



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 03:13 PM BST

PDB ID : 5C4J  
Title : Crystal structure of a transcribing RNA Polymerase II complex reveals a complete transcription bubble  
Authors : Barnes, C.O.; Calero, M.; Malik, I.; Spahr, H.; Zhang, Q.; Pullara, F.; Kaplan, C.D.; Calero, G.  
Deposited on : 2015-06-18  
Resolution : 4.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

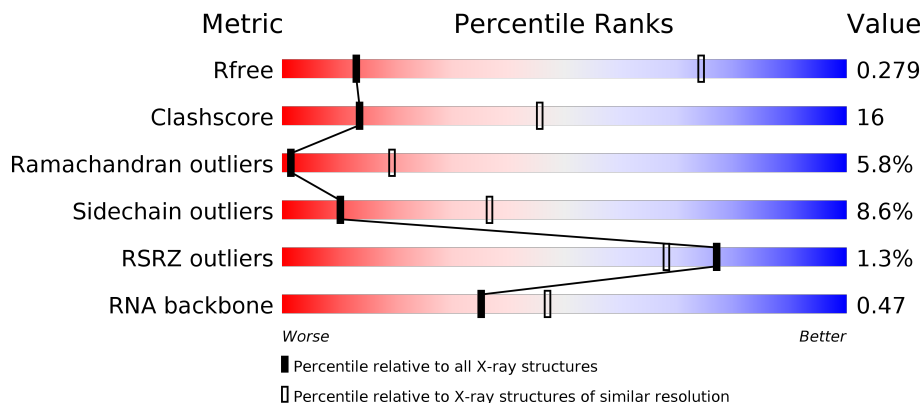
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.








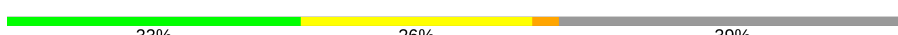

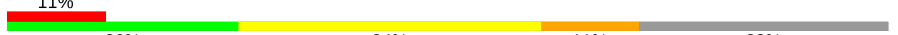

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	 52% 25% 5% 17%
2	B	1224	 60% 30% 5% 5%
3	C	318	 53% 28% 17%
4	E	215	 67% 29% 4% 2%

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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	S	53	
13	U	53	

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
14	ZN	C	402	-	-	X	-

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 30496 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
			Total	C	N	O	S			
1	A	1432	11240	7079	1964	2136	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1157	9145	5776	1599	1714	56	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	265	2074	1304	345	412	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	212	1735	1102	306	316	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	87	705	451	119	132	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	143	1102	689	189	220	4	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	114	927	571	168	178	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	J	66	540	345	94	95	6	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	K	115	924	593	157	172	2	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	43	344	211	69	60	4	0	0	0

- Molecule 11 is a RNA chain called RNA (5'-R(P\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	R	9	197	88	40	60	9	0	0	0

- Molecule 12 is a DNA chain called NON-TEMPLATE STRAND DNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	S	38	782	371	142	231	38	0	0	0

- Molecule 13 is a DNA chain called TEMPLATE STRAND DNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	U	38	771	366	144	223	38	0	0	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

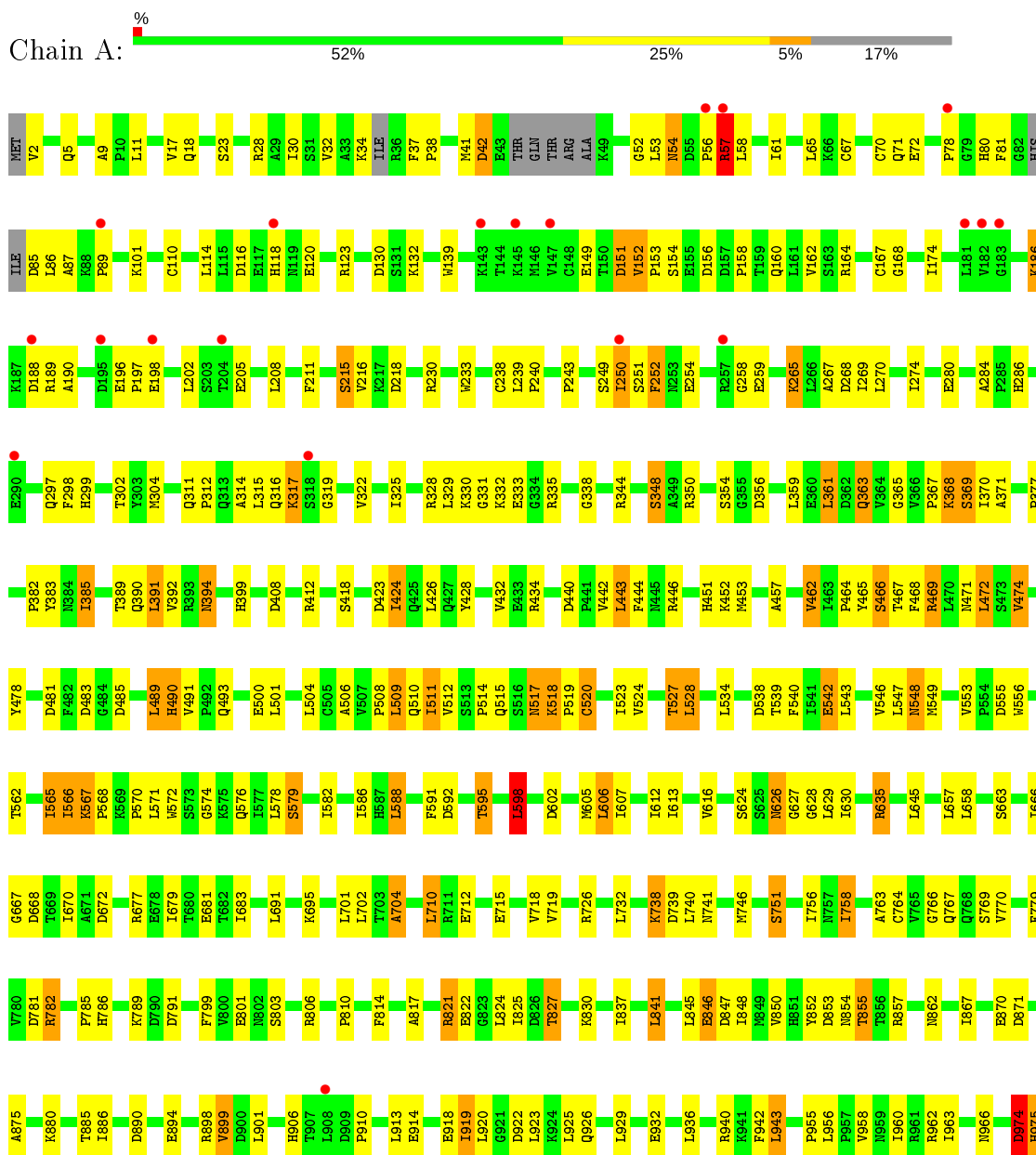
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

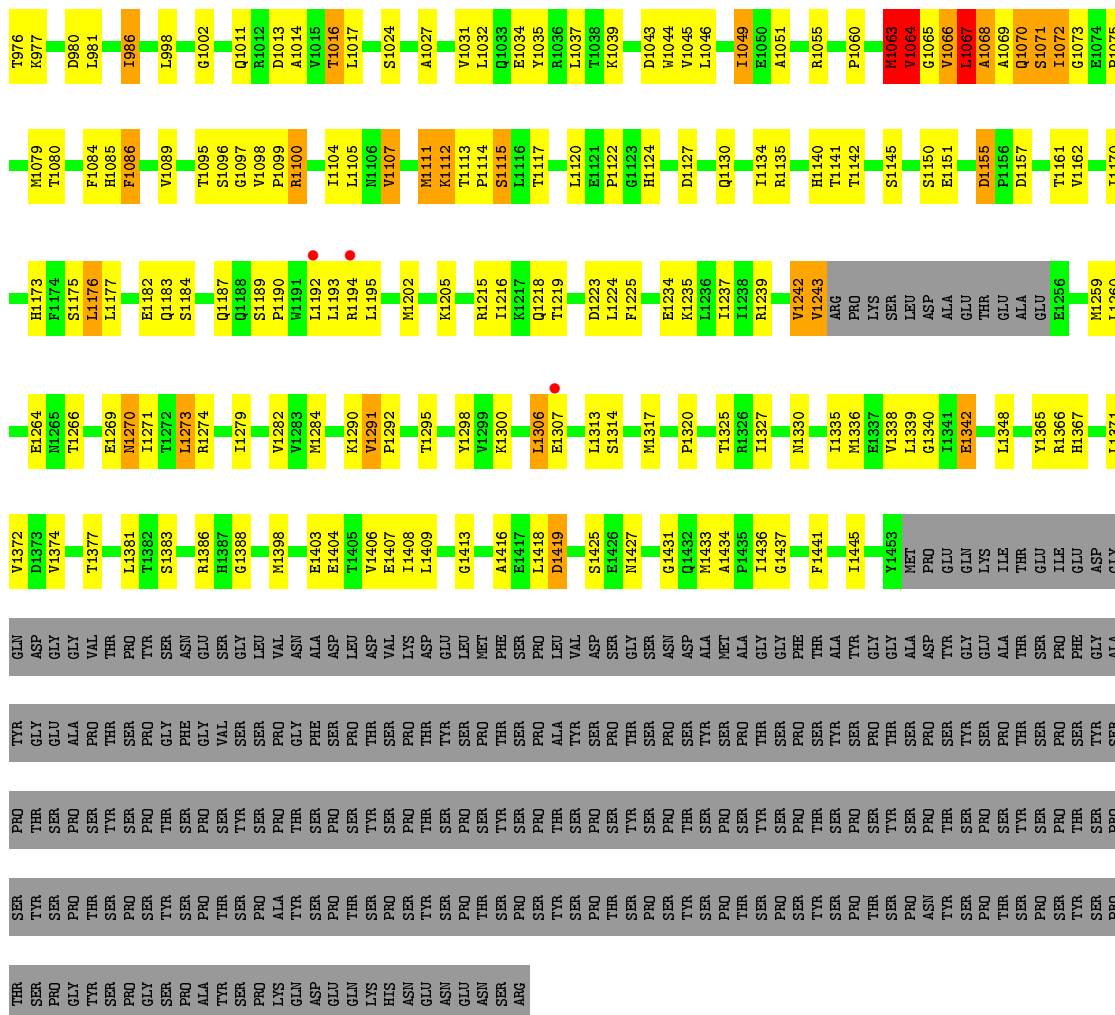
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	R	1	Total 1	Mg 1	0	0

### 3 Residue-property plots

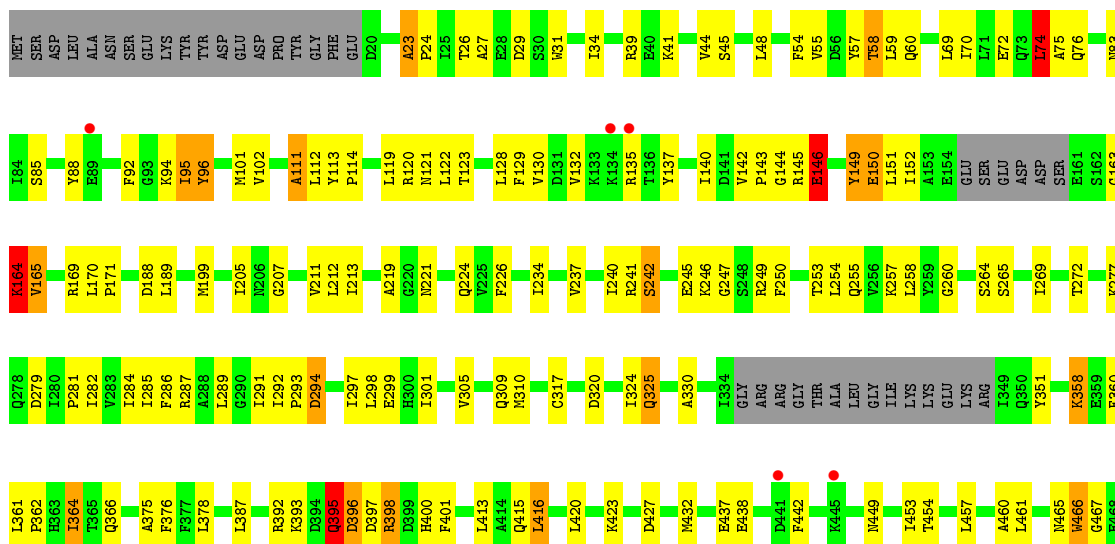
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

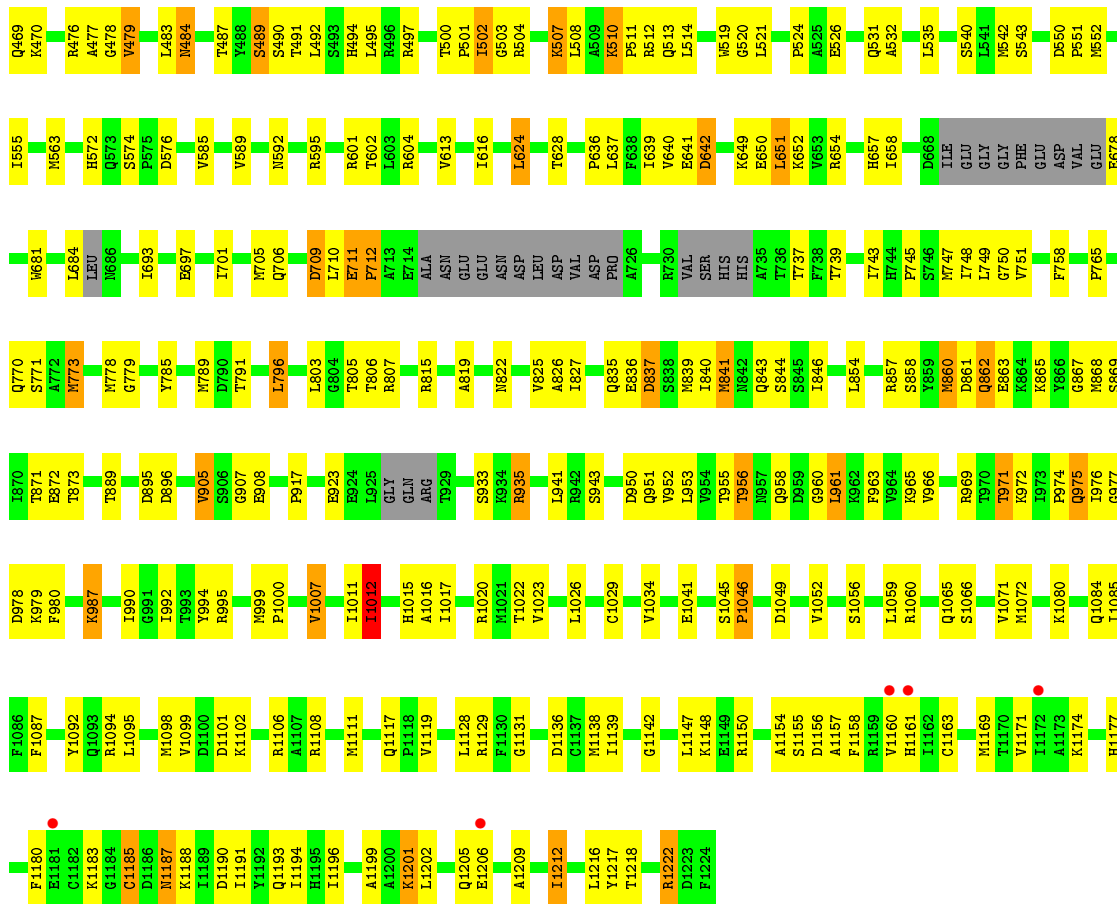




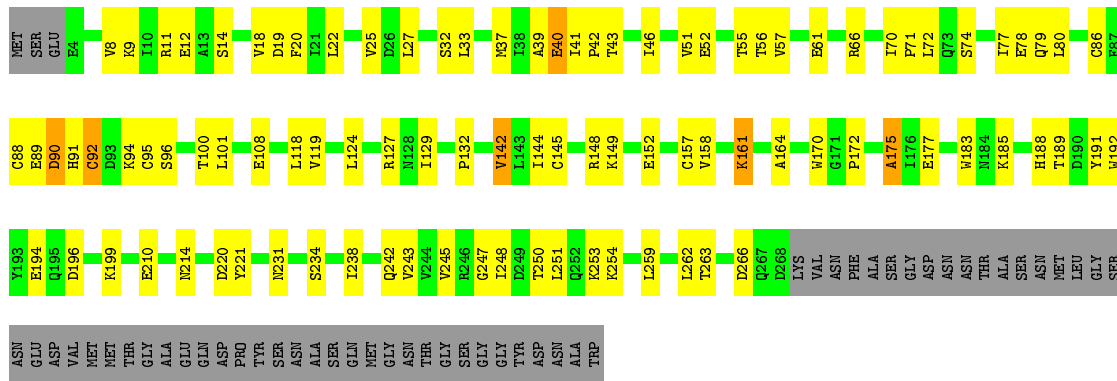
● Molecule 2: DNA-directed RNA polymerase II subunit RPB2



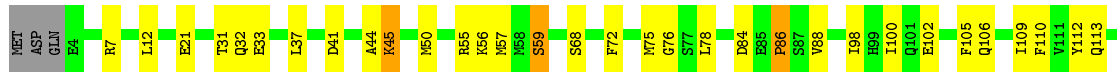




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



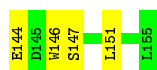
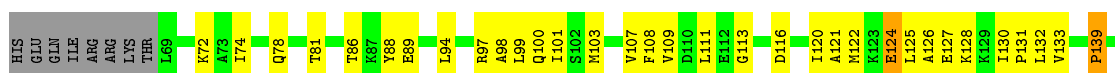
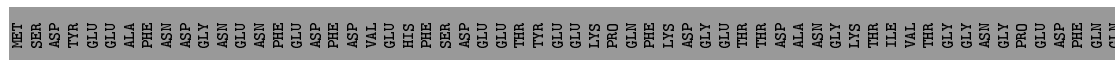
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1





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

Chain F:



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

Chain H:



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

Chain I:



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

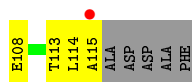
Chain J:



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

Chain K:

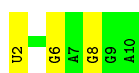




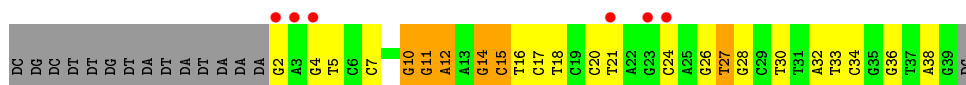
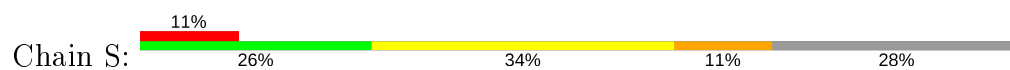
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



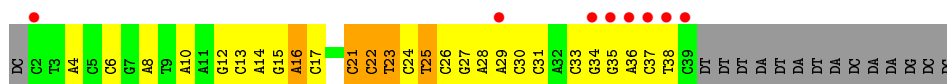
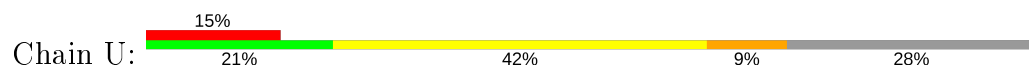
- Molecule 11: RNA (5'-R(P\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3')



- Molecule 12: NON-TEMPLATE STRAND DNA (38-MER)



- Molecule 13: TEMPLATE STRAND DNA (38-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	280.71Å 223.38Å 156.42Å 90.00° 98.14° 90.00°	Depositor
Resolution (Å)	174.08 – 4.00 48.89 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (174.08-4.00) 97.7 (48.89-4.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 4.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.212 , 0.271 0.229 , 0.279	Depositor DCC
$R_{free}$ test set	2689 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	155.3	Xtrriage
Anisotropy	0.326	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 186.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	30496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	231.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.46	0/11441	0.77	5/15470 (0.0%)
2	B	0.45	0/9320	0.74	3/12568 (0.0%)
3	C	0.43	0/2112	0.68	0/2866
4	E	0.45	0/1771	0.74	1/2383 (0.0%)
5	F	0.43	0/717	0.77	1/967 (0.1%)
6	H	0.43	0/1120	0.81	1/1513 (0.1%)
7	I	0.42	0/945	0.78	1/1273 (0.1%)
8	J	0.45	0/549	0.73	0/738
9	K	0.42	0/942	0.69	0/1272
10	L	0.40	0/346	0.75	0/457
11	R	0.46	0/221	0.72	0/343
12	S	1.05	0/876	1.88	31/1351 (2.3%)
13	U	1.02	0/864	1.83	34/1328 (2.6%)
All	All	0.50	0/31224	0.86	77/42529 (0.2%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	S	15	DC	O4'-C1'-N1	12.27	116.59	108.00
13	U	25	DT	P-O3'-C3'	12.22	134.36	119.70
12	S	10	DG	P-O3'-C3'	11.81	133.88	119.70
13	U	27	DG	P-O3'-C3'	11.61	133.64	119.70
13	U	35	DG	P-O3'-C3'	11.16	133.09	119.70
13	U	17	DC	P-O3'-C3'	10.91	132.79	119.70
13	U	30	DC	O4'-C1'-N1	9.59	114.72	108.00
12	S	17	DC	O4'-C1'-N1	9.38	114.56	108.00
12	S	30	DT	O4'-C1'-N1	9.35	114.55	108.00
12	S	12	DA	P-O3'-C3'	9.28	130.84	119.70
13	U	14	DA	P-O3'-C3'	8.83	130.29	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	35	DG	O4'-C1'-N9	8.62	114.03	108.00
12	S	28	DG	P-O3'-C3'	8.31	129.67	119.70
12	S	7	DC	O4'-C1'-N1	7.95	113.57	108.00
12	S	11	DG	P-O3'-C3'	7.73	128.97	119.70
12	S	4	DG	P-O3'-C3'	7.51	128.71	119.70
12	S	34	DC	O4'-C1'-N1	7.29	113.10	108.00
12	S	18	DT	O4'-C1'-N1	7.19	113.04	108.00
13	U	16	DA	O4'-C1'-N9	7.00	112.90	108.00
12	S	14	DG	P-O3'-C3'	6.89	127.96	119.70
12	S	10	DG	O4'-C1'-N9	6.72	112.70	108.00
12	S	28	DG	O4'-C1'-N9	6.68	112.68	108.00
5	F	98	ALA	N-CA-CB	6.66	119.42	110.10
6	H	134	ASN	N-CA-CB	6.63	122.53	110.60
12	S	34	DC	C1'-O4'-C4'	-6.58	103.52	110.10
13	U	6	DC	O4'-C1'-N1	6.53	112.57	108.00
2	B	74	LEU	N-CA-C	6.50	128.54	111.00
13	U	33	DC	P-O3'-C3'	6.49	127.48	119.70
13	U	13	DC	P-O3'-C3'	6.43	127.41	119.70
13	U	37	DC	P-O3'-C3'	6.42	127.40	119.70
12	S	27	DT	P-O3'-C3'	6.41	127.39	119.70
13	U	22	DC	O4'-C1'-N1	6.40	112.48	108.00
13	U	34	DG	O4'-C1'-N9	6.28	112.40	108.00
13	U	22	DC	O4'-C4'-C3'	-6.17	102.03	104.50
13	U	28	DA	P-O3'-C3'	6.10	127.02	119.70
13	U	34	DG	P-O3'-C3'	6.10	127.02	119.70
13	U	30	DC	C1'-O4'-C4'	-5.88	104.22	110.10
2	B	149	TYR	C-N-CA	5.84	136.31	121.70
13	U	4	DA	P-O3'-C3'	5.83	126.69	119.70
13	U	29	DA	P-O3'-C3'	5.80	126.66	119.70
12	S	36	DG	O4'-C1'-N9	5.76	112.03	108.00
12	S	38	DA	P-O3'-C3'	5.75	126.60	119.70
13	U	13	DC	O4'-C1'-N1	5.72	112.00	108.00
13	U	24	DC	O4'-C1'-N1	5.72	112.00	108.00
1	A	1063	MET	C-N-CA	5.66	135.86	121.70
13	U	15	DG	O4'-C1'-N9	5.63	111.94	108.00
12	S	11	DG	O4'-C1'-N9	5.62	111.93	108.00
12	S	16	DT	P-O3'-C3'	5.60	126.42	119.70
13	U	6	DC	C1'-O4'-C4'	-5.60	104.50	110.10
12	S	36	DG	C1'-O4'-C4'	-5.54	104.56	110.10
1	A	151	ASP	C-N-CA	5.49	135.41	121.70
12	S	5	DT	P-O3'-C3'	5.48	126.28	119.70
1	A	974	ASP	C-N-CA	5.46	135.35	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	S	18	DT	P-O3'-C3'	5.41	126.19	119.70
4	E	205	SER	N-CA-C	5.40	125.58	111.00
12	S	21	DT	P-O3'-C3'	5.40	126.18	119.70
13	U	21	DC	O4'-C1'-N1	5.33	111.73	108.00
2	B	164	LYS	C-N-CA	5.29	134.93	121.70
1	A	1066	VAL	C-N-CA	5.27	134.88	121.70
13	U	30	DC	P-O3'-C3'	5.23	125.98	119.70
12	S	24	DC	P-O3'-C3'	5.21	125.95	119.70
12	S	32	DA	P-O3'-C3'	5.20	125.94	119.70
12	S	30	DT	C1'-O4'-C4'	-5.20	104.91	110.10
12	S	14	DG	O4'-C1'-N9	5.18	111.63	108.00
12	S	15	DC	C1'-O4'-C4'	-5.18	104.92	110.10
13	U	36	DA	P-O3'-C3'	5.17	125.91	119.70
13	U	6	DC	P-O3'-C3'	5.17	125.90	119.70
1	A	1071	SER	C-N-CA	5.16	134.60	121.70
12	S	2	DG	P-O3'-C3'	5.16	125.89	119.70
13	U	12	DG	O4'-C1'-N9	5.14	111.60	108.00
13	U	38	DT	P-O3'-C3'	5.14	125.86	119.70
13	U	21	DC	O4'-C4'-C3'	-5.13	102.45	104.50
12	S	7	DC	C1'-O4'-C4'	-5.12	104.98	110.10
7	I	18	GLU	N-CA-CB	-5.12	101.38	110.60
13	U	23	DT	O4'-C1'-N1	5.11	111.58	108.00
13	U	22	DC	C4'-C3'-C2'	-5.04	98.56	103.10
13	U	10	DA	P-O3'-C3'	5.03	125.73	119.70

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	11240	0	11270	290	0
2	B	9145	0	9117	267	0
3	C	2074	0	2020	159	0
4	E	1735	0	1762	83	0
5	F	705	0	731	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1102	0	1035	58	0
7	I	927	0	886	34	0
8	J	540	0	554	25	0
9	K	924	0	934	73	0
10	L	344	0	366	26	0
11	R	197	0	96	6	0
12	S	782	0	429	7	0
13	U	771	0	425	6	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	2	0	0	2	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	1	0
15	R	1	0	0	0	0
All	All	30496	0	29625	957	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 16.

All (957) 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)
4:E:151:PRO:HD2	4:E:153:HIS:CE1	1.30	1.65
4:E:151:PRO:CD	4:E:153:HIS:HE1	1.24	1.50
7:I:56:ALA:HB2	7:I:89:GLN:CD	1.35	1.47
7:I:56:ALA:CB	7:I:89:GLN:OE1	1.64	1.46
3:C:221:TYR:CB	6:H:46:LEU:HD22	1.44	1.43
1:A:53:LEU:HD23	1:A:54:ASN:N	1.45	1.30
3:C:221:TYR:CA	6:H:46:LEU:CD2	2.10	1.29
1:A:116:ASP:OD1	1:A:164:ARG:CG	1.78	1.29
1:A:116:ASP:OD1	1:A:164:ARG:HG2	1.17	1.28
3:C:221:TYR:HA	6:H:46:LEU:CD2	1.60	1.28
3:C:8:VAL:HG23	9:K:108:GLU:OE1	1.26	1.27
3:C:70:ILE:HD12	3:C:142:VAL:CG1	1.66	1.23
7:I:56:ALA:CB	7:I:89:GLN:NE2	2.03	1.22
7:I:56:ALA:CB	7:I:89:GLN:CD	2.03	1.18
3:C:88:CYS:SG	3:C:91:HIS:O	2.00	1.18
3:C:221:TYR:CA	6:H:46:LEU:HD21	1.72	1.17
3:C:259:LEU:HG	9:K:91:CYS:SG	1.85	1.16
3:C:70:ILE:HD12	3:C:142:VAL:HG11	1.23	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:TYR:HB3	6:H:46:LEU:CD2	1.77	1.15
7:I:56:ALA:HB3	7:I:89:GLN:OE1	1.45	1.15
3:C:91:HIS:CD2	3:C:96:SER:CB	2.31	1.14
1:A:870:GLU:O	4:E:205:SER:HB2	1.48	1.12
6:H:41:ASP:O	6:H:42:ILE:HG13	1.49	1.12
10:L:57:LEU:HD23	10:L:59:ALA:N	1.63	1.12
3:C:221:TYR:CA	6:H:46:LEU:HD22	1.75	1.10
7:I:56:ALA:HB2	7:I:89:GLN:NE2	1.65	1.10
3:C:118:LEU:HD11	3:C:132:PRO:HG3	1.27	1.08
1:A:1067:LEU:O	1:A:1069:ALA:N	1.86	1.08
3:C:70:ILE:CD1	3:C:142:VAL:HG11	1.83	1.07
7:I:56:ALA:CB	7:I:89:GLN:HE22	1.65	1.07
7:I:56:ALA:HB2	7:I:89:GLN:OE1	1.34	1.07
3:C:8:VAL:CG2	9:K:108:GLU:OE1	2.03	1.05
2:B:289:LEU:CD2	2:B:375:ALA:HB2	1.85	1.05
4:E:151:PRO:CD	4:E:153:HIS:CE1	2.11	1.04
2:B:285:ILE:HD13	2:B:378:LEU:HD11	1.37	1.04
9:K:75:ILE:HD13	9:K:83:PRO:HB2	1.06	1.04
9:K:94:ILE:O	9:K:98:LEU:HD13	1.58	1.03
5:F:94:LEU:HD12	5:F:121:ALA:CB	1.89	1.02
3:C:91:HIS:CD2	3:C:96:SER:OG	2.12	1.02
9:K:75:ILE:CD1	9:K:83:PRO:HB2	1.91	1.01
6:H:22:LYS:O	6:H:43:ASN:ND2	1.92	1.01
10:L:57:LEU:HD23	10:L:59:ALA:H	0.87	1.00
9:K:19:LEU:HD21	9:K:35:PHE:CE2	1.97	1.00
5:F:94:LEU:CD1	5:F:121:ALA:HB3	1.91	1.00
3:C:262:LEU:HD22	9:K:88:LYS:NZ	1.77	0.99
3:C:43:THR:HG21	3:C:172:PRO:HG3	1.42	0.99
2:B:282:ILE:O	2:B:285:ILE:HG22	1.63	0.98
2:B:130:VAL:HG23	2:B:132:VAL:HG23	1.42	0.98
5:F:97:ARG:HG3	5:F:101:ILE:HD12	1.44	0.97
3:C:100:THR:OG1	3:C:119:VAL:HG23	1.64	0.97
8:J:20:SER:O	8:J:24:LEU:HG	1.64	0.97
3:C:43:THR:CG2	3:C:172:PRO:HG3	1.94	0.96
4:E:178:ILE:HD11	4:E:182:ASP:OD1	1.66	0.95
9:K:75:ILE:HD13	9:K:83:PRO:CB	1.96	0.95
3:C:221:TYR:HB3	6:H:46:LEU:HD22	0.96	0.94
4:E:110:PHE:HE2	4:E:116:ILE:HD11	1.32	0.94
9:K:11:LEU:HD23	9:K:12:LEU:N	1.83	0.94
10:L:57:LEU:CD2	10:L:59:ALA:H	1.79	0.94
3:C:70:ILE:CD1	3:C:142:VAL:CG1	2.42	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:TYR:CB	6:H:46:LEU:CD2	2.29	0.93
3:C:78:GLU:OE1	3:C:78:GLU:N	2.01	0.93
1:A:53:LEU:HD23	1:A:54:ASN:H	1.33	0.93
4:E:184:VAL:O	4:E:188:LEU:HD13	1.66	0.93
3:C:70:ILE:HD12	3:C:142:VAL:HG12	1.49	0.93
3:C:259:LEU:CG	9:K:91:CYS:SG	2.56	0.92
2:B:285:ILE:HD13	2:B:378:LEU:CD1	2.00	0.91
3:C:91:HIS:CD2	3:C:96:SER:HB2	2.03	0.91
5:F:94:LEU:HD12	5:F:121:ALA:HB1	1.52	0.91
4:E:151:PRO:O	4:E:153:HIS:ND1	2.02	0.91
1:A:565:ILE:HD11	1:A:571:LEU:H	1.36	0.91
5:F:125:LEU:HD12	5:F:126:ALA:N	1.85	0.91
7:I:56:ALA:HB1	7:I:89:GLN:HE22	1.33	0.90
2:B:44:VAL:HG23	2:B:48:LEU:HD11	1.51	0.90
3:C:71:PRO:C	3:C:72:LEU:HD12	1.93	0.89
8:J:30:LEU:HD13	8:J:34:THR:OG1	1.72	0.89
3:C:251:LEU:HD22	9:K:98:LEU:HD21	1.54	0.89
5:F:130:ILE:CG2	5:F:132:LEU:HD13	2.03	0.89
3:C:221:TYR:HA	6:H:46:LEU:HD21	0.90	0.89
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.06	0.88
6:H:6:PHE:O	6:H:7:ASP:OD1	1.92	0.88
10:L:33:GLU:OE2	10:L:53:HIS:CD2	2.26	0.88
3:C:91:HIS:NE2	3:C:96:SER:OG	2.05	0.88
4:E:151:PRO:CG	4:E:153:HIS:CE1	2.57	0.88
1:A:354:SER:HB2	1:A:469:ARG:HD3	1.55	0.87
2:B:360:PHE:CE1	2:B:361:LEU:HD13	2.09	0.87
9:K:91:CYS:O	9:K:94:ILE:HG22	1.74	0.87
1:A:1067:LEU:HD23	1:A:1068:ALA:H	1.38	0.87
5:F:86:THR:HG22	5:F:89:GLU:OE1	1.74	0.86
2:B:289:LEU:HD23	2:B:375:ALA:HB2	1.56	0.86
1:A:565:ILE:HD11	1:A:571:LEU:N	1.91	0.86
5:F:94:LEU:CD1	5:F:121:ALA:CB	2.49	0.86
2:B:74:LEU:HD12	2:B:75:ALA:H	1.41	0.86
1:A:116:ASP:OD1	1:A:164:ARG:HG3	1.71	0.85
3:C:92:CYS:SG	14:C:402:ZN:ZN	1.64	0.85
3:C:262:LEU:HD22	9:K:88:LYS:HZ3	1.40	0.85
3:C:92:CYS:HG	14:C:402:ZN:ZN	0.56	0.85
3:C:9:LYS:HA	9:K:108:GLU:OE2	1.77	0.84
2:B:254:LEU:HD12	2:B:272:THR:O	1.76	0.84
2:B:44:VAL:HG23	2:B:48:LEU:CD1	2.06	0.84
5:F:94:LEU:HD11	5:F:121:ALA:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:45:LEU:HD13	9:K:94:ILE:CD1	2.07	0.83
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.60	0.82
4:E:110:PHE:CE2	4:E:116:ILE:HD11	2.14	0.82
3:C:92:CYS:O	3:C:96:SER:OG	1.98	0.82
2:B:285:ILE:CD1	2:B:378:LEU:HD11	2.10	0.81
1:A:53:LEU:CD2	1:A:54:ASN:N	2.39	0.81
3:C:118:LEU:HD12	3:C:118:LEU:O	1.81	0.81
8:J:43:ARG:O	8:J:46:CYS:SG	2.38	0.80
4:E:151:PRO:HG2	4:E:153:HIS:CE1	2.17	0.80
9:K:75:ILE:O	9:K:75:ILE:HD12	1.81	0.80
3:C:91:HIS:CE1	3:C:96:SER:OG	2.34	0.80
7:I:18:GLU:HG3	7:I:20:LYS:CD	2.11	0.80
1:A:845:LEU:HB3	1:A:1065:GLY:O	1.81	0.80
3:C:100:THR:OG1	3:C:119:VAL:CG2	2.29	0.80
2:B:44:VAL:CG2	2:B:48:LEU:HD11	2.11	0.79
5:F:97:ARG:HA	5:F:100:GLN:HB2	1.64	0.79
1:A:152:VAL:HG12	1:A:160:GLN:O	1.83	0.79
3:C:145:CYS:HA	8:J:2:ILE:HD11	1.64	0.78
2:B:254:LEU:CD2	2:B:361:LEU:HD11	2.13	0.78
3:C:91:HIS:NE2	3:C:96:SER:CB	2.46	0.78
3:C:259:LEU:HD21	9:K:91:CYS:HB3	1.65	0.78
4:E:118:PRO:HA	4:E:121:MET:HB2	1.65	0.78
1:A:311:GLN:HB2	1:A:312:PRO:HD2	1.66	0.78
5:F:131:PRO:C	5:F:132:LEU:HD12	2.04	0.78
7:I:18:GLU:HG3	7:I:20:LYS:HD3	1.65	0.77
2:B:149:TYR:HA	2:B:150:GLU:HB2	1.65	0.77
2:B:387:LEU:CD2	2:B:392:ARG:HB2	2.15	0.77
5:F:99:LEU:HD23	5:F:103:MET:HG2	1.65	0.77
7:I:78:CYS:SG	7:I:106:CYS:HB3	2.24	0.77
1:A:1071:SER:O	1:A:1072:ILE:HG13	1.85	0.76
1:A:870:GLU:O	4:E:205:SER:CB	2.32	0.76
2:B:282:ILE:O	2:B:285:ILE:CG2	2.31	0.76
3:C:144:ILE:O	8:J:2:ILE:HD13	1.85	0.76
1:A:467:THR:HG23	1:A:469:ARG:HH12	1.49	0.76
2:B:289:LEU:HD23	2:B:291:ILE:HD13	1.67	0.76
10:L:64:LEU:HD12	10:L:64:LEU:O	1.84	0.76
2:B:142:VAL:HB	2:B:143:PRO:HD2	1.66	0.75
3:C:27:LEU:H	3:C:27:LEU:HD23	1.51	0.75
4:E:78:LEU:HD11	4:E:109:ILE:HG12	1.68	0.75
1:A:712:GLU:HG3	7:I:93:LYS:HE2	1.68	0.75
2:B:130:VAL:CG2	2:B:132:VAL:HG23	2.14	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:HB3	2:B:1201:LYS:HD2	1.69	0.75
3:C:145:CYS:HA	8:J:2:ILE:CD1	2.17	0.74
10:L:34:CYS:SG	14:L:101:ZN:ZN	1.76	0.74
5:F:86:THR:HG23	5:F:89:GLU:H	1.52	0.74
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.51	0.74
1:A:566:ILE:HB	6:H:96:VAL:HG23	1.69	0.74
4:E:144:ILE:CD1	4:E:183:PRO:HB2	2.18	0.74
1:A:1067:LEU:C	1:A:1069:ALA:H	1.88	0.73
9:K:11:LEU:HD23	9:K:12:LEU:H	1.50	0.73
2:B:26:THR:HG22	2:B:27:ALA:N	2.03	0.73
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.70	0.72
9:K:45:LEU:HD13	9:K:94:ILE:HD11	1.69	0.72
2:B:213:ILE:HD11	2:B:497:ARG:HB3	1.71	0.72
2:B:254:LEU:HD23	2:B:361:LEU:HD11	1.71	0.72
5:F:94:LEU:HD12	5:F:121:ALA:HB3	1.57	0.72
6:H:40:LEU:HD23	6:H:41:ASP:N	2.03	0.72
1:A:252:PHE:HZ	11:R:2:U:C1'	2.02	0.72
9:K:94:ILE:O	9:K:98:LEU:CD1	2.36	0.72
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.72	0.72
4:E:151:PRO:HG2	4:E:198:ILE:CG2	2.21	0.71
1:A:37:PHE:H	1:A:52:GLY:HA3	1.55	0.71
3:C:259:LEU:CD1	9:K:91:CYS:SG	2.78	0.71
3:C:33:LEU:O	3:C:33:LEU:HD23	1.90	0.71
3:C:91:HIS:CG	3:C:96:SER:OG	2.44	0.71
1:A:1342:GLU:HB3	4:E:151:PRO:HG3	1.72	0.70
3:C:91:HIS:NE2	3:C:96:SER:HB2	2.04	0.70
1:A:770:VAL:HG23	1:A:822:GLU:HG3	1.73	0.70
2:B:74:LEU:HD12	2:B:75:ALA:N	2.06	0.70
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.72	0.70
2:B:101:MET:HG2	2:B:111:ALA:HA	1.73	0.70
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.73	0.70
3:C:221:TYR:N	6:H:46:LEU:CD2	2.53	0.70
1:A:443:LEU:HG	1:A:501:LEU:HD21	1.74	0.70
2:B:360:PHE:CZ	2:B:361:LEU:HD13	2.26	0.70
3:C:70:ILE:O	3:C:72:LEU:CD1	2.40	0.70
2:B:285:ILE:CD1	2:B:378:LEU:CD1	2.66	0.70
10:L:30:ILE:CG2	10:L:57:LEU:HB3	2.22	0.70
10:L:57:LEU:CD2	10:L:59:ALA:N	2.46	0.70
6:H:96:VAL:HG12	6:H:143:LEU:HA	1.75	0.69
1:A:446:ARG:HB3	1:A:478:TYR:HD2	1.57	0.69
7:I:78:CYS:SG	7:I:106:CYS:CB	2.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:57:LEU:CD2	10:L:59:ALA:HA	2.23	0.69
1:A:1170:ILE:HD11	1:A:1239:ARG:HH11	1.57	0.69
8:J:36:LEU:HA	8:J:41:LEU:HD12	1.75	0.69
1:A:252:PHE:CE2	11:R:2:U:H4'	2.28	0.68
1:A:738:LYS:HE3	3:C:194:GLU:HA	1.73	0.68
5:F:130:ILE:HG23	5:F:132:LEU:HD13	1.74	0.68
9:K:11:LEU:O	9:K:37:LYS:HG3	1.92	0.68
9:K:19:LEU:HD21	9:K:35:PHE:CD2	2.27	0.68
3:C:33:LEU:HD21	3:C:37:MET:SD	2.33	0.68
4:E:185:ALA:O	4:E:190:LEU:HD23	1.93	0.68
10:L:30:ILE:HG22	10:L:57:LEU:HB3	1.74	0.68
4:E:206:GLY:O	4:E:207:ARG:HG2	1.94	0.68
2:B:69:LEU:O	2:B:69:LEU:HD12	1.93	0.68
1:A:1067:LEU:HD23	1:A:1068:ALA:N	2.08	0.68
1:A:1155:ASP:HB3	1:A:1162:VAL:HG23	1.76	0.68
2:B:654:ARG:H	2:B:657:HIS:HD2	1.42	0.68
1:A:369:SER:O	1:A:371:ALA:N	2.28	0.67
3:C:262:LEU:O	3:C:262:LEU:HD23	1.94	0.67
1:A:855:THR:CG2	1:A:857:ARG:HE	2.07	0.67
2:B:137:TYR:CE1	2:B:151:LEU:HD13	2.28	0.67
3:C:100:THR:HG1	3:C:119:VAL:HG23	1.57	0.67
3:C:57:VAL:HG21	8:J:60:PHE:HB3	1.76	0.67
9:K:21:ILE:HA	9:K:33:ILE:HG22	1.77	0.67
2:B:955:THR:HG22	2:B:956:THR:H	1.60	0.67
3:C:72:LEU:N	3:C:72:LEU:HD12	2.10	0.67
12:S:14:DG:H4'	12:S:15:DC:H5'	1.76	0.67
1:A:515:GLN:NE2	1:A:1075:PRO:HD3	2.09	0.67
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.76	0.67
2:B:416:LEU:HD22	2:B:466:TRP:CE3	2.29	0.67
1:A:348:SER:HB3	2:B:1128:LEU:HB2	1.76	0.67
4:E:188:LEU:N	4:E:188:LEU:HD12	2.10	0.67
1:A:252:PHE:HZ	11:R:2:U:H1'	1.60	0.66
2:B:387:LEU:HD23	2:B:392:ARG:HB2	1.77	0.66
5:F:130:ILE:HG22	5:F:132:LEU:HD13	1.77	0.66
1:A:367:PRO:HB3	9:K:2:ASN:ND2	2.11	0.66
3:C:27:LEU:N	3:C:27:LEU:HD23	2.11	0.66
4:E:37:LEU:HD21	4:E:45:LYS:NZ	2.11	0.66
1:A:810:PRO:HB3	2:B:745:PRO:HB3	1.76	0.66
2:B:397:ASP:HB3	2:B:400:HIS:HB2	1.77	0.66
1:A:53:LEU:HD23	1:A:54:ASN:CA	2.26	0.66
4:E:190:LEU:N	4:E:190:LEU:HD22	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:91:CYS:O	9:K:94:ILE:CG2	2.44	0.66
1:A:382:PRO:HD3	1:A:428:TYR:HE1	1.61	0.65
1:A:53:LEU:HD23	1:A:53:LEU:C	2.17	0.65
2:B:254:LEU:CD2	2:B:361:LEU:CD1	2.74	0.65
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.77	0.65
3:C:51:VAL:HB	10:L:65:VAL:CG2	2.26	0.65
9:K:12:LEU:N	9:K:12:LEU:HD12	2.10	0.65
9:K:87:LEU:HD23	9:K:87:LEU:O	1.95	0.65
1:A:1071:SER:HB3	1:A:1367:HIS:CD2	2.31	0.65
3:C:27:LEU:H	3:C:27:LEU:CD2	2.09	0.65
2:B:858:SER:HA	2:B:966:VAL:O	1.96	0.65
1:A:974:ASP:HA	1:A:975:HIS:HB2	1.77	0.65
2:B:511:PRO:HD2	2:B:512:ARG:HG3	1.78	0.65
3:C:33:LEU:CD2	3:C:37:MET:SD	2.85	0.65
3:C:262:LEU:CD2	9:K:88:LYS:NZ	2.58	0.65
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.61	0.65
9:K:87:LEU:HD23	9:K:87:LEU:C	2.17	0.65
1:A:855:THR:HG21	1:A:857:ARG:HE	1.62	0.64
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.79	0.64
1:A:846:GLU:O	1:A:1066:VAL:HG12	1.97	0.64
3:C:33:LEU:HD23	3:C:33:LEU:C	2.18	0.64
1:A:335:ARG:HE	2:B:1202:LEU:HD23	1.61	0.64
4:E:151:PRO:O	4:E:153:HIS:CE1	2.49	0.64
3:C:80:LEU:HD12	3:C:94:LYS:O	1.98	0.64
2:B:526:GLU:HG2	2:B:771:SER:HB2	1.80	0.64
3:C:259:LEU:HD21	9:K:91:CYS:CB	2.28	0.64
8:J:10:CYS:SG	8:J:11:GLY:N	2.70	0.64
2:B:26:THR:HG22	2:B:27:ALA:H	1.62	0.63
5:F:99:LEU:C	5:F:99:LEU:HD23	2.18	0.63
2:B:826:ALA:HB3	2:B:1011:ILE:HG12	1.81	0.63
2:B:387:LEU:HD23	2:B:387:LEU:O	1.99	0.63
3:C:262:LEU:HD22	9:K:88:LYS:HZ1	1.62	0.63
3:C:9:LYS:CA	9:K:108:GLU:OE2	2.46	0.63
1:A:781:ASP:HB2	1:A:789:LYS:HG2	1.79	0.63
2:B:289:LEU:HD21	2:B:375:ALA:HB2	1.78	0.63
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.81	0.63
4:E:188:LEU:HB2	4:E:190:LEU:HD21	1.81	0.63
1:A:1063:MET:O	1:A:1066:VAL:HG13	1.99	0.62
1:A:451:HIS:CD2	1:A:453:MET:HB2	2.34	0.62
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.80	0.62
6:H:44:VAL:HA	6:H:47:PHE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1182:GLU:HB2	1:A:1183:GLN:HB3	1.81	0.62
3:C:262:LEU:HD23	3:C:262:LEU:C	2.20	0.62
2:B:387:LEU:C	2:B:387:LEU:HD23	2.19	0.62
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.81	0.62
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.81	0.62
3:C:66:ARG:NH2	8:J:2:ILE:HG22	2.14	0.62
2:B:1142:GLY:HA3	5:F:88:TYR:CE2	2.34	0.62
2:B:867:GLY:HA3	2:B:869:SER:H	1.63	0.62
4:E:182:ASP:OD1	4:E:184:VAL:HG22	2.00	0.62
4:E:179:GLN:HA	4:E:215:MET:HG2	1.81	0.62
1:A:1016:THR:HB	4:E:206:GLY:HA3	1.82	0.62
2:B:26:THR:CG2	2:B:27:ALA:H	2.13	0.62
10:L:43:THR:O	10:L:44:ASP:OD1	2.16	0.62
6:H:44:VAL:O	6:H:45:GLU:C	2.37	0.62
3:C:70:ILE:HD13	3:C:142:VAL:HG11	1.78	0.61
6:H:43:ASN:ND2	6:H:44:VAL:H	1.98	0.61
2:B:1080:LYS:HE3	3:C:188:HIS:HB2	1.82	0.61
2:B:254:LEU:HD22	2:B:361:LEU:CD1	2.30	0.61
1:A:1111:MET:HG3	1:A:1112:LYS:H	1.65	0.61
2:B:358:LYS:HA	2:B:366:GLN:HB2	1.82	0.61
2:B:309:GLN:HE21	2:B:392:ARG:HH21	1.49	0.61
2:B:72:GLU:OE1	2:B:74:LEU:HD23	1.99	0.61
1:A:85:ASP:N	1:A:238:CYS:HG	1.99	0.61
2:B:74:LEU:HB3	2:B:85:SER:HA	1.83	0.61
3:C:221:TYR:HB3	6:H:46:LEU:CG	2.30	0.61
6:H:40:LEU:HD23	6:H:40:LEU:C	2.21	0.61
7:I:56:ALA:CA	7:I:89:GLN:OE1	2.45	0.61
10:L:57:LEU:CD2	10:L:59:ALA:CA	2.78	0.61
1:A:89:PRO:HD2	1:A:205:GLU:HG2	1.82	0.61
2:B:642:ASP:HA	2:B:649:LYS:HG2	1.83	0.61
4:E:144:ILE:HD12	4:E:183:PRO:HB2	1.82	0.61
4:E:37:LEU:HD11	4:E:45:LYS:NZ	2.16	0.61
5:F:130:ILE:CG2	5:F:132:LEU:CD1	2.78	0.61
8:J:30:LEU:HD12	8:J:31:ASP:O	2.01	0.61
1:A:901:LEU:H	1:A:926:GLN:NE2	1.99	0.61
5:F:99:LEU:HD23	5:F:99:LEU:O	2.02	0.60
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.82	0.60
2:B:542:MET:HG2	2:B:747:MET:HB3	1.84	0.60
1:A:472:LEU:HD22	2:B:835:GLN:HE22	1.67	0.60
2:B:221:ASN:HB3	2:B:242:SER:HA	1.83	0.60
1:A:974:ASP:HB3	1:A:976:THR:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:LEU:HD11	9:K:91:CYS:SG	2.42	0.60
12:S:10:DG:H1	13:U:31:DC:H42	1.47	0.60
5:F:111:LEU:HG	5:F:113:GLY:H	1.66	0.60
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.83	0.60
1:A:252:PHE:HE2	11:R:2:U:H4'	1.64	0.60
1:A:489:LEU:HG	1:A:490:HIS:H	1.67	0.60
3:C:91:HIS:CG	3:C:92:CYS:H	2.20	0.60
1:A:81:PHE:HE2	2:B:1209:ALA:HB2	1.66	0.59
4:E:144:ILE:CD1	4:E:183:PRO:CB	2.80	0.59
3:C:32:SER:CB	9:K:45:LEU:HD23	2.32	0.59
2:B:26:THR:CG2	2:B:27:ALA:N	2.65	0.59
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.84	0.59
4:E:37:LEU:HD21	4:E:45:LYS:HZ3	1.66	0.59
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.84	0.59
1:A:446:ARG:HB3	1:A:478:TYR:CD2	2.38	0.59
7:I:78:CYS:HG	7:I:106:CYS:CB	2.16	0.59
3:C:66:ARG:NH1	8:J:2:ILE:CG2	2.65	0.59
1:A:359:LEU:HD22	1:A:363:GLN:HB3	1.84	0.59
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.83	0.59
4:E:187:TYR:HB3	4:E:188:LEU:HD12	1.85	0.59
3:C:66:ARG:CZ	8:J:2:ILE:HG22	2.32	0.59
3:C:89:GLU:O	3:C:90:ASP:OD1	2.20	0.59
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.38	0.59
4:E:187:TYR:C	4:E:188:LEU:HD12	2.23	0.58
9:K:45:LEU:HD13	9:K:94:ILE:HD12	1.84	0.58
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.86	0.58
3:C:92:CYS:SG	3:C:95:CYS:SG	3.01	0.58
1:A:1063:MET:HB3	1:A:1066:VAL:HG13	1.84	0.58
2:B:291:ILE:HG22	2:B:297:ILE:HG12	1.85	0.58
2:B:213:ILE:HG22	2:B:479:VAL:H	1.68	0.58
4:E:151:PRO:HG2	4:E:198:ILE:HG23	1.86	0.58
1:A:9:ALA:HB3	2:B:1161:HIS:CD2	2.39	0.58
2:B:487:THR:H	2:B:490:SER:HB3	1.68	0.58
3:C:66:ARG:NH1	8:J:2:ILE:HG21	2.18	0.58
2:B:484:ASN:HD22	2:B:494:HIS:HD2	1.51	0.58
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.34	0.58
4:E:118:PRO:HA	4:E:121:MET:CB	2.33	0.58
4:E:172:GLU:HG3	4:E:213:ILE:HD13	1.86	0.58
3:C:90:ASP:O	3:C:91:HIS:HB3	2.04	0.58
2:B:511:PRO:HD2	2:B:512:ARG:H	1.69	0.57
1:A:1014:ALA:HA	4:E:205:SER:OG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:LEU:CD2	1:A:1068:ALA:H	2.15	0.57
1:A:270:LEU:O	1:A:274:ILE:HG22	2.05	0.57
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.86	0.57
6:H:26:ILE:N	6:H:40:LEU:O	2.32	0.57
5:F:101:ILE:HG12	5:F:107:VAL:HG22	1.86	0.57
2:B:144:GLY:HA2	2:B:146:GLU:HB2	1.85	0.57
2:B:170:LEU:HA	2:B:457:LEU:HD13	1.86	0.57
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.40	0.57
1:A:845:LEU:HD12	1:A:1065:GLY:O	2.04	0.57
1:A:28:ARG:HH22	1:A:34:LYS:HA	1.68	0.57
4:E:12:LEU:HD21	4:E:55:ARG:HH11	1.68	0.57
1:A:467:THR:HG21	2:B:976:ILE:HG22	1.86	0.57
1:A:546:VAL:HG21	1:A:572:TRP:CD1	2.40	0.57
3:C:91:HIS:CG	3:C:92:CYS:N	2.73	0.57
9:K:94:ILE:HG12	9:K:98:LEU:HD13	1.87	0.57
1:A:1013:ASP:O	4:E:205:SER:OG	2.22	0.57
2:B:129:PHE:O	2:B:130:VAL:HG13	2.04	0.57
3:C:262:LEU:HD21	9:K:88:LYS:HE2	1.86	0.57
2:B:770:GLN:HA	2:B:773:MET:HG3	1.87	0.56
6:H:63:LEU:HB2	6:H:89:LEU:HD22	1.87	0.56
1:A:58:LEU:HG	1:A:80:HIS:O	2.05	0.56
2:B:241:ARG:HH21	12:S:20:DC:H41	1.53	0.56
4:E:144:ILE:HD13	4:E:183:PRO:CB	2.35	0.56
2:B:130:VAL:HG22	2:B:165:VAL:HG23	1.87	0.56
1:A:841:LEU:O	1:A:845:LEU:HD23	2.06	0.56
4:E:41:ASP:O	4:E:45:LYS:HG3	2.04	0.56
1:A:151:ASP:HA	1:A:152:VAL:HB	1.86	0.56
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.87	0.56
2:B:466:TRP:HE1	2:B:479:VAL:HG21	1.70	0.56
2:B:520:GLY:H	2:B:748:ILE:HG23	1.71	0.56
3:C:263:THR:O	3:C:266:ASP:HB3	2.05	0.56
1:A:330:LYS:HG3	1:A:1406:VAL:HG23	1.88	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.88	0.56
2:B:532:ALA:HA	2:B:535:LEU:HD12	1.88	0.56
2:B:654:ARG:H	2:B:657:HIS:CD2	2.24	0.56
2:B:863:GLU:HB3	2:B:961:LEU:HD22	1.88	0.56
3:C:55:THR:HB	3:C:152:GLU:H	1.71	0.56
4:E:31:THR:HG22	4:E:32:GLN:N	2.21	0.56
9:K:19:LEU:CD2	9:K:35:PHE:CE2	2.81	0.56
4:E:144:ILE:HD13	4:E:183:PRO:HB3	1.86	0.55
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:SER:HB3	7:I:46:HIS:HB2	1.88	0.55
7:I:56:ALA:N	7:I:89:GLN:OE1	2.38	0.55
1:A:30:ILE:HA	2:B:1183:LYS:O	2.05	0.55
1:A:333:GLU:HA	1:A:338:GLY:HA3	1.88	0.55
1:A:523:ILE:HG23	1:A:527:THR:HG23	1.88	0.55
2:B:130:VAL:HG23	2:B:132:VAL:CG2	2.27	0.55
2:B:502:ILE:HG22	2:B:503:GLY:H	1.71	0.55
2:B:364:ILE:HG22	2:B:585:VAL:HG13	1.89	0.55
4:E:151:PRO:HG2	4:E:198:ILE:HG21	1.88	0.55
4:E:44:ALA:O	4:E:45:LYS:HG3	2.06	0.55
2:B:137:TYR:CD1	2:B:151:LEU:HD13	2.41	0.55
2:B:286:PHE:CG	2:B:297:ILE:HG23	2.41	0.55
1:A:746:MET:HE1	2:B:1015:HIS:HA	1.88	0.55
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.89	0.55
2:B:492:LEU:HA	2:B:495:LEU:HD12	1.89	0.55
5:F:86:THR:HG22	5:F:89:GLU:CD	2.28	0.55
1:A:467:THR:HG23	1:A:469:ARG:NH1	2.21	0.55
5:F:74:ILE:HD12	5:F:144:GLU:HG3	1.89	0.55
1:A:1070:GLN:C	1:A:1072:ILE:H	2.09	0.54
2:B:289:LEU:HD23	2:B:291:ILE:CD1	2.36	0.54
2:B:510:LYS:HB2	2:B:511:PRO:HA	1.88	0.54
10:L:64:LEU:HD12	10:L:64:LEU:C	2.28	0.54
2:B:1158:PHE:HE2	2:B:1201:LYS:HD3	1.71	0.54
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.89	0.54
2:B:149:TYR:CA	2:B:150:GLU:HB2	2.37	0.54
4:E:21:GLU:OE2	4:E:146:HIS:HE1	1.90	0.54
2:B:872:GLU:HA	2:B:917:PRO:HD3	1.89	0.54
12:S:10:DG:H1'	12:S:11:DG:H5'	1.90	0.54
1:A:1013:ASP:O	4:E:205:SER:O	2.26	0.54
1:A:1313:LEU:HD23	1:A:1338:VAL:HG11	1.89	0.54
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.90	0.54
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.90	0.54
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.89	0.54
2:B:130:VAL:CG2	2:B:132:VAL:CG2	2.85	0.54
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.88	0.54
5:F:130:ILE:HG22	5:F:132:LEU:CD1	2.37	0.54
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.90	0.54
1:A:252:PHE:CZ	11:R:2:U:H1'	2.40	0.54
1:A:32:VAL:HB	1:A:57:ARG:HB3	1.90	0.53
1:A:61:ILE:HG21	1:A:250:ILE:HG13	1.89	0.53
10:L:60:ARG:HG2	10:L:61:THR:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLN:HE22	1:A:1075:PRO:HD3	1.73	0.53
1:A:53:LEU:CD2	1:A:54:ASN:H	2.16	0.53
3:C:55:THR:O	3:C:55:THR:HG22	2.08	0.53
1:A:1383:SER:HB2	1:A:1388:GLY:HA3	1.91	0.53
1:A:534:LEU:O	1:A:539:THR:HG21	2.08	0.53
2:B:305:VAL:O	2:B:305:VAL:HG12	2.08	0.53
6:H:4:THR:HG21	6:H:7:ASP:OD1	2.07	0.53
7:I:83:ASN:HD21	7:I:101:PHE:HD2	1.55	0.53
1:A:845:LEU:CB	1:A:1065:GLY:O	2.56	0.53
2:B:637:LEU:HB2	2:B:693:ILE:HD13	1.90	0.53
6:H:6:PHE:C	6:H:7:ASP:OD1	2.45	0.53
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.91	0.53
1:A:314:ALA:HB1	1:A:322:VAL:HG12	1.89	0.53
2:B:140:ILE:O	2:B:140:ILE:HG13	2.09	0.53
4:E:118:PRO:HA	4:E:121:MET:CG	2.39	0.53
4:E:55:ARG:HE	4:E:84:ASP:HA	1.73	0.53
6:H:56:THR:HB	6:H:145:ARG:HB3	1.91	0.53
1:A:240:PRO:HB2	2:B:1209:ALA:HA	1.89	0.53
3:C:43:THR:OG1	3:C:170:TRP:HB3	2.08	0.53
1:A:315:LEU:HD12	1:A:316:GLN:H	1.74	0.53
2:B:164:LYS:O	2:B:165:VAL:HG22	2.08	0.53
2:B:420:LEU:HD23	2:B:453:ILE:HA	1.89	0.53
2:B:510:LYS:HD2	2:B:513:GLN:HB2	1.90	0.53
3:C:118:LEU:HD11	3:C:132:PRO:CG	2.18	0.53
3:C:66:ARG:CZ	8:J:2:ILE:CG2	2.86	0.53
2:B:260:GLY:HA2	2:B:264:SER:HB3	1.91	0.53
2:B:1171:VAL:HG21	2:B:1191:ILE:HG12	1.90	0.53
10:L:30:ILE:HG21	10:L:57:LEU:HD22	1.90	0.53
1:A:18:GLN:HB3	1:A:1418:LEU:HG	1.90	0.53
1:A:298:PHE:O	1:A:302:THR:HG22	2.08	0.53
3:C:118:LEU:CD1	3:C:132:PRO:HG3	2.19	0.53
9:K:42:LEU:O	9:K:46:ILE:HG12	2.08	0.53
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.73	0.52
1:A:591:PHE:HA	1:A:595:THR:HG21	1.91	0.52
5:F:122:MET:O	5:F:125:LEU:HG	2.08	0.52
1:A:1107:VAL:HG12	1:A:1383:SER:HA	1.90	0.52
1:A:565:ILE:CD1	1:A:571:LEU:H	2.14	0.52
2:B:415:GLN:HE22	2:B:476:ARG:HH22	1.57	0.52
4:E:183:PRO:HA	4:E:186:LEU:HD12	1.89	0.52
1:A:377:PRO:HA	1:A:432:VAL:O	2.10	0.52
2:B:129:PHE:HB3	2:B:163:GLY:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:58:THR:HB	6:H:143:LEU:HB2	1.92	0.52
1:A:368:LYS:HA	1:A:462:VAL:HG12	1.91	0.52
2:B:860:MET:HB3	2:B:965:LYS:HG3	1.90	0.52
6:H:8:ASP:OD2	6:H:129:TYR:OH	2.17	0.52
1:A:464:PRO:HB2	9:K:4:PRO:HD3	1.92	0.52
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	1.92	0.52
7:I:56:ALA:HB3	7:I:89:GLN:CD	2.03	0.52
10:L:60:ARG:HG2	10:L:61:THR:O	2.09	0.52
1:A:489:LEU:CG	1:A:490:HIS:H	2.22	0.52
3:C:46:ILE:HG21	3:C:157:CYS:HB2	1.91	0.52
4:E:188:LEU:N	4:E:188:LEU:CD1	2.73	0.52
5:F:133:VAL:HG12	5:F:147:SER:HA	1.91	0.52
5:F:86:THR:HG22	5:F:89:GLU:CG	2.40	0.52
1:A:606:LEU:HB3	1:A:613:ILE:HB	1.90	0.52
1:A:919:ILE:O	1:A:922:ASP:HB2	2.10	0.52
1:A:1035:TYR:HB3	1:A:1037:LEU:HD23	1.91	0.52
1:A:216:VAL:HG12	1:A:230:ARG:HH21	1.74	0.52
4:E:72:PHE:HB2	4:E:75:MET:SD	2.50	0.52
9:K:27:ALA:HB3	9:K:74:ARG:HH21	1.75	0.52
1:A:845:LEU:HA	1:A:848:ILE:HD12	1.91	0.52
1:A:901:LEU:H	1:A:926:GLN:HE22	1.58	0.52
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.92	0.52
9:K:12:LEU:N	9:K:12:LEU:CD1	2.73	0.52
2:B:1158:PHE:CE2	2:B:1160:VAL:HG13	2.45	0.52
3:C:72:LEU:N	3:C:72:LEU:CD1	2.73	0.52
4:E:151:PRO:CG	4:E:198:ILE:CG2	2.88	0.52
4:E:187:TYR:HB3	4:E:188:LEU:CD1	2.40	0.52
1:A:471:ASN:HB3	1:A:474:VAL:HG12	1.91	0.51
2:B:123:THR:HG23	2:B:205:ILE:HA	1.92	0.51
6:H:38:LEU:CD2	6:H:40:LEU:HB2	2.40	0.51
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.93	0.51
2:B:129:PHE:O	2:B:130:VAL:CG1	2.59	0.51
3:C:80:LEU:HD11	3:C:95:CYS:HA	1.92	0.51
2:B:737:THR:O	7:I:66:PRO:HB2	2.11	0.51
9:K:32:VAL:O	9:K:32:VAL:HG23	2.10	0.51
2:B:1171:VAL:CG2	2:B:1191:ILE:HG12	2.40	0.51
2:B:74:LEU:CD1	2:B:75:ALA:N	2.73	0.51
5:F:97:ARG:HG3	5:F:101:ILE:CD1	2.29	0.51
6:H:133:ASN:OD1	6:H:134:ASN:N	2.44	0.51
3:C:14:SER:HA	9:K:115:ALA:HB3	1.92	0.51
9:K:65:HIS:HD2	9:K:67:PHE:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:SER:HA	2:B:492:LEU:HD12	1.93	0.51
6:H:6:PHE:CE1	6:H:8:ASP:HB2	2.44	0.51
1:A:899:VAL:HB	1:A:929:LEU:HD13	1.93	0.51
2:B:1023:VAL:HA	2:B:1026:LEU:HD12	1.92	0.51
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.51
2:B:1142:GLY:HA3	5:F:88:TYR:HE2	1.71	0.51
2:B:955:THR:HG22	2:B:956:THR:N	2.25	0.51
2:B:706:GLN:HB3	2:B:709:ASP:HB2	1.93	0.51
6:H:41:ASP:O	6:H:42:ILE:CG1	2.40	0.51
10:L:38:LEU:HD21	10:L:49:LYS:H	1.76	0.51
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.10	0.51
1:A:58:LEU:HD23	1:A:243:PRO:HA	1.93	0.51
2:B:540:SER:HA	2:B:750:GLY:HA2	1.93	0.51
3:C:46:ILE:H	3:C:46:ILE:HD12	1.76	0.51
5:F:130:ILE:HG23	5:F:132:LEU:CD1	2.38	0.51
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.93	0.50
3:C:79:GLN:HG3	3:C:127:ARG:HH11	1.76	0.50
5:F:116:ASP:O	5:F:120:ILE:HG13	2.10	0.50
1:A:1117:THR:HG22	1:A:1307:GLU:HG2	1.93	0.50
2:B:282:ILE:C	2:B:285:ILE:HG22	2.30	0.50
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.94	0.50
10:L:60:ARG:NH1	10:L:61:THR:O	2.44	0.50
2:B:128:LEU:HD11	2:B:170:LEU:HB2	1.94	0.50
2:B:791:THR:O	2:B:857:ARG:HG3	2.12	0.50
2:B:974:PRO:HB3	2:B:980:PHE:HZ	1.75	0.50
3:C:79:GLN:HG3	3:C:127:ARG:NH1	2.26	0.50
4:E:182:ASP:OD1	4:E:184:VAL:CG2	2.59	0.50
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.92	0.50
2:B:298:LEU:O	2:B:301:ILE:N	2.45	0.50
2:B:269:ILE:H	2:B:317:CYS:HB3	1.75	0.50
6:H:43:ASN:HD21	6:H:45:GLU:HG2	1.77	0.50
1:A:361:LEU:HA	1:A:471:ASN:HD22	1.77	0.50
1:A:663:SER:HB2	2:B:1085:ILE:HA	1.94	0.50
4:E:151:PRO:HD2	4:E:153:HIS:HE1	0.39	0.50
5:F:99:LEU:CD2	5:F:103:MET:HG2	2.40	0.50
6:H:43:ASN:ND2	6:H:44:VAL:N	2.60	0.49
13:U:25:DT:H2''	13:U:26:DC:H5'	1.93	0.49
3:C:11:ARG:NH2	3:C:19:ASP:OD1	2.44	0.49
1:A:1161:THR:HG21	1:A:1239:ARG:NH1	2.27	0.49
2:B:44:VAL:HG23	2:B:48:LEU:HD12	1.92	0.49
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:92:ARG:HB2	7:I:95:THR:HG23	1.94	0.49
2:B:511:PRO:CD	2:B:512:ARG:H	2.25	0.49
2:B:1158:PHE:CE2	2:B:1201:LYS:HD3	2.46	0.49
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.93	0.49
3:C:40:GLU:HG2	3:C:254:LYS:NZ	2.27	0.49
3:C:91:HIS:ND1	3:C:92:CYS:N	2.61	0.49
3:C:92:CYS:O	3:C:96:SER:N	2.45	0.49
4:E:190:LEU:N	4:E:190:LEU:CD2	2.75	0.49
12:S:26:DG:N3	12:S:27:DT:N3	2.60	0.49
1:A:1413:GLY:HA3	2:B:1212:ILE:HD12	1.94	0.49
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.94	0.49
2:B:31:TRP:HA	2:B:34:ILE:HD12	1.94	0.49
2:B:975:GLN:O	2:B:990:ILE:HD13	2.12	0.49
1:A:86:LEU:HD21	1:A:239:LEU:H	1.78	0.49
1:A:391:LEU:HA	1:A:394:ASN:HB2	1.94	0.49
1:A:1115:SER:O	1:A:1330:ASN:HB2	2.13	0.49
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.48	0.49
5:F:125:LEU:O	5:F:126:ALA:C	2.50	0.49
7:I:4:PHE:CE2	7:I:14:LEU:HB2	2.47	0.49
2:B:867:GLY:HA3	2:B:869:SER:N	2.27	0.49
4:E:155:ARG:HA	4:E:196:VAL:HG12	1.95	0.49
2:B:552:MET:HA	2:B:555:ILE:HD12	1.95	0.49
3:C:101:LEU:C	3:C:101:LEU:HD23	2.34	0.49
9:K:33:ILE:HG13	9:K:73:LEU:HB3	1.96	0.48
1:A:986:ILE:HD11	1:A:1032:LEU:HD21	1.95	0.48
6:H:105:GLU:HB3	6:H:113:ALA:HB3	1.95	0.48
8:J:56:LEU:O	8:J:57:ILE:C	2.51	0.48
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.96	0.48
2:B:69:LEU:CD1	2:B:432:MET:CE	2.91	0.48
3:C:185:LYS:HE3	3:C:220:ASP:HB2	1.95	0.48
5:F:109:VAL:HG11	5:F:124:GLU:HA	1.95	0.48
1:A:101:LYS:HG2	1:A:139:TRP:CD1	2.49	0.48
1:A:966:ASN:HB3	1:A:1044:TRP:HH2	1.78	0.48
10:L:30:ILE:CG2	10:L:57:LEU:HD22	2.43	0.48
2:B:1117:GLN:OE1	2:B:1199:ALA:HB2	2.14	0.48
2:B:524:PRO:HD2	2:B:749:LEU:HD23	1.95	0.48
12:S:33:DT:H3	13:U:8:DA:H61	1.61	0.48
1:A:216:VAL:HG12	1:A:230:ARG:NH2	2.28	0.48
1:A:579:SER:HA	1:A:582:ILE:HD12	1.96	0.48
2:B:1174:LYS:HG2	2:B:1177:HIS:HB2	1.95	0.48
2:B:293:PRO:O	2:B:297:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASP:O	2:B:298:LEU:HG	2.13	0.48
3:C:91:HIS:O	3:C:92:CYS:HB3	2.13	0.48
1:A:367:PRO:HB3	9:K:2:ASN:HD21	1.76	0.48
1:A:663:SER:CB	2:B:1085:ILE:HA	2.43	0.48
2:B:1016:ALA:O	2:B:1020:ARG:HG2	2.14	0.48
2:B:1160:VAL:HG23	2:B:1194:ILE:HG13	1.96	0.48
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.49	0.48
2:B:484:ASN:HD22	2:B:494:HIS:CD2	2.31	0.48
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.95	0.48
1:A:1170:ILE:HD11	1:A:1239:ARG:NH1	2.25	0.48
1:A:53:LEU:CD2	1:A:54:ASN:CG	2.82	0.48
1:A:1068:ALA:HA	1:A:1071:SER:HB2	1.95	0.47
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.96	0.47
1:A:880:LYS:HA	1:A:955:PRO:HA	1.96	0.47
2:B:640:VAL:HA	2:B:651:LEU:HA	1.96	0.47
7:I:77:LYS:HD2	7:I:108:HIS:HB2	1.95	0.47
3:C:127:ARG:HG3	3:C:129:ILE:HG22	1.95	0.47
1:A:1404:GLU:HB3	1:A:1407:GLU:HB2	1.97	0.47
1:A:846:GLU:O	1:A:848:ILE:N	2.47	0.47
2:B:601:ARG:HH21	2:B:639:ILE:HD11	1.80	0.47
1:A:280:GLU:HA	1:A:284:ALA:HB2	1.94	0.47
2:B:640:VAL:HG22	2:B:651:LEU:HB3	1.96	0.47
5:F:147:SER:O	5:F:151:LEU:HD12	2.15	0.47
7:I:56:ALA:HB3	7:I:89:GLN:NE2	2.16	0.47
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	1.97	0.47
1:A:715:GLU:HA	1:A:718:VAL:HG22	1.96	0.47
3:C:221:TYR:HB3	6:H:46:LEU:CD1	2.44	0.47
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.97	0.47
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.97	0.47
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.95	0.47
9:K:56:VAL:HA	9:K:77:THR:HG22	1.96	0.47
1:A:1107:VAL:HG21	1:A:1381:LEU:HD23	1.96	0.47
3:C:262:LEU:CD2	9:K:88:LYS:HE2	2.45	0.47
5:F:131:PRO:O	5:F:132:LEU:HG	2.15	0.47
2:B:60:GLN:HE22	2:B:94:LYS:NZ	2.13	0.47
3:C:221:TYR:HB3	6:H:46:LEU:HD13	1.96	0.47
2:B:1060:ARG:HB2	2:B:1066:SER:HB3	1.96	0.47
2:B:284:ILE:HG12	2:B:324:ILE:HD11	1.97	0.47
2:B:521:LEU:HA	2:B:543:SER:HB3	1.95	0.47
4:E:168:TYR:HB2	4:E:170:LEU:HD12	1.97	0.47
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:31:VAL:HB	9:K:75:ILE:HD11	1.97	0.47
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.96	0.46
1:A:960:ILE:C	1:A:962:ARG:H	2.18	0.46
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.96	0.46
1:A:446:ARG:HG2	1:A:478:TYR:HB3	1.97	0.46
1:A:817:ALA:HB1	2:B:524:PRO:HB2	1.98	0.46
5:F:125:LEU:O	5:F:127:GLU:N	2.49	0.46
5:F:97:ARG:NH2	5:F:131:PRO:HG2	2.30	0.46
9:K:75:ILE:CD1	9:K:83:PRO:CB	2.73	0.46
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.80	0.46
2:B:120:ARG:HB3	2:B:122:LEU:HD13	1.97	0.46
1:A:1043:ASP:HA	1:A:1046:LEU:HD12	1.98	0.46
1:A:32:VAL:HG21	1:A:57:ARG:O	2.16	0.46
3:C:145:CYS:HA	8:J:2:ILE:HD13	1.96	0.46
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.80	0.46
5:F:86:THR:CG2	5:F:89:GLU:HG3	2.45	0.46
6:H:5:LEU:HD22	6:H:133:ASN:O	2.15	0.46
1:A:542:GLU:CD	1:A:542:GLU:H	2.19	0.46
3:C:88:CYS:SG	3:C:92:CYS:SG	3.14	0.46
5:F:97:ARG:O	5:F:101:ILE:N	2.28	0.46
5:F:146:TRP:HB3	5:F:151:LEU:HD11	1.97	0.46
1:A:1063:MET:HB3	1:A:1066:VAL:CG1	2.45	0.46
1:A:265:LYS:HD3	1:A:302:THR:HG23	1.98	0.46
2:B:364:ILE:H	2:B:364:ILE:HG13	1.62	0.46
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.97	0.46
2:B:805:THR:HG21	2:B:815:ARG:HD3	1.98	0.46
6:H:102:TYR:CZ	6:H:115:TYR:HB3	2.51	0.46
1:A:365:GLY:HA3	1:A:469:ARG:HB3	1.98	0.46
1:A:451:HIS:HA	1:A:1070:GLN:HB2	1.98	0.46
1:A:452:LYS:HE2	1:A:510:GLN:HE22	1.80	0.46
1:A:534:LEU:O	1:A:574:GLY:HA3	2.16	0.46
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.98	0.46
1:A:738:LYS:HG3	1:A:740:LEU:HG	1.98	0.46
2:B:285:ILE:HD13	2:B:378:LEU:HD13	1.94	0.46
1:A:827:THR:HA	1:A:830:LYS:HB2	1.98	0.46
5:F:99:LEU:O	5:F:103:MET:HG2	2.15	0.46
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.98	0.46
1:A:208:LEU:HA	1:A:211:PHE:HB2	1.98	0.46
1:A:56:PRO:HD2	1:A:58:LEU:HD13	1.98	0.46
4:E:31:THR:CG2	4:E:32:GLN:N	2.78	0.46
9:K:31:VAL:HB	9:K:75:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:ILE:HA	1:A:1219:THR:HG22	1.98	0.45
1:A:1284:MET:HA	1:A:1306:LEU:HG	1.98	0.45
1:A:855:THR:HG23	1:A:857:ARG:HE	1.79	0.45
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.20	0.45
3:C:70:ILE:O	3:C:72:LEU:HD12	2.16	0.45
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.98	0.45
2:B:711:GLU:HB3	2:B:712:PRO:HD3	1.97	0.45
1:A:1120:LEU:HB3	1:A:1124:HIS:HB2	1.98	0.45
1:A:524:VAL:O	1:A:527:THR:HG22	2.16	0.45
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	1.98	0.45
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.46	0.45
1:A:1398:MET:HA	1:A:1425:SER:HB3	1.97	0.45
1:A:304:MET:HA	1:A:325:ILE:HD12	1.99	0.45
1:A:821:ARG:O	1:A:825:ILE:HG12	2.16	0.45
2:B:803:LEU:H	2:B:822:ASN:HD21	1.64	0.45
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.98	0.45
2:B:975:GLN:HE21	2:B:976:ILE:H	1.64	0.45
7:I:18:GLU:HG3	7:I:20:LYS:HD2	1.94	0.45
8:J:6:ARG:HA	8:J:12:LYS:O	2.16	0.45
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.97	0.45
1:A:325:ILE:HA	1:A:328:ARG:HD2	1.98	0.45
1:A:779:PHE:HB2	1:A:782:ARG:HG2	1.98	0.45
1:A:683:ILE:HG12	1:A:801:GLU:HG3	1.99	0.45
2:B:827:ILE:HG13	2:B:1012:ILE:HD11	1.99	0.45
3:C:41:ILE:HD11	3:C:247:GLY:HA2	1.98	0.45
9:K:19:LEU:CD2	9:K:35:PHE:CD2	2.97	0.45
2:B:95:ILE:HD12	2:B:96:TYR:H	1.81	0.45
3:C:234:SER:HB2	3:C:243:VAL:HG21	1.98	0.45
3:C:74:SER:HA	3:C:129:ILE:HG13	1.99	0.45
6:H:6:PHE:HE1	6:H:57:VAL:HG23	1.81	0.45
7:I:49:ILE:HG23	7:I:92:ARG:HH22	1.82	0.45
10:L:33:GLU:OE2	10:L:53:HIS:HD2	1.93	0.45
2:B:285:ILE:HD11	2:B:360:PHE:CZ	2.52	0.45
2:B:469:GLN:HA	2:B:470:LYS:HA	1.68	0.45
4:E:56:LYS:O	4:E:59:SER:N	2.50	0.45
6:H:40:LEU:C	6:H:40:LEU:CD2	2.86	0.45
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.99	0.45
3:C:33:LEU:C	3:C:33:LEU:CD2	2.86	0.45
3:C:91:HIS:CD2	3:C:158:VAL:CG1	3.00	0.45
5:F:99:LEU:CD2	5:F:99:LEU:C	2.85	0.45
7:I:25:LEU:HB3	7:I:38:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:VAL:CB	9:K:108:GLU:OE1	2.64	0.45
1:A:466:SER:HA	9:K:2:ASN:HD22	1.82	0.45
1:A:547:LEU:HD23	9:K:59:ALA:H	1.81	0.45
1:A:1111:MET:HB2	1:A:1114:PRO:HG3	1.99	0.45
1:A:382:PRO:HA	1:A:385:ILE:HD12	1.99	0.45
3:C:51:VAL:HB	10:L:65:VAL:HG23	1.98	0.45
6:H:63:LEU:HD13	6:H:89:LEU:HD13	1.99	0.45
8:J:38:ARG:C	8:J:40:GLY:H	2.20	0.45
1:A:981:LEU:HD23	1:A:1039:LYS:HA	1.99	0.44
1:A:354:SER:HB2	1:A:469:ARG:CD	2.36	0.44
3:C:250:THR:HA	3:C:253:LYS:HE3	1.98	0.44
1:A:17:VAL:HG13	1:A:1419:ASP:HB2	1.99	0.44
1:A:758:ILE:H	1:A:758:ILE:HG13	1.60	0.44
1:A:974:ASP:HB3	1:A:977:LYS:H	1.83	0.44
2:B:129:PHE:C	2:B:130:VAL:HG13	2.37	0.44
2:B:709:ASP:HB3	2:B:710:LEU:HD12	1.99	0.44
10:L:30:ILE:HB	10:L:59:ALA:HB2	1.99	0.44
1:A:635:ARG:HE	1:A:635:ARG:HA	1.81	0.44
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.99	0.44
4:E:112:TYR:HE1	4:E:134:THR:HB	1.81	0.44
6:H:4:THR:HG22	6:H:6:PHE:H	1.81	0.44
9:K:18:LYS:HE3	9:K:38:GLU:HG2	1.99	0.44
3:C:70:ILE:CD1	3:C:142:VAL:HG12	2.26	0.44
1:A:1100:ARG:HE	1:A:1104:ILE:HD11	1.82	0.44
1:A:252:PHE:CZ	11:R:2:U:H4'	2.53	0.44
1:A:514:PRO:HB3	1:A:875:ALA:HB3	1.99	0.44
2:B:1171:VAL:HG11	2:B:1180:PHE:HD1	1.81	0.44
2:B:387:LEU:HD21	2:B:392:ARG:HB2	1.99	0.44
10:L:43:THR:C	10:L:44:ASP:OD1	2.55	0.44
1:A:1051:ALA:O	1:A:1055:ARG:HB2	2.17	0.44
1:A:1194:ARG:CZ	1:A:1237:ILE:HG21	2.47	0.44
1:A:38:PRO:HB3	1:A:267:ALA:HB1	1.99	0.44
1:A:442:VAL:HG22	1:A:491:VAL:HG22	1.99	0.44
4:E:118:PRO:CA	4:E:121:MET:HB2	2.44	0.44
1:A:1194:ARG:HH22	1:A:1235:LYS:HE2	1.83	0.44
1:A:565:ILE:CD1	1:A:570:PRO:HA	2.47	0.44
1:A:691:LEU:HD11	1:A:695:LYS:HE3	1.99	0.44
2:B:70:ILE:HA	2:B:88:TYR:O	2.18	0.44
2:B:908:GLU:HA	2:B:941:LEU:HB3	1.99	0.44
9:K:87:LEU:CD2	9:K:87:LEU:C	2.86	0.44
13:U:22:DC:H2'	13:U:23:DT:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:905:VAL:HB	2:B:941:LEU:HD22	1.99	0.44
1:A:315:LEU:HB2	12:S:12:DA:H61	1.83	0.44
2:B:170:LEU:HD12	2:B:171:PRO:CD	2.48	0.44
2:B:551:PRO:HB3	2:B:628:THR:HG21	1.99	0.44
4:E:86:PRO:HA	4:E:113:GLN:HB2	2.00	0.44
1:A:579:SER:HB2	1:A:612:ILE:H	1.83	0.43
9:K:113:THR:HB	9:K:114:LEU:HB2	1.99	0.43
1:A:845:LEU:CG	1:A:1065:GLY:O	2.66	0.43
1:A:1124:HIS:CG	1:A:1130:GLN:HG2	2.54	0.43
2:B:1106:ARG:NH2	2:B:1111:MET:SD	2.91	0.43
2:B:286:PHE:CD2	2:B:297:ILE:HG23	2.53	0.43
2:B:778:MET:HG3	2:B:1094:ARG:HB3	2.00	0.43
3:C:11:ARG:HB3	3:C:12:GLU:OE1	2.18	0.43
5:F:108:PHE:CZ	5:F:131:PRO:HG3	2.53	0.43
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.99	0.43
1:A:528:LEU:HD13	1:A:751:SER:H	1.82	0.43
6:H:41:ASP:C	6:H:42:ILE:HG13	2.32	0.43
2:B:1129:ARG:HD3	13:U:21:DC:H5"	1.99	0.43
1:A:86:LEU:HG	1:A:238:CYS:HA	2.01	0.43
1:A:553:VAL:HB	1:A:556:TRP:HB2	2.00	0.43
1:A:741:ASN:HA	3:C:192:TRP:HE1	1.84	0.43
3:C:74:SER:HB2	3:C:238:ILE:HG23	2.00	0.43
1:A:1135:ARG:HD2	1:A:1282:VAL:O	2.19	0.43
1:A:265:LYS:HD2	1:A:322:VAL:HG11	1.99	0.43
1:A:845:LEU:O	1:A:846:GLU:C	2.57	0.43
2:B:825:VAL:HG21	2:B:1092:TYR:CE1	2.54	0.43
8:J:14:VAL:HA	8:J:17:LYS:HG3	2.00	0.43
1:A:1223:ASP:HA	1:A:1243:VAL:HG13	2.01	0.43
2:B:977:GLY:HA3	2:B:1099:VAL:CB	2.48	0.43
1:A:1189:SER:HB2	1:A:1190:PRO:CD	2.49	0.43
1:A:562:THR:HG22	6:H:79:TRP:HD1	1.84	0.43
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	2.00	0.43
2:B:1180:PHE:HB2	2:B:1188:LYS:HB2	2.01	0.43
2:B:253:THR:O	2:B:253:THR:HG23	2.19	0.43
2:B:305:VAL:O	2:B:305:VAL:CG1	2.67	0.43
9:K:91:CYS:C	9:K:94:ILE:HG22	2.37	0.43
1:A:512:VAL:HA	1:A:519:PRO:HA	2.00	0.43
1:A:824:LEU:HA	1:A:827:THR:HG22	2.01	0.43
1:A:886:ILE:HB	1:A:943:LEU:HD23	2.00	0.43
2:B:57:TYR:O	2:B:59:LEU:N	2.51	0.43
3:C:148:ARG:NH2	8:J:61:LEU:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1163:CYS:HA	2:B:1191:ILE:HG13	2.01	0.43
2:B:865:LYS:HA	2:B:871:THR:HG22	2.00	0.43
6:H:26:ILE:HD12	6:H:42:ILE:HB	2.00	0.43
6:H:4:THR:HG22	6:H:5:LEU:N	2.33	0.43
1:A:1070:GLN:C	1:A:1073:GLY:H	2.22	0.43
1:A:377:PRO:HD3	1:A:493:GLN:NE2	2.34	0.43
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.00	0.43
2:B:254:LEU:HD22	2:B:361:LEU:HD12	2.01	0.43
2:B:840:ILE:HG12	2:B:994:TYR:HE1	1.83	0.43
3:C:175:ALA:HB2	8:J:10:CYS:HB2	2.00	0.43
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.01	0.43
3:C:262:LEU:C	3:C:262:LEU:CD2	2.86	0.43
2:B:1169:MET:HG3	2:B:1205:GLN:HG3	2.01	0.42
3:C:66:ARG:NH1	8:J:2:ILE:HG22	2.31	0.42
1:A:1290:LYS:HD3	1:A:1298:TYR:HB3	2.01	0.42
1:A:1292:PRO:HA	1:A:1298:TYR:HA	1.99	0.42
2:B:102:VAL:HB	2:B:112:LEU:HD13	2.01	0.42
1:A:70:CYS:HB2	2:B:1174:LYS:HD2	2.01	0.42
2:B:119:LEU:HD22	2:B:789:MET:H	1.84	0.42
8:J:56:LEU:O	8:J:58:GLU:N	2.51	0.42
9:K:36:GLU:OE1	9:K:36:GLU:HA	2.18	0.42
1:A:857:ARG:NH2	5:F:139:PRO:HG2	2.34	0.42
2:B:246:LYS:HG2	2:B:249:ARG:HA	2.00	0.42
1:A:1016:THR:HB	4:E:205:SER:O	2.19	0.42
10:L:32:ALA:O	10:L:33:GLU:HB2	2.18	0.42
1:A:1066:VAL:O	1:A:1069:ALA:HB3	2.18	0.42
1:A:1175:SER:HA	1:A:1176:LEU:HA	1.78	0.42
1:A:1386:ARG:HH12	13:U:16:DA:H1'	1.84	0.42
2:B:1071:VAL:HG13	3:C:189:THR:HG21	2.00	0.42
1:A:1418:LEU:HD13	2:B:1222:ARG:HE	1.84	0.42
2:B:234:ILE:HG12	2:B:257:LYS:HD2	2.02	0.42
1:A:1317:MET:HG2	4:E:142:VAL:HG11	2.02	0.42
1:A:786:HIS:HE2	2:B:519:TRP:HE1	1.67	0.42
2:B:398:ARG:HH11	2:B:507:LYS:HD3	1.85	0.42
1:A:1161:THR:HG21	1:A:1239:ARG:HH12	1.83	0.42
1:A:174:ILE:HG12	1:A:202:LEU:CD1	2.49	0.42
1:A:508:PRO:HA	1:A:511:ILE:HD12	2.01	0.42
2:B:1071:VAL:HG22	2:B:1084:GLN:HG2	2.02	0.42
2:B:487:THR:HG21	2:B:819:ALA:HB2	2.02	0.42
1:A:1320:PRO:HD3	4:E:7:ARG:HH21	1.85	0.42
3:C:221:TYR:CG	6:H:46:LEU:HD22	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:ARG:HD3	9:K:6:ARG:HH12	1.85	0.42
1:A:41:MET:HB3	1:A:42:ASP:H	1.59	0.42
1:A:588:LEU:HB3	1:A:607:ILE:HB	2.01	0.42
1:A:2:VAL:N	2:B:1157:ALA:HB1	2.35	0.42
2:B:1017:ILE:HG22	2:B:1022:THR:HG23	2.01	0.42
3:C:183:TRP:CD1	3:C:210:GLU:HB3	2.55	0.42
1:A:1140:HIS:HB2	1:A:1279:ILE:HB	2.02	0.42
2:B:57:TYR:HB2	2:B:58:THR:H	1.72	0.42
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.02	0.42
1:A:814:PHE:HA	1:A:817:ALA:HB3	2.01	0.42
2:B:119:LEU:HD22	2:B:789:MET:HB2	2.01	0.42
2:B:212:LEU:HA	2:B:479:VAL:O	2.20	0.42
2:B:242:SER:HB3	2:B:362:PRO:HD2	2.01	0.42
3:C:124:LEU:O	3:C:127:ARG:HG2	2.19	0.42
4:E:76:GLY:HA3	4:E:106:GLN:HB2	2.02	0.42
5:F:132:LEU:HD12	5:F:132:LEU:N	2.35	0.42
1:A:120:GLU:HA	1:A:123:ARG:HB3	2.02	0.41
1:A:1215:ARG:HG2	1:A:1273:LEU:HD23	2.02	0.41
1:A:598:LEU:HD23	6:H:25:ARG:HH22	1.84	0.41
2:B:862:GLN:HB3	2:B:963:PHE:HD2	1.84	0.41
2:B:789:MET:HG3	2:B:953:LEU:HD23	2.02	0.41
3:C:70:ILE:O	3:C:72:LEU:HD11	2.17	0.41
3:C:86:CYS:SG	3:C:92:CYS:SG	3.18	0.41
4:E:98:ILE:HG23	4:E:102:GLU:HG3	2.01	0.41
5:F:125:LEU:HD12	5:F:126:ALA:H	1.76	0.41
6:H:38:LEU:HD11	6:H:123:MET:HE3	2.01	0.41
7:I:78:CYS:SG	7:I:106:CYS:SG	3.18	0.41
1:A:23:SER:HB3	1:A:233:TRP:CH2	2.55	0.41
2:B:224:GLN:HE21	2:B:396:ASP:HB3	1.86	0.41
3:C:259:LEU:HD11	9:K:91:CYS:CB	2.50	0.41
6:H:130:ARG:HB3	6:H:134:ASN:HB2	2.02	0.41
9:K:33:ILE:HD11	9:K:73:LEU:HD23	2.01	0.41
9:K:94:ILE:HG12	9:K:98:LEU:CD1	2.50	0.41
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.35	0.41
1:A:239:LEU:HD11	1:A:304:MET:CE	2.50	0.41
1:A:763:ALA:O	1:A:803:SER:HB2	2.20	0.41
2:B:1158:PHE:HB3	2:B:1196:ILE:O	2.19	0.41
2:B:254:LEU:CD1	2:B:272:THR:O	2.60	0.41
4:E:88:VAL:HG11	4:E:110:PHE:HZ	1.84	0.41
5:F:125:LEU:C	5:F:125:LEU:HD12	2.39	0.41
8:J:30:LEU:CD1	8:J:31:ASP:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:262:LEU:CD2	9:K:88:LYS:CE	2.97	0.41
3:C:259:LEU:HD11	9:K:91:CYS:HB3	2.01	0.41
1:A:453:MET:HG2	1:A:520:CYS:SG	2.60	0.41
1:A:853:ASP:C	1:A:855:THR:H	2.24	0.41
1:A:960:ILE:HA	1:A:963:ILE:HD12	2.03	0.41
1:A:974:ASP:HA	1:A:975:HIS:CB	2.46	0.41
3:C:242:GLN:HA	3:C:245:VAL:HG12	2.03	0.41
4:E:110:PHE:CE2	4:E:116:ILE:CD1	2.96	0.41
1:A:1340:GLY:HA2	4:E:182:ASP:OD2	2.20	0.41
1:A:1427:ASN:O	1:A:1431:GLY:N	2.53	0.41
2:B:1099:VAL:HA	2:B:1102:LYS:HB2	2.02	0.41
2:B:54:PHE:HA	2:B:58:THR:HB	2.03	0.41
2:B:971:THR:HG21	3:C:61:GLU:HG3	2.01	0.41
4:E:68:SER:HB3	4:E:75:MET:SD	2.60	0.41
2:B:979:LYS:HE2	2:B:1095:LEU:HD22	2.03	0.41
2:B:237:VAL:HG12	2:B:255:GLN:HB2	2.02	0.41
2:B:299:GLU:HG3	2:B:572:HIS:NE2	2.35	0.41
4:E:151:PRO:HB2	4:E:198:ILE:CG2	2.51	0.41
4:E:170:LEU:HD13	4:E:175:LEU:HD23	2.02	0.41
1:A:186:LYS:HG2	1:A:197:PRO:HB3	2.02	0.41
2:B:130:VAL:CG2	2:B:165:VAL:CG2	2.98	0.41
2:B:387:LEU:C	2:B:387:LEU:CD2	2.86	0.41
3:C:108:GLU:OE1	3:C:149:LYS:HE2	2.20	0.41
1:A:1269:GLU:O	1:A:1270:ASN:HB2	2.20	0.41
2:B:1034:VAL:HG22	2:B:1059:LEU:HD13	2.03	0.41
2:B:1187:ASN:HD22	2:B:1190:ASP:H	1.69	0.41
2:B:145:ARG:HA	2:B:146:GLU:CB	2.51	0.41
3:C:90:ASP:O	3:C:91:HIS:CB	2.67	0.41
3:C:221:TYR:CB	6:H:46:LEU:HD13	2.51	0.41
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.03	0.41
2:B:69:LEU:CD1	2:B:432:MET:HE1	2.51	0.41
3:C:43:THR:OG1	3:C:170:TRP:CB	2.67	0.41
3:C:56:THR:HG21	3:C:145:CYS:SG	2.61	0.41
4:E:37:LEU:HD21	4:E:45:LYS:HZ2	1.85	0.41
7:I:18:GLU:CG	7:I:20:LYS:HD3	2.45	0.41
10:L:47:ARG:HB3	10:L:54:ARG:HG2	2.03	0.41
1:A:1151:GLU:HG2	7:I:45:ARG:HE	1.86	0.41
3:C:32:SER:HB2	9:K:45:LEU:HD23	2.01	0.41
1:A:508:PRO:O	1:A:511:ILE:HB	2.21	0.41
1:A:540:PHE:HB3	1:A:571:LEU:HB3	2.02	0.41
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:HE22	2:B:1177:HIS:CD2	2.39	0.41
2:B:135:ARG:CB	2:B:151:LEU:HD11	2.51	0.41
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.25	0.41
3:C:91:HIS:CD2	3:C:158:VAL:HG11	2.56	0.41
4:E:56:LYS:O	4:E:57:MET:C	2.58	0.41
5:F:81:THR:OG1	5:F:146:TRP:NE1	2.53	0.41
1:A:785:PRO:HD2	1:A:786:HIS:HD2	1.85	0.40
2:B:245:GLU:N	2:B:246:LYS:HA	2.36	0.40
2:B:29:ASP:HB3	2:B:658:ILE:HG21	2.02	0.40
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.95	0.40
7:I:18:GLU:CG	7:I:20:LYS:HD2	2.51	0.40
7:I:59:VAL:C	7:I:61:ASP:H	2.25	0.40
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.56	0.40
1:A:837:ILE:HD11	1:A:1098:VAL:HG13	2.04	0.40
1:A:1141:THR:HG22	1:A:1274:ARG:HB2	2.03	0.40
2:B:616:ILE:O	2:B:624:LEU:HA	2.21	0.40
4:E:145:THR:HA	4:E:150:VAL:HG11	2.03	0.40
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.87	0.40
1:A:1404:GLU:HB2	1:A:1408:ILE:HD12	2.03	0.40
2:B:287:ARG:HD3	2:B:325:GLN:HA	2.04	0.40
2:B:309:GLN:NE2	2:B:392:ARG:HH21	2.16	0.40
2:B:613:VAL:HG22	2:B:628:THR:HA	2.03	0.40
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.50	0.40
4:E:116:ILE:CG2	4:E:120:ALA:HB3	2.52	0.40
1:A:1142:THR:O	1:A:1145:SER:HB3	2.21	0.40
1:A:506:ALA:O	1:A:509:LEU:HB2	2.21	0.40
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.86	0.40
3:C:33:LEU:HD23	3:C:37:MET:SD	2.62	0.40
5:F:97:ARG:HH21	5:F:131:PRO:HG2	1.86	0.40
1:A:565:ILE:HA	6:H:97:MET:HA	2.03	0.40
1:A:311:GLN:HB2	1:A:312:PRO:CD	2.46	0.40
1:A:704:ALA:HB2	1:A:710:LEU:HD12	2.04	0.40
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.51	0.40
3:C:43:THR:HG1	3:C:170:TRP:HD1	1.67	0.40
3:C:79:GLN:HA	3:C:79:GLN:OE1	2.21	0.40
6:H:26:ILE:O	6:H:40:LEU:N	2.31	0.40
9:K:37:LYS:HD3	9:K:37:LYS:N	2.37	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	1422/1733 (82%)	1129 (79%)	199 (14%)	94 (7%)	1	17
2	B	1141/1224 (93%)	919 (80%)	158 (14%)	64 (6%)	2	20
3	C	263/318 (83%)	226 (86%)	30 (11%)	7 (3%)	5	34
4	E	210/215 (98%)	186 (89%)	17 (8%)	7 (3%)	4	30
5	F	85/155 (55%)	72 (85%)	9 (11%)	4 (5%)	2	23
6	H	139/146 (95%)	97 (70%)	26 (19%)	16 (12%)	0	6
7	I	112/122 (92%)	88 (79%)	16 (14%)	8 (7%)	1	16
8	J	64/70 (91%)	49 (77%)	11 (17%)	4 (6%)	1	18
9	K	113/120 (94%)	99 (88%)	12 (11%)	2 (2%)	8	41
10	L	41/70 (59%)	31 (76%)	6 (15%)	4 (10%)	0	10
All	All	3590/4173 (86%)	2896 (81%)	484 (14%)	210 (6%)	1	19

All (210) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	65	LEU
1	A	152	VAL
1	A	153	PRO
1	A	162	VAL
1	A	190	ALA
1	A	370	ILE
1	A	399	HIS
1	A	465	TYR
1	A	466	SER
1	A	629	LEU
1	A	751	SER
1	A	846	GLU
1	A	847	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1064	VAL
1	A	1067	LEU
1	A	1068	ALA
1	A	1072	ILE
1	A	1111	MET
1	A	1270	ASN
1	A	1365	TYR
1	A	1416	ALA
2	B	45	SER
2	B	58	THR
2	B	150	GLU
2	B	165	VAL
2	B	242	SER
2	B	477	ALA
2	B	531	GLN
2	B	785	TYR
2	B	807	ARG
2	B	895	ASP
2	B	933	SER
2	B	987	LYS
2	B	992	ILE
2	B	1046	PRO
2	B	1212	ILE
3	C	90	ASP
3	C	92	CYS
3	C	142	VAL
3	C	161	LYS
4	E	207	ARG
6	H	64	ASN
6	H	67	ASP
6	H	94	ASP
8	J	6	ARG
1	A	42	ASP
1	A	87	ALA
1	A	110	CYS
1	A	168	GLY
1	A	249	SER
1	A	252	PHE
1	A	258	GLY
1	A	490	HIS
1	A	566	ILE
1	A	567	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	595	THR
1	A	624	SER
1	A	626	ASN
1	A	975	HIS
1	A	1016	THR
1	A	1079	MET
1	A	1084	PHE
1	A	1085	HIS
1	A	1097	GLY
1	A	1377	THR
1	A	1433	MET
1	A	1437	GLY
2	B	76	GLN
2	B	95	ILE
2	B	146	GLU
2	B	152	ILE
2	B	164	LYS
2	B	247	GLY
2	B	351	TYR
2	B	442	PHE
2	B	478	GLY
2	B	479	VAL
2	B	507	LYS
2	B	705	MET
2	B	907	GLY
2	B	935	ARG
2	B	1216	LEU
3	C	175	ALA
4	E	59	SER
5	F	128	LYS
6	H	73	SER
6	H	77	ARG
6	H	96	VAL
6	H	107	VAL
6	H	109	LYS
7	I	3	THR
8	J	2	ILE
8	J	49	MET
10	L	69	ALA
1	A	130	ASP
1	A	154	SER
1	A	186	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	286	HIS
1	A	331	GLY
1	A	423	ASP
1	A	517	ASN
1	A	543	LEU
1	A	704	ALA
1	A	1127	ASP
2	B	55	VAL
2	B	96	TYR
2	B	111	ALA
2	B	358	LYS
2	B	510	LYS
2	B	711	GLU
2	B	751	VAL
2	B	836	GLU
2	B	896	ASP
2	B	943	SER
2	B	951	GLN
4	E	45	LYS
4	E	50	MET
6	H	85	GLY
7	I	88	SER
7	I	113	ASP
10	L	38	LEU
10	L	39	SER
1	A	54	ASN
1	A	72	GLU
1	A	156	ASP
1	A	167	CYS
1	A	215	SER
1	A	317	LYS
1	A	319	GLY
1	A	332	LYS
1	A	369	SER
1	A	598	LEU
1	A	628	GLY
1	A	854	ASN
1	A	958	VAL
1	A	1086	PHE
1	A	1115	SER
1	A	1184	SER
1	A	1327	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1403	GLU
2	B	41	LYS
2	B	219	ALA
2	B	265	SER
2	B	395	GLN
2	B	504	ARG
2	B	514	LEU
2	B	1041	GLU
2	B	1155	SER
2	B	1185	CYS
3	C	40	GLU
3	C	214	ASN
4	E	86	PRO
5	F	72	LYS
5	F	78	GLN
5	F	139	PRO
6	H	45	GLU
6	H	84	ALA
6	H	87	ARG
6	H	129	TYR
7	I	10	CYS
7	I	11	ASN
7	I	95	THR
8	J	57	ILE
1	A	5	GLN
1	A	67	CYS
1	A	118	HIS
1	A	251	SER
1	A	254	GLU
1	A	385	ILE
1	A	418	SER
1	A	424	ILE
1	A	1002	GLY
1	A	1063	MET
1	A	1122	PRO
1	A	1300	LYS
2	B	652	LYS
2	B	712	PRO
2	B	868	MET
2	B	1108	ARG
2	B	1156	ASP
4	E	151	PRO

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Mol	Chain	Res	Type
4	E	164	LEU
7	I	60	GLN
9	K	41	THR
10	L	30	ILE
1	A	114	LEU
1	A	565	ILE
1	A	986	ILE
1	A	1107	VAL
2	B	23	ALA
2	B	250	PHE
2	B	467	GLY
6	H	60	ALA
6	H	76	THR
7	I	28	GLU
1	A	250	ILE
1	A	910	PRO
2	B	960	GLY
1	A	158	PRO
9	K	23	PRO
1	A	474	VAL
2	B	1012	ILE
2	B	1045	SER
6	H	17	PRO
1	A	627	GLY
1	A	1089	VAL
2	B	501	PRO
2	B	1131	GLY
2	B	1119	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1244/1520 (82%)	1081 (87%)	163 (13%)	4 21
2	B	991/1061 (93%)	889 (90%)	102 (10%)	7 28
3	C	230/274 (84%)	229 (100%)	1 (0%)	91 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	194/197 (98%)	193 (100%)	1 (0%)	88	93
5	F	77/137 (56%)	76 (99%)	1 (1%)	69	82
6	H	115/128 (90%)	115 (100%)	0	100	100
7	I	108/116 (93%)	106 (98%)	2 (2%)	57	75
8	J	61/65 (94%)	60 (98%)	1 (2%)	62	79
9	K	99/102 (97%)	99 (100%)	0	100	100
10	L	38/57 (67%)	37 (97%)	1 (3%)	46	67
All	All	3157/3657 (86%)	2885 (91%)	272 (9%)	10	37

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	132	LYS
1	A	149	GLU
1	A	188	ASP
1	A	189	ARG
1	A	196	GLU
1	A	198	GLU
1	A	215	SER
1	A	218	ASP
1	A	259	GLU
1	A	265	LYS
1	A	268	ASP
1	A	297	GLN
1	A	317	LYS
1	A	329	LEU
1	A	348	SER
1	A	361	LEU
1	A	363	GLN
1	A	368	LYS
1	A	383	TYR
1	A	389	THR
1	A	390	GLN
1	A	391	LEU
1	A	394	ASN
1	A	408	ASP
1	A	412	ARG
1	A	426	LEU
1	A	434	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	440	ASP
1	A	443	LEU
1	A	444	PHE
1	A	462	VAL
1	A	468	PHE
1	A	469	ARG
1	A	472	LEU
1	A	481	ASP
1	A	485	ASP
1	A	489	LEU
1	A	500	GLU
1	A	504	LEU
1	A	509	LEU
1	A	511	ILE
1	A	517	ASN
1	A	518	LYS
1	A	520	CYS
1	A	527	THR
1	A	528	LEU
1	A	538	ASP
1	A	542	GLU
1	A	548	ASN
1	A	549	MET
1	A	555	ASP
1	A	576	GLN
1	A	578	LEU
1	A	579	SER
1	A	586	ILE
1	A	588	LEU
1	A	592	ASP
1	A	598	LEU
1	A	605	MET
1	A	606	LEU
1	A	626	ASN
1	A	630	ILE
1	A	635	ARG
1	A	645	LEU
1	A	657	LEU
1	A	658	LEU
1	A	666	ILE
1	A	668	ASP
1	A	672	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	677	ARG
1	A	679	ILE
1	A	681	GLU
1	A	701	LEU
1	A	702	LEU
1	A	710	LEU
1	A	719	VAL
1	A	732	LEU
1	A	738	LYS
1	A	739	ASP
1	A	756	ILE
1	A	758	ILE
1	A	764	CYS
1	A	769	SER
1	A	782	ARG
1	A	791	ASP
1	A	806	ARG
1	A	821	ARG
1	A	827	THR
1	A	841	LEU
1	A	855	THR
1	A	862	ASN
1	A	867	ILE
1	A	885	THR
1	A	890	ASP
1	A	894	GLU
1	A	898	ARG
1	A	899	VAL
1	A	906	HIS
1	A	913	LEU
1	A	914	GLU
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	925	LEU
1	A	932	GLU
1	A	936	LEU
1	A	940	ARG
1	A	942	PHE
1	A	943	LEU
1	A	974	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	980	ASP
1	A	998	LEU
1	A	1011	GLN
1	A	1024	SER
1	A	1034	GLU
1	A	1049	ILE
1	A	1064	VAL
1	A	1067	LEU
1	A	1070	GLN
1	A	1080	THR
1	A	1086	PHE
1	A	1096	SER
1	A	1100	ARG
1	A	1105	LEU
1	A	1112	LYS
1	A	1113	THR
1	A	1134	ILE
1	A	1155	ASP
1	A	1157	ASP
1	A	1173	HIS
1	A	1176	LEU
1	A	1177	LEU
1	A	1187	GLN
1	A	1192	LEU
1	A	1193	LEU
1	A	1195	LEU
1	A	1202	MET
1	A	1205	LYS
1	A	1218	GLN
1	A	1224	LEU
1	A	1225	PHE
1	A	1234	GLU
1	A	1242	VAL
1	A	1243	VAL
1	A	1259	MET
1	A	1260	LEU
1	A	1264	GLU
1	A	1266	THR
1	A	1271	ILE
1	A	1273	LEU
1	A	1291	VAL
1	A	1295	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1306	LEU
1	A	1314	SER
1	A	1325	THR
1	A	1342	GLU
1	A	1371	LEU
1	A	1374	VAL
1	A	1409	LEU
1	A	1419	ASP
1	A	1445	ILE
2	B	39	ARG
2	B	74	LEU
2	B	83	ASN
2	B	92	PHE
2	B	146	GLU
2	B	188	ASP
2	B	189	LEU
2	B	199	MET
2	B	258	LEU
2	B	277	LYS
2	B	279	ASP
2	B	294	ASP
2	B	310	MET
2	B	320	ASP
2	B	325	GLN
2	B	364	ILE
2	B	376	PHE
2	B	393	LYS
2	B	395	GLN
2	B	396	ASP
2	B	398	ARG
2	B	401	PHE
2	B	413	LEU
2	B	416	LEU
2	B	423	LYS
2	B	427	ASP
2	B	437	GLU
2	B	438	GLU
2	B	449	ASN
2	B	461	LEU
2	B	465	ASN
2	B	466	TRP
2	B	484	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	489	SER
2	B	491	THR
2	B	500	THR
2	B	502	ILE
2	B	508	LEU
2	B	550	ASP
2	B	563	MET
2	B	574	SER
2	B	576	ASP
2	B	589	VAL
2	B	592	ASN
2	B	595	ARG
2	B	602	THR
2	B	624	LEU
2	B	641	GLU
2	B	642	ASP
2	B	650	GLU
2	B	651	LEU
2	B	678	GLU
2	B	701	ILE
2	B	709	ASP
2	B	739	THR
2	B	743	ILE
2	B	758	PHE
2	B	773	MET
2	B	796	LEU
2	B	837	ASP
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	854	LEU
2	B	860	MET
2	B	861	ASP
2	B	862	GLN
2	B	873	THR
2	B	889	THR
2	B	905	VAL
2	B	923	GLU
2	B	935	ARG
2	B	950	ASP
2	B	956	THR
2	B	958	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	961	LEU
2	B	969	ARG
2	B	971	THR
2	B	972	LYS
2	B	975	GLN
2	B	978	ASP
2	B	987	LYS
2	B	1007	VAL
2	B	1012	ILE
2	B	1029	CYS
2	B	1049	ASP
2	B	1052	VAL
2	B	1065	GLN
2	B	1072	MET
2	B	1087	PHE
2	B	1098	MET
2	B	1101	ASP
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1185	CYS
2	B	1187	ASN
2	B	1201	LYS
2	B	1206	GLU
2	B	1217	TYR
2	B	1218	THR
2	B	1222	ARG
3	C	52	GLU
4	E	33	GLU
5	F	124	GLU
7	I	4	PHE
7	I	46	HIS
8	J	31	ASP
10	L	28	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	71	GLN
1	A	306	ASN
1	A	316	GLN
1	A	363	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	390	GLN
1	A	479	ASN
1	A	493	GLN
1	A	515	GLN
1	A	768	GLN
1	A	854	ASN
1	A	865	GLN
1	A	881	GLN
1	A	926	GLN
1	A	1070	GLN
1	A	1130	GLN
1	A	1183	GLN
1	A	1188	GLN
1	A	1203	ASN
1	A	1211	GLN
1	A	1218	GLN
1	A	1354	ASN
1	A	1387	HIS
1	A	1427	ASN
2	B	46	GLN
2	B	60	GLN
2	B	224	GLN
2	B	309	GLN
2	B	350	GLN
2	B	415	GLN
2	B	494	HIS
2	B	518	HIS
2	B	610	ASN
2	B	761	HIS
2	B	842	ASN
2	B	975	GLN
2	B	1177	HIS
2	B	1195	HIS
3	C	112	ASN
4	E	146	HIS
6	H	43	ASN
6	H	131	ASN
6	H	134	ASN
9	K	2	ASN
9	K	65	HIS
9	K	110	ASN
10	L	53	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	7/9 (77%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	6	G
11	R	8	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	1432/1733 (82%)	-0.21	23 (1%) 72 62	28, 216, 298, 382	0
2	B	1157/1224 (94%)	-0.22	10 (0%) 84 77	115, 221, 304, 366	0
3	C	265/318 (83%)	-0.50	0 100 100	134, 213, 270, 315	0
4	E	212/215 (98%)	-0.35	0 100 100	153, 232, 298, 322	0
5	F	87/155 (56%)	-0.36	0 100 100	134, 193, 260, 341	0
6	H	143/146 (97%)	-0.33	0 100 100	176, 258, 312, 334	0
7	I	114/122 (93%)	-0.35	0 100 100	177, 240, 306, 334	0
8	J	66/70 (94%)	-0.40	0 100 100	125, 223, 286, 318	0
9	K	115/120 (95%)	-0.31	1 (0%) 84 77	131, 202, 271, 293	0
10	L	43/70 (61%)	-0.30	0 100 100	170, 228, 283, 364	0
11	R	9/9 (100%)	0.18	0 100 100	285, 306, 337, 338	0
12	S	38/53 (71%)	0.98	6 (15%) 2 2	338, 360, 380, 381	0
13	U	38/53 (71%)	0.96	8 (21%) 1 1	275, 348, 378, 380	0
All	All	3719/4288 (86%)	-0.24	48 (1%) 77 68	28, 221, 309, 382	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	THR	6.9
1	A	183	GLY	4.3
13	U	35	DG	3.8
1	A	1194	ARG	3.7
2	B	1181	GLU	3.7
1	A	182	VAL	3.7
13	U	36	DA	3.5
1	A	89	PRO	3.4
1	A	257	ARG	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	S	3	DA	3.3
1	A	1192	LEU	3.2
2	B	445	LYS	3.1
13	U	38	DT	3.1
2	B	1172	ILE	2.9
1	A	56	PRO	2.9
1	A	290	GLU	2.9
1	A	188	ASP	2.8
1	A	1307	GLU	2.8
12	S	24	DC	2.6
13	U	37	DC	2.6
9	K	115	ALA	2.6
1	A	118	HIS	2.6
2	B	135	ARG	2.6
12	S	23	DG	2.5
13	U	2	DC	2.5
1	A	250	ILE	2.5
1	A	78	PRO	2.5
13	U	39	DC	2.4
13	U	34	DG	2.4
1	A	145	LYS	2.4
1	A	908	LEU	2.3
13	U	29	DA	2.3
1	A	198	GLU	2.2
1	A	143	LYS	2.2
12	S	4	DG	2.2
2	B	89	GLU	2.2
2	B	1206	GLU	2.1
1	A	57	ARG	2.1
1	A	318	SER	2.1
2	B	441	ASP	2.1
12	S	2	DG	2.1
1	A	181	LEU	2.1
2	B	1160	VAL	2.1
12	S	21	DT	2.1
2	B	1161	HIS	2.0
1	A	147	VAL	2.0
1	A	195	ASP	2.0
2	B	134	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
15	MG	R	101	1/1	0.56	0.16	201,201,201,201	0
14	ZN	I	202	1/1	0.87	0.03	213,213,213,213	0
14	ZN	J	101	1/1	0.92	0.32	207,207,207,207	0
14	ZN	A	1801	1/1	0.96	0.04	205,205,205,205	0
14	ZN	L	101	1/1	0.97	0.11	202,202,202,202	0
14	ZN	C	401	1/1	0.97	0.22	226,226,226,226	0
14	ZN	A	1802	1/1	0.97	0.10	200,200,200,200	0
14	ZN	B	1301	1/1	0.98	0.11	214,214,214,214	0
14	ZN	I	201	1/1	0.99	0.13	201,201,201,201	0
14	ZN	C	402	1/1	1.00	0.14	186,186,186,186	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.