Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:36 pm BST

PDB ID	:	4X67
Title	:	Crystal structure of elongating yeast RNA polymerase II stalled at oxidative Cyclopurine DNA lesions.
Authors	:	Wang, L.; Chong, J.; Wang, D.
Deposited on	:	2014-12-07
Resolution	:	4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

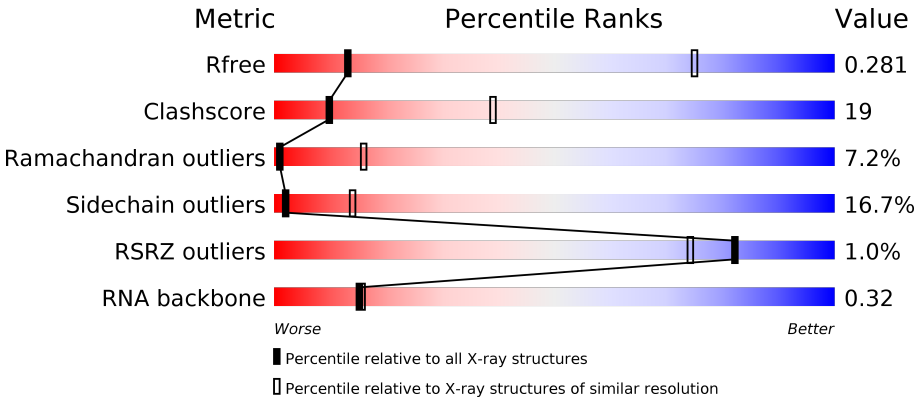
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)
RNA backbone	3102	1049 (5.04-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	% 46% 26% 8% • 20%
2	B	1224	49% 33% 8% • 10%
3	C	318	52% 26% 6% 16%
4	E	215	3% 59% 34% 6%

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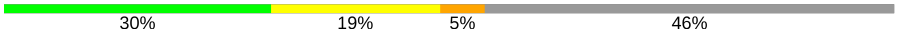
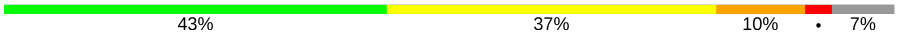
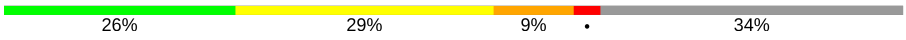
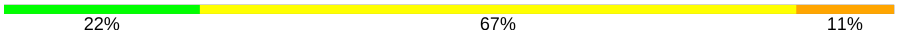
Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	9	
12	T	29	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28521 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	1394	Total	C	N	O	S	0	0	0
			10961	6911	1922	2067	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	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	119	Total	C	N	O	S	0	0	0
			971	596	179	186	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 RNA chain called RNA_9 mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	9	Total	C	N	O	P	0	0	0
			176	77	32	58	9			

- Molecule 12 is a DNA chain called Template DNA _29 mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	10	Total	C	N	O	P	0	0	0
			205	98	37	60	10			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		
13	B	1	Total	Zn	0	0
			1	1		

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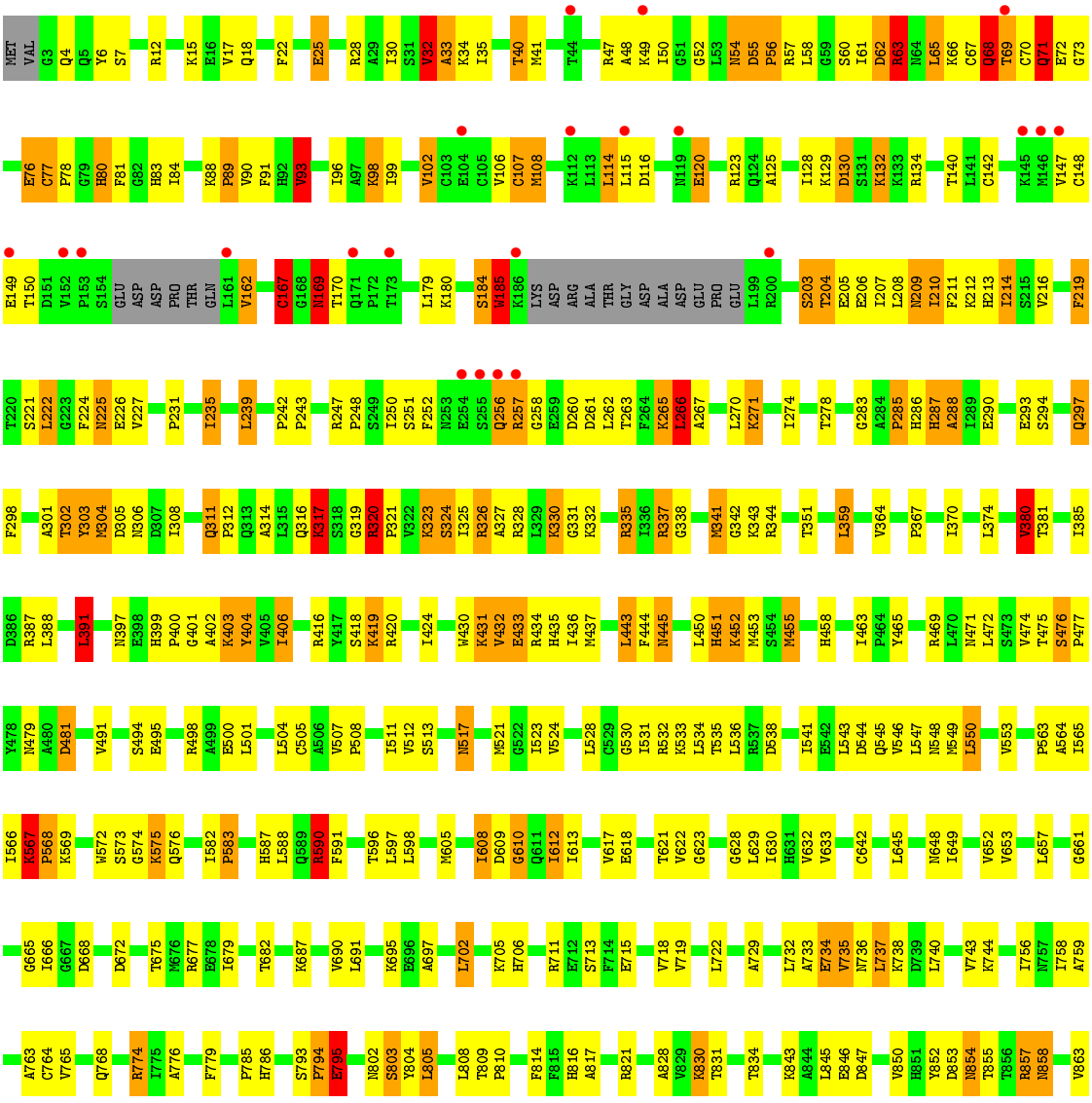
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	I	2	Total Zn 2 2	0	0
13	C	1	Total Zn 1 1	0	0
13	A	2	Total Zn 2 2	0	0
13	L	1	Total Zn 1 1	0	0

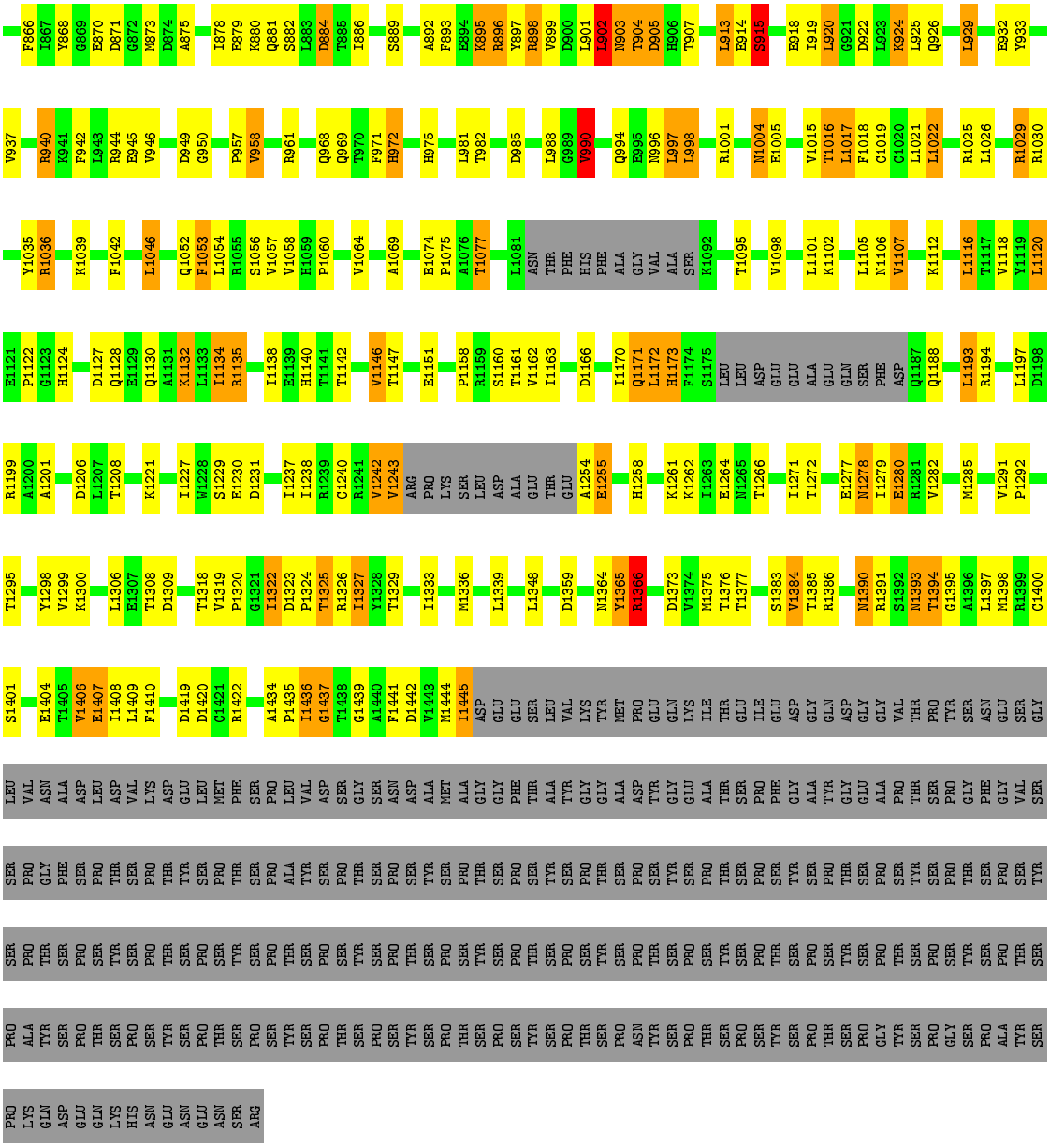
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

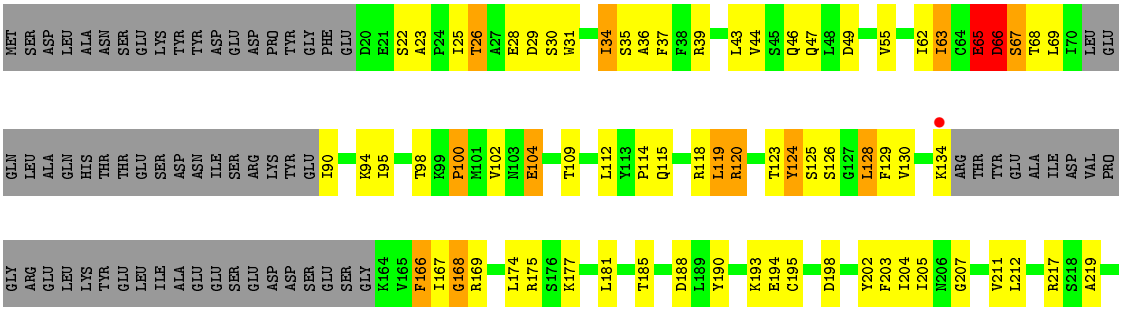
Chain A:

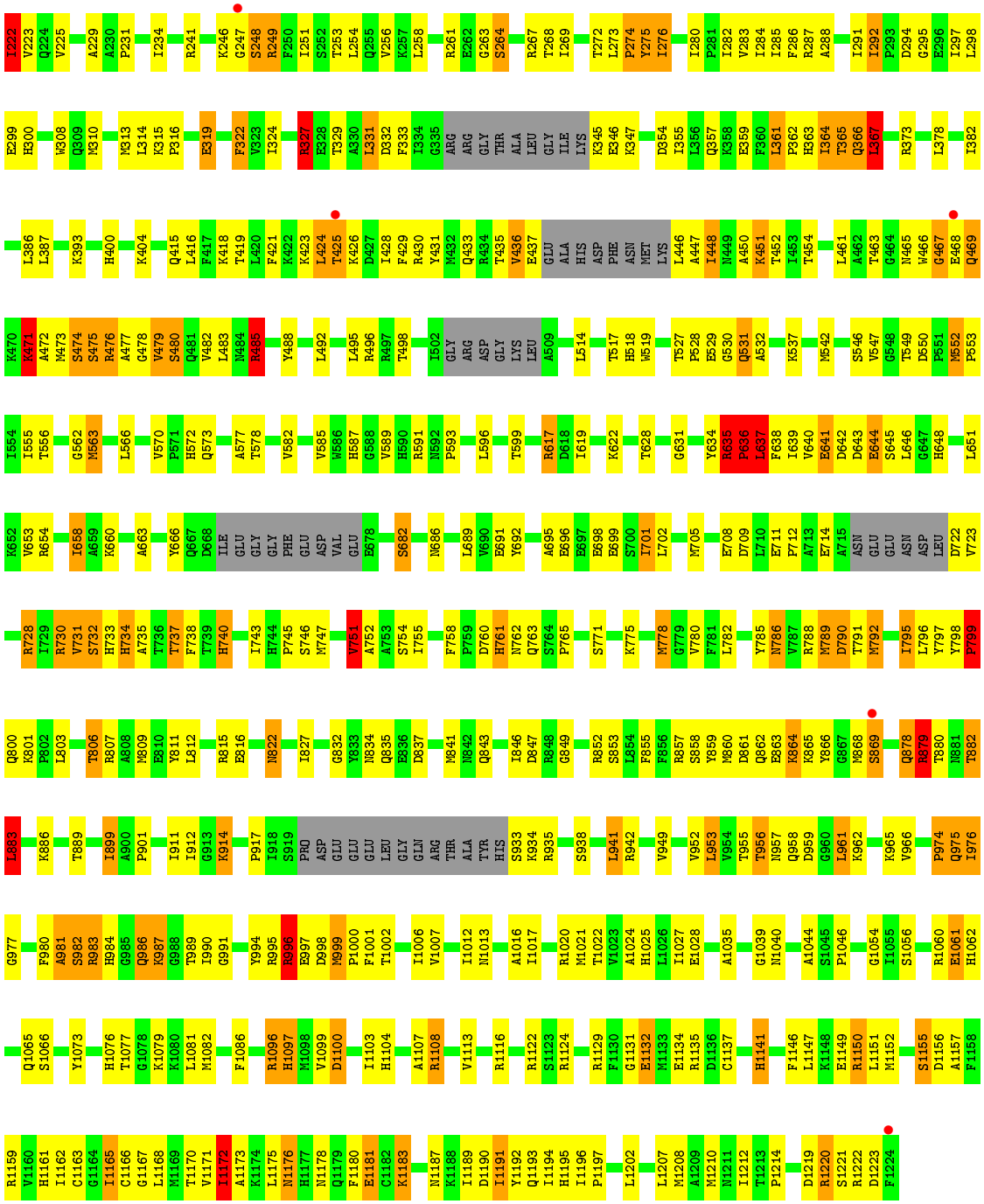




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

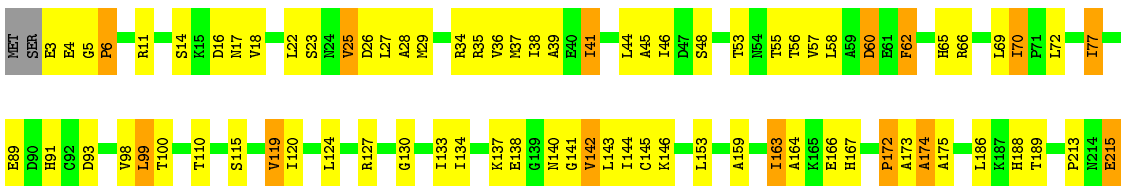
Chain B:

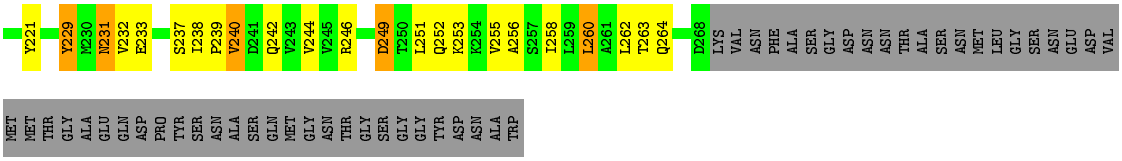




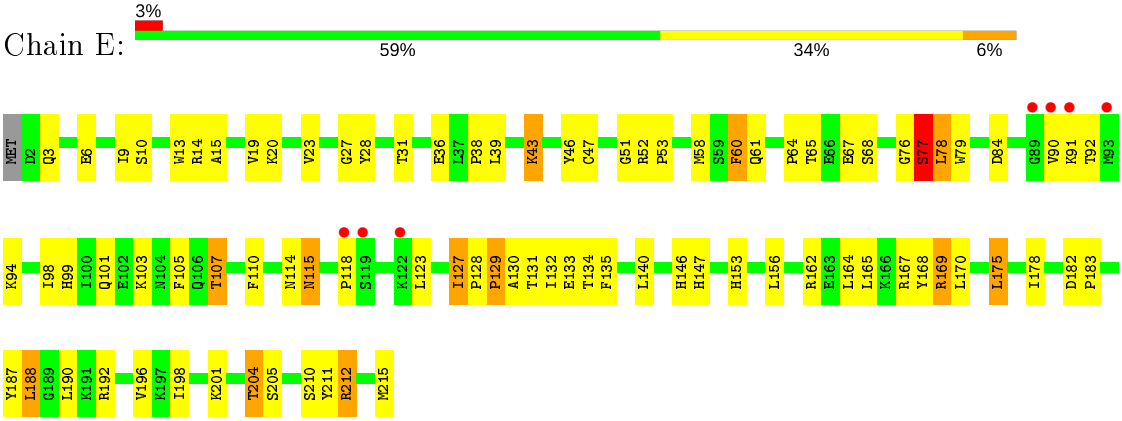
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

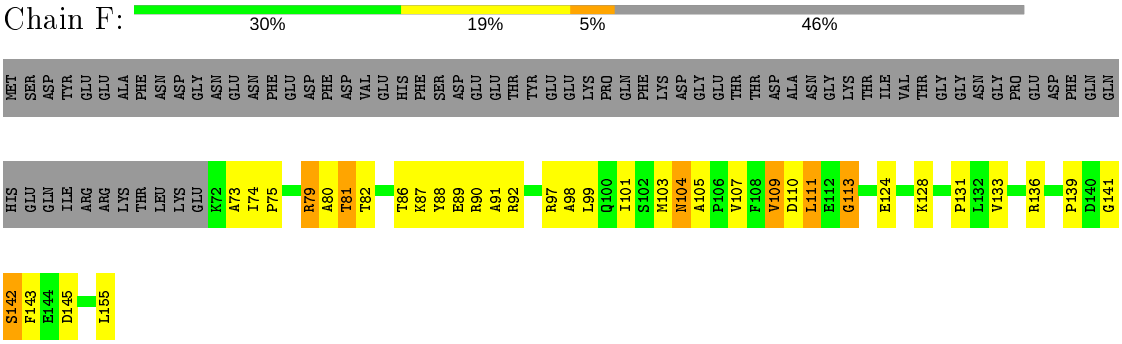




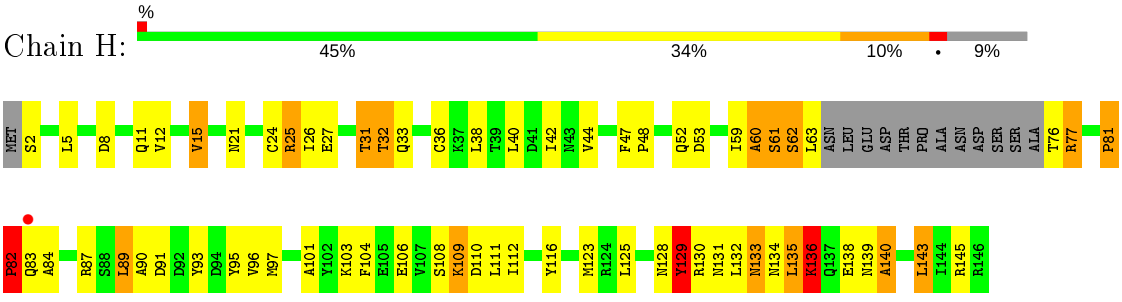
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



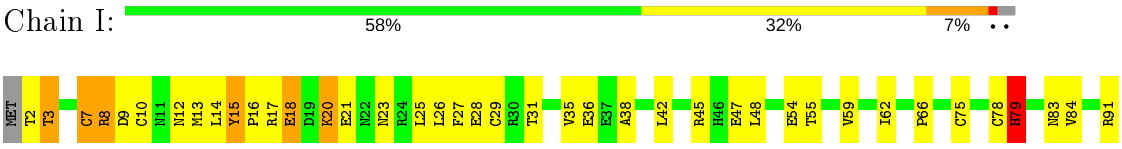
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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

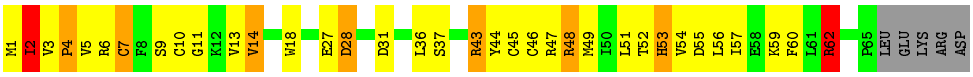


• Molecule 7: DNA-directed RNA polymerase II subunit RPB9



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

Chain J:

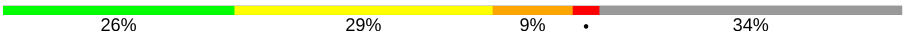


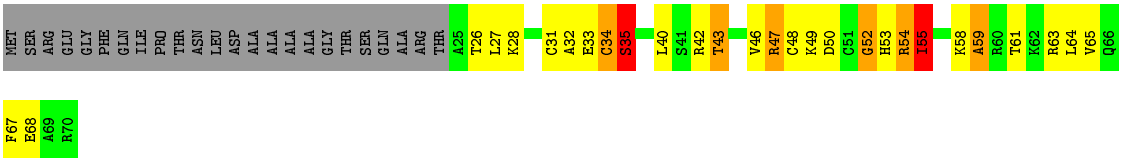
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:

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

Chain L:





• Molecule 11: RNA_9 mer

Chain R:

• Molecule 12: Template DNA _29 mer

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	167.15Å 220.80Å 193.92Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	50.00 – 4.10 49.44 – 4.10	Depositor EDS
% Data completeness (in resolution range)	75.9 (50.00-4.10) 76.0 (49.44-4.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 4.14Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.289 0.238 , 0.281	Depositor DCC
R_{free} test set	2105 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	28521	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 02I

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	0.41	1/11155 (0.0%)	0.73	3/15080 (0.0%)
2	B	0.41	0/8963	0.74	2/12086 (0.0%)
3	C	0.40	0/2133	0.70	0/2891
4	E	0.41	0/1788	0.72	0/2406
5	F	0.39	0/691	0.69	0/933
6	H	0.41	0/1086	0.73	0/1470
7	I	0.45	0/989	0.75	1/1331 (0.1%)
8	J	0.42	0/541	0.74	0/727
9	K	0.39	0/937	0.69	1/1265 (0.1%)
10	L	0.44	0/365	0.78	0/485
11	R	0.22	0/196	0.60	0/304
12	T	0.22	0/204	0.56	0/310
All	All	0.41	1/29048 (0.0%)	0.73	7/39288 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	9
3	C	0	1
6	H	0	3
7	I	0	1
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	CYS	CB-SG	5.70	1.92	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	637	LEU	CA-CB-CG	9.71	137.63	115.30
9	K	47	ARG	NE-CZ-NH1	6.97	123.79	120.30
2	B	485	ARG	NE-CZ-NH1	5.76	123.18	120.30
7	I	79	HIS	N-CA-CB	5.66	120.79	110.60
1	A	239	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	590	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	391	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	CYS	Peptide
1	A	120	GLU	Peptide
1	A	169	ASN	Peptide
1	A	324	SER	Peptide
1	A	451	HIS	Peptide
1	A	997	LEU	Peptide
2	B	1221	SER	Peptide
2	B	222	ILE	Peptide
2	B	474	SER	Peptide
2	B	635	ARG	Peptide
2	B	636	PRO	Peptide
2	B	730	ARG	Peptide
2	B	879	ARG	Peptide
2	B	883	LEU	Peptide
2	B	980	PHE	Peptide
3	C	172	PRO	Peptide
6	H	129	TYR	Peptide
6	H	136	LYS	Peptide
6	H	82	PRO	Peptide
7	I	20	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10961	0	11059	442	0
2	B	8792	0	8823	389	0
3	C	2095	0	2051	79	0
4	E	1752	0	1776	57	0
5	F	679	0	701	19	0
6	H	1068	0	1040	61	0
7	I	971	0	927	29	0
8	J	532	0	542	46	0
9	K	919	0	929	45	0
10	L	363	0	386	23	0
11	R	176	0	86	6	0
12	T	205	0	112	9	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	28521	0	28432	1091	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 19.

All (1091) 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)
6:H:109:LYS:HB3	6:H:110:ASP:CB	1.71	1.21
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.28	1.14
6:H:109:LYS:HB3	6:H:110:ASP:HB2	1.32	1.12
6:H:109:LYS:CB	6:H:110:ASP:HB2	1.80	1.11
2:B:472:ALA:HB3	2:B:473:MET:HB2	1.43	0.97
2:B:882:THR:HG21	2:B:935:ARG:HA	1.42	0.97
1:A:1173:HIS:CD2	1:A:1227:ILE:HG12	2.02	0.95
1:A:804:TYR:O	2:B:761:HIS:HB3	1.67	0.94
6:H:109:LYS:CA	6:H:110:ASP:HB2	1.98	0.93
1:A:327:ALA:HA	1:A:330:LYS:HB2	1.51	0.92
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.10	0.91
1:A:128:ILE:HG22	1:A:134:ARG:HG3	1.50	0.90
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.08	0.89
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.56	0.87
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.14	0.87
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:108:SER:O	6:H:109:LYS:HB2	1.73	0.86
4:E:132:ILE:HG22	4:E:133:GLU:H	1.41	0.84
4:E:46:TYR:CD2	4:E:58:MET:HG3	2.11	0.84
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.44	0.83
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.08	0.82
2:B:280:ILE:HG21	2:B:285:ILE:HG12	1.62	0.82
6:H:109:LYS:HB3	6:H:110:ASP:CA	2.09	0.81
4:E:132:ILE:HG22	4:E:133:GLU:N	1.93	0.81
1:A:257:ARG:HB2	1:A:258:GLY:CA	2.10	0.81
1:A:855:THR:HG21	1:A:857:ARG:HE	1.46	0.81
1:A:107:CYS:SG	1:A:114:LEU:HD22	2.22	0.80
2:B:1175:LEU:O	2:B:1176:ASN:HB2	1.79	0.80
1:A:649:ILE:O	1:A:653:VAL:HG23	1.82	0.79
4:E:46:TYR:CE2	4:E:58:MET:HG3	2.17	0.79
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.64	0.79
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.13	0.78
4:E:130:ALA:HB1	4:E:131:THR:HB	1.66	0.78
5:F:107:VAL:HG11	5:F:111:LEU:HD11	1.66	0.78
3:C:56:THR:HG21	3:C:145:CYS:SG	2.24	0.78
1:A:56:PRO:HD2	1:A:58:LEU:HD13	1.64	0.78
2:B:129:PHE:CE1	2:B:166:PHE:HB2	2.20	0.77
1:A:256:GLN:HA	1:A:257:ARG:O	1.83	0.77
2:B:800:GLN:HG2	8:J:52:THR:HG21	1.67	0.77
2:B:115:GLN:O	2:B:119:LEU:HD12	1.85	0.77
11:R:3:C:H2'	11:R:4:G:C8	2.20	0.76
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.66	0.76
1:A:67:CYS:SG	1:A:70:CYS:HB3	2.25	0.76
2:B:806:THR:HG23	2:B:809:MET:CE	2.15	0.76
10:L:48:CYS:SG	10:L:49:LYS:N	2.57	0.76
2:B:834:ASN:O	2:B:1013:ASN:HB2	1.85	0.76
1:A:76:GLU:O	1:A:78:PRO:HD3	1.87	0.75
10:L:53:HIS:O	10:L:55:ILE:HG12	1.86	0.75
3:C:66:ARG:NH2	8:J:5:VAL:HG23	2.02	0.75
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.53	0.74
2:B:120:ARG:HD2	2:B:955:THR:HG21	1.68	0.74
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.69	0.74
1:A:451:HIS:O	2:B:1137:CYS:SG	2.43	0.74
2:B:754:SER:O	2:B:806:THR:HG21	1.87	0.74
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.69	0.73
6:H:109:LYS:HA	6:H:110:ASP:HB2	1.68	0.73
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASP:HB3	1:A:323:LYS:CE	2.18	0.73
2:B:1129:ARG:HH21	2:B:1131:GLY:HA2	1.53	0.73
3:C:41:ILE:HG12	3:C:172:PRO:HG3	1.70	0.73
11:R:7:A:H2'	11:R:8:U:O4'	1.88	0.73
6:H:109:LYS:HB3	6:H:110:ASP:C	2.10	0.73
2:B:287:ARG:HG2	2:B:292:ILE:HD13	1.70	0.72
2:B:806:THR:HG23	2:B:809:MET:HE2	1.70	0.72
2:B:733:HIS:O	2:B:735:ALA:N	2.23	0.71
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.21	0.71
4:E:130:ALA:CB	4:E:131:THR:HB	2.20	0.71
1:A:901:LEU:HA	1:A:907:THR:HG23	1.71	0.71
2:B:475:SER:O	2:B:477:ALA:N	2.23	0.70
4:E:132:ILE:CG2	4:E:133:GLU:H	2.03	0.70
2:B:477:ALA:HB3	2:B:479:VAL:HG22	1.73	0.70
3:C:70:ILE:HD12	3:C:144:ILE:HD11	1.74	0.70
6:H:134:ASN:O	6:H:135:LEU:O	2.09	0.70
10:L:48:CYS:HB3	10:L:52:GLY:HA2	1.74	0.70
1:A:129:LYS:O	1:A:130:ASP:HB2	1.90	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.17	0.70
7:I:7:CYS:HB3	7:I:14:LEU:HD21	1.73	0.70
2:B:1103:ILE:N	2:B:1103:ILE:HD13	2.07	0.69
1:A:893:PHE:CE2	1:A:940:ARG:HG3	2.27	0.69
4:E:168:TYR:C	4:E:169:ARG:HG2	2.12	0.69
1:A:546:VAL:HG12	1:A:550:LEU:CD2	2.22	0.69
2:B:1099:VAL:CG1	2:B:1103:ILE:HD11	2.22	0.69
1:A:1173:HIS:NE2	1:A:1227:ILE:HG12	2.07	0.69
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.74	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.75	0.69
4:E:170:LEU:HD13	4:E:175:LEU:CD2	2.23	0.69
1:A:54:ASN:O	1:A:55:ASP:HB2	1.93	0.68
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.57	0.68
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.76	0.68
4:E:20:LYS:HE2	4:E:60:PHE:CZ	2.29	0.68
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.07	0.68
1:A:590:ARG:HH21	1:A:621:THR:HA	1.59	0.68
2:B:977:GLY:CA	2:B:1099:VAL:HG21	2.24	0.68
5:F:109:VAL:CG2	5:F:124:GLU:HG2	2.24	0.68
7:I:10:CYS:SG	7:I:31:THR:HB	2.34	0.68
1:A:913:LEU:HD11	1:A:981:LEU:O	1.94	0.67
2:B:329:THR:HA	2:B:332:ASP:HB2	1.76	0.67
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:HB2	1:A:324:SER:CA	2.24	0.67
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.76	0.67
3:C:36:VAL:HG23	9:K:41:THR:HG21	1.76	0.67
8:J:43:ARG:CG	8:J:46:CYS:SG	2.83	0.67
6:H:108:SER:O	6:H:109:LYS:CB	2.43	0.67
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.82	0.66
2:B:1155:SER:OG	2:B:1156:ASP:N	2.28	0.66
2:B:316:PRO:HA	2:B:319:GLU:HG3	1.76	0.66
2:B:617:ARG:HH11	2:B:617:ARG:HG2	1.59	0.66
2:B:737:THR:HG21	7:I:66:PRO:O	1.95	0.66
6:H:61:SER:O	6:H:62:SER:HB2	1.94	0.66
12:T:21:02I:H12'	12:T:22:DT:C6	2.30	0.66
1:A:257:ARG:CB	1:A:258:GLY:HA2	2.24	0.66
1:A:257:ARG:CB	1:A:258:GLY:CA	2.73	0.66
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.77	0.66
6:H:47:PHE:HB3	6:H:95:TYR:HD2	1.60	0.66
6:H:129:TYR:C	6:H:131:ASN:H	1.99	0.66
2:B:638:PHE:O	2:B:740:HIS:HB2	1.95	0.66
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.11	0.66
1:A:35:ILE:HG22	1:A:270:LEU:HD13	1.78	0.65
2:B:43:LEU:HD11	2:B:811:TYR:O	1.95	0.65
4:E:132:ILE:O	4:E:133:GLU:HG3	1.94	0.65
10:L:58:LYS:O	10:L:59:ALA:HB3	1.95	0.65
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.30	0.65
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.26	0.65
1:A:1436:ILE:O	1:A:1437:GLY:C	2.33	0.65
2:B:976:ILE:O	2:B:990:ILE:HB	1.97	0.65
2:B:981:ALA:O	2:B:982:SER:O	2.13	0.65
10:L:33:GLU:HG3	10:L:53:HIS:CB	2.27	0.65
2:B:981:ALA:HB3	2:B:987:LYS:HA	1.79	0.65
1:A:278:THR:O	1:A:278:THR:HG22	1.96	0.65
2:B:34:ILE:HD12	2:B:542:MET:HE1	1.79	0.65
2:B:635:ARG:CG	2:B:636:PRO:HD3	2.27	0.65
6:H:109:LYS:CB	6:H:110:ASP:CB	2.49	0.65
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.79	0.65
10:L:46:VAL:O	10:L:47:ARG:CB	2.45	0.65
9:K:65:HIS:HD2	9:K:67:PHE:H	1.45	0.65
1:A:203:SER:O	1:A:205:GLU:N	2.29	0.64
4:E:132:ILE:CG2	4:E:133:GLU:N	2.60	0.64
2:B:701:ILE:HG13	2:B:740:HIS:HE1	1.62	0.64
1:A:54:ASN:O	1:A:55:ASP:CB	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:THR:HG23	7:I:66:PRO:CB	2.27	0.64
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.78	0.64
3:C:133:ILE:HD11	3:C:237:SER:HA	1.77	0.64
2:B:546:SER:OG	2:B:631:GLY:N	2.31	0.64
2:B:555:ILE:HD11	2:B:582:VAL:HG11	1.80	0.64
1:A:344:ARG:CZ	2:B:1129:ARG:HG3	2.27	0.63
2:B:357:GLN:O	2:B:366:GLN:HA	1.98	0.63
1:A:532:ARG:O	1:A:535:THR:N	2.30	0.63
2:B:65:GLU:HG2	2:B:66:ASP:N	2.14	0.63
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.28	0.63
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.79	0.63
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.81	0.63
4:E:15:ALA:O	4:E:19:VAL:HG23	1.98	0.63
1:A:675:THR:HG21	1:A:736:ASN:HD21	1.63	0.62
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.81	0.62
1:A:68:GLN:OE1	1:A:80:HIS:CE1	2.53	0.62
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.81	0.62
4:E:64:PRO:CG	4:E:76:GLY:HA2	2.30	0.62
2:B:801:LYS:HG2	8:J:52:THR:HG23	1.81	0.62
1:A:1434:ALA:HB1	1:A:1436:ILE:HD12	1.82	0.62
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.34	0.62
7:I:17:ARG:HG2	7:I:18:GLU:H	1.65	0.62
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.81	0.62
1:A:648:ASN:O	1:A:652:VAL:HG23	2.00	0.62
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.81	0.62
2:B:635:ARG:HB2	2:B:636:PRO:HD3	1.82	0.62
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.35	0.61
1:A:316:GLN:O	1:A:317:LYS:O	2.18	0.61
1:A:89:PRO:O	1:A:204:THR:HG21	2.01	0.61
1:A:320:ARG:HB2	1:A:321:PRO:HA	1.82	0.61
8:J:52:THR:O	8:J:53:HIS:C	2.38	0.61
1:A:1172:LEU:O	1:A:1173:HIS:HB2	1.99	0.61
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.35	0.61
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.83	0.61
1:A:257:ARG:HB2	1:A:258:GLY:HA3	1.82	0.61
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.36	0.60
1:A:261:ASP:HB3	1:A:323:LYS:HD3	1.83	0.60
1:A:566:ILE:O	1:A:567:LYS:O	2.19	0.60
2:B:640:VAL:HG23	2:B:740:HIS:CA	2.29	0.60
2:B:322:PHE:CD1	2:B:322:PHE:O	2.55	0.60
2:B:25:ILE:HD12	2:B:651:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:CG	2:B:66:ASP:N	2.65	0.60
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.83	0.60
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.17	0.60
2:B:129:PHE:CD1	2:B:166:PHE:HB2	2.37	0.60
2:B:1081:LEU:O	3:C:189:THR:HG23	2.02	0.60
1:A:71:GLN:O	1:A:73:GLY:N	2.35	0.60
10:L:33:GLU:HG3	10:L:53:HIS:CG	2.36	0.60
10:L:33:GLU:HG3	10:L:53:HIS:HB2	1.82	0.59
1:A:302:THR:HA	1:A:305:ASP:O	2.02	0.59
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.85	0.59
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.83	0.59
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.32	0.59
2:B:471:LYS:N	2:B:472:ALA:HA	2.17	0.59
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.84	0.59
2:B:882:THR:HG22	2:B:883:LEU:N	2.18	0.59
6:H:44:VAL:O	6:H:44:VAL:HG12	2.03	0.59
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.84	0.59
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.49	0.59
9:K:63:VAL:HG23	9:K:63:VAL:O	2.02	0.59
1:A:805:LEU:C	1:A:805:LEU:HD12	2.23	0.59
1:A:125:ALA:O	1:A:134:ARG:CG	2.51	0.58
2:B:167:ILE:HG23	2:B:424:LEU:HD13	1.84	0.58
2:B:273:LEU:O	2:B:274:PRO:O	2.21	0.58
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.86	0.58
2:B:635:ARG:CB	2:B:636:PRO:HD3	2.33	0.58
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.69	0.58
1:A:1004:ASN:CG	1:A:1005:GLU:H	2.07	0.58
4:E:130:ALA:CA	4:E:131:THR:HB	2.34	0.58
4:E:192:ARG:O	4:E:192:ARG:HG3	2.03	0.58
1:A:262:LEU:O	1:A:266:LEU:HB2	2.03	0.58
2:B:617:ARG:NH1	2:B:619:ILE:HD13	2.18	0.58
3:C:3:GLU:HG3	3:C:4:GLU:H	1.68	0.58
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.69	0.58
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.38	0.58
2:B:1187:ASN:HD21	2:B:1190:ASP:CB	2.16	0.58
4:E:187:TYR:HD1	4:E:188:LEU:HD23	1.68	0.58
8:J:51:LEU:O	8:J:51:LEU:HD12	2.04	0.58
1:A:402:ALA:HB1	1:A:433:GLU:O	2.04	0.57
2:B:847:ASP:HB3	3:C:167:HIS:CE1	2.39	0.57
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.57
1:A:134:ARG:HD2	1:A:221:SER:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:VAL:CG1	8:J:60:PHE:HB2	2.32	0.57
1:A:391:LEU:HD13	1:A:400:PRO:O	2.04	0.57
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.04	0.57
2:B:31:TRP:HA	2:B:34:ILE:HG12	1.87	0.57
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.86	0.57
2:B:996:ARG:NH2	3:C:38:ILE:HD12	2.20	0.57
2:B:118:ARG:HA	2:B:207:GLY:HA2	1.87	0.57
2:B:701:ILE:HG12	2:B:702:LEU:N	2.19	0.57
4:E:28:TYR:HE2	4:E:78:LEU:HD13	1.70	0.57
1:A:452:LYS:HB2	2:B:1141:HIS:HE1	1.67	0.57
2:B:635:ARG:CD	2:B:636:PRO:HD3	2.34	0.57
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.86	0.57
2:B:274:PRO:O	2:B:276:ILE:N	2.38	0.57
2:B:638:PHE:O	2:B:740:HIS:CB	2.53	0.57
2:B:917:PRO:HA	2:B:933:SER:O	2.04	0.57
8:J:57:ILE:HA	8:J:60:PHE:HD1	1.70	0.57
10:L:58:LYS:O	10:L:59:ALA:CB	2.53	0.57
1:A:323:LYS:HB2	1:A:324:SER:O	2.05	0.57
3:C:141:GLY:O	3:C:142:VAL:O	2.23	0.57
3:C:98:VAL:C	3:C:99:LEU:HD23	2.25	0.57
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.70	0.57
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.35	0.57
1:A:128:ILE:CG2	1:A:134:ARG:HG3	2.31	0.56
1:A:528:LEU:O	1:A:528:LEU:HD12	2.05	0.56
1:A:530:GLY:C	1:A:532:ARG:N	2.58	0.56
3:C:251:LEU:O	3:C:255:VAL:HG23	2.05	0.56
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.87	0.56
2:B:428:ILE:HG13	2:B:448:ILE:HD13	1.88	0.56
2:B:563:MET:HG3	2:B:563:MET:O	2.04	0.56
2:B:798:TYR:CD2	8:J:4:PRO:HB3	2.41	0.56
1:A:267:ALA:O	1:A:271:LYS:N	2.38	0.56
2:B:822:ASN:O	8:J:48:ARG:NH1	2.39	0.56
1:A:511:ILE:HA	1:A:521:MET:HE2	1.85	0.56
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.87	0.56
2:B:1099:VAL:HG12	2:B:1103:ILE:CD1	2.30	0.56
4:E:130:ALA:HB1	4:E:131:THR:CB	2.33	0.56
7:I:17:ARG:HG2	7:I:18:GLU:N	2.21	0.56
1:A:583:PRO:O	1:A:610:GLY:HA3	2.06	0.56
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.87	0.56
8:J:3:VAL:HG12	8:J:4:PRO:HD2	1.88	0.56
1:A:89:PRO:O	1:A:204:THR:CG2	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.87	0.56
7:I:25:LEU:HB3	7:I:38:ALA:HB2	1.88	0.56
2:B:636:PRO:HD2	2:B:637:LEU:HB3	1.87	0.56
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.88	0.56
1:A:568:PRO:HB3	3:C:221:TYR:CE2	2.40	0.56
1:A:225:ASN:O	1:A:227:VAL:N	2.37	0.55
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	2.22	0.55
2:B:479:VAL:O	2:B:480:SER:HB3	2.05	0.55
4:E:23:VAL:HG13	4:E:28:TYR:HD2	1.71	0.55
6:H:59:ILE:O	6:H:60:ALA:HB3	2.07	0.55
1:A:834:THR:HG21	1:A:1077:THR:CA	2.37	0.55
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.88	0.55
2:B:901:PRO:O	2:B:949:VAL:O	2.24	0.55
4:E:129:PRO:O	4:E:130:ALA:HB3	2.06	0.55
2:B:128:LEU:HB3	2:B:167:ILE:O	2.06	0.55
1:A:1021:LEU:HD11	1:A:1025:ARG:NH1	2.22	0.55
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.05	0.55
2:B:957:ASN:O	2:B:959:ASP:N	2.39	0.55
6:H:106:GLU:C	6:H:108:SER:H	2.10	0.55
2:B:634:TYR:CE1	2:B:692:TYR:CD2	2.94	0.55
2:B:857:ARG:NH2	12:T:26:DG:OP2	2.39	0.55
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.88	0.55
1:A:265:LYS:CE	1:A:323:LYS:HE2	2.36	0.55
2:B:363:HIS:O	2:B:364:ILE:HB	2.07	0.55
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.39	0.55
6:H:109:LYS:CB	6:H:110:ASP:C	2.75	0.55
1:A:203:SER:O	1:A:206:GLU:N	2.39	0.55
2:B:1006:ILE:HD13	8:J:45:CYS:SG	2.47	0.55
2:B:698:GLU:O	2:B:701:ILE:HD12	2.07	0.55
4:E:64:PRO:HG3	4:E:76:GLY:HA2	1.89	0.55
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.87	0.55
2:B:284:ILE:HD12	2:B:324:ILE:HD12	1.88	0.55
2:B:378:LEU:O	2:B:382:ILE:HG12	2.07	0.55
3:C:173:ALA:O	3:C:233:GLU:O	2.25	0.55
4:E:28:TYR:CE2	4:E:78:LEU:HD13	2.42	0.55
1:A:120:GLU:HG2	1:A:120:GLU:O	2.07	0.55
1:A:323:LYS:HB2	1:A:324:SER:HA	1.88	0.55
1:A:469:ARG:NH2	2:B:991:GLY:O	2.40	0.55
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.89	0.55
9:K:49:GLU:HG3	9:K:94:ILE:HD11	1.88	0.55
1:A:1319:VAL:HB	1:A:1322:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:ILE:O	1:A:1439:GLY:N	2.40	0.54
2:B:471:LYS:CB	2:B:472:ALA:HA	2.38	0.54
6:H:93:TYR:CD2	6:H:143:LEU:HB3	2.42	0.54
12:T:24:DT:H2'	12:T:24:DT:O2	2.07	0.54
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.88	0.54
2:B:461:LEU:O	2:B:480:SER:OG	2.21	0.54
12:T:28:DT:OP1	12:T:28:DT:H4'	2.06	0.54
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.88	0.54
1:A:567:LYS:O	1:A:569:LYS:N	2.41	0.54
1:A:531:ILE:N	1:A:653:VAL:HG11	2.21	0.54
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	1.89	0.54
1:A:548:ASN:HD21	9:K:47:ARG:HE	1.56	0.54
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.54
2:B:211:VAL:O	2:B:480:SER:HA	2.08	0.54
2:B:638:PHE:CE2	2:B:743:ILE:HA	2.42	0.54
2:B:640:VAL:O	2:B:641:GLU:C	2.45	0.54
1:A:1021:LEU:CD1	1:A:1025:ARG:NH1	2.71	0.54
1:A:406:ILE:HD13	1:A:431:LYS:HB2	1.89	0.54
2:B:701:ILE:HG13	2:B:740:HIS:CE1	2.41	0.54
3:C:60:ASP:HB3	10:L:67:PHE:CE2	2.42	0.54
3:C:145:CYS:HA	8:J:2:ILE:HD11	1.89	0.54
9:K:32:VAL:HG23	9:K:74:ARG:HG3	1.88	0.54
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.88	0.54
2:B:273:LEU:HB3	2:B:274:PRO:HD2	1.89	0.54
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.37	0.54
3:C:37:MET:SD	3:C:232:VAL:HG21	2.48	0.54
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.74	0.54
1:A:481:ASP:OD1	1:A:481:ASP:N	2.41	0.54
2:B:863:GLU:O	2:B:864:LYS:HG3	2.08	0.54
3:C:120:ILE:HD11	3:C:130:GLY:O	2.07	0.54
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.08	0.53
1:A:331:GLY:O	1:A:332:LYS:HB3	2.08	0.53
9:K:49:GLU:CB	9:K:94:ILE:HD11	2.37	0.53
10:L:53:HIS:O	10:L:55:ILE:N	2.40	0.53
1:A:903:ASN:O	1:A:905:ASP:N	2.42	0.53
2:B:35:SER:O	2:B:39:ARG:HG3	2.08	0.53
1:A:265:LYS:HZ2	1:A:302:THR:HG23	1.73	0.53
1:A:544:ASP:OD1	1:A:545:GLN:N	2.41	0.53
1:A:737:LEU:HD11	1:A:758:ILE:HG21	1.91	0.53
6:H:109:LYS:CB	6:H:110:ASP:CA	2.81	0.53
6:H:32:THR:HG22	6:H:33:GLN:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:6:ARG:O	9:K:9:LEU:HG	2.07	0.53
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.44	0.53
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.90	0.53
1:A:1364:ASN:HD22	1:A:1366:ARG:CG	2.18	0.53
1:A:216:VAL:O	1:A:219:PHE:HB2	2.09	0.53
6:H:31:THR:O	6:H:32:THR:CB	2.56	0.53
11:R:2:U:H6	11:R:2:U:O5'	1.92	0.53
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.44	0.53
4:E:52:ARG:HB3	4:E:53:PRO:HD2	1.91	0.53
5:F:142:SER:O	5:F:143:PHE:HB3	2.08	0.53
7:I:7:CYS:SG	7:I:10:CYS:HB2	2.48	0.53
2:B:254:LEU:HD12	2:B:272:THR:O	2.08	0.53
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.74	0.53
2:B:882:THR:CG2	2:B:935:ARG:HA	2.29	0.53
3:C:16:ASP:HA	3:C:240:VAL:HG22	1.91	0.53
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.38	0.53
2:B:863:GLU:HG3	2:B:962:LYS:HB3	1.91	0.53
4:E:10:SER:O	4:E:14:ARG:HG3	2.08	0.53
1:A:630:ILE:HD12	1:A:630:ILE:H	1.74	0.52
1:A:67:CYS:O	1:A:68:GLN:OE1	2.27	0.52
2:B:114:PRO:CG	2:B:181:LEU:HD11	2.38	0.52
12:T:23:DC:H2'	12:T:23:DC:O2	2.08	0.52
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.89	0.52
6:H:104:PHE:CZ	6:H:136:LYS:HA	2.44	0.52
1:A:1101:LEU:HG	1:A:1105:LEU:HD12	1.92	0.52
2:B:800:GLN:CG	8:J:52:THR:HG21	2.38	0.52
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.43	0.52
1:A:332:LYS:H	1:A:337:ARG:CB	2.23	0.52
3:C:99:LEU:HD23	3:C:99:LEU:N	2.24	0.52
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.90	0.52
1:A:852:TYR:HH	1:A:1441:PHE:HD2	1.56	0.52
1:A:1188:GLN:NE2	1:A:1188:GLN:H	2.07	0.52
2:B:44:VAL:HG11	2:B:495:LEU:HD13	1.92	0.52
7:I:8:ARG:O	7:I:10:CYS:N	2.43	0.52
10:L:34:CYS:SG	10:L:35:SER:N	2.80	0.52
1:A:219:PHE:O	1:A:222:LEU:O	2.27	0.52
2:B:119:LEU:HD23	2:B:953:LEU:HD13	1.92	0.52
2:B:701:ILE:CG1	2:B:740:HIS:HE1	2.23	0.52
4:E:78:LEU:HA	4:E:107:THR:HG22	1.92	0.52
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.92	0.52
11:R:1:A:H8	11:R:1:A:O5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:O	1:A:243:PRO:HG3	2.09	0.52
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.92	0.52
1:A:622:VAL:HG22	1:A:622:VAL:O	2.10	0.52
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.10	0.52
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.39	0.52
2:B:701:ILE:CB	2:B:740:HIS:HE1	2.23	0.52
2:B:933:SER:OG	2:B:934:LYS:N	2.41	0.52
1:A:1171:GLN:HB2	1:A:1172:LEU:HD23	1.91	0.51
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.92	0.51
1:A:30:ILE:O	2:B:1183:LYS:NZ	2.43	0.51
2:B:977:GLY:C	2:B:1099:VAL:CG2	2.78	0.51
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.92	0.51
2:B:862:GLN:O	2:B:914:LYS:NZ	2.42	0.51
5:F:73:ALA:O	5:F:74:ILE:HG12	2.10	0.51
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.51	0.51
1:A:125:ALA:O	1:A:134:ARG:HG3	2.11	0.51
1:A:387:ARG:O	1:A:391:LEU:HD23	2.10	0.51
1:A:853:ASP:OD2	1:A:855:THR:CG2	2.58	0.51
2:B:868:MET:O	2:B:869:SER:CB	2.58	0.51
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.51
1:A:919:ILE:HG21	1:A:925:LEU:HD12	1.91	0.51
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.91	0.51
2:B:957:ASN:HB3	2:B:961:LEU:HD12	1.90	0.51
3:C:145:CYS:SG	3:C:146:LYS:N	2.83	0.51
2:B:123:THR:HG23	2:B:205:ILE:HD13	1.92	0.51
2:B:34:ILE:HD11	2:B:743:ILE:HG22	1.92	0.51
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.75	0.51
1:A:1022:LEU:CD1	1:A:1026:LEU:HD12	2.40	0.51
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.92	0.51
2:B:682:SER:O	2:B:686:ASN:ND2	2.44	0.51
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.25	0.51
8:J:10:CYS:SG	8:J:11:GLY:N	2.83	0.51
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.50	0.51
1:A:852:TYR:CD1	1:A:1060:PRO:HB2	2.45	0.51
2:B:34:ILE:N	2:B:34:ILE:HD13	2.24	0.51
1:A:567:LYS:HB3	6:H:96:VAL:N	2.25	0.51
9:K:47:ARG:HH11	9:K:47:ARG:HG2	1.75	0.51
1:A:1022:LEU:O	1:A:1026:LEU:HB2	2.11	0.51
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.93	0.51
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.92	0.51
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1006:ILE:CD1	8:J:45:CYS:SG	2.98	0.51
3:C:134:ILE:CD1	3:C:141:GLY:HA3	2.41	0.51
2:B:660:LYS:O	2:B:663:ALA:HB3	2.10	0.51
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.93	0.51
2:B:899:ILE:HD11	2:B:911:ILE:HG12	1.93	0.51
4:E:36:GLU:O	4:E:38:PRO:HD3	2.11	0.51
1:A:1188:GLN:CD	1:A:1188:GLN:H	2.14	0.51
1:A:167:CYS:SG	1:A:167:CYS:O	2.69	0.51
1:A:530:GLY:C	1:A:532:ARG:H	2.12	0.51
2:B:34:ILE:HD12	2:B:542:MET:CE	2.41	0.51
2:B:809:MET:HE1	2:B:983:ARG:NH2	2.26	0.51
4:E:130:ALA:HB1	4:E:131:THR:CG2	2.40	0.51
1:A:32:VAL:HB	1:A:57:ARG:HB2	1.93	0.51
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.75	0.51
2:B:65:GLU:CG	2:B:66:ASP:H	2.24	0.51
3:C:41:ILE:CG1	3:C:172:PRO:HG3	2.40	0.51
5:F:81:THR:CG2	5:F:136:ARG:HD3	2.41	0.51
1:A:857:ARG:CZ	5:F:139:PRO:HG2	2.41	0.51
8:J:28:ASP:N	8:J:28:ASP:OD1	2.44	0.51
1:A:1053:PHE:O	1:A:1056:SER:N	2.36	0.50
2:B:463:THR:HG21	2:B:465:ASN:ND2	2.27	0.50
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.41	0.50
4:E:43:LYS:O	4:E:47:CYS:HB2	2.12	0.50
6:H:89:LEU:C	6:H:91:ASP:H	2.14	0.50
7:I:7:CYS:C	7:I:8:ARG:O	2.49	0.50
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.42	0.50
1:A:547:LEU:HD22	9:K:58:PHE:HD1	1.77	0.50
1:A:432:VAL:O	1:A:433:GLU:C	2.49	0.50
1:A:567:LYS:HB3	6:H:96:VAL:H	1.75	0.50
1:A:892:ALA:HA	1:A:895:LYS:HD3	1.93	0.50
2:B:1162:ILE:HD13	2:B:1168:LEU:C	2.32	0.50
2:B:841:MET:SD	2:B:990:ILE:HD11	2.51	0.50
3:C:260:LEU:O	3:C:264:GLN:HG3	2.12	0.50
6:H:31:THR:O	6:H:32:THR:OG1	2.29	0.50
6:H:76:THR:HG22	6:H:76:THR:O	2.12	0.50
4:E:204:THR:HG22	4:E:205:SER:N	2.27	0.50
1:A:705:LYS:HG3	1:A:713:SER:HB3	1.93	0.50
2:B:1170:THR:O	2:B:1170:THR:HG22	2.10	0.50
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.50
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.43	0.50
2:B:274:PRO:HG2	2:B:359:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:PRO:HB2	2:B:701:ILE:HD11	1.94	0.50
2:B:760:ASP:OD1	2:B:760:ASP:N	2.44	0.50
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.94	0.50
10:L:43:THR:O	10:L:43:THR:HG22	2.12	0.50
2:B:104:GLU:HG3	10:L:54:ARG:NH2	2.27	0.50
4:E:130:ALA:HA	4:E:131:THR:HB	1.92	0.50
6:H:93:TYR:CD2	6:H:143:LEU:CB	2.94	0.50
3:C:145:CYS:HA	8:J:2:ILE:CD1	2.41	0.50
1:A:1166:ASP:O	1:A:1170:ILE:HG12	2.11	0.50
1:A:265:LYS:HE3	1:A:323:LYS:HE2	1.93	0.50
1:A:472:LEU:HD11	2:B:835:GLN:HE22	1.76	0.50
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.75	0.50
5:F:103:MET:O	5:F:105:ALA:N	2.45	0.50
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.93	0.50
1:A:1292:PRO:HD3	1:A:1298:TYR:CE2	2.47	0.50
1:A:1434:ALA:CB	1:A:1436:ILE:HD12	2.40	0.50
1:A:404:TYR:HB2	1:A:433:GLU:HG3	1.93	0.50
1:A:61:ILE:O	1:A:63:ARG:N	2.44	0.50
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.12	0.50
2:B:472:ALA:CB	2:B:473:MET:HB2	2.29	0.50
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.94	0.50
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.79	0.50
10:L:46:VAL:O	10:L:47:ARG:HB2	2.11	0.50
1:A:902:LEU:O	1:A:903:ASN:CB	2.60	0.49
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.47	0.49
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.12	0.49
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.77	0.49
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.94	0.49
7:I:119:THR:O	7:I:119:THR:HG22	2.12	0.49
2:B:1076:HIS:CG	9:K:40:HIS:CD2	2.99	0.49
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.47	0.49
1:A:257:ARG:HB2	1:A:258:GLY:HA2	1.83	0.49
1:A:403:LYS:O	1:A:404:TYR:O	2.30	0.49
1:A:56:PRO:CD	1:A:57:ARG:H	2.25	0.49
1:A:881:GLN:NE2	1:A:958:VAL:O	2.45	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.94	0.49
1:A:1101:LEU:HG	1:A:1105:LEU:CD1	2.42	0.49
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.48	0.49
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.42	0.49
1:A:107:CYS:SG	1:A:107:CYS:O	2.71	0.49
1:A:590:ARG:HB3	1:A:605:MET:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.95	0.49
4:E:128:PRO:HA	4:E:130:ALA:H	1.78	0.49
1:A:1004:ASN:HD22	4:E:167:ARG:HD2	1.76	0.49
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.41	0.49
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.42	0.49
1:A:946:VAL:HG22	4:E:201:LYS:HB3	1.94	0.49
2:B:562:GLY:O	2:B:563:MET:C	2.51	0.49
2:B:63:ILE:CD1	2:B:95:ILE:HD12	2.43	0.49
2:B:30:SER:O	2:B:34:ILE:HD13	2.12	0.49
2:B:430:ARG:HA	2:B:433:GLN:HB2	1.95	0.49
2:B:788:ARG:NH1	2:B:790:ASP:OD2	2.41	0.49
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.48	0.49
6:H:109:LYS:CA	6:H:110:ASP:CB	2.77	0.49
9:K:47:ARG:HH11	9:K:47:ARG:CG	2.26	0.49
2:B:100:PRO:HA	2:B:126:SER:HA	1.94	0.49
2:B:361:LEU:O	2:B:363:HIS:O	2.31	0.49
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.95	0.49
1:A:213:HIS:O	1:A:214:ILE:O	2.30	0.49
1:A:380:VAL:CG2	1:A:430:TRP:H	2.25	0.49
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.95	0.49
1:A:1266:THR:O	1:A:1271:ILE:HG12	2.13	0.48
1:A:257:ARG:HB3	1:A:258:GLY:HA2	1.94	0.48
2:B:868:MET:O	2:B:869:SER:HB3	2.13	0.48
3:C:175:ALA:HB3	8:J:43:ARG:NH2	2.27	0.48
1:A:530:GLY:O	1:A:532:ARG:N	2.46	0.48
1:A:633:VAL:HG11	1:A:645:LEU:HD22	1.95	0.48
2:B:313:MET:O	2:B:316:PRO:HD2	2.13	0.48
5:F:79:ARG:NH2	5:F:145:ASP:O	2.47	0.48
1:A:1437:GLY:HA3	5:F:88:TYR:CD1	2.48	0.48
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.95	0.48
8:J:3:VAL:HG12	8:J:4:PRO:CD	2.43	0.48
1:A:1404:GLU:O	1:A:1408:ILE:HG12	2.13	0.48
1:A:56:PRO:CD	1:A:58:LEU:HD13	2.37	0.48
1:A:623:GLY:O	1:A:630:ILE:HD13	2.13	0.48
2:B:1104:HIS:HB2	2:B:1122:ARG:HB2	1.95	0.48
2:B:34:ILE:HD12	2:B:743:ILE:HG21	1.95	0.48
2:B:639:ILE:HA	2:B:740:HIS:HB3	1.96	0.48
9:K:46:ILE:HG23	9:K:50:LEU:HD12	1.94	0.48
1:A:274:ILE:HG22	1:A:274:ILE:O	2.13	0.48
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.79	0.48
2:B:366:GLN:O	2:B:367:LEU:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:MET:HE3	2:B:853:SER:HB3	1.94	0.48
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.28	0.48
1:A:990:VAL:CG2	1:A:1026:LEU:HB3	2.44	0.48
2:B:46:GLN:HG3	2:B:47:GLN:H	1.79	0.48
2:B:479:VAL:O	2:B:480:SER:CB	2.61	0.48
2:B:485:ARG:HG3	2:B:485:ARG:HH11	1.77	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.13	0.48
1:A:91:PHE:HD2	1:A:297:GLN:OE1	1.97	0.48
2:B:637:LEU:HA	2:B:743:ILE:HG12	1.96	0.48
5:F:80:ALA:O	5:F:81:THR:C	2.51	0.48
1:A:1172:LEU:HD23	1:A:1172:LEU:N	2.29	0.48
1:A:1238:ILE:HG22	1:A:1240:CYS:SG	2.54	0.48
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.44	0.48
1:A:919:ILE:CG2	1:A:925:LEU:HD12	2.43	0.48
4:E:204:THR:CG2	4:E:205:SER:N	2.76	0.48
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.48	0.48
1:A:265:LYS:NZ	1:A:302:THR:CG2	2.76	0.48
1:A:290:GLU:HA	1:A:293:GLU:HG3	1.96	0.48
2:B:956:THR:HA	2:B:961:LEU:O	2.14	0.48
4:E:164:LEU:HD13	4:E:211:TYR:CE2	2.49	0.48
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.95	0.48
8:J:57:ILE:HA	8:J:60:PHE:CD1	2.49	0.48
1:A:319:GLY:O	1:A:320:ARG:HG3	2.14	0.48
1:A:351:THR:CG2	2:B:1103:ILE:HD12	2.42	0.48
2:B:552:MET:N	2:B:553:PRO:HD2	2.29	0.48
2:B:976:ILE:HG22	2:B:977:GLY:N	2.29	0.48
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.96	0.48
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.95	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.96	0.48
2:B:471:LYS:HB2	2:B:472:ALA:HA	1.96	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.96	0.48
4:E:127:ILE:HG12	4:E:127:ILE:O	2.13	0.48
1:A:67:CYS:O	1:A:70:CYS:HB3	2.13	0.47
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.96	0.47
7:I:26:LEU:HD22	7:I:35:VAL:CG1	2.44	0.47
8:J:7:CYS:HA	8:J:49:MET:HE3	1.96	0.47
1:A:1021:LEU:CD1	1:A:1025:ARG:HH11	2.27	0.47
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.44	0.47
2:B:797:TYR:C	2:B:799:PRO:HD2	2.34	0.47
2:B:809:MET:HE1	2:B:983:ARG:HH21	1.78	0.47
2:B:863:GLU:HG3	2:B:962:LYS:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:129:TYR:C	6:H:131:ASN:N	2.66	0.47
2:B:778:MET:CE	2:B:853:SER:HB3	2.45	0.47
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.96	0.47
9:K:92:ASN:O	9:K:93:SER:C	2.52	0.47
1:A:1120:LEU:HB3	1:A:1124:HIS:O	2.13	0.47
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.96	0.47
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.47
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.96	0.47
2:B:363:HIS:O	2:B:364:ILE:CB	2.62	0.47
2:B:435:THR:O	2:B:437:GLU:N	2.47	0.47
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.39	0.47
1:A:40:THR:HG22	1:A:41:MET:SD	2.55	0.47
1:A:469:ARG:HE	9:K:67:PHE:HZ	1.63	0.47
1:A:830:LYS:HG3	1:A:1098:VAL:HG21	1.96	0.47
2:B:761:HIS:CD2	2:B:761:HIS:N	2.82	0.47
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.49	0.47
2:B:167:ILE:HD12	2:B:424:LEU:HD11	1.95	0.47
2:B:994:TYR:HB2	2:B:999:MET:CE	2.45	0.47
8:J:37:SER:OG	8:J:47:ARG:NH2	2.48	0.47
9:K:49:GLU:HB2	9:K:94:ILE:HD11	1.96	0.47
1:A:1042:PHE:CE2	1:A:1046:LEU:HD12	2.50	0.47
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.49	0.47
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.48	0.47
1:A:278:THR:CG2	1:A:278:THR:O	2.61	0.47
1:A:179:LEU:HD13	1:A:297:GLN:HG3	1.95	0.47
1:A:314:ALA:O	1:A:321:PRO:O	2.32	0.47
1:A:990:VAL:CG2	1:A:1026:LEU:HD13	2.45	0.47
2:B:114:PRO:HG3	2:B:181:LEU:CD1	2.44	0.47
2:B:977:GLY:CA	2:B:1099:VAL:CG2	2.92	0.47
2:B:1076:HIS:CG	9:K:40:HIS:HD2	2.32	0.47
2:B:446:LEU:O	2:B:447:ALA:HB3	2.14	0.47
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.97	0.47
8:J:2:ILE:C	8:J:53:HIS:NE2	2.68	0.47
1:A:261:ASP:HB3	1:A:323:LYS:HE3	1.96	0.47
1:A:535:THR:HG21	1:A:617:VAL:H	1.80	0.47
1:A:1134:ILE:O	1:A:1135:ARG:C	2.54	0.47
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.97	0.47
1:A:1393:ASN:O	1:A:1394:THR:O	2.33	0.46
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.45	0.46
2:B:34:ILE:CD1	2:B:743:ILE:CG2	2.93	0.46
6:H:42:ILE:HD12	6:H:95:TYR:CE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:H	1:A:1308:THR:HB	1.80	0.46
1:A:548:ASN:HA	9:K:60:ALA:HB1	1.96	0.46
1:A:737:LEU:HB2	1:A:744:LYS:HD2	1.97	0.46
1:A:942:PHE:C	1:A:942:PHE:CD1	2.89	0.46
2:B:475:SER:C	2:B:477:ALA:H	2.18	0.46
2:B:617:ARG:NH1	2:B:617:ARG:HG2	2.27	0.46
3:C:163:ILE:CD1	9:K:10:PHE:CZ	2.98	0.46
3:C:163:ILE:HD11	9:K:10:PHE:CZ	2.50	0.46
1:A:1327:ILE:O	1:A:1327:ILE:HG23	2.16	0.46
1:A:169:ASN:HD22	1:A:169:ASN:N	2.13	0.46
1:A:323:LYS:CB	1:A:324:SER:HA	2.45	0.46
1:A:919:ILE:O	1:A:920:LEU:C	2.54	0.46
4:E:114:ASN:O	4:E:115:ASN:CB	2.64	0.46
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.98	0.46
7:I:7:CYS:SG	7:I:8:ARG:O	2.74	0.46
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.15	0.46
1:A:108:MET:N	1:A:108:MET:SD	2.89	0.46
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.46	0.46
2:B:25:ILE:HG22	2:B:26:THR:N	2.30	0.46
3:C:262:LEU:HD21	9:K:19:LEU:HD12	1.97	0.46
1:A:1021:LEU:HD11	1:A:1025:ARG:HH11	1.80	0.46
1:A:990:VAL:HG22	1:A:1026:LEU:CD1	2.45	0.46
1:A:706:HIS:CG	1:A:1135:ARG:HH21	2.33	0.46
1:A:495:GLU:HA	1:A:498:ARG:HG3	1.98	0.46
4:E:77:SER:HB3	4:E:105:PHE:HD1	1.81	0.46
6:H:129:TYR:O	6:H:131:ASN:N	2.45	0.46
6:H:139:ASN:O	6:H:140:ALA:HB2	2.16	0.46
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.97	0.46
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	2.14	0.46
1:A:531:ILE:HD13	1:A:649:ILE:CG2	2.46	0.46
1:A:65:LEU:O	1:A:67:CYS:N	2.44	0.46
1:A:351:THR:HG23	2:B:1103:ILE:HG23	1.97	0.46
2:B:1146:PHE:CZ	2:B:1150:ARG:HG3	2.51	0.46
6:H:109:LYS:HB3	6:H:110:ASP:HB3	1.81	0.46
7:I:15:TYR:O	7:I:27:PHE:HA	2.16	0.46
1:A:1132:LYS:O	1:A:1135:ARG:HB3	2.16	0.46
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.30	0.46
1:A:304:MET:CG	2:B:1210:MET:HG3	2.45	0.46
1:A:765:VAL:HG23	1:A:802:ASN:O	2.16	0.46
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.15	0.46
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:MET:HB2	9:K:45:LEU:CD1	2.46	0.46
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.16	0.46
1:A:1146:VAL:HG12	1:A:1201:ALA:HB3	1.98	0.46
1:A:517:ASN:ND2	1:A:1364:ASN:OD1	2.48	0.46
1:A:367:PRO:HA	1:A:463:ILE:HD12	1.98	0.46
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.97	0.46
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.16	0.46
2:B:354:ASP:O	2:B:357:GLN:N	2.49	0.46
2:B:745:PRO:C	2:B:747:MET:H	2.19	0.46
2:B:752:ALA:O	2:B:755:ILE:HB	2.15	0.46
1:A:265:LYS:HZ3	1:A:302:THR:HG23	1.80	0.46
1:A:608:ILE:HG12	1:A:613:ILE:HG13	1.98	0.46
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.98	0.46
1:A:763:ALA:O	1:A:803:SER:HB3	2.15	0.46
1:A:975:HIS:HA	1:A:1036:ARG:HD2	1.98	0.46
2:B:1024:ALA:O	2:B:1025:HIS:C	2.54	0.46
2:B:219:ALA:HB3	2:B:222:ILE:HD11	1.98	0.46
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.51	0.46
7:I:119:THR:C	7:I:120:GLN:CG	2.84	0.46
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.98	0.45
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.97	0.45
1:A:134:ARG:NH1	1:A:221:SER:HA	2.30	0.45
1:A:247:ARG:CG	1:A:247:ARG:O	2.64	0.45
1:A:892:ALA:HA	1:A:895:LYS:HB2	1.97	0.45
1:A:933:TYR:O	1:A:937:VAL:HG23	2.16	0.45
2:B:288:ALA:O	2:B:327:ARG:NH2	2.48	0.45
2:B:698:GLU:O	2:B:701:ILE:CD1	2.63	0.45
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.51	0.45
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.45
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.46	0.45
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.98	0.45
5:F:111:LEU:N	5:F:111:LEU:CD1	2.79	0.45
6:H:47:PHE:HB3	6:H:95:TYR:CD2	2.45	0.45
12:T:21:02I:C8	12:T:22:DT:H72	2.45	0.45
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.98	0.45
1:A:294:SER:O	1:A:298:PHE:HB3	2.16	0.45
1:A:808:LEU:O	2:B:728:ARG:NH1	2.49	0.45
1:A:997:LEU:O	1:A:1053:PHE:CE1	2.70	0.45
2:B:800:GLN:HG2	8:J:52:THR:CG2	2.43	0.45
5:F:98:ALA:HA	5:F:101:ILE:HD12	1.99	0.45
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:VAL:O	1:A:722:LEU:HD12	2.17	0.45
1:A:913:LEU:HD12	1:A:915:SER:H	1.80	0.45
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.99	0.45
8:J:45:CYS:SG	8:J:46:CYS:N	2.90	0.45
1:A:56:PRO:HD2	1:A:57:ARG:H	1.81	0.45
1:A:605:MET:SD	1:A:621:THR:HG21	2.57	0.45
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.56	0.45
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.98	0.45
1:A:990:VAL:HG21	1:A:1026:LEU:HB3	1.99	0.45
2:B:128:LEU:HD12	2:B:128:LEU:HA	1.84	0.45
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.97	0.45
2:B:832:GLY:O	2:B:835:GLN:NE2	2.49	0.45
6:H:5:LEU:HD22	6:H:133:ASN:O	2.17	0.45
9:K:57:LEU:HD12	9:K:76:GLN:CG	2.46	0.45
1:A:675:THR:HG21	1:A:736:ASN:ND2	2.28	0.45
2:B:287:ARG:HG2	2:B:292:ILE:CD1	2.44	0.45
2:B:635:ARG:HD2	2:B:636:PRO:HD3	1.98	0.45
11:R:5:A:N1	12:T:24:DT:O4	2.50	0.45
1:A:209:ASN:O	1:A:210:ILE:C	2.54	0.45
1:A:341:MET:HE3	1:A:341:MET:HB3	1.53	0.45
1:A:338:GLY:O	1:A:342:GLY:O	2.34	0.45
2:B:1024:ALA:O	2:B:1027:ILE:N	2.50	0.45
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.98	0.45
2:B:364:ILE:O	2:B:365:THR:HB	2.17	0.45
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.98	0.45
2:B:421:PHE:O	2:B:425:THR:HB	2.15	0.45
2:B:737:THR:HG23	7:I:66:PRO:HB3	1.98	0.45
2:B:780:VAL:HA	2:B:795:ILE:HG23	1.98	0.45
1:A:870:GLU:CB	4:E:204:THR:HG21	2.47	0.45
4:E:65:THR:C	4:E:67:GLU:H	2.20	0.45
7:I:75:CYS:HB3	7:I:103:CYS:HB2	1.99	0.45
1:A:323:LYS:HB2	1:A:324:SER:C	2.37	0.45
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.97	0.45
3:C:124:LEU:O	3:C:127:ARG:HG2	2.17	0.45
4:E:78:LEU:HD12	4:E:107:THR:HG21	1.99	0.45
1:A:805:LEU:C	1:A:805:LEU:CD1	2.85	0.45
1:A:98:LYS:O	1:A:102:VAL:HG22	2.17	0.45
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.17	0.45
2:B:628:THR:O	2:B:628:THR:CG2	2.64	0.45
2:B:798:TYR:N	2:B:799:PRO:CD	2.80	0.45
10:L:31:CYS:SG	10:L:32:ALA:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.99	0.45
2:B:291:ILE:HG21	2:B:300:HIS:CD2	2.51	0.45
1:A:326:ARG:O	1:A:330:LYS:N	2.50	0.44
2:B:22:SER:O	2:B:654:ARG:HD2	2.17	0.44
3:C:134:ILE:HD12	3:C:141:GLY:N	2.32	0.44
3:C:17:ASN:OD1	3:C:233:GLU:HG3	2.17	0.44
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.98	0.44
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.82	0.44
1:A:971:PHE:O	1:A:972:HIS:C	2.55	0.44
2:B:636:PRO:CD	2:B:637:LEU:HB3	2.47	0.44
2:B:104:GLU:HG3	10:L:54:ARG:HH21	1.82	0.44
1:A:120:GLU:HG3	1:A:123:ARG:HD3	2.00	0.44
1:A:265:LYS:HZ3	1:A:302:THR:CG2	2.30	0.44
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.52	0.44
1:A:380:VAL:HG23	1:A:430:TRP:H	1.82	0.44
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.50	0.44
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.97	0.44
2:B:745:PRO:O	2:B:747:MET:N	2.50	0.44
1:A:99:ILE:HA	1:A:102:VAL:CG2	2.47	0.44
1:A:543:LEU:O	1:A:547:LEU:HG	2.17	0.44
1:A:90:VAL:HG13	1:A:297:GLN:HB2	1.99	0.44
2:B:1180:PHE:O	2:B:1181:GLU:O	2.35	0.44
1:A:15:LYS:HB3	2:B:1220:ARG:HA	2.00	0.44
2:B:737:THR:HG23	7:I:66:PRO:HB2	1.99	0.44
4:E:114:ASN:O	4:E:115:ASN:HB3	2.18	0.44
1:A:1057:VAL:HG12	1:A:1058:VAL:O	2.18	0.44
2:B:295:GLY:HA2	2:B:298:LEU:HG	1.98	0.44
2:B:701:ILE:HB	2:B:740:HIS:CE1	2.52	0.44
2:B:785:TYR:CD1	2:B:785:TYR:C	2.90	0.44
2:B:849:GLY:HA2	2:B:852:ARG:HD2	2.00	0.44
2:B:955:THR:HG22	2:B:956:THR:N	2.32	0.44
3:C:46:ILE:HA	3:C:159:ALA:HA	1.98	0.44
7:I:2:THR:O	7:I:3:THR:C	2.56	0.44
1:A:546:VAL:HG12	1:A:550:LEU:HD23	1.97	0.44
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.66	0.44
6:H:40:LEU:CD2	6:H:42:ILE:HD11	2.48	0.44
1:A:265:LYS:C	1:A:267:ALA:H	2.21	0.44
1:A:476:SER:N	1:A:477:PRO:HD2	2.33	0.44
1:A:507:VAL:N	1:A:508:PRO:CD	2.80	0.44
1:A:733:ALA:O	1:A:735:VAL:N	2.51	0.44
2:B:174:LEU:HD23	2:B:202:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:634:TYR:HE1	2:B:692:TYR:CD2	2.34	0.44
2:B:635:ARG:CB	2:B:636:PRO:CD	2.95	0.44
7:I:17:ARG:CG	7:I:18:GLU:H	2.27	0.44
1:A:1158:PRO:HB3	1:A:1188:GLN:HG3	1.99	0.44
1:A:54:ASN:OD1	1:A:54:ASN:O	2.36	0.44
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.52	0.44
1:A:913:LEU:HD12	1:A:914:GLU:N	2.33	0.44
2:B:1161:HIS:CD2	2:B:1173:ALA:HB2	2.53	0.44
2:B:314:LEU:C	2:B:316:PRO:HD2	2.38	0.44
2:B:361:LEU:N	2:B:362:PRO:CD	2.80	0.44
2:B:485:ARG:HH11	2:B:485:ARG:CG	2.31	0.44
6:H:82:PRO:O	6:H:83:GLN:HB2	2.17	0.44
3:C:6:PRO:HG2	9:K:97:LYS:HB3	2.00	0.44
1:A:1004:ASN:CG	1:A:1005:GLU:N	2.70	0.44
1:A:129:LYS:O	1:A:130:ASP:CB	2.62	0.44
1:A:242:PRO:O	1:A:247:ARG:NH2	2.44	0.44
1:A:532:ARG:HG2	1:A:533:LYS:N	2.33	0.44
2:B:247:GLY:O	2:B:248:SER:CB	2.66	0.44
2:B:642:ASP:O	2:B:644:GLU:N	2.51	0.44
3:C:39:ALA:HA	3:C:164:ALA:CB	2.47	0.44
6:H:42:ILE:HD12	6:H:95:TYR:CZ	2.53	0.44
3:C:166:GLU:O	9:K:6:ARG:NH1	2.50	0.44
1:A:1004:ASN:ND2	4:E:167:ARG:CD	2.80	0.43
1:A:1422:ARG:HH21	2:B:1220:ARG:HD3	1.83	0.43
1:A:314:ALA:HB1	1:A:321:PRO:HB2	2.00	0.43
1:A:325:ILE:O	1:A:328:ARG:HB2	2.18	0.43
1:A:834:THR:HG21	1:A:1077:THR:HA	2.00	0.43
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.00	0.43
2:B:640:VAL:O	2:B:640:VAL:HG12	2.17	0.43
4:E:135:PHE:CB	4:E:140:LEU:HD11	2.48	0.43
6:H:101:ALA:HB2	6:H:116:TYR:CE1	2.53	0.43
11:R:2:U:C6	11:R:2:U:O5'	2.71	0.43
1:A:1015:VAL:O	1:A:1016:THR:C	2.56	0.43
1:A:209:ASN:O	1:A:212:LYS:N	2.51	0.43
1:A:582:ILE:CG2	1:A:610:GLY:HA2	2.49	0.43
2:B:1168:LEU:HD22	2:B:1208:MET:SD	2.58	0.43
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.28	0.43
2:B:36:ALA:C	2:B:37:PHE:O	2.53	0.43
2:B:473:MET:C	2:B:475:SER:H	2.21	0.43
1:A:148:CYS:HB3	1:A:167:CYS:O	2.17	0.43
1:A:553:VAL:HG22	1:A:652:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:792:MET:HE3	12:T:26:DG:OP1	2.18	0.43
3:C:144:ILE:HD13	3:C:144:ILE:HA	1.89	0.43
9:K:91:CYS:O	9:K:94:ILE:HB	2.19	0.43
10:L:34:CYS:O	10:L:35:SER:CB	2.66	0.43
1:A:1160:SER:HA	1:A:1170:ILE:HG21	2.00	0.43
2:B:1134:GLU:N	2:B:1134:GLU:OE1	2.51	0.43
2:B:203:PHE:HE2	2:B:212:LEU:HD12	1.84	0.43
2:B:333:PHE:O	2:B:333:PHE:CD1	2.71	0.43
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.53	0.43
2:B:596:LEU:O	2:B:599:THR:HB	2.18	0.43
2:B:728:ARG:NH2	2:B:760:ASP:OD2	2.49	0.43
2:B:790:ASP:N	2:B:790:ASP:OD1	2.51	0.43
2:B:806:THR:CG2	2:B:809:MET:HE2	2.44	0.43
12:T:22:DT:H5"	12:T:22:DT:H6	1.83	0.43
1:A:33:ALA:HA	1:A:56:PRO:CG	2.48	0.43
1:A:399:HIS:O	1:A:435:HIS:ND1	2.52	0.43
1:A:690:VAL:HG13	1:A:718:VAL:HG22	2.00	0.43
3:C:36:VAL:HG23	9:K:41:THR:CG2	2.45	0.43
8:J:43:ARG:O	8:J:47:ARG:HD2	2.19	0.43
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.00	0.43
1:A:567:LYS:CB	1:A:568:PRO:CD	2.82	0.43
2:B:203:PHE:CE2	2:B:212:LEU:HD12	2.54	0.43
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.43	0.43
3:C:62:PHE:O	3:C:65:HIS:HB3	2.18	0.43
6:H:101:ALA:HB2	6:H:116:TYR:CD1	2.53	0.43
2:B:1039:GLY:HA2	8:J:51:LEU:CD2	2.49	0.43
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.19	0.43
1:A:884:ASP:N	1:A:884:ASP:OD1	2.46	0.43
1:A:924:LYS:HE3	1:A:924:LYS:HB2	1.91	0.43
2:B:315:LYS:N	2:B:316:PRO:CD	2.82	0.43
1:A:1173:HIS:CD2	1:A:1227:ILE:CG1	2.90	0.43
1:A:1386:ARG:HA	1:A:1390:ASN:HB2	2.01	0.43
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.49	0.43
1:A:588:LEU:HD13	1:A:632:VAL:HG21	1.99	0.43
2:B:451:LYS:O	2:B:452:THR:C	2.56	0.43
2:B:461:LEU:HD12	2:B:466:TRP:CZ3	2.53	0.43
1:A:786:HIS:CE1	2:B:705:MET:HE1	2.54	0.43
2:B:711:GLU:N	2:B:712:PRO:HD3	2.33	0.43
2:B:701:ILE:HB	2:B:740:HIS:HE1	1.84	0.43
2:B:806:THR:CG2	2:B:809:MET:CE	2.93	0.43
3:C:238:ILE:HG22	3:C:239:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.18	0.43
10:L:42:ARG:O	10:L:43:THR:CB	2.67	0.43
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.51	0.43
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.33	0.43
1:A:1105:LEU:CD2	1:A:1384:VAL:HG21	2.49	0.43
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.34	0.43
1:A:359:LEU:O	1:A:471:ASN:ND2	2.51	0.43
2:B:984:HIS:CD2	2:B:1024:ALA:HB3	2.54	0.43
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.18	0.43
2:B:549:THR:HG22	2:B:550:ASP:H	1.84	0.43
9:K:49:GLU:CG	9:K:94:ILE:HD11	2.48	0.43
10:L:46:VAL:O	10:L:47:ARG:HB3	2.18	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.00	0.43
1:A:715:GLU:O	1:A:719:VAL:HG23	2.19	0.43
1:A:675:THR:CG2	1:A:736:ASN:HD21	2.31	0.43
1:A:875:ALA:HA	1:A:878:ILE:HD12	2.01	0.43
1:A:90:VAL:O	1:A:235:ILE:HG22	2.19	0.43
2:B:751:VAL:HG12	2:B:752:ALA:N	2.34	0.43
4:E:98:ILE:O	4:E:99:HIS:C	2.57	0.43
1:A:902:LEU:O	1:A:903:ASN:HB2	2.18	0.42
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.49	0.42
2:B:473:MET:C	2:B:475:SER:N	2.71	0.42
1:A:451:HIS:HB3	1:A:453:MET:N	2.33	0.42
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.34	0.42
2:B:732:SER:CB	2:B:734:HIS:CD2	3.02	0.42
1:A:106:VAL:CG1	1:A:107:CYS:N	2.82	0.42
1:A:630:ILE:HD12	1:A:630:ILE:N	2.33	0.42
1:A:863:VAL:HG11	1:A:866:PHE:CE1	2.54	0.42
1:A:940:ARG:O	1:A:944:ARG:HG3	2.20	0.42
2:B:476:ARG:O	2:B:478:GLY:N	2.52	0.42
2:B:986:GLN:OE1	2:B:986:GLN:CA	2.67	0.42
1:A:1242:VAL:O	1:A:1243:VAL:HG23	2.20	0.42
1:A:1397:LEU:O	1:A:1400:CYS:HB2	2.19	0.42
1:A:1406:VAL:HG12	1:A:1407:GLU:N	2.34	0.42
1:A:314:ALA:HB1	1:A:321:PRO:CB	2.50	0.42
1:A:573:SER:O	1:A:576:GLN:HB2	2.19	0.42
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.42
2:B:771:SER:O	2:B:775:LYS:HE3	2.20	0.42
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.84	0.42
3:C:18:VAL:HG23	3:C:240:VAL:HG11	2.01	0.42
6:H:125:LEU:HD12	6:H:125:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ARG:HG3	1:A:247:ARG:O	2.19	0.42
1:A:471:ASN:O	1:A:474:VAL:HG12	2.19	0.42
2:B:310:MET:O	2:B:313:MET:HB2	2.20	0.42
1:A:211:PHE:CG	1:A:231:PRO:HB2	2.54	0.42
1:A:261:ASP:CB	1:A:323:LYS:HD3	2.48	0.42
1:A:41:MET:HE2	1:A:61:ILE:CD1	2.49	0.42
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.55	0.42
1:A:845:LEU:O	1:A:847:ASP:N	2.52	0.42
2:B:286:PHE:HB3	2:B:297:ILE:CD1	2.48	0.42
5:F:97:ARG:HG3	5:F:101:ILE:HD11	2.01	0.42
7:I:25:LEU:HD12	7:I:26:LEU:H	1.85	0.42
1:A:852:TYR:CD1	1:A:1060:PRO:CB	3.02	0.42
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.02	0.42
1:A:494:SER:N	2:B:1149:GLU:OE2	2.53	0.42
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.01	0.42
3:C:260:LEU:O	3:C:263:THR:HB	2.20	0.42
7:I:106:CYS:O	7:I:107:SER:C	2.58	0.42
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.50	0.42
1:A:99:ILE:HA	1:A:102:VAL:HG23	2.01	0.42
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.50	0.42
1:A:1410:PHE:CD1	2:B:1212:ILE:HD11	2.54	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.42
2:B:263:GLY:O	2:B:264:SER:C	2.58	0.42
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.55	0.42
3:C:258:ILE:HD12	9:K:42:LEU:HD21	1.97	0.42
1:A:283:GLY:O	1:A:285:PRO:HD3	2.20	0.42
1:A:56:PRO:CD	1:A:57:ARG:N	2.83	0.42
1:A:12:ARG:HD3	2:B:1192:TYR:CE1	2.55	0.42
2:B:488:TYR:CE2	2:B:492:LEU:HD11	2.55	0.42
2:B:636:PRO:CB	2:B:637:LEU:HB3	2.50	0.42
3:C:242:GLN:O	3:C:246:ARG:HG3	2.19	0.42
9:K:17:SER:O	9:K:18:LYS:C	2.57	0.42
1:A:1022:LEU:CD1	1:A:1026:LEU:CD1	2.97	0.42
1:A:287:HIS:O	1:A:288:ALA:HB2	2.19	0.42
1:A:690:VAL:HG21	1:A:722:LEU:HD11	2.00	0.42
1:A:759:ALA:O	1:A:763:ALA:HB3	2.19	0.42
1:A:853:ASP:OD2	1:A:855:THR:HG22	2.20	0.42
1:A:929:LEU:HA	1:A:929:LEU:HD13	1.91	0.42
1:A:950:GLY:HA3	1:A:1298:TYR:CE2	2.54	0.42
2:B:123:THR:HG22	2:B:125:SER:HB3	2.01	0.42
6:H:44:VAL:HG13	6:H:48:PRO:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:75:CYS:CB	7:I:103:CYS:HB2	2.50	0.42
1:A:107:CYS:O	1:A:108:MET:O	2.37	0.41
1:A:858:ASN:HD22	1:A:858:ASN:C	2.23	0.41
2:B:1060:ARG:C	2:B:1062:HIS:N	2.73	0.41
2:B:461:LEU:HD12	2:B:466:TRP:CH2	2.55	0.41
2:B:585:VAL:HG12	2:B:587:HIS:CD2	2.55	0.41
2:B:34:ILE:CD1	2:B:743:ILE:HG21	2.50	0.41
3:C:70:ILE:HD11	3:C:115:SER:HB3	2.02	0.41
3:C:249:ASP:O	3:C:252:GLN:HB3	2.20	0.41
4:E:90:VAL:HG13	4:E:91:LYS:N	2.34	0.41
1:A:1140:HIS:HB3	1:A:1279:ILE:O	2.20	0.41
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.67	0.41
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.36	0.41
1:A:857:ARG:HB3	1:A:863:VAL:HA	2.02	0.41
2:B:1022:THR:HG23	2:B:1022:THR:O	2.20	0.41
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.54	0.41
3:C:229:TYR:N	3:C:229:TYR:CD1	2.87	0.41
4:E:178:ILE:HB	4:E:212:ARG:HD3	2.01	0.41
1:A:809:THR:HB	1:A:810:PRO:HD2	2.01	0.41
1:A:893:PHE:C	1:A:893:PHE:CD1	2.93	0.41
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.55	0.41
7:I:59:VAL:O	7:I:62:ILE:HB	2.20	0.41
7:I:96:SER:HB2	7:I:98:VAL:HG23	2.02	0.41
2:B:816:GLU:O	8:J:56:LEU:HD21	2.20	0.41
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.20	0.41
1:A:332:LYS:H	1:A:337:ARG:HB2	1.84	0.41
1:A:505:CYS:SG	2:B:1141:HIS:HD2	2.43	0.41
2:B:167:ILE:HG23	2:B:424:LEU:CD1	2.50	0.41
3:C:14:SER:OG	3:C:17:ASN:N	2.53	0.41
5:F:111:LEU:C	5:F:113:GLY:N	2.71	0.41
1:A:1025:ARG:O	1:A:1035:TYR:OH	2.39	0.41
1:A:33:ALA:HA	1:A:56:PRO:HG2	2.02	0.41
1:A:898:ARG:HB2	1:A:933:TYR:CE2	2.56	0.41
2:B:1171:VAL:HG12	2:B:1172:ILE:H	1.85	0.41
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.55	0.41
2:B:696:GLU:O	2:B:699:GLU:HB2	2.21	0.41
3:C:100:THR:O	3:C:119:VAL:HB	2.20	0.41
6:H:38:LEU:HD13	6:H:125:LEU:HD13	2.02	0.41
6:H:24:CYS:HB2	6:H:44:VAL:HG21	2.01	0.41
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.61	0.41
1:A:1404:GLU:HB3	1:A:1407:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:HB3	1:A:312:PRO:CD	2.50	0.41
1:A:88:LYS:O	1:A:89:PRO:O	2.38	0.41
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.55	0.41
1:A:795:GLU:OE1	2:B:731:VAL:HG11	2.21	0.41
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.35	0.41
1:A:380:VAL:HG21	1:A:430:TRP:HB2	2.01	0.41
1:A:657:LEU:O	1:A:661:GLY:N	2.50	0.41
1:A:343:LYS:HE3	2:B:1151:LEU:HG	2.02	0.41
2:B:785:TYR:CD1	2:B:786:ASN:N	2.89	0.41
6:H:82:PRO:HA	6:H:84:ALA:HB3	2.01	0.41
2:B:104:GLU:CD	10:L:54:ARG:NH2	2.74	0.41
1:A:120:GLU:CG	1:A:120:GLU:O	2.69	0.41
1:A:128:ILE:O	1:A:128:ILE:CG2	2.68	0.41
2:B:1146:PHE:CE2	2:B:1150:ARG:HG3	2.56	0.41
2:B:258:LEU:HD11	2:B:267:ARG:HB3	2.02	0.41
2:B:431:TYR:CG	2:B:447:ALA:HB1	2.56	0.41
2:B:69:LEU:HB2	2:B:90:ILE:HB	2.03	0.41
2:B:912:ILE:O	2:B:938:SER:HB2	2.20	0.41
3:C:57:VAL:CG1	8:J:60:PHE:CB	2.98	0.41
4:E:127:ILE:O	4:E:127:ILE:CG1	2.69	0.41
8:J:59:LYS:O	8:J:62:ARG:HB2	2.21	0.41
3:C:166:GLU:O	9:K:6:ARG:HG3	2.20	0.41
2:B:1163:CYS:SG	2:B:1166:CYS:N	2.90	0.41
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.36	0.41
2:B:806:THR:HG23	2:B:809:MET:HE3	2.00	0.41
3:C:120:ILE:CD1	3:C:130:GLY:O	2.69	0.41
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.20	0.41
1:A:317:LYS:HD2	1:A:317:LYS:N	2.36	0.41
1:A:370:ILE:HG22	1:A:374:LEU:HD12	2.01	0.41
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.41
2:B:431:TYR:CG	2:B:447:ALA:CB	3.04	0.41
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.36	0.41
3:C:142:VAL:HG13	8:J:5:VAL:HG22	2.03	0.41
1:A:1444:MET:HB3	1:A:1445:ILE:H	1.72	0.41
1:A:549:MET:O	1:A:550:LEU:C	2.60	0.41
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.51	0.41
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.21	0.41
4:E:182:ASP:HA	4:E:183:PRO:HD2	1.88	0.41
7:I:17:ARG:O	7:I:25:LEU:HD12	2.19	0.41
8:J:59:LYS:O	8:J:62:ARG:CB	2.69	0.41
10:L:32:ALA:HB3	10:L:55:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:TYR:O	1:A:1366:ARG:C	2.60	0.40
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.21	0.40
1:A:665:GLY:HA2	2:B:1086:PHE:CD1	2.56	0.40
2:B:299:GLU:OE1	2:B:572:HIS:HB3	2.21	0.40
2:B:467:GLY:HA3	2:B:473:MET:SD	2.61	0.40
2:B:800:GLN:CG	8:J:52:THR:CG2	2.99	0.40
6:H:15:VAL:O	6:H:15:VAL:CG1	2.69	0.40
6:H:81:PRO:CB	6:H:82:PRO:HD2	2.51	0.40
1:A:1022:LEU:HD11	1:A:1026:LEU:HD12	2.03	0.40
1:A:1107:VAL:HG23	1:A:1383:SER:HA	2.02	0.40
1:A:364:VAL:HG12	1:A:458:HIS:HB3	2.03	0.40
1:A:541:ILE:CD1	1:A:574:GLY:HA2	2.51	0.40
2:B:986:GLN:HE22	2:B:1016:ALA:HB1	1.86	0.40
2:B:1183:LYS:O	2:B:1183:LYS:HE2	2.21	0.40
2:B:190:TYR:CE2	8:J:62:ARG:HG2	2.56	0.40
2:B:530:GLY:O	2:B:531:GLN:C	2.59	0.40
2:B:737:THR:CG2	7:I:66:PRO:HB2	2.51	0.40
2:B:803:LEU:N	2:B:822:ASN:HD21	2.19	0.40
2:B:789:MET:HE3	2:B:965:LYS:HB3	2.03	0.40
4:E:198:ILE:N	4:E:210:SER:O	2.53	0.40
6:H:93:TYR:HD1	6:H:145:ARG:HB3	1.86	0.40
7:I:35:VAL:HG12	7:I:36:GLU:N	2.36	0.40
1:A:184:SER:O	1:A:185:TRP:CG	2.75	0.40
1:A:311:GLN:HB3	1:A:312:PRO:HD2	2.04	0.40
1:A:401:GLY:C	1:A:435:HIS:ND1	2.75	0.40
1:A:532:ARG:O	1:A:535:THR:HB	2.21	0.40
2:B:1129:ARG:HH21	2:B:1131:GLY:CA	2.27	0.40
2:B:46:GLN:HG3	2:B:47:GLN:N	2.36	0.40
3:C:175:ALA:HB3	8:J:43:ARG:HH22	1.86	0.40
5:F:74:ILE:HG23	5:F:75:PRO:HD2	2.03	0.40
6:H:76:THR:O	6:H:77:ARG:O	2.39	0.40
9:K:49:GLU:HG3	9:K:94:ILE:CD1	2.52	0.40
9:K:71:PHE:CD1	9:K:71:PHE:C	2.94	0.40
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.86	0.40
1:A:734:GLU:O	1:A:734:GLU:HG3	2.20	0.40
1:A:814:PHE:O	1:A:817:ALA:HB3	2.22	0.40
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.57	0.40
3:C:253:LYS:O	3:C:256:ALA:HB3	2.21	0.40
6:H:11:GLN:HA	6:H:53:ASP:O	2.21	0.40
6:H:63:LEU:N	6:H:63:LEU:HD12	2.36	0.40
1:A:834:THR:HB	1:A:1077:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HB3	1:A:465:TYR:O	2.22	0.40
1:A:564:ALA:O	6:H:97:MET:HA	2.22	0.40
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.90	0.40
2:B:639:ILE:HD11	2:B:691:GLU:HG3	2.04	0.40
2:B:860:MET:HG2	2:B:861:ASP:N	2.36	0.40
3:C:174:ALA:O	8:J:10:CYS:O	2.39	0.40
3:C:231:ASN:C	3:C:231:ASN:HD22	2.25	0.40
4:E:78:LEU:HG	4:E:79:TRP:N	2.37	0.40
9:K:12:LEU:N	9:K:12:LEU:HD12	2.36	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	1382/1733 (80%)	1069 (77%)	203 (15%)	110 (8%)	1 14
2	B	1088/1224 (89%)	869 (80%)	143 (13%)	76 (7%)	1 16
3	C	264/318 (83%)	212 (80%)	42 (16%)	10 (4%)	3 26
4	E	212/215 (99%)	174 (82%)	30 (14%)	8 (4%)	3 26
5	F	82/155 (53%)	62 (76%)	14 (17%)	6 (7%)	1 16
6	H	129/146 (88%)	89 (69%)	26 (20%)	14 (11%)	0 7
7	I	117/122 (96%)	88 (75%)	17 (14%)	12 (10%)	0 8
8	J	63/70 (90%)	49 (78%)	8 (13%)	6 (10%)	0 11
9	K	112/120 (93%)	98 (88%)	12 (11%)	2 (2%)	8 40
10	L	44/70 (63%)	26 (59%)	9 (20%)	9 (20%)	0 2
All	All	3493/4173 (84%)	2736 (78%)	504 (14%)	253 (7%)	1 16

All (253) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	63	ARG
1	A	72	GLU
1	A	76	GLU
1	A	89	PRO
1	A	93	VAL
1	A	108	MET
1	A	130	ASP
1	A	167	CYS
1	A	204	THR
1	A	209	ASN
1	A	210	ILE
1	A	214	ILE
1	A	250	ILE
1	A	257	ARG
1	A	285	PRO
1	A	286	HIS
1	A	288	ALA
1	A	317	LYS
1	A	335	ARG
1	A	404	TYR
1	A	517	ASN
1	A	567	LYS
1	A	568	PRO
1	A	575	LYS
1	A	628	GLY
1	A	776	ALA
1	A	795	GLU
1	A	889	SER
1	A	903	ASN
1	A	904	THR
1	A	998	LEU
1	A	1054	LEU
1	A	1173	HIS
1	A	1255	GLU
1	A	1280	GLU
1	A	1327	ILE
1	A	1394	THR
1	A	1437	GLY
2	B	23	ALA
2	B	66	ASP
2	B	67	SER
2	B	223	VAL

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Mol	Chain	Res	Type
2	B	248	SER
2	B	274	PRO
2	B	367	LEU
2	B	451	LYS
2	B	476	ARG
2	B	531	GLN
2	B	635	ARG
2	B	643	ASP
2	B	695	ALA
2	B	708	GLU
2	B	709	ASP
2	B	734	HIS
2	B	869	SER
2	B	880	THR
2	B	958	GLN
2	B	961	LEU
2	B	981	ALA
2	B	982	SER
2	B	1167	GLY
2	B	1178	ASN
2	B	1181	GLU
3	C	142	VAL
3	C	215	GLU
4	E	115	ASN
5	F	81	THR
5	F	104	ASN
5	F	128	LYS
6	H	32	THR
6	H	77	ARG
6	H	82	PRO
6	H	109	LYS
6	H	130	ARG
6	H	135	LEU
6	H	140	ALA
7	I	8	ARG
7	I	20	LYS
7	I	21	GLU
7	I	78	CYS
7	I	79	HIS
8	J	2	ILE
10	L	35	SER
10	L	43	THR

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Mol	Chain	Res	Type
10	L	47	ARG
10	L	59	ALA
10	L	64	LEU
1	A	34	LYS
1	A	52	GLY
1	A	56	PRO
1	A	62	ASP
1	A	69	THR
1	A	203	SER
1	A	248	PRO
1	A	385	ILE
1	A	418	SER
1	A	846	GLU
1	A	854	ASN
1	A	880	LYS
1	A	915	SER
1	A	922	ASP
1	A	958	VAL
1	A	972	HIS
1	A	994	GLN
1	A	1016	THR
1	A	1036	ARG
1	A	1365	TYR
1	A	1366	ARG
2	B	249	ARG
2	B	275	TYR
2	B	294	ASP
2	B	327	ARG
2	B	436	VAL
2	B	448	ILE
2	B	645	SER
2	B	737	THR
2	B	738	PHE
2	B	746	SER
2	B	751	VAL
2	B	878	GLN
2	B	1054	GLY
2	B	1061	GLU
2	B	1132	GLU
2	B	1165	ILE
2	B	1172	ILE
2	B	1176	ASN

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Mol	Chain	Res	Type
3	C	6	PRO
3	C	110	THR
4	E	77	SER
5	F	113	GLY
6	H	62	SER
6	H	81	PRO
7	I	3	THR
7	I	9	ASP
7	I	16	PRO
7	I	54	GLU
9	K	90	ALA
10	L	52	GLY
1	A	33	ALA
1	A	48	ALA
1	A	54	ASN
1	A	71	GLN
1	A	132	LYS
1	A	185	TRP
1	A	251	SER
1	A	734	GLU
1	A	794	PRO
1	A	895	LYS
1	A	902	LEU
1	A	949	ASP
1	A	1221	LYS
1	A	1231	ASP
1	A	1393	ASN
1	A	1401	SER
2	B	65	GLU
2	B	94	LYS
2	B	264	SER
2	B	364	ILE
2	B	450	ALA
2	B	471	LYS
2	B	474	SER
2	B	480	SER
2	B	636	PRO
2	B	641	GLU
2	B	1046	PRO
2	B	1100	ASP
3	C	5	GLY
7	I	23	ASN

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Mol	Chain	Res	Type
7	I	47	GLU
8	J	62	ARG
9	K	28	PRO
10	L	34	CYS
10	L	54	ARG
1	A	25	GLU
1	A	149	GLU
1	A	184	SER
1	A	219	PHE
1	A	326	ARG
1	A	380	VAL
1	A	1135	ARG
1	A	1261	LYS
1	A	1278	ASN
2	B	308	TRP
2	B	467	GLY
2	B	792	MET
2	B	1017	ILE
2	B	1097	HIS
3	C	28	ALA
3	C	174	ALA
4	E	118	PRO
5	F	131	PRO
5	F	141	GLY
6	H	52	GLN
6	H	60	ALA
6	H	90	ALA
8	J	6	ARG
8	J	53	HIS
1	A	32	VAL
1	A	66	LYS
1	A	77	CYS
1	A	266	LEU
1	A	424	ILE
1	A	985	ASP
1	A	1004	ASN
1	A	1122	PRO
1	A	1242	VAL
1	A	1407	GLU
2	B	124	TYR
2	B	469	GLN
2	B	483	LEU

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Mol	Chain	Res	Type
2	B	799	PRO
2	B	879	ARG
2	B	1220	ARG
3	C	48	SER
4	E	31	THR
4	E	103	LYS
6	H	111	LEU
1	A	68	GLN
1	A	226	GLU
1	A	320	ARG
1	A	432	VAL
1	A	536	LEU
1	A	583	PRO
1	A	591	PHE
1	A	609	ASP
1	A	1053	PHE
2	B	168	GLY
2	B	292	ILE
2	B	355	ILE
2	B	996	ARG
3	C	60	ASP
6	H	133	ASN
10	L	55	ILE
1	A	1435	PRO
4	E	27	GLY
8	J	4	PRO
1	A	162	VAL
1	A	308	ILE
2	B	731	VAL
4	E	51	GLY
4	E	129	PRO
1	A	610	GLY
2	B	55	VAL
2	B	100	PRO
2	B	974	PRO
2	B	1214	PRO
3	C	213	PRO
8	J	14	VAL
1	A	990	VAL
1	A	1107	VAL
2	B	482	VAL
7	I	15	TYR

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	1217/1520 (80%)	1005 (83%)	212 (17%)	2 12
2	B	960/1061 (90%)	799 (83%)	161 (17%)	2 14
3	C	234/274 (85%)	204 (87%)	30 (13%)	4 21
4	E	196/197 (100%)	165 (84%)	31 (16%)	2 16
5	F	74/137 (54%)	61 (82%)	13 (18%)	2 12
6	H	117/128 (91%)	99 (85%)	18 (15%)	2 16
7	I	113/116 (97%)	97 (86%)	16 (14%)	3 19
8	J	60/65 (92%)	45 (75%)	15 (25%)	0 4
9	K	99/102 (97%)	87 (88%)	12 (12%)	5 23
10	L	40/57 (70%)	29 (72%)	11 (28%)	0 3
All	All	3110/3657 (85%)	2591 (83%)	519 (17%)	2 14

All (519) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	TYR
1	A	18	GLN
1	A	22	PHE
1	A	25	GLU
1	A	28	ARG
1	A	32	VAL
1	A	40	THR
1	A	47	ARG
1	A	49	LYS
1	A	50	ILE
1	A	60	SER
1	A	62	ASP
1	A	63	ARG
1	A	65	LEU
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	69	THR
1	A	71	GLN
1	A	80	HIS
1	A	81	PHE
1	A	83	HIS
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	98	LYS
1	A	102	VAL
1	A	114	LEU
1	A	115	LEU
1	A	116	ASP
1	A	132	LYS
1	A	140	THR
1	A	142	CYS
1	A	147	VAL
1	A	150	THR
1	A	162	VAL
1	A	167	CYS
1	A	169	ASN
1	A	170	THR
1	A	180	LYS
1	A	185	TRP
1	A	207	ILE
1	A	208	LEU
1	A	222	LEU
1	A	225	ASN
1	A	235	ILE
1	A	239	LEU
1	A	252	PHE
1	A	256	GLN
1	A	260	ASP
1	A	263	THR
1	A	265	LYS
1	A	266	LEU
1	A	271	LYS
1	A	287	HIS
1	A	297	GLN
1	A	302	THR
1	A	303	TYR
1	A	304	MET

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Mol	Chain	Res	Type
1	A	306	ASN
1	A	311	GLN
1	A	317	LYS
1	A	320	ARG
1	A	323	LYS
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	341	MET
1	A	359	LEU
1	A	380	VAL
1	A	381	THR
1	A	388	LEU
1	A	391	LEU
1	A	397	ASN
1	A	403	LYS
1	A	406	ILE
1	A	416	ARG
1	A	419	LYS
1	A	431	LYS
1	A	433	GLU
1	A	434	ARG
1	A	437	MET
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	455	MET
1	A	475	THR
1	A	476	SER
1	A	479	ASN
1	A	481	ASP
1	A	500	GLU
1	A	501	LEU
1	A	512	VAL
1	A	513	SER
1	A	524	VAL
1	A	538	ASP
1	A	550	LEU
1	A	567	LYS
1	A	590	ARG
1	A	596	THR

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Mol	Chain	Res	Type
1	A	597	LEU
1	A	608	ILE
1	A	612	ILE
1	A	618	GLU
1	A	629	LEU
1	A	666	ILE
1	A	677	ARG
1	A	682	THR
1	A	687	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	711	ARG
1	A	732	LEU
1	A	735	VAL
1	A	737	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	774	ARG
1	A	795	GLU
1	A	803	SER
1	A	805	LEU
1	A	816	HIS
1	A	821	ARG
1	A	830	LYS
1	A	831	THR
1	A	854	ASN
1	A	857	ARG
1	A	858	ASN
1	A	879	GLU
1	A	882	SER
1	A	884	ASP
1	A	886	ILE
1	A	896	ARG
1	A	898	ARG
1	A	902	LEU
1	A	904	THR
1	A	905	ASP
1	A	913	LEU

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Mol	Chain	Res	Type
1	A	915	SER
1	A	918	GLU
1	A	920	LEU
1	A	924	LYS
1	A	929	LEU
1	A	932	GLU
1	A	940	ARG
1	A	945	GLU
1	A	961	ARG
1	A	968	GLN
1	A	982	THR
1	A	988	LEU
1	A	990	VAL
1	A	996	ASN
1	A	998	LEU
1	A	1001	ARG
1	A	1017	LEU
1	A	1022	LEU
1	A	1029	ARG
1	A	1030	ARG
1	A	1046	LEU
1	A	1052	GLN
1	A	1077	THR
1	A	1095	THR
1	A	1112	LYS
1	A	1116	LEU
1	A	1120	LEU
1	A	1128	GLN
1	A	1132	LYS
1	A	1134	ILE
1	A	1142	THR
1	A	1146	VAL
1	A	1162	VAL
1	A	1171	GLN
1	A	1172	LEU
1	A	1193	LEU
1	A	1199	ARG
1	A	1206	ASP
1	A	1208	THR
1	A	1229	SER
1	A	1230	GLU
1	A	1243	VAL

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Mol	Chain	Res	Type
1	A	1258	HIS
1	A	1262	LYS
1	A	1264	GLU
1	A	1272	THR
1	A	1280	GLU
1	A	1282	VAL
1	A	1285	MET
1	A	1295	THR
1	A	1299	VAL
1	A	1300	LYS
1	A	1318	THR
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1359	ASP
1	A	1366	ARG
1	A	1376	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1390	ASN
1	A	1391	ARG
1	A	1406	VAL
1	A	1420	ASP
1	A	1436	ILE
1	A	1442	ASP
1	A	1445	ILE
2	B	26	THR
2	B	28	GLU
2	B	34	ILE
2	B	49	ASP
2	B	63	ILE
2	B	65	GLU
2	B	66	ASP
2	B	67	SER
2	B	68	THR
2	B	98	THR
2	B	104	GLU
2	B	109	THR
2	B	119	LEU
2	B	120	ARG

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Mol	Chain	Res	Type
2	B	128	LEU
2	B	130	VAL
2	B	134	LYS
2	B	166	PHE
2	B	175	ARG
2	B	177	LYS
2	B	185	THR
2	B	188	ASP
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	225	VAL
2	B	234	ILE
2	B	241	ARG
2	B	246	LYS
2	B	249	ARG
2	B	251	ILE
2	B	253	THR
2	B	261	ARG
2	B	268	THR
2	B	275	TYR
2	B	276	ILE
2	B	283	VAL
2	B	319	GLU
2	B	322	PHE
2	B	327	ARG
2	B	331	LEU
2	B	345	LYS
2	B	346	GLU
2	B	347	LYS
2	B	361	LEU
2	B	365	THR
2	B	366	GLN
2	B	367	LEU
2	B	387	LEU
2	B	393	LYS
2	B	404	LYS
2	B	415	GLN
2	B	416	LEU
2	B	419	THR
2	B	423	LYS
2	B	424	LEU

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Mol	Chain	Res	Type
2	B	425	THR
2	B	426	LYS
2	B	429	PHE
2	B	436	VAL
2	B	468	GLU
2	B	469	GLN
2	B	471	LYS
2	B	475	SER
2	B	479	VAL
2	B	485	ARG
2	B	498	THR
2	B	529	GLU
2	B	537	LYS
2	B	547	VAL
2	B	552	MET
2	B	556	THR
2	B	563	MET
2	B	570	VAL
2	B	573	GLN
2	B	591	ARG
2	B	617	ARG
2	B	622	LYS
2	B	637	LEU
2	B	644	GLU
2	B	646	LEU
2	B	648	HIS
2	B	658	ILE
2	B	666	TYR
2	B	682	SER
2	B	701	ILE
2	B	714	GLU
2	B	722	ASP
2	B	723	VAL
2	B	728	ARG
2	B	730	ARG
2	B	732	SER
2	B	740	HIS
2	B	751	VAL
2	B	761	HIS
2	B	762	ASN
2	B	778	MET
2	B	786	ASN

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Mol	Chain	Res	Type
2	B	789	MET
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	799	PRO
2	B	806	THR
2	B	807	ARG
2	B	812	LEU
2	B	815	ARG
2	B	822	ASN
2	B	837	ASP
2	B	858	SER
2	B	864	LYS
2	B	865	LYS
2	B	866	TYR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	886	LYS
2	B	889	THR
2	B	899	ILE
2	B	914	LYS
2	B	941	LEU
2	B	942	ARG
2	B	953	LEU
2	B	956	THR
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	987	LYS
2	B	989	THR
2	B	995	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1020	ARG
2	B	1021	MET
2	B	1061	GLU
2	B	1065	GLN

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Mol	Chain	Res	Type
2	B	1082	MET
2	B	1096	ARG
2	B	1108	ARG
2	B	1113	VAL
2	B	1116	ARG
2	B	1124	ARG
2	B	1141	HIS
2	B	1147	LEU
2	B	1150	ARG
2	B	1155	SER
2	B	1172	ILE
2	B	1183	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE
2	B	1195	HIS
2	B	1196	ILE
2	B	1202	LEU
2	B	1219	ASP
2	B	1222	ARG
2	B	1223	ASP
3	C	11	ARG
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG
3	C	41	ILE
3	C	53	THR
3	C	55	THR
3	C	62	PHE
3	C	69	LEU
3	C	70	ILE
3	C	77	ILE
3	C	89	GLU
3	C	91	HIS
3	C	99	LEU
3	C	119	VAL
3	C	137	LYS
3	C	138	GLU
3	C	140	ASN
3	C	143	LEU

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Mol	Chain	Res	Type
3	C	153	LEU
3	C	163	ILE
3	C	215	GLU
3	C	229	TYR
3	C	231	ASN
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	260	LEU
4	E	3	GLN
4	E	6	GLU
4	E	9	ILE
4	E	43	LYS
4	E	60	PHE
4	E	61	GLN
4	E	68	SER
4	E	77	SER
4	E	78	LEU
4	E	84	ASP
4	E	92	THR
4	E	94	LYS
4	E	101	GLN
4	E	107	THR
4	E	110	PHE
4	E	123	LEU
4	E	127	ILE
4	E	134	THR
4	E	146	HIS
4	E	153	HIS
4	E	156	LEU
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	175	LEU
4	E	188	LEU
4	E	190	LEU
4	E	196	VAL
4	E	204	THR
4	E	212	ARG
4	E	215	MET
5	F	79	ARG
5	F	82	THR

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Mol	Chain	Res	Type
5	F	87	LYS
5	F	90	ARG
5	F	92	ARG
5	F	99	LEU
5	F	104	ASN
5	F	109	VAL
5	F	110	ASP
5	F	111	LEU
5	F	133	VAL
5	F	142	SER
5	F	155	LEU
6	H	2	SER
6	H	8	ASP
6	H	15	VAL
6	H	21	ASN
6	H	25	ARG
6	H	27	GLU
6	H	31	THR
6	H	36	CYS
6	H	61	SER
6	H	89	LEU
6	H	103	LYS
6	H	112	ILE
6	H	128	ASN
6	H	129	TYR
6	H	132	LEU
6	H	136	LYS
6	H	138	GLU
6	H	143	LEU
7	I	7	CYS
7	I	12	ASN
7	I	13	MET
7	I	18	GLU
7	I	28	GLU
7	I	29	CYS
7	I	42	LEU
7	I	48	LEU
7	I	55	THR
7	I	79	HIS
7	I	83	ASN
7	I	84	VAL
7	I	91	ARG

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Mol	Chain	Res	Type
7	I	107	SER
7	I	118	ARG
7	I	120	GLN
8	J	1	MET
8	J	2	ILE
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	14	VAL
8	J	27	GLU
8	J	28	ASP
8	J	31	ASP
8	J	36	LEU
8	J	43	ARG
8	J	48	ARG
8	J	54	VAL
8	J	55	ASP
8	J	62	ARG
9	K	5	ASP
9	K	31	VAL
9	K	32	VAL
9	K	47	ARG
9	K	50	LEU
9	K	64	GLU
9	K	71	PHE
9	K	81	TYR
9	K	101	LEU
9	K	111	LEU
9	K	113	THR
9	K	114	LEU
10	L	26	THR
10	L	27	LEU
10	L	28	LYS
10	L	35	SER
10	L	40	LEU
10	L	50	ASP
10	L	55	ILE
10	L	61	THR
10	L	63	ARG
10	L	65	VAL
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	83	HIS
1	A	92	HIS
1	A	169	ASN
1	A	171	GLN
1	A	313	GLN
1	A	339	ASN
1	A	451	HIS
1	A	493	GLN
1	A	517	ASN
1	A	587	HIS
1	A	736	ASN
1	A	757	ASN
1	A	760	GLN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN
1	A	965	GLN
1	A	1106	ASN
1	A	1188	GLN
1	A	1364	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	366	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	590	HIS
2	B	686	ASN
2	B	734	HIS
2	B	740	HIS
2	B	794	ASN
2	B	822	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1187	ASN
2	B	1193	GLN
3	C	73	GLN

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Mol	Chain	Res	Type
3	C	112	ASN
3	C	123	ASN
3	C	231	ASN
3	C	242	GLN
6	H	128	ASN
6	H	137	GLN
7	I	22	ASN
7	I	83	ASN
9	K	29	ASN
9	K	40	HIS
9	K	65	HIS
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	7/9 (77%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	8	U

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
12	02I	T	21	12	16,24,25	3.36	7 (43%)	15,37,40	4.13	6 (40%)

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
12	02I	T	21	12	-	0/0/28/29	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	21	02I	O4'-C1'	-7.61	1.25	1.42
12	T	21	02I	O4'-C4'	-7.28	1.33	1.44
12	T	21	02I	C2-N3	3.92	1.38	1.32
12	T	21	02I	C4'-C5'	-3.75	1.45	1.52
12	T	21	02I	O3'-C3'	-3.73	1.35	1.43
12	T	21	02I	C8-C5'	3.32	1.57	1.51
12	T	21	02I	C2-N1	2.31	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	21	02I	C5-C6-N6	11.30	137.52	120.35
12	T	21	02I	N6-C6-N1	-7.79	102.41	118.57
12	T	21	02I	N3-C2-N1	-5.54	120.03	128.68
12	T	21	02I	O4'-C1'-C2'	-4.48	97.79	106.25
12	T	21	02I	C2'-C1'-N9	-2.45	105.70	109.56
12	T	21	02I	C4'-O4'-C1'	2.19	115.06	108.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	21	02I	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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	1394/1733 (80%)	-0.33	22 (1%) 72 62	35, 79, 170, 246	0
2	B	1106/1224 (90%)	-0.43	6 (0%) 91 85	37, 71, 142, 225	0
3	C	266/318 (83%)	-0.55	0 100 100	43, 70, 109, 146	0
4	E	214/215 (99%)	-0.21	7 (3%) 46 37	55, 119, 208, 230	0
5	F	84/155 (54%)	-0.62	0 100 100	52, 80, 114, 146	0
6	H	133/146 (91%)	-0.17	1 (0%) 86 79	64, 102, 154, 189	0
7	I	119/122 (97%)	-0.41	0 100 100	53, 93, 125, 166	0
8	J	65/70 (92%)	-0.66	0 100 100	40, 63, 90, 116	0
9	K	114/120 (95%)	-0.45	0 100 100	43, 75, 104, 119	0
10	L	46/70 (65%)	-0.08	0 100 100	57, 113, 169, 193	0
11	R	9/9 (100%)	-0.35	0 100 100	62, 81, 116, 136	0
12	T	9/29 (31%)	-0.40	0 100 100	65, 83, 154, 163	0
All	All	3559/4211 (84%)	-0.38	36 (1%) 82 74	35, 78, 162, 246	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	4.8
1	A	44	THR	3.7
4	E	118	PRO	3.5
1	A	254	GLU	3.3
1	A	161	LEU	3.3
1	A	255	SER	3.2
1	A	186	LYS	3.1
4	E	119	SER	3.0
1	A	147	VAL	2.9
4	E	122	LYS	2.7
1	A	145	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	2.6
1	A	104	GLU	2.4
1	A	173	THR	2.4
1	A	171	GLN	2.4
1	A	256	GLN	2.4
1	A	119	ASN	2.4
2	B	1224	PHE	2.3
1	A	153	PRO	2.3
2	B	134	LYS	2.2
1	A	69	THR	2.2
1	A	49	LYS	2.2
1	A	257	ARG	2.2
4	E	89	GLY	2.2
1	A	152	VAL	2.2
1	A	112	LYS	2.1
2	B	247	GLY	2.1
4	E	91	LYS	2.1
2	B	468	GLU	2.1
1	A	146	MET	2.1
4	E	90	VAL	2.1
2	B	425	THR	2.1
1	A	200	ARG	2.0
2	B	869	SER	2.0
4	E	93	MET	2.0
6	H	83	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
12	02I	T	21	21/22	0.93	0.18	87,93,115,121	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
13	ZN	A	1801	1/1	0.92	0.14	199,199,199,199	0
13	ZN	B	1301	1/1	0.95	0.05	127,127,127,127	0
13	ZN	L	101	1/1	0.96	0.07	111,111,111,111	0
13	ZN	C	401	1/1	0.97	0.03	78,78,78,78	0
13	ZN	I	201	1/1	0.98	0.07	118,118,118,118	0
13	ZN	A	1802	1/1	0.99	0.07	120,120,120,120	0
13	ZN	J	101	1/1	0.99	0.11	61,61,61,61	0
13	ZN	I	202	1/1	0.99	0.07	74,74,74,74	0

6.5 Other polymers

There are no such residues in this entry.