Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:59 AM GMT

PDB ID	:	3K7A
Title	:	Crystal Structure of an RNA polymerase II-TFIIB complex
Authors	:	Liu, X.; Bushnell, D.A.; Wang, D.; Calero, G.; Kornberg, R.D.
Deposited on	:	2009-10-12
Resolution	:	3.80 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 ⓘ symbol.

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

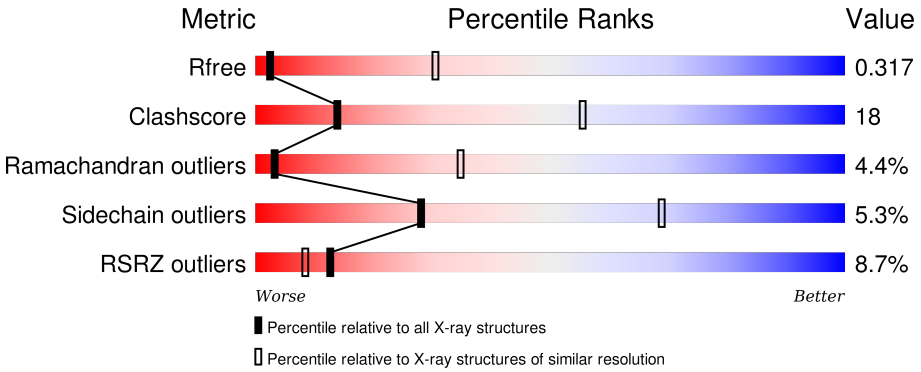
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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	4% 49% 29% • 19%
2	B	1224	13% 53% 33% • 8%
3	C	318	55% 27% • 16%
4	E	215	9% 79% 21%
5	F	155	34% 18% • 46%

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Mol	Chain	Length	Quality of chain
6	H	146	5% 48% 38% 5% 9%
7	I	122	30% 53% 38% 6%
8	J	70	9% 64% 23% 6% 7%
9	K	120	63% 25% 7% 5%
10	L	70	9% 36% 23% 7% 34%
11	M	345	7% 45% 9% 46%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	ZN	M	346	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29029 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 subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1408	Total	C	N	O	S	0	0	0
			11052	6966	1936	2089	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1122	Total	C	N	O	S	0	0	0
			8845	5595	1551	1644	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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 subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	118	Total	C	N	O	S	0	0	0
			967	594	178	185	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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 subunit RPB11.

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 subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	187	Total	C	N	O	0	0	0
			748	374	187	187			

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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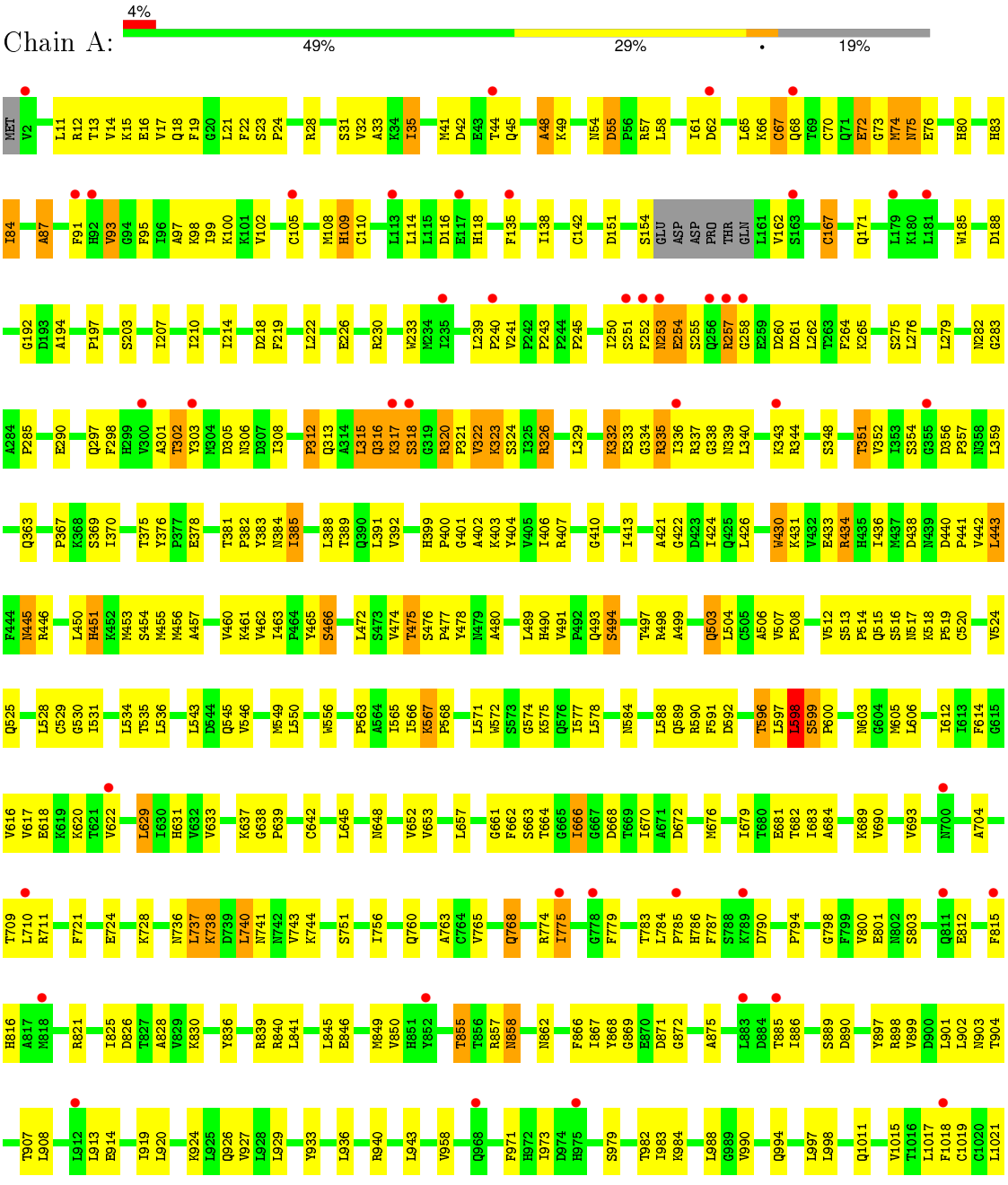
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total Zn 1 1	0	0
12	M	1	Total Zn 1 1	0	0

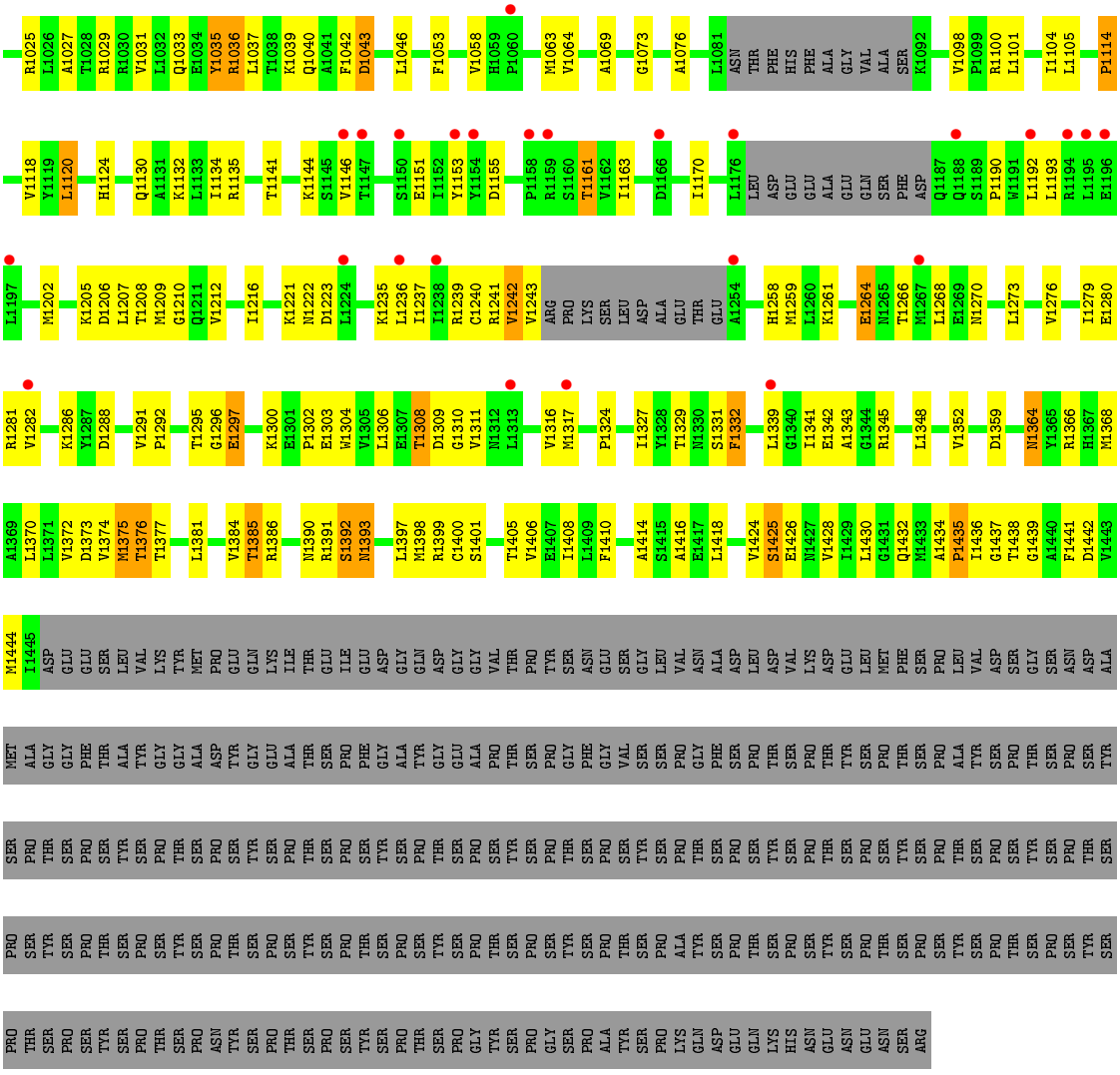
3 Residue-property plots (i)

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 subunit RPB1

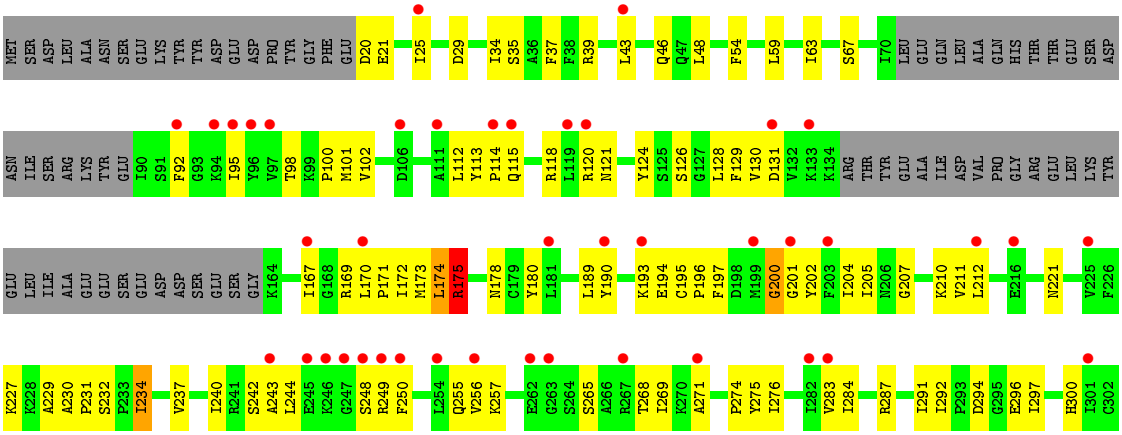
Chain A:

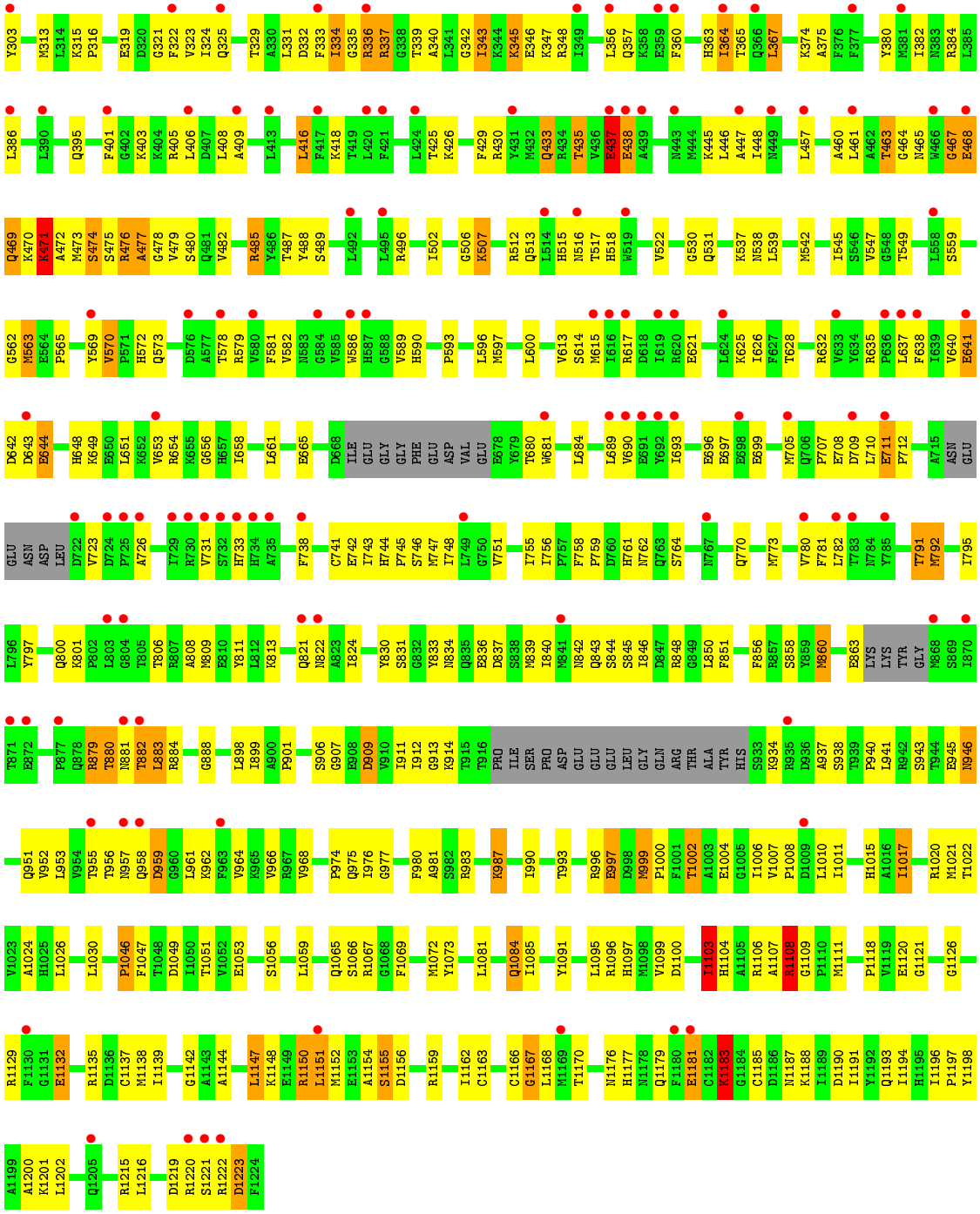




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

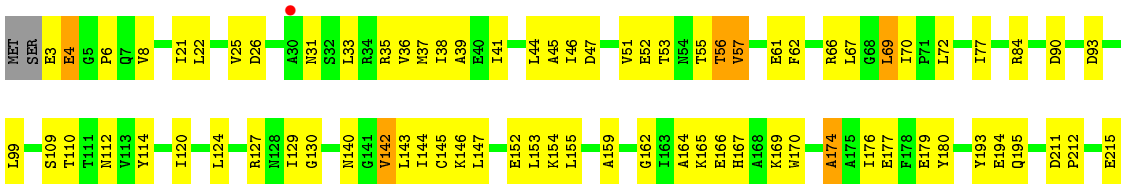
Chain B:

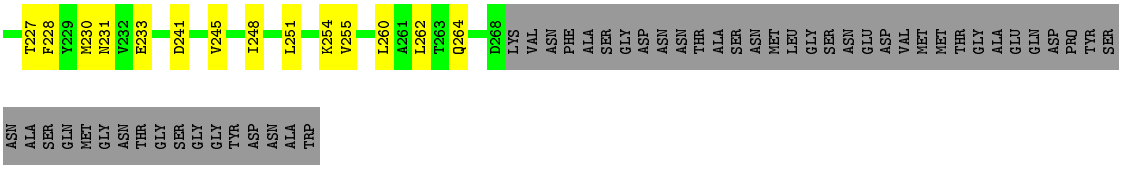




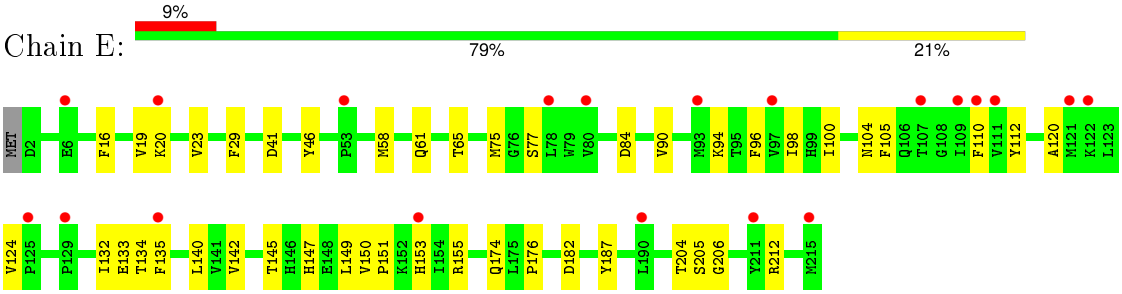
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

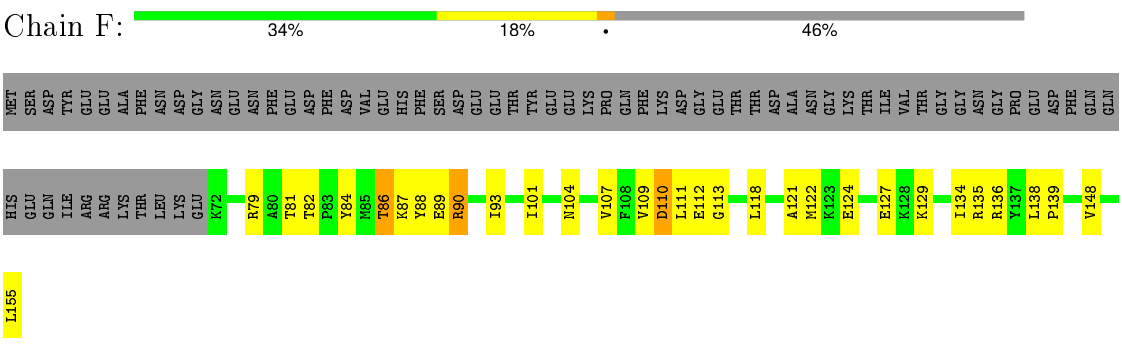




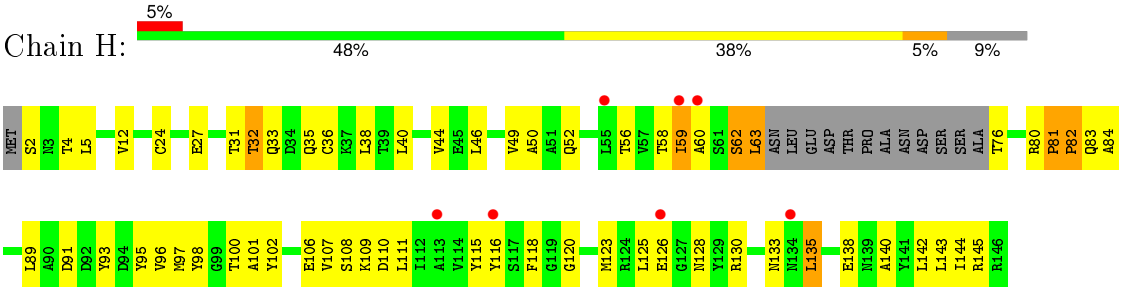
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



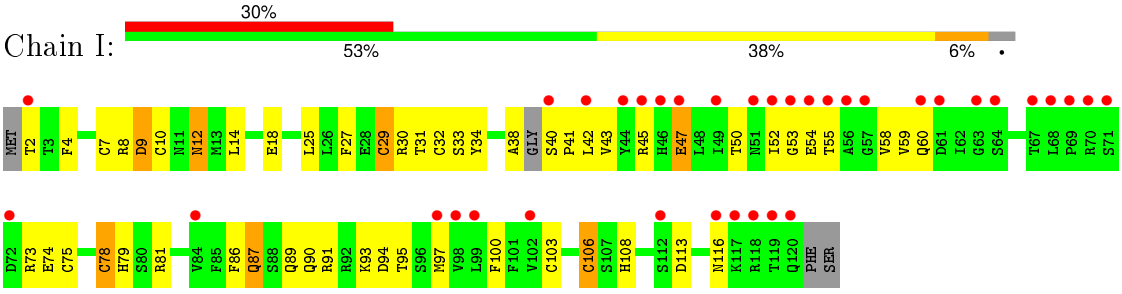
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



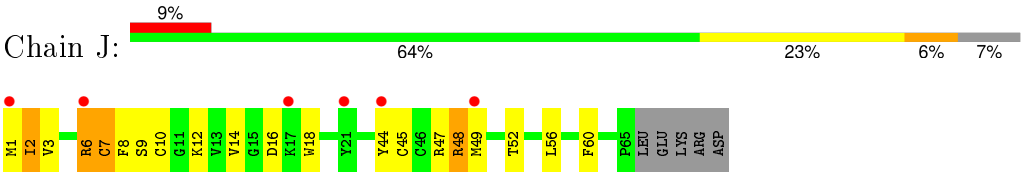
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



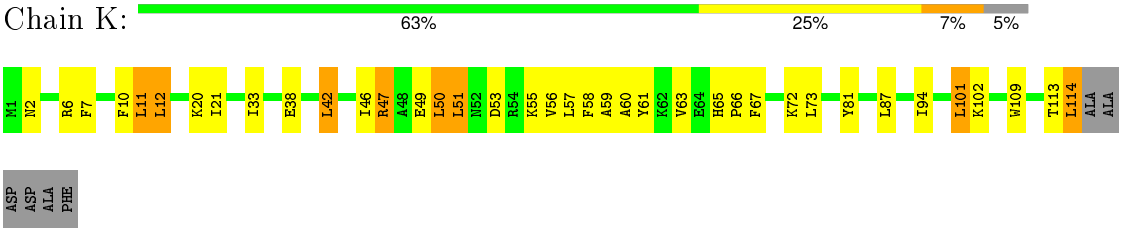
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9



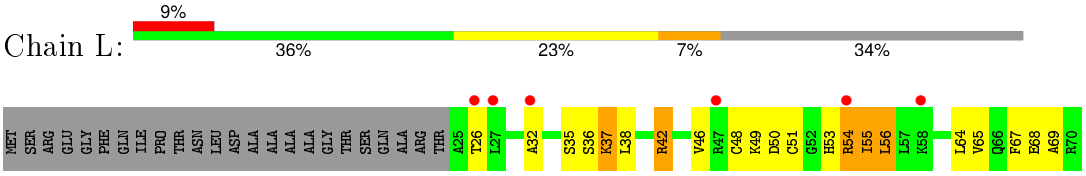
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



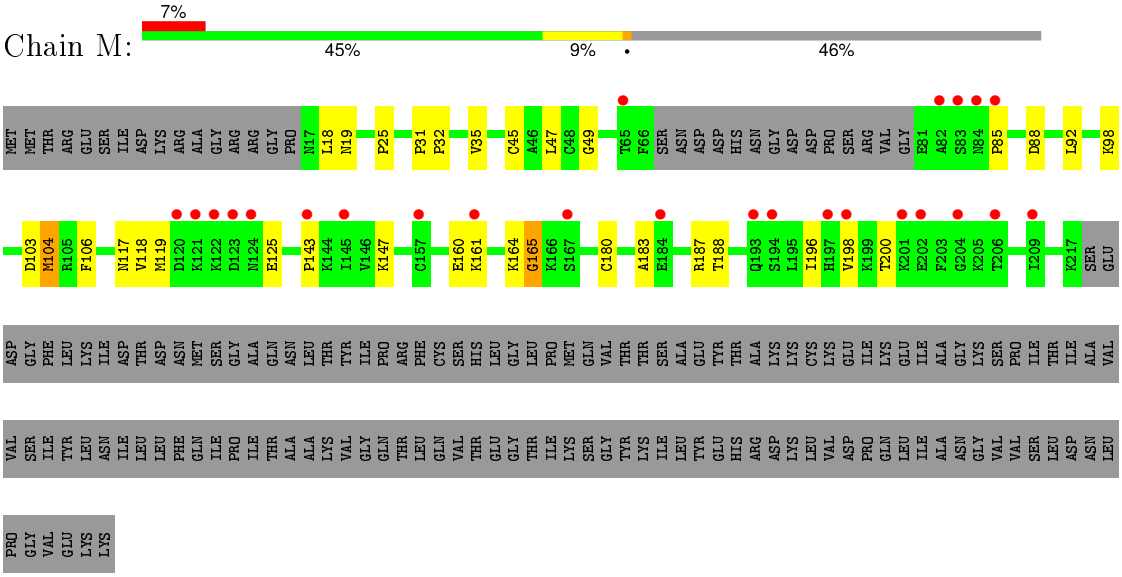
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



• Molecule 11: Transcription initiation factor IIB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	204.15Å 216.21Å 420.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 148.44 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-3.80) 95.5 (148.44-3.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.78Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.263 , 0.313 0.265 , 0.317	Depositor DCC
R_{free} test set	4320 reflections (4.94%)	DCC
Wilson B-factor (Å^2)	126.3	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 152.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 168084 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	29029	wwPDB-VP
Average B, all atoms (Å^2)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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

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	0.52	0/11248	0.67	0/15211
2	B	0.50	0/9016	0.65	0/12165
3	C	0.47	0/2133	0.64	0/2891
4	E	0.41	0/1788	0.56	0/2406
5	F	0.61	0/691	0.72	0/933
6	H	0.45	0/1086	0.61	0/1470
7	I	0.44	0/984	0.61	0/1323
8	J	0.50	0/541	0.66	0/727
9	K	0.55	0/937	0.68	0/1265
10	L	0.52	0/365	0.78	0/485
11	M	0.34	0/746	0.80	2/929 (0.2%)
All	All	0.50	0/29535	0.66	2/39805 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	165	GLY	N-CA-C	-5.23	100.03	113.10
11	M	161	LYS	N-CA-C	5.08	124.73	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	11052	0	11130	470	0
2	B	8845	0	8816	373	0
3	C	2095	0	2051	71	0
4	E	1752	0	1776	33	0
5	F	679	0	701	24	0
6	H	1068	0	1040	51	0
7	I	967	0	925	45	0
8	J	532	0	542	32	0
9	K	919	0	929	46	0
10	L	363	0	386	12	0
11	M	748	0	200	22	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
12	M	1	0	0	0	0
All	All	29029	0	28496	1060	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 18.

All (1060) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.23	1.10
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.29	1.07
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.83	1.06
1:A:441:PRO:HD2	1:A:498:ARG:NH2	1.69	1.05
1:A:855:THR:HG21	1:A:857:ARG:HE	0.94	1.05
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.70	1.04
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.40	1.02
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.41	1.02
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.00	1.00
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.94	0.97
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.47	0.97
1:A:567:LYS:HB3	6:H:96:VAL:H	1.27	0.96
1:A:855:THR:HG21	1:A:857:ARG:NE	1.78	0.96
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.31	0.96
2:B:437:GLU:HG2	2:B:438:GLU:H	1.31	0.95
2:B:174:LEU:O	2:B:175:ARG:HB2	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:THR:HG22	2:B:956:THR:H	1.30	0.93
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.00	0.90
2:B:334:ILE:HG22	2:B:336:ARG:O	1.72	0.90
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.02	0.89
7:I:75:CYS:SG	7:I:108:HIS:HB3	2.12	0.89
1:A:312:PRO:HG3	11:M:98:LYS:H	1.37	0.89
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.35	0.88
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.56	0.87
1:A:1329:THR:HG22	1:A:1331:SER:H	1.38	0.87
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.38	0.87
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.57	0.86
1:A:672:ASP:H	1:A:736:ASN:HD21	1.22	0.86
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.56	0.85
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.56	0.85
1:A:901:LEU:H	1:A:926:GLN:NE2	1.75	0.84
9:K:113:THR:O	9:K:114:LEU:HB2	1.77	0.84
2:B:801:LYS:O	8:J:52:THR:HG23	1.78	0.84
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.59	0.83
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.61	0.83
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.44	0.82
3:C:56:THR:HG21	3:C:145:CYS:SG	2.20	0.82
2:B:322:PHE:CZ	7:I:30:ARG:HG3	2.15	0.82
1:A:66:LYS:HE3	11:M:18:LEU:N	1.95	0.82
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.25	0.81
1:A:15:LYS:HB3	2:B:1220:ARG:HG2	1.63	0.81
2:B:1084:GLN:CD	2:B:1084:GLN:H	1.84	0.81
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.10	0.81
1:A:1370:LEU:O	1:A:1374:VAL:HG23	1.81	0.81
3:C:56:THR:HG22	3:C:57:VAL:H	1.46	0.81
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.28	0.81
1:A:913:LEU:HD12	1:A:914:GLU:H	1.46	0.80
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.61	0.80
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.16	0.80
1:A:65:LEU:CD1	11:M:19:ASN:O	2.31	0.79
3:C:124:LEU:O	3:C:127:ARG:HG2	1.83	0.79
1:A:830:LYS:HG3	1:A:1098:VAL:HG21	1.65	0.78
1:A:472:LEU:O	1:A:475:THR:HB	1.82	0.78
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.12	0.78
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.64	0.78
1:A:1021:LEU:O	1:A:1025:ARG:HG2	1.84	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:59:ILE:HG22	6:H:60:ALA:N	2.00	0.76
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.51	0.76
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.00	0.76
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.68	0.76
2:B:515:HIS:H	2:B:518:HIS:HD2	1.33	0.76
2:B:227:LYS:HB2	2:B:395:GLN:OE1	1.86	0.75
1:A:61:ILE:HG22	1:A:62:ASP:H	1.51	0.75
2:B:1106:ARG:HH21	2:B:1109:GLY:H	1.34	0.75
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.69	0.75
2:B:101:MET:HB2	2:B:169:ARG:HH12	1.51	0.75
2:B:843:GLN:HB2	2:B:993:THR:HB	1.68	0.74
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.69	0.74
7:I:75:CYS:SG	7:I:108:HIS:CD2	2.81	0.74
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.68	0.73
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.54	0.73
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.70	0.73
1:A:567:LYS:HB3	6:H:96:VAL:N	2.01	0.73
1:A:1153:TYR:HA	7:I:41:PRO:HB2	1.69	0.73
10:L:48:CYS:SG	10:L:49:LYS:N	2.61	0.73
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.71	0.73
2:B:335:GLY:HA2	2:B:348:ARG:HD2	1.70	0.73
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.18	0.72
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.71	0.72
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.70	0.72
1:A:524:VAL:HG12	1:A:525:GLN:H	1.54	0.72
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.70	0.72
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.25	0.72
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.71	0.72
2:B:25:ILE:HD12	2:B:651:LEU:HD12	1.70	0.71
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.26	0.71
1:A:672:ASP:H	1:A:736:ASN:ND2	1.87	0.71
9:K:60:ALA:O	9:K:73:LEU:HD12	1.91	0.71
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.72	0.71
1:A:265:LYS:HZ1	1:A:322:VAL:HB	1.56	0.71
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.56	0.71
1:A:413:ILE:HA	11:M:49:GLY:O	1.91	0.71
1:A:441:PRO:CD	1:A:498:ARG:NH2	2.51	0.70
7:I:75:CYS:SG	7:I:108:HIS:HD2	2.14	0.70
1:A:66:LYS:HE3	11:M:18:LEU:H	1.55	0.70
1:A:262:LEU:HG	1:A:323:LYS:CE	2.21	0.70
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:ILE:HG22	1:A:1437:GLY:N	2.06	0.70
2:B:912:ILE:O	2:B:938:SER:HB2	1.90	0.70
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.73	0.70
1:A:1397:LEU:O	1:A:1400:CYS:HB2	1.91	0.70
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.89	0.70
1:A:367:PRO:CG	1:A:370:ILE:HD12	2.21	0.70
2:B:1072:MET:HE2	2:B:1085:ILE:HB	1.73	0.70
1:A:1436:ILE:HG22	1:A:1437:GLY:H	1.57	0.70
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.57	0.70
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.74	0.70
1:A:49:LYS:HB3	1:A:55:ASP:HB2	1.72	0.70
2:B:437:GLU:CG	2:B:438:GLU:H	2.05	0.69
1:A:58:LEU:HD22	1:A:80:HIS:O	1.92	0.69
1:A:913:LEU:HD12	1:A:914:GLU:N	2.07	0.69
1:A:343:LYS:HE3	2:B:1151:LEU:O	1.93	0.69
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.74	0.69
2:B:842:ASN:ND2	2:B:845:SER:H	1.91	0.69
1:A:253:ASN:O	1:A:254:GLU:HB2	1.93	0.69
1:A:445:ASN:HB2	1:A:454:SER:O	1.93	0.69
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.56	0.69
2:B:559:SER:HA	2:B:563:MET:HB3	1.75	0.69
2:B:474:SER:HA	2:B:476:ARG:HG2	1.76	0.68
1:A:907:THR:HG22	1:A:908:LEU:N	2.09	0.68
1:A:230:ARG:HD2	1:A:233:TRP:CZ2	2.28	0.68
1:A:438:ASP:OD1	1:A:462:VAL:HG23	1.93	0.68
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.74	0.68
5:F:127:GLU:O	5:F:129:LYS:HG3	1.94	0.68
1:A:869:GLY:O	4:E:204:THR:HG21	1.95	0.67
2:B:465:ASN:HA	2:B:476:ARG:HA	1.77	0.67
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.77	0.67
3:C:66:ARG:NH2	8:J:3:VAL:O	2.28	0.67
2:B:744:HIS:HD2	2:B:746:SER:H	1.41	0.67
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	1.95	0.67
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.76	0.67
1:A:914:GLU:HB2	1:A:979:SER:O	1.95	0.67
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.43	0.66
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.76	0.66
6:H:106:GLU:C	6:H:108:SER:H	1.96	0.66
1:A:535:THR:HG21	1:A:617:VAL:H	1.60	0.66
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.78	0.66
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HB3	1:A:466:SER:HA	1.78	0.66
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.78	0.66
1:A:332:LYS:H	1:A:337:ARG:HB2	1.61	0.66
2:B:296:GLU:O	2:B:300:HIS:HD2	1.79	0.66
1:A:1444:MET:HE1	5:F:135:ARG:HE	1.59	0.65
2:B:955:THR:HG22	2:B:956:THR:N	2.09	0.65
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.78	0.65
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.79	0.65
9:K:65:HIS:HD2	9:K:67:PHE:H	1.40	0.65
10:L:55:ILE:HG13	10:L:56:LEU:H	1.61	0.65
2:B:569:TYR:CD1	2:B:589:VAL:HG21	2.31	0.65
3:C:93:ASP:O	3:C:127:ARG:NH2	2.29	0.65
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.31	0.65
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.78	0.65
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.31	0.65
1:A:1276:VAL:HB	1:A:1279:ILE:HD12	1.78	0.65
8:J:9:SER:HB2	8:J:45:CYS:HB2	1.78	0.65
2:B:1106:ARG:NH1	2:B:1118:PRO:HB3	2.12	0.65
1:A:1368:MET:O	1:A:1372:VAL:HG23	1.96	0.65
2:B:1107:ALA:O	2:B:1108:ARG:HG2	1.97	0.65
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.79	0.65
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.26	0.64
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.31	0.64
1:A:1132:LYS:O	1:A:1135:ARG:HB3	1.97	0.64
1:A:1428:VAL:HG13	2:B:1151:LEU:HD23	1.79	0.64
1:A:982:THR:HG22	1:A:984:LYS:H	1.62	0.64
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.32	0.64
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.27	0.64
1:A:578:LEU:O	1:A:578:LEU:HG	1.96	0.64
6:H:81:PRO:CB	6:H:82:PRO:HD3	2.16	0.64
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.79	0.64
1:A:1341:ILE:HG22	4:E:182:ASP:OD2	1.98	0.64
1:A:57:ARG:HB3	1:A:68:GLN:HG3	1.79	0.64
1:A:590:ARG:NH2	1:A:620:LYS:HB3	2.13	0.64
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.63	0.64
6:H:81:PRO:CB	6:H:82:PRO:CD	2.72	0.64
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.78	0.64
1:A:391:LEU:HD22	1:A:400:PRO:O	1.97	0.64
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.31	0.64
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.78	0.64
1:A:826:ASP:O	1:A:830:LYS:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.81	0.63
11:M:187:ARG:CA	11:M:188:THR:C	2.66	0.63
2:B:882:THR:O	2:B:883:LEU:HB2	1.97	0.63
1:A:512:VAL:HA	1:A:519:PRO:HA	1.79	0.63
1:A:382:PRO:HD2	5:F:104:ASN:OD1	1.99	0.63
7:I:29:CYS:SG	7:I:31:THR:HG22	2.38	0.63
1:A:75:ASN:O	1:A:76:GLU:HB3	1.98	0.63
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.81	0.63
2:B:1181:GLU:HG2	2:B:1188:LYS:HE2	1.81	0.63
1:A:265:LYS:NZ	1:A:322:VAL:HB	2.12	0.63
7:I:7:CYS:SG	7:I:8:ARG:O	2.56	0.63
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.99	0.62
7:I:7:CYS:HB2	7:I:14:LEU:HD21	1.80	0.62
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	1.80	0.62
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.79	0.62
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	1.96	0.62
1:A:381:THR:HG22	1:A:383:TYR:H	1.64	0.62
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.35	0.62
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.99	0.62
1:A:32:VAL:HG21	1:A:68:GLN:NE2	2.14	0.62
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.81	0.62
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.81	0.62
6:H:56:THR:HB	6:H:145:ARG:HG2	1.81	0.62
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.14	0.62
2:B:945:GLU:O	2:B:946:ASN:HB3	1.99	0.62
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.81	0.62
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.80	0.62
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.35	0.61
2:B:406:LEU:HD12	2:B:545:ILE:HD11	1.81	0.61
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.80	0.61
2:B:705:MET:H	2:B:710:LEU:HD12	1.64	0.61
1:A:323:LYS:HZ2	1:A:324:SER:H	1.47	0.61
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.65	0.61
6:H:32:THR:HG22	6:H:33:GLN:HG3	1.82	0.61
3:C:166:GLU:HG3	9:K:10:PHE:CZ	2.35	0.61
1:A:298:PHE:O	1:A:302:THR:HB	1.99	0.61
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.83	0.61
1:A:253:ASN:H	1:A:253:ASN:HD22	1.46	0.61
1:A:251:SER:HB3	1:A:258:GLY:HA3	1.83	0.61
1:A:711:ARG:NH1	7:I:95:THR:HB	2.15	0.61
1:A:1153:TYR:HA	7:I:41:PRO:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.64	0.61
8:J:1:MET:H2	8:J:56:LEU:H	1.48	0.61
2:B:515:HIS:H	2:B:518:HIS:CD2	2.18	0.60
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.01	0.60
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.83	0.60
1:A:1444:MET:HE1	5:F:135:ARG:NE	2.16	0.60
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.32	0.60
1:A:214:ILE:HG22	1:A:218:ASP:HB2	1.82	0.60
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.84	0.60
1:A:323:LYS:HZ2	1:A:324:SER:N	1.98	0.60
3:C:46:ILE:HD12	3:C:67:LEU:O	2.01	0.60
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.67	0.60
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.83	0.60
2:B:726:ALA:HB1	2:B:1051:THR:CG2	2.24	0.60
7:I:75:CYS:HB2	7:I:103:CYS:SG	2.38	0.60
1:A:65:LEU:HG	11:M:19:ASN:O	2.01	0.60
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.37	0.60
1:A:855:THR:CG2	1:A:857:ARG:HE	1.89	0.60
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.66	0.60
1:A:516:SER:O	1:A:518:LYS:N	2.35	0.60
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.83	0.60
11:M:103:ASP:O	11:M:106:PHE:N	2.35	0.60
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.67	0.60
1:A:534:LEU:O	1:A:574:GLY:HA3	2.02	0.59
2:B:542:MET:CE	2:B:747:MET:HG3	2.32	0.59
6:H:82:PRO:O	6:H:84:ALA:N	2.32	0.59
1:A:376:TYR:OH	1:A:498:ARG:HD2	2.03	0.59
2:B:957:ASN:O	2:B:959:ASP:N	2.35	0.59
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.66	0.59
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.11	0.59
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.37	0.59
3:C:167:HIS:CD2	3:C:169:LYS:H	2.16	0.59
2:B:516:ASN:HD22	2:B:516:ASN:H	1.51	0.59
5:F:82:THR:HG22	5:F:84:TYR:H	1.68	0.59
1:A:1436:ILE:CG2	2:B:1142:GLY:HA2	2.33	0.59
1:A:1151:GLU:HG2	7:I:42:LEU:HD13	1.85	0.59
1:A:709:THR:CG2	7:I:94:ASP:HA	2.32	0.59
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.59
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.37	0.59
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.84	0.59
6:H:100:THR:HG23	6:H:138:GLU:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:VAL:O	2:B:480:SER:HA	2.03	0.59
1:A:1329:THR:HG22	1:A:1331:SER:N	2.16	0.58
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.17	0.58
9:K:47:ARG:HD3	9:K:59:ALA:O	2.03	0.58
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.84	0.58
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.18	0.58
1:A:262:LEU:HG	1:A:323:LYS:NZ	2.17	0.58
3:C:248:ILE:HD11	9:K:101:LEU:HD22	1.83	0.58
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.85	0.58
2:B:446:LEU:O	2:B:448:ILE:HG12	2.03	0.58
4:E:176:PRO:O	4:E:212:ARG:HA	2.02	0.58
2:B:342:GLY:O	2:B:343:ILE:CB	2.51	0.58
1:A:48:ALA:O	1:A:49:LYS:HG3	2.03	0.58
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.85	0.58
1:A:451:HIS:HB3	1:A:453:MET:H	1.68	0.58
2:B:614:SER:H	2:B:632:ARG:HH12	1.52	0.58
1:A:1372:VAL:O	1:A:1376:THR:HB	2.03	0.58
1:A:1398:MET:HG2	1:A:1425:SER:OG	2.03	0.58
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.85	0.58
2:B:363:HIS:O	2:B:364:ILE:HB	2.04	0.58
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.33	0.58
11:M:180:CYS:O	11:M:183:ALA:O	2.21	0.58
1:A:1031:VAL:HG13	1:A:1037:LEU:HD12	1.85	0.58
2:B:842:ASN:HD22	2:B:845:SER:H	1.51	0.58
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.38	0.58
1:A:262:LEU:HD22	1:A:303:TYR:CE1	2.39	0.58
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.86	0.58
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.86	0.58
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.36	0.58
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.85	0.58
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.39	0.57
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.85	0.57
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.68	0.57
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.85	0.57
2:B:426:LYS:HZ1	2:B:430:ARG:HH22	1.52	0.57
1:A:629:LEU:O	1:A:633:VAL:HG23	2.04	0.57
4:E:147:HIS:CD2	4:E:149:LEU:H	2.22	0.57
1:A:1223:ASP:HA	1:A:1243:VAL:HG12	1.86	0.57
1:A:11:LEU:O	1:A:12:ARG:HG2	2.03	0.57
1:A:369:SER:CB	9:K:2:ASN:HD21	2.18	0.57
1:A:1384:VAL:HG12	1:A:1384:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG23	7:I:94:ASP:HA	1.86	0.57
2:B:549:THR:HB	2:B:628:THR:CG2	2.34	0.57
7:I:75:CYS:SG	7:I:108:HIS:CB	2.91	0.57
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.70	0.57
2:B:506:GLY:O	2:B:507:LYS:CB	2.52	0.57
3:C:56:THR:HG23	3:C:147:LEU:HD23	1.85	0.57
11:M:45:CYS:O	11:M:49:GLY:HA2	2.05	0.57
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.86	0.57
6:H:62:SER:OG	6:H:63:LEU:N	2.37	0.57
1:A:441:PRO:HD2	1:A:498:ARG:HH21	1.61	0.57
1:A:605:MET:HE3	1:A:614:PHE:O	2.04	0.57
1:A:367:PRO:CB	1:A:466:SER:HA	2.34	0.56
2:B:46:GLN:NE2	2:B:496:ARG:HA	2.20	0.56
1:A:332:LYS:H	1:A:337:ARG:CB	2.16	0.56
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.35	0.56
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.35	0.56
2:B:345:LYS:HA	2:B:348:ARG:HE	1.70	0.56
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.87	0.56
6:H:24:CYS:HB2	6:H:44:VAL:HG21	1.87	0.56
1:A:95:PHE:HE2	1:A:1414:ALA:HB2	1.69	0.56
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.87	0.56
1:A:907:THR:CG2	1:A:908:LEU:N	2.68	0.56
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.88	0.56
2:B:1084:GLN:N	2:B:1084:GLN:CD	2.56	0.56
1:A:535:THR:HG21	1:A:616:VAL:HA	1.87	0.56
1:A:73:GLY:O	1:A:75:ASN:N	2.37	0.56
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.20	0.56
2:B:745:PRO:O	2:B:748:ILE:HG12	2.06	0.56
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.33	0.56
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.68	0.56
6:H:59:ILE:HG22	6:H:60:ALA:H	1.71	0.56
2:B:792:MET:HA	2:B:856:PHE:O	2.06	0.56
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.70	0.56
1:A:351:THR:CG2	2:B:1103:ILE:HG23	2.35	0.56
1:A:351:THR:HG21	1:A:466:SER:O	2.06	0.56
1:A:210:ILE:O	1:A:214:ILE:HG13	2.06	0.56
2:B:256:VAL:HG11	2:B:382:ILE:HG12	1.87	0.56
1:A:65:LEU:CG	11:M:19:ASN:O	2.54	0.55
1:A:648:ASN:O	1:A:652:VAL:HG23	2.06	0.55
7:I:74:GLU:HB3	7:I:79:HIS:HA	1.88	0.55
2:B:642:ASP:HB3	2:B:649:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:O	1:A:254:GLU:CB	2.55	0.55
2:B:899:ILE:HG13	2:B:911:ILE:O	2.06	0.55
1:A:738:LYS:HG3	1:A:740:LEU:HG	1.88	0.55
1:A:528:LEU:O	1:A:531:ILE:HG22	2.06	0.55
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.07	0.55
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.89	0.55
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.46	0.55
2:B:1135:ARG:HG3	2:B:1147:LEU:HD21	1.87	0.55
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.37	0.55
2:B:437:GLU:HG2	2:B:438:GLU:N	2.13	0.55
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.06	0.55
1:A:312:PRO:HG3	11:M:98:LYS:N	2.15	0.55
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.22	0.55
1:A:1391:ARG:O	1:A:1393:ASN:N	2.40	0.55
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.54	0.54
1:A:65:LEU:HD11	11:M:19:ASN:O	2.07	0.54
1:A:1376:THR:HG23	4:E:212:ARG:NH2	2.21	0.54
2:B:475:SER:C	2:B:477:ALA:H	2.09	0.54
2:B:470:LYS:O	2:B:471:LYS:HG3	2.07	0.54
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.71	0.54
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.52	0.54
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.89	0.54
11:M:143:PRO:O	11:M:147:LYS:CA	2.56	0.54
10:L:51:CYS:SG	10:L:51:CYS:O	2.66	0.54
9:K:65:HIS:CD2	9:K:67:PHE:H	2.23	0.54
6:H:80:ARG:HG2	9:K:57:LEU:HD22	1.89	0.54
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.42	0.54
1:A:1039:LYS:O	1:A:1043:ASP:HB2	2.07	0.54
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.88	0.54
6:H:106:GLU:C	6:H:108:SER:N	2.61	0.54
1:A:31:SER:CB	1:A:83:HIS:HB2	2.38	0.54
1:A:1392:SER:O	1:A:1393:ASN:HB2	2.07	0.54
1:A:1235:LYS:HB3	1:A:1237:ILE:HD11	1.89	0.54
2:B:801:LYS:O	8:J:52:THR:CG2	2.52	0.54
6:H:24:CYS:HB2	6:H:44:VAL:CG2	2.38	0.54
1:A:549:MET:SD	1:A:577:ILE:HD12	2.48	0.54
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.89	0.54
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.90	0.54
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.88	0.54
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.91	0.54
2:B:496:ARG:HH11	2:B:539:LEU:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:31:THR:O	6:H:32:THR:CB	2.55	0.54
7:I:78:CYS:SG	7:I:106:CYS:HB3	2.48	0.54
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.73	0.54
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.70	0.54
1:A:442:VAL:O	1:A:457:ALA:HA	2.08	0.54
1:A:1308:THR:CG2	1:A:1310:GLY:H	2.21	0.53
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.48	0.53
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.90	0.53
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.71	0.53
4:E:135:PHE:HD2	4:E:140:LEU:HD21	1.73	0.53
3:C:180:TYR:HB3	3:C:228:PHE:CD2	2.43	0.53
3:C:62:PHE:O	3:C:66:ARG:HG3	2.08	0.53
1:A:336:ILE:HD12	1:A:1405:THR:CG2	2.38	0.53
1:A:1436:ILE:CG2	1:A:1437:GLY:H	2.21	0.53
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.73	0.53
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.33	0.53
8:J:1:MET:H1	8:J:56:LEU:HB2	1.73	0.53
9:K:7:PHE:O	9:K:11:LEU:HB2	2.08	0.53
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.91	0.53
8:J:8:PHE:H	8:J:49:MET:CE	2.20	0.53
6:H:31:THR:O	6:H:32:THR:HB	2.07	0.53
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.89	0.53
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.91	0.53
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.91	0.53
5:F:90:ARG:HD3	5:F:155:LEU:HD12	1.90	0.53
2:B:1084:GLN:NE2	2:B:1084:GLN:H	2.07	0.53
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.37	0.53
2:B:291:ILE:HD12	2:B:375:ALA:HB1	1.89	0.53
2:B:34:ILE:O	2:B:37:PHE:HB3	2.09	0.53
2:B:597:MET:SD	2:B:617:ARG:HB2	2.49	0.53
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.37	0.53
2:B:467:GLY:HA3	2:B:473:MET:HE3	1.91	0.53
6:H:125:LEU:HG	6:H:130:ARG:NH1	2.24	0.52
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.92	0.52
2:B:975:GLN:HG2	2:B:976:ILE:H	1.74	0.52
2:B:98:THR:O	2:B:126:SER:HB2	2.09	0.52
3:C:55:THR:HB	3:C:152:GLU:H	1.75	0.52
1:A:741:ASN:HD22	1:A:744:LYS:H	1.56	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.52
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.90	0.52
1:A:369:SER:HB3	9:K:2:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ILE:HD11	6:H:98:TYR:HB2	1.92	0.52
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.91	0.52
1:A:1114:PRO:HB2	1:A:1311:VAL:CG2	2.40	0.52
1:A:1161:THR:HG23	1:A:1239:ARG:HH21	1.74	0.52
1:A:1190:PRO:HG3	7:I:18:GLU:OE2	2.10	0.52
1:A:1291:VAL:CG1	1:A:1292:PRO:HD2	2.40	0.52
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.75	0.52
1:A:1434:ALA:O	1:A:1436:ILE:N	2.39	0.52
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.91	0.52
6:H:12:VAL:O	6:H:52:GLN:HA	2.10	0.52
3:C:99:LEU:CD2	3:C:120:ILE:HG12	2.40	0.52
2:B:839:MET:HE1	2:B:1010:LEU:HD11	1.91	0.52
1:A:33:ALA:O	1:A:83:HIS:HB3	2.10	0.52
1:A:709:THR:HG21	7:I:93:LYS:O	2.09	0.52
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.74	0.52
6:H:58:THR:HB	6:H:143:LEU:HB2	1.90	0.52
1:A:340:LEU:HD21	2:B:1200:ALA:HB2	1.92	0.52
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.92	0.52
1:A:783:THR:O	1:A:784:LEU:HD23	2.10	0.52
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.92	0.52
2:B:1154:ALA:O	2:B:1155:SER:CB	2.58	0.52
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.52
2:B:487:THR:HG22	2:B:489:SER:H	1.75	0.52
3:C:174:ALA:O	8:J:10:CYS:O	2.28	0.52
1:A:535:THR:CG2	1:A:616:VAL:HA	2.40	0.51
11:M:103:ASP:O	11:M:104:MET:C	2.48	0.51
2:B:128:LEU:HB3	2:B:167:ILE:O	2.09	0.51
5:F:93:ILE:HD13	5:F:148:VAL:CG2	2.40	0.51
2:B:173:MET:O	2:B:175:ARG:N	2.44	0.51
2:B:542:MET:HE1	2:B:743:ILE:CB	2.40	0.51
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.57	0.51
2:B:955:THR:HG23	10:L:54:ARG:O	2.10	0.51
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.93	0.51
1:A:262:LEU:HG	1:A:323:LYS:HZ3	1.74	0.51
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.45	0.51
1:A:494:SER:O	1:A:498:ARG:HG3	2.09	0.51
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.93	0.51
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.92	0.51
1:A:690:VAL:HG11	1:A:794:PRO:HD3	1.91	0.51
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.46	0.51
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:GLU:N	2:B:712:PRO:CD	2.74	0.51
4:E:145:THR:HG21	4:E:187:TYR:CE2	2.45	0.51
1:A:1343:ALA:HB2	4:E:150:VAL:HG22	1.92	0.51
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.11	0.51
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
2:B:542:MET:HE1	2:B:743:ILE:HB	1.92	0.51
1:A:499:ALA:O	1:A:503:GLN:HB2	2.11	0.51
7:I:73:ARG:O	7:I:81:ARG:HA	2.10	0.51
5:F:138:LEU:HB3	5:F:139:PRO:HD2	1.93	0.51
2:B:336:ARG:O	2:B:337:ARG:CB	2.59	0.51
1:A:575:LYS:HB3	1:A:612:ILE:HG21	1.93	0.51
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.93	0.51
8:J:7:CYS:SG	8:J:49:MET:HE3	2.51	0.51
3:C:180:TYR:HB3	3:C:228:PHE:HD2	1.76	0.51
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.41	0.51
1:A:283:GLY:O	1:A:285:PRO:HD3	2.11	0.51
2:B:955:THR:CG2	2:B:956:THR:H	2.12	0.51
1:A:262:LEU:HD22	1:A:303:TYR:HE1	1.76	0.51
2:B:640:VAL:O	2:B:640:VAL:HG12	2.11	0.51
8:J:12:LYS:O	8:J:14:VAL:HG23	2.11	0.51
1:A:670:ILE:O	1:A:737:LEU:HD21	2.10	0.50
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.93	0.50
2:B:426:LYS:NZ	2:B:430:ARG:HH22	2.10	0.50
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.73	0.50
1:A:451:HIS:HB3	1:A:453:MET:N	2.27	0.50
1:A:348:SER:HA	1:A:489:LEU:O	2.11	0.50
2:B:244:LEU:O	2:B:249:ARG:HG2	2.12	0.50
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.92	0.50
6:H:59:ILE:CG2	6:H:60:ALA:N	2.71	0.50
2:B:274:PRO:HB2	2:B:275:TYR:HD1	1.76	0.50
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	1.94	0.50
1:A:605:MET:CE	1:A:614:PHE:O	2.59	0.50
6:H:91:ASP:C	6:H:93:TYR:H	2.13	0.50
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.93	0.50
2:B:43:LEU:HD11	2:B:811:TYR:O	2.11	0.50
1:A:388:LEU:O	1:A:392:VAL:HG23	2.10	0.50
1:A:546:VAL:HG13	1:A:577:ILE:HG21	1.92	0.50
3:C:142:VAL:H	8:J:16:ASP:HB3	1.77	0.50
1:A:787:PHE:HE1	1:A:815:PHE:HZ	1.58	0.50
2:B:1220:ARG:O	2:B:1222:ARG:N	2.44	0.50
2:B:781:PHE:CE2	2:B:795:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.47	0.50
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.41	0.50
3:C:56:THR:HG22	3:C:57:VAL:N	2.21	0.50
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.12	0.50
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.41	0.50
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.93	0.50
2:B:130:VAL:HG12	2:B:131:ASP:N	2.27	0.50
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.41	0.50
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.77	0.50
8:J:8:PHE:H	8:J:49:MET:HE1	1.77	0.50
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.93	0.50
1:A:1170:ILE:HD11	1:A:1239:ARG:NH1	2.27	0.50
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.46	0.50
1:A:736:ASN:O	1:A:737:LEU:HB2	2.12	0.50
1:A:709:THR:HG22	1:A:711:ARG:H	1.76	0.50
2:B:640:VAL:O	2:B:641:GLU:C	2.50	0.50
1:A:868:TYR:HD2	1:A:1058:VAL:CG2	2.16	0.49
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.46	0.49
2:B:243:ALA:HA	2:B:250:PHE:O	2.12	0.49
1:A:973:ILE:HG21	1:A:1036:ARG:O	2.11	0.49
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.94	0.49
6:H:5:LEU:O	6:H:133:ASN:HB3	2.12	0.49
2:B:205:ILE:CD1	2:B:461:LEU:HD23	2.39	0.49
1:A:317:LYS:O	1:A:318:SER:O	2.30	0.49
5:F:81:THR:HG22	5:F:82:THR:N	2.27	0.49
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.46	0.49
2:B:705:MET:N	2:B:710:LEU:HD12	2.27	0.49
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.77	0.49
3:C:248:ILE:HG21	9:K:102:LYS:HB2	1.92	0.49
1:A:1281:ARG:O	1:A:1282:VAL:HG23	2.13	0.49
1:A:108:MET:O	1:A:109:HIS:HB2	2.13	0.49
2:B:380:TYR:O	2:B:384:ARG:HG2	2.12	0.49
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.93	0.49
1:A:711:ARG:HH11	7:I:95:THR:HB	1.76	0.49
2:B:1194:ILE:HD12	2:B:1196:ILE:HG23	1.93	0.49
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.95	0.49
1:A:359:LEU:HD22	1:A:363:GLN:HB2	1.94	0.49
1:A:376:TYR:CZ	1:A:498:ARG:HD2	2.47	0.49
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.43	0.49
2:B:237:VAL:HG22	2:B:257:LYS:HG2	1.94	0.49
2:B:836:GLU:O	2:B:837:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.27	0.49
2:B:839:MET:O	2:B:990:ILE:HA	2.12	0.49
2:B:1166:CYS:HB2	2:B:1215:ARG:HH11	1.77	0.49
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.93	0.49
1:A:1105:LEU:HA	1:A:1375:MET:HE3	1.94	0.49
1:A:858:ASN:HD22	1:A:858:ASN:C	2.16	0.49
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.13	0.49
6:H:89:LEU:C	6:H:91:ASP:H	2.15	0.49
2:B:600:LEU:HB3	2:B:615:MET:SD	2.53	0.49
1:A:351:THR:HG23	2:B:1103:ILE:HG23	1.93	0.49
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.44	0.49
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.12	0.49
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.12	0.49
1:A:825:ILE:HD11	2:B:512:ARG:O	2.12	0.49
2:B:981:ALA:HB2	2:B:1095:LEU:HD11	1.94	0.49
2:B:899:ILE:HD12	2:B:911:ILE:HG23	1.93	0.49
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.48	0.49
5:F:101:ILE:HD11	5:F:124:GLU:OE1	2.13	0.49
1:A:849:MET:HB3	1:A:1063:MET:SD	2.53	0.49
2:B:240:ILE:HG23	2:B:240:ILE:O	2.13	0.49
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.11	0.48
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.93	0.48
5:F:86:THR:HG23	5:F:89:GLU:CD	2.32	0.48
1:A:590:ARG:HB3	1:A:605:MET:N	2.28	0.48
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.78	0.48
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.27	0.48
2:B:642:ASP:O	2:B:644:GLU:N	2.46	0.48
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.13	0.48
7:I:113:ASP:OD2	7:I:116:ASN:HB2	2.13	0.48
2:B:248:SER:H	2:B:418:LYS:NZ	2.12	0.48
4:E:90:VAL:HA	4:E:120:ALA:HB2	1.93	0.48
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.66	0.48
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.47	0.48
1:A:1317:MET:HG2	1:A:1327:ILE:HG21	1.94	0.48
1:A:1261:LYS:HE2	7:I:43:VAL:HG11	1.95	0.48
1:A:1266:THR:HA	1:A:1270:ASN:HD22	1.79	0.48
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.48
2:B:1017:ILE:HD13	2:B:1026:LEU:HD21	1.95	0.48
1:A:855:THR:HG23	1:A:857:ARG:CG	2.39	0.48
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.96	0.48
1:A:839:ARG:NH1	2:B:1132:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:93:ILE:HD13	5:F:148:VAL:HG21	1.95	0.48
1:A:114:LEU:HD12	1:A:142:CYS:O	2.12	0.48
2:B:806:THR:HG22	2:B:808:ALA:H	1.76	0.48
1:A:901:LEU:H	1:A:926:GLN:HE21	1.55	0.48
2:B:516:ASN:ND2	2:B:516:ASN:H	2.12	0.48
1:A:84:ILE:HG22	1:A:239:LEU:O	2.14	0.48
9:K:47:ARG:HB3	9:K:47:ARG:NH1	2.29	0.48
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.96	0.48
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.78	0.48
1:A:105:CYS:SG	1:A:138:ILE:HG22	2.53	0.48
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.44	0.48
2:B:879:ARG:HD2	2:B:883:LEU:HD23	1.94	0.48
1:A:866:PHE:C	1:A:867:ILE:HG13	2.34	0.48
1:A:257:ARG:NH2	11:M:88:ASP:O	2.46	0.48
3:C:255:VAL:HG21	9:K:94:ILE:HG21	1.96	0.48
1:A:997:LEU:HB3	1:A:1053:PHE:CE2	2.49	0.48
2:B:696:GLU:O	2:B:699:GLU:HB2	2.13	0.48
1:A:42:ASP:OD1	1:A:45:GLN:O	2.32	0.48
2:B:48:LEU:HD21	2:B:175:ARG:HB3	1.96	0.47
2:B:95:ILE:HG13	2:B:129:PHE:O	2.14	0.47
2:B:303:TYR:HH	2:B:586:TRP:HZ3	1.60	0.47
2:B:806:THR:HB	2:B:809:MET:HG3	1.96	0.47
1:A:116:ASP:HB2	1:A:118:HIS:CD2	2.49	0.47
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.14	0.47
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.29	0.47
1:A:76:GLU:O	1:A:76:GLU:CG	2.62	0.47
2:B:705:MET:H	2:B:710:LEU:CD1	2.28	0.47
2:B:470:LYS:C	2:B:472:ALA:H	2.17	0.47
1:A:315:LEU:O	1:A:317:LYS:O	2.32	0.47
2:B:315:LYS:HE3	7:I:4:PHE:CD2	2.48	0.47
1:A:70:CYS:O	1:A:72:GLU:HG2	2.14	0.47
1:A:872:GLY:C	1:A:1058:VAL:HG23	2.35	0.47
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.96	0.47
2:B:405:ARG:NH1	2:B:632:ARG:HG2	2.30	0.47
1:A:724:GLU:O	1:A:728:LYS:HG2	2.15	0.47
11:M:143:PRO:O	11:M:147:LYS:N	2.47	0.47
1:A:1390:ASN:ND2	1:A:1399:ARG:HA	2.30	0.47
2:B:821:GLN:HE22	2:B:851:PHE:H	1.62	0.47
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	2.13	0.47
2:B:276:ILE:HG23	2:B:337:ARG:CB	2.44	0.47
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.15	0.47
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.63	0.47
4:E:205:SER:O	4:E:206:GLY:C	2.52	0.47
2:B:54:PHE:O	2:B:59:LEU:HB2	2.14	0.47
7:I:53:GLY:O	7:I:89:GLN:HB2	2.14	0.47
1:A:1288:ASP:OD1	1:A:1300:LYS:NZ	2.47	0.47
3:C:37:MET:HA	3:C:41:ILE:HD11	1.96	0.47
3:C:241:ASP:O	3:C:245:VAL:HG23	2.15	0.47
2:B:773:MET:SD	2:B:987:LYS:HD2	2.55	0.47
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.96	0.47
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.79	0.47
1:A:1207:LEU:HD13	1:A:1273:LEU:HD23	1.96	0.47
1:A:984:LYS:O	1:A:988:LEU:HB2	2.15	0.47
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.97	0.47
1:A:1130:GLN:HE21	1:A:1134:ILE:HD11	1.80	0.47
1:A:49:LYS:HB3	1:A:55:ASP:CB	2.44	0.47
1:A:207:ILE:HA	1:A:210:ILE:HD12	1.96	0.47
11:M:164:LYS:O	11:M:165:GLY:C	2.52	0.47
1:A:663:SER:OG	1:A:664:THR:N	2.48	0.47
3:C:31:ASN:O	3:C:35:ARG:HG3	2.14	0.47
6:H:4:THR:HA	6:H:60:ALA:HB2	1.96	0.46
1:A:367:PRO:HB3	1:A:465:TYR:O	2.15	0.46
3:C:46:ILE:HA	3:C:159:ALA:HA	1.95	0.46
1:A:302:THR:HA	1:A:305:ASP:O	2.15	0.46
2:B:363:HIS:O	2:B:364:ILE:CB	2.63	0.46
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.50	0.46
5:F:111:LEU:C	5:F:113:GLY:H	2.18	0.46
3:C:8:VAL:HA	3:C:21:ILE:O	2.15	0.46
1:A:367:PRO:HG2	1:A:370:ILE:CD1	2.41	0.46
11:M:45:CYS:C	11:M:47:LEU:H	2.16	0.46
1:A:257:ARG:NH1	11:M:85:PRO:O	2.48	0.46
1:A:14:VAL:HB	1:A:1430:LEU:HD13	1.97	0.46
1:A:456:MET:HB2	1:A:478:TYR:OH	2.15	0.46
1:A:514:PRO:O	1:A:875:ALA:HB1	2.15	0.46
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.15	0.46
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.15	0.46
1:A:324:SER:O	1:A:326:ARG:N	2.45	0.46
7:I:29:CYS:HB3	7:I:34:TYR:HB3	1.98	0.46
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.98	0.46
1:A:763:ALA:O	1:A:803:SER:HB3	2.14	0.46
9:K:20:LYS:HB2	9:K:20:LYS:HE3	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HD12	2:B:651:LEU:CD1	2.43	0.46
4:E:61:GLN:HE21	4:E:105:PHE:HE2	1.64	0.46
2:B:693:ILE:HG23	2:B:697:GLU:HB3	1.97	0.46
3:C:55:THR:O	3:C:55:THR:HG22	2.16	0.46
1:A:507:VAL:O	1:A:508:PRO:C	2.52	0.46
7:I:86:PHE:HD1	7:I:87:GLN:O	1.99	0.46
1:A:800:VAL:HA	1:A:812:GLU:OE2	2.16	0.46
1:A:638:GLY:O	1:A:639:PRO:C	2.54	0.46
5:F:118:LEU:O	5:F:122:MET:HG3	2.15	0.46
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.97	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.46
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.76	0.46
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.51	0.46
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.56	0.46
2:B:34:ILE:HG12	2:B:542:MET:HE2	1.98	0.46
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.16	0.46
3:C:44:LEU:HD23	3:C:130:GLY:HA2	1.98	0.46
2:B:614:SER:N	2:B:632:ARG:HH12	2.14	0.46
3:C:251:LEU:O	3:C:255:VAL:HG23	2.16	0.46
7:I:75:CYS:SG	7:I:103:CYS:HB2	2.55	0.46
7:I:8:ARG:HG3	7:I:9:ASP:CG	2.36	0.46
1:A:451:HIS:O	2:B:1137:CYS:SG	2.68	0.46
5:F:109:VAL:CG1	5:F:110:ASP:N	2.79	0.46
2:B:365:THR:HG23	2:B:367:LEU:H	1.81	0.46
2:B:357:GLN:O	2:B:374:LYS:NZ	2.49	0.46
1:A:32:VAL:HG21	1:A:68:GLN:HE22	1.79	0.46
1:A:243:PRO:HB2	1:A:245:PRO:CD	2.44	0.46
2:B:468:GLU:O	2:B:470:LYS:N	2.49	0.46
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.16	0.46
1:A:1385:THR:HG22	1:A:1386:ARG:HG2	1.98	0.45
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.82	0.45
2:B:880:THR:HA	2:B:881:ASN:HA	1.74	0.45
2:B:1190:ASP:O	2:B:1191:ILE:HG13	2.16	0.45
1:A:329:LEU:HD23	1:A:335:ARG:HG3	1.98	0.45
1:A:1120:LEU:HD23	1:A:1124:HIS:O	2.16	0.45
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.98	0.45
3:C:53:THR:O	3:C:153:LEU:HA	2.16	0.45
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.52	0.45
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.98	0.45
2:B:345:LYS:O	2:B:347:LYS:N	2.49	0.45
1:A:1436:ILE:HB	2:B:1144:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:HE2	2:B:747:MET:HG3	1.99	0.45
1:A:1291:VAL:HG12	1:A:1292:PRO:HD2	1.96	0.45
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.16	0.45
2:B:325:GLN:HE22	7:I:12:ASN:ND2	2.14	0.45
10:L:53:HIS:C	10:L:55:ILE:H	2.20	0.45
2:B:437:GLU:CG	2:B:438:GLU:N	2.77	0.45
2:B:938:SER:O	2:B:940:PRO:HD3	2.17	0.45
2:B:463:THR:HB	2:B:464:GLY:H	1.55	0.45
1:A:676:MET:HA	1:A:679:ILE:HD12	1.98	0.45
2:B:743:ILE:H	2:B:743:ILE:HG12	1.64	0.45
2:B:542:MET:HE3	2:B:747:MET:HG3	1.98	0.45
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.52	0.45
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.56	0.45
1:A:584:ASN:O	1:A:637:LYS:HE3	2.16	0.45
1:A:850:VAL:HG23	1:A:1064:VAL:CG2	2.45	0.45
2:B:1106:ARG:NH2	2:B:1109:GLY:H	2.07	0.45
3:C:177:GLU:O	3:C:230:MET:HA	2.16	0.45
1:A:185:TRP:O	1:A:197:PRO:HB3	2.16	0.45
2:B:955:THR:HA	10:L:54:ARG:O	2.17	0.45
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.16	0.45
1:A:1035:TYR:O	1:A:1037:LEU:N	2.50	0.45
2:B:842:ASN:ND2	2:B:845:SER:N	2.62	0.45
1:A:475:THR:HG22	1:A:476:SER:N	2.32	0.45
1:A:1399:ARG:HB2	1:A:1408:ILE:HG21	1.99	0.45
1:A:399:HIS:C	1:A:401:GLY:H	2.20	0.45
2:B:755:ILE:HG22	2:B:755:ILE:O	2.17	0.45
3:C:165:LYS:O	9:K:6:ARG:NH1	2.49	0.45
2:B:570:VAL:HG12	2:B:572:HIS:CE1	2.52	0.45
1:A:74:MET:O	1:A:75:ASN:HB2	2.17	0.45
1:A:97:ALA:HA	1:A:100:LYS:HE3	1.98	0.45
2:B:21:GLU:HB2	2:B:656:GLY:HA3	1.99	0.45
9:K:12:LEU:HD12	9:K:12:LEU:H	1.82	0.45
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.99	0.45
6:H:106:GLU:O	6:H:108:SER:N	2.50	0.45
1:A:535:THR:HG21	1:A:617:VAL:N	2.30	0.45
1:A:335:ARG:O	1:A:339:ASN:N	2.49	0.45
1:A:1406:VAL:HG12	1:A:1410:PHE:HE1	1.80	0.44
3:C:84:ARG:NE	9:K:11:LEU:HD21	2.32	0.44
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.98	0.44
1:A:440:ASP:O	1:A:460:VAL:HG23	2.17	0.44
2:B:1170:THR:HG22	2:B:1183:LYS:HZ2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LYS:HE3	3:C:193:TYR:O	2.17	0.44
1:A:384:ASN:O	1:A:385:ILE:C	2.54	0.44
1:A:320:ARG:HA	1:A:321:PRO:C	2.38	0.44
1:A:642:CYS:O	1:A:645:LEU:HB3	2.16	0.44
3:C:260:LEU:O	3:C:264:GLN:HG3	2.17	0.44
1:A:661:GLY:HA3	2:B:1081:LEU:HD22	2.00	0.44
1:A:17:VAL:HA	2:B:1215:ARG:O	2.18	0.44
2:B:1163:CYS:HB3	2:B:1166:CYS:O	2.16	0.44
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.52	0.44
8:J:1:MET:N	8:J:56:LEU:HB2	2.31	0.44
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.00	0.44
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.98	0.44
1:A:1170:ILE:HD11	1:A:1239:ARG:CZ	2.47	0.44
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	1.99	0.44
4:E:75:MET:CE	4:E:155:ARG:HH22	2.31	0.44
1:A:841:LEU:O	1:A:845:LEU:HG	2.17	0.44
1:A:352:VAL:HB	2:B:1099:VAL:CG2	2.47	0.44
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.83	0.44
2:B:661:LEU:HD11	2:B:684:LEU:HD21	1.99	0.44
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.53	0.44
2:B:324:ILE:HG23	2:B:329:THR:HB	2.00	0.44
2:B:283:VAL:HG13	2:B:297:ILE:HD13	1.99	0.44
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.82	0.44
1:A:590:ARG:O	1:A:591:PHE:HB2	2.17	0.44
1:A:1235:LYS:HB3	1:A:1237:ILE:CD1	2.48	0.44
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.99	0.44
4:E:46:TYR:CE2	4:E:58:MET:HA	2.53	0.44
2:B:35:SER:O	2:B:39:ARG:HG3	2.17	0.44
1:A:666:ILE:H	1:A:666:ILE:HD12	1.82	0.44
2:B:830:TYR:HB3	2:B:831:SER:H	1.56	0.44
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.99	0.44
2:B:1166:CYS:HB2	2:B:1215:ARG:NH1	2.33	0.44
1:A:1033:GLN:O	1:A:1036:ARG:NH1	2.49	0.44
2:B:380:TYR:CE1	2:B:384:ARG:HD3	2.52	0.44
7:I:45:ARG:HE	7:I:47:GLU:HG3	1.82	0.44
4:E:19:VAL:O	4:E:23:VAL:HG23	2.18	0.44
1:A:323:LYS:NZ	1:A:324:SER:H	2.16	0.44
3:C:33:LEU:O	3:C:37:MET:HE2	2.16	0.44
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.98	0.44
2:B:487:THR:CG2	2:B:488:TYR:N	2.80	0.44
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:61:TYR:HA	9:K:72:LYS:O	2.18	0.44
1:A:924:LYS:O	1:A:927:VAL:HB	2.18	0.44
2:B:956:THR:HA	2:B:961:LEU:O	2.18	0.44
1:A:867:ILE:HG22	1:A:872:GLY:N	2.33	0.44
1:A:689:LYS:O	1:A:693:VAL:HG23	2.17	0.44
3:C:99:LEU:HD22	3:C:120:ILE:HG12	2.00	0.44
2:B:221:ASN:OD1	2:B:242:SER:HA	2.18	0.44
1:A:260:ASP:OD1	1:A:261:ASP:N	2.51	0.44
7:I:54:GLU:HB3	7:I:100:PHE:CZ	2.53	0.44
3:C:67:LEU:HD23	3:C:70:ILE:HD12	2.00	0.43
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.99	0.43
2:B:201:GLY:H	2:B:202:TYR:HD2	1.66	0.43
1:A:243:PRO:CB	1:A:245:PRO:HD2	2.46	0.43
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.17	0.43
3:C:38:ILE:HG13	3:C:176:ILE:HD12	2.00	0.43
7:I:59:VAL:HG12	7:I:60:GLN:H	1.83	0.43
1:A:567:LYS:CB	1:A:568:PRO:CD	2.67	0.43
6:H:95:TYR:HE2	6:H:97:MET:CG	2.24	0.43
1:A:41:MET:HA	1:A:49:LYS:HA	1.99	0.43
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.12	0.43
9:K:58:PHE:CD2	9:K:59:ALA:N	2.86	0.43
4:E:46:TYR:CD2	4:E:58:MET:HG2	2.53	0.43
1:A:599:SER:HB2	1:A:603:ASN:H	1.82	0.43
2:B:313:MET:O	2:B:316:PRO:HD2	2.18	0.43
2:B:1187:ASN:OD1	2:B:1190:ASP:HB3	2.19	0.43
10:L:36:SER:O	10:L:37:LYS:C	2.56	0.43
2:B:433:GLN:O	2:B:435:THR:N	2.51	0.43
1:A:550:LEU:HB3	1:A:556:TRP:CE2	2.54	0.43
2:B:174:LEU:O	2:B:175:ARG:CB	2.50	0.43
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.90	0.43
1:A:605:MET:HA	1:A:605:MET:HE3	1.99	0.43
3:C:33:LEU:HD11	3:C:248:ILE:HG13	2.00	0.43
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.47	0.43
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.52	0.43
9:K:10:PHE:CD2	9:K:10:PHE:N	2.86	0.43
1:A:588:LEU:O	1:A:606:LEU:HA	2.19	0.43
9:K:53:ASP:HB3	9:K:56:VAL:HG23	2.01	0.43
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.53	0.43
1:A:1042:PHE:HE2	1:A:1046:LEU:HD11	1.84	0.43
2:B:467:GLY:HA3	2:B:473:MET:CE	2.47	0.43
2:B:860:MET:HA	2:B:964:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:107:VAL:HG12	5:F:109:VAL:H	1.83	0.43
1:A:219:PHE:O	1:A:222:LEU:O	2.37	0.43
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.00	0.43
7:I:2:THR:HA	7:I:40:SER:OG	2.18	0.43
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.44	0.43
1:A:253:ASN:ND2	1:A:253:ASN:H	2.15	0.43
9:K:11:LEU:HD12	9:K:11:LEU:HA	1.76	0.43
9:K:51:LEU:HD13	9:K:59:ALA:HB3	2.00	0.43
2:B:426:LYS:HZ3	2:B:430:ARG:HH12	1.65	0.43
6:H:143:LEU:N	6:H:143:LEU:HD12	2.34	0.43
2:B:1046:PRO:HB2	2:B:1047:PHE:H	1.63	0.43
1:A:760:GLN:HE21	1:A:765:VAL:HG13	1.83	0.43
2:B:476:ARG:C	2:B:478:GLY:H	2.22	0.43
1:A:599:SER:HA	1:A:600:PRO:HD2	1.87	0.43
2:B:212:LEU:HD13	2:B:409:ALA:HA	2.01	0.43
6:H:82:PRO:HB2	6:H:83:GLN:H	1.67	0.43
2:B:1222:ARG:O	2:B:1223:ASP:C	2.58	0.43
2:B:227:LYS:H	2:B:395:GLN:CD	2.23	0.43
2:B:169:ARG:O	2:B:457:LEU:HD12	2.19	0.43
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.34	0.43
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.49	0.43
6:H:35:GLN:HB3	6:H:111:LEU:HD21	2.01	0.43
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.19	0.43
9:K:38:GLU:HA	9:K:38:GLU:OE1	2.19	0.43
2:B:850:LEU:HD12	8:J:8:PHE:CD1	2.54	0.42
1:A:351:THR:HG21	2:B:1103:ILE:HG23	1.99	0.42
6:H:56:THR:O	6:H:144:ILE:HA	2.20	0.42
2:B:248:SER:H	2:B:418:LYS:HE3	1.84	0.42
3:C:44:LEU:HD22	3:C:129:ILE:HG12	2.00	0.42
2:B:329:THR:HA	2:B:332:ASP:HB3	2.01	0.42
7:I:59:VAL:HG12	7:I:60:GLN:N	2.34	0.42
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.53	0.42
1:A:389:THR:OG1	1:A:426:LEU:HD12	2.19	0.42
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.52	0.42
1:A:711:ARG:HA	7:I:97:MET:HE1	2.01	0.42
1:A:443:LEU:HD21	1:A:455:MET:HB3	2.01	0.42
3:C:61:GLU:HB3	10:L:67:PHE:CE2	2.55	0.42
4:E:29:PHE:HB2	4:E:65:THR:HG22	2.00	0.42
6:H:102:TYR:CZ	6:H:115:TYR:HB3	2.54	0.42
1:A:1424:VAL:CG1	2:B:1139:ILE:HD13	2.47	0.42
1:A:31:SER:OG	1:A:83:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:710:LEU:HD22	2:B:733:HIS:HB3	2.00	0.42
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.83	0.42
1:A:114:LEU:HD13	1:A:171:GLN:HE22	1.83	0.42
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.84	0.42
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.54	0.42
2:B:1167:GLY:HA3	2:B:1216:LEU:N	2.34	0.42
6:H:97:MET:HB3	6:H:118:PHE:CD2	2.54	0.42
4:E:133:GLU:HB3	4:E:135:PHE:HE1	1.83	0.42
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.77	0.42
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.55	0.42
1:A:359:LEU:HD22	1:A:363:GLN:CB	2.49	0.42
2:B:833:TYR:CE1	9:K:66:PRO:HG3	2.54	0.42
2:B:321:GLY:C	2:B:323:VAL:H	2.23	0.42
11:M:117:ASN:C	11:M:119:MET:H	2.23	0.42
1:A:575:LYS:HD2	6:H:120:GLY:HA3	2.00	0.42
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.01	0.42
1:A:737:LEU:HB3	1:A:738:LYS:H	1.63	0.42
1:A:65:LEU:HD12	11:M:19:ASN:O	2.15	0.42
1:A:406:ILE:HG22	1:A:407:ARG:N	2.34	0.42
2:B:473:MET:C	2:B:475:SER:H	2.23	0.42
1:A:334:GLY:O	1:A:335:ARG:C	2.57	0.42
1:A:315:LEU:O	1:A:316:GLN:C	2.58	0.42
1:A:19:PHE:O	1:A:1416:ALA:HA	2.19	0.42
1:A:275:SER:O	1:A:279:LEU:HG	2.19	0.42
1:A:98:LYS:O	1:A:102:VAL:HG23	2.20	0.42
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	2.01	0.42
8:J:1:MET:N	8:J:56:LEU:H	2.17	0.42
1:A:41:MET:HE1	1:A:257:ARG:HG2	2.02	0.42
1:A:337:ARG:HD3	1:A:839:ARG:HH12	1.85	0.42
4:E:77:SER:HB2	4:E:105:PHE:HD2	1.84	0.42
1:A:1392:SER:O	1:A:1393:ASN:CB	2.67	0.42
2:B:316:PRO:HA	2:B:319:GLU:HG3	2.02	0.42
4:E:96:PHE:CE2	4:E:110:PHE:HB2	2.55	0.42
4:E:94:LYS:HG3	4:E:98:ILE:CD1	2.50	0.42
2:B:845:SER:HB2	8:J:8:PHE:HB3	2.02	0.42
1:A:332:LYS:HG3	1:A:333:GLU:HG2	2.02	0.42
2:B:856:PHE:HA	2:B:968:VAL:O	2.20	0.42
2:B:416:LEU:HD11	2:B:460:ALA:HB2	2.01	0.42
2:B:843:GLN:HG3	9:K:6:ARG:HH21	1.84	0.42
1:A:1332:PHE:CD1	1:A:1348:LEU:HD13	2.55	0.42
1:A:1348:LEU:HD22	1:A:1381:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:THR:HG23	1:A:1239:ARG:NH2	2.35	0.42
2:B:711:GLU:N	2:B:712:PRO:HD3	2.35	0.42
1:A:1101:LEU:O	1:A:1105:LEU:HG	2.20	0.42
2:B:429:PHE:O	2:B:433:GLN:HG3	2.20	0.42
1:A:513:SER:HB3	1:A:520:CYS:HB3	2.01	0.42
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.19	0.42
4:E:112:TYR:CE2	4:E:134:THR:HB	2.54	0.42
2:B:999:MET:HB3	2:B:1007:VAL:HG21	2.01	0.42
1:A:95:PHE:O	1:A:99:ILE:HG13	2.20	0.42
2:B:791:THR:O	2:B:792:MET:HB2	2.20	0.42
4:E:150:VAL:HA	4:E:151:PRO:HD3	1.91	0.42
1:A:67:CYS:O	1:A:70:CYS:SG	2.77	0.42
1:A:261:ASP:O	1:A:264:PHE:HB2	2.19	0.42
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.19	0.42
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.55	0.42
2:B:1177:HIS:C	2:B:1179:GLN:H	2.23	0.42
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.53	0.41
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.83	0.41
1:A:340:LEU:HD21	2:B:1200:ALA:CA	2.50	0.41
1:A:1141:THR:O	1:A:1273:LEU:HB2	2.19	0.41
1:A:589:GLN:HG2	1:A:606:LEU:HD13	2.02	0.41
1:A:530:GLY:HA3	1:A:657:LEU:HD22	2.02	0.41
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.60	0.41
7:I:25:LEU:HB3	7:I:38:ALA:HB2	2.01	0.41
3:C:3:GLU:HB3	3:C:4:GLU:H	1.69	0.41
8:J:1:MET:H2	8:J:56:LEU:N	2.16	0.41
3:C:254:LYS:HB3	9:K:42:LEU:HD11	2.03	0.41
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.02	0.41
2:B:255:GLN:O	2:B:271:ALA:HA	2.20	0.41
9:K:63:VAL:HG23	9:K:63:VAL:O	2.19	0.41
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.86	0.41
2:B:476:ARG:O	2:B:478:GLY:N	2.53	0.41
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.02	0.41
1:A:442:VAL:HB	1:A:489:LEU:HD11	2.02	0.41
2:B:880:THR:O	2:B:934:LYS:HB2	2.20	0.41
1:A:668:ASP:HB3	1:A:743:VAL:HG23	2.03	0.41
2:B:913:GLY:HA2	2:B:938:SER:HB2	2.01	0.41
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.50	0.41
1:A:203:SER:O	1:A:207:ILE:HG12	2.20	0.41
1:A:453:MET:HB3	1:A:477:PRO:HB3	2.01	0.41
2:B:711:GLU:H	2:B:712:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.55	0.41
7:I:75:CYS:SG	7:I:108:HIS:CG	3.13	0.41
3:C:167:HIS:CD2	3:C:169:LYS:CG	3.04	0.41
1:A:516:SER:C	1:A:518:LYS:H	2.23	0.41
1:A:402:ALA:HB1	1:A:433:GLU:O	2.20	0.41
2:B:1168:LEU:HD21	2:B:1215:ARG:HD3	2.02	0.41
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.21	0.41
3:C:194:GLU:O	3:C:195:GLN:HG3	2.21	0.41
1:A:885:THR:O	1:A:940:ARG:HG3	2.20	0.41
1:A:571:LEU:HD22	6:H:46:LEU:HD11	2.02	0.41
1:A:872:GLY:O	1:A:1058:VAL:HG23	2.20	0.41
1:A:515:GLN:HG3	1:A:516:SER:N	2.36	0.41
7:I:29:CYS:SG	7:I:32:CYS:N	2.94	0.41
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.55	0.41
1:A:1205:LYS:O	1:A:1207:LEU:N	2.54	0.41
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.51	0.41
2:B:210:LYS:NZ	2:B:482:VAL:HG22	2.35	0.41
4:E:124:VAL:HG13	4:E:132:ILE:HB	2.03	0.41
1:A:494:SER:HB2	1:A:497:THR:OG1	2.20	0.41
9:K:7:PHE:CD1	9:K:7:PHE:C	2.94	0.41
2:B:121:ASN:HD22	2:B:121:ASN:N	2.18	0.41
5:F:90:ARG:HD3	5:F:155:LEU:CD1	2.49	0.41
1:A:885:THR:HG22	1:A:940:ARG:HA	2.02	0.41
1:A:596:THR:O	1:A:598:LEU:N	2.52	0.41
6:H:49:VAL:HG12	6:H:50:ALA:N	2.35	0.41
7:I:91:ARG:HD3	7:I:91:ARG:HA	1.85	0.41
7:I:50:THR:C	7:I:90:GLN:HE22	2.24	0.41
2:B:842:ASN:HD22	2:B:845:SER:N	2.17	0.41
1:A:1017:LEU:HB3	4:E:205:SER:HA	2.01	0.41
2:B:487:THR:HG22	2:B:488:TYR:N	2.35	0.41
2:B:914:LYS:HB3	2:B:937:ALA:O	2.21	0.41
2:B:1202:LEU:HA	2:B:1202:LEU:HD23	1.69	0.41
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.21	0.41
1:A:855:THR:CG2	1:A:857:ARG:CG	2.98	0.41
10:L:55:ILE:H	10:L:55:ILE:HG12	1.70	0.41
2:B:999:MET:HA	2:B:999:MET:CE	2.51	0.41
1:A:344:ARG:O	2:B:1118:PRO:HG2	2.20	0.41
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	2.02	0.41
2:B:287:ARG:HA	2:B:291:ILE:O	2.21	0.41
1:A:711:ARG:HA	7:I:97:MET:CE	2.51	0.41
2:B:475:SER:C	2:B:477:ALA:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:708:GLU:O	2:B:712:PRO:HD3	2.21	0.41
5:F:101:ILE:HD12	5:F:121:ALA:HB2	2.02	0.41
1:A:456:MET:HB3	1:A:507:VAL:HG22	2.03	0.41
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.56	0.41
9:K:46:ILE:HG22	9:K:50:LEU:HD12	2.03	0.41
2:B:638:PHE:HB2	2:B:741:CYS:HB3	2.02	0.41
1:A:188:ASP:HB3	1:A:192:GLY:HA3	2.03	0.41
2:B:1103:ILE:HG13	2:B:1103:ILE:H	1.70	0.41
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.68	0.41
1:A:1259:MET:C	1:A:1261:LYS:H	2.24	0.41
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	2.01	0.41
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.03	0.41
2:B:329:THR:O	2:B:333:PHE:N	2.54	0.41
2:B:844:SER:O	2:B:848:ARG:HG3	2.21	0.41
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.41
1:A:110:CYS:SG	1:A:167:CYS:SG	3.15	0.41
1:A:565:ILE:HG23	1:A:567:LYS:HG2	2.03	0.40
2:B:401:PHE:C	2:B:403:LYS:H	2.24	0.40
10:L:48:CYS:HB3	10:L:51:CYS:O	2.21	0.40
2:B:640:VAL:HG12	2:B:649:LYS:HG2	2.03	0.40
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.55	0.40
3:C:69:LEU:O	8:J:6:ARG:HD2	2.22	0.40
2:B:906:SER:O	2:B:909:ASP:OD1	2.39	0.40
5:F:87:LYS:HE2	5:F:88:TYR:CZ	2.56	0.40
1:A:13:THR:HB	1:A:15:LYS:HE2	2.02	0.40
1:A:343:LYS:CE	2:B:1151:LEU:O	2.66	0.40
1:A:1376:THR:CG2	4:E:212:ARG:NH2	2.84	0.40
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.86	0.40
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.56	0.40
3:C:255:VAL:HG21	9:K:94:ILE:CG2	2.51	0.40
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.51	0.40
9:K:63:VAL:O	9:K:63:VAL:CG2	2.69	0.40
6:H:36:CYS:HA	6:H:126:GLU:O	2.20	0.40
1:A:436:ILE:HD11	1:A:491:VAL:HG11	2.04	0.40
2:B:621:GLU:OE2	2:B:621:GLU:HA	2.21	0.40
2:B:170:LEU:HA	2:B:171:PRO:HD2	1.80	0.40
2:B:563:MET:O	2:B:565:PRO:HD3	2.20	0.40
2:B:1104:HIS:CE1	2:B:1126:GLY:O	2.74	0.40
2:B:479:VAL:O	2:B:480:SER:HB3	2.20	0.40
1:A:1291:VAL:HA	1:A:1292:PRO:HD3	1.89	0.40
5:F:109:VAL:HG21	5:F:124:GLU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:VAL:HG11	2:B:537:LYS:HD2	2.02	0.40
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.55	0.40
8:J:48:ARG:HE	8:J:49:MET:HE2	1.87	0.40
2:B:997:GLU:CD	3:C:39:ALA:HB2	2.41	0.40
7:I:8:ARG:O	7:I:10:CYS:N	2.54	0.40
3:C:37:MET:HA	3:C:41:ILE:CD1	2.51	0.40
1:A:661:GLY:O	1:A:662:PHE:HB2	2.22	0.40
2:B:230:ALA:N	2:B:231:PRO:HD2	2.37	0.40
2:B:232:SER:OG	2:B:234:ILE:HD12	2.22	0.40
2:B:1030:LEU:HD12	2:B:1059:LEU:HD22	2.04	0.40
1:A:990:VAL:O	1:A:994:GLN:HG3	2.21	0.40
1:A:929:LEU:HD21	1:A:983:ILE:HG21	2.04	0.40
1:A:681:GLU:HA	1:A:684:ALA:HB3	2.03	0.40
8:J:1:MET:HG3	8:J:60:PHE:CE2	2.45	0.40
5:F:138:LEU:HD23	5:F:138:LEU:HA	1.84	0.40
1:A:44:THR:O	1:A:45:GLN:HB2	2.21	0.40
1:A:151:ASP:HA	1:A:162:VAL:O	2.20	0.40
2:B:323:VAL:HG12	2:B:323:VAL:O	2.21	0.40
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.87	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	1398/1733 (81%)	1184 (85%)	154 (11%)	60 (4%)	3 35
2	B	1108/1224 (90%)	943 (85%)	105 (10%)	60 (5%)	2 30
3	C	264/318 (83%)	236 (89%)	20 (8%)	8 (3%)	5 46
4	E	212/215 (99%)	194 (92%)	18 (8%)	0	100 100
5	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	16 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	H	129/146 (88%)	98 (76%)	22 (17%)	9 (7%)	1 23
7	I	114/122 (93%)	97 (85%)	15 (13%)	2 (2%)	11 55
8	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	5 44
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100 100
10	L	44/70 (63%)	22 (50%)	14 (32%)	8 (18%)	0 3
11	M	183/345 (53%)	152 (83%)	19 (10%)	12 (7%)	1 25
All	All	3709/4518 (82%)	3162 (85%)	385 (10%)	162 (4%)	3 35

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ALA
1	A	54	ASN
1	A	55	ASP
1	A	109	HIS
1	A	250	ILE
1	A	254	GLU
1	A	318	SER
1	A	335	ARG
1	A	424	ILE
1	A	517	ASN
1	A	543	LEU
1	A	567	LYS
1	A	846	GLU
1	A	903	ASN
1	A	1036	ARG
1	A	1206	ASP
1	A	1392	SER
2	B	175	ARG
2	B	337	ARG
2	B	339	THR
2	B	343	ILE
2	B	364	ILE
2	B	367	LEU
2	B	447	ALA
2	B	469	GLN
2	B	507	LYS
2	B	531	GLN
2	B	643	ASP
2	B	648	HIS

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Mol	Chain	Res	Type
2	B	731	VAL
2	B	958	GLN
2	B	1046	PRO
2	B	1155	SER
2	B	1176	ASN
2	B	1183	LYS
2	B	1221	SER
2	B	1223	ASP
3	C	215	GLU
6	H	32	THR
6	H	81	PRO
8	J	2	ILE
8	J	6	ARG
10	L	64	LEU
11	M	25	PRO
11	M	31	PRO
11	M	32	PRO
11	M	35	VAL
11	M	104	MET
11	M	125	GLU
11	M	200	THR
1	A	67	CYS
1	A	74	MET
1	A	75	ASN
1	A	167	CYS
1	A	312	PRO
1	A	316	GLN
1	A	404	TYR
1	A	597	LEU
1	A	904	THR
1	A	1114	PRO
1	A	1393	ASN
2	B	174	LEU
2	B	200	GLY
2	B	346	GLU
2	B	445	LYS
2	B	477	ALA
2	B	502	ILE
2	B	882	THR
2	B	946	ASN
2	B	1108	ARG
3	C	110	THR

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Mol	Chain	Res	Type
3	C	142	VAL
6	H	82	PRO
10	L	55	ILE
1	A	35	ILE
1	A	87	ALA
1	A	257	ARG
1	A	421	ALA
1	A	422	GLY
1	A	430	TRP
1	A	536	LEU
1	A	598	LEU
1	A	920	LEU
1	A	1221	LYS
1	A	1280	GLU
2	B	345	LYS
2	B	435	THR
2	B	467	GLY
2	B	471	LYS
2	B	476	ARG
2	B	880	THR
2	B	959	ASP
2	B	1017	ILE
2	B	1103	ILE
3	C	4	GLU
6	H	128	ASN
6	H	135	LEU
7	I	9	ASP
7	I	47	GLU
10	L	42	ARG
10	L	56	LEU
11	M	160	GLU
1	A	194	ALA
1	A	282	ASN
1	A	290	GLU
1	A	308	ILE
1	A	592	ASP
1	A	737	LEU
1	A	998	LEU
2	B	336	ARG
2	B	474	SER
2	B	751	VAL
2	B	879	ARG

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Mol	Chain	Res	Type
2	B	883	LEU
2	B	1156	ASP
2	B	1181	GLU
3	C	6	PRO
3	C	90	ASP
3	C	174	ALA
3	C	227	THR
6	H	62	SER
6	H	140	ALA
10	L	35	SER
11	M	196	ILE
1	A	72	GLU
1	A	255	SER
1	A	317	LYS
1	A	322	VAL
1	A	332	LYS
1	A	599	SER
1	A	790	ASP
2	B	340	ALA
2	B	438	GLU
2	B	463	THR
2	B	468	GLU
2	B	641	GLU
2	B	738	PHE
2	B	888	GLY
2	B	1167	GLY
5	F	112	GLU
6	H	59	ILE
10	L	26	THR
10	L	37	LYS
10	L	46	VAL
11	M	118	VAL
1	A	653	VAL
1	A	958	VAL
1	A	1242	VAL
2	B	433	GLN
2	B	437	GLU
2	B	792	MET
2	B	884	ARG
11	M	92	LEU
11	M	198	VAL
1	A	84	ILE

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Mol	Chain	Res	Type
2	B	711	GLU
2	B	901	PRO
1	A	775	ILE
6	H	107	VAL
1	A	1435	PRO
2	B	907	GLY
1	A	410	GLY

5.3.2 Protein sidechains

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	1224/1520 (80%)	1158 (95%)	66 (5%)	27 68
2	B	953/1061 (90%)	901 (94%)	52 (6%)	27 68
3	C	234/274 (85%)	225 (96%)	9 (4%)	40 76
4	E	196/197 (100%)	192 (98%)	4 (2%)	63 87
5	F	74/137 (54%)	70 (95%)	4 (5%)	27 68
6	H	117/128 (91%)	110 (94%)	7 (6%)	24 65
7	I	113/116 (97%)	106 (94%)	7 (6%)	23 64
8	J	60/65 (92%)	57 (95%)	3 (5%)	30 70
9	K	99/102 (97%)	91 (92%)	8 (8%)	15 54
10	L	40/57 (70%)	34 (85%)	6 (15%)	3 26
All	All	3110/3657 (85%)	2944 (95%)	166 (5%)	28 69

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	93	VAL
1	A	226	GLU
1	A	252	PHE
1	A	253	ASN
1	A	302	THR

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Mol	Chain	Res	Type
1	A	306	ASN
1	A	313	GLN
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	326	ARG
1	A	351	THR
1	A	354	SER
1	A	385	ILE
1	A	403	LYS
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	463	ILE
1	A	466	SER
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	494	SER
1	A	503	GLN
1	A	504	LEU
1	A	529	CYS
1	A	545	GLN
1	A	596	THR
1	A	598	LEU
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	666	ILE
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	768	GLN
1	A	774	ARG
1	A	821	ARG
1	A	855	THR
1	A	858	ASN
1	A	1035	TYR
1	A	1043	ASP

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Mol	Chain	Res	Type
1	A	1120	LEU
1	A	1155	ASP
1	A	1161	THR
1	A	1222	ASN
1	A	1258	HIS
1	A	1264	GLU
1	A	1297	GLU
1	A	1303	GLU
1	A	1308	THR
1	A	1332	PHE
1	A	1359	ASP
1	A	1364	ASN
1	A	1375	MET
1	A	1376	THR
1	A	1385	THR
1	A	1401	SER
1	A	1425	SER
1	A	1442	ASP
2	B	20	ASP
2	B	63	ILE
2	B	175	ARG
2	B	194	GLU
2	B	234	ILE
2	B	265	SER
2	B	268	THR
2	B	331	LEU
2	B	334	ILE
2	B	408	LEU
2	B	416	LEU
2	B	425	THR
2	B	437	GLU
2	B	469	GLN
2	B	471	LYS
2	B	485	ARG
2	B	513	GLN
2	B	538	ASN
2	B	547	VAL
2	B	563	MET
2	B	570	VAL
2	B	644	GLU
2	B	680	THR
2	B	709	ASP

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Mol	Chain	Res	Type
2	B	723	VAL
2	B	762	ASN
2	B	764	SER
2	B	791	THR
2	B	797	TYR
2	B	858	SER
2	B	860	MET
2	B	909	ASP
2	B	943	SER
2	B	951	GLN
2	B	953	LEU
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1021	MET
2	B	1049	ASP
2	B	1084	GLN
2	B	1103	ILE
2	B	1108	ARG
2	B	1111	MET
2	B	1132	GLU
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1183	LYS
2	B	1185	CYS
2	B	1219	ASP
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	56	THR
3	C	57	VAL
3	C	69	LEU
3	C	77	ILE
3	C	109	SER
3	C	233	GLU
4	E	41	ASP
4	E	84	ASP
4	E	104	ASN
4	E	153	HIS
5	F	79	ARG

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Mol	Chain	Res	Type
5	F	86	THR
5	F	90	ARG
5	F	110	ASP
6	H	2	SER
6	H	27	GLU
6	H	63	LEU
6	H	76	THR
6	H	109	LYS
6	H	110	ASP
6	H	135	LEU
7	I	12	ASN
7	I	29	CYS
7	I	33	SER
7	I	52	ILE
7	I	78	CYS
7	I	87	GLN
7	I	106	CYS
8	J	2	ILE
8	J	7	CYS
8	J	48	ARG
9	K	11	LEU
9	K	12	LEU
9	K	42	LEU
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	101	LEU
9	K	114	LEU
10	L	38	LEU
10	L	42	ARG
10	L	50	ASP
10	L	54	ARG
10	L	65	VAL
10	L	68	GLU

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS

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Mol	Chain	Res	Type
1	A	118	HIS
1	A	225	ASN
1	A	253	ASN
1	A	313	GLN
1	A	316	GLN
1	A	339	ASN
1	A	435	HIS
1	A	445	ASN
1	A	503	GLN
1	A	517	ASN
1	A	736	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	965	GLN
1	A	968	GLN
1	A	1130	GLN
1	A	1173	HIS
1	A	1270	ASN
1	A	1364	ASN
1	A	1390	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	121	ASN
2	B	236	HIS
2	B	300	HIS
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	744	HIS
2	B	822	ASN
2	B	842	ASN
2	B	975	GLN
2	B	986	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1093	GLN
2	B	1117	GLN

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Mol	Chain	Res	Type
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
3	C	252	GLN
4	E	5	ASN
4	E	101	GLN
4	E	104	ASN
4	E	114	ASN
4	E	147	HIS
7	I	12	ASN
7	I	90	GLN
7	I	108	HIS
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1408/1733 (81%)	0.47	70 (4%) 32 21	82, 172, 267, 498	0
2	B	1122/1224 (91%)	0.85	157 (13%) 4 3	68, 183, 297, 489	0
3	C	266/318 (83%)	0.36	1 (0%) 93 87	93, 166, 244, 317	0
4	E	214/215 (99%)	0.48	20 (9%) 11 7	109, 202, 304, 500	0
5	F	84/155 (54%)	0.25	0 100 100	82, 135, 188, 256	0
6	H	133/146 (91%)	0.37	7 (5%) 30 20	118, 220, 305, 358	0
7	I	118/122 (96%)	1.52	36 (30%) 1 1	132, 237, 353, 412	0
8	J	65/70 (92%)	0.60	6 (9%) 11 7	106, 169, 237, 266	0
9	K	114/120 (95%)	0.25	0 100 100	94, 148, 208, 270	0
10	L	46/70 (65%)	0.64	6 (13%) 5 4	137, 208, 293, 359	0
11	M	187/345 (54%)	0.56	25 (13%) 4 4	111, 242, 373, 500	0
All	All	3757/4518 (83%)	0.60	328 (8%) 13 8	68, 181, 296, 500	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	M	121	LYS	15.7
7	I	119	THR	10.1
7	I	120	GLN	10.1
11	M	83	SER	9.3
7	I	53	GLY	9.2
11	M	120	ASP	9.1
2	B	882	THR	8.9
7	I	118	ARG	8.7
7	I	52	ILE	8.5
11	M	84	ASN	8.2
7	I	40	SER	8.1
4	E	93	MET	7.5

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Mol	Chain	Res	Type	RSRZ
11	M	124	ASN	7.0
2	B	637	LEU	6.7
1	A	318	SER	6.7
2	B	730	ARG	6.4
7	I	60	GLN	6.3
7	I	55	THR	6.2
1	A	44	THR	6.1
1	A	1197	LEU	6.1
2	B	735	ALA	6.0
7	I	49	ILE	5.9
2	B	868	MET	5.8
2	B	1220	ARG	5.7
2	B	732	SER	5.7
11	M	122	LYS	5.5
1	A	252	PHE	5.3
7	I	2	THR	5.2
2	B	247	GLY	5.2
1	A	1150	SER	5.1
2	B	731	VAL	5.1
2	B	638	PHE	5.1
2	B	729	ILE	5.0
2	B	325	GLN	5.0
2	B	283	VAL	5.0
11	M	194	SER	4.8
1	A	1159	ARG	4.8
2	B	322	PHE	4.7
2	B	726	ALA	4.7
1	A	1317	MET	4.7
7	I	57	GLY	4.6
1	A	2	VAL	4.6
2	B	615	MET	4.6
7	I	71	SER	4.5
2	B	734	HIS	4.4
1	A	1153	TYR	4.4
6	H	60	ALA	4.3
2	B	804	GLY	4.3
2	B	431	TYR	4.3
7	I	117	LYS	4.2
7	I	116	ASN	4.2
2	B	705	MET	4.2
2	B	576	ASP	4.2
2	B	785	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	303	TYR	4.0
7	I	67	THR	4.0
2	B	267	ARG	4.0
2	B	689	LEU	4.0
2	B	349	ILE	3.9
4	E	109	ILE	3.9
1	A	1339	LEU	3.8
2	B	246	LYS	3.8
4	E	53	PRO	3.8
2	B	360	PHE	3.8
2	B	636	PRO	3.8
2	B	243	ALA	3.7
1	A	251	SER	3.7
7	I	42	LEU	3.7
2	B	1180	PHE	3.7
7	I	70	ARG	3.7
1	A	1254	ALA	3.7
11	M	201	LYS	3.7
2	B	587	HIS	3.6
2	B	495	LEU	3.6
2	B	698	GLU	3.6
11	M	206	THR	3.6
2	B	620	ARG	3.5
2	B	437	GLU	3.5
2	B	106	ASP	3.5
2	B	578	THR	3.5
2	B	725	PRO	3.5
2	B	390	LEU	3.5
8	J	1	MET	3.5
2	B	356	LEU	3.5
2	B	468	GLU	3.5
4	E	110	PHE	3.4
2	B	1221	SER	3.4
1	A	62	ASP	3.4
1	A	1154	TYR	3.4
2	B	733	HIS	3.4
2	B	617	ARG	3.4
2	B	420	LEU	3.4
2	B	457	LEU	3.4
1	A	818	MET	3.4
1	A	258	GLY	3.4
1	A	975	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	692	TYR	3.3
2	B	738	PHE	3.3
2	B	461	LEU	3.3
7	I	84	VAL	3.3
1	A	710	LEU	3.3
2	B	693	ILE	3.3
2	B	643	ASP	3.3
2	B	514	LEU	3.3
10	L	47	ARG	3.3
1	A	253	ASN	3.2
7	I	112	SER	3.2
2	B	569	TYR	3.2
6	H	134	ASN	3.2
7	I	51	ASN	3.2
7	I	68	LEU	3.2
2	B	111	ALA	3.2
1	A	1192	LEU	3.2
2	B	181	LEU	3.2
1	A	179	LEU	3.1
2	B	443	ASN	3.1
11	M	82	ALA	3.1
2	B	92	PHE	3.1
2	B	120	ARG	3.1
4	E	125	PRO	3.1
1	A	1282	VAL	3.1
1	A	1146	VAL	3.1
1	A	117	GLU	3.0
2	B	935	ARG	3.0
2	B	377	PHE	3.0
1	A	1188	GLN	3.0
4	E	135	PHE	3.0
1	A	1195	LEU	3.0
7	I	56	ALA	3.0
2	B	586	TRP	3.0
7	I	64	SER	3.0
2	B	43	LEU	3.0
2	B	449	ASN	3.0
2	B	955	THR	3.0
1	A	778	GLY	3.0
2	B	263	GLY	3.0
2	B	96	TYR	2.9
6	H	116	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	333	PHE	2.9
11	M	184	GLU	2.9
2	B	1181	GLU	2.9
1	A	1313	LEU	2.9
11	M	197	HIS	2.9
2	B	201	GLY	2.9
1	A	811	GLN	2.9
7	I	72	ASP	2.9
11	M	65	THR	2.9
2	B	271	ALA	2.9
2	B	199	MET	2.8
1	A	257	ARG	2.8
2	B	193	LYS	2.8
2	B	1222	ARG	2.8
1	A	1267	MET	2.8
2	B	386	LEU	2.8
6	H	59	ILE	2.8
10	L	32	ALA	2.8
2	B	245	GLU	2.8
10	L	58	LYS	2.8
2	B	131	ASP	2.8
4	E	107	THR	2.8
11	M	193	GLN	2.8
11	M	143	PRO	2.8
11	M	157	CYS	2.7
2	B	439	ALA	2.7
2	B	584	GLY	2.7
2	B	1169	MET	2.7
2	B	558	LEU	2.7
2	B	877	PRO	2.7
1	A	852	TYR	2.7
7	I	61	ASP	2.7
2	B	94	LYS	2.7
1	A	1147	THR	2.7
2	B	97	VAL	2.7
7	I	99	LEU	2.7
8	J	44	TYR	2.7
2	B	633	VAL	2.7
2	B	167	ILE	2.7
2	B	424	LEU	2.7
2	B	466	TRP	2.7
1	A	235	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
11	M	145	ILE	2.7
2	B	114	PRO	2.7
11	M	123	ASP	2.7
2	B	248	SER	2.7
1	A	1158	PRO	2.7
2	B	681	TRP	2.7
4	E	97	VAL	2.6
1	A	785	PRO	2.6
1	A	1196	GLU	2.6
7	I	63	GLY	2.6
2	B	709	ASP	2.6
2	B	1009	ASP	2.6
2	B	421	PHE	2.6
7	I	102	VAL	2.6
1	A	343	LYS	2.6
11	M	85	PRO	2.6
1	A	163	SER	2.6
4	E	111	VAL	2.6
2	B	803	LEU	2.6
2	B	95	ILE	2.6
1	A	700	ASN	2.6
2	B	767	ASN	2.6
1	A	256	GLN	2.6
11	M	204	GLY	2.6
4	E	80	VAL	2.6
2	B	881	ASN	2.6
1	A	135	PHE	2.6
2	B	957	ASN	2.5
2	B	871	THR	2.5
10	L	26	THR	2.5
2	B	364	ILE	2.5
11	M	167	SER	2.5
2	B	691	GLU	2.5
2	B	872	GLU	2.5
2	B	841	MET	2.5
2	B	406	LEU	2.5
2	B	722	ASP	2.5
3	C	30	ALA	2.5
2	B	724	ASP	2.5
2	B	381	MET	2.5
2	B	25	ILE	2.5
2	B	336	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	203	PHE	2.5
1	A	336	ILE	2.5
1	A	912	LEU	2.4
4	E	122	LYS	2.4
2	B	822	ASN	2.4
7	I	44	TYR	2.4
7	I	54	GLU	2.4
2	B	1151	LEU	2.4
2	B	516	ASN	2.4
7	I	97	MET	2.4
2	B	133	LYS	2.4
4	E	129	PRO	2.4
2	B	119	LEU	2.4
1	A	789	LYS	2.4
1	A	113	LEU	2.4
1	A	1018	PHE	2.4
2	B	262	GLU	2.4
1	A	775	ILE	2.4
1	A	300	VAL	2.4
2	B	301	ILE	2.3
1	A	1176	LEU	2.3
2	B	963	PHE	2.3
7	I	45	ARG	2.3
2	B	580	VAL	2.3
11	M	198	VAL	2.3
1	A	91	PHE	2.3
1	A	1238	ILE	2.3
2	B	783	THR	2.3
2	B	212	LEU	2.3
2	B	409	ALA	2.3
2	B	417	PHE	2.3
2	B	958	GLN	2.3
6	H	55	LEU	2.3
2	B	250	PHE	2.3
2	B	447	ALA	2.3
4	E	215	MET	2.3
7	I	98	VAL	2.3
6	H	113	ALA	2.3
7	I	47	GLU	2.3
4	E	190	LEU	2.3
2	B	616	ILE	2.3
1	A	1224	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	190	TYR	2.2
2	B	641	GLU	2.2
2	B	780	VAL	2.2
2	B	870	ILE	2.2
2	B	653	VAL	2.2
2	B	619	ILE	2.2
2	B	690	VAL	2.2
1	A	105	CYS	2.2
1	A	883	LEU	2.2
2	B	711	GLU	2.2
2	B	249	ARG	2.2
2	B	216	GLU	2.2
2	B	254	LEU	2.2
2	B	749	LEU	2.2
11	M	161	LYS	2.2
1	A	181	LEU	2.2
1	A	1236	LEU	2.2
2	B	366	GLN	2.2
2	B	782	LEU	2.2
1	A	303	TYR	2.2
2	B	1205	GLN	2.2
1	A	355	GLY	2.2
11	M	202	GLU	2.2
2	B	401	PHE	2.2
1	A	92	HIS	2.1
2	B	519	TRP	2.1
1	A	1166	ASP	2.1
10	L	27	LEU	2.1
4	E	211	TYR	2.1
1	A	1194	ARG	2.1
2	B	282	ILE	2.1
1	A	1060	PRO	2.1
2	B	492	LEU	2.1
2	B	413	LEU	2.1
4	E	78	LEU	2.1
10	L	54	ARG	2.1
2	B	225	VAL	2.1
2	B	170	LEU	2.1
6	H	126	GLU	2.1
1	A	68	GLN	2.1
4	E	20	LYS	2.1
2	B	256	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	E	153	HIS	2.1
1	A	968	GLN	2.1
2	B	115	GLN	2.1
4	E	121	MET	2.0
8	J	49	MET	2.0
7	I	46	HIS	2.0
2	B	359	GLU	2.0
2	B	821	GLN	2.0
8	J	6	ARG	2.0
1	A	885	THR	2.0
2	B	1130	PHE	2.0
8	J	21	TYR	2.0
7	I	69	PRO	2.0
1	A	317	LYS	2.0
1	A	622	VAL	2.0
2	B	624	LEU	2.0
2	B	438	GLU	2.0
11	M	209	ILE	2.0
1	A	815	PHE	2.0
4	E	6	GLU	2.0
1	A	240	PRO	2.0
8	J	17	LYS	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
12	ZN	M	346	1/1	0.89	0.50	3.14	193,193,193,193	0
12	ZN	C	319	1/1	0.98	0.31	1.16	191,191,191,191	0
12	ZN	A	1734	1/1	0.98	0.24	0.12	205,205,205,205	0
12	ZN	I	204	1/1	0.94	0.18	0.05	311,311,311,311	0
12	ZN	L	105	1/1	0.98	0.18	0.02	215,215,215,215	0
12	ZN	J	101	1/1	1.00	0.22	-0.72	177,177,177,177	0
12	ZN	A	1735	1/1	0.99	0.20	-0.73	183,183,183,183	0
12	ZN	B	1307	1/1	0.88	0.27	-	195,195,195,195	0
12	ZN	I	203	1/1	0.98	0.25	-	218,218,218,218	0

6.5 Other polymers

There are no such residues in this entry.