS:NZ	2.29	0.52
3:D:290:ILE:HD12	3:D:290:ILE:H	1.75	0.52
1:H:74:VAL:HG22	1:H:133:LEU:HD12	1.91	0.52
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.75	0.52
3:J:94:GLN:O	3:J:97:VAL:HG23	2.10	0.52
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.92	0.52
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.92	0.52
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1286:THR:N	3:J:479:GLU:OE2	2.39	0.52
3:J:1165:PHE:HE1	3:J:1200:GLU:HB3	1.75	0.52
4:K:25:ARG:NH2	4:K:68:GLU:OE1	2.43	0.52
3:J:709:ARG:C	3:J:711:GLY:H	2.13	0.52
3:J:1184:ASP:O	3:J:1186:TYR:N	2.42	0.52
5:L:314:THR:O	5:L:318:ALA:HB3	2.10	0.52
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.75	0.51
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.92	0.51
3:D:19:ALA:O	3:D:20:ILE:HG13	2.11	0.51
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.36	0.51
2:I:1247:SER:HB3	3:J:375:GLU:O	2.09	0.51
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.90	0.51
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.92	0.51
2:C:778:GLU:O	2:C:781:ASP:HB2	2.10	0.51
2:C:878:THR:OG1	2:C:879:GLY:N	2.42	0.51
2:I:462:ASN:O	2:I:466:VAL:HG23	2.09	0.51
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.10	0.51
2:I:170:VAL:HG23	2:I:171:LEU:N	2.25	0.51
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.92	0.51
2:I:1246:ARG:HH11	2:I:1266:GLY:HA2	1.75	0.51
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.09	0.51
4:K:13:ILE:HD12	4:K:19:LEU:HA	1.92	0.51
1:A:49:SER:OG	1:A:50:SER:N	2.43	0.51
2:C:4:SER:HB2	2:C:7:GLU:HG3	1.93	0.51
2:C:516:ASP:HB2	6:C:3001:RFP:H20C	1.92	0.51
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.46	0.51
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.92	0.51
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.93	0.51
3:J:748:ALA:HA	3:J:754:ILE:HA	1.93	0.51
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.40	0.51
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.31	0.51
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.43	0.51
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.92	0.51
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.92	0.51
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.93	0.51
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.10	0.51
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.93	0.51
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.11	0.51
2:C:91:THR:HG21	2:C:503:LYS:HZ1	1.75	0.51
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.92	0.51
3:D:557:LYS:HA	3:D:563:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:789:LYS:NZ	3:D:931:THR:O	2.37	0.51
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.44	0.51
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.93	0.51
2:C:452:ARG:NH1	2:C:584:TYR:O	2.43	0.51
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.50	0.51
5:F:507:MET:HG2	5:F:520:GLY:CA	2.41	0.51
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.26	0.51
2:I:778:GLU:O	2:I:781:ASP:HB2	2.11	0.51
5:L:585:GLU:O	5:L:589:GLN:HG3	2.11	0.51
2:C:180:ARG:NH2	2:C:465:ARG:HH22	2.09	0.51
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.74	0.51
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.44	0.51
2:I:963:GLU:O	2:I:967:LEU:HB2	2.10	0.51
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.51	0.51
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.75	0.51
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.93	0.51
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.44	0.50
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.45	0.50
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.25	0.50
3:D:356:THR:OG1	3:D:357:VAL:N	2.44	0.50
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.93	0.50
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.77	0.50
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.60	0.50
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.93	0.50
2:C:170:VAL:HG23	2:C:171:LEU:N	2.26	0.50
3:D:103:GLY:CA	3:D:244:VAL:HG22	2.41	0.50
3:D:362:ARG:H	3:D:365:GLN:HE21	1.60	0.50
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.93	0.50
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.32	0.50
1:H:62:ASP:OD1	1:H:141:SER:OG	2.28	0.50
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.93	0.50
2:I:516:ASP:H	2:I:526:HIS:HD1	1.57	0.50
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.12	0.50
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.93	0.50
1:H:31:LEU:HB2	1:H:199:ASP:O	2.11	0.50
2:I:23:ASP:OD1	2:I:23:ASP:N	2.45	0.50
3:J:19:ALA:O	3:J:20:ILE:HG13	2.11	0.50
2:C:510:GLN:HE21	6:C:3001:RFP:H131	1.76	0.50
3:D:1295:ASN:OD1	3:J:1206:ARG:NH2	2.45	0.50
2:I:168:GLY:C	2:I:170:VAL:H	2.14	0.50
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:96:ASP:O	5:L:98:VAL:N	2.44	0.50
1:B:182:ARG:HG3	3:D:534:GLU:OE1	2.10	0.50
2:I:617:ALA:HA	2:I:636:CYS:SG	2.51	0.50
2:I:1327:LEU:HD23	2:I:1331:ARG:HH21	1.76	0.50
3:J:1165:PHE:CE1	3:J:1200:GLU:HB3	2.47	0.50
1:A:233:ASP:C	1:A:234:LEU:HD22	2.32	0.50
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	1.94	0.50
5:F:139:GLU:HG2	5:F:351:THR:HA	1.94	0.50
1:G:9:LEU:HD21	1:G:195:ARG:NH2	2.27	0.50
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.93	0.50
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.27	0.50
5:L:127:ILE:O	5:L:130:VAL:HG22	2.12	0.50
1:H:90:VAL:HG23	1:H:123:ILE:HD13	1.93	0.50
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.47	0.50
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.10	0.50
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.93	0.49
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.76	0.49
3:D:42:GLU:CG	5:F:451:ARG:HE	2.25	0.49
3:D:1371:ARG:HH21	3:J:854:ALA:HA	1.77	0.49
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.93	0.49
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.77	0.49
2:I:490:GLN:HG2	2:I:491:ASP:N	2.26	0.49
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.47	0.49
1:B:35:PHE:HA	1:B:38:THR:HG22	1.92	0.49
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.94	0.49
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.94	0.49
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.47	0.49
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.47	0.49
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.94	0.49
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.94	0.49
2:I:466:VAL:O	2:I:470:ARG:HG2	2.13	0.49
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.77	0.49
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.94	0.49
5:L:166:VAL:O	5:L:167:ASP:HB2	2.12	0.49
5:L:343:LYS:H	5:L:343:LYS:HD2	1.76	0.49
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.93	0.49
6:C:3001:RFP:O9	6:C:3001:RFP:O10	2.26	0.49
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.94	0.49
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.93	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.95	0.49
1:B:183:ILE:CD1	1:B:205:MET:HG3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:529:ARG:HH12	6:C:3001:RFP:C18	2.26	0.49
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.47	0.49
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.94	0.49
3:D:473:THR:HG23	3:D:476:ALA:H	1.77	0.49
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.27	0.49
2:I:396:ASP:HA	2:I:418:GLY:O	2.13	0.49
3:D:11:GLN:HG2	3:D:15:GLU:HG2	1.95	0.49
3:D:363:LEU:HG	3:D:363:LEU:O	2.12	0.49
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.26	0.49
3:J:70:CYS:SG	3:J:71:LEU:N	2.85	0.49
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.49
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.28	0.49
1:A:73:GLY:O	1:A:134:THR:HG22	2.12	0.49
2:C:101:ARG:HG3	2:C:118:LYS:HD2	1.93	0.49
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.93	0.49
3:J:362:ARG:H	3:J:365:GLN:HE21	1.60	0.49
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.94	0.49
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.48	0.49
2:C:566:GLY:O	2:C:569:ILE:HG13	2.11	0.49
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.24	0.49
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.13	0.49
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.48	0.49
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.26	0.49
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.28	0.49
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.22	0.49
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.95	0.49
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.95	0.49
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.12	0.49
3:J:110:PRO:HG2	3:J:183:GLU:HG2	1.94	0.49
2:C:44:GLU:HA	2:C:54:ARG:NH1	2.28	0.48
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.47	0.48
3:D:514:THR:OG1	3:D:594:GLN:O	2.31	0.48
3:D:517:CYS:HA	3:D:716:GLN:NE2	2.28	0.48
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.95	0.48
1:G:10:LYS:HA	1:H:227:GLN:NE2	2.28	0.48
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.93	0.48
2:I:262:TYR:HE1	2:I:280:ASP:OD2	1.96	0.48
3:J:914:ALA:O	3:J:918:ILE:HG23	2.13	0.48
1:A:185:TYR:HE1	2:C:1087:TYR:HH	1.59	0.48
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.94	0.48
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:94:GLN:O	3:D:97:VAL:HG23	2.12	0.48
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.95	0.48
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.28	0.48
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.48	0.48
3:J:290:ILE:H	3:J:290:ILE:HD12	1.77	0.48
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.95	0.48
3:J:838:ARG:NH1	3:J:1250:ASP:OD1	2.46	0.48
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.44	0.48
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.95	0.48
3:D:418:GLU:HG3	4:E:45:LYS:H	1.79	0.48
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.79	0.48
5:F:244:THR:O	5:F:247:GLU:HG2	2.11	0.48
1:H:83:LEU:HD11	3:J:526:VAL:CG2	2.43	0.48
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.95	0.48
3:J:209:ASN:HA	3:J:214:ARG:HE	1.77	0.48
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.95	0.48
2:C:513:GLN:OE1	6:C:3001:RFP:H343	2.14	0.48
3:D:214:ARG:HA	3:D:217:LEU:HB2	1.95	0.48
5:F:466:ILE:HG22	5:F:470:MET:HG3	1.95	0.48
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.96	0.48
3:J:748:ALA:O	3:J:777:HIS:HD2	1.97	0.48
2:C:548:ARG:HB3	2:C:569:ILE:O	2.13	0.48
2:C:1281:TYR:OH	3:D:431:ARG:O	2.30	0.48
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.95	0.48
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.14	0.48
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.13	0.48
1:G:45:ARG:HG2	1:H:38:THR:CB	2.39	0.48
1:G:73:GLY:O	1:G:134:THR:HG22	2.13	0.48
2:I:138:ILE:HB	2:I:143:ARG:HD3	1.95	0.48
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.32	0.48
5:L:483:LEU:HD12	5:L:483:LEU:H	1.76	0.48
2:C:490:GLN:HE21	5:F:472:GLN:HE21	1.60	0.48
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.94	0.48
1:H:182:ARG:NH1	3:J:581:MET:SD	2.87	0.48
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.95	0.48
3:J:525:MET:O	3:J:548:VAL:HG13	2.12	0.48
1:B:153:VAL:H	1:B:175:ALA:HB3	1.78	0.48
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	1.95	0.48
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.77	0.48
2:I:1285:TYR:CD2	3:J:1356:LEU:HD21	2.48	0.48
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.96	0.48
1:B:47:LEU:O	1:B:180:VAL:HG21	2.13	0.48
1:B:57:THR:HG21	1:B:158:ARG:HE	1.78	0.48
3:D:827:GLU:O	3:D:829:GLY:N	2.37	0.48
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.43	0.48
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.78	0.48
4:K:60:ASN:H	4:K:63:ILE:HB	1.79	0.48
1:A:9:LEU:HD21	1:A:195:ARG:HH21	1.79	0.48
3:J:34:SER:HB2	3:J:104:HIS:HB3	1.95	0.48
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.44	0.48
5:L:354:THR:O	5:L:358:VAL:HG23	2.14	0.48
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.95	0.48
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.96	0.48
5:F:571:TYR:CD1	5:F:575:GLU:HG2	2.48	0.48
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.95	0.48
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.96	0.48
2:I:886:LYS:H	2:I:917:SER:HB3	1.78	0.48
3:J:1154:ALA:N	3:J:1214:PRO:O	2.43	0.48
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.96	0.47
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.29	0.47
1:H:13:LEU:HD23	1:H:13:LEU:H	1.78	0.47
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.78	0.47
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.95	0.47
3:J:317:THR:HB	3:J:324:LEU:HB3	1.95	0.47
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.96	0.47
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.95	0.47
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.95	0.47
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.95	0.47
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.96	0.47
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.95	0.47
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.96	0.47
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.13	0.47
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.14	0.47
3:J:518:VAL:N	3:J:716:GLN:HE22	2.12	0.47
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.47	0.47
3:D:1174:ARG:HG2	3:D:1189:MET:SD	2.54	0.47
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.49	0.47
4:E:10:VAL:HG13	4:E:16:ARG:HB2	1.96	0.47
5:F:470:MET:HA	5:F:473:GLU:HB3	1.96	0.47
1:H:51:MET:O	1:H:150:ARG:HA	2.13	0.47
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.95	0.47
3:J:1307:LEU:HB3	3:J:1312:ALA:HB2	1.97	0.47
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.96	0.47
2:C:42:ASP:OD2	2:C:44:GLU:HG2	2.14	0.47
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.49	0.47
3:D:11:GLN:HG3	3:D:12:THR:H	1.79	0.47
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.78	0.47
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.44	0.47
3:J:592:VAL:HA	3:J:596:LEU:HD21	1.95	0.47
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.96	0.47
3:D:748:ALA:O	3:D:777:HIS:HD2	1.98	0.47
5:F:388:ILE:O	5:F:392:LYS:HG3	2.14	0.47
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.96	0.47
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.49	0.47
5:L:532:LEU:HD12	5:L:532:LEU:H	1.79	0.47
2:C:231:GLU:O	2:C:238:GLN:N	2.46	0.47
2:C:632:ASP:O	2:C:647:ARG:HB2	2.14	0.47
1:B:113:ALA:HB2	1:B:126:PRO:HB3	1.97	0.47
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.49	0.47
5:F:499:LYS:HA	5:F:502:LYS:HE2	1.96	0.47
2:I:739:ASP:OD1	2:I:739:ASP:N	2.47	0.47
2:I:1272:GLU:H	3:J:343:LEU:HD12	1.79	0.47
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.97	0.47
3:J:35:PHE:HD1	3:J:101:ARG:HB3	1.80	0.47
4:K:29:GLN:CD	4:K:35:LYS:HE2	2.35	0.47
2:C:468:LEU:O	2:C:471:VAL:HG12	2.15	0.47
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.62	0.47
3:D:741:ALA:O	3:D:762:ASN:ND2	2.48	0.47
1:H:19:VAL:HG23	1:H:24:ALA:HA	1.96	0.47
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.96	0.47
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.80	0.47
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.14	0.47
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	1.97	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.96	0.47
3:D:513:MET:HE3	3:D:579:LEU:HD22	1.97	0.47
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.97	0.47
1:H:20:SER:OG	1:H:21:SER:N	2.48	0.47
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.49	0.47
5:L:148:TYR:OH	5:L:218:ARG:HA	2.15	0.47
2:C:18:ARG:NH1	2:C:621:SER:O	2.47	0.47
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.47
3:D:1198:VAL:HG11	3:D:1210:ILE:HG23	1.96	0.47
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.29	0.47
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.96	0.47
3:J:262:THR:C	5:L:507:MET:HB2	2.36	0.47
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.97	0.47
1:B:125:LYS:HG3	1:B:128:HIS:HB2	1.96	0.46
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.50	0.46
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.97	0.46
2:C:891:GLY:O	2:C:892:GLU:HG3	2.15	0.46
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.15	0.46
3:D:121:PRO:HG2	3:D:123:ARG:HH21	1.80	0.46
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.44	0.46
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.96	0.46
3:J:338:PHE:C	3:J:340:GLN:H	2.18	0.46
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.96	0.46
3:J:544:LEU:O	3:J:574:VAL:HB	2.15	0.46
3:J:587:LEU:HD23	3:J:591:ILE:HG21	1.95	0.46
1:A:90:VAL:HG22	1:A:91:ARG:H	1.80	0.46
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.97	0.46
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.50	0.46
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.49	0.46
3:J:425:ARG:HG2	3:J:426:ALA:H	1.80	0.46
2:C:13:LYS:O	2:C:1183:ALA:N	2.42	0.46
2:C:452:ARG:HH21	2:C:458:GLU:CD	2.18	0.46
3:D:334:LYS:HA	3:D:335:GLN:HA	1.57	0.46
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.98	0.46
3:D:1227:HIS:CB	3:J:1293:GLU:HG2	2.44	0.46
5:F:486:ARG:CZ	5:F:486:ARG:HB2	2.46	0.46
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.98	0.46
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.97	0.46
1:A:39:LEU:O	1:A:43:LEU:N	2.40	0.46
1:B:190:ALA:N	1:B:198:LEU:O	2.40	0.46
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.97	0.46
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.16	0.46
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.80	0.46
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.96	0.46
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.45	0.46
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.61	0.46
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.49	0.46
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:O	3:D:545:HIS:HB3	2.15	0.46
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.96	0.46
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.81	0.46
2:I:4:SER:HB2	2:I:7:GLU:HG3	1.97	0.46
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.97	0.46
3:J:34:SER:HG	3:J:104:HIS:CG	2.27	0.46
3:J:338:PHE:O	3:J:340:GLN:N	2.48	0.46
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.98	0.46
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.98	0.46
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.97	0.46
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.16	0.46
3:D:598:LYS:O	3:D:601:ILE:HG22	2.16	0.46
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.51	0.46
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	1.97	0.46
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.98	0.46
2:I:387:ASN:HA	2:I:391:SER:HB2	1.96	0.46
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.16	0.46
3:J:733:SER:O	3:J:737:ILE:HG12	2.14	0.46
2:C:55:SER:OG	2:C:56:VAL:N	2.49	0.46
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.97	0.46
3:J:451:PRO:O	3:J:454:CYS:HB2	2.15	0.46
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.97	0.46
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.98	0.46
2:C:60:GLN:HA	2:C:67:GLU:HA	1.98	0.46
2:C:149:LEU:HD12	2:C:452:ARG:O	2.15	0.46
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.80	0.46
5:F:343:LYS:O	5:F:347:ILE:HG13	2.16	0.46
1:H:213:PRO:O	1:H:217:ILE:HG13	2.16	0.46
2:I:169:LYS:O	2:I:170:VAL:HG22	2.15	0.46
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.51	0.46
3:J:121:PRO:HG2	3:J:123:ARG:HH21	1.80	0.46
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.98	0.46
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.98	0.46
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.97	0.46
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.50	0.46
1:B:19:VAL:O	1:B:20:SER:HB3	2.15	0.46
1:B:74:VAL:HG22	1:B:133:LEU:HD12	1.96	0.46
2:C:1298:VAL:HG11	3:D:96:LYS:HE3	1.98	0.46
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.16	0.46
3:D:658:GLU:O	3:D:661:VAL:HG13	2.16	0.46
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:697:MET:SD	3:D:741:ALA:HB3	2.56	0.46
5:F:575:GLU:OE2	5:F:578:LYS:NZ	2.43	0.46
1:G:118:ASP:H	1:G:121:VAL:HB	1.81	0.46
2:I:132:ASP:OD1	2:I:132:ASP:N	2.38	0.46
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.48	0.46
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.15	0.46
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.96	0.46
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.96	0.46
3:D:133:ARG:HD2	3:D:133:ARG:HA	1.77	0.46
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.98	0.46
3:D:748:ALA:O	3:D:777:HIS:CD2	2.69	0.46
1:H:101:THR:H	1:H:116:THR:CG2	2.28	0.46
1:H:118:ASP:H	1:H:121:VAL:HB	1.81	0.46
2:I:1211:ARG:HE	2:I:1220:GLN:HE21	1.63	0.46
3:J:473:THR:HG23	3:J:476:ALA:H	1.81	0.46
2:C:670:PHE:CD1	2:C:1184:THR:HG21	2.51	0.45
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.50	0.45
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.98	0.45
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.98	0.45
3:D:1165:PHE:CE1	3:D:1200:GLU:HB3	2.52	0.45
5:F:127:ILE:O	5:F:130:VAL:HG22	2.15	0.45
3:J:620:PHE:CE1	3:J:624:ILE:HD11	2.51	0.45
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.97	0.45
5:L:316:PHE:CZ	5:L:337:VAL:HB	2.50	0.45
1:A:56:VAL:HG11	1:A:85:LEU:HB3	1.99	0.45
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.97	0.45
1:G:19:VAL:HG13	1:G:20:SER:H	1.80	0.45
1:G:77:ASP:O	1:G:81:ILE:HG13	2.16	0.45
1:H:41:ASN:O	1:H:45:ARG:HG3	2.15	0.45
1:H:183:ILE:HG13	1:H:205:MET:HG3	1.96	0.45
2:I:138:ILE:HG22	2:I:139:ASN:N	2.31	0.45
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.30	0.45
3:J:336:GLY:O	3:J:337:ARG:HB2	2.16	0.45
1:A:172:LEU:HD12	1:A:172:LEU:H	1.81	0.45
2:C:138:ILE:HG22	2:C:139:ASN:N	2.30	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.16	0.45
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.98	0.45
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.30	0.45
2:C:1248:THR:HG21	5:F:531:PRO:HG2	1.98	0.45
3:D:122:SER:O	3:D:126:LEU:HG	2.16	0.45
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:VAL:HG22	1:G:91:ARG:H	1.81	0.45
1:H:11:PRO:HB2	1:H:28:LEU:HD11	1.97	0.45
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.31	0.45
2:C:195:PHE:CG	2:C:203:LYS:HD3	2.51	0.45
2:C:745:GLU:HG3	2:C:1017:GLN:CB	2.36	0.45
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.17	0.45
3:D:489:ASN:HA	3:D:904:ALA:CB	2.46	0.45
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.97	0.45
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.73	0.45
3:J:215:LYS:O	3:J:218:THR:HG22	2.17	0.45
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.17	0.45
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.99	0.45
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.50	0.45
3:D:797:THR:O	3:D:801:VAL:HG13	2.16	0.45
1:H:105:SER:HA	1:H:138:ALA:O	2.17	0.45
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.97	0.45
3:J:222:LYS:HE2	3:J:1276:GLU:OE1	2.16	0.45
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.98	0.45
2:C:239:MET:O	2:C:284:LEU:HD12	2.17	0.45
2:C:498:ILE:HD12	2:C:498:ILE:H	1.81	0.45
2:C:499:SER:O	2:C:503:LYS:HB2	2.17	0.45
2:C:675:ASP:HB3	2:C:1107:MET:O	2.15	0.45
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.98	0.45
3:D:331:ILE:CG2	3:D:1328:THR:HG21	2.47	0.45
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	1.99	0.45
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.97	0.45
2:I:180:ARG:NH2	2:I:396:ASP:HB2	2.32	0.45
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.99	0.45
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.32	0.45
1:A:62:ASP:OD1	1:A:141:SER:OG	2.29	0.45
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.49	0.45
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.83	0.45
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.72	0.45
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.98	0.45
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.52	0.45
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.99	0.45
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.99	0.45
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.17	0.45
3:J:56:LEU:HD12	3:J:56:LEU:H	1.82	0.45
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.98	0.45
3:J:905:ARG:HH21	3:J:907:HIS:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.99	0.45
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.82	0.45
2:C:701:GLY:O	2:C:1184:THR:N	2.37	0.45
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.46	0.45
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.50	0.45
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.82	0.45
1:G:9:LEU:HD21	1:G:195:ARG:HH21	1.81	0.45
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.99	0.45
3:J:77:ARG:HG3	3:J:79:LYS:H	1.81	0.45
2:C:132:ASP:OD1	2:C:132:ASP:N	2.37	0.45
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.99	0.45
2:I:15:PHE:CG	2:I:1190:ALA:HB2	2.52	0.45
3:J:364:HIS:CD2	4:K:4:VAL:HG23	2.52	0.45
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.98	0.45
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.32	0.45
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.52	0.45
2:I:27:LEU:HB2	2:I:524:ILE:HD11	1.98	0.45
2:I:703:GLY:N	2:I:705:GLU:OE2	2.43	0.45
2:I:1099:ASN:HD21	3:J:505:ASP:CG	2.20	0.45
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.52	0.45
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.17	0.45
3:J:432:LEU:HD13	3:J:499:ILE:HG21	1.98	0.45
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.80	0.45
1:B:57:THR:O	1:B:173:VAL:HG22	2.17	0.44
1:B:175:ALA:HB1	1:B:177:TYR:CZ	2.52	0.44
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.44
3:D:343:LEU:HD22	3:D:343:LEU:HA	1.42	0.44
1:H:73:GLY:C	1:H:134:THR:HG22	2.38	0.44
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.99	0.44
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.52	0.44
3:J:746:LEU:HB2	3:J:754:ILE:HD11	2.00	0.44
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.82	0.44
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.32	0.44
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.32	0.44
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.44
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.83	0.44
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.51	0.44
3:J:759:ILE:HG23	3:J:771:GLN:HB3	1.98	0.44
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.50	0.44
5:L:515:GLU:HG2	5:L:516:ASP:N	2.32	0.44
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:VAL:HG12	1:B:76:GLU:H	1.82	0.44
1:B:93:GLN:HB2	1:B:120:ASP:OD1	2.16	0.44
1:B:194:GLN:O	1:B:195:ARG:HG2	2.18	0.44
2:C:867:GLU:H	2:C:867:GLU:HG3	1.52	0.44
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.99	0.44
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.82	0.44
1:H:13:LEU:HD12	1:H:16:ILE:HD11	1.98	0.44
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.18	0.44
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.52	0.44
3:J:849:LEU:HD13	3:J:849:LEU:H	1.82	0.44
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.82	0.44
5:L:372:ALA:O	5:L:376:LYS:HG3	2.17	0.44
2:C:168:GLY:C	2:C:170:VAL:H	2.20	0.44
2:C:494:ASN:HB3	2:C:497:PRO:HD2	2.00	0.44
2:C:782:VAL:HG11	2:C:792:GLY:HA2	1.99	0.44
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.45	0.44
3:D:113:HIS:HB3	3:D:116:PHE:HD2	1.82	0.44
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.99	0.44
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.98	0.44
3:D:903:LEU:HD23	3:D:905:ARG:HD3	1.99	0.44
5:F:555:GLU:OE2	5:F:597:LYS:NZ	2.46	0.44
1:H:84:ASN:OD1	3:J:551:ARG:NH2	2.51	0.44
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.99	0.44
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.99	0.44
2:I:1272:GLU:H	3:J:343:LEU:CD1	2.30	0.44
2:I:1288:GLN:HG2	2:I:1315:MET:HE1	1.99	0.44
3:J:79:LYS:HG3	3:J:80:HIS:N	2.32	0.44
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.98	0.44
5:L:139:GLU:HG2	5:L:351:THR:HA	2.00	0.44
1:A:90:VAL:HG23	1:A:123:ILE:HD13	2.00	0.44
3:D:646:ILE:H	3:D:646:ILE:HG12	1.57	0.44
3:D:799:ARG:NH1	3:D:1146:GLU:OE1	2.50	0.44
2:I:98:VAL:C	2:I:121:GLU:HA	2.38	0.44
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.47	0.44
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.99	0.44
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.99	0.44
2:C:62:TYR:C	2:C:64:GLY:H	2.21	0.44
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.99	0.44
2:C:980:VAL:O	2:C:984:VAL:HB	2.17	0.44
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.98	0.44
3:D:892:PHE:CE1	3:D:1281:GLU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:LYS:HG2	1:H:110:VAL:HG22	2.00	0.44
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.52	0.44
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.18	0.44
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.17	0.44
5:L:226:ALA:O	5:L:229:VAL:HG22	2.18	0.44
1:B:214:GLU:HG2	1:B:218:ARG:NH2	2.32	0.44
2:C:356:THR:HG21	2:C:362:ALA:HA	2.00	0.44
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	2.00	0.44
3:D:612:LEU:HB3	3:D:616:PRO:HG2	2.00	0.44
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.83	0.44
2:I:91:THR:HG21	2:I:503:LYS:HZ1	1.82	0.44
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.17	0.44
1:B:12:ARG:H	1:B:30:PRO:HD2	1.81	0.44
2:C:23:ASP:OD1	2:C:23:ASP:N	2.48	0.44
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.32	0.44
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.17	0.44
3:D:903:LEU:HD12	3:D:903:LEU:HA	1.91	0.44
5:F:281:ARG:O	5:F:285:ARG:HG3	2.18	0.44
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.00	0.44
1:H:90:VAL:HG22	1:H:91:ARG:H	1.82	0.44
2:I:90:VAL:HG12	2:I:91:THR:H	1.81	0.44
3:J:232:ASN:HA	3:J:236:TRP:HZ3	1.83	0.44
4:K:26:ARG:HH22	4:K:38:LEU:HD13	1.83	0.44
2:C:732:ILE:HG21	2:C:783:LEU:HD12	2.00	0.44
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.29	0.44
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.87	0.44
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.99	0.44
5:F:94:THR:O	5:F:95:THR:OG1	2.27	0.44
1:G:9:LEU:HD23	1:G:9:LEU:H	1.83	0.44
2:I:225:PHE:CE2	2:I:347:ILE:HB	2.52	0.44
2:I:808:ASN:H	3:J:633:ALA:HB2	1.83	0.44
5:L:528:LEU:HD23	5:L:528:LEU:HA	1.85	0.44
5:L:547:VAL:HG23	5:L:603:ARG:NH1	2.31	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.77	0.43
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.00	0.43
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.00	0.43
1:G:75:GLN:HA	2:I:729:ALA:N	2.33	0.43
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.73	0.43
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.72	0.43
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.82	0.43
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1333:LEU:HD22	3:J:307:LEU:HD22	2.00	0.43
3:J:334:LYS:HA	3:J:335:GLN:HA	1.54	0.43
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.82	0.43
1:B:20:SER:OG	1:B:21:SER:N	2.51	0.43
2:C:104:ILE:O	2:C:113:THR:HA	2.18	0.43
2:C:724:VAL:HG11	2:C:727:VAL:HG22	2.00	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.98	0.43
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.30	0.43
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.48	0.43
5:F:507:MET:HG2	5:F:520:GLY:HA3	2.00	0.43
1:G:12:ARG:HA	1:H:230:ALA:HB2	1.99	0.43
1:G:74:VAL:HG22	1:G:76:GLU:H	1.82	0.43
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.19	0.43
2:I:896:THR:HB	2:I:897:PRO:HD2	1.99	0.43
2:I:967:LEU:HD12	2:I:967:LEU:HA	1.87	0.43
3:J:514:THR:CB	3:J:576:ARG:HG2	2.47	0.43
3:J:801:VAL:O	3:J:805:GLN:HB2	2.18	0.43
1:A:83:LEU:HD23	2:C:694:ARG:NH2	2.33	0.43
1:A:118:ASP:H	1:A:121:VAL:HB	1.83	0.43
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.89	0.43
2:I:559:CYS:CB	2:I:662:SER:HB3	2.47	0.43
5:L:569:THR:OG1	5:L:570:ASP:N	2.48	0.43
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.00	0.43
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.54	0.43
2:C:806:PRO:HB3	3:D:505:ASP:OD1	2.18	0.43
3:D:708:ASN:OD1	3:D:708:ASN:N	2.49	0.43
3:D:1344:LEU:HB3	3:D:1350:ASN:ND2	2.30	0.43
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.99	0.43
1:H:93:GLN:H	1:H:120:ASP:HB3	1.83	0.43
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.54	0.43
2:I:757:THR:HG23	2:I:765:ILE:HG23	2.00	0.43
2:I:1109:ILE:HD12	2:I:1109:ILE:HA	1.88	0.43
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.99	0.43
3:J:682:VAL:O	3:J:685:ILE:HG12	2.17	0.43
4:K:58:LEU:O	4:K:63:ILE:HG21	2.18	0.43
5:L:461:ASN:O	5:L:465:ARG:HG2	2.19	0.43
1:B:153:VAL:O	1:B:175:ALA:N	2.28	0.43
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.54	0.43
2:C:642:SER:HB2	3:D:770:LEU:HD21	2.01	0.43
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.99	0.43
3:D:931:THR:O	3:D:931:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.18	0.43
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.68	0.43
1:G:73:GLY:C	1:G:134:THR:HG22	2.39	0.43
2:I:316:GLU:H	2:I:316:GLU:CD	2.22	0.43
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.53	0.43
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.54	0.43
5:L:227:GLN:HG2	5:L:252:LEU:HA	2.00	0.43
1:A:47:LEU:O	1:A:180:VAL:HG21	2.19	0.43
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.49	0.43
2:C:696:ASP:O	2:C:697:LYS:HB3	2.18	0.43
2:C:972:PHE:HD1	2:C:994:ARG:HH21	1.65	0.43
5:F:463:LEU:HD23	5:F:463:LEU:HA	1.86	0.43
3:J:800:LEU:O	3:J:803:VAL:HG12	2.19	0.43
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.83	0.43
3:J:1246:VAL:HG12	3:J:1248:ILE:HG13	2.01	0.43
5:L:316:PHE:O	5:L:320:ILE:HG13	2.18	0.43
2:C:660:VAL:HG13	2:C:661:VAL:HG13	2.00	0.43
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.00	0.43
5:F:512:GLY:O	5:F:514:ASP:N	2.52	0.43
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.84	0.43
2:I:62:TYR:C	2:I:64:GLY:H	2.22	0.43
2:I:159:SER:HB2	2:I:442:VAL:HG21	2.01	0.43
3:J:546:ALA:O	3:J:573:THR:HA	2.18	0.43
3:J:698:MET:O	3:J:702:GLN:HB3	2.18	0.43
2:C:687:ARG:HH22	6:C:3001:RFP:H301	1.83	0.43
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.84	0.43
2:C:1142:ARG:HD3	2:C:1161:LEU:CD1	2.48	0.43
3:D:822:MET:SD	3:D:838:ARG:HB3	2.58	0.43
5:F:499:LYS:HB2	5:F:499:LYS:HE3	1.77	0.43
2:I:10:ARG:HA	2:I:1172:LEU:HD23	2.00	0.43
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.74	0.43
3:J:317:THR:HG22	3:J:322:ARG:O	2.19	0.43
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.49	0.43
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.84	0.43
2:C:735:LYS:HA	2:C:748:ILE:HG22	2.00	0.43
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.63	0.43
2:C:1250:SER:OG	5:F:524:GLU:OE1	2.37	0.43
3:D:513:MET:HE1	3:D:579:LEU:HD13	2.01	0.43
3:D:1237:VAL:HG11	3:D:1253:ILE:HG21	2.01	0.43
5:F:227:GLN:HG2	5:F:252:LEU:HA	2.01	0.43
2:I:69:GLN:HG3	2:I:101:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:ARG:HG3	2:I:118:LYS:HD2	2.01	0.43
2:I:149:LEU:HD11	2:I:451:ARG:HB3	2.00	0.43
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.58	0.43
3:J:661:VAL:HB	3:J:682:VAL:HG13	2.01	0.43
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.18	0.43
2:C:463:GLN:HG3	2:C:505:PHE:HB2	2.01	0.43
2:C:619:ALA:HB1	2:C:657:THR:HA	2.00	0.43
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.41	0.43
2:C:992:LEU:H	2:C:992:LEU:HD23	1.84	0.43
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.51	0.43
3:D:546:ALA:O	3:D:573:THR:HA	2.18	0.43
3:D:647:PRO:CG	3:D:697:MET:HB3	2.46	0.43
3:D:689:ALA:O	3:D:693:VAL:HG23	2.19	0.43
3:D:1184:ASP:O	3:D:1186:TYR:N	2.52	0.43
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.32	0.43
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.81	0.43
1:H:55:ALA:HB3	1:H:177:TYR:CD1	2.54	0.43
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.54	0.42
2:C:565:GLU:HB2	2:C:680:LEU:HD21	1.99	0.42
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.49	0.42
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.84	0.42
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.84	0.42
5:F:559:LEU:HD22	5:F:594:ALA:HB1	2.01	0.42
1:G:90:VAL:HG23	1:G:123:ILE:HD13	2.00	0.42
3:J:64:PRO:HB3	3:J:69:GLU:O	2.19	0.42
3:J:536:LEU:HD12	3:J:542:ALA:HB2	2.00	0.42
3:J:708:ASN:OD1	3:J:708:ASN:N	2.51	0.42
3:J:793:SER:O	3:J:797:THR:HG23	2.18	0.42
1:B:41:ASN:OD1	2:C:1217:THR:HG22	2.19	0.42
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.19	0.42
5:F:96:ASP:O	5:F:98:VAL:N	2.52	0.42
2:I:498:ILE:HD12	2:I:498:ILE:H	1.83	0.42
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	2.01	0.42
2:I:816:ILE:HG22	2:I:818:VAL:HG23	2.01	0.42
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	2.00	0.42
1:A:177:TYR:O	1:A:178:SER:HB2	2.19	0.42
1:B:154:PRO:HA	1:B:174:ASP:HB3	2.01	0.42
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.23	0.42
2:C:496:LYS:HB3	2:C:496:LYS:HE3	1.61	0.42
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.91	0.42
5:F:532:LEU:HD12	5:F:532:LEU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:519:ASN:ND2	2:I:796:LEU:HD23	2.31	0.42
2:I:980:VAL:O	2:I:984:VAL:HB	2.19	0.42
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.02	0.42
1:A:19:VAL:HG13	1:A:20:SER:H	1.84	0.42
1:A:219:ARG:O	1:A:223:ILE:HG13	2.19	0.42
1:A:228:LEU:HD23	1:A:231:PHE:HD2	1.83	0.42
2:C:221:LEU:HD11	2:C:314:ASN:HB2	2.01	0.42
2:C:488:MET:O	2:C:490:GLN:N	2.46	0.42
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.34	0.42
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.84	0.42
3:D:93:THR:HG22	3:D:94:GLN:H	1.83	0.42
3:D:218:THR:HA	3:D:221:ILE:HG22	2.01	0.42
3:D:824:PRO:HD3	3:D:835:LEU:HB2	2.01	0.42
5:F:462:LYS:O	5:F:466:ILE:HG13	2.18	0.42
5:F:512:GLY:C	5:F:514:ASP:H	2.23	0.42
1:G:38:THR:HG23	1:H:45:ARG:HB2	2.02	0.42
1:G:47:LEU:O	1:G:180:VAL:HG21	2.20	0.42
2:I:37:LYS:HA	2:I:37:LYS:HD3	1.80	0.42
2:I:503:LYS:HA	2:I:503:LYS:HD2	1.85	0.42
5:L:292:VAL:HG21	5:L:299:LYS:HG2	2.00	0.42
2:C:618:GLN:HG3	2:C:620:ASN:H	1.83	0.42
3:D:114:ILE:HG22	3:D:307:LEU:HD12	2.01	0.42
3:D:137:ARG:HD3	3:D:143:SER:OG	2.19	0.42
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.19	0.42
4:K:15:ASN:HB3	4:K:18:ASP:HB2	2.01	0.42
5:L:561:MET:HA	5:L:567:MET:HE1	2.01	0.42
2:C:516:ASP:H	2:C:526:HIS:HD1	1.68	0.42
2:C:593:LYS:HA	2:C:652:TYR:CD2	2.55	0.42
2:C:854:ILE:O	2:C:857:VAL:HG22	2.18	0.42
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.55	0.42
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.02	0.42
3:D:598:LYS:N	3:D:728:SER:O	2.41	0.42
3:D:1283:SER:O	3:D:1286:LYS:N	2.52	0.42
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.35	0.42
3:J:42:GLU:HG3	5:L:451:ARG:HE	1.83	0.42
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.78	0.42
1:A:38:THR:OG1	1:B:45:ARG:HG2	2.20	0.42
1:B:155:ALA:HB2	1:B:173:VAL:C	2.39	0.42
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.85	0.42
2:C:196:VAL:HG12	2:C:206:ALA:HA	2.00	0.42
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:324:LYS:O	2:C:327:GLN:NE2	2.51	0.42
2:C:1114:GLU:OE1	2:C:1230:MET:HA	2.20	0.42
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.48	0.42
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.84	0.42
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.84	0.42
5:F:409:ASN:O	5:F:413:MET:HG3	2.20	0.42
1:G:71:LYS:HB2	1:G:78:ILE:HD11	2.01	0.42
2:I:791:LEU:HD23	2:I:791:LEU:HA	1.84	0.42
3:J:806:ASP:HA	3:J:1347:LEU:HD13	2.01	0.42
2:C:615:VAL:HG13	2:C:651:ASP:N	2.33	0.42
3:D:27:PRO:HB3	3:D:241:VAL:HG23	2.00	0.42
5:F:98:VAL:HB	5:F:402:LEU:HD11	2.02	0.42
1:H:192:VAL:HG21	1:H:198:LEU:HD12	2.02	0.42
2:I:194:LEU:HA	2:I:194:LEU:HD12	1.77	0.42
2:I:402:ARG:HG2	2:I:416:GLY:N	2.35	0.42
2:I:1174:GLU:OE2	2:I:1177:ARG:NH1	2.51	0.42
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	2.01	0.42
2:I:1285:TYR:CE2	3:J:1356:LEU:HD11	2.55	0.42
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.85	0.42
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.35	0.42
3:J:342:LEU:HA	3:J:343:LEU:HA	1.57	0.42
3:J:598:LYS:O	3:J:601:ILE:HG22	2.19	0.42
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	2.02	0.42
5:L:552:THR:OG1	5:L:555:GLU:HG3	2.20	0.42
5:L:582:VAL:CG1	5:L:586:ARG:HG2	2.49	0.42
2:C:810:TYR:CD2	3:D:359:PRO:HG2	2.55	0.42
2:C:985:GLU:HB3	2:C:988:LYS:HB2	2.02	0.42
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.83	0.42
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.19	0.42
3:D:623:GLN:O	3:D:627:THR:HG22	2.19	0.42
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.33	0.42
3:J:825:VAL:C	3:J:826:ILE:HG13	2.39	0.42
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.50	0.42
1:B:177:TYR:O	1:B:178:SER:C	2.58	0.42
3:D:682:VAL:O	3:D:685:ILE:HG12	2.20	0.42
3:D:825:VAL:C	3:D:826:ILE:HG13	2.39	0.42
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.02	0.42
2:I:61:SER:HB3	2:I:479:LEU:HB3	2.02	0.42
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.50	0.42
2:I:1114:GLU:OE1	2:I:1230:MET:HA	2.20	0.42
2:I:1314:GLN:HG2	4:K:28:ARG:NE	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.85	0.42
5:L:493:LYS:HA	5:L:496:LYS:HE2	2.02	0.42
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.23	0.41
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.85	0.41
2:C:808:ASN:H	3:D:633:ALA:HB2	1.85	0.41
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.85	0.41
3:D:526:VAL:HA	3:D:549:LYS:O	2.19	0.41
3:D:641:ILE:HD13	3:D:641:ILE:O	2.20	0.41
3:D:849:LEU:HB3	3:D:853:THR:HG23	2.01	0.41
5:F:276:MET:O	5:F:280:VAL:HG23	2.20	0.41
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.20	0.41
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.49	0.41
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.20	0.41
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.01	0.41
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.85	0.41
5:L:476:ARG:HG3	5:L:477:GLU:N	2.35	0.41
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.49	0.41
5:L:603:ARG:H	5:L:603:ARG:HG2	1.65	0.41
1:B:212:ASP:OD1	1:B:215:GLU:HB2	2.20	0.41
2:C:169:LYS:O	2:C:169:LYS:HG2	2.19	0.41
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.77	0.41
2:C:722:GLY:HA2	2:C:737:ASN:OD1	2.20	0.41
2:C:953:LEU:HD12	2:C:953:LEU:HA	1.85	0.41
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.35	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.84	0.41
3:D:875:ASN:OD1	3:D:875:ASN:N	2.54	0.41
1:G:211:ILE:HD13	1:G:211:ILE:HA	1.95	0.41
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.84	0.41
2:I:593:LYS:HE3	2:I:595:THR:HG22	2.02	0.41
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.35	0.41
3:J:850:LYS:HB3	3:J:851:PRO:HD2	2.01	0.41
3:J:850:LYS:HG2	3:J:857:LEU:HD23	2.02	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
1:A:228:LEU:HD11	1:B:224:LEU:HD22	2.01	0.41
1:B:35:PHE:O	1:B:38:THR:HG22	2.20	0.41
2:C:41:GLN:NE2	2:C:73:TYR:O	2.54	0.41
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.38	0.41
2:C:1328:LYS:O	2:C:1332:SER:N	2.52	0.41
3:D:859:PRO:HG2	3:D:862:THR:HG21	2.01	0.41
5:F:316:PHE:CZ	5:F:334:SER:HA	2.45	0.41
2:I:587:LEU:HA	2:I:587:LEU:HD23	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:985:GLU:HB3	2:I:988:LYS:HB2	2.00	0.41
3:J:19:ALA:CB	3:J:1373:ARG:HH22	2.33	0.41
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.35	0.41
3:J:441:LEU:HD13	3:J:441:LEU:HA	1.91	0.41
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.85	0.41
2:C:796:LEU:O	2:C:1233:LEU:HD12	2.20	0.41
2:C:996:ARG:HA	2:C:996:ARG:HD3	1.81	0.41
2:C:1038:GLN:O	2:C:1038:GLN:HG3	2.20	0.41
3:D:451:PRO:O	3:D:454:CYS:HB2	2.19	0.41
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.20	0.41
2:I:86:GLN:HA	2:I:140:GLY:HA2	2.02	0.41
2:I:705:GLU:HB2	2:I:794:LEU:H	1.86	0.41
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.28	0.41
3:J:214:ARG:HA	3:J:217:LEU:HB2	2.02	0.41
3:J:332:LYS:HB2	3:J:332:LYS:HE3	1.82	0.41
3:J:689:ALA:O	3:J:693:VAL:HG23	2.21	0.41
3:J:810:THR:HG23	3:J:811:GLU:H	1.86	0.41
3:J:860:ARG:HB3	3:J:861:ASN:H	1.73	0.41
5:L:457:ILE:HA	5:L:460:ILE:HD12	2.02	0.41
5:L:586:ARG:O	5:L:590:ILE:HG13	2.21	0.41
1:A:167:PRO:HB2	1:A:170:ARG:HB2	2.02	0.41
1:A:181:GLU:HB3	1:A:206:GLU:HG3	2.02	0.41
1:B:64:VAL:HG11	1:B:69:SER:HB2	2.02	0.41
1:B:118:ASP:H	1:B:121:VAL:HB	1.84	0.41
1:B:201:LEU:HG	1:B:203:ILE:HG13	2.02	0.41
2:C:590:PRO:HG3	2:C:605:TYR:OH	2.21	0.41
2:C:791:LEU:HA	2:C:791:LEU:HD23	1.79	0.41
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.51	0.41
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.86	0.41
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.87	0.41
1:G:227:GLN:HE21	1:H:35:PHE:HD2	1.68	0.41
3:J:461:PHE:HD2	3:J:461:PHE:HA	1.72	0.41
3:J:818:GLU:HB3	3:J:887:SER:HB2	2.03	0.41
1:B:79:LEU:HD11	3:D:526:VAL:HG21	2.03	0.41
2:C:396:ASP:HA	2:C:418:GLY:O	2.20	0.41
2:C:519:ASN:ND2	2:C:796:LEU:HD23	2.34	0.41
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.55	0.41
3:D:30:ILE:HD13	3:D:243:PRO:HD3	2.03	0.41
3:D:317:THR:HG22	3:D:322:ARG:O	2.20	0.41
3:D:362:ARG:H	3:D:365:GLN:NE2	2.17	0.41
2:I:98:VAL:O	2:I:121:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:607:SER:N	2:I:610:GLU:HB2	2.35	0.41
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.02	0.41
5:L:584:ARG:HH11	5:L:584:ARG:HA	1.86	0.41
1:A:83:LEU:HD23	2:C:694:ARG:HH21	1.85	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.02	0.41
2:C:980:VAL:HA	2:C:984:VAL:HA	2.03	0.41
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.53	0.41
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.36	0.41
5:F:226:ALA:O	5:F:229:VAL:HG22	2.20	0.41
1:G:35:PHE:CE1	1:H:46:ILE:HG23	2.55	0.41
1:H:47:LEU:HD23	1:H:47:LEU:HA	1.70	0.41
2:I:198:ILE:O	2:I:201:ARG:HB2	2.20	0.41
3:J:1174:ARG:HG2	3:J:1189:MET:SD	2.60	0.41
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.20	0.41
5:L:233:ASP:O	5:L:236:LYS:HE2	2.21	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.68	0.41
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.55	0.41
2:C:206:ALA:O	2:C:209:ILE:HG22	2.21	0.41
3:D:18:ASP:HB2	3:D:1373:ARG:CZ	2.50	0.41
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.41
3:D:422:LEU:HB2	3:D:469:HIS:HB2	2.03	0.41
1:G:27:THR:HA	1:G:201:LEU:O	2.21	0.41
1:G:38:THR:HA	1:H:45:ARG:HD3	2.03	0.41
1:G:83:LEU:HD23	2:I:694:ARG:HH21	1.85	0.41
2:I:202:ARG:NH2	2:I:368:ARG:HH12	2.19	0.41
2:I:299:LYS:HB3	2:I:299:LYS:HE2	1.91	0.41
2:I:896:THR:OG1	2:I:899:GLU:HG3	2.20	0.41
2:I:1198:LEU:HD22	2:I:1198:LEU:HA	1.84	0.41
2:I:1309:VAL:HA	3:J:383:GLY:HA3	2.01	0.41
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	2.03	0.41
1:B:82:LEU:HD13	1:B:173:VAL:HG12	2.02	0.41
2:C:149:LEU:HD13	2:C:453:ILE:HG12	2.01	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.21	0.41
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.39	0.41
2:C:1136:GLN:O	2:C:1137:GLU:HB3	2.21	0.41
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.56	0.41
3:D:839:VAL:HG13	3:D:882:VAL:HG21	2.01	0.41
3:D:844:THR:HG23	3:D:864:LEU:HD11	2.03	0.41
5:F:230:VAL:HG13	5:F:231:THR:H	1.83	0.41
5:F:320:ILE:HG12	5:F:330:LEU:HD12	2.02	0.41
5:F:572:THR:O	5:F:576:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:588:ARG:H	5:F:588:ARG:HG3	1.58	0.41
1:G:61:ILE:HB	1:G:64:VAL:CG2	2.51	0.41
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.56	0.41
1:H:57:THR:HG21	1:H:158:ARG:NH2	2.35	0.41
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.88	0.41
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.93	0.41
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.86	0.41
2:I:675:ASP:HB3	2:I:1107:MET:O	2.21	0.41
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.41
2:I:805:MET:HB2	2:I:805:MET:HE2	1.92	0.41
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.54	0.41
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.55	0.41
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.56	0.41
3:J:325:LYS:HG3	3:J:329:ASP:HB2	2.02	0.41
3:J:363:LEU:O	3:J:363:LEU:HG	2.21	0.41
3:J:600:ALA:O	3:J:603:LYS:HG2	2.21	0.41
3:J:701:LEU:CD1	3:J:723:TYR:HB2	2.51	0.41
1:A:137:ASN:OD1	1:A:137:ASN:N	2.53	0.41
2:C:57:PHE:CD1	2:C:59:ILE:HG13	2.55	0.41
2:C:269:ILE:HG22	2:C:274:ILE:HG13	2.03	0.41
3:D:11:GLN:NE2	3:D:15:GLU:OE2	2.54	0.41
3:D:647:PRO:HG3	3:D:697:MET:CB	2.47	0.41
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.20	0.41
4:E:15:ASN:O	4:E:16:ARG:HB3	2.20	0.41
1:H:198:LEU:HD23	1:H:198:LEU:HA	1.86	0.41
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.21	0.41
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.56	0.41
3:J:809:VAL:HA	3:J:894:VAL:O	2.21	0.41
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.80	0.40
1:A:73:GLY:C	1:A:134:THR:HG22	2.42	0.40
2:C:187:GLU:OE2	2:C:203:LYS:HE2	2.21	0.40
2:C:1178:LYS:HD3	2:C:1178:LYS:HA	1.96	0.40
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.40	0.40
3:D:369:PRO:HB3	3:D:444:GLY:O	2.21	0.40
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.95	0.40
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.51	0.40
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	2.02	0.40
2:I:94:ALA:HB2	2:I:129:LEU:HD11	2.02	0.40
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.56	0.40
5:L:281:ARG:HG2	5:L:285:ARG:HD2	2.03	0.40
5:L:296:LYS:HA	5:L:296:LYS:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:653:MET:HG2	2:C:654:ASP:N	2.37	0.40
3:D:339:ARG:O	3:D:344:GLY:HA2	2.21	0.40
1:G:177:TYR:O	1:G:178:SER:HB2	2.21	0.40
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	2.03	0.40
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.03	0.40
3:J:77:ARG:HA	3:J:77:ARG:HD2	1.85	0.40
3:J:189:LEU:HD22	3:J:234:PRO:HB3	2.01	0.40
3:J:526:VAL:HA	3:J:549:LYS:O	2.21	0.40
4:K:15:ASN:O	4:K:16:ARG:HB3	2.22	0.40
1:A:233:ASP:OD2	1:A:233:ASP:N	2.55	0.40
2:C:62:TYR:O	2:C:64:GLY:N	2.54	0.40
2:C:232:ILE:HD12	2:C:330:HIS:O	2.20	0.40
2:C:646:SER:HB3	2:C:649:GLN:HG3	2.02	0.40
2:C:819:SER:HB2	2:C:1085:MET:CG	2.51	0.40
3:D:232:ASN:HA	3:D:236:TRP:HZ3	1.84	0.40
3:D:901:ARG:HD2	3:D:906:GLY:O	2.22	0.40
5:F:372:ALA:O	5:F:376:LYS:HG3	2.21	0.40
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.04	0.40
1:H:92:VAL:HA	1:H:120:ASP:O	2.21	0.40
2:I:496:LYS:HB3	2:I:497:PRO:HD3	2.02	0.40
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.22	0.40
3:J:294:ASN:HB2	5:L:101:TYR:CD1	2.56	0.40
3:J:785:ASP:O	3:J:789:LYS:HG3	2.21	0.40
3:J:805:GLN:OE1	3:J:1348:LYS:HD3	2.21	0.40
5:L:437:GLN:HG3	5:L:438:ALA:N	2.35	0.40
5:L:547:VAL:CG2	5:L:603:ARG:HB3	2.51	0.40
2:C:27:LEU:HG	2:C:711:ASP:OD2	2.21	0.40
2:C:678:ARG:HD3	2:C:678:ARG:HA	1.92	0.40
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.92	0.40
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	2.03	0.40
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.19	0.40
5:F:105:MET:HE1	5:F:385:ARG:HG2	2.02	0.40
3:J:1183:SER:OG	3:J:1185:PRO:HD3	2.21	0.40
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.57	0.40
1:B:211:ILE:HD13	1:B:211:ILE:HA	1.90	0.40
2:C:444:ASP:OD1	2:C:447:HIS:HB2	2.22	0.40
2:C:606:LEU:HD23	2:C:611:GLU:HA	2.03	0.40
2:C:1131:MET:CE	2:C:1141:LEU:HD12	2.51	0.40
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	2.04	0.40
3:D:705:THR:OG1	3:D:718:SER:HA	2.21	0.40
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.52	0.40
5:F:235:ILE:HA	5:F:245:ALA:HB2	2.04	0.40
1:G:219:ARG:O	1:G:223:ILE:HG13	2.22	0.40
2:I:564:PRO:HG3	2:I:572:ILE:HG13	2.04	0.40
2:I:722:GLY:HA2	2:I:737:ASN:OD1	2.21	0.40
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.36	0.40
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.21	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%)	195 (87%)	26 (12%)	4 (2%)	8	41
1	B	210/329 (64%)	180 (86%)	25 (12%)	5 (2%)	6	37
1	G	222/329 (68%)	192 (86%)	24 (11%)	6 (3%)	5	35
1	H	211/329 (64%)	185 (88%)	21 (10%)	5 (2%)	6	37
2	C	1328/1342 (99%)	1220 (92%)	101 (8%)	7 (0%)	29	67
2	I	1324/1342 (99%)	1220 (92%)	97 (7%)	7 (0%)	29	67
3	D	1162/1407 (83%)	1070 (92%)	85 (7%)	7 (1%)	25	63
3	J	1151/1407 (82%)	1059 (92%)	80 (7%)	12 (1%)	15	52
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
5	F	462/613 (75%)	424 (92%)	37 (8%)	1 (0%)	47	79
5	L	463/613 (76%)	426 (92%)	36 (8%)	1 (0%)	47	79
All	All	6922/8222 (84%)	6328 (91%)	539 (8%)	55 (1%)	19	57

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	B	13	LEU
2	C	3	TYR
2	C	1159	VAL
3	D	10	ALA
3	D	332	LYS
2	I	1159	VAL
1	A	167	PRO
1	B	136	GLU
2	C	170	VAL
2	C	697	LYS
1	G	162	GLU
1	G	167	PRO
1	H	20	SER
1	H	135	ASP
2	I	170	VAL
2	I	697	LYS
3	J	332	LYS
3	J	334	LYS
3	J	339	ARG
1	B	20	SER
1	H	136	GLU
1	A	14	VAL
2	C	484	LEU
2	C	1158	LYS
3	D	710	ASP
3	D	806	ASP
2	I	484	LEU
2	I	1158	LYS
3	J	333	GLY
3	J	338	PHE
3	J	710	ASP
1	A	62	ASP
1	G	14	VAL
1	G	62	ASP
1	G	229	GLU
1	H	138	ALA
3	J	344	GLY
3	J	806	ASP
1	B	14	VAL
1	B	62	ASP
3	D	831	VAL
1	G	196	THR

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Mol	Chain	Res	Type
1	H	62	ASP
2	I	63	SER
3	J	831	VAL
5	F	477	GLU
2	I	1186	VAL
2	C	1186	VAL
3	D	826	ILE
3	D	1180	VAL
3	J	826	ILE
3	J	1180	VAL
5	L	477	GLU
3	J	336	GLY

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	46
1	B	182/286 (64%)	172 (94%)	10 (6%)	21	52
1	G	191/286 (67%)	179 (94%)	12 (6%)	18	47
1	H	184/286 (64%)	175 (95%)	9 (5%)	25	54
2	C	1150/1157 (99%)	1050 (91%)	100 (9%)	10	37
2	I	1147/1157 (99%)	1045 (91%)	102 (9%)	9	37
3	D	970/1168 (83%)	871 (90%)	99 (10%)	7	30
3	J	960/1168 (82%)	864 (90%)	96 (10%)	7	31
4	E	72/75 (96%)	65 (90%)	7 (10%)	8	32
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	49
5	F	417/540 (77%)	376 (90%)	41 (10%)	8	31
5	L	418/540 (77%)	378 (90%)	40 (10%)	8	32
All	All	5952/7024 (85%)	5419 (91%)	533 (9%)	9	36

All (533) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	19	VAL
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	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	115	ILE
1	B	133	LEU
1	B	215	GLU
2	C	11	ILE
2	C	22	LEU
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

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Mol	Chain	Res	Type
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	518	ASN
2	C	554	HIS
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
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

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Mol	Chain	Res	Type
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	919	ARG
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
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

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Mol	Chain	Res	Type
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	98	ARG
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	343	LEU
3	D	352	ARG
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	425	ARG
3	D	454	CYS
3	D	490	ILE
3	D	506	VAL
3	D	507	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

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Mol	Chain	Res	Type
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	704	GLU
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	764	ARG
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
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

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Mol	Chain	Res	Type
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
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	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	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	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

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Mol	Chain	Res	Type
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	19	VAL
1	G	50	SER
1	G	61	ILE
1	G	74	VAL
1	G	115	ILE
1	G	133	LEU
1	G	145	LYS
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	9	LEU
1	H	13	LEU
1	H	22	THR
1	H	26	VAL
1	H	44	ARG
1	H	50	SER
1	H	61	ILE
1	H	115	ILE
1	H	215	GLU
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	60	GLN

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Mol	Chain	Res	Type
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	124	MET
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
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	518	ASN
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

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Mol	Chain	Res	Type
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	817	LEU
2	I	819	SER
2	I	826	ASP
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

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Mol	Chain	Res	Type
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
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	98	ARG
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	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	507	VAL

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
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	606	VAL
5	L	612	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	510	GLN
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1288	GLN

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Mol	Chain	Res	Type
2	C	1314	GLN
3	D	11	GLN
3	D	94	GLN
3	D	200	GLN
3	D	365	GLN
3	D	419	HIS
3	D	450	HIS
3	D	469	HIS
3	D	594	GLN
3	D	665	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1259	GLN
5	F	131	GLN
5	F	246	GLN
5	F	309	ASN
5	F	383	ASN
5	F	446	GLN
5	F	472	GLN
5	F	518	HIS
1	H	186	ASN
2	I	69	GLN
2	I	139	ASN
2	I	343	HIS
2	I	494	ASN
2	I	513	GLN
2	I	628	HIS
2	I	688	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1220	GLN
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	206	ASN
3	J	365	GLN
3	J	665	GLN

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Mol	Chain	Res	Type
3	J	702	GLN
3	J	716	GLN
3	J	777	HIS
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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	RFP	C	3001	-	63,63,63	2.16	11 (17%)	94,94,94	2.00	29 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RFP	C	3001	-	-	21/60/85/85	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O3-C6	9.91	1.56	1.37
6	C	3001	RFP	C15-N1	6.41	1.49	1.35
6	C	3001	RFP	O7-C25	-4.90	1.37	1.44
6	C	3001	RFP	C12-C11	-4.66	1.36	1.54
6	C	3001	RFP	C3-C43	3.85	1.54	1.46
6	C	3001	RFP	C18-C17	3.76	1.55	1.43
6	C	3001	RFP	C6-C7	-2.53	1.35	1.39
6	C	3001	RFP	O6-C27	-2.44	1.37	1.43
6	C	3001	RFP	C17-C16	2.31	1.41	1.34
6	C	3001	RFP	C43-N2	2.24	1.34	1.27
6	C	3001	RFP	C2-N1	2.11	1.47	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	3001	RFP	C2-C3-C43	-5.02	119.06	124.17
6	C	3001	RFP	O4-C11-C5	-5.02	122.23	131.81
6	C	3001	RFP	C41-N3-N2	4.85	138.90	113.86
6	C	3001	RFP	C12-C11-C5	4.65	116.41	107.30
6	C	3001	RFP	C38-N4-C42	4.57	117.50	110.66
6	C	3001	RFP	C38-N4-C39	4.34	117.16	110.66
6	C	3001	RFP	C24-C23-C22	-4.15	108.47	115.43
6	C	3001	RFP	O7-C35-C36	4.09	118.61	111.09
6	C	3001	RFP	C20-C19-C18	-3.59	118.62	126.16
6	C	3001	RFP	C4-C3-C43	3.27	120.43	116.52
6	C	3001	RFP	C42-N4-C39	3.10	113.86	109.52
6	C	3001	RFP	C5-C10-C9	-3.04	114.11	119.66
6	C	3001	RFP	C3-C2-N1	-2.91	114.41	119.25
6	C	3001	RFP	C18-C17-C16	-2.89	118.11	126.61
6	C	3001	RFP	C40-C39-N4	2.84	114.02	110.80
6	C	3001	RFP	C40-N3-N2	-2.82	99.28	113.86
6	C	3001	RFP	C41-C42-N4	2.64	113.79	110.80
6	C	3001	RFP	C17-C16-C15	-2.62	113.07	121.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	3001	RFP	C12-O3-C6	-2.56	103.36	107.68
6	C	3001	RFP	C5-C10-C4	2.54	126.68	124.03
6	C	3001	RFP	C41-N3-C40	2.41	120.01	113.74
6	C	3001	RFP	C3-C43-N2	-2.34	118.14	121.54
6	C	3001	RFP	C13-C12-C11	-2.34	108.11	113.90
6	C	3001	RFP	C37-O6-C27	2.32	118.57	113.01
6	C	3001	RFP	O1-C1-C2	2.31	123.87	119.26
6	C	3001	RFP	O7-C35-O8	-2.19	118.61	122.96
6	C	3001	RFP	C20-C21-C22	-2.02	110.84	114.96
6	C	3001	RFP	C2-C3-C4	2.01	120.49	119.20
6	C	3001	RFP	O5-C12-C13	2.01	112.24	106.99

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3001	RFP	C2-C3-C43-N2
6	C	3001	RFP	C4-C3-C43-N2
6	C	3001	RFP	C30-C16-C17-C18
6	C	3001	RFP	C3-C2-N1-C15
6	C	3001	RFP	C17-C18-C19-C20
6	C	3001	RFP	C18-C19-C20-C31
6	C	3001	RFP	C23-C24-C25-O7
6	C	3001	RFP	C21-C22-C23-C24
6	C	3001	RFP	C1-C2-N1-C15
6	C	3001	RFP	C33-C24-C25-O7
6	C	3001	RFP	C32-C22-C23-O9
6	C	3001	RFP	C32-C22-C23-C24
6	C	3001	RFP	C21-C22-C23-O9
6	C	3001	RFP	C28-C27-O6-C37
6	C	3001	RFP	C33-C24-C25-C26
6	C	3001	RFP	O11-C15-C16-C30
6	C	3001	RFP	C16-C17-C18-C19
6	C	3001	RFP	C18-C19-C20-C21
6	C	3001	RFP	C43-N2-N3-C40
6	C	3001	RFP	N1-C15-C16-C30
6	C	3001	RFP	C26-C27-O6-C37

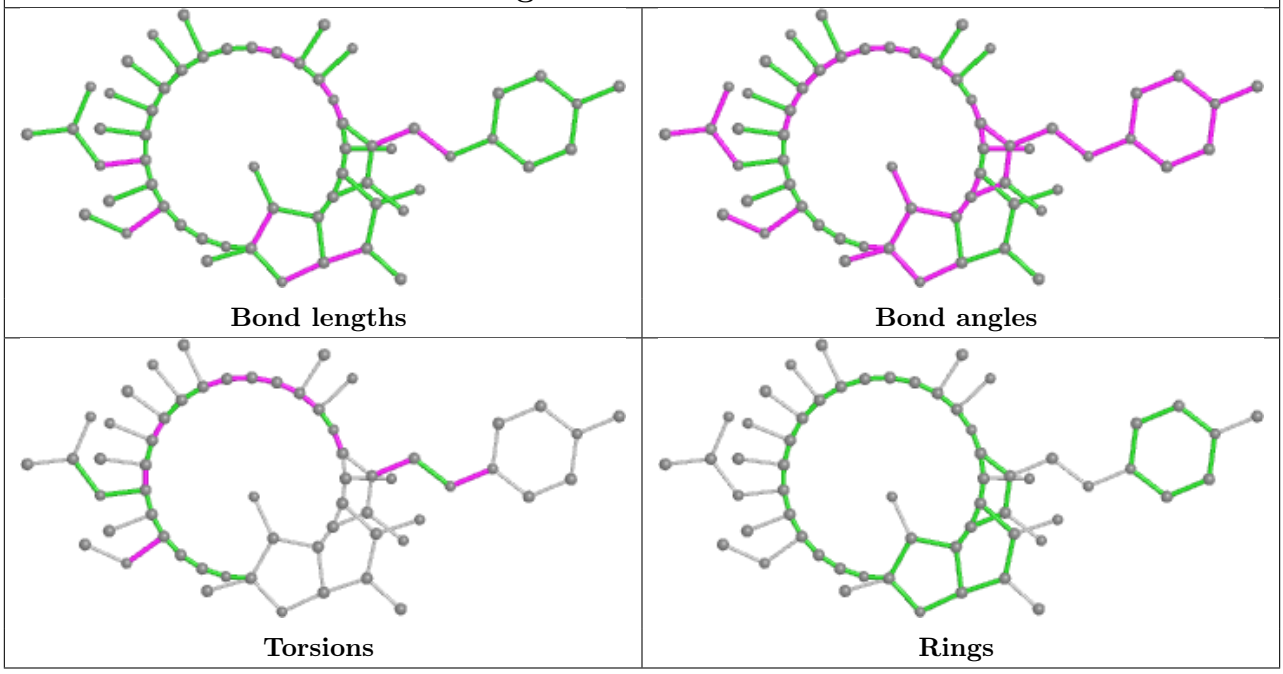
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand RFP C 3001



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%)	-0.30	3 (1%)	77	70	134, 178, 241, 363	0
1	B	214/329 (65%)	0.04	8 (3%)	41	33	141, 222, 328, 396	0
1	G	224/329 (68%)	-0.11	5 (2%)	62	52	175, 225, 285, 364	0
1	H	215/329 (65%)	0.20	8 (3%)	41	33	179, 247, 312, 401	0
2	C	1332/1342 (99%)	-0.11	62 (4%)	31	26	101, 169, 396, 542	0
2	I	1328/1342 (98%)	0.06	64 (4%)	30	25	139, 219, 353, 523	0
3	D	1166/1407 (82%)	-0.25	10 (0%)	84	78	93, 151, 275, 441	0
3	J	1155/1407 (82%)	-0.09	41 (3%)	44	35	128, 181, 311, 455	0
4	E	89/91 (97%)	-0.14	1 (1%)	80	73	144, 205, 237, 275	0
4	K	79/91 (86%)	0.91	19 (24%)	0	0	255, 318, 411, 416	0
5	F	468/613 (76%)	-0.15	16 (3%)	45	36	139, 222, 362, 481	0
5	L	469/613 (76%)	-0.15	16 (3%)	45	36	161, 231, 357, 487	0
All	All	6966/8222 (84%)	-0.08	253 (3%)	42	34	93, 196, 346, 542	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	311	CYS	14.4
2	C	252	SER	11.6
2	I	981	ALA	8.0
2	I	982	GLY	7.8
2	I	1000	LEU	7.6
2	C	283	LYS	7.4
2	C	323	ALA	7.3
2	I	978	VAL	7.0
2	C	376	PRO	6.9
2	C	1	MET	6.4
2	I	979	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
2	C	258	ASN	6.3
1	H	96	ASP	6.1
2	I	1011	LEU	5.9
2	C	284	LEU	5.5
5	L	490	PRO	5.2
2	C	377	THR	5.2
2	C	234	ASP	4.9
2	C	236	LYS	4.7
2	I	975	ILE	4.6
2	I	1004	ASP	4.6
2	C	265	LYS	4.6
5	F	314	THR	4.5
2	C	322	LEU	4.5
2	C	378	ARG	4.5
2	C	312	ALA	4.5
2	I	999	GLU	4.4
2	I	983	GLY	4.4
2	I	998	LEU	4.4
2	C	120	GLN	4.3
3	J	542	ALA	4.3
2	I	311	CYS	4.2
2	C	235	ASN	4.2
5	F	319	ALA	4.2
5	F	167	ASP	4.2
2	I	1006	GLU	4.2
5	F	318	ALA	4.2
1	B	147	GLN	4.1
5	F	325	PRO	4.1
3	J	712	GLN	4.0
1	G	95	LYS	4.0
2	C	330	HIS	4.0
2	C	329	GLY	3.9
4	K	37	PRO	3.9
1	B	172	LEU	3.9
2	I	1005	GLU	3.8
2	C	301	TYR	3.8
3	D	1203	ARG	3.8
2	I	413	GLU	3.8
2	I	980	VAL	3.7
2	C	288	PRO	3.7
2	C	314	ASN	3.7
3	J	218	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	J	518	VAL	3.6
3	J	175	GLU	3.5
4	K	38	LEU	3.5
3	J	1202	GLU	3.5
2	C	240	GLU	3.4
2	I	1010	GLN	3.4
5	F	324	LYS	3.4
3	J	827	GLU	3.4
4	K	41	GLU	3.4
2	C	310	ILE	3.3
1	H	135	ASP	3.3
3	J	212	THR	3.3
2	I	727	VAL	3.3
1	H	148	ARG	3.3
3	D	1202	GLU	3.3
5	L	488	LEU	3.3
3	J	1204	VAL	3.3
5	L	315	TRP	3.2
2	I	376	PRO	3.2
3	J	209	ASN	3.2
4	K	14	GLY	3.2
3	J	857	LEU	3.2
2	I	163	LYS	3.2
2	C	251	ALA	3.2
3	J	1203	ARG	3.2
4	K	36	ASP	3.2
2	C	1000	LEU	3.2
3	J	208	THR	3.2
2	C	262	TYR	3.2
2	I	412	GLU	3.2
4	K	77	ALA	3.2
4	K	75	GLN	3.2
1	H	107	ILE	3.1
2	I	374	GLU	3.1
4	K	79	GLU	3.1
2	I	247	ARG	3.1
2	C	229	ILE	3.1
4	K	78	ALA	3.1
1	H	14	VAL	3.1
5	F	315	TRP	3.1
2	C	248	GLY	3.1
5	F	313	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	1001	GLY	3.1
2	I	1014	LEU	3.1
5	L	322	MET	3.0
3	J	176	PHE	3.0
2	I	185	ASP	3.0
2	C	250	THR	3.0
2	C	259	GLY	3.0
3	J	207	GLU	3.0
2	I	234	ASP	3.0
2	I	1020	GLU	3.0
5	L	487	MET	3.0
2	C	169	LYS	3.0
2	I	375	PRO	3.0
3	J	830	ASP	2.9
2	C	267	ARG	2.9
2	I	985	GLU	2.9
2	I	891	GLY	2.9
2	I	110	PRO	2.8
3	D	1173	ARG	2.8
4	E	2	ALA	2.8
4	K	13	ILE	2.8
1	B	158	ARG	2.8
5	L	319	ALA	2.8
5	L	321	ALA	2.8
2	C	325	LEU	2.8
3	J	677	GLU	2.8
2	C	273	HIS	2.8
5	F	421	TYR	2.8
2	I	112	GLY	2.7
3	J	931	THR	2.7
2	C	264	GLU	2.7
2	I	233	ARG	2.7
5	F	321	ALA	2.7
4	K	40	PRO	2.7
3	D	1161	GLY	2.7
2	C	305	SER	2.7
3	D	1172	LYS	2.7
1	A	194	GLN	2.7
3	J	708	ASN	2.7
2	I	258	ASN	2.6
4	K	56	GLU	2.6
2	I	1022	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	373	GLY	2.6
2	C	260	LYS	2.6
4	K	35	LYS	2.6
2	I	600	THR	2.6
2	C	327	GLN	2.6
2	I	1068	GLY	2.6
2	C	318	SER	2.6
2	I	414	ILE	2.6
5	F	155	GLU	2.5
3	J	204	GLU	2.5
2	I	974	ARG	2.5
2	I	231	GLU	2.5
3	J	828	GLY	2.5
2	C	321	LEU	2.5
4	K	26	ARG	2.5
2	C	332	ARG	2.5
3	J	675	ALA	2.5
2	C	333	ILE	2.5
4	K	74	GLU	2.5
2	C	543	ALA	2.5
2	I	66	SER	2.5
3	J	1250	ASP	2.4
2	I	302	ILE	2.4
3	J	930	LEU	2.4
2	I	1007	LYS	2.4
2	I	174	ALA	2.4
2	I	1025	PHE	2.4
3	J	566	LYS	2.4
4	K	2	ALA	2.4
2	I	1137	GLU	2.4
2	I	1154	ASP	2.4
5	F	326	TRP	2.4
3	J	707	ILE	2.4
2	C	268	ARG	2.4
2	I	190	PRO	2.4
1	B	143	ARG	2.4
3	J	1148	ARG	2.4
2	C	249	GLU	2.4
3	J	213	LYS	2.4
1	B	41	ASN	2.4
1	A	162	GLU	2.4
2	I	254	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
5	L	423	ARG	2.3
3	J	1166	GLY	2.3
5	L	167	ASP	2.3
5	F	157	ARG	2.3
3	J	849	LEU	2.3
2	C	320	ASP	2.3
5	L	613	ASP	2.3
5	L	489	MET	2.3
1	G	194	GLN	2.3
3	D	209	ASN	2.3
5	L	294	GLN	2.3
1	H	204	GLU	2.3
3	J	1198	VAL	2.3
1	G	193	GLU	2.3
2	I	633	LEU	2.3
3	J	831	VAL	2.3
3	J	715	LYS	2.3
1	A	41	ASN	2.3
2	C	261	VAL	2.2
2	C	373	GLY	2.2
1	B	146	VAL	2.2
2	C	164	THR	2.2
2	I	117	ILE	2.2
2	C	117	ILE	2.2
2	C	253	PHE	2.2
2	C	116	ASP	2.2
2	I	991	LYS	2.2
2	I	1003	THR	2.2
5	L	422	ARG	2.2
4	K	58	LEU	2.2
4	K	72	GLN	2.2
1	G	191	ARG	2.2
2	C	414	ILE	2.2
2	C	302	ILE	2.2
3	J	76	LYS	2.2
2	I	107	ARG	2.2
2	C	270	THR	2.2
3	J	714	GLU	2.2
3	J	1375	ALA	2.1
1	B	66	HIS	2.1
2	C	271	ALA	2.1
3	J	314	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	108	GLU	2.1
3	J	335	GLN	2.1
2	C	233	ARG	2.1
5	L	421	TYR	2.1
3	J	1249	ASN	2.1
5	F	310	GLU	2.1
2	C	102	LEU	2.1
4	K	80	LEU	2.1
2	I	1015	ALA	2.1
2	C	1002	LEU	2.1
3	D	1165	PHE	2.1
3	D	149	GLY	2.1
1	H	211	ILE	2.1
5	F	514	ASP	2.1
5	F	323	ASN	2.1
2	I	1021	LEU	2.1
1	H	25	LYS	2.1
2	I	269	ILE	2.1
3	J	471	PRO	2.1
1	B	135	ASP	2.1
2	I	720	ARG	2.1
2	I	732	ILE	2.1
2	I	912	ASP	2.1
5	L	514	ASP	2.1
3	D	712	GLN	2.0
2	I	599	VAL	2.0
3	J	669	GLN	2.0
1	G	192	VAL	2.0
5	L	425	TYR	2.0
3	D	1296	GLY	2.0
2	C	291	TYR	2.0
2	I	1070	HIS	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)

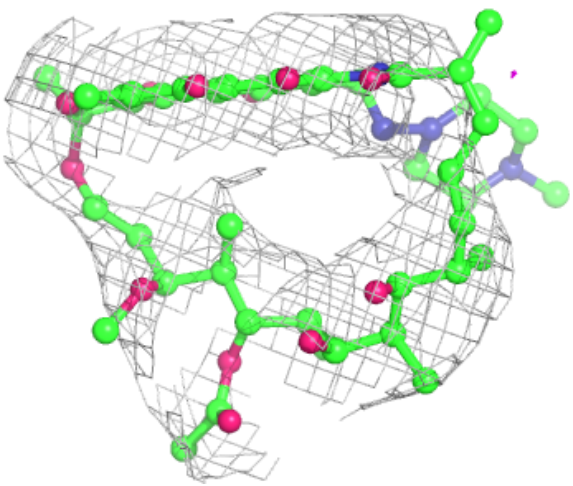
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

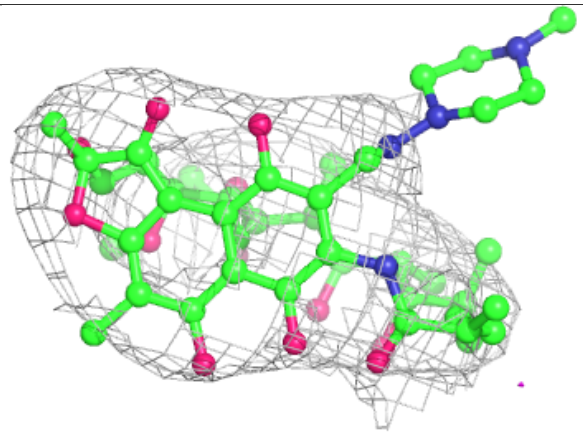
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	D	1501	1/1	0.94	0.39	77,77,77,77	0
6	RFP	C	3001	59/59	0.95	0.21	91,139,195,202	0
7	MG	J	1501	1/1	0.95	0.42	121,121,121,121	0
8	ZN	J	1502	1/1	0.96	0.06	174,174,174,174	0
8	ZN	D	1502	1/1	0.97	0.07	150,150,150,150	0
8	ZN	J	1503	1/1	0.98	0.14	126,126,126,126	0
8	ZN	D	1503	1/1	0.99	0.12	82,82,82,82	0

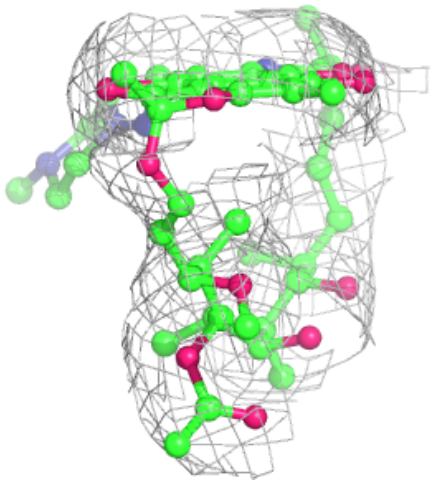
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RFP C 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.