Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:31 PM GMT

PDB ID	:	1TWF
Title	:	RNA polymerase II complexed with UTP at 2.3 A resolution
Authors	:	Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2004-06-30
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

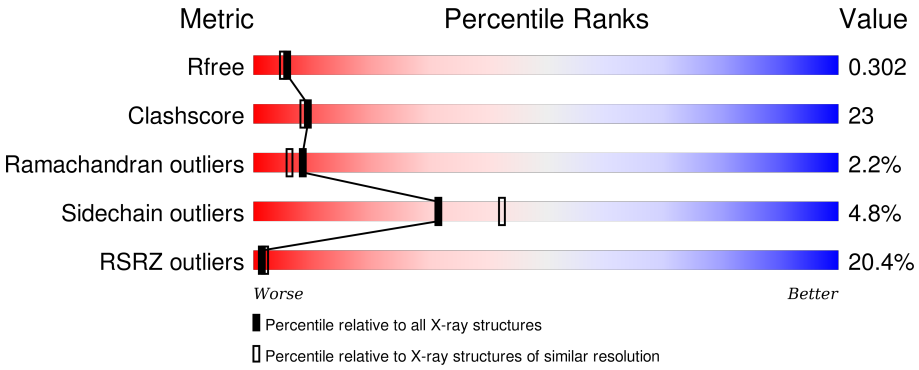
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	1733	15% 47% 31% • 18%
2	B	1224	18% 51% 36% • 11%
3	C	318	12% 44% 37% • 16%
4	E	215	23% 66% 33% •
5	F	155	6% 33% 21% • 46%

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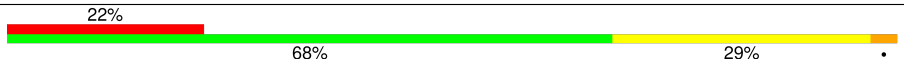
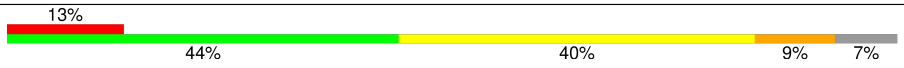
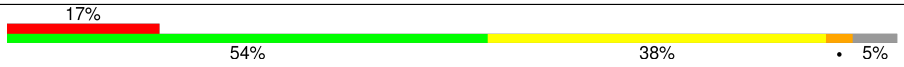
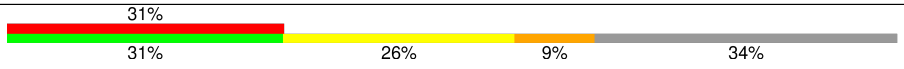
Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28318 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 II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1419	11154	7023	1952	2118	61	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1094	8711	5525	1519	1614	53	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	215	1760	1116	310	322	12	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	84	679	434	115	127	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	C	1	Total	Zn	0	0
			1	1		
11	A	2	Total	Zn	0	0
			2	2		

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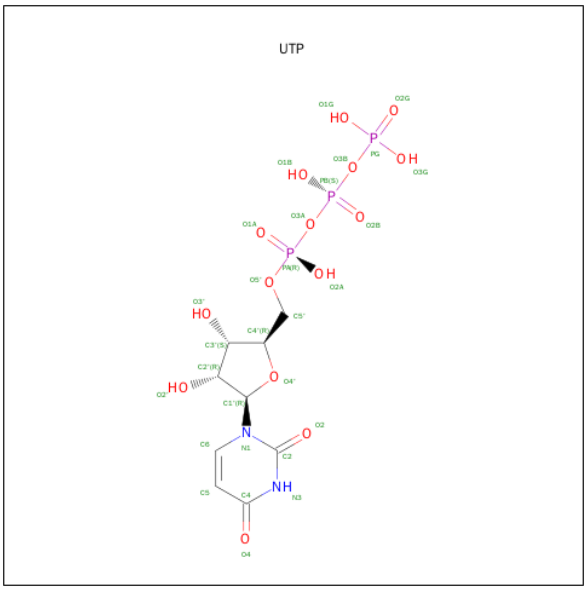
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total Zn 1 1	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	2	Total Mn 2 2	0	0

- Molecule 13 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



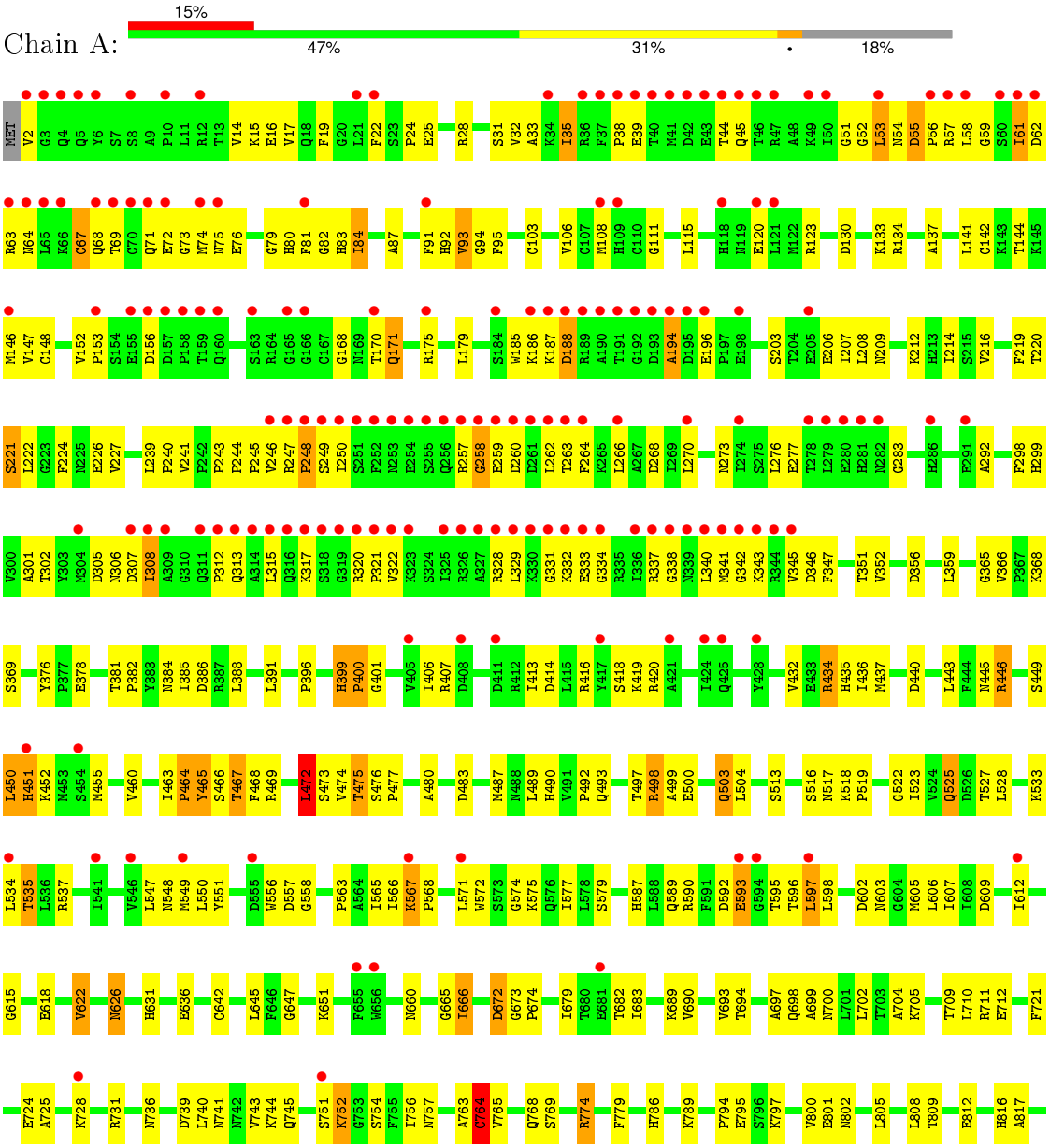
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O P 29 9 2 15 3	0	0

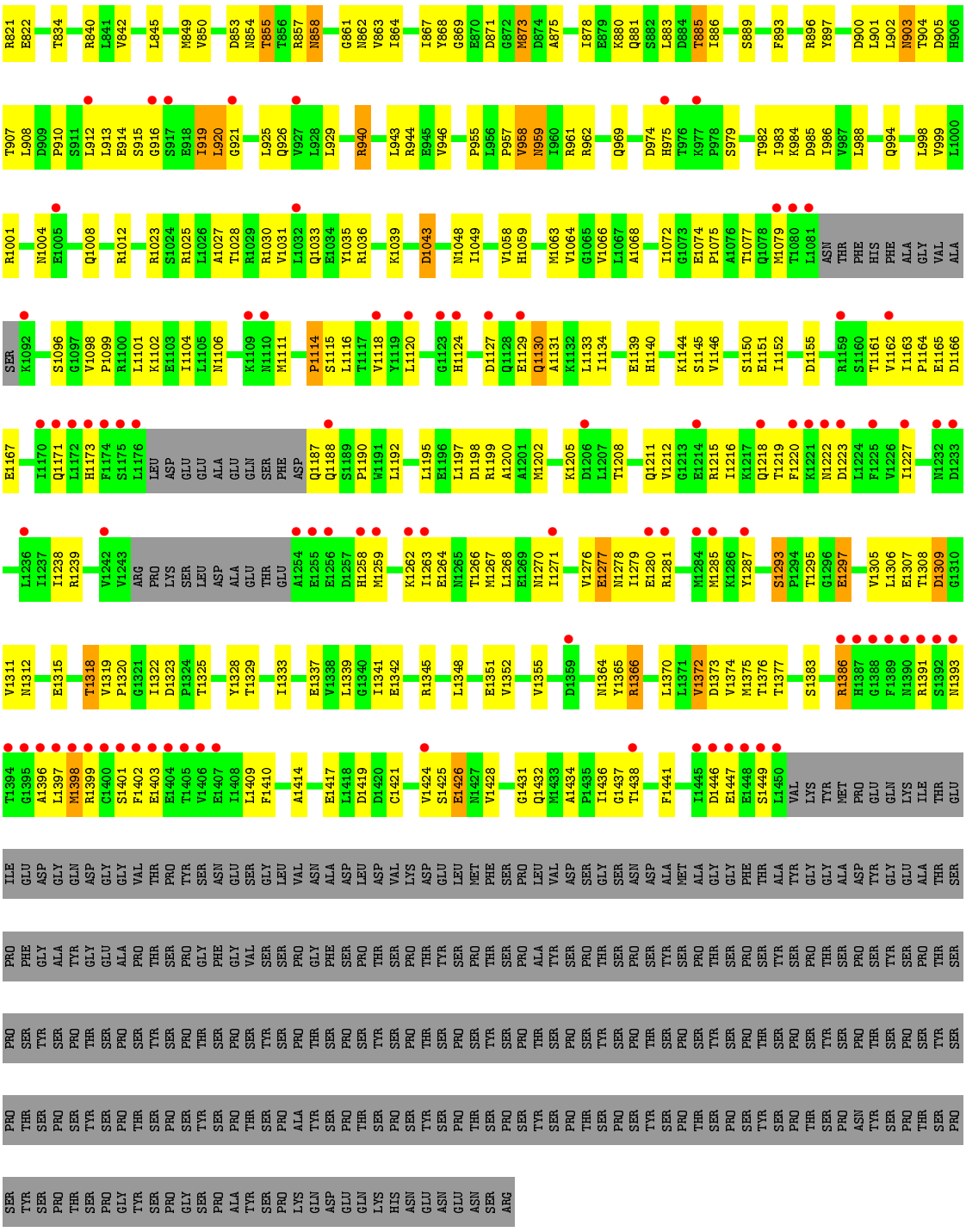
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

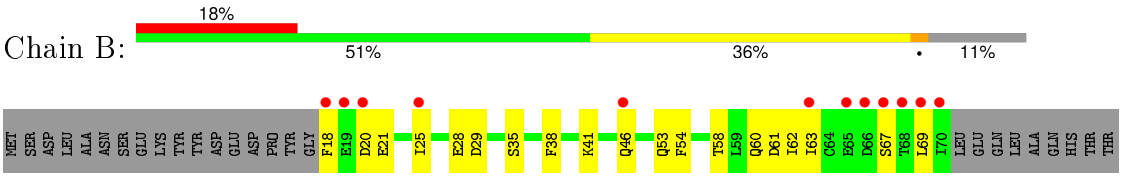
- Molecule 1: DNA-directed RNA polymerase II largest subunit

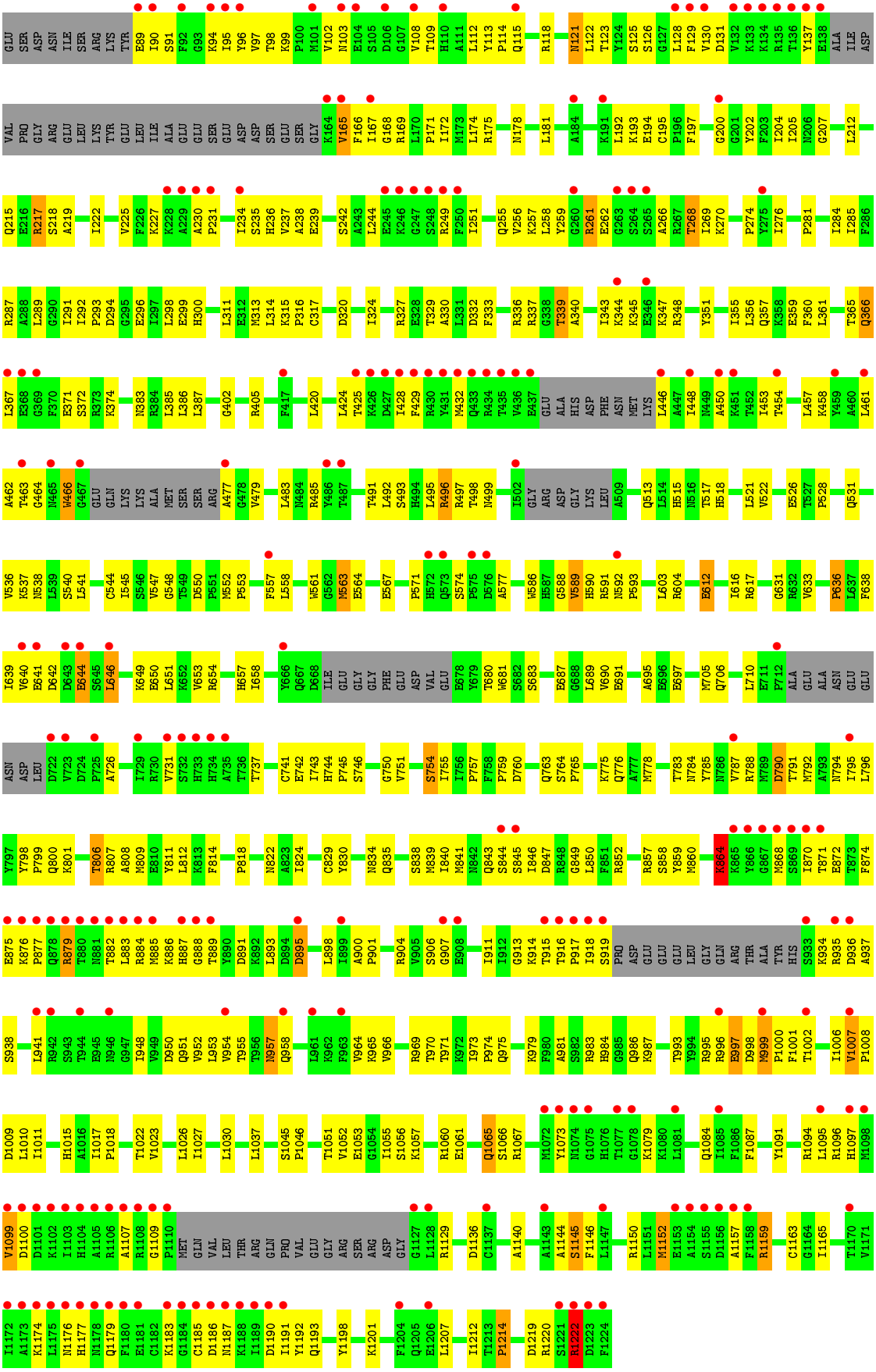
Chain A:





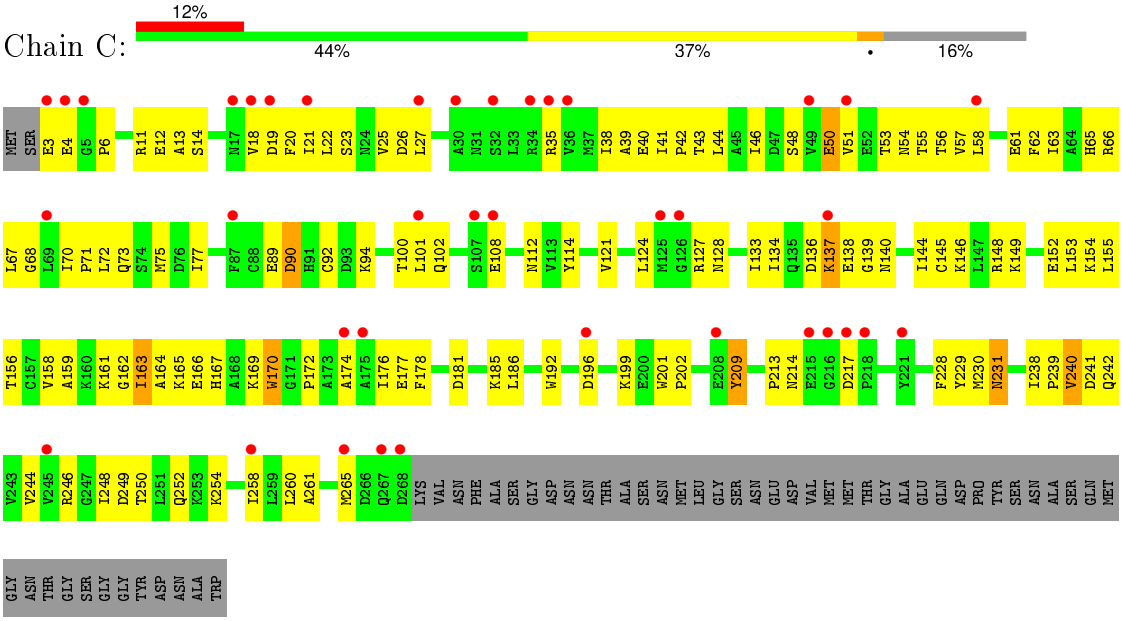
• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide




GLU SER ASP ASN ILE SER ARG LYS TYR E89 I90 S91 F92 G93 K94 I95 Y96 V97 T98 K99 P100 M101 V102 N103 E104 S105 D106 G107 V108 T109 H110 A111 L112 Y113 P114 Q115 R118 N121 L122 T123 Y124 S125 S126 G127 L128 F129 V130 D131 V132 K133 K134 R135 T136 Y137 E138 ALA ILE ASP
VAL PRO GLY ARG GLU LEU LYS TYR GLU LEU ILE ALA GLU GLU SER GLU ASP ASP SER GLU SER GLY K164 V165 F166 I167 G168 R169 L170 P171 I172 M173 L174 R175 N178 L181 A184 K191 L192 K193 E194 C195 P196 F197 G200 G201 Y202 F203 I204 I205 N206 G207 L212
Q215 E216 R217 S218 A219 I222 V225 F226 K227 K228 A229 A230 P231 I234 S235 H236 V237 A238 E239 S242 A243 L244 E245 K246 G247 S248 R249 F250 I251 Q255 V256 K257 L258 Y259 G260 R261 E262 G263 S264 S265 A266 R267 T268 I269 K270 P274 Y275 I276 P281 I284 I285 F286
R287 A288 L289 G290 I291 T292 P293 D294 G295 E296 I297 L298 E299 H300 L311 E312 M313 L314 K315 P316 C317 D320 I324 R327 E328 T329 A330 L331 D332 F333 R336 R337 G338 T339 A340 I343 K344 K345 E346 K347 R348 Y351 I355 L356 Q357 K358 E359 F360 L361 T365 Q366
L367 E368 G369 F370 E371 S372 R373 K374 N383 R384 L385 L386 L387 G402 R405 F417 L420 L424 T425 K426 D427 I428 F429 R430 Y431 M432 Q433 R434 T435 V436 E437 GLU ALA HIS ASP PHE ASN MET LYS L446 A447 I448 N449 A450 K451 T452 I453 T454 L457 K458 Y459 A460 L461
A462 T463 G464 N465 W466 G467 GLU GLN LYS LYS ALA MET SER SER ARG A477 G478 V479 L483 N484 R485 Y486 T487 T491 L492 S493 H494 L495 R496 R497 T498 N499 I502 GLY ARG ASP GLY LYS LEU A509 Q513 L514 H515 N516 T517 H518 L521 V522 E526 T527 P528 Q531
V536 K537 N538 L539 S540 L541 C544 I545 S546 V547 G548 T549 D550 P551 M552 P553 F557 L558 W561 G562 M563 E564 E567 P571 H572 Q573 S574 P575 D576 A577 W586 H587 G588 V589 H590 R591 N592 P593 L603 R604 R612 I616 R617 G631 R632 V633 F636 L637 F638
I639 V640 E641 D642 D643 E644 S645 L646 K649 E650 L651 K652 V653 R654 H657 I658 Y666 Q667 D668 ILE GLU GLY GLY PHE GLU ASP VAL GLU E678 Y679 T680 W681 S682 S683 E687 G688 L689 V690 E691 A695 E696 E697 M705 Q706 L710 E711 P712 ALA GLU ALA ASN GLU GLU
ASN ASP LEU D722 V723 D724 P725 A726 I729 R730 V731 S732 H733 H734 A735 T736 T737 C741 E742 I743 H744 P745 S746 G750 V751 S754 I755 I756 P757 F758 P759 D760 Q763 S764 P765 K775 Q776 A777 M778 T783 N784 Y785 N786 V787 R788 M789 D790 T791 M792 A793 N794 I795 L796
Y797 Y798 P799 Q800 K801 T806 R807 A808 M809 E810 Y811 L812 K813 F814 P818 M822 A823 I824 C829 Y830 N834 Q835 S838 M839 I840 M841 N842 Q843 S844 S845 I846 D847 R848 G849 L850 F851 R852 R857 S858 Y859 M860 K864 K865 Y866 G867 M868 S869 I870 T871 E872 T873 F874
E875 K876 P877 Q878 R879 T880 N881 T882 L883 R884 M885 K886 H887 G888 T889 Y890 D891 K892 L893 D894 D895 L898 I899 A900 P901 R904 V905 S906 G907 E908 I911 I912 G913 K914 T915 T916 P917 I918 S919 PRO ASP GLU GLU GLU LEU GLY GLN ARG THR ALA TYR HIS S933 K934 R935 D936 A937
S938 L941 R942 S943 T944 E945 N946 G947 I948 V949 D950 Q951 V952 L953 V954 T955 T956 N957 Q958 L961 K962 F963 V964 K965 V966 R969 T970 T971 K972 I973 P974 Q975 K979 F980 A981 S982 R983 H984 G985 Q986 K987 T993 Y994 R995 R996 E997 D998 M999 P1000 F1001 T1002 I1006 V1007 P1008
D1009 L1010 I1011 H1015 A1016 I1017 P1018 T1022 V1023 L1026 I1027 L1030 L1037 S1045 P1046 T1051 V1052 E1053 G1054 I1055 S1056 K1057 R1060 E1061 Q1065 S1066 R1067 M1072 Y1073 N1074 G1075 H1076 T1077 G1078 K1079 K1080 L1081 Q1084 I1085 F1086 F1087 Y1091 R1094 L1095 R1096 H1097 M1098
V1099 D1100 D1101 K1102 I1103 H1104 A1105 R1106 A1107 R1108 G1109 P1110 MET GLN VAL LEU THR ARG GLN PRO VAL GLU GLY ARG SER ARG ASP GLY G1127 L1128 R1129 D1136 C1137 A1140 A1143 A1144 S1145 F1146 L1147 R1150 L1151 M1152 E1153 A1154 S1155 D1156 A1157 F1158 R1159 C1163 G1164 I1165 T1170 V1171
I1172 A1173 K1174 L1175 N1176 H1177 N1178 Q1179 F1180 E1181 C1182 K1183 G1184 C1185 D1186 N1187 K1188 I1189 D1190 I1191 Y1192 Q1193 Y1198 K1201 F1204 Q1205 E1206 L1207 I1212 T1213 P1214 D1219 R1220 S1221 R1222 D1223 F1224

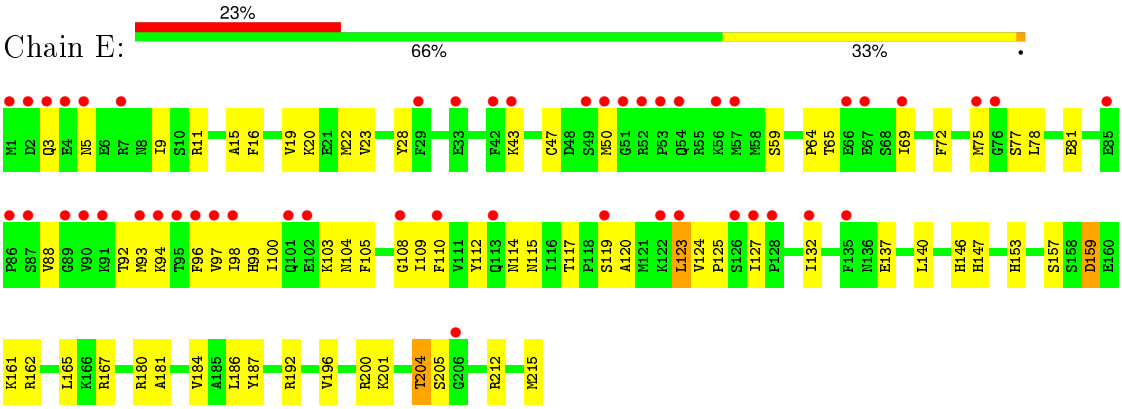
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:



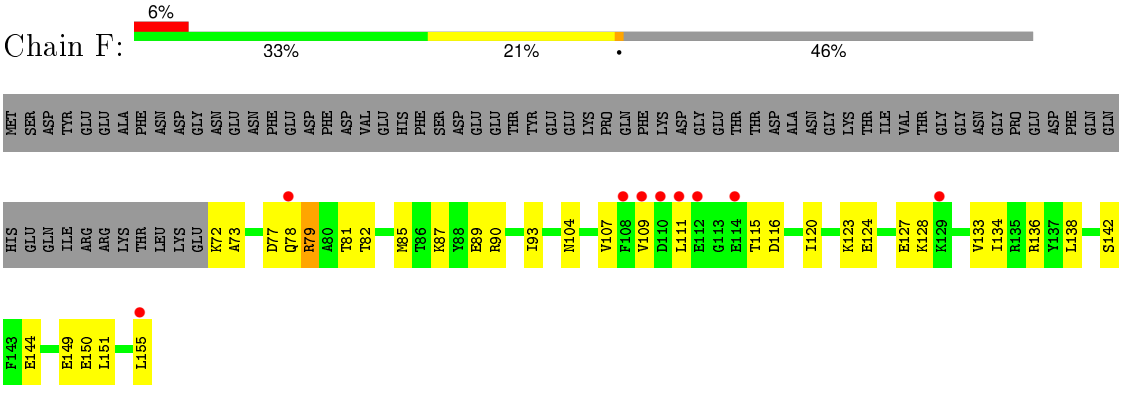
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:



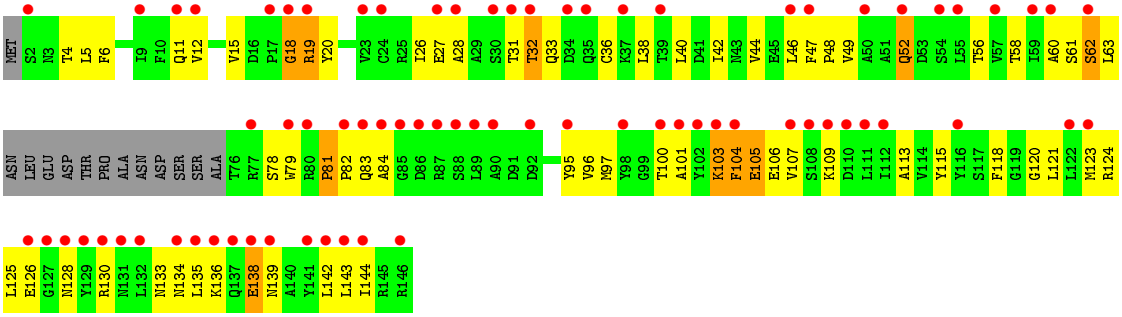
• Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



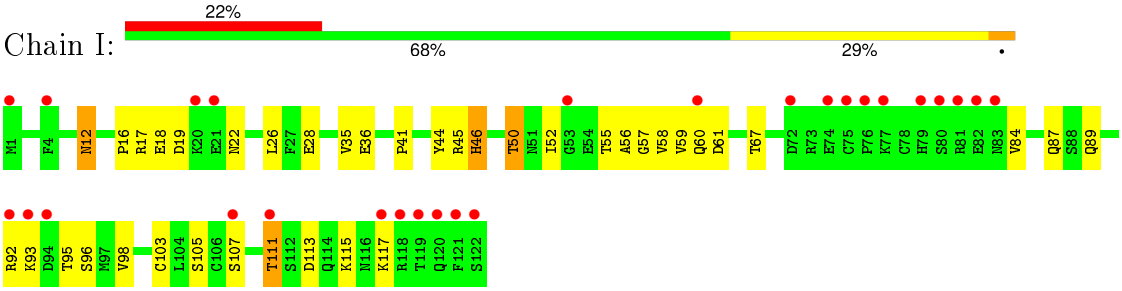
• Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



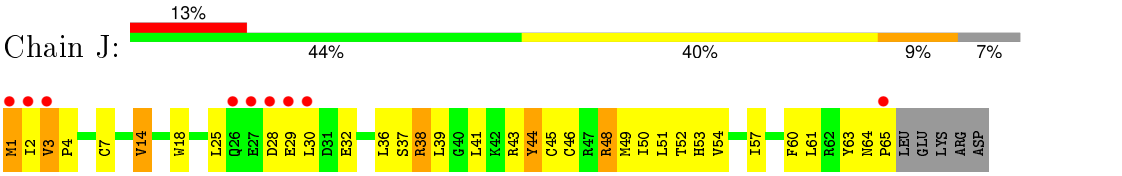
• Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide

Chain I:



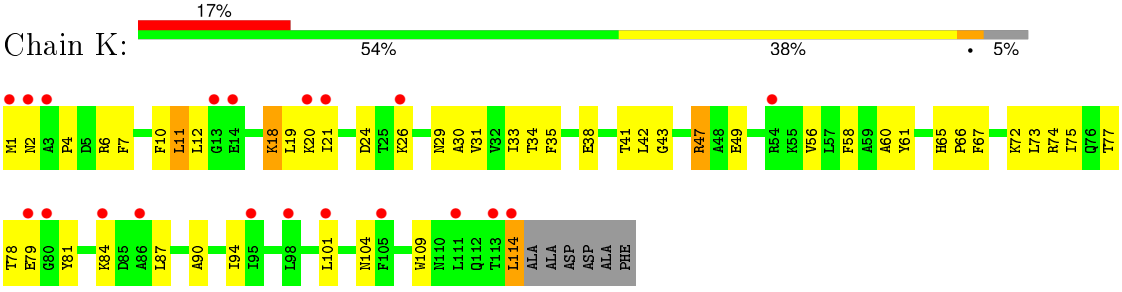
• Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J:



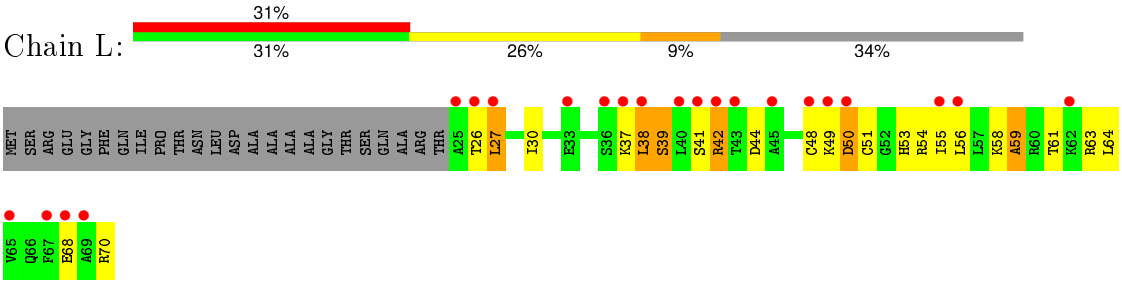
• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



• Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 39.69 – 2.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.30) 90.5 (39.69-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.294 0.301 , 0.302	Depositor DCC
R_{free} test set	4190 reflections (2.01%)	DCC
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 258084 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28318	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.43	1/11352 (0.0%)	0.66	2/15352 (0.0%)
2	B	0.41	0/8882	0.64	1/11976 (0.0%)
3	C	0.41	0/2133	0.60	0/2891
4	E	0.41	0/1796	0.63	1/2416 (0.0%)
5	F	0.44	0/691	0.63	0/933
6	H	0.30	0/1086	0.58	0/1470
7	I	0.40	0/1016	0.60	0/1365
8	J	0.41	0/541	0.65	0/727
9	K	0.39	0/937	0.56	0/1265
10	L	0.37	0/366	0.55	0/485
All	All	0.41	1/28800 (0.0%)	0.64	4/38880 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	764	CYS	CB-SG	-7.44	1.69	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	472	LEU	CA-CB-CG	-7.72	97.54	115.30
2	B	829	CYS	N-CA-C	-6.17	94.35	111.00
4	E	200	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	779	PHE	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

There are no planarity outliers.

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	11154	0	11224	555	0
2	B	8711	0	8738	427	0
3	C	2095	0	2051	139	0
4	E	1760	0	1788	53	0
5	F	679	0	701	34	0
6	H	1068	0	1040	57	0
7	I	997	0	953	40	0
8	J	532	0	542	53	0
9	K	919	0	929	62	0
10	L	364	0	389	33	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
13	B	29	0	11	1	0
All	All	28318	0	28366	1291	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 23.

All (1291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.09	1.14
6:H:130:ARG:HA	6:H:133:ASN:HD22	1.11	1.11
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.53	1.05
1:A:351:THR:HG22	1:A:352:VAL:H	1.20	1.05
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.58	0.99
1:A:901:LEU:H	1:A:926:GLN:NE2	1.60	0.98
2:B:680:THR:HG22	2:B:681:TRP:H	1.28	0.98
1:A:725:ALA:HA	1:A:728:LYS:HE3	1.48	0.95
9:K:65:HIS:HD2	9:K:67:PHE:H	1.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.32	0.93
2:B:118:ARG:NH1	2:B:204:ILE:HD11	1.83	0.93
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.51	0.92
3:C:137:LYS:HD2	3:C:137:LYS:H	1.35	0.91
8:J:48:ARG:HG2	8:J:48:ARG:HH11	1.34	0.91
1:A:337:ARG:HG2	1:A:341:MET:HE2	1.51	0.91
1:A:901:LEU:H	1:A:926:GLN:HE21	1.19	0.90
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.53	0.90
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.37	0.89
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.55	0.89
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.03	0.88
1:A:446:ARG:HD3	1:A:480:ALA:HB2	1.52	0.88
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.87	0.88
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.55	0.87
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.09	0.87
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.23	0.87
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.57	0.86
1:A:313:GLN:HE21	1:A:322:VAL:HG12	1.40	0.86
1:A:55:ASP:H	1:A:56:PRO:HD2	1.40	0.86
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.57	0.86
1:A:351:THR:HG22	1:A:352:VAL:N	1.90	0.86
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.57	0.86
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.56	0.85
1:A:1376:THR:HG22	4:E:212:ARG:NH2	1.91	0.85
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	0.86	0.85
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.58	0.85
1:A:246:VAL:HG12	1:A:328:ARG:HH12	1.39	0.85
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.57	0.85
5:F:90:ARG:HD3	5:F:155:LEU:HD12	1.58	0.85
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.58	0.85
1:A:317:LYS:HD2	1:A:321:PRO:HG2	1.57	0.85
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.59	0.85
3:C:167:HIS:HD2	3:C:169:LYS:H	1.21	0.85
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.76	0.85
9:K:65:HIS:CD2	9:K:67:PHE:H	1.93	0.84
3:C:73:GLN:HE21	3:C:75:MET:H	1.25	0.84
6:H:101:ALA:HB1	6:H:103:LYS:HG3	1.58	0.84
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.58	0.84
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.58	0.84
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.43	0.83
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.60	0.83
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.08	0.83
2:B:526:GLU:HG2	2:B:538:ASN:ND2	1.93	0.83
3:C:56:THR:HG23	3:C:58:LEU:H	1.42	0.83
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.60	0.83
2:B:864:LYS:HB3	2:B:871:THR:HA	1.58	0.83
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.59	0.83
5:F:81:THR:HG22	5:F:136:ARG:NH1	1.93	0.82
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.61	0.82
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.44	0.82
2:B:25:ILE:HD12	2:B:653:VAL:HG23	1.62	0.82
3:C:54:ASN:OD1	3:C:56:THR:HG22	1.80	0.82
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.62	0.81
1:A:869:GLY:O	4:E:204:THR:HG21	1.80	0.81
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.63	0.81
1:A:1398:MET:HG3	1:A:1426:GLU:HG2	1.62	0.81
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.64	0.80
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.63	0.80
1:A:982:THR:O	1:A:985:ASP:HB2	1.82	0.80
1:A:855:THR:CG2	1:A:857:ARG:HE	1.91	0.80
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.64	0.79
2:B:871:THR:HG22	2:B:872:GLU:H	1.44	0.79
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.29	0.79
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.13	0.79
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.48	0.79
3:C:258:ILE:HD13	9:K:35:PHE:HE2	1.48	0.78
1:A:741:ASN:HD22	1:A:744:LYS:H	1.31	0.78
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.49	0.78
1:A:1446:ASP:HB2	5:F:133:VAL:HG23	1.63	0.78
2:B:882:THR:HG21	2:B:935:ARG:HG2	1.67	0.77
1:A:1398:MET:HG2	1:A:1425:SER:HB2	1.65	0.77
2:B:193:LYS:HE2	8:J:65:PRO:HG3	1.66	0.77
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.30	0.77
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.49	0.77
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.67	0.77
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.00	0.77
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.65	0.76
1:A:472:LEU:HD13	2:B:835:GLN:NE2	1.98	0.76
1:A:709:THR:HB	1:A:712:GLU:HG3	1.66	0.76
1:A:672:ASP:H	1:A:736:ASN:ND2	1.84	0.76
2:B:801:LYS:O	8:J:52:THR:HG23	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:O	1:A:401:GLY:N	2.18	0.76
1:A:855:THR:HG21	1:A:857:ARG:NE	1.94	0.76
2:B:515:HIS:HD2	2:B:517:THR:H	1.33	0.75
1:A:840:ARG:HH11	1:A:1386:ARG:HB3	1.51	0.75
1:A:108:MET:H	1:A:171:GLN:NE2	1.83	0.75
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.69	0.74
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.68	0.74
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.52	0.74
3:C:124:LEU:O	3:C:127:ARG:HG2	1.87	0.74
1:A:55:ASP:N	1:A:56:PRO:HD2	2.02	0.74
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.69	0.74
2:B:809:MET:HG2	2:B:814:PHE:HB3	1.70	0.74
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.69	0.74
2:B:680:THR:HG22	2:B:681:TRP:N	2.02	0.74
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.50	0.74
1:A:179:LEU:HG	1:A:308:ILE:HG21	1.67	0.74
1:A:1215:ARG:HA	1:A:1218:GLN:HE21	1.53	0.74
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.69	0.74
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.69	0.73
2:B:324:ILE:HG12	2:B:329:THR:HG22	1.70	0.73
1:A:450:LEU:H	1:A:450:LEU:HD12	1.50	0.73
10:L:38:LEU:HG	10:L:39:SER:H	1.53	0.73
2:B:953:LEU:HD21	2:B:955:THR:HG23	1.68	0.73
2:B:914:LYS:HB3	2:B:937:ALA:O	1.87	0.73
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.71	0.73
1:A:907:THR:HG22	1:A:908:LEU:H	1.53	0.73
1:A:79:GLY:HA3	1:A:245:PRO:HG3	1.71	0.73
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.24	0.72
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.69	0.72
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.71	0.72
2:B:46:GLN:HE22	2:B:496:ARG:HB3	1.54	0.72
1:A:567:LYS:HB3	6:H:96:VAL:N	2.05	0.72
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.72	0.72
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.71	0.72
9:K:43:GLY:O	9:K:47:ARG:HB2	1.89	0.72
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.23	0.72
2:B:294:ASP:H	7:I:12:ASN:ND2	1.87	0.72
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.90	0.71
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.71	0.71
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.54	0.71
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.72	0.71
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.31	0.71
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.04	0.71
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.19	0.71
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.73	0.71
2:B:1222:ARG:H	2:B:1222:ARG:HD2	1.55	0.71
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.72	0.71
5:F:72:LYS:N	5:F:142:SER:HA	2.06	0.71
1:A:567:LYS:HB3	6:H:96:VAL:H	1.55	0.71
1:A:55:ASP:H	1:A:56:PRO:CD	2.04	0.71
2:B:644:GLU:HB2	2:B:654:ARG:HH22	1.55	0.70
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.56	0.70
1:A:1192:LEU:HD11	1:A:1239:ARG:HB2	1.73	0.70
1:A:587:HIS:HA	1:A:607:ILE:O	1.91	0.70
2:B:806:THR:HG22	2:B:809:MET:H	1.57	0.70
1:A:567:LYS:HE2	6:H:95:TYR:CZ	2.27	0.70
1:A:246:VAL:HG12	1:A:328:ARG:NH1	2.06	0.70
2:B:705:MET:CE	2:B:745:PRO:HB3	2.21	0.70
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.72	0.70
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.89	0.70
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.72	0.70
1:A:754:SER:H	1:A:757:ASN:HD22	1.38	0.70
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.73	0.70
1:A:574:GLY:O	1:A:577:ILE:HG13	1.92	0.70
1:A:340:LEU:HD13	1:A:1399:ARG:HG2	1.74	0.70
2:B:824:ILE:HD11	8:J:48:ARG:NH1	2.07	0.70
1:A:1059:HIS:HE1	5:F:155:LEU:HD22	1.56	0.70
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.72	0.70
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.73	0.69
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.27	0.69
1:A:134:ARG:HD2	1:A:221:SER:O	1.91	0.69
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.75	0.69
2:B:824:ILE:HD11	8:J:48:ARG:HH12	1.57	0.69
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.73	0.69
3:C:20:PHE:HE1	3:C:22:LEU:HG	1.58	0.69
1:A:264:PHE:HD1	1:A:315:LEU:HB3	1.58	0.69
2:B:755:ILE:HG22	2:B:755:ILE:O	1.91	0.69
2:B:957:ASN:ND2	2:B:958:GLN:H	1.91	0.69
3:C:56:THR:HG21	3:C:63:ILE:HD11	1.73	0.68
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.74	0.68
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:THR:HG22	10:L:55:ILE:HA	1.73	0.68
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.75	0.68
1:A:381:THR:HG22	5:F:104:ASN:OD1	1.93	0.68
2:B:955:THR:HG22	10:L:54:ARG:O	1.94	0.68
1:A:533:LYS:NZ	1:A:660:ASN:HD21	1.92	0.68
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.75	0.68
2:B:67:SER:O	2:B:91:SER:HA	1.93	0.68
1:A:351:THR:CG2	1:A:352:VAL:H	2.01	0.68
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.73	0.68
1:A:914:GLU:HG3	1:A:979:SER:O	1.94	0.68
1:A:567:LYS:HE2	6:H:95:TYR:CE1	2.29	0.68
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.29	0.68
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.76	0.67
1:A:53:LEU:HD23	1:A:54:ASN:H	1.58	0.67
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.60	0.67
1:A:1277:GLU:O	1:A:1278:ASN:HB2	1.92	0.67
1:A:853:ASP:OD1	1:A:855:THR:HB	1.95	0.67
1:A:786:HIS:HE1	2:B:742:GLU:OE2	1.76	0.67
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.77	0.67
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.76	0.67
3:C:73:GLN:HE21	3:C:75:MET:N	1.92	0.67
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.77	0.67
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.76	0.67
2:B:268:THR:HG21	2:B:270:LYS:HE3	1.76	0.67
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.77	0.67
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.25	0.67
1:A:907:THR:HG22	1:A:908:LEU:N	2.09	0.67
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.76	0.66
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.77	0.66
1:A:1066:VAL:HG12	2:B:1140:ALA:HB2	1.77	0.66
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.77	0.66
6:H:79:TRP:CZ3	6:H:81:PRO:HG3	2.30	0.66
2:B:324:ILE:HD11	2:B:333:PHE:HB2	1.76	0.66
3:C:35:ARG:NH1	9:K:41:THR:N	2.43	0.66
3:C:166:GLU:HG2	10:L:70:ARG:NH1	2.09	0.66
2:B:876:LYS:HE3	2:B:893:LEU:O	1.96	0.66
1:A:203:SER:OG	1:A:206:GLU:HG3	1.95	0.66
1:A:472:LEU:O	1:A:475:THR:HB	1.96	0.66
6:H:103:LYS:HB3	6:H:105:GLU:OE2	1.96	0.66
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.77	0.66
6:H:130:ARG:HA	6:H:133:ASN:ND2	1.97	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.76	0.66
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.78	0.65
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.77	0.65
1:A:1145:SER:HB2	1:A:1205:LYS:NZ	2.10	0.65
1:A:1124:HIS:HB3	1:A:1130:GLN:HG3	1.77	0.65
2:B:175:ARG:HB3	2:B:175:ARG:HH11	1.61	0.65
2:B:841:MET:HE2	2:B:1010:LEU:HD11	1.79	0.65
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.93	0.65
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.12	0.65
1:A:694:THR:O	1:A:698:GLN:HG3	1.96	0.65
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.65
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.78	0.65
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.77	0.65
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.78	0.65
1:A:834:THR:HG21	1:A:1077:THR:HA	1.79	0.65
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.26	0.65
2:B:864:LYS:CG	2:B:871:THR:HG23	2.27	0.65
1:A:567:LYS:CB	1:A:568:PRO:CD	2.75	0.65
2:B:89:GLU:HB2	2:B:137:TYR:HB2	1.79	0.65
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.79	0.65
1:A:1279:ILE:HD11	1:A:1312:ASN:HB3	1.77	0.65
1:A:998:LEU:HD12	1:A:1001:ARG:NH1	2.10	0.64
5:F:87:LYS:HA	5:F:155:LEU:HD13	1.78	0.64
1:A:1068:ALA:O	1:A:1072:ILE:HG13	1.97	0.64
1:A:1263:ILE:O	1:A:1267:MET:HG3	1.96	0.64
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.80	0.64
2:B:276:ILE:HG23	2:B:337:ARG:HB2	1.80	0.64
1:A:347:PHE:H	2:B:1107:ALA:HA	1.63	0.64
1:A:673:GLY:N	1:A:674:PRO:HD2	2.12	0.64
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.59	0.64
2:B:872:GLU:HB3	2:B:914:LYS:HD3	1.78	0.64
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.78	0.64
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.78	0.64
1:A:1449:SER:HB3	5:F:149:GLU:OE2	1.97	0.64
2:B:125:SER:HA	2:B:171:PRO:HA	1.80	0.64
1:A:903:ASN:ND2	1:A:905:ASP:H	1.95	0.64
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.80	0.63
2:B:577:ALA:HB1	2:B:589:VAL:HG22	1.80	0.63
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.80	0.63
3:C:248:ILE:HD13	9:K:101:LEU:HD13	1.80	0.63
1:A:1258:HIS:O	1:A:1262:LYS:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:SER:N	1:A:757:ASN:HD22	1.95	0.63
6:H:4:THR:HA	6:H:60:ALA:HA	1.79	0.63
1:A:986:ILE:HG21	1:A:1028:THR:HA	1.81	0.63
2:B:464:GLY:O	2:B:477:ALA:HB3	1.98	0.63
1:A:789:LYS:HE3	7:I:67:THR:OG1	1.98	0.63
1:A:864:ILE:HD13	1:A:1374:VAL:HG22	1.80	0.63
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.28	0.63
2:B:550:ASP:OD1	2:B:552:MET:HG3	1.98	0.63
2:B:839:MET:CE	2:B:1010:LEU:HG	2.28	0.63
2:B:195:CYS:SG	2:B:783:THR:HG23	2.38	0.63
1:A:567:LYS:HD3	6:H:96:VAL:H	1.64	0.63
1:A:672:ASP:H	1:A:736:ASN:HD21	1.47	0.63
3:C:22:LEU:HD12	3:C:230:MET:CE	2.29	0.63
1:A:443:LEU:HB3	1:A:490:HIS:HB2	1.80	0.63
2:B:130:VAL:HG12	2:B:131:ASP:H	1.63	0.63
4:E:43:LYS:O	4:E:47:CYS:HB2	1.98	0.63
4:E:64:PRO:HG2	4:E:75:MET:O	1.98	0.63
3:C:242:GLN:NE2	3:C:246:ARG:HH21	1.94	0.62
10:L:27:LEU:HD13	10:L:37:LYS:HE2	1.81	0.62
1:A:728:LYS:HA	1:A:731:ARG:HD2	1.80	0.62
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.34	0.62
2:B:58:THR:O	2:B:62:ILE:HG13	1.98	0.62
2:B:839:MET:HE1	2:B:1010:LEU:HG	1.82	0.62
1:A:873:MET:HE2	1:A:957:PRO:HG3	1.80	0.62
7:I:59:VAL:HG12	7:I:60:GLN:H	1.65	0.62
1:A:329:LEU:O	1:A:333:GLU:HG2	2.00	0.62
1:A:31:SER:CB	1:A:83:HIS:HB2	2.30	0.62
1:A:873:MET:CE	1:A:957:PRO:HG3	2.30	0.62
1:A:665:GLY:C	2:B:1026:LEU:HD13	2.20	0.62
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.00	0.62
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.40	0.62
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.35	0.62
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.03	0.62
1:A:901:LEU:N	1:A:926:GLN:NE2	2.43	0.62
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.65	0.62
2:B:477:ALA:HB1	2:B:479:VAL:HG23	1.82	0.62
1:A:1025:ARG:HD3	1:A:1030:ARG:HH21	1.64	0.62
1:A:867:ILE:HD11	1:A:999:VAL:CG1	2.30	0.61
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.83	0.61
7:I:50:THR:HG22	7:I:52:ILE:HG22	1.81	0.61
1:A:1164:PRO:O	1:A:1167:GLU:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.15	0.61
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.81	0.61
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.82	0.61
1:A:137:ALA:O	1:A:141:LEU:HD13	2.00	0.61
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.36	0.61
1:A:32:VAL:HG11	1:A:68:GLN:HE22	1.65	0.61
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.41	0.61
1:A:579:SER:OG	1:A:612:ILE:HG22	2.01	0.61
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.30	0.61
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.13	0.61
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.81	0.61
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.81	0.61
3:C:58:LEU:HD11	8:J:2:ILE:CD1	2.31	0.61
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.66	0.60
10:L:26:THR:HG22	10:L:27:LEU:H	1.65	0.60
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.82	0.60
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.66	0.60
7:I:59:VAL:HG12	7:I:60:GLN:N	2.16	0.60
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.65	0.60
1:A:187:LYS:HB2	1:A:194:ALA:CB	2.31	0.60
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.31	0.60
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.82	0.60
7:I:56:ALA:O	7:I:89:GLN:HG3	2.02	0.60
1:A:345:VAL:HG11	2:B:1129:ARG:HA	1.84	0.60
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.82	0.60
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.82	0.60
1:A:535:THR:CG2	1:A:575:LYS:HG2	2.31	0.60
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.65	0.60
7:I:45:ARG:HH11	7:I:45:ARG:HG2	1.65	0.60
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.67	0.60
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.82	0.60
2:B:531:GLN:H	2:B:531:GLN:CD	2.05	0.60
2:B:515:HIS:H	2:B:518:HIS:CD2	2.19	0.60
1:A:535:THR:O	1:A:575:LYS:HE2	2.02	0.60
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.02	0.60
3:C:166:GLU:HG2	10:L:70:ARG:HH12	1.67	0.60
2:B:60:GLN:HA	2:B:95:ILE:HD12	1.84	0.60
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.31	0.59
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.83	0.59
2:B:365:THR:HG22	2:B:367:LEU:H	1.65	0.59
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.03	0.59
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.84	0.59
2:B:25:ILE:HD12	2:B:653:VAL:CG2	2.32	0.59
1:A:35:ILE:HD12	1:A:35:ILE:N	2.18	0.59
8:J:48:ARG:NH1	8:J:48:ARG:HG2	2.11	0.59
4:E:117:THR:HG22	4:E:119:SER:H	1.67	0.59
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.84	0.59
1:A:903:ASN:HD22	1:A:904:THR:N	2.00	0.59
9:K:29:ASN:HD21	9:K:79:GLU:HA	1.67	0.59
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.85	0.59
1:A:61:ILE:HG22	1:A:62:ASP:H	1.67	0.59
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.84	0.59
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.32	0.59
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.83	0.59
1:A:80:HIS:O	1:A:243:PRO:HB3	2.02	0.59
1:A:903:ASN:C	1:A:903:ASN:HD22	2.06	0.59
2:B:885:MET:HA	2:B:936:ASP:HB2	1.85	0.59
10:L:27:LEU:HB3	10:L:37:LYS:HD3	1.84	0.59
1:A:523:ILE:N	1:A:523:ILE:HD12	2.17	0.59
2:B:755:ILE:CG2	2:B:755:ILE:O	2.50	0.59
1:A:883:LEU:O	1:A:886:ILE:HG22	2.03	0.58
3:C:71:PRO:O	3:C:72:LEU:HD23	2.03	0.58
6:H:6:PHE:O	6:H:58:THR:HG23	2.03	0.58
2:B:874:PHE:O	2:B:875:GLU:HG3	2.04	0.58
2:B:239:GLU:CD	2:B:255:GLN:HE21	2.07	0.58
2:B:651:LEU:CD2	2:B:710:LEU:HD11	2.33	0.58
1:A:587:HIS:CE1	1:A:609:ASP:H	2.21	0.58
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.03	0.58
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.85	0.58
2:B:792:MET:SD	2:B:857:ARG:NH2	2.76	0.58
1:A:598:LEU:HG	6:H:115:TYR:CE2	2.38	0.58
1:A:264:PHE:HB3	1:A:315:LEU:HD22	1.85	0.58
1:A:858:ASN:HD22	1:A:858:ASN:C	2.06	0.58
1:A:537:ARG:NH1	6:H:120:GLY:O	2.36	0.58
3:C:62:PHE:O	3:C:66:ARG:HG3	2.03	0.58
2:B:953:LEU:HD21	2:B:955:THR:CG2	2.33	0.58
1:A:1064:VAL:HG12	1:A:1370:LEU:CD2	2.34	0.58
3:C:39:ALA:O	3:C:163:ILE:HG23	2.04	0.58
1:A:914:GLU:C	1:A:916:GLY:H	2.06	0.58
2:B:791:THR:HG22	2:B:792:MET:HG3	1.85	0.58
1:A:739:ASP:OD2	6:H:19:ARG:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.85	0.58
1:A:523:ILE:HB	1:A:622:VAL:CG1	2.33	0.58
1:A:317:LYS:CD	1:A:321:PRO:HG2	2.31	0.58
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.38	0.58
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.02	0.58
4:E:180:ARG:HH21	4:E:192:ARG:HB2	1.69	0.57
1:A:986:ILE:HD12	1:A:1028:THR:HG23	1.86	0.57
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.39	0.57
1:A:451:HIS:CG	1:A:1074:GLU:HG3	2.40	0.57
7:I:17:ARG:HG3	7:I:28:GLU:HG2	1.86	0.57
1:A:913:LEU:HD12	1:A:914:GLU:N	2.19	0.57
1:A:1066:VAL:CG1	2:B:1140:ALA:HB2	2.34	0.57
9:K:20:LYS:HB2	9:K:34:THR:HB	1.86	0.57
4:E:15:ALA:O	4:E:19:VAL:HG23	2.03	0.57
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.34	0.57
8:J:2:ILE:HG22	8:J:3:VAL:N	2.20	0.57
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.20	0.57
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.70	0.57
1:A:1220:PHE:O	1:A:1223:ASP:HB2	2.05	0.57
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.52	0.57
1:A:329:LEU:HB3	1:A:333:GLU:HB3	1.86	0.57
1:A:550:LEU:HD22	1:A:556:TRP:NE1	2.19	0.57
2:B:824:ILE:CD1	8:J:48:ARG:HH12	2.18	0.57
1:A:244:PRO:N	1:A:245:PRO:HD2	2.20	0.57
2:B:834:ASN:HA	2:B:838:SER:OG	2.05	0.57
2:B:754:SER:HB3	2:B:812:LEU:HD11	1.87	0.57
2:B:785:TYR:CD2	2:B:795:ILE:HG12	2.40	0.57
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.85	0.57
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.40	0.57
2:B:230:ALA:N	2:B:231:PRO:HD2	2.20	0.56
7:I:103:CYS:O	7:I:107:SER:HA	2.05	0.56
2:B:172:ILE:HD11	2:B:178:ASN:HD22	1.70	0.56
1:A:1366:ARG:CZ	1:A:1366:ARG:HB3	2.36	0.56
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.53	0.56
1:A:913:LEU:HD12	1:A:914:GLU:H	1.68	0.56
2:B:879:ARG:HD3	2:B:883:LEU:HD22	1.88	0.56
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.87	0.56
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.88	0.56
1:A:243:PRO:C	1:A:245:PRO:HD2	2.26	0.56
2:B:1065:GLN:O	2:B:1065:GLN:HG3	2.05	0.56
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.00	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.86	0.56
1:A:679:ILE:HD13	1:A:763:ALA:HB2	1.88	0.56
2:B:215:GLN:HE22	2:B:499:ASN:ND2	2.03	0.56
2:B:175:ARG:HB3	2:B:175:ARG:NH1	2.21	0.56
1:A:858:ASN:ND2	1:A:862:ASN:H	2.03	0.56
1:A:1127:ASP:HB2	1:A:1130:GLN:HB2	1.87	0.56
1:A:489:LEU:HD23	1:A:489:LEU:C	2.26	0.56
4:E:19:VAL:HG22	4:E:140:LEU:HD13	1.87	0.56
1:A:849:MET:CE	1:A:1436:ILE:HA	2.35	0.56
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.71	0.56
3:C:6:PRO:HG2	9:K:101:LEU:HB2	1.87	0.56
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.36	0.56
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.40	0.56
2:B:809:MET:HG2	2:B:814:PHE:CB	2.36	0.56
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.21	0.56
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.87	0.55
1:A:1025:ARG:HD3	1:A:1030:ARG:NH2	2.20	0.55
2:B:871:THR:HG22	2:B:872:GLU:N	2.17	0.55
8:J:48:ARG:NE	8:J:49:MET:HE2	2.22	0.55
10:L:38:LEU:HG	10:L:39:SER:N	2.21	0.55
3:C:56:THR:HG23	3:C:58:LEU:N	2.18	0.55
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.88	0.55
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.88	0.55
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.88	0.55
2:B:680:THR:O	2:B:683:SER:HB2	2.07	0.55
2:B:871:THR:O	2:B:917:PRO:HD2	2.07	0.55
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.21	0.55
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.89	0.55
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.87	0.55
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.89	0.55
2:B:680:THR:CG2	2:B:681:TRP:H	2.09	0.55
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.55	0.55
2:B:193:LYS:CE	8:J:65:PRO:HG3	2.35	0.55
2:B:800:GLN:CB	8:J:52:THR:HG22	2.37	0.55
6:H:113:ALA:HB1	6:H:124:ARG:HE	1.72	0.55
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.35	0.55
3:C:248:ILE:HD13	9:K:101:LEU:CD1	2.37	0.55
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.39	0.55
1:A:901:LEU:O	1:A:920:LEU:HD23	2.07	0.54
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.88	0.54
3:C:258:ILE:HD13	9:K:35:PHE:CE2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:MET:HG3	2:B:1010:LEU:HD12	1.90	0.54
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.08	0.54
7:I:115:LYS:O	7:I:117:LYS:HG3	2.06	0.54
1:A:15:LYS:O	1:A:1421:CYS:HB2	2.07	0.54
1:A:273:ASN:O	1:A:277:GLU:HG3	2.07	0.54
7:I:55:THR:O	7:I:58:VAL:HG23	2.07	0.54
1:A:709:THR:HG22	1:A:710:LEU:N	2.22	0.54
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.07	0.54
4:E:5:ASN:O	4:E:9:ILE:HG13	2.07	0.54
3:C:11:ARG:HD2	3:C:21:ILE:HD11	1.89	0.54
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.89	0.54
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.90	0.54
1:A:313:GLN:HB3	1:A:320:ARG:C	2.27	0.54
2:B:1051:THR:O	2:B:1055:ILE:HG13	2.07	0.54
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.73	0.54
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.73	0.54
8:J:48:ARG:NH1	8:J:48:ARG:CG	2.71	0.54
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.89	0.54
3:C:43:THR:HG22	3:C:44:LEU:N	2.23	0.54
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.37	0.54
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.20	0.54
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.23	0.54
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.88	0.54
2:B:757:PRO:HD3	2:B:983:ARG:NH2	2.23	0.54
1:A:208:LEU:HD23	1:A:208:LEU:C	2.28	0.54
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.43	0.54
1:A:697:ALA:HB2	1:A:702:LEU:HD23	1.89	0.54
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.43	0.54
10:L:26:THR:HG22	10:L:27:LEU:N	2.23	0.54
7:I:57:GLY:O	7:I:59:VAL:HG23	2.08	0.54
1:A:464:PRO:O	1:A:465:TYR:O	2.25	0.54
2:B:205:ILE:HG21	2:B:462:ALA:HB2	1.89	0.54
2:B:644:GLU:CD	2:B:646:LEU:HB2	2.29	0.54
4:E:96:PHE:CE2	4:E:110:PHE:HB2	2.43	0.54
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.90	0.54
1:A:689:LYS:O	1:A:693:VAL:HG23	2.08	0.54
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.90	0.54
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.90	0.54
9:K:56:VAL:HA	9:K:77:THR:HG22	1.89	0.54
2:B:41:LYS:HE2	2:B:544:CYS:SG	2.48	0.54
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.08	0.53
2:B:339:THR:HG23	2:B:343:ILE:HD12	1.89	0.53
5:F:77:ASP:O	5:F:78:GLN:HB2	2.07	0.53
1:A:1102:LYS:HD3	1:A:1106:ASN:HD21	1.73	0.53
2:B:281:PRO:HG2	2:B:284:ILE:CD1	2.38	0.53
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.09	0.53
1:A:69:THR:O	2:B:1174:LYS:HG2	2.08	0.53
7:I:50:THR:HB	7:I:92:ARG:HH22	1.73	0.53
8:J:48:ARG:CG	8:J:48:ARG:HH11	2.10	0.53
1:A:523:ILE:HG23	1:A:527:THR:HB	1.90	0.53
3:C:25:VAL:HG23	3:C:228:PHE:HE1	1.73	0.53
5:F:107:VAL:HG11	5:F:111:LEU:HD11	1.90	0.53
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.90	0.53
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.71	0.53
1:A:320:ARG:N	1:A:321:PRO:HD3	2.24	0.53
1:A:709:THR:HG22	1:A:711:ARG:H	1.74	0.53
4:E:114:ASN:OD1	4:E:115:ASN:N	2.42	0.53
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.91	0.53
1:A:434:ARG:HH21	1:A:437:MET:HG3	1.74	0.53
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.38	0.53
2:B:868:MET:O	2:B:870:ILE:HG13	2.08	0.53
2:B:515:HIS:H	2:B:518:HIS:HD2	1.56	0.53
2:B:954:VAL:O	10:L:55:ILE:O	2.26	0.53
2:B:845:SER:HB3	2:B:850:LEU:HD22	1.91	0.53
3:C:258:ILE:HD11	9:K:42:LEU:CD2	2.38	0.53
1:A:1199:ARG:HA	1:A:1202:MET:HB2	1.91	0.53
4:E:161:LYS:HE2	4:E:165:LEU:HD11	1.91	0.53
8:J:25:LEU:O	8:J:29:GLU:HA	2.09	0.53
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.91	0.53
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.44	0.53
1:A:858:ASN:HD21	1:A:862:ASN:H	1.56	0.53
1:A:499:ALA:O	1:A:503:GLN:HB2	2.08	0.53
3:C:58:LEU:HD11	8:J:2:ILE:HD12	1.91	0.53
1:A:849:MET:HE3	1:A:1063:MET:SD	2.49	0.53
1:A:366:VAL:HG11	1:A:436:ILE:HD11	1.90	0.53
2:B:429:PHE:HA	2:B:432:MET:CE	2.39	0.53
2:B:344:LYS:H	2:B:347:LYS:HE3	1.74	0.53
1:A:55:ASP:N	1:A:56:PRO:CD	2.69	0.52
5:F:128:LYS:HD2	5:F:149:GLU:HA	1.91	0.52
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.44	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:GLU:OE1	7:I:44:TYR:HE2	1.93	0.52
1:A:1279:ILE:N	1:A:1279:ILE:HD12	2.24	0.52
5:F:107:VAL:HG12	5:F:109:VAL:H	1.74	0.52
7:I:50:THR:CB	7:I:92:ARG:HH22	2.22	0.52
2:B:636:PRO:HA	2:B:691:GLU:O	2.08	0.52
3:C:21:ILE:HG12	3:C:229:TYR:HD2	1.74	0.52
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.91	0.52
1:A:528:LEU:HD23	1:A:751:SER:HB3	1.91	0.52
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.92	0.52
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.90	0.52
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.38	0.52
1:A:533:LYS:NZ	1:A:660:ASN:ND2	2.56	0.52
2:B:296:GLU:O	2:B:300:HIS:HD2	1.93	0.52
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.92	0.52
1:A:516:SER:O	1:A:518:LYS:HG2	2.10	0.52
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.92	0.52
9:K:1:MET:HG3	9:K:2:ASN:N	2.25	0.52
2:B:249:ARG:O	2:B:251:ILE:HG13	2.10	0.52
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.10	0.52
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.91	0.52
4:E:124:VAL:HB	4:E:125:PRO:CD	2.40	0.52
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.24	0.52
1:A:817:ALA:HA	2:B:764:SER:OG	2.09	0.52
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	2.23	0.52
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.43	0.52
1:A:492:PRO:CB	1:A:497:THR:HG22	2.40	0.52
1:A:1162:VAL:CG1	7:I:41:PRO:HG3	2.34	0.52
2:B:864:LYS:NZ	2:B:864:LYS:HB2	2.25	0.52
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.92	0.52
2:B:552:MET:N	2:B:553:PRO:HD2	2.25	0.52
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.92	0.52
2:B:846:ILE:HG12	2:B:974:PRO:HB2	1.92	0.52
2:B:528:PRO:HG3	2:B:536:VAL:HB	1.92	0.52
1:A:795:GLU:HG2	2:B:731:VAL:CG2	2.40	0.52
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.92	0.52
1:A:575:LYS:HD3	1:A:612:ILE:CD1	2.40	0.51
2:B:292:ILE:N	2:B:293:PRO:HD2	2.26	0.51
5:F:109:VAL:HG21	5:F:124:GLU:HA	1.92	0.51
3:C:145:CYS:SG	3:C:146:LYS:N	2.83	0.51
2:B:885:MET:HA	2:B:936:ASP:CB	2.40	0.51
2:B:314:LEU:O	2:B:317:CYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PRO:HG2	1:A:25:GLU:OE2	2.10	0.51
2:B:852:ARG:NH2	10:L:70:ARG:O	2.38	0.51
2:B:128:LEU:HB3	2:B:167:ILE:O	2.11	0.51
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.41	0.51
3:C:53:THR:O	3:C:153:LEU:HA	2.10	0.51
1:A:1376:THR:O	1:A:1376:THR:HG22	2.09	0.51
1:A:673:GLY:N	1:A:674:PRO:CD	2.73	0.51
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.10	0.51
1:A:465:TYR:CE2	9:K:4:PRO:HD2	2.45	0.51
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.93	0.51
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.75	0.51
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.25	0.51
2:B:859:TYR:O	2:B:965:LYS:HA	2.11	0.51
2:B:1037:LEU:HD21	8:J:44:TYR:HD2	1.75	0.51
2:B:574:SER:HB3	2:B:591:ARG:NH2	2.26	0.51
4:E:93:MET:O	4:E:97:VAL:HG23	2.10	0.51
2:B:653:VAL:HG13	2:B:689:LEU:HB3	1.92	0.51
1:A:840:ARG:NH1	1:A:1386:ARG:HB3	2.23	0.51
1:A:523:ILE:CG2	1:A:527:THR:HB	2.41	0.51
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.39	0.51
2:B:577:ALA:HB1	2:B:589:VAL:CG2	2.39	0.51
1:A:32:VAL:HG23	1:A:33:ALA:N	2.24	0.51
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.46	0.51
1:A:705:LYS:HD2	1:A:705:LYS:H	1.75	0.51
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.26	0.51
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.44	0.51
5:F:81:THR:HB	5:F:144:GLU:OE1	2.11	0.51
3:C:58:LEU:HD11	8:J:2:ILE:HD11	1.92	0.51
8:J:57:ILE:O	8:J:61:LEU:HG	2.10	0.51
7:I:98:VAL:CG2	7:I:113:ASP:HB2	2.39	0.51
1:A:903:ASN:HD22	1:A:905:ASP:H	1.58	0.51
2:B:847:ASP:O	3:C:65:HIS:HE1	1.94	0.51
1:A:1348:LEU:HD21	1:A:1375:MET:CE	2.40	0.51
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.11	0.51
1:A:2:VAL:HG21	2:B:1157:ALA:O	2.11	0.51
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.46	0.51
1:A:313:GLN:HB2	1:A:320:ARG:HB3	1.93	0.51
1:A:95:PHE:CE2	1:A:1414:ALA:HB2	2.46	0.51
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.93	0.51
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.41	0.50
6:H:104:PHE:O	6:H:106:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:SER:HA	9:K:114:LEU:O	2.10	0.50
2:B:913:GLY:HA2	2:B:938:SER:CB	2.41	0.50
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.93	0.50
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.76	0.50
10:L:30:ILE:HG13	10:L:59:ALA:HB2	1.93	0.50
2:B:914:LYS:HD2	2:B:937:ALA:HB3	1.92	0.50
1:A:208:LEU:CD2	1:A:212:LYS:HE3	2.41	0.50
1:A:605:MET:HE2	1:A:606:LEU:H	1.75	0.50
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.59	0.50
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.92	0.50
2:B:558:LEU:O	2:B:563:MET:HB2	2.12	0.50
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.26	0.50
8:J:64:ASN:N	8:J:65:PRO:HD2	2.26	0.50
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.92	0.50
1:A:849:MET:HE3	1:A:1436:ILE:HA	1.92	0.50
4:E:65:THR:O	4:E:69:ILE:HG13	2.12	0.50
1:A:1391:ARG:NH2	1:A:1417:GLU:OE2	2.44	0.50
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.12	0.50
1:A:1376:THR:O	1:A:1376:THR:CG2	2.59	0.50
3:C:73:GLN:NE2	3:C:75:MET:CB	2.74	0.50
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.77	0.50
2:B:168:GLY:H	2:B:450:ALA:HB1	1.77	0.50
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.34	0.50
2:B:169:ARG:O	2:B:457:LEU:HD12	2.11	0.50
1:A:53:LEU:CD2	1:A:54:ASN:H	2.23	0.50
1:A:147:VAL:HG22	1:A:170:THR:HG22	1.93	0.50
10:L:38:LEU:HD13	10:L:48:CYS:HA	1.94	0.49
1:A:1399:ARG:HH11	1:A:1401:SER:HA	1.75	0.49
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.23	0.49
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.92	0.49
4:E:100:ILE:HD13	4:E:108:GLY:HA3	1.94	0.49
1:A:338:GLY:HA2	1:A:343:LYS:HD2	1.94	0.49
4:E:112:TYR:O	4:E:137:GLU:HG3	2.12	0.49
1:A:1120:LEU:HG	1:A:1134:ILE:HD12	1.94	0.49
2:B:901:PRO:CD	10:L:58:LYS:HB3	2.40	0.49
3:C:50:GLU:HB2	3:C:156:THR:HB	1.93	0.49
2:B:492:LEU:O	2:B:496:ARG:HG2	2.12	0.49
1:A:786:HIS:CE1	2:B:742:GLU:OE2	2.62	0.49
1:A:219:PHE:O	1:A:224:PHE:HB2	2.13	0.49
2:B:870:ILE:HG23	2:B:917:PRO:O	2.13	0.49
3:C:46:ILE:HB	3:C:68:GLY:HA2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:HZ	1:A:1397:LEU:HG	1.78	0.49
6:H:11:GLN:HE21	6:H:52:GLN:HA	1.77	0.49
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.28	0.49
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.94	0.49
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.13	0.49
1:A:724:GLU:O	1:A:728:LYS:HG2	2.13	0.49
2:B:204:ILE:C	2:B:205:ILE:HD12	2.32	0.49
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.45	0.49
1:A:17:VAL:HB	1:A:1419:ASP:HB2	1.94	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.95	0.49
1:A:71:GLN:HG2	2:B:1176:ASN:ND2	2.27	0.49
3:C:73:GLN:NE2	3:C:75:MET:N	2.60	0.49
2:B:806:THR:CG2	2:B:808:ALA:H	2.26	0.49
1:A:58:LEU:HD22	1:A:80:HIS:O	2.12	0.49
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.12	0.49
2:B:332:ASP:O	2:B:336:ARG:HG3	2.13	0.49
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.13	0.49
1:A:75:ASN:HB2	1:A:76:GLU:OE2	2.13	0.49
3:C:137:LYS:CD	3:C:137:LYS:H	2.10	0.49
1:A:1438:THR:HG23	2:B:1144:ALA:HB3	1.95	0.49
2:B:650:GLU:HG3	2:B:651:LEU:N	2.28	0.49
1:A:376:TYR:CZ	1:A:498:ARG:HD2	2.48	0.49
2:B:219:ALA:HB3	2:B:222:ILE:HD12	1.94	0.49
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.41	0.49
2:B:54:PHE:HA	2:B:58:THR:HB	1.95	0.49
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.94	0.49
1:A:148:CYS:O	1:A:168:GLY:HA2	2.13	0.49
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.95	0.49
3:C:12:GLU:HB2	3:C:19:ASP:HB3	1.94	0.49
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.48	0.49
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.39	0.48
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.95	0.48
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.48	0.48
1:A:984:LYS:HB3	1:A:988:LEU:HD12	1.94	0.48
2:B:1022:THR:HG23	2:B:1022:THR:O	2.13	0.48
9:K:47:ARG:C	9:K:47:ARG:HD2	2.32	0.48
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.95	0.48
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.95	0.48
2:B:591:ARG:O	2:B:592:ASN:HB2	2.13	0.48
2:B:843:GLN:HB2	2:B:993:THR:HB	1.94	0.48
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.49	0.48
1:A:1116:LEU:HD13	1:A:1311:VAL:HG13	1.94	0.48
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.43	0.48
3:C:163:ILE:HG23	3:C:165:LYS:H	1.78	0.48
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.95	0.48
2:B:545:ILE:HG12	2:B:633:VAL:HG22	1.94	0.48
9:K:20:LYS:O	9:K:33:ILE:HA	2.13	0.48
9:K:12:LEU:N	9:K:12:LEU:HD12	2.28	0.48
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.11	0.48
1:A:597:LEU:H	1:A:597:LEU:HD12	1.78	0.48
10:L:48:CYS:SG	10:L:49:LYS:N	2.87	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.14	0.48
2:B:122:LEU:CD2	2:B:958:GLN:HG2	2.43	0.48
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	1.94	0.48
1:A:38:PRO:HB3	1:A:270:LEU:HD23	1.95	0.48
1:A:338:GLY:CA	1:A:343:LYS:HD2	2.44	0.48
10:L:42:ARG:C	10:L:44:ASP:H	2.17	0.48
6:H:26:ILE:HD13	6:H:49:VAL:HG11	1.95	0.48
2:B:864:LYS:HB2	2:B:864:LYS:HZ2	1.77	0.48
2:B:979:LYS:CE	2:B:987:LYS:HD2	2.44	0.48
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.95	0.48
1:A:849:MET:CE	1:A:1063:MET:SD	3.01	0.48
2:B:298:LEU:HD22	2:B:314:LEU:HD13	1.93	0.48
1:A:765:VAL:HG23	1:A:802:ASN:O	2.14	0.48
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.13	0.48
9:K:61:TYR:HA	9:K:72:LYS:O	2.12	0.48
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.13	0.48
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.96	0.48
2:B:806:THR:HG23	2:B:808:ALA:H	1.79	0.48
1:A:517:ASN:HB2	1:A:878:ILE:O	2.13	0.48
1:A:1102:LYS:HD3	1:A:1106:ASN:ND2	2.28	0.48
2:B:315:LYS:N	2:B:316:PRO:HD2	2.27	0.48
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.48	0.48
2:B:497:ARG:HH22	2:B:775:LYS:HE3	1.78	0.48
2:B:324:ILE:HD11	2:B:333:PHE:CB	2.43	0.48
1:A:1434:ALA:O	1:A:1436:ILE:N	2.41	0.48
9:K:30:ALA:HA	9:K:75:ILE:O	2.14	0.48
2:B:429:PHE:HA	2:B:432:MET:HE3	1.95	0.48
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.96	0.48
1:A:1447:GLU:OE1	1:A:1447:GLU:HA	2.14	0.48
6:H:125:LEU:C	6:H:130:ARG:HH12	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.78	0.48
2:B:953:LEU:C	2:B:953:LEU:HD23	2.34	0.48
1:A:249:SER:HB2	1:A:258:GLY:O	2.13	0.48
2:B:98:THR:HG22	2:B:99:LYS:N	2.28	0.48
1:A:857:ARG:HD3	1:A:861:GLY:O	2.14	0.48
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.96	0.48
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.96	0.48
1:A:51:GLY:O	1:A:56:PRO:HB3	2.13	0.48
2:B:564:GLU:HB2	2:B:589:VAL:HG12	1.96	0.48
3:C:209:TYR:N	3:C:209:TYR:CD1	2.82	0.48
2:B:294:ASP:H	7:I:12:ASN:HD22	1.57	0.47
7:I:50:THR:CB	7:I:92:ARG:HH12	2.27	0.47
3:C:108:GLU:OE1	3:C:149:LYS:HD3	2.14	0.47
2:B:776:GLN:HA	2:B:1096:ARG:NH1	2.29	0.47
3:C:121:VAL:HG12	3:C:121:VAL:O	2.14	0.47
1:A:740:LEU:HD12	1:A:740:LEU:N	2.29	0.47
3:C:166:GLU:CG	10:L:70:ARG:HH12	2.27	0.47
1:A:1145:SER:HB2	1:A:1205:LYS:HZ3	1.78	0.47
4:E:99:HIS:O	4:E:103:LYS:HG2	2.15	0.47
2:B:285:ILE:O	2:B:289:LEU:HG	2.13	0.47
3:C:73:GLN:NE2	3:C:75:MET:H	2.05	0.47
1:A:1118:VAL:CG2	1:A:1306:LEU:HD12	2.44	0.47
3:C:22:LEU:HD12	3:C:230:MET:HE1	1.95	0.47
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.44	0.47
1:A:602:ASP:O	1:A:615:GLY:HA2	2.14	0.47
10:L:58:LYS:O	10:L:59:ALA:HB3	2.14	0.47
1:A:1279:ILE:HD11	1:A:1312:ASN:CB	2.43	0.47
2:B:202:TYR:N	2:B:202:TYR:CD2	2.83	0.47
3:C:244:VAL:O	3:C:248:ILE:HG13	2.14	0.47
2:B:528:PRO:CG	2:B:536:VAL:HB	2.44	0.47
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.79	0.47
1:A:144:THR:O	1:A:146:MET:HG3	2.14	0.47
2:B:108:VAL:HG12	2:B:109:THR:N	2.29	0.47
1:A:483:ASP:OD1	13:B:3571:UTP:O1B	2.32	0.47
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	1.97	0.47
1:A:346:ASP:O	1:A:347:PHE:HB2	2.15	0.47
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.95	0.47
3:C:169:LYS:HZ3	10:L:70:ARG:HG2	1.79	0.47
2:B:914:LYS:HG2	2:B:915:THR:N	2.28	0.47
2:B:955:THR:CG2	10:L:55:ILE:HA	2.43	0.47
7:I:50:THR:CG2	7:I:52:ILE:HG22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LYS:O	1:A:988:LEU:HB2	2.14	0.47
7:I:95:THR:HG22	7:I:96:SER:O	2.14	0.47
2:B:1165:ILE:HG13	2:B:1187:ASN:ND2	2.29	0.47
1:A:598:LEU:HD11	6:H:124:ARG:CB	2.44	0.47
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.96	0.47
3:C:167:HIS:CD2	3:C:169:LYS:H	2.13	0.47
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.45	0.47
7:I:98:VAL:HG22	7:I:111:THR:HG22	1.97	0.47
6:H:40:LEU:CD1	6:H:123:MET:HB2	2.42	0.47
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.15	0.47
1:A:1167:GLU:O	1:A:1171:GLN:HG3	2.14	0.47
1:A:440:ASP:O	1:A:460:VAL:HG23	2.15	0.47
1:A:44:THR:O	1:A:45:GLN:HB2	2.14	0.47
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.35	0.47
6:H:100:THR:HG23	6:H:138:GLU:HG3	1.96	0.47
1:A:1431:GLY:HA2	2:B:1152:MET:CE	2.45	0.47
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.96	0.47
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.96	0.47
5:F:134:ILE:HD12	5:F:151:LEU:CD1	2.45	0.47
2:B:1060:ARG:NH2	3:C:202:PRO:HG3	2.30	0.47
2:B:461:LEU:HD12	2:B:466:TRP:HH2	1.80	0.47
1:A:381:THR:HB	1:A:382:PRO:HD2	1.97	0.47
1:A:880:LYS:HA	1:A:955:PRO:HA	1.95	0.47
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.55	0.47
1:A:516:SER:O	1:A:517:ASN:C	2.52	0.47
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.14	0.47
1:A:365:GLY:O	1:A:468:PHE:HA	2.14	0.47
3:C:55:THR:HB	3:C:152:GLU:H	1.80	0.47
4:E:120:ALA:O	4:E:123:LEU:HB2	2.15	0.47
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.31	0.46
2:B:683:SER:O	2:B:687:GLU:HG3	2.14	0.46
6:H:96:VAL:HG13	6:H:143:LEU:CD2	2.45	0.46
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.97	0.46
3:C:35:ARG:NH1	9:K:41:THR:H	2.12	0.46
1:A:1124:HIS:CB	1:A:1130:GLN:HG3	2.45	0.46
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.51	0.46
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.50	0.46
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.51	0.46
2:B:287:ARG:NH1	2:B:324:ILE:O	2.48	0.46
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.61	0.46
1:A:115:LEU:CD1	1:A:141:LEU:HB3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:95:THR:HG22	7:I:96:SER:N	2.31	0.46
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.97	0.46
2:B:889:THR:HG22	2:B:891:ASP:H	1.80	0.46
1:A:907:THR:CG2	1:A:908:LEU:H	2.26	0.46
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.44	0.46
2:B:60:GLN:O	2:B:63:ILE:HG22	2.16	0.46
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.97	0.46
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.80	0.46
2:B:420:LEU:HD13	2:B:453:ILE:HA	1.97	0.46
2:B:98:THR:O	2:B:126:SER:HB3	2.15	0.46
2:B:778:MET:SD	2:B:1094:ARG:HD3	2.56	0.46
1:A:418:SER:C	1:A:420:ARG:H	2.17	0.46
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.51	0.46
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.15	0.46
2:B:651:LEU:HD23	2:B:710:LEU:HD11	1.96	0.46
1:A:1293:SER:HB3	1:A:1297:GLU:O	2.15	0.46
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.98	0.46
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.98	0.46
1:A:401:GLY:H	1:A:435:HIS:HD1	1.64	0.46
1:A:345:VAL:CG1	2:B:1129:ARG:HA	2.46	0.46
8:J:30:LEU:HD11	8:J:38:ARG:NH2	2.31	0.46
6:H:130:ARG:HD3	6:H:134:ASN:HD21	1.81	0.46
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.98	0.46
2:B:103:ASN:HB2	2:B:169:ARG:NH1	2.31	0.46
2:B:884:ARG:O	2:B:936:ASP:HB2	2.16	0.46
2:B:859:TYR:CD1	2:B:859:TYR:N	2.83	0.46
3:C:11:ARG:HD2	3:C:21:ILE:CD1	2.46	0.46
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.97	0.46
1:A:1039:LYS:O	1:A:1043:ASP:OD1	2.34	0.46
3:C:242:GLN:HE21	3:C:246:ARG:NH2	2.03	0.46
2:B:25:ILE:HG13	2:B:654:ARG:HA	1.97	0.46
2:B:174:LEU:O	2:B:200:GLY:O	2.33	0.46
1:A:1396:ALA:HB2	1:A:1417:GLU:OE1	2.16	0.46
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.51	0.46
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.98	0.46
1:A:226:GLU:HG3	1:A:227:VAL:HG23	1.98	0.46
3:C:102:GLN:OE1	3:C:154:LYS:HE2	2.16	0.46
6:H:12:VAL:HA	6:H:28:ALA:CB	2.46	0.46
3:C:89:GLU:O	3:C:90:ASP:HB3	2.16	0.46
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.46
1:A:666:ILE:HG12	2:B:1026:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.97	0.46
2:B:493:SER:OG	2:B:497:ARG:NH2	2.49	0.46
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.16	0.46
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.50	0.46
2:B:705:MET:HB3	2:B:706:GLN:NE2	2.31	0.45
10:L:49:LYS:O	10:L:50:ASP:HB2	2.16	0.45
1:A:35:ILE:HD13	1:A:83:HIS:H	1.81	0.45
1:A:795:GLU:HG2	2:B:731:VAL:HG22	1.98	0.45
1:A:752:LYS:HG2	2:B:1015:HIS:O	2.17	0.45
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.30	0.45
3:C:42:PRO:HG3	3:C:163:ILE:HD11	1.97	0.45
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.16	0.45
3:C:55:THR:O	3:C:55:THR:HG22	2.16	0.45
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.15	0.45
2:B:1191:ILE:HG22	2:B:1192:TYR:N	2.30	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.97	0.45
2:B:1051:THR:HG22	2:B:1053:GLU:N	2.23	0.45
6:H:105:GLU:O	6:H:107:VAL:HG23	2.15	0.45
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.15	0.45
3:C:6:PRO:CB	9:K:101:LEU:HD23	2.46	0.45
1:A:62:ASP:HB2	1:A:64:ASN:ND2	2.31	0.45
1:A:239:LEU:HD23	1:A:240:PRO:N	2.31	0.45
3:C:100:THR:HG22	3:C:101:LEU:N	2.32	0.45
1:A:853:ASP:O	1:A:854:ASN:HB2	2.17	0.45
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.98	0.45
1:A:489:LEU:HD23	1:A:490:HIS:N	2.31	0.45
6:H:31:THR:HG22	6:H:32:THR:N	2.31	0.45
3:C:57:VAL:O	3:C:57:VAL:HG12	2.17	0.45
1:A:1386:ARG:HG3	1:A:1386:ARG:O	2.16	0.45
3:C:6:PRO:HA	3:C:25:VAL:HG13	1.98	0.45
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.97	0.45
10:L:41:SER:HB2	10:L:42:ARG:HH21	1.82	0.45
1:A:1295:THR:HB	1:A:1297:GLU:OE1	2.17	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.45
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.51	0.45
6:H:56:THR:O	6:H:144:ILE:HA	2.17	0.45
2:B:904:ARG:HH21	2:B:948:ILE:HD11	1.81	0.45
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.51	0.45
10:L:38:LEU:O	10:L:39:SER:HB2	2.17	0.45
2:B:879:ARG:HG3	2:B:885:MET:HE1	1.97	0.45
2:B:276:ILE:CD1	2:B:355:ILE:HD13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1322:ILE:HG13	1:A:1323:ASP:N	2.31	0.45
1:A:464:PRO:HB2	9:K:4:PRO:HD3	1.98	0.45
1:A:765:VAL:HB	1:A:800:VAL:CG1	2.47	0.45
1:A:71:GLN:HG2	2:B:1176:ASN:HD22	1.82	0.45
1:A:822:GLU:HG3	2:B:513:GLN:HE22	1.81	0.45
1:A:84:ILE:O	1:A:84:ILE:HG23	2.17	0.45
1:A:1364:ASN:ND2	1:A:1366:ARG:CG	2.79	0.45
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.49	0.45
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.65	0.45
9:K:12:LEU:HD12	9:K:12:LEU:H	1.82	0.45
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.31	0.45
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.98	0.45
2:B:638:PHE:HB2	2:B:741:CYS:O	2.17	0.45
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.98	0.45
3:C:48:SER:HB3	3:C:158:VAL:HB	1.99	0.45
1:A:368:LYS:HB2	1:A:368:LYS:NZ	2.32	0.45
1:A:329:LEU:HA	1:A:332:LYS:HB2	1.99	0.45
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.47	0.45
4:E:88:VAL:HG13	4:E:92:THR:HB	1.99	0.45
2:B:1079:LYS:HB2	3:C:27:LEU:HD21	1.97	0.45
8:J:36:LEU:HD21	8:J:50:ILE:HB	1.99	0.45
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.17	0.45
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.50	0.45
6:H:31:THR:HG22	6:H:32:THR:H	1.81	0.45
8:J:14:VAL:HG23	8:J:41:LEU:HD21	1.99	0.45
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.46	0.45
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.97	0.45
2:B:98:THR:HG22	2:B:99:LYS:H	1.82	0.45
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.99	0.45
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.32	0.45
1:A:682:THR:HG23	1:A:728:LYS:NZ	2.32	0.44
5:F:85:MET:O	5:F:155:LEU:HD21	2.17	0.44
10:L:68:GLU:C	10:L:70:ARG:H	2.21	0.44
3:C:261:ALA:O	3:C:265:MET:HB2	2.17	0.44
1:A:709:THR:HG21	7:I:93:LYS:O	2.17	0.44
2:B:757:PRO:HD3	2:B:983:ARG:CZ	2.47	0.44
3:C:71:PRO:C	3:C:72:LEU:HD23	2.38	0.44
3:C:239:PRO:O	3:C:242:GLN:HB2	2.16	0.44
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.98	0.44
2:B:872:GLU:HG2	2:B:916:THR:OG1	2.17	0.44
3:C:35:ARG:HH12	9:K:41:THR:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:O	1:A:1035:TYR:HE1	2.00	0.44
1:A:849:MET:CE	1:A:1437:GLY:H	2.31	0.44
1:A:1348:LEU:HD21	1:A:1375:MET:HE2	1.99	0.44
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.99	0.44
1:A:208:LEU:HD23	1:A:208:LEU:O	2.17	0.44
1:A:1150:SER:HB3	1:A:1195:LEU:HD22	2.00	0.44
1:A:35:ILE:HA	1:A:52:GLY:O	2.17	0.44
1:A:1190:PRO:HG3	7:I:18:GLU:OE2	2.18	0.44
1:A:589:GLN:HB2	1:A:961:ARG:NH2	2.32	0.44
1:A:854:ASN:O	1:A:867:ILE:HA	2.17	0.44
1:A:472:LEU:HD13	2:B:835:GLN:HE21	1.82	0.44
1:A:54:ASN:HD21	1:A:259:GLU:HG2	1.83	0.44
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.18	0.44
2:B:405:ARG:HA	2:B:631:GLY:O	2.17	0.44
4:E:159:ASP:HA	4:E:162:ARG:NH1	2.32	0.44
8:J:45:CYS:O	8:J:48:ARG:HG3	2.18	0.44
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.53	0.44
2:B:654:ARG:N	2:B:657:HIS:HD2	2.16	0.44
1:A:1220:PHE:HE1	1:A:1267:MET:HG2	1.83	0.44
1:A:549:MET:HE1	1:A:577:ILE:HD13	1.99	0.44
2:B:1159:ARG:CG	2:B:1193:GLN:HE21	2.31	0.44
2:B:744:HIS:HD2	2:B:746:SER:H	1.66	0.44
1:A:940:ARG:O	1:A:944:ARG:HG3	2.18	0.44
2:B:849:GLY:HA2	2:B:852:ARG:HG3	1.99	0.44
3:C:66:ARG:NH2	8:J:3:VAL:O	2.51	0.44
1:A:1079:MET:HE3	1:A:1098:VAL:HG22	1.99	0.44
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.81	0.44
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.00	0.44
1:A:247:ARG:HD3	1:A:263:THR:OG1	2.17	0.44
2:B:53:GLN:HB2	2:B:547:VAL:CG2	2.48	0.44
10:L:61:THR:HB	10:L:63:ARG:HG2	1.99	0.44
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.17	0.44
2:B:46:GLN:HE21	2:B:496:ARG:HH11	1.66	0.44
5:F:138:LEU:HD12	5:F:142:SER:OG	2.18	0.44
2:B:1009:ASP:O	2:B:1010:LEU:HD12	2.18	0.44
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.17	0.44
1:A:57:ARG:O	1:A:68:GLN:HG3	2.16	0.44
1:A:1295:THR:O	1:A:1295:THR:HG22	2.18	0.44
1:A:16:GLU:HG3	2:B:1220:ARG:HA	1.99	0.44
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.17	0.44
1:A:248:PRO:O	1:A:260:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TRP:O	1:A:186:LYS:HB2	2.18	0.44
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.99	0.44
2:B:791:THR:O	2:B:857:ARG:HA	2.18	0.44
1:A:302:THR:HG21	1:A:312:PRO:CG	2.48	0.44
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.98	0.44
1:A:445:ASN:ND2	1:A:446:ARG:N	2.65	0.44
5:F:81:THR:HG21	5:F:136:ARG:CD	2.48	0.44
7:I:50:THR:HB	7:I:92:ARG:HH12	1.82	0.44
6:H:62:SER:O	6:H:63:LEU:C	2.56	0.44
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.15	0.43
8:J:64:ASN:N	8:J:65:PRO:CD	2.81	0.43
2:B:979:LYS:NZ	2:B:987:LYS:HD2	2.33	0.43
1:A:768:GLN:HG3	1:A:816:HIS:HA	2.00	0.43
1:A:647:GLY:O	1:A:651:LYS:HG3	2.18	0.43
2:B:491:THR:O	2:B:495:LEU:HD12	2.18	0.43
2:B:900:ALA:HB2	10:L:58:LYS:HD2	2.00	0.43
3:C:62:PHE:CD2	3:C:66:ARG:HD2	2.53	0.43
8:J:64:ASN:H	8:J:65:PRO:HD2	1.81	0.43
1:A:523:ILE:HD13	1:A:622:VAL:HG13	2.00	0.43
2:B:235:SER:OG	2:B:236:HIS:HD2	2.01	0.43
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.99	0.43
1:A:1328:TYR:CG	1:A:1329:THR:N	2.86	0.43
3:C:148:ARG:HD2	8:J:61:LEU:O	2.19	0.43
7:I:45:ARG:NH1	7:I:45:ARG:HG2	2.28	0.43
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.18	0.43
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.83	0.43
4:E:93:MET:HG3	4:E:97:VAL:HG23	2.00	0.43
1:A:800:VAL:HG22	1:A:812:GLU:HB3	2.00	0.43
3:C:136:ASP:C	3:C:138:GLU:H	2.21	0.43
1:A:642:CYS:O	1:A:645:LEU:HB3	2.19	0.43
2:B:548:GLY:N	2:B:612:GLU:OE2	2.51	0.43
1:A:1341:ILE:CG1	1:A:1376:THR:HG23	2.48	0.43
1:A:1438:THR:CG2	2:B:1144:ALA:H	2.29	0.43
1:A:276:LEU:HD13	1:A:292:ALA:HB3	2.01	0.43
3:C:38:ILE:CG1	3:C:176:ILE:HD12	2.48	0.43
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.33	0.43
2:B:785:TYR:CE2	2:B:795:ILE:HG12	2.53	0.43
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.54	0.43
2:B:973:ILE:O	2:B:975:GLN:HG3	2.18	0.43
5:F:116:ASP:O	5:F:120:ILE:HG13	2.18	0.43
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HB2	1:A:487:MET:HE2	2.00	0.43
1:A:313:GLN:HG2	1:A:322:VAL:HB	2.00	0.43
4:E:204:THR:CG2	4:E:205:SER:N	2.81	0.43
1:A:79:GLY:HA3	1:A:245:PRO:CG	2.45	0.43
2:B:46:GLN:HE21	2:B:496:ARG:NH1	2.16	0.43
5:F:109:VAL:HG23	5:F:124:GLU:HG2	2.00	0.43
2:B:979:LYS:HE2	2:B:1095:LEU:HD12	2.00	0.43
1:A:1104:ILE:HD13	1:A:1351:GLU:HB3	2.01	0.43
3:C:185:LYS:HG2	3:C:213:PRO:HB3	2.00	0.43
2:B:446:LEU:O	2:B:448:ILE:HG13	2.18	0.43
1:A:774:ARG:HB2	1:A:797:LYS:HB3	2.00	0.43
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.16	0.43
2:B:800:GLN:O	2:B:818:PRO:HB2	2.18	0.43
2:B:274:PRO:HG3	2:B:359:GLU:HB3	2.00	0.43
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.34	0.43
2:B:212:LEU:HD11	2:B:461:LEU:HD11	2.00	0.43
2:B:877:PRO:HB3	2:B:915:THR:CG2	2.48	0.43
1:A:1264:GLU:HA	1:A:1267:MET:HE2	2.01	0.43
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.59	0.43
2:B:860:MET:HA	2:B:964:VAL:O	2.18	0.43
1:A:881:GLN:CD	1:A:959:ASN:HA	2.39	0.43
2:B:1222:ARG:H	2:B:1222:ARG:CD	2.21	0.43
1:A:605:MET:HE3	1:A:612:ILE:HG13	2.01	0.43
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.52	0.43
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.54	0.43
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.54	0.43
2:B:561:TRP:O	2:B:590:HIS:HE1	2.02	0.43
3:C:260:LEU:O	3:C:260:LEU:HD12	2.18	0.43
4:E:22:MET:HA	4:E:187:TYR:CZ	2.54	0.43
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.54	0.43
1:A:566:ILE:O	1:A:567:LYS:O	2.37	0.43
1:A:1118:VAL:O	1:A:1118:VAL:HG23	2.18	0.43
3:C:58:LEU:HD22	3:C:62:PHE:CE2	2.53	0.43
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.19	0.43
2:B:281:PRO:CG	2:B:284:ILE:HD12	2.46	0.43
2:B:796:LEU:O	2:B:799:PRO:HD3	2.18	0.43
1:A:262:LEU:O	1:A:266:LEU:HG	2.19	0.43
6:H:18:GLY:O	6:H:20:TYR:N	2.52	0.43
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.19	0.43
1:A:329:LEU:C	1:A:331:GLY:H	2.21	0.43
1:A:187:LYS:O	1:A:188:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:O	3:C:161:LYS:HA	2.19	0.43
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.47	0.43
7:I:50:THR:HB	7:I:92:ARG:NH2	2.33	0.43
2:B:986:GLN:NE2	2:B:987:LYS:O	2.48	0.43
4:E:153:HIS:CG	4:E:184:VAL:HG11	2.54	0.43
3:C:169:LYS:NZ	10:L:70:ARG:HG2	2.34	0.42
3:C:63:ILE:O	3:C:67:LEU:HG	2.19	0.42
1:A:914:GLU:C	1:A:916:GLY:N	2.72	0.42
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.54	0.42
3:C:13:ALA:O	9:K:114:LEU:HB3	2.18	0.42
1:A:73:GLY:C	1:A:75:ASN:H	2.22	0.42
2:B:497:ARG:HG3	2:B:498:THR:H	1.84	0.42
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.83	0.42
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.34	0.42
4:E:77:SER:HG	4:E:105:PHE:HD2	1.64	0.42
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.19	0.42
1:A:914:GLU:O	1:A:916:GLY:N	2.52	0.42
2:B:268:THR:CG2	2:B:270:LYS:HE3	2.46	0.42
9:K:78:THR:HG22	9:K:79:GLU:N	2.35	0.42
2:B:750:GLY:O	2:B:754:SER:HB2	2.19	0.42
2:B:794:ASN:C	2:B:795:ILE:HD12	2.39	0.42
2:B:225:VAL:HA	2:B:237:VAL:O	2.20	0.42
2:B:424:LEU:O	2:B:428:ILE:HG13	2.19	0.42
1:A:1173:HIS:NE2	1:A:1227:ILE:HG23	2.35	0.42
2:B:875:GLU:HG2	2:B:895:ASP:O	2.20	0.42
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.34	0.42
2:B:953:LEU:CD2	2:B:955:THR:HG23	2.43	0.42
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.84	0.42
2:B:983:ARG:HH11	2:B:1091:TYR:CB	2.32	0.42
1:A:1436:ILE:O	1:A:1437:GLY:C	2.58	0.42
1:A:38:PRO:C	1:A:39:GLU:HG3	2.38	0.42
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.84	0.42
1:A:974:ASP:HA	6:H:136:LYS:HE2	2.01	0.42
2:B:784:ASN:HB3	8:J:63:TYR:OH	2.19	0.42
1:A:557:ASP:HA	9:K:26:LYS:HD2	2.02	0.42
2:B:760:ASP:OD1	2:B:760:ASP:N	2.53	0.42
1:A:853:ASP:OD1	1:A:855:THR:CB	2.66	0.42
1:A:450:LEU:N	1:A:450:LEU:HD12	2.25	0.42
2:B:46:GLN:NE2	2:B:496:ARG:HB3	2.28	0.42
2:B:1023:VAL:HG12	2:B:1027:ILE:CD1	2.49	0.42
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:GLU:OE2	1:A:962:ARG:HD3	2.19	0.42
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.85	0.42
1:A:1008:GLN:O	1:A:1012:ARG:HG3	2.18	0.42
1:A:699:ALA:O	1:A:700:ASN:HB3	2.20	0.42
3:C:57:VAL:CG1	3:C:57:VAL:O	2.67	0.42
2:B:957:ASN:ND2	2:B:958:GLN:N	2.65	0.42
1:A:342:GLY:O	1:A:345:VAL:HG13	2.20	0.42
7:I:17:ARG:CG	7:I:28:GLU:HG2	2.48	0.42
9:K:90:ALA:O	9:K:94:ILE:HG13	2.19	0.42
2:B:315:LYS:HB2	2:B:315:LYS:HE3	1.80	0.42
1:A:808:LEU:HD12	1:A:808:LEU:N	2.34	0.42
2:B:586:TRP:NE1	2:B:588:GLY:O	2.52	0.42
2:B:653:VAL:HG12	2:B:689:LEU:HD13	2.02	0.42
2:B:654:ARG:H	2:B:657:HIS:HD2	1.67	0.42
2:B:950:ASP:O	2:B:951:GLN:HB2	2.20	0.42
9:K:21:ILE:HG23	9:K:31:VAL:CG1	2.50	0.42
1:A:551:TYR:CE1	9:K:74:ARG:HD3	2.55	0.42
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.40	0.42
8:J:32:GLU:CD	8:J:32:GLU:H	2.23	0.42
1:A:329:LEU:HD23	1:A:332:LYS:HB2	2.00	0.42
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	2.01	0.42
2:B:174:LEU:HD12	2:B:174:LEU:N	2.35	0.42
2:B:102:VAL:HG11	2:B:122:LEU:HD13	2.01	0.42
1:A:92:HIS:CD2	1:A:94:GLY:H	2.38	0.42
4:E:78:LEU:HD11	4:E:109:ILE:HG13	2.02	0.42
1:A:337:ARG:HH12	1:A:1403:GLU:HA	1.85	0.42
3:C:58:LEU:HD12	3:C:145:CYS:SG	2.60	0.42
1:A:2:VAL:HG13	1:A:2:VAL:O	2.20	0.42
7:I:35:VAL:HG22	7:I:36:GLU:N	2.35	0.42
2:B:383:ASN:O	2:B:387:LEU:HB2	2.20	0.42
6:H:97:MET:CE	6:H:142:LEU:HD23	2.50	0.41
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.02	0.41
3:C:42:PRO:HA	3:C:163:ILE:HD12	2.02	0.41
3:C:43:THR:CG2	3:C:44:LEU:N	2.83	0.41
1:A:834:THR:HG21	1:A:1077:THR:CA	2.47	0.41
2:B:844:SER:OG	2:B:996:ARG:N	2.43	0.41
2:B:35:SER:HA	2:B:811:TYR:CE2	2.55	0.41
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.43	0.41
2:B:858:SER:HA	2:B:966:VAL:O	2.20	0.41
4:E:204:THR:HG22	4:E:205:SER:N	2.36	0.41
2:B:94:LYS:HD3	2:B:96:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:18:LYS:HE3	9:K:38:GLU:HG2	2.02	0.41
1:A:1115:SER:HA	1:A:1308:THR:O	2.21	0.41
6:H:125:LEU:HB3	6:H:130:ARG:CZ	2.50	0.41
3:C:166:GLU:HA	9:K:6:ARG:HB3	2.01	0.41
8:J:52:THR:O	8:J:52:THR:HG22	2.19	0.41
1:A:391:LEU:HD23	1:A:400:PRO:O	2.20	0.41
4:E:88:VAL:HG21	4:E:110:PHE:CE2	2.55	0.41
9:K:21:ILE:HD13	9:K:84:LYS:HE2	2.01	0.41
1:A:925:LEU:HD13	1:A:983:ILE:HD12	2.02	0.41
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.61	0.41
4:E:59:SER:OG	4:E:81:GLU:HA	2.21	0.41
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.35	0.41
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	2.03	0.41
3:C:265:MET:HE1	9:K:19:LEU:O	2.20	0.41
1:A:103:CYS:SG	1:A:207:ILE:HG23	2.60	0.41
6:H:82:PRO:O	6:H:84:ALA:N	2.52	0.41
3:C:35:ARG:HH11	9:K:41:THR:N	2.18	0.41
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.50	0.41
2:B:339:THR:CG2	2:B:343:ILE:HB	2.50	0.41
1:A:369:SER:CB	9:K:2:ASN:HD21	2.33	0.41
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.49	0.41
4:E:94:LYS:O	4:E:98:ILE:HG13	2.20	0.41
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.04	0.41
1:A:246:VAL:O	1:A:328:ARG:NH2	2.54	0.41
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.02	0.41
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.55	0.41
2:B:875:GLU:O	2:B:877:PRO:HD3	2.21	0.41
1:A:605:MET:CE	1:A:612:ILE:HG13	2.51	0.41
3:C:22:LEU:CD2	9:K:101:LEU:HD21	2.50	0.41
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.85	0.41
1:A:106:VAL:CG2	1:A:111:GLY:C	2.89	0.41
2:B:121:ASN:HA	2:B:207:GLY:CA	2.51	0.41
2:B:235:SER:HA	2:B:261:ARG:NH2	2.35	0.41
2:B:995:ARG:HD2	2:B:997:GLU:OE2	2.20	0.41
2:B:361:LEU:O	2:B:374:LYS:HE2	2.21	0.41
1:A:63:ARG:HA	1:A:74:MET:HE2	2.02	0.41
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.55	0.41
2:B:515:HIS:CD2	2:B:517:THR:H	2.23	0.41
2:B:324:ILE:HD11	2:B:333:PHE:CG	2.56	0.41
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.56	0.41
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:SER:O	2:B:251:ILE:HA	2.19	0.41
1:A:476:SER:N	1:A:477:PRO:HD2	2.36	0.41
7:I:16:PRO:HA	7:I:26:LEU:O	2.21	0.41
3:C:258:ILE:HG23	9:K:19:LEU:HD11	2.02	0.41
1:A:32:VAL:HG23	1:A:33:ALA:H	1.85	0.41
2:B:757:PRO:HD3	2:B:983:ARG:HH21	1.86	0.41
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.21	0.41
2:B:123:THR:OG1	2:B:458:LYS:HE3	2.21	0.41
6:H:5:LEU:HD11	6:H:135:LEU:HG	2.03	0.41
2:B:886:LYS:C	2:B:888:GLY:H	2.24	0.41
2:B:1183:LYS:C	2:B:1185:CYS:H	2.24	0.41
1:A:406:ILE:N	1:A:406:ILE:HD12	2.36	0.41
6:H:113:ALA:HA	6:H:125:LEU:O	2.21	0.41
1:A:186:LYS:HG2	1:A:187:LYS:H	1.86	0.41
6:H:12:VAL:HG13	6:H:26:ILE:CG2	2.51	0.41
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.50	0.41
2:B:870:ILE:HD11	2:B:919:SER:OG	2.21	0.41
7:I:98:VAL:CG2	7:I:111:THR:HG22	2.50	0.41
1:A:81:PHE:HA	1:A:243:PRO:HD3	2.03	0.41
10:L:26:THR:C	10:L:27:LEU:HD23	2.41	0.41
7:I:103:CYS:SG	7:I:105:SER:HB2	2.60	0.41
2:B:339:THR:HG22	2:B:340:ALA:O	2.20	0.41
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.21	0.41
6:H:15:VAL:HG22	6:H:26:ILE:HG12	2.03	0.41
1:A:313:GLN:CB	1:A:320:ARG:HB3	2.51	0.41
3:C:62:PHE:CE2	3:C:66:ARG:HD2	2.55	0.41
2:B:1006:ILE:HD11	8:J:43:ARG:CB	2.46	0.41
3:C:163:ILE:CG2	3:C:165:LYS:H	2.33	0.41
1:A:91:PHE:HZ	1:A:207:ILE:HG13	1.86	0.41
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.35	0.41
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.55	0.41
2:B:165:VAL:HG12	2:B:167:ILE:HG13	2.03	0.41
1:A:1104:ILE:CD1	1:A:1351:GLU:HB3	2.51	0.41
8:J:41:LEU:HD22	8:J:46:CYS:HB3	2.02	0.41
4:E:72:PHE:HE2	4:E:157:SER:HA	1.85	0.41
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.44	0.41
8:J:39:LEU:HD23	8:J:39:LEU:HA	1.92	0.41
6:H:36:CYS:HA	6:H:126:GLU:O	2.21	0.41
2:B:129:PHE:CZ	2:B:166:PHE:HB2	2.56	0.41
1:A:850:VAL:HG21	1:A:1058:VAL:HG21	2.03	0.41
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:HG2	1:A:590:ARG:HH11	1.86	0.41
1:A:220:THR:O	1:A:222:LEU:O	2.39	0.41
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.36	0.41
1:A:901:LEU:HA	1:A:907:THR:HG23	2.03	0.41
1:A:1059:HIS:CE1	5:F:155:LEU:HD22	2.45	0.41
1:A:946:VAL:CG2	4:E:201:LYS:HD2	2.45	0.41
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.51	0.41
9:K:21:ILE:HG21	9:K:84:LYS:HE2	2.03	0.41
2:B:795:ILE:HD12	2:B:795:ILE:N	2.36	0.41
1:A:120:GLU:HG3	1:A:123:ARG:NH2	2.36	0.41
2:B:906:SER:O	2:B:907:GLY:C	2.58	0.41
1:A:334:GLY:HA2	1:A:337:ARG:HB3	2.02	0.40
2:B:324:ILE:HG12	2:B:329:THR:CG2	2.45	0.40
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.35	0.40
1:A:463:ILE:HB	1:A:464:PRO:HD2	2.03	0.40
1:A:24:PRO:O	1:A:28:ARG:HG3	2.21	0.40
1:A:473:SER:OG	1:A:522:GLY:O	2.23	0.40
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.02	0.40
6:H:27:GLU:HA	6:H:38:LEU:O	2.20	0.40
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.21	0.40
1:A:849:MET:HE1	1:A:1436:ILE:HA	2.00	0.40
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	2.02	0.40
4:E:201:LYS:HA	4:E:201:LYS:HD3	1.92	0.40
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.21	0.40
1:A:115:LEU:HD12	1:A:142:CYS:SG	2.61	0.40
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.54	0.40
1:A:302:THR:HG23	1:A:306:ASN:ND2	2.36	0.40
9:K:18:LYS:HE3	9:K:38:GLU:CG	2.52	0.40
2:B:217:ARG:HG2	2:B:218:SER:O	2.21	0.40
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.21	0.40
1:A:1376:THR:CG2	4:E:212:ARG:NH2	2.76	0.40
3:C:73:GLN:HA	3:C:133:ILE:HD11	2.02	0.40
2:B:882:THR:HB	2:B:934:LYS:O	2.22	0.40
1:A:305:ASP:O	1:A:308:ILE:HD11	2.21	0.40
5:F:107:VAL:HG13	5:F:124:GLU:OE2	2.22	0.40
2:B:344:LYS:HB2	2:B:347:LYS:HE2	2.02	0.40
2:B:483:LEU:HD11	2:B:491:THR:HG23	2.04	0.40
2:B:1057:LYS:O	2:B:1061:GLU:HG3	2.21	0.40
1:A:1365:TYR:C	1:A:1365:TYR:CD2	2.94	0.40
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.03	0.40
1:A:901:LEU:CD2	1:A:907:THR:HG23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLU:O	1:A:337:ARG:HB2	2.22	0.40
2:B:259:TYR:HB2	2:B:268:THR:HG22	2.04	0.40
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.04	0.40
2:B:311:LEU:HA	2:B:314:LEU:HD12	2.04	0.40
6:H:32:THR:HB	6:H:33:GLN:H	1.54	0.40
1:A:298:PHE:CZ	1:A:312:PRO:HD3	2.57	0.40
2:B:996:ARG:NH2	3:C:174:ALA:O	2.54	0.40
3:C:250:THR:O	3:C:254:LYS:HG3	2.22	0.40
8:J:53:HIS:CG	8:J:54:VAL:N	2.90	0.40
1:A:592:ASP:O	1:A:593:GLU:C	2.60	0.40
3:C:3:GLU:HB2	9:K:104:ASN:OD1	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	1411/1733 (81%)	1250 (89%)	123 (9%)	38 (3%)	6 4
2	B	1074/1224 (88%)	950 (88%)	110 (10%)	14 (1%)	15 15
3	C	264/318 (83%)	236 (89%)	24 (9%)	4 (2%)	13 12
4	E	213/215 (99%)	189 (89%)	22 (10%)	2 (1%)	21 24
5	F	82/155 (53%)	76 (93%)	5 (6%)	1 (1%)	16 16
6	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0 0
7	I	120/122 (98%)	103 (86%)	17 (14%)	0	100 100
8	J	63/70 (90%)	59 (94%)	3 (5%)	1 (2%)	12 11
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100 100
10	L	44/70 (63%)	25 (57%)	16 (36%)	3 (7%)	1 0
All	All	3512/4173 (84%)	3087 (88%)	347 (10%)	78 (2%)	8 6

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	464	PRO
1	A	465	TYR
1	A	466	SER
1	A	567	LYS
1	A	593	GLU
1	A	1393	ASN
2	B	1222	ARG
6	H	128	ASN
1	A	35	ILE
1	A	307	ASP
1	A	467	THR
1	A	525	GLN
1	A	1398	MET
2	B	646	LEU
2	B	879	ARG
2	B	887	HIS
3	C	4	GLU
3	C	231	ASN
4	E	3	GLN
4	E	50	MET
6	H	18	GLY
6	H	19	ARG
6	H	61	SER
6	H	78	SER
6	H	105	GLU
6	H	138	GLU
1	A	67	CYS
1	A	156	ASP
1	A	258	GLY
1	A	283	GLY
1	A	626	ASN
1	A	915	SER
1	A	958	VAL
1	A	1386	ARG
2	B	165	VAL
2	B	262	GLU
2	B	266	ALA
2	B	1190	ASP
3	C	90	ASP
3	C	137	LYS
5	F	73	ALA

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Mol	Chain	Res	Type
6	H	52	GLN
6	H	81	PRO
6	H	103	LYS
8	J	44	TYR
10	L	39	SER
1	A	72	GLU
1	A	188	ASP
1	A	194	ALA
1	A	196	GLU
1	A	248	PRO
1	A	752	LYS
1	A	764	CYS
2	B	864	LYS
2	B	1100	ASP
6	H	62	SER
10	L	56	LEU
10	L	59	ALA
1	A	257	ARG
1	A	308	ILE
1	A	419	LYS
1	A	959	ASN
1	A	1402	PHE
2	B	90	ILE
2	B	1099	VAL
6	H	83	GLN
6	H	109	LYS
6	H	139	ASN
1	A	250	ILE
6	H	47	PHE
1	A	84	ILE
1	A	399	HIS
2	B	1214	PRO
1	A	61	ILE
2	B	1109	GLY
1	A	1114	PRO
1	A	400	PRO

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	1239/1520 (82%)	1180 (95%)	59 (5%)	31	42
2	B	950/1061 (90%)	903 (95%)	47 (5%)	31	41
3	C	234/274 (85%)	226 (97%)	8 (3%)	44	59
4	E	197/197 (100%)	191 (97%)	6 (3%)	48	65
5	F	74/137 (54%)	71 (96%)	3 (4%)	37	50
6	H	117/128 (91%)	115 (98%)	2 (2%)	68	83
7	I	116/116 (100%)	109 (94%)	7 (6%)	24	31
8	J	60/65 (92%)	52 (87%)	8 (13%)	5	5
9	K	99/102 (97%)	93 (94%)	6 (6%)	23	30
10	L	40/57 (70%)	35 (88%)	5 (12%)	6	6
All	All	3126/3657 (86%)	2975 (95%)	151 (5%)	31	42

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	53	LEU
1	A	93	VAL
1	A	171	GLN
1	A	175	ARG
1	A	209	ASN
1	A	221	SER
1	A	385	ILE
1	A	386	ASP
1	A	434	ARG
1	A	446	ARG
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	467	THR
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	498	ARG
1	A	503	GLN

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Mol	Chain	Res	Type
1	A	504	LEU
1	A	513	SER
1	A	535	THR
1	A	596	THR
1	A	597	LEU
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	666	ILE
1	A	672	ASP
1	A	756	ILE
1	A	769	SER
1	A	774	ARG
1	A	821	ARG
1	A	855	THR
1	A	858	ASN
1	A	873	MET
1	A	885	THR
1	A	903	ASN
1	A	919	ILE
1	A	920	LEU
1	A	940	ARG
1	A	1043	ASP
1	A	1048	ASN
1	A	1130	GLN
1	A	1166	ASP
1	A	1222	ASN
1	A	1277	GLU
1	A	1293	SER
1	A	1297	GLU
1	A	1309	ASP
1	A	1318	THR
1	A	1366	ARG
1	A	1372	VAL
1	A	1377	THR
1	A	1383	SER
1	A	1426	GLU
2	B	18	PHE
2	B	20	ASP
2	B	21	GLU
2	B	61	ASP
2	B	121	ASN

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Mol	Chain	Res	Type
2	B	194	GLU
2	B	217	ARG
2	B	261	ARG
2	B	268	THR
2	B	313	MET
2	B	339	THR
2	B	357	GLN
2	B	366	GLN
2	B	372	SER
2	B	463	THR
2	B	466	TRP
2	B	485	ARG
2	B	496	ARG
2	B	540	SER
2	B	563	MET
2	B	567	GLU
2	B	589	VAL
2	B	612	GLU
2	B	636	PRO
2	B	641	GLU
2	B	644	GLU
2	B	737	THR
2	B	754	SER
2	B	790	ASP
2	B	806	THR
2	B	864	LYS
2	B	895	ASP
2	B	957	ASN
2	B	970	THR
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1065	GLN
2	B	1097	HIS
2	B	1099	VAL
2	B	1145	SER
2	B	1150	ARG
2	B	1152	MET
2	B	1159	ARG
2	B	1186	ASP
2	B	1219	ASP
2	B	1222	ARG

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Mol	Chain	Res	Type
3	C	23	SER
3	C	26	ASP
3	C	50	GLU
3	C	77	ILE
3	C	163	ILE
3	C	170	TRP
3	C	209	TYR
3	C	240	VAL
4	E	104	ASN
4	E	123	LEU
4	E	146	HIS
4	E	159	ASP
4	E	196	VAL
4	E	204	THR
5	F	79	ARG
5	F	82	THR
5	F	115	THR
6	H	32	THR
6	H	104	PHE
7	I	12	ASN
7	I	46	HIS
7	I	50	THR
7	I	61	ASP
7	I	84	VAL
7	I	87	GLN
7	I	111	THR
8	J	1	MET
8	J	3	VAL
8	J	7	CYS
8	J	14	VAL
8	J	28	ASP
8	J	37	SER
8	J	38	ARG
8	J	48	ARG
9	K	11	LEU
9	K	18	LYS
9	K	47	ARG
9	K	73	LEU
9	K	81	TYR
9	K	114	LEU
10	L	27	LEU
10	L	38	LEU

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Mol	Chain	Res	Type
10	L	42	ARG
10	L	50	ASP
10	L	64	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS
1	A	171	GLN
1	A	313	GLN
1	A	390	GLN
1	A	394	ASN
1	A	397	ASN
1	A	479	ASN
1	A	503	GLN
1	A	517	ASN
1	A	660	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	854	ASN
1	A	858	ASN
1	A	903	ASN
1	A	906	HIS
1	A	926	GLN
1	A	994	GLN
1	A	1048	ASN
1	A	1052	GLN
1	A	1218	GLN
1	A	1265	ASN
1	A	1270	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1432	GLN
2	B	46	GLN
2	B	178	ASN

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Mol	Chain	Res	Type
2	B	215	GLN
2	B	236	HIS
2	B	255	GLN
2	B	325	GLN
2	B	363	HIS
2	B	366	GLN
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	587	HIS
2	B	590	HIS
2	B	657	HIS
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	786	ASN
2	B	957	ASN
2	B	1015	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1179	GLN
2	B	1187	ASN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
4	E	101	GLN
4	E	104	ASN
4	E	113	GLN
4	E	147	HIS
6	H	11	GLN
6	H	133	ASN
6	H	134	ASN
7	I	12	ASN

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Mol	Chain	Res	Type
7	I	116	ASN
8	J	53	HIS
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 10 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	$\#\|Z\| > 2$
13	UTP	B	3571	12	20,30,30	1.39	3 (15%)	30,47,47	2.82	5 (16%)

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
13	UTP	B	3571	12	-	0/18/38/38	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3571	UTP	PB-O1B	-2.21	1.45	1.54
13	B	3571	UTP	C6-N1	2.76	1.39	1.35
13	B	3571	UTP	C4-N3	4.07	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	3571	UTP	C4'-O4'-C1'	-4.09	105.22	109.72
13	B	3571	UTP	C5-C4-N3	-3.34	114.55	123.12
13	B	3571	UTP	O3A-PA-O5'	-2.89	95.27	102.94
13	B	3571	UTP	O1B-PB-O3A	2.39	115.93	105.09
13	B	3571	UTP	C4-N3-C2	13.37	127.38	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	3571	UTP	1	0

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1419/1733 (81%)	1.38	257 (18%) 2 3	15, 54, 147, 169	0
2	B	1094/1224 (89%)	1.49	221 (20%) 1 2	16, 50, 129, 158	0
3	C	266/318 (83%)	1.12	38 (14%) 4 6	27, 58, 95, 144	0
4	E	215/215 (100%)	1.37	49 (22%) 1 1	23, 67, 113, 149	0
5	F	84/155 (54%)	0.84	9 (10%) 8 12	20, 49, 77, 98	0
6	H	133/146 (91%)	2.90	75 (56%) 0 0	63, 99, 141, 150	0
7	I	122/122 (100%)	1.34	27 (22%) 1 1	41, 64, 108, 130	0
8	J	65/70 (92%)	0.99	9 (13%) 4 6	29, 49, 80, 94	0
9	K	114/120 (95%)	1.27	20 (17%) 2 3	31, 67, 86, 97	0
10	L	46/70 (65%)	2.62	22 (47%) 0 0	52, 105, 132, 137	0
All	All	3558/4173 (85%)	1.44	727 (20%) 1 2	15, 56, 135, 169	0

All (727) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1390	ASN	20.6
1	A	188	ASP	19.7
1	A	1176	LEU	18.6
1	A	1175	SER	17.8
6	H	85	GLY	17.5
1	A	340	LEU	17.1
1	A	249	SER	17.0
2	B	919	SER	14.8
1	A	251	SER	14.6
6	H	84	ALA	14.3
1	A	341	MET	14.3
10	L	27	LEU	14.1
1	A	190	ALA	14.0

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Mol	Chain	Res	Type	RSRZ
1	A	318	SER	13.8
1	A	344	ARG	13.8
2	B	137	TYR	13.8
2	B	870	ILE	13.8
1	A	2	VAL	13.4
1	A	314	ALA	13.3
1	A	1389	PHE	13.2
2	B	883	LEU	13.2
1	A	1402	PHE	13.2
1	A	189	ARG	12.7
1	A	343	LYS	12.6
1	A	253	ASN	12.6
1	A	194	ALA	12.5
2	B	866	TYR	12.1
1	A	254	GLU	12.1
2	B	643	ASP	12.0
1	A	44	THR	11.2
2	B	1184	GLY	11.1
2	B	70	ILE	11.0
2	B	1189	ILE	10.9
1	A	319	GLY	10.8
2	B	918	ILE	10.8
1	A	69	THR	10.8
2	B	1106	ARG	10.7
1	A	258	GLY	10.7
1	A	252	PHE	10.6
1	A	1391	ARG	10.6
6	H	104	PHE	10.4
1	A	250	ILE	10.3
1	A	1387	HIS	10.2
2	B	1105	ALA	10.2
1	A	1450	LEU	10.2
2	B	882	THR	10.1
2	B	1223	ASP	9.9
2	B	1110	PRO	9.8
1	A	1386	ARG	9.8
6	H	146	ARG	9.8
2	B	1109	GLY	9.8
2	B	250	PHE	9.7
1	A	315	LEU	9.6
2	B	69	LEU	9.6
2	B	1100	ASP	9.6

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Mol	Chain	Res	Type	RSRZ
1	A	257	ARG	9.5
2	B	868	MET	9.5
1	A	1449	SER	9.5
6	H	83	GLN	9.4
1	A	259	GLU	9.4
2	B	869	SER	9.4
2	B	1224	PHE	9.3
1	A	45	GLN	9.2
4	E	1	MET	9.1
1	A	320	ARG	9.1
1	A	1400	CYS	9.1
1	A	321	PRO	8.9
1	A	191	THR	8.9
1	A	339	ASN	8.9
2	B	132	VAL	8.9
1	A	1392	SER	8.7
2	B	136	THR	8.6
10	L	50	ASP	8.6
2	B	734	HIS	8.6
1	A	345	VAL	8.6
2	B	1156	ASP	8.5
2	B	867	GLY	8.5
1	A	311	GLN	8.3
1	A	1399	ARG	8.3
1	A	65	LEU	8.3
1	A	3	GLY	8.3
6	H	88	SER	8.2
1	A	316	GLN	8.2
2	B	434	ARG	8.1
1	A	312	PRO	7.9
6	H	132	LEU	7.9
1	A	193	ASP	7.8
2	B	733	HIS	7.8
7	I	1	MET	7.7
1	A	46	THR	7.6
4	E	50	MET	7.6
1	A	1092	LYS	7.6
7	I	119	THR	7.6
2	B	732	SER	7.5
4	E	2	ASP	7.5
1	A	62	ASP	7.4
7	I	121	PHE	7.4

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Mol	Chain	Res	Type	RSRZ
2	B	265	SER	7.4
1	A	1388	GLY	7.4
2	B	432	MET	7.4
1	A	1174	PHE	7.4
6	H	131	ASN	7.4
7	I	120	GLN	7.3
10	L	26	THR	7.3
9	K	1	MET	7.2
2	B	712	PRO	7.2
2	B	935	ARG	7.2
1	A	329	LEU	7.2
2	B	65	GLU	7.1
1	A	248	PRO	7.0
1	A	323	LYS	7.0
1	A	1448	GLU	6.9
1	A	342	GLY	6.8
6	H	87	ARG	6.8
2	B	92	PHE	6.8
2	B	1175	LEU	6.8
6	H	82	PRO	6.8
7	I	122	SER	6.8
1	A	66	LYS	6.7
2	B	89	GLU	6.7
3	C	268	ASP	6.7
1	A	158	PRO	6.7
2	B	1098	MET	6.7
2	B	865	LYS	6.7
2	B	1107	ALA	6.7
2	B	246	LYS	6.6
2	B	1101	ASP	6.6
1	A	166	GLY	6.6
1	A	313	GLN	6.6
2	B	1103	ILE	6.6
1	A	68	GLN	6.5
2	B	1108	ARG	6.5
2	B	884	ARG	6.5
1	A	1396	ALA	6.4
2	B	367	LEU	6.4
10	L	40	LEU	6.4
2	B	249	ARG	6.3
10	L	43	THR	6.3
1	A	192	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	42	ASP	6.2
1	A	71	GLN	6.2
2	B	90	ILE	6.2
6	H	139	ASN	6.2
2	B	917	PRO	6.2
2	B	436	VAL	6.2
2	B	723	VAL	6.2
7	I	74	GLU	6.2
1	A	6	TYR	6.2
2	B	1181	GLU	6.1
2	B	134	LYS	6.1
4	E	90	VAL	6.1
6	H	107	VAL	6.0
1	A	282	ASN	6.0
1	A	1256	GLU	6.0
2	B	944	THR	6.0
3	C	265	MET	6.0
6	H	110	ASP	6.0
5	F	111	LEU	5.9
1	A	317	LYS	5.9
1	A	1397	LEU	5.9
2	B	1176	ASN	5.8
1	A	327	ALA	5.8
6	H	127	GLY	5.8
1	A	255	SER	5.8
2	B	247	GLY	5.7
2	B	1186	ASP	5.7
2	B	135	ARG	5.7
2	B	1221	SER	5.7
5	F	155	LEU	5.6
2	B	67	SER	5.6
7	I	118	ARG	5.6
1	A	256	GLN	5.6
2	B	1104	HIS	5.6
1	A	1080	THR	5.6
2	B	1102	LYS	5.5
7	I	93	LYS	5.5
7	I	79	HIS	5.5
2	B	248	SER	5.4
2	B	1172	ILE	5.4
2	B	106	ASP	5.4
3	C	216	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
6	H	126	GLU	5.4
2	B	96	TYR	5.4
1	A	1232	ASN	5.4
2	B	129	PHE	5.4
2	B	245	GLU	5.3
1	A	1170	ILE	5.3
2	B	433	GLN	5.3
2	B	1155	SER	5.3
2	B	1099	VAL	5.2
7	I	76	PRO	5.2
1	A	1081	LEU	5.2
2	B	138	GLU	5.2
2	B	68	THR	5.2
6	H	137	GLN	5.2
2	B	1180	PHE	5.2
6	H	111	LEU	5.1
2	B	108	VAL	5.1
6	H	136	LYS	5.0
1	A	72	GLU	5.0
2	B	164	LYS	5.0
6	H	2	SER	5.0
1	A	330	LYS	5.0
1	A	1447	GLU	4.9
2	B	437	GLU	4.9
1	A	186	LYS	4.9
2	B	887	HIS	4.9
1	A	64	ASN	4.9
2	B	130	VAL	4.9
9	K	2	ASN	4.8
5	F	109	VAL	4.8
6	H	77	ARG	4.8
1	A	421	ALA	4.8
1	A	187	LYS	4.8
2	B	888	GLY	4.8
1	A	279	LEU	4.7
1	A	63	ARG	4.7
4	E	7	ARG	4.7
1	A	195	ASP	4.7
4	E	51	GLY	4.7
4	E	52	ARG	4.6
1	A	1221	LYS	4.6
1	A	157	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	1403	GLU	4.6
2	B	230	ALA	4.6
6	H	130	ARG	4.6
1	A	57	ARG	4.6
1	A	1254	ALA	4.5
3	C	267	GLN	4.5
2	B	167	ILE	4.5
1	A	4	GLN	4.5
2	B	448	ILE	4.5
2	B	465	ASN	4.5
1	A	41	MET	4.5
6	H	35	GLN	4.5
4	E	57	MET	4.5
2	B	646	LEU	4.4
2	B	871	THR	4.4
6	H	134	ASN	4.4
1	A	120	GLU	4.4
2	B	1188	LYS	4.3
1	A	1255	GLU	4.3
1	A	308	ILE	4.3
1	A	593	GLU	4.3
1	A	334	GLY	4.3
10	L	49	LYS	4.3
10	L	25	ALA	4.3
6	H	54	SER	4.3
1	A	1393	ASN	4.3
4	E	123	LEU	4.2
1	A	1359	ASP	4.2
2	B	427	ASP	4.2
2	B	916	THR	4.2
2	B	908	GLU	4.2
1	A	322	VAL	4.2
1	A	8	SER	4.2
1	A	260	ASP	4.2
1	A	1225	PHE	4.2
4	E	102	GLU	4.2
6	H	30	SER	4.1
2	B	429	PHE	4.1
3	C	4	GLU	4.1
10	L	33	GLU	4.1
4	E	29	PHE	4.1
4	E	53	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
4	E	54	GLN	4.0
6	H	142	LEU	4.0
2	B	18	PHE	4.0
2	B	165	VAL	4.0
1	A	196	GLU	4.0
4	E	66	GLU	4.0
2	B	428	ILE	4.0
4	E	91	LYS	4.0
9	K	3	ALA	4.0
2	B	1128	LEU	4.0
1	A	49	LYS	4.0
2	B	19	GLU	4.0
1	A	338	GLY	3.9
1	A	261	ASP	3.9
2	B	1075	GLY	3.9
6	H	109	LYS	3.9
6	H	32	THR	3.9
6	H	89	LEU	3.9
1	A	198	GLU	3.9
2	B	101	MET	3.8
1	A	70	CYS	3.8
2	B	941	LEU	3.8
6	H	55	LEU	3.8
7	I	77	LYS	3.7
10	L	56	LEU	3.7
1	A	921	GLY	3.7
2	B	231	PRO	3.7
2	B	477	ALA	3.7
9	K	111	LEU	3.7
1	A	58	LEU	3.7
1	A	1123	GLY	3.7
4	E	67	GLU	3.7
1	A	47	ARG	3.7
1	A	336	ILE	3.6
4	E	94	LYS	3.6
6	H	103	LYS	3.6
1	A	281	HIS	3.6
6	H	12	VAL	3.6
1	A	1446	ASP	3.6
1	A	1401	SER	3.6
9	K	14	GLU	3.6
6	H	112	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	722	ASP	3.6
1	A	278	THR	3.6
1	A	247	ARG	3.6
2	B	881	ASN	3.6
6	H	129	TYR	3.6
2	B	644	GLU	3.5
1	A	307	ASP	3.5
10	L	45	ALA	3.5
1	A	1404	GLU	3.5
3	C	215	GLU	3.5
4	E	4	GLU	3.5
1	A	264	PHE	3.5
4	E	122	LYS	3.5
1	A	1172	LEU	3.5
1	A	1218	GLN	3.5
2	B	1177	HIS	3.5
1	A	1220	PHE	3.4
8	J	65	PRO	3.4
9	K	113	THR	3.4
1	A	428	TYR	3.4
6	H	18	GLY	3.4
2	B	1077	THR	3.4
2	B	1222	ARG	3.4
1	A	1395	GLY	3.4
1	A	912	LEU	3.4
2	B	880	THR	3.4
1	A	325	ILE	3.4
2	B	666	TYR	3.4
3	C	218	PRO	3.4
1	A	40	THR	3.4
10	L	36	SER	3.4
1	A	408	ASP	3.4
4	E	128	PRO	3.4
6	H	31	THR	3.3
7	I	92	ARG	3.3
2	B	229	ALA	3.3
2	B	1173	ALA	3.3
1	A	121	LEU	3.3
1	A	266	LEU	3.3
2	B	961	LEU	3.3
2	B	1178	ASN	3.3
1	A	1394	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	304	MET	3.3
1	A	309	ALA	3.3
2	B	889	THR	3.3
4	E	49	SER	3.3
8	J	29	GLU	3.2
1	A	728	LYS	3.2
3	C	175	ALA	3.2
1	A	38	PRO	3.2
2	B	426	LYS	3.2
6	H	116	TYR	3.2
4	E	56	LYS	3.2
6	H	52	GLN	3.2
2	B	1185	CYS	3.2
2	B	999	MET	3.2
1	A	1162	VAL	3.2
2	B	592	ASN	3.2
6	H	47	PHE	3.1
4	E	132	ILE	3.1
1	A	1223	ASP	3.1
2	B	467	GLY	3.1
1	A	597	LEU	3.1
3	C	137	LYS	3.1
2	B	1174	LYS	3.1
1	A	43	GLU	3.1
9	K	98	LEU	3.1
6	H	57	VAL	3.1
6	H	128	ASN	3.1
4	E	101	GLN	3.1
6	H	95	TYR	3.1
2	B	1179	GLN	3.1
1	A	37	PHE	3.1
1	A	56	PRO	3.1
2	B	1072	MET	3.1
2	B	942	ARG	3.1
2	B	435	THR	3.0
9	K	79	GLU	3.0
2	B	95	ILE	3.0
3	C	18	VAL	3.0
3	C	3	GLU	3.0
4	E	85	GLU	3.0
7	I	53	GLY	3.0
9	K	80	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
6	H	144	ILE	3.0
1	A	411	ASP	3.0
2	B	877	PRO	3.0
2	B	875	GLU	3.0
1	A	1271	ILE	3.0
6	H	100	THR	3.0
2	B	94	LYS	3.0
2	B	451	LYS	3.0
6	H	86	ASP	3.0
6	H	60	ALA	3.0
1	A	160	GLN	3.0
1	A	1281	ARG	3.0
9	K	101	LEU	3.0
4	E	127	ILE	2.9
4	E	5	ASN	2.9
1	A	146	MET	2.9
1	A	270	LEU	2.9
2	B	575	PRO	2.9
10	L	38	LEU	2.9
2	B	66	ASP	2.9
9	K	13	GLY	2.9
6	H	108	SER	2.9
1	A	1214	GLU	2.9
5	F	114	GLU	2.9
2	B	876	LYS	2.9
2	B	907	GLY	2.9
1	A	156	ASP	2.9
6	H	19	ARG	2.9
1	A	1398	MET	2.9
1	A	1287	TYR	2.9
2	B	1085	ILE	2.9
2	B	264	SER	2.9
2	B	1154	ALA	2.8
1	A	74	MET	2.8
1	A	60	SER	2.8
1	A	163	SER	2.8
1	A	5	GLN	2.8
1	A	1222	ASN	2.8
4	E	3	GLN	2.8
6	H	59	ILE	2.8
6	H	37	LYS	2.8
4	E	86	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
6	H	80	ARG	2.8
1	A	1120	LEU	2.8
4	E	87	SER	2.8
2	B	1073	TYR	2.8
2	B	450	ALA	2.8
1	A	280	GLU	2.8
1	A	1129	GLU	2.8
4	E	126	SER	2.8
1	A	1173	HIS	2.8
2	B	1190	ASP	2.8
10	L	37	LYS	2.8
2	B	63	ILE	2.8
1	A	36	ARG	2.8
2	B	369	GLY	2.8
1	A	274	ILE	2.7
6	H	9	ILE	2.7
8	J	30	LEU	2.7
2	B	184	ALA	2.7
3	C	174	ALA	2.7
3	C	217	ASP	2.7
2	B	640	VAL	2.7
9	K	21	ILE	2.7
7	I	20	LYS	2.7
1	A	917	SER	2.7
3	C	5	GLY	2.7
1	A	612	ILE	2.7
5	F	108	PHE	2.7
2	B	879	ARG	2.7
6	H	141	TYR	2.7
7	I	111	THR	2.7
1	A	262	LEU	2.7
8	J	1	MET	2.7
2	B	963	PHE	2.7
1	A	205	GLU	2.7
2	B	1157	ALA	2.7
7	I	80	SER	2.7
2	B	1097	HIS	2.7
1	A	1079	MET	2.7
1	A	655	PHE	2.7
3	C	35	ARG	2.7
2	B	446	LEU	2.6
4	E	119	SER	2.6

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Mol	Chain	Res	Type	RSRZ
7	I	4	PHE	2.6
8	J	26	GLN	2.6
1	A	1262	LYS	2.6
2	B	200	GLY	2.6
1	A	1109	LYS	2.6
2	B	128	LEU	2.6
2	B	1095	LEU	2.6
2	B	1002	THR	2.6
2	B	573	GLN	2.6
4	E	113	GLN	2.6
6	H	11	GLN	2.6
2	B	946	ASN	2.6
2	B	1074	ASN	2.6
1	A	50	ILE	2.6
4	E	69	ILE	2.6
1	A	291	GLU	2.6
3	C	108	GLU	2.6
2	B	731	VAL	2.6
2	B	958	GLN	2.6
4	E	110	PHE	2.6
1	A	286	HIS	2.6
2	B	368	GLU	2.6
1	A	1259	MET	2.6
7	I	83	ASN	2.6
10	L	48	CYS	2.6
1	A	541	ILE	2.6
2	B	844	SER	2.5
3	C	126	GLY	2.5
1	A	425	GLN	2.5
2	B	425	THR	2.5
7	I	21	GLU	2.5
2	B	263	GLY	2.5
9	K	54	ARG	2.5
2	B	1081	LEU	2.5
1	A	405	VAL	2.5
1	A	159	THR	2.5
1	A	328	ARG	2.5
8	J	3	VAL	2.5
1	A	1258	HIS	2.5
2	B	25	ILE	2.5
9	K	20	LYS	2.5
3	C	245	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	735	ALA	2.5
6	H	24	CYS	2.5
6	H	28	ALA	2.5
2	B	463	THR	2.5
1	A	61	ILE	2.5
1	A	1445	ILE	2.5
1	A	175	ARG	2.5
6	H	138	GLU	2.5
2	B	557	PHE	2.5
10	L	69	ALA	2.4
1	A	751	SER	2.4
2	B	1137	CYS	2.4
1	A	555	ASP	2.4
1	A	1280	GLU	2.4
1	A	1285	MET	2.4
2	B	431	TYR	2.4
2	B	936	ASP	2.4
3	C	196	ASP	2.4
6	H	34	ASP	2.4
7	I	81	ARG	2.4
1	A	546	VAL	2.4
2	B	1206	GLU	2.4
1	A	53	LEU	2.4
3	C	49	VAL	2.4
1	A	22	PHE	2.4
1	A	81	PHE	2.4
1	A	916	GLY	2.4
2	B	417	PHE	2.4
4	E	135	PHE	2.4
7	I	60	GLN	2.4
1	A	263	THR	2.4
2	B	725	PRO	2.4
3	C	125	MET	2.4
2	B	346	GLU	2.4
1	A	1242	VAL	2.4
1	A	567	LYS	2.4
5	F	112	GLU	2.4
6	H	102	TYR	2.4
3	C	17	ASN	2.4
9	K	84	LYS	2.4
1	A	451	HIS	2.4
2	B	915	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	21	LEU	2.4
6	H	122	LEU	2.4
1	A	424	ILE	2.4
1	A	975	HIS	2.4
4	E	98	ILE	2.4
8	J	27	GLU	2.4
4	E	95	THR	2.4
1	A	332	LYS	2.4
1	A	1407	GLU	2.3
4	E	33	GLU	2.3
1	A	454	SER	2.3
2	B	1183	LYS	2.3
2	B	1187	ASN	2.3
2	B	1078	GLY	2.3
2	B	191	LYS	2.3
2	B	430	ARG	2.3
1	A	1406	VAL	2.3
2	B	1170	THR	2.3
7	I	72	ASP	2.3
2	B	275	TYR	2.3
2	B	459	TYR	2.3
8	J	2	ILE	2.3
1	A	1171	GLN	2.3
7	I	82	GLU	2.3
4	E	108	GLY	2.3
1	A	34	LYS	2.3
6	H	46	LEU	2.3
6	H	143	LEU	2.3
1	A	333	GLU	2.3
1	A	1438	THR	2.3
2	B	729	ILE	2.3
3	C	34	ARG	2.3
2	B	954	VAL	2.3
4	E	89	GLY	2.3
2	B	228	LYS	2.3
1	A	337	ARG	2.3
1	A	153	PRO	2.2
2	B	1127	GLY	2.2
3	C	258	ILE	2.2
7	I	75	CYS	2.2
10	L	41	SER	2.2
1	A	1233	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
6	H	101	ALA	2.2
1	A	246	VAL	2.2
3	C	208	GLU	2.2
1	A	75	ASN	2.2
9	K	26	LYS	2.2
2	B	885	MET	2.2
1	A	10	PRO	2.2
3	C	30	ALA	2.2
6	H	50	ALA	2.2
2	B	502	ILE	2.2
1	A	1424	VAL	2.2
2	B	103	ASN	2.2
1	A	417	TYR	2.2
10	L	67	PHE	2.2
1	A	39	GLU	2.2
1	A	681	GLU	2.2
1	A	1405	THR	2.2
3	C	107	SER	2.2
6	H	39	THR	2.2
2	B	899	ILE	2.2
10	L	55	ILE	2.2
4	E	97	VAL	2.2
1	A	1005	GLU	2.2
9	K	105	PHE	2.2
4	E	76	GLY	2.2
5	F	110	ASP	2.2
2	B	996	ARG	2.2
2	B	878	GLN	2.2
2	B	933	SER	2.2
2	B	104	GLU	2.2
2	B	1143	ALA	2.2
2	B	1191	ILE	2.2
1	A	656	TRP	2.2
1	A	331	GLY	2.2
6	H	92	ASP	2.2
2	B	486	TYR	2.2
5	F	129	LYS	2.2
1	A	1110	ASN	2.2
2	B	461	LEU	2.2
3	C	58	LEU	2.2
1	A	1124	HIS	2.2
6	H	90	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1206	ASP	2.1
2	B	20	ASP	2.1
8	J	28	ASP	2.1
1	A	326	ARG	2.1
2	B	260	GLY	2.1
3	C	36	VAL	2.1
1	A	1188	GLN	2.1
6	H	79	TRP	2.1
1	A	109	HIS	2.1
1	A	1032	LEU	2.1
2	B	572	HIS	2.1
1	A	594	GLY	2.1
1	A	1263	ILE	2.1
2	B	115	GLN	2.1
2	B	1007	VAL	2.1
3	C	51	VAL	2.1
4	E	96	PHE	2.1
1	A	977	LYS	2.1
3	C	27	LEU	2.1
4	E	93	MET	2.1
1	A	1159	ARG	2.1
2	B	576	ASP	2.1
2	B	1153	GLU	2.1
6	H	27	GLU	2.1
2	B	234	ILE	2.1
2	B	344	LYS	2.1
6	H	62	SER	2.1
1	A	1127	ASP	2.1
2	B	641	GLU	2.1
2	B	895	ASP	2.1
3	C	221	TYR	2.1
10	L	68	GLU	2.1
6	H	135	LEU	2.1
1	A	1227	ILE	2.1
1	A	118	HIS	2.1
1	A	927	VAL	2.1
6	H	23	VAL	2.1
7	I	94	ASP	2.1
10	L	65	VAL	2.1
2	B	454	THR	2.1
3	C	69	LEU	2.1
9	K	114	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	133	LYS	2.1
4	E	206	GLY	2.1
1	A	184	SER	2.1
5	F	78	GLN	2.1
2	B	487	THR	2.1
4	E	42	PHE	2.1
1	A	155	GLU	2.1
1	A	534	LEU	2.1
9	K	86	ALA	2.1
10	L	42	ARG	2.1
6	H	17	PRO	2.1
2	B	795	ILE	2.1
3	C	21	ILE	2.1
9	K	95	ILE	2.1
1	A	1118	VAL	2.1
2	B	787	VAL	2.1
1	A	91	PHE	2.0
2	B	1204	PHE	2.0
3	C	87	PHE	2.0
1	A	1236	LEU	2.0
2	B	1147	LEU	2.0
6	H	98	TYR	2.0
7	I	117	LYS	2.0
7	I	107	SER	2.0
1	A	170	THR	2.0
2	B	46	GLN	2.0
1	A	108	MET	2.0
1	A	1284	MET	2.0
2	B	1158	PHE	2.0
4	E	43	LYS	2.0
6	H	123	MET	2.0
10	L	62	LYS	2.0
2	B	110	HIS	2.0
2	B	845	SER	2.0
3	C	32	SER	2.0
1	A	12	ARG	2.0
1	A	165	GLY	2.0
3	C	19	ASP	2.0
1	A	549	MET	2.0
1	A	571	LEU	2.0
3	C	101	LEU	2.0
4	E	75	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
11	ZN	I	3003	1/1	0.69	0.12	-0.16	58,58,58,58	0
13	UTP	B	3571	29/29	0.85	0.15	-0.56	53,61,64,65	0
11	ZN	C	3002	1/1	0.97	0.08	-1.14	48,48,48,48	0
11	ZN	A	3008	1/1	0.89	0.08	-1.47	97,97,97,97	0
11	ZN	I	3004	1/1	0.93	0.07	-1.60	74,74,74,74	0
11	ZN	A	3006	1/1	0.79	0.08	-1.68	53,53,53,53	0
11	ZN	J	3001	1/1	0.93	0.13	-1.69	45,45,45,45	0
11	ZN	L	3005	1/1	0.81	0.06	-1.78	89,89,89,89	0
11	ZN	B	3007	1/1	0.90	0.06	-2.21	55,55,55,55	0
12	MN	A	3010	1/1	0.95	0.16	-	40,40,40,40	0
12	MN	A	3009	1/1	0.95	0.25	-	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.