



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2022 – 04:31 PM EST

PDB ID : 7RIM
Title : RNA polymerase II elongation complex with hairpin polyamide Py-Im 1, scaffold 1
Authors : Oh, J.; Dervan, P.B.; Wang, D.
Deposited on : 2021-07-20
Resolution : 2.90 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 ⓘ](#)) 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	:	2.25
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.25

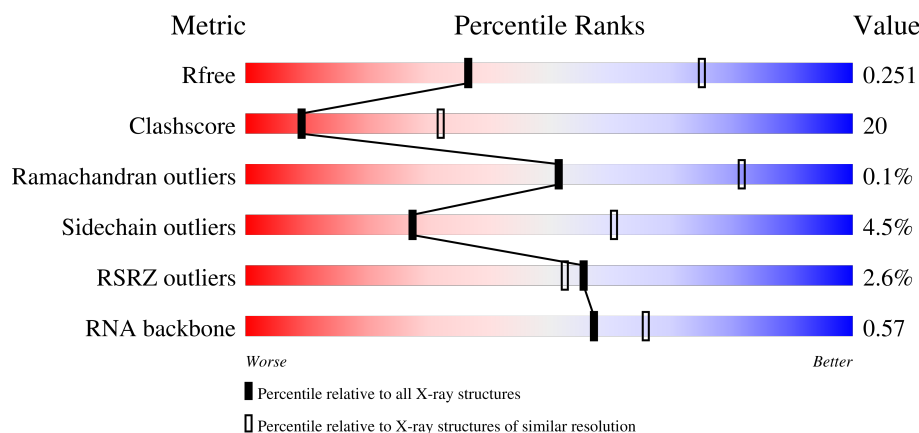
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	R	9	<div> <div>89%</div> <div>11%</div> </div>
2	T	30	<div> <div>20%</div> <div>63%</div> <div>13%</div> </div>
3	N	20	<div> <div>10%</div> <div>65%</div> <div>25%</div> </div>
4	A	1733	<div> <div>3%</div> <div>50%</div> <div>28%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
5	B	1224	<div><div></div><div>2%61%30%8%</div></div>
6	C	318	<div><div></div><div>52%30%16%</div></div>
7	E	215	<div><div></div><div>7%49%45%</div></div>
8	F	155	<div><div></div><div>%32%20%45%</div></div>
9	H	146	<div><div></div><div>8%42%46%9%</div></div>
10	I	122	<div><div></div><div>65%29%</div></div>
11	J	70	<div><div></div><div>60%30%7%</div></div>
12	K	120	<div><div></div><div>63%32%5%</div></div>
13	L	70	<div><div></div><div>%40%20%39%</div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29191 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			525	252	84	163	26			

- Molecule 3 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	15	Total	C	N	O	P	0	0	0
			312	147	66	84	15			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10828	6831	1896	2041	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1129	Total	C	N	O	S	0	0	0
			8899	5630	1561	1655	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

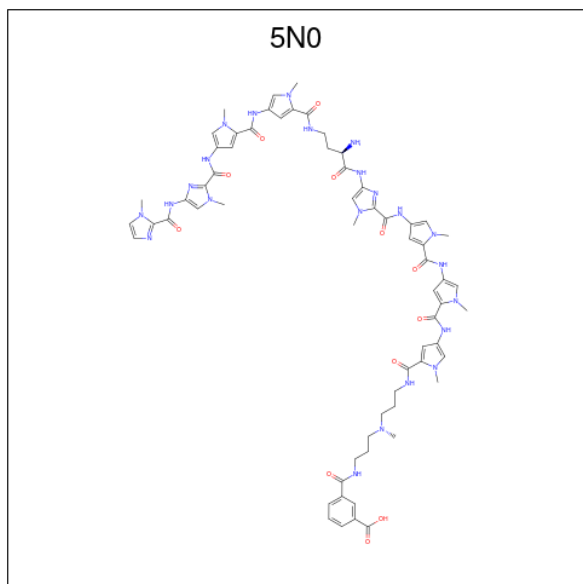
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

- Molecule 14 is 3-({3-[(3-{[4-({4-[(4-{[4-((2R)-2-amino-4-[(1-methyl-4-{[1-methyl-4-({1-met

hyl-4-[(1-methyl-1H-imidazole-2-carbonyl)amino]-1H-imidazole-2-carbonyl}amino)-1H-pyrrole-2-carbonyl]amino}-1H-pyrrole-2-carbonyl)amino]butanoyl}amino)-1-methyl-1H-imidazole-2-carbonyl]amino}-1-methyl-1H-pyrrole-2-carbonyl)amino]-1-methyl-1H-pyrrole-2-carbonyl}amino)-1-methyl-1H-pyrrole-2-carbonyl]amino}propyl)(methylamino)propyl}carbamoyl)benzoic acid (three-letter code: 5N0) (formula: C₆₄H₇₅N₂₃O₁₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	T	1	Total	C	N	O	0	0
			99	64	23	12		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

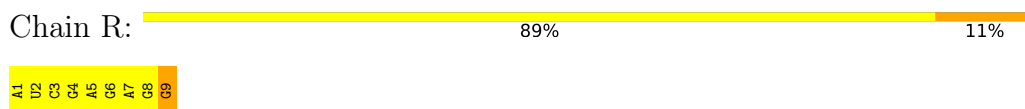
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

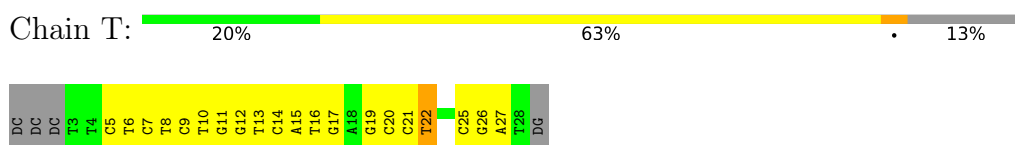
3 Residue-property plots [i](#)

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

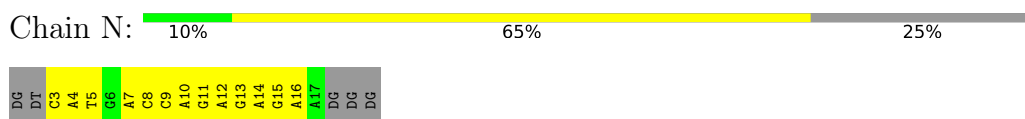
- Molecule 1: RNA



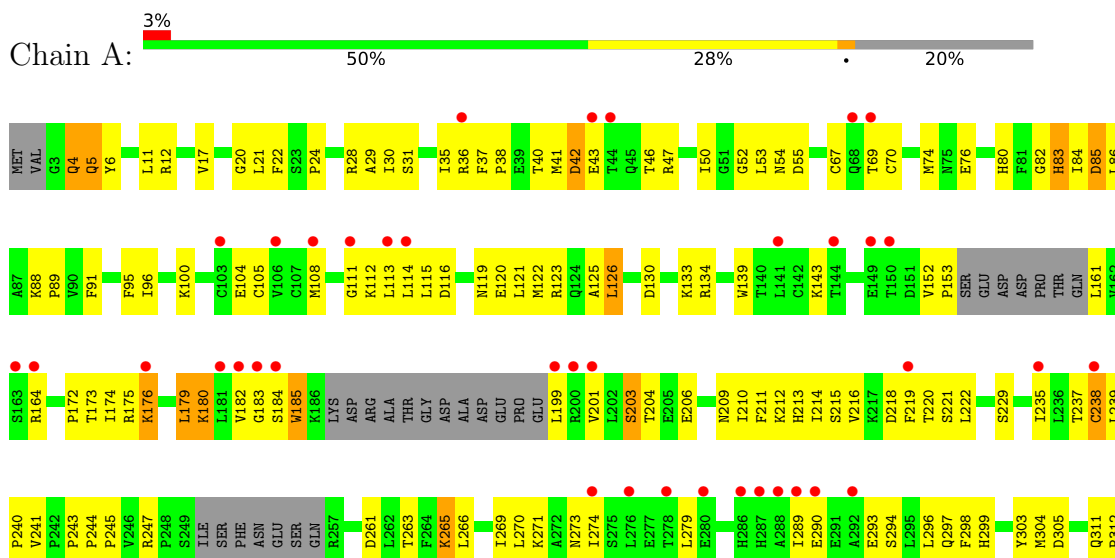
- Molecule 2: Template strand DNA



- Molecule 3: Non-template DNA



- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

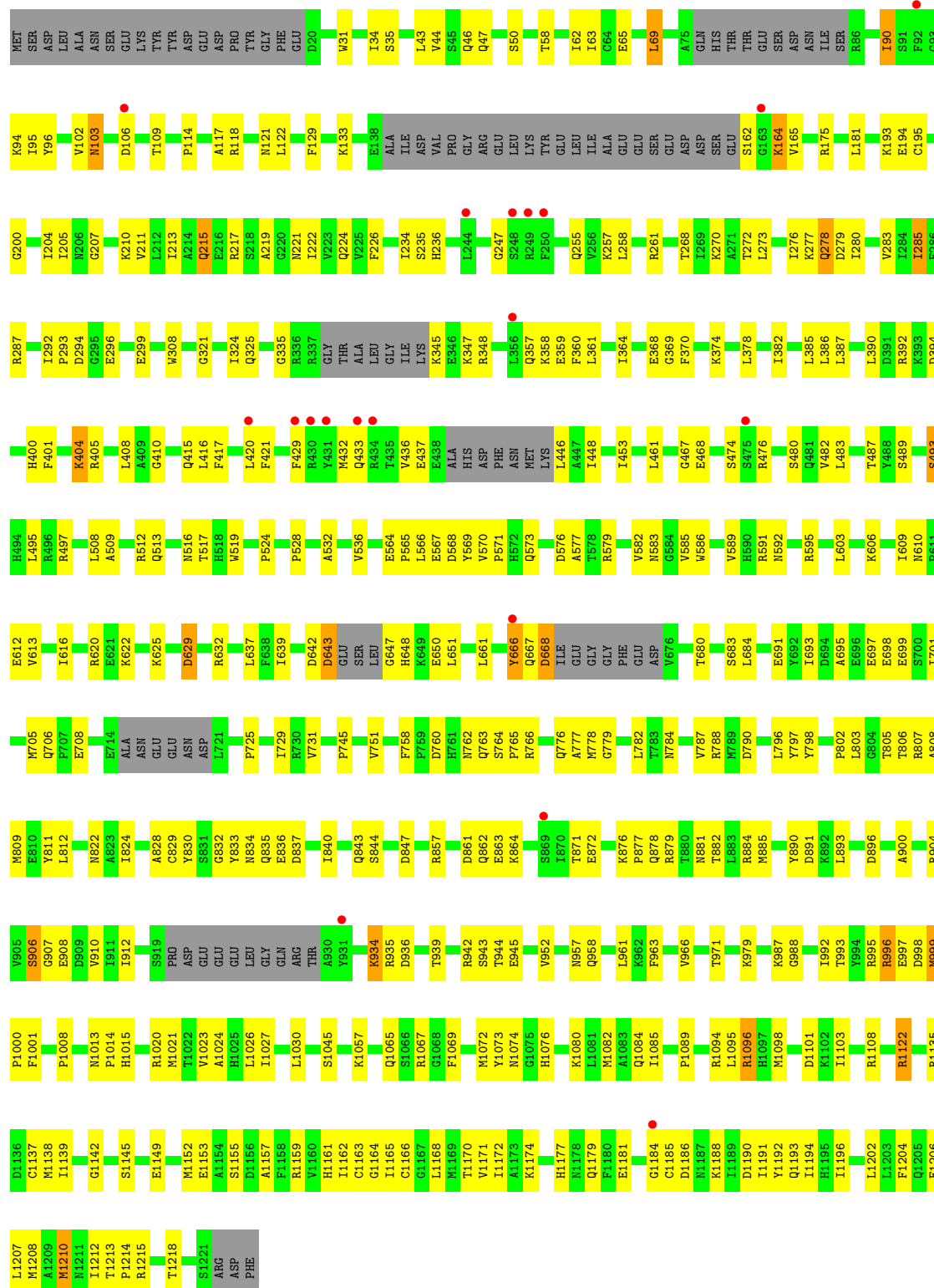


WORLDWIDE
PDB
PROTEIN DATA BANK

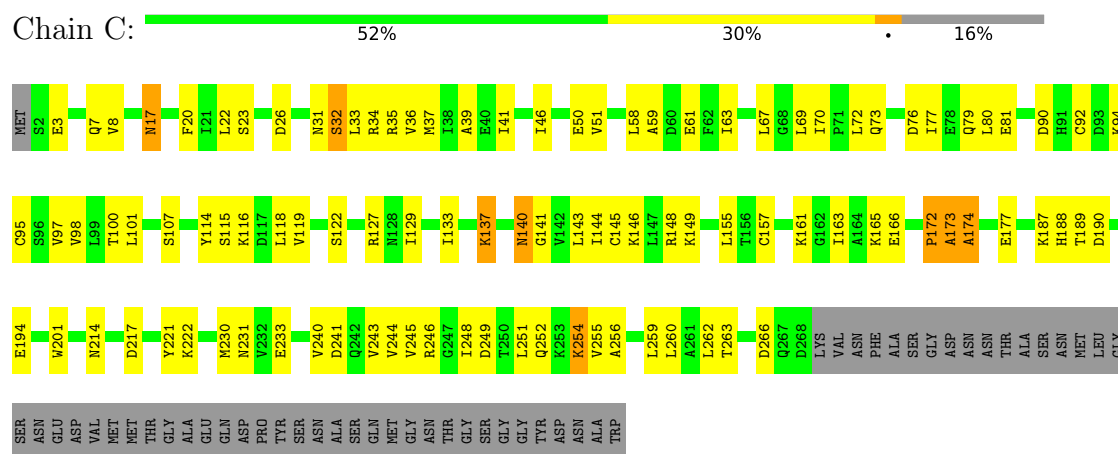
PRO
LYS
GLN
ASP
GLU
GLN
LYS
HIS
ASN
GLU
ASN
GLU
SER
ARG

• Molecule 5: DNA-directed RNA polymerase II subunit RPB2

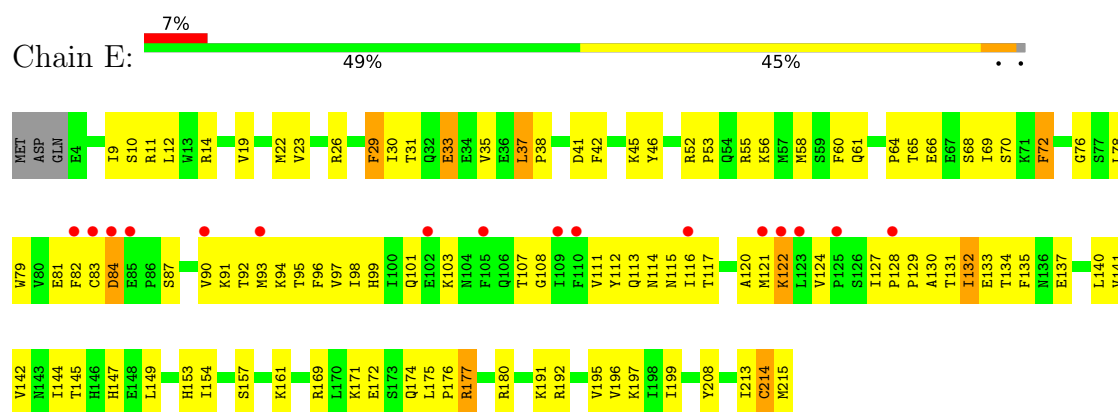
Chain B: 2% 61% 30% 8%



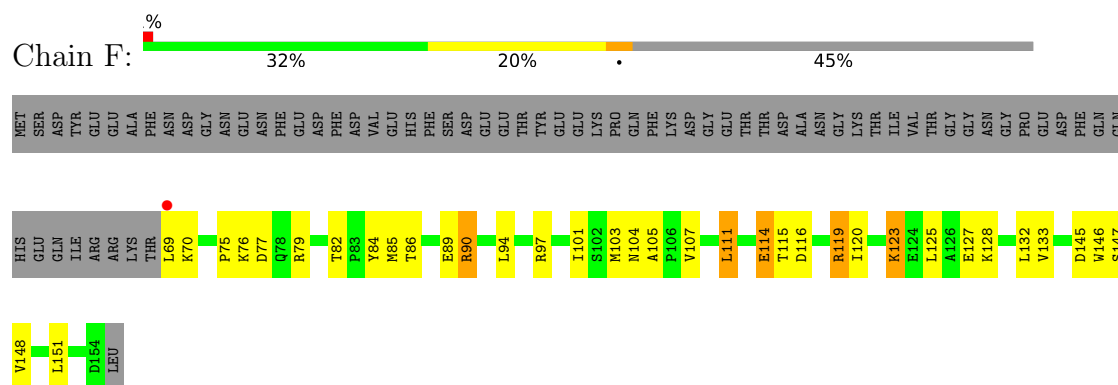
- Molecule 6: DNA-directed RNA polymerase II subunit RPB3



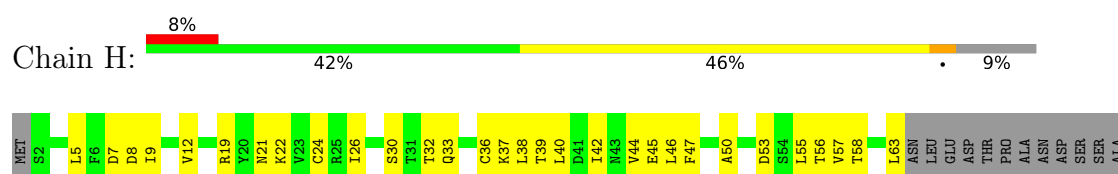
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

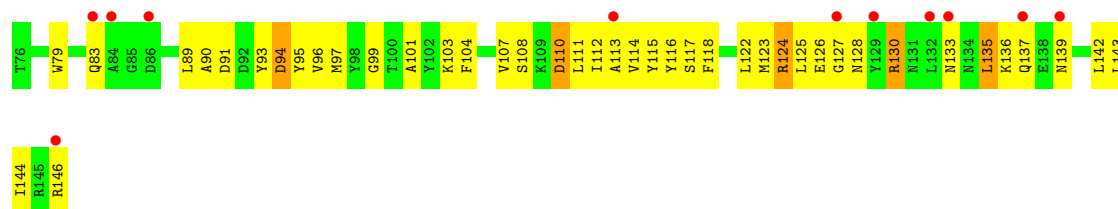


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



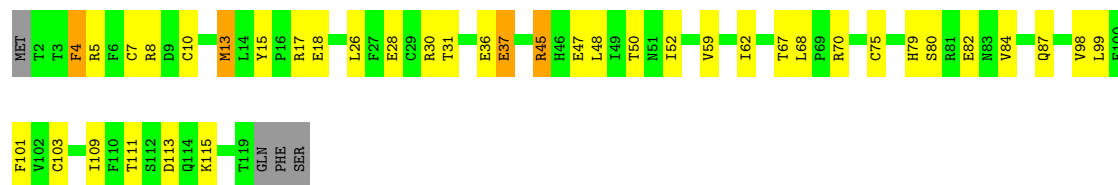
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3





- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I: 65% 29%



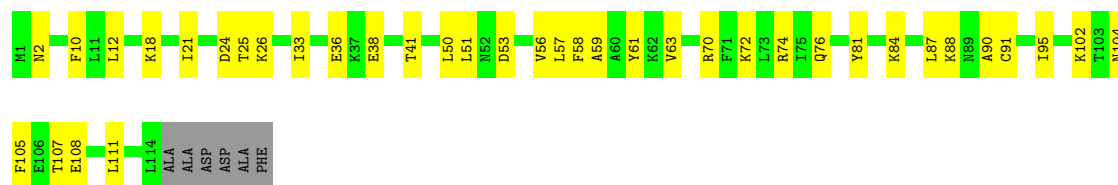
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 60% 30% 7%



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11

Chain K: 63% 32% 5%



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 40% 20% 39%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.22Å 221.93Å 193.71Å 90.00° 99.63° 90.00°	Depositor
Resolution (Å)	82.43 – 2.90 95.49 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (82.43-2.90) 100.0 (95.49-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.215 , 0.251 0.215 , 0.251	Depositor DCC
R_{free} test set	7776 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29191	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5N0, 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	R	0.86	1/223 (0.4%)	1.04	0/345
2	T	0.78	0/584	1.21	2/898 (0.2%)
3	N	0.76	0/352	1.00	0/541
4	A	0.35	0/11020	0.59	5/14907 (0.0%)
5	B	0.32	1/9071 (0.0%)	0.54	2/12242 (0.0%)
6	C	0.32	0/2139	0.56	0/2899
7	E	0.36	0/1767	0.60	2/2378 (0.1%)
8	F	0.33	0/696	0.61	2/943 (0.2%)
9	H	0.44	0/1082	0.77	3/1466 (0.2%)
10	I	0.43	0/970	0.58	0/1308
11	J	0.28	0/541	0.51	0/727
12	K	0.33	0/937	0.55	0/1265
13	L	0.37	0/339	0.69	0/450
All	All	0.37	2/29721 (0.0%)	0.61	16/40369 (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
4	A	0	5
6	C	0	2
9	H	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1	A	OP3-P	-10.91	1.48	1.61
5	B	278	GLN	CG-CD	5.12	1.62	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	179	LEU	CB-CG-CD1	-8.51	96.53	111.00
2	T	22	DT	O4'-C4'-C3'	-8.40	100.96	106.00
5	B	90	ILE	CG1-CB-CG2	-6.57	96.94	111.40
7	E	37	LEU	CA-CB-CG	6.31	129.81	115.30
9	H	130	ARG	NE-CZ-NH1	-5.92	117.34	120.30
4	A	936	LEU	CB-CG-CD2	-5.80	101.14	111.00
5	B	285	ILE	CG1-CB-CG2	-5.78	98.67	111.40
2	T	22	DT	C4'-C3'-C2'	-5.61	98.05	103.10
9	H	7	ASP	CB-CG-OD2	5.59	123.33	118.30
4	A	126	LEU	CB-CG-CD1	-5.49	101.67	111.00
4	A	398	GLU	C-N-CA	5.34	135.06	121.70
9	H	135	LEU	CA-CB-CG	5.24	127.34	115.30
8	F	119	ARG	NE-CZ-NH2	5.21	122.90	120.30
7	E	132	ILE	CG1-CB-CG2	-5.19	99.98	111.40
8	F	119	ARG	NE-CZ-NH1	-5.12	117.74	120.30
4	A	1217	LYS	CD-CE-NZ	-5.01	100.17	111.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1106	ASN	Peptide
4	A	4	GLN	Peptide
4	A	524	VAL	Peptide
4	A	55	ASP	Peptide
4	A	592	ASP	Peptide
6	C	172	PRO	Peptide
6	C	174	ALA	Peptide
9	H	83	GLN	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	R	199	0	98	9	0
2	T	525	0	297	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	312	0	167	15	0
4	A	10828	0	10876	478	1
5	B	8899	0	8853	329	0
6	C	2101	0	2056	87	1
7	E	1731	0	1758	97	0
8	F	684	0	692	40	0
9	H	1064	0	1029	81	0
10	I	952	0	897	43	0
11	J	532	0	542	18	0
12	K	919	0	929	37	0
13	L	337	0	352	15	0
14	T	99	0	0	2	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	29191	0	28546	1147	1

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 20.

All (1147) 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)
12:K:107:THR:O	12:K:111:LEU:HD12	1.29	1.30
5:B:1165:ILE:HD12	5:B:1166:CYS:N	1.50	1.27
9:H:89:LEU:HD13	9:H:91:ASP:O	1.07	1.20
5:B:1101:ASP:O	5:B:1122:ARG:NH2	1.76	1.18
5:B:118:ARG:NH2	5:B:194:GLU:OE2	1.79	1.16
8:F:114:GLU:HG3	8:F:119:ARG:NH2	1.59	1.16
5:B:280:ILE:HD11	5:B:285:ILE:HG13	1.24	1.14
8:F:114:GLU:HG3	8:F:119:ARG:HH22	0.97	1.11
4:A:1143:LEU:HB2	4:A:1271:ILE:HD11	1.32	1.11
5:B:882:THR:HG22	5:B:934:LYS:CE	1.81	1.10
9:H:89:LEU:CD1	9:H:91:ASP:O	1.98	1.09
10:I:4:PHE:CZ	10:I:13:MET:HG3	1.89	1.06
4:A:789:LYS:HG3	10:I:67:THR:HG22	1.34	1.04
5:B:1165:ILE:HD12	5:B:1166:CYS:H	1.04	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:59:VAL:H	10:I:62:ILE:HD13	1.23	1.02
5:B:234:ILE:HD12	5:B:257:LYS:HB3	1.43	1.01
4:A:567:LYS:HB2	9:H:96:VAL:HG12	1.41	1.01
5:B:234:ILE:CD1	5:B:257:LYS:HB3	1.91	1.00
4:A:179:LEU:HD11	4:A:297:GLN:HG2	1.42	1.00
4:A:42:ASP:HA	4:A:50:ILE:HB	1.43	0.98
4:A:424:ILE:HD12	4:A:424:ILE:O	1.64	0.97
6:C:41:ILE:HD11	6:C:246:ARG:HB3	1.45	0.97
5:B:1000:PRO:HB2	5:B:1072:MET:HE3	1.43	0.97
4:A:28:ARG:HH12	4:A:85:ASP:HB3	1.27	0.97
5:B:882:THR:HG22	5:B:934:LYS:HE2	1.46	0.96
9:H:107:VAL:HG23	9:H:111:LEU:HB3	1.48	0.96
12:K:107:THR:O	12:K:111:LEU:CD1	2.15	0.93
4:A:666:ILE:HG23	5:B:1026:LEU:HB3	1.51	0.92
4:A:50:ILE:HG12	4:A:52:GLY:H	1.36	0.91
4:A:1300:LYS:HD3	4:A:1300:LYS:H	1.35	0.90
4:A:152:VAL:HB	4:A:153:PRO:HD2	1.53	0.90
5:B:1101:ASP:C	5:B:1122:ARG:HH12	1.75	0.89
5:B:996:ARG:HH22	6:C:173:ALA:HB1	1.36	0.89
4:A:697:ALA:HA	4:A:702:LEU:CD1	2.03	0.88
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.56	0.87
9:H:89:LEU:HD13	9:H:91:ASP:C	1.94	0.86
8:F:114:GLU:CG	8:F:119:ARG:NH2	2.38	0.86
4:A:660:ASN:ND2	5:B:1082:MET:HB2	1.90	0.86
4:A:1118:VAL:HG12	4:A:1327:ILE:HD11	1.56	0.86
4:A:114:LEU:O	4:A:164:ARG:NH2	2.09	0.86
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.55	0.85
5:B:1194:ILE:HD13	5:B:1196:ILE:HG23	1.56	0.85
6:C:41:ILE:CD1	6:C:246:ARG:HB3	2.07	0.84
7:E:124:VAL:HG13	7:E:132:ILE:CD1	2.08	0.83
5:B:1162:ILE:HD12	5:B:1162:ILE:O	1.78	0.83
12:K:107:THR:HG22	12:K:111:LEU:HD11	1.61	0.83
9:H:26:ILE:HD11	9:H:40:LEU:HB3	1.60	0.82
5:B:1165:ILE:CD1	5:B:1166:CYS:H	1.90	0.81
4:A:247:ARG:NH1	4:A:263:THR:HG22	1.96	0.81
4:A:913:LEU:HD22	4:A:915:SER:H	1.45	0.81
5:B:882:THR:HG22	5:B:934:LYS:NZ	1.96	0.81
4:A:86:LEU:HD12	4:A:238:CYS:HA	1.63	0.81
10:I:4:PHE:HZ	10:I:13:MET:HG3	1.46	0.81
4:A:100:LYS:O	4:A:104:GLU:N	2.14	0.80
4:A:247:ARG:CZ	4:A:263:THR:HG22	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:143:LEU:HD21	6:C:146:LYS:HE2	1.63	0.79
7:E:56:LYS:HZ3	7:E:84:ASP:CB	1.94	0.79
5:B:1161:HIS:HB3	5:B:1171:VAL:HG11	1.65	0.79
5:B:1072:MET:HE2	5:B:1085:ILE:HD12	1.63	0.79
7:E:132:ILE:HD12	7:E:132:ILE:O	1.82	0.78
3:N:3:DC:H4'	5:B:508:LEU:HD21	1.63	0.78
4:A:24:PRO:HG3	4:A:237:THR:HG21	1.65	0.78
4:A:86:LEU:HD23	4:A:296:LEU:HD11	1.65	0.78
4:A:524:VAL:HG12	4:A:525:GLN:H	1.49	0.78
5:B:1194:ILE:CD1	5:B:1196:ILE:HG23	2.13	0.78
4:A:697:ALA:HA	4:A:702:LEU:HD13	1.64	0.78
5:B:661:LEU:HD11	5:B:684:LEU:HD11	1.66	0.78
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.17	0.77
8:F:146:TRP:HB3	8:F:151:LEU:HD21	1.67	0.77
4:A:30:ILE:HD12	5:B:1170:THR:HG21	1.67	0.77
5:B:1165:ILE:CD1	5:B:1166:CYS:N	2.43	0.77
7:E:117:THR:HG23	7:E:120:ALA:H	1.49	0.77
6:C:35:ARG:HH11	12:K:41:THR:HG23	1.48	0.77
4:A:105:CYS:SG	4:A:143:LYS:HA	2.26	0.76
4:A:1116:LEU:HD21	4:A:1316:VAL:HG11	1.64	0.76
6:C:133:ILE:N	6:C:133:ILE:HD12	1.98	0.76
4:A:67:CYS:HB3	4:A:70:CYS:HB2	1.67	0.76
7:E:55:ARG:HH22	7:E:113:GLN:HE21	1.31	0.76
4:A:569:LYS:HD2	4:A:571:LEU:HD21	1.66	0.76
5:B:751:VAL:HG23	5:B:812:LEU:HD22	1.67	0.76
5:B:278:GLN:HG3	5:B:279:ASP:O	1.86	0.75
5:B:971:THR:HB	6:C:61:GLU:OE2	1.85	0.75
5:B:493:SER:OG	5:B:497:ARG:NH2	2.19	0.75
4:A:607:ILE:HG12	4:A:612:ILE:HG22	1.68	0.75
4:A:660:ASN:HD21	5:B:1082:MET:HB2	1.50	0.74
6:C:50:GLU:HB3	13:L:64:LEU:HD11	1.67	0.74
10:I:4:PHE:CZ	10:I:13:MET:CG	2.68	0.74
6:C:50:GLU:OE2	13:L:64:LEU:HD21	1.86	0.74
2:T:19:DG:H2'	2:T:20:DC:C6	2.22	0.74
10:I:111:THR:HG22	10:I:113:ASP:H	1.51	0.74
4:A:789:LYS:HE3	10:I:67:THR:HG21	1.70	0.74
7:E:169:ARG:HH11	7:E:169:ARG:HB2	1.53	0.74
5:B:1101:ASP:CA	5:B:1122:ARG:HH12	2.00	0.74
4:A:961:ARG:HH11	4:A:1025:ARG:HH22	1.36	0.73
4:A:113:LEU:HD21	4:A:222:LEU:HD21	1.69	0.73
4:A:471:ASN:O	4:A:474:VAL:HG12	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:75:PRO:HB2	8:F:77:ASP:OD2	1.88	0.73
5:B:979:LYS:HG2	5:B:1095:LEU:HD12	1.71	0.73
4:A:46:THR:HG22	4:A:47:ARG:H	1.53	0.73
4:A:565:ILE:HB	4:A:571:LEU:HB2	1.70	0.73
6:C:41:ILE:HG23	6:C:172:PRO:HG2	1.70	0.73
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.71	0.73
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.71	0.72
9:H:94:ASP:OD2	9:H:146:ARG:HG2	1.88	0.72
5:B:616:ILE:CG2	5:B:697:GLU:HA	2.19	0.72
5:B:1082:MET:HE3	6:C:190:ASP:HB2	1.72	0.72
6:C:241:ASP:O	6:C:245:VAL:HG12	1.90	0.72
5:B:234:ILE:HD11	5:B:257:LYS:HB3	1.71	0.72
5:B:213:ILE:O	5:B:215:GLN:NE2	2.22	0.72
6:C:98:VAL:H	6:C:122:SER:HB2	1.55	0.72
10:I:59:VAL:N	10:I:62:ILE:HD13	2.02	0.71
2:T:8:DT:H2''	2:T:9:DC:H2'	1.72	0.71
5:B:564:GLU:OE2	5:B:591:ARG:NH1	2.22	0.71
5:B:1065:GLN:HE22	5:B:1067:ARG:HB2	1.53	0.71
7:E:153:HIS:HB3	7:E:196:VAL:HG21	1.71	0.71
12:K:21:ILE:HD13	12:K:33:ILE:HG12	1.72	0.71
4:A:789:LYS:HG3	10:I:67:THR:CG2	2.17	0.71
7:E:180:ARG:NH2	7:E:191:LYS:HA	2.05	0.71
4:A:664:THR:HG22	5:B:1014:PRO:HB3	1.72	0.70
6:C:256:ALA:HA	6:C:259:LEU:HD23	1.73	0.70
10:I:13:MET:CE	10:I:15:TYR:HE1	2.04	0.70
9:H:8:ASP:OD2	9:H:9:ILE:N	2.24	0.70
4:A:606:LEU:HG	4:A:613:ILE:HD13	1.73	0.70
4:A:514:PRO:HB3	4:A:875:ALA:HB3	1.73	0.70
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.24	0.70
4:A:356:ASP:HB3	4:A:359:LEU:HD12	1.74	0.70
4:A:475:THR:HG21	5:B:836:GLU:OE2	1.92	0.70
4:A:91:PHE:N	4:A:297:GLN:OE1	2.25	0.70
5:B:762:ASN:HD21	5:B:1024:ALA:HB3	1.56	0.70
7:E:56:LYS:NZ	7:E:84:ASP:H	1.90	0.70
5:B:1094:ARG:NH2	5:B:1098:MET:SD	2.65	0.69
4:A:113:LEU:HD12	4:A:113:LEU:H	1.58	0.69
6:C:146:LYS:HE3	11:J:57:ILE:HD11	1.75	0.69
7:E:81:GLU:HB3	7:E:96:PHE:HE1	1.56	0.69
4:A:88:LYS:HG2	4:A:89:PRO:HD2	1.74	0.69
5:B:996:ARG:NH2	6:C:173:ALA:HB1	2.06	0.69
6:C:35:ARG:NH1	12:K:41:THR:HG23	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:124:VAL:HG13	7:E:132:ILE:HD11	1.73	0.69
4:A:211:PHE:HA	4:A:214:ILE:CD1	2.22	0.69
5:B:1101:ASP:O	5:B:1122:ARG:CZ	2.41	0.69
7:E:99:HIS:CD2	7:E:103:LYS:HD2	2.28	0.69
4:A:46:THR:HG22	4:A:47:ARG:N	2.07	0.69
5:B:884:ARG:HH21	5:B:935:ARG:HH22	1.39	0.69
4:A:24:PRO:HB3	4:A:237:THR:HG21	1.74	0.68
4:A:1394:THR:OG1	4:A:1399:ARG:HD3	1.93	0.68
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.75	0.68
7:E:175:LEU:HD12	7:E:176:PRO:HD2	1.75	0.68
5:B:582:VAL:O	5:B:585:VAL:HG12	1.92	0.68
5:B:667:GLN:O	5:B:668:ASP:OD2	2.11	0.68
5:B:824:ILE:HG22	5:B:1008:PRO:HA	1.76	0.68
4:A:1167:GLU:CD	4:A:1170:ILE:HD11	2.14	0.68
12:K:107:THR:C	12:K:111:LEU:HD12	2.13	0.68
5:B:637:LEU:HD12	5:B:693:ILE:HG13	1.75	0.68
7:E:90:VAL:HA	7:E:120:ALA:HB2	1.74	0.68
4:A:848:ILE:HG21	4:A:1370:LEU:HD21	1.75	0.67
5:B:1181:GLU:HG3	5:B:1188:LYS:HD2	1.76	0.67
4:A:899:VAL:HG21	4:A:908:LEU:HG	1.74	0.67
10:I:17:ARG:HD2	10:I:28:GLU:OE2	1.95	0.67
3:N:15:DG:H2'	3:N:16:DA:C8	2.29	0.67
4:A:237:THR:HG23	4:A:238:CYS:H	1.59	0.67
4:A:179:LEU:O	4:A:179:LEU:HD12	1.94	0.67
4:A:1300:LYS:H	4:A:1300:LYS:CD	2.07	0.67
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.76	0.67
4:A:961:ARG:NH1	4:A:1025:ARG:HH22	1.91	0.67
4:A:1195:LEU:HD11	4:A:1267:MET:HE1	1.77	0.67
5:B:577:ALA:HB1	5:B:589:VAL:HG13	1.77	0.67
4:A:809:THR:OG1	4:A:812:GLU:HG3	1.96	0.66
4:A:1100:ARG:NH2	4:A:1351:GLU:OE2	2.24	0.66
4:A:567:LYS:HB2	9:H:96:VAL:CG1	2.20	0.66
5:B:118:ARG:NH1	5:B:204:ILE:HD11	2.10	0.66
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.78	0.66
5:B:778:MET:C	5:B:796:LEU:CD1	2.63	0.66
5:B:995:ARG:NH1	5:B:997:GLU:OE1	2.28	0.66
4:A:381:THR:HA	8:F:104:ASN:HD21	1.61	0.66
6:C:41:ILE:CG2	6:C:172:PRO:HG2	2.26	0.66
4:A:115:LEU:HB2	4:A:122:MET:SD	2.36	0.66
4:A:879:GLU:OE2	4:A:962:ARG:NH2	2.28	0.66
4:A:1004:ASN:HD21	4:A:1007:ILE:HD12	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:82:GLY:CA	4:A:241:VAL:HG22	2.25	0.66
7:E:180:ARG:HH22	7:E:191:LYS:HA	1.61	0.66
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.77	0.66
5:B:806:THR:HG22	5:B:808:ALA:H	1.61	0.65
4:A:1116:LEU:H	4:A:1308:THR:HB	1.61	0.65
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.77	0.65
4:A:1279:ILE:HG23	4:A:1308:THR:HG23	1.78	0.65
4:A:175:ARG:HG2	4:A:176:LYS:N	2.10	0.65
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.79	0.65
4:A:1215:ARG:NH2	4:A:1218:GLN:OE1	2.30	0.65
8:F:85:MET:HG3	8:F:89:GLU:HG3	1.77	0.65
1:R:9:G:O2'	4:A:485:ASP:OD1	2.14	0.65
3:N:12:DA:H2''	3:N:13:DG:C8	2.32	0.65
5:B:1162:ILE:HD12	5:B:1162:ILE:C	2.16	0.65
10:I:59:VAL:H	10:I:62:ILE:CD1	2.07	0.65
5:B:1194:ILE:C	5:B:1194:ILE:HD12	2.18	0.65
4:A:38:PRO:HG3	4:A:271:LYS:HG2	1.79	0.64
4:A:697:ALA:CA	4:A:702:LEU:CD1	2.76	0.64
5:B:776:GLN:HB3	5:B:1096:ARG:HG3	1.79	0.64
5:B:805:THR:HB	5:B:809:MET:SD	2.38	0.64
5:B:877:PRO:HB2	5:B:882:THR:HG21	1.78	0.64
4:A:116:ASP:OD1	4:A:164:ARG:NH1	2.31	0.64
4:A:1215:ARG:HH21	4:A:1218:GLN:CD	2.00	0.64
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.79	0.64
4:A:601:LYS:HB2	4:A:603:ASN:OD1	1.97	0.64
4:A:179:LEU:CD1	4:A:297:GLN:HG2	2.23	0.63
5:B:429:PHE:HA	5:B:432:MET:HE3	1.79	0.63
4:A:183:GLY:O	4:A:199:LEU:N	2.32	0.63
12:K:84:LYS:O	12:K:88:LYS:HG3	1.98	0.63
4:A:1130:GLN:O	4:A:1134:ILE:HG12	1.98	0.63
5:B:807:ARG:H	5:B:1045:SER:HB3	1.63	0.63
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.80	0.63
10:I:13:MET:HE3	10:I:15:TYR:HE1	1.63	0.63
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.81	0.63
4:A:237:THR:HG23	4:A:238:CYS:N	2.14	0.63
11:J:36:LEU:HD11	11:J:51:LEU:HB2	1.81	0.63
4:A:913:LEU:CD2	4:A:915:SER:H	2.11	0.63
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.28	0.63
7:E:65:THR:HG23	7:E:68:SER:H	1.64	0.63
9:H:47:PHE:HE1	9:H:146:ARG:HD3	1.62	0.63
4:A:689:LYS:O	4:A:693:VAL:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:8:DT:H1'	2:T:9:DC:H5'	1.82	0.62
4:A:877:HIS:CD2	4:A:1056:SER:HA	2.34	0.62
4:A:1140:HIS:HE1	4:A:1142:THR:HG23	1.65	0.62
5:B:1101:ASP:HA	5:B:1122:ARG:HH12	1.63	0.62
13:L:61:THR:HB	13:L:63:ARG:HG3	1.81	0.62
4:A:88:LYS:NZ	4:A:293:GLU:HB2	2.15	0.62
4:A:756:ILE:O	4:A:760:GLN:HG3	1.99	0.62
5:B:643:ASP:O	5:B:647:GLY:N	2.32	0.62
7:E:107:THR:HA	7:E:131:THR:O	1.98	0.62
9:H:47:PHE:HE1	9:H:146:ARG:CD	2.13	0.62
10:I:4:PHE:HZ	10:I:13:MET:CG	2.08	0.62
4:A:28:ARG:NH1	4:A:85:ASP:HB3	2.09	0.62
6:C:73:GLN:N	6:C:133:ILE:HD11	2.14	0.62
12:K:21:ILE:CD1	12:K:33:ILE:HG12	2.29	0.62
12:K:107:THR:C	12:K:111:LEU:CD1	2.66	0.62
5:B:779:GLY:HA2	5:B:796:LEU:HD13	1.81	0.62
4:A:24:PRO:CG	4:A:237:THR:HG21	2.29	0.62
4:A:868:TYR:CD2	4:A:1058:VAL:HG11	2.34	0.62
5:B:219:ALA:HB2	5:B:405:ARG:HD3	1.81	0.62
2:T:12:DG:H2''	2:T:13:DT:H5''	1.80	0.62
4:A:424:ILE:HD12	4:A:424:ILE:C	2.20	0.62
5:B:257:LYS:HE2	5:B:272:THR:HG23	1.81	0.62
5:B:280:ILE:HD11	5:B:285:ILE:CG1	2.17	0.62
7:E:78:LEU:HD12	7:E:107:THR:OG1	1.99	0.62
8:F:111:LEU:HD23	8:F:111:LEU:H	1.65	0.62
7:E:56:LYS:NZ	7:E:84:ASP:N	2.47	0.61
3:N:8:DC:H2''	3:N:9:DC:H5''	1.83	0.61
6:C:133:ILE:N	6:C:133:ILE:CD1	2.63	0.61
4:A:17:VAL:HG23	4:A:1421:CYS:SG	2.40	0.61
4:A:1063:MET:SD	4:A:1436:ILE:HD12	2.40	0.61
5:B:698:GLU:HA	5:B:701:ILE:HG12	1.81	0.61
5:B:1000:PRO:CB	5:B:1072:MET:HE3	2.23	0.61
7:E:101:GLN:OE1	7:E:127:ILE:HD13	2.01	0.61
5:B:882:THR:CG2	5:B:934:LYS:HE2	2.24	0.61
2:T:15:DA:H2''	2:T:16:DT:C6	2.36	0.61
4:A:1171:GLN:HG2	4:A:1172:LEU:HD23	1.81	0.61
5:B:882:THR:CG2	5:B:934:LYS:NZ	2.63	0.61
4:A:1370:LEU:O	4:A:1374:VAL:HG23	2.00	0.61
5:B:579:ARG:HG2	5:B:586:TRP:CE2	2.36	0.61
4:A:36:ARG:O	4:A:270:LEU:HD21	2.01	0.61
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:100:THR:HG22	6:C:119:VAL:HG23	1.83	0.61
9:H:89:LEU:CD1	9:H:91:ASP:C	2.61	0.61
10:I:82:GLU:OE1	10:I:82:GLU:N	2.34	0.61
2:T:6:DT:H1'	2:T:7:DC:H5'	1.82	0.60
4:A:424:ILE:HD13	4:A:426:LEU:HG	1.83	0.60
5:B:58:THR:O	5:B:62:ILE:HG13	2.00	0.60
5:B:487:THR:OG1	5:B:777:ALA:O	2.20	0.60
11:J:36:LEU:HD13	11:J:47:ARG:HG2	1.83	0.60
3:N:4:DA:H2''	3:N:5:DT:H71	1.81	0.60
4:A:1355:VAL:HG13	4:A:1356:ILE:HD12	1.83	0.60
4:A:1436:ILE:O	4:A:1439:GLY:N	2.34	0.60
4:A:873:MET:HG3	4:A:957:PRO:HG3	1.83	0.60
5:B:882:THR:HG22	5:B:934:LYS:CD	2.32	0.60
4:A:1424:VAL:HG21	5:B:1139:ILE:HD12	1.82	0.60
4:A:113:LEU:HD11	4:A:218:ASP:HB3	1.84	0.60
4:A:919:ILE:HD11	4:A:925:LEU:HD12	1.83	0.60
5:B:509:ALA:O	5:B:513:GLN:HG3	2.02	0.60
5:B:763:GLN:HG3	5:B:765:PRO:HD2	1.83	0.60
8:F:77:ASP:OD2	8:F:77:ASP:N	2.29	0.60
4:A:38:PRO:HD3	4:A:270:LEU:HD22	1.84	0.60
4:A:298:PHE:HE1	4:A:312:PRO:HB2	1.67	0.60
4:A:1276:VAL:HB	4:A:1279:ILE:HD13	1.82	0.60
5:B:778:MET:O	5:B:796:LEU:CD1	2.50	0.60
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.35	0.60
4:A:1138:ILE:HG23	4:A:1282:VAL:HG21	1.84	0.59
6:C:77:ILE:HG13	6:C:161:LYS:HE3	1.83	0.59
10:I:26:LEU:HD23	10:I:37:GLU:HA	1.84	0.59
4:A:100:LYS:NZ	4:A:174:ILE:HB	2.16	0.59
5:B:133:LYS:HZ1	5:B:162:SER:N	2.00	0.59
5:B:224:GLN:HE21	5:B:226:PHE:HZ	1.49	0.59
4:A:1050:GLU:O	4:A:1054:LEU:HD12	2.02	0.59
7:E:12:LEU:HD11	7:E:58:MET:SD	2.42	0.59
4:A:567:LYS:HB3	4:A:568:PRO:HD3	1.84	0.59
4:A:1220:PHE:O	4:A:1223:ASP:HB2	2.02	0.59
6:C:240:VAL:HA	6:C:243:VAL:HG12	1.84	0.59
10:I:10:CYS:SG	10:I:31:THR:OG1	2.61	0.59
4:A:53:LEU:HD21	4:A:247:ARG:NH2	2.17	0.59
5:B:896:ASP:OD2	13:L:58:LYS:NZ	2.32	0.59
5:B:1072:MET:CE	5:B:1085:ILE:HD12	2.30	0.59
10:I:50:THR:HG22	10:I:52:ILE:H	1.66	0.59
4:A:337:ARG:HH21	4:A:337:ARG:HG2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:56:LYS:HZ2	7:E:84:ASP:N	1.99	0.59
9:H:94:ASP:OD2	9:H:146:ARG:CG	2.50	0.59
4:A:1215:ARG:NH2	4:A:1218:GLN:CD	2.56	0.59
9:H:24:CYS:HB2	9:H:44:VAL:CG2	2.32	0.59
4:A:112:LYS:HG2	4:A:113:LEU:N	2.17	0.59
4:A:1025:ARG:HE	4:A:1030:ARG:HH12	1.51	0.59
5:B:1153:GLU:OE1	5:B:1153:GLU:N	2.34	0.58
9:H:47:PHE:CE1	9:H:146:ARG:CD	2.85	0.58
4:A:122:MET:CE	4:A:126:LEU:HD11	2.33	0.58
4:A:380:VAL:HG23	4:A:428:TYR:HA	1.84	0.58
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.84	0.58
4:A:464:PRO:O	12:K:2:ASN:HB3	2.03	0.58
4:A:1239:ARG:HH22	4:A:1241:ARG:HH12	1.49	0.58
4:A:1288:ASP:OD1	4:A:1288:ASP:N	2.33	0.58
1:R:2:U:H2'	1:R:3:C:C6	2.38	0.58
9:H:47:PHE:CE1	9:H:146:ARG:HD2	2.38	0.58
9:H:89:LEU:HD12	9:H:91:ASP:H	1.69	0.58
4:A:795:GLU:HG3	5:B:731:VAL:HG21	1.84	0.58
6:C:17:ASN:HA	6:C:240:VAL:HG11	1.86	0.58
4:A:20:GLY:C	5:B:1213:THR:HG22	2.25	0.58
4:A:24:PRO:CB	4:A:237:THR:HG21	2.33	0.58
4:A:524:VAL:HG12	4:A:525:GLN:HG2	1.86	0.58
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.37	0.58
7:E:56:LYS:HZ2	7:E:84:ASP:H	1.50	0.58
7:E:92:THR:O	7:E:95:THR:HB	2.04	0.58
7:E:93:MET:O	7:E:97:VAL:HG12	2.04	0.58
12:K:57:LEU:HB2	12:K:76:GLN:HG2	1.86	0.58
5:B:763:GLN:CG	5:B:765:PRO:HD2	2.34	0.57
8:F:119:ARG:HH21	8:F:119:ARG:HB3	1.69	0.57
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.86	0.57
4:A:1404:GLU:O	4:A:1408:ILE:HG12	2.02	0.57
10:I:4:PHE:CZ	10:I:13:MET:SD	2.97	0.57
12:K:18:LYS:HE2	12:K:36:GLU:O	2.04	0.57
4:A:176:LYS:HD2	4:A:176:LYS:O	2.04	0.57
4:A:88:LYS:HZ1	4:A:293:GLU:HB2	1.69	0.57
4:A:913:LEU:HD22	4:A:915:SER:N	2.17	0.57
6:C:79:GLN:OE1	6:C:127:ARG:HG2	2.04	0.57
9:H:38:LEU:HD11	9:H:123:MET:HE3	1.85	0.57
5:B:446:LEU:HB3	5:B:448:ILE:HD11	1.87	0.57
5:B:680:THR:O	5:B:683:SER:OG	2.21	0.57
9:H:112:ILE:HG13	9:H:113:ALA:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:464:PRO:HB2	4:A:465:TYR:CD1	2.39	0.57
5:B:287:ARG:NH1	5:B:324:ILE:O	2.38	0.57
4:A:739:ASP:OD2	9:H:19:ARG:NH1	2.38	0.57
4:A:864:ILE:HG21	4:A:1374:VAL:HG22	1.86	0.57
4:A:1390:ASN:HD22	4:A:1399:ARG:HG3	1.70	0.57
5:B:1194:ILE:HD12	5:B:1194:ILE:O	2.05	0.57
6:C:36:VAL:HG21	6:C:251:LEU:HB2	1.86	0.57
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.22	0.57
9:H:126:GLU:CA	9:H:130:ARG:HH12	2.18	0.57
5:B:884:ARG:NH2	5:B:935:ARG:HH22	2.01	0.56
4:A:642:CYS:O	4:A:645:LEU:HB3	2.05	0.56
4:A:1412:ALA:HA	4:A:1417:GLU:HG3	1.86	0.56
7:E:197:LYS:HE2	7:E:199:ILE:HD11	1.86	0.56
10:I:75:CYS:HB3	10:I:79:HIS:H	1.70	0.56
4:A:21:LEU:HD21	4:A:95:PHE:CE1	2.40	0.56
4:A:500:GLU:OE2	5:B:1145:SER:OG	2.23	0.56
4:A:793:SER:OG	4:A:795:GLU:OE1	2.22	0.56
4:A:1120:LEU:HD23	4:A:1125:ALA:HA	1.86	0.56
6:C:251:LEU:O	6:C:255:VAL:HG23	2.04	0.56
7:E:113:GLN:HG3	7:E:114:ASN:OD1	2.06	0.56
7:E:127:ILE:HD12	7:E:128:PRO:HD2	1.87	0.56
7:E:60:PHE:C	7:E:79:TRP:CD1	2.79	0.56
8:F:107:VAL:HG21	8:F:111:LEU:HD22	1.88	0.56
1:R:9:G:OP1	5:B:987:LYS:NZ	2.28	0.56
7:E:61:GLN:CA	7:E:79:TRP:HD1	2.19	0.56
2:T:7:DC:H2''	2:T:8:DT:H5''	1.87	0.56
4:A:119:ASN:OD1	4:A:122:MET:N	2.31	0.56
4:A:211:PHE:HA	4:A:214:ILE:HD11	1.87	0.56
5:B:1082:MET:HA	6:C:189:THR:HA	1.88	0.56
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.86	0.56
4:A:1297:GLU:OE2	4:A:1297:GLU:N	2.33	0.56
5:B:912:ILE:HB	5:B:939:THR:HB	1.88	0.56
1:R:7:A:O2'	1:R:8:G:H5'	2.06	0.56
4:A:525:GLN:HB3	5:B:1015:HIS:CD2	2.40	0.56
4:A:562:THR:O	4:A:576:GLN:NE2	2.39	0.56
5:B:1149:GLU:HA	5:B:1153:GLU:OE1	2.06	0.56
4:A:821:ARG:NH1	5:B:524:PRO:O	2.39	0.56
4:A:1079:MET:HG2	4:A:1098:VAL:HG23	1.88	0.56
5:B:650:GLU:OE2	5:B:651:LEU:HD23	2.06	0.56
10:I:15:TYR:HD2	10:I:30:ARG:NE	2.04	0.55
4:A:203:SER:O	4:A:206:GLU:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:843:GLN:HG2	5:B:993:THR:OG1	2.06	0.55
5:B:361:LEU:HD23	5:B:364:ILE:HG13	1.89	0.55
11:J:7:CYS:HA	11:J:49:MET:HG3	1.87	0.55
2:T:13:DT:H2'	2:T:14:DC:C6	2.42	0.55
4:A:374:LEU:C	4:A:436:ILE:HD13	2.27	0.55
4:A:569:LYS:NZ	6:C:221:TYR:HB2	2.21	0.55
8:F:132:LEU:O	8:F:148:VAL:HG23	2.06	0.55
4:A:394:ASN:ND2	4:A:398:GLU:OE1	2.40	0.55
7:E:91:LYS:HA	7:E:94:LYS:HB2	1.89	0.55
5:B:803:LEU:H	5:B:822:ASN:HD21	1.54	0.55
4:A:244:PRO:HA	4:A:247:ARG:HG3	1.89	0.55
4:A:494:SER:HB2	4:A:497:THR:HG23	1.87	0.55
4:A:1308:THR:HG22	4:A:1309:ASP:N	2.22	0.55
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.89	0.55
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.88	0.55
4:A:598:LEU:HD11	9:H:39:THR:HG21	1.89	0.55
5:B:69:LEU:HD11	5:B:90:ILE:HB	1.88	0.55
6:C:249:ASP:OD1	12:K:102:LYS:NZ	2.39	0.55
9:H:57:VAL:HG22	9:H:144:ILE:HG13	1.89	0.55
4:A:69:THR:HB	5:B:1172:ILE:HG21	1.88	0.54
4:A:825:ILE:O	4:A:829:VAL:HG22	2.07	0.54
4:A:943:LEU:HD11	4:A:1020:CYS:HB3	1.89	0.54
4:A:1005:GLU:HG3	4:A:1009:ASN:ND2	2.22	0.54
10:I:4:PHE:HZ	10:I:13:MET:SD	2.30	0.54
4:A:42:ASP:OD1	4:A:46:THR:HB	2.06	0.54
4:A:179:LEU:CD1	4:A:297:GLN:HE21	2.20	0.54
4:A:525:GLN:NE2	5:B:836:GLU:HG3	2.22	0.54
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.89	0.54
5:B:46:GLN:HG2	5:B:47:GLN:N	2.22	0.54
5:B:1101:ASP:C	5:B:1122:ARG:NH1	2.53	0.54
6:C:76:ASP:C	6:C:129:ILE:HD11	2.27	0.54
4:A:472:LEU:HD21	5:B:835:GLN:HB2	1.89	0.54
4:A:1215:ARG:HH21	4:A:1218:GLN:CG	2.19	0.54
5:B:235:SER:OG	5:B:236:HIS:ND1	2.40	0.54
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.41	0.54
6:C:17:ASN:HB3	6:C:233:GLU:HG2	1.90	0.54
10:I:45:ARG:NH1	10:I:47:GLU:OE2	2.40	0.54
4:A:1318:THR:HG22	7:E:142:VAL:HG23	1.88	0.54
9:H:135:LEU:HD23	9:H:136:LYS:N	2.21	0.54
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.90	0.54
4:A:1120:LEU:O	4:A:1323:ASP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1161:HIS:HB3	5:B:1171:VAL:CG1	2.36	0.54
4:A:82:GLY:C	4:A:241:VAL:HG22	2.28	0.54
7:E:14:ARG:HH11	7:E:141:VAL:HG12	1.72	0.54
7:E:169:ARG:HB2	7:E:169:ARG:NH1	2.20	0.54
4:A:1094:VAL:HG12	4:A:1113:THR:HG21	1.90	0.54
6:C:100:THR:CG2	6:C:119:VAL:HG23	2.37	0.54
8:F:114:GLU:CD	8:F:119:ARG:NH2	2.61	0.54
4:A:112:LYS:HG2	4:A:113:LEU:H	1.73	0.53
4:A:182:VAL:HG12	4:A:201:VAL:HG12	1.89	0.53
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.90	0.53
4:A:1138:ILE:HD11	4:A:1316:VAL:HG13	1.91	0.53
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.91	0.53
2:T:17:DG:OP1	4:A:1403:GLU:HG2	2.09	0.53
4:A:761:MET:HG3	5:B:1021:MET:HG2	1.90	0.53
5:B:603:LEU:HB3	5:B:609:ILE:HG13	1.90	0.53
5:B:1194:ILE:HD13	5:B:1196:ILE:CG2	2.33	0.53
4:A:28:ARG:HH12	4:A:85:ASP:CB	2.13	0.53
4:A:36:ARG:HH21	4:A:270:LEU:HD21	1.72	0.53
4:A:587:HIS:NE2	4:A:969:GLN:HG3	2.24	0.53
4:A:870:GLU:HG2	7:E:208:TYR:CG	2.43	0.53
6:C:3:GLU:HB2	12:K:104:ASN:HD21	1.74	0.53
4:A:100:LYS:HD3	4:A:174:ILE:CG2	2.39	0.53
4:A:1444:MET:HG3	8:F:133:VAL:CG1	2.38	0.53
7:E:55:ARG:HH22	7:E:113:GLN:NE2	2.04	0.53
10:I:80:SER:OG	10:I:103:CYS:SG	2.66	0.53
4:A:311:GLN:N	4:A:312:PRO:HD3	2.24	0.53
4:A:1118:VAL:HG22	4:A:1306:LEU:HB2	1.91	0.53
5:B:612:GLU:O	5:B:632:ARG:NH2	2.42	0.53
7:E:124:VAL:CG1	7:E:132:ILE:CD1	2.85	0.53
4:A:46:THR:CG2	4:A:47:ARG:H	2.20	0.53
4:A:372:LYS:HG2	4:A:399:HIS:HB2	1.90	0.53
4:A:112:LYS:HG3	4:A:218:ASP:OD1	2.09	0.53
2:T:11:DG:H2"	2:T:12:DG:C8	2.44	0.53
4:A:85:ASP:HA	4:A:238:CYS:HB2	1.90	0.53
4:A:388:LEU:O	4:A:392:VAL:HG23	2.09	0.53
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.40	0.53
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.91	0.52
4:A:1390:ASN:ND2	4:A:1399:ARG:HG3	2.24	0.52
7:E:56:LYS:HZ3	7:E:84:ASP:HB3	1.74	0.52
7:E:56:LYS:HZ3	7:E:84:ASP:CA	2.22	0.52
4:A:1407:GLU:OE2	4:A:1407:GLU:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.45	0.52
5:B:1101:ASP:O	5:B:1122:ARG:NH1	2.43	0.52
4:A:705:LYS:HD2	4:A:706:HIS:H	1.74	0.52
4:A:836:TYR:OH	4:A:1403:GLU:OE2	2.19	0.52
4:A:919:ILE:HD11	4:A:925:LEU:CD1	2.39	0.52
4:A:1295:THR:HB	4:A:1297:GLU:OE2	2.09	0.52
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.91	0.52
7:E:55:ARG:O	7:E:82:PHE:HB2	2.09	0.52
7:E:161:LYS:HD2	7:E:195:VAL:HG23	1.91	0.52
4:A:591:PHE:HB3	4:A:595:THR:OG1	2.09	0.52
5:B:864:LYS:HG2	5:B:872:GLU:OE1	2.09	0.52
5:B:1082:MET:CE	6:C:190:ASP:HB2	2.40	0.52
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.92	0.52
4:A:803:SER:OG	4:A:806:ARG:HG3	2.09	0.52
7:E:91:LYS:O	7:E:94:LYS:HB3	2.10	0.52
4:A:4:GLN:O	4:A:5:GLN:O	2.28	0.52
4:A:216:VAL:O	4:A:219:PHE:HB2	2.09	0.52
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.91	0.52
8:F:114:GLU:OE1	8:F:115:THR:N	2.42	0.52
10:I:13:MET:HE2	10:I:15:TYR:HE1	1.74	0.52
5:B:1174:LYS:HD2	5:B:1177:HIS:HB2	1.91	0.52
11:J:57:ILE:O	11:J:61:LEU:HG	2.10	0.52
4:A:782:ARG:NH1	10:I:67:THR:HG23	2.24	0.52
4:A:20:GLY:O	4:A:21:LEU:HD12	2.09	0.52
4:A:179:LEU:HD12	4:A:297:GLN:HE21	1.75	0.52
6:C:72:LEU:C	6:C:133:ILE:HD11	2.30	0.52
7:E:69:ILE:HD12	7:E:70:SER:N	2.25	0.52
8:F:128:LYS:NZ	8:F:151:LEU:O	2.42	0.52
8:F:146:TRP:HB3	8:F:151:LEU:CD2	2.39	0.52
9:H:37:LYS:O	9:H:125:LEU:HD12	2.10	0.52
4:A:443:LEU:HD21	5:B:1138:MET:HE3	1.92	0.52
4:A:449:SER:HB3	5:B:1137:CYS:SG	2.50	0.52
5:B:579:ARG:HG2	5:B:586:TRP:CZ2	2.45	0.52
4:A:122:MET:O	4:A:125:ALA:N	2.43	0.51
4:A:134:ARG:NH2	4:A:221:SER:HA	2.25	0.51
5:B:666:TYR:O	5:B:668:ASP:N	2.43	0.51
6:C:114:TYR:CG	6:C:140:ASN:HB3	2.45	0.51
9:H:39:THR:HG22	9:H:124:ARG:HB3	1.92	0.51
4:A:119:ASN:OD1	4:A:121:LEU:HB3	2.10	0.51
4:A:204:THR:HG23	4:A:235:ILE:HD12	1.92	0.51
4:A:351:THR:OG1	4:A:352:VAL:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:535:THR:HG21	4:A:578:LEU:HD23	1.91	0.51
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.93	0.51
5:B:620:ARG:HD3	10:I:68:LEU:HD11	1.93	0.51
5:B:1065:GLN:HE22	5:B:1069:PHE:HD1	1.58	0.51
5:B:1162:ILE:HD11	5:B:1192:TYR:HB2	1.93	0.51
6:C:259:LEU:O	6:C:263:THR:HG23	2.10	0.51
8:F:97:ARG:NH2	8:F:101:ILE:HD11	2.26	0.51
9:H:110:ASP:C	9:H:128:ASN:HD22	2.14	0.51
4:A:446:ARG:NH1	4:A:447:GLN:O	2.44	0.51
4:A:1239:ARG:HH22	4:A:1241:ARG:NH1	2.08	0.51
5:B:276:ILE:HD11	5:B:335:GLY:N	2.25	0.51
5:B:577:ALA:HB1	5:B:589:VAL:CG1	2.40	0.51
6:C:115:SER:OG	6:C:141:GLY:HA3	2.10	0.51
8:F:79:ARG:NH1	8:F:145:ASP:O	2.44	0.51
9:H:32:THR:HG22	9:H:32:THR:O	2.11	0.51
2:T:25:DC:P	5:B:942:ARG:HH22	2.34	0.51
4:A:830:LYS:HD2	4:A:1079:MET:O	2.11	0.51
4:A:12:ARG:HG3	5:B:1192:TYR:CD2	2.46	0.51
4:A:54:ASN:OD1	4:A:244:PRO:HG3	2.09	0.51
4:A:874:ASP:HA	4:A:1058:VAL:HG12	1.92	0.51
5:B:944:THR:HG23	5:B:945:GLU:HG3	1.92	0.51
9:H:47:PHE:CE1	9:H:146:ARG:HD3	2.43	0.51
12:K:25:THR:O	12:K:26:LYS:HG2	2.10	0.51
2:T:10:DT:H2"	2:T:11:DG:N7	2.26	0.51
4:A:1134:ILE:HB	4:A:1306:LEU:HD11	1.92	0.51
5:B:437:GLU:N	5:B:437:GLU:OE1	2.43	0.51
5:B:760:ASP:OD1	5:B:760:ASP:N	2.40	0.51
6:C:107:SER:O	6:C:149:LYS:HB2	2.11	0.51
7:E:19:VAL:O	7:E:23:VAL:HG22	2.11	0.51
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.46	0.51
5:B:69:LEU:HD12	5:B:69:LEU:O	2.11	0.51
9:H:63:LEU:HB3	9:H:90:ALA:HB2	1.93	0.51
4:A:216:VAL:O	4:A:220:THR:HG23	2.11	0.51
7:E:195:VAL:HG22	7:E:213:ILE:HG13	1.93	0.51
10:I:87:GLN:HG2	10:I:99:LEU:CD2	2.40	0.51
11:J:64:ASN:N	11:J:65:PRO:HD2	2.26	0.51
4:A:175:ARG:HG2	4:A:176:LYS:H	1.76	0.50
4:A:443:LEU:HD11	4:A:455:MET:HB3	1.93	0.50
5:B:802:PRO:HG2	5:B:805:THR:HG22	1.93	0.50
4:A:913:LEU:HD23	4:A:914:GLU:N	2.27	0.50
9:H:12:VAL:HG22	9:H:53:ASP:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:130:ASP:OD1	4:A:133:LYS:HG3	2.11	0.50
5:B:420:LEU:HD13	5:B:453:ILE:HG12	1.93	0.50
6:C:262:LEU:HD11	12:K:87:LEU:HD23	1.94	0.50
2:T:22:DT:OP1	4:A:344:ARG:NH1	2.44	0.50
5:B:582:VAL:O	5:B:583:ASN:HB2	2.11	0.50
5:B:778:MET:O	5:B:796:LEU:HD11	2.12	0.50
7:E:132:ILE:HD12	7:E:132:ILE:C	2.32	0.50
4:A:17:VAL:HA	5:B:1215:ARG:O	2.12	0.50
4:A:36:ARG:HH22	4:A:273:ASN:HD22	1.60	0.50
4:A:587:HIS:HA	4:A:607:ILE:O	2.11	0.50
4:A:1193:LEU:HD11	4:A:1264:GLU:HB2	1.92	0.50
4:A:382:PRO:HD3	8:F:104:ASN:ND2	2.27	0.50
4:A:556:TRP:O	12:K:26:LYS:CE	2.60	0.50
5:B:1213:THR:HG21	5:B:1215:ARG:NH2	2.26	0.50
4:A:88:LYS:HG2	4:A:89:PRO:CD	2.41	0.49
4:A:452:LYS:HG2	4:A:453:MET:HE2	1.94	0.49
2:T:9:DC:H2''	2:T:10:DT:H71	1.94	0.49
2:T:19:DG:H2'	2:T:20:DC:H6	1.72	0.49
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.93	0.49
4:A:780:VAL:HG22	5:B:699:GLU:OE2	2.11	0.49
5:B:762:ASN:ND2	5:B:1024:ALA:HB3	2.25	0.49
4:A:175:ARG:HD3	4:A:176:LYS:O	2.12	0.49
4:A:472:LEU:O	4:A:475:THR:HG23	2.12	0.49
4:A:1268:LEU:HD13	10:I:48:LEU:HD21	1.93	0.49
4:A:1341:ILE:HD13	4:A:1380:GLY:HA2	1.94	0.49
5:B:357:GLN:HE21	5:B:369:GLY:H	1.59	0.49
5:B:446:LEU:HB3	5:B:448:ILE:CD1	2.41	0.49
8:F:94:LEU:HD21	8:F:125:LEU:HD22	1.95	0.49
9:H:139:ASN:HD22	9:H:139:ASN:N	2.10	0.49
4:A:343:LYS:HD2	5:B:1155:SER:HB3	1.94	0.49
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.45	0.49
5:B:629:ASP:O	5:B:632:ARG:NH1	2.45	0.49
2:T:13:DT:H1'	14:T:101:5N0:N6	2.28	0.49
6:C:163:ILE:HD12	6:C:165:LYS:HB2	1.94	0.49
7:E:99:HIS:NE2	7:E:103:LYS:HD2	2.27	0.49
4:A:36:ARG:CZ	4:A:274:ILE:HD12	2.43	0.49
4:A:304:MET:CE	5:B:1210:MET:HA	2.43	0.49
4:A:686:ALA:O	4:A:690:VAL:HG13	2.13	0.49
5:B:1162:ILE:C	5:B:1162:ILE:CD1	2.80	0.49
9:H:42:ILE:HD12	9:H:95:TYR:CE1	2.47	0.49
4:A:464:PRO:HB2	4:A:465:TYR:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1410:PHE:HE2	5:B:1210:MET:HG2	1.76	0.49
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.11	0.49
9:H:5:LEU:HG	9:H:133:ASN:HB3	1.95	0.49
9:H:101:ALA:HB2	9:H:116:TYR:HE2	1.76	0.49
4:A:433:GLU:OE2	5:B:1108:ARG:NH2	2.45	0.49
4:A:598:LEU:O	9:H:122:LEU:HD12	2.12	0.49
7:E:124:VAL:CG1	7:E:132:ILE:HD11	2.43	0.49
5:B:360:PHE:HE2	5:B:374:LYS:HB3	1.77	0.49
6:C:8:VAL:HG22	6:C:22:LEU:HD22	1.95	0.49
4:A:382:PRO:HD3	8:F:104:ASN:HD22	1.78	0.49
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.38	0.49
4:A:544:ASP:OD1	4:A:544:ASP:N	2.42	0.49
6:C:50:GLU:CD	13:L:64:LEU:HD21	2.32	0.49
9:H:118:PHE:HE1	9:H:123:MET:HB3	1.78	0.49
4:A:662:PHE:O	5:B:828:ALA:HA	2.12	0.48
4:A:697:ALA:HB2	4:A:702:LEU:HD11	1.95	0.48
4:A:40:THR:HG23	4:A:41:MET:H	1.78	0.48
4:A:672:ASP:OD1	4:A:672:ASP:N	2.44	0.48
4:A:1118:VAL:HA	4:A:1327:ILE:HD12	1.94	0.48
5:B:942:ARG:HB2	5:B:945:GLU:OE1	2.14	0.48
6:C:166:GLU:HG3	12:K:10:PHE:CZ	2.48	0.48
7:E:46:TYR:CE2	7:E:58:MET:HA	2.48	0.48
5:B:400:HIS:CD2	5:B:517:THR:HG21	2.48	0.48
5:B:433:GLN:O	5:B:436:VAL:HG13	2.13	0.48
5:B:881:ASN:HB3	5:B:934:LYS:NZ	2.27	0.48
5:B:1101:ASP:HA	5:B:1122:ARG:NH1	2.29	0.48
7:E:115:ASN:OD1	7:E:116:ILE:N	2.46	0.48
4:A:46:THR:CG2	4:A:47:ARG:N	2.74	0.48
4:A:289:ILE:HG22	4:A:290:GLU:OE2	2.12	0.48
4:A:821:ARG:HG3	4:A:825:ILE:HD11	1.95	0.48
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.12	0.48
8:F:147:SER:O	8:F:151:LEU:HD23	2.13	0.48
9:H:24:CYS:HB2	9:H:44:VAL:HG21	1.96	0.48
4:A:4:GLN:OE1	5:B:1159:ARG:HB3	2.14	0.48
4:A:35:ILE:O	4:A:84:ILE:HG22	2.14	0.48
4:A:82:GLY:HA3	4:A:241:VAL:HG22	1.93	0.48
4:A:608:ILE:N	4:A:613:ILE:HD11	2.29	0.48
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.47	0.48
4:A:1129:GLU:O	4:A:1133:LEU:HD23	2.14	0.48
4:A:1159:ARG:HB2	4:A:1159:ARG:CZ	2.42	0.48
5:B:695:ALA:HA	5:B:698:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:882:THR:CG2	5:B:934:LYS:HZ3	2.25	0.48
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.13	0.48
6:C:244:VAL:HG11	12:K:105:PHE:CZ	2.49	0.48
8:F:123:LYS:O	8:F:127:GLU:HG3	2.14	0.48
4:A:215:SER:OG	4:A:218:ASP:OD1	2.31	0.48
4:A:776:ALA:O	4:A:783:THR:HG22	2.14	0.48
4:A:982:THR:O	4:A:985:ASP:HB2	2.13	0.48
1:R:9:G:P	5:B:987:LYS:HZ1	2.36	0.48
4:A:446:ARG:HB2	4:A:487:MET:SD	2.54	0.48
4:A:567:LYS:NZ	9:H:93:TYR:O	2.39	0.48
4:A:949:ASP:OD1	4:A:949:ASP:N	2.45	0.48
5:B:1084:GLN:HG2	6:C:201:TRP:CH2	2.49	0.48
6:C:41:ILE:HD11	6:C:246:ARG:CB	2.31	0.48
4:A:36:ARG:O	4:A:36:ARG:NE	2.35	0.48
4:A:1217:LYS:HZ3	4:A:1222:ASN:H	1.60	0.48
5:B:706:GLN:HG3	5:B:708:GLU:HB3	1.96	0.48
5:B:857:ARG:HH12	5:B:942:ARG:NH2	2.12	0.48
9:H:38:LEU:HB2	9:H:125:LEU:HD13	1.95	0.48
4:A:586:ILE:HD11	4:A:637:LYS:HG2	1.96	0.48
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.54	0.48
5:B:369:GLY:C	5:B:370:PHE:HD1	2.15	0.48
5:B:415:GLN:HE22	5:B:476:ARG:NH1	2.11	0.48
5:B:595:ARG:HE	5:B:595:ARG:HB2	1.53	0.48
12:K:21:ILE:HD12	12:K:21:ILE:HA	1.63	0.48
4:A:1443:VAL:HG12	8:F:132:LEU:HD22	1.95	0.48
5:B:1057:LYS:O	5:B:1057:LYS:HD3	2.13	0.48
7:E:61:GLN:N	7:E:79:TRP:HD1	2.12	0.48
7:E:121:MET:O	7:E:124:VAL:HG23	2.14	0.48
7:E:124:VAL:HG13	7:E:132:ILE:HD12	1.95	0.48
7:E:154:ILE:C	7:E:196:VAL:HG23	2.34	0.48
4:A:868:TYR:HD2	4:A:1058:VAL:HG11	1.79	0.47
4:A:1390:ASN:OD1	4:A:1402:PHE:CD2	2.67	0.47
7:E:180:ARG:HH21	7:E:192:ARG:H	1.62	0.47
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	1.97	0.47
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.49	0.47
4:A:1444:MET:HG3	8:F:133:VAL:HG13	1.95	0.47
7:E:171:LYS:HB2	7:E:174:GLN:HE21	1.79	0.47
7:E:192:ARG:HA	7:E:214:CYS:HB3	1.97	0.47
9:H:94:ASP:CG	9:H:146:ARG:HG2	2.34	0.47
4:A:884:ASP:HB3	4:A:896:ARG:NH1	2.29	0.47
4:A:1314:SER:O	4:A:1318:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.48	0.47
7:E:87:SER:HA	7:E:115:ASN:HB3	1.96	0.47
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.47	0.47
6:C:51:VAL:HG23	6:C:155:LEU:HB3	1.96	0.47
9:H:126:GLU:C	9:H:130:ARG:HH12	2.16	0.47
5:B:616:ILE:HG21	5:B:697:GLU:HA	1.95	0.47
5:B:1065:GLN:NE2	5:B:1069:PHE:HD1	2.12	0.47
2:T:25:DC:H2''	2:T:26:DG:H5'	1.95	0.47
4:A:67:CYS:SG	4:A:80:HIS:CD2	3.07	0.47
4:A:328:ARG:HD3	5:B:1206:GLU:OE1	2.14	0.47
4:A:424:ILE:O	4:A:424:ILE:CD1	2.51	0.47
4:A:635:ARG:CZ	4:A:877:HIS:HB3	2.43	0.47
4:A:690:VAL:HG21	4:A:794:PRO:HG3	1.96	0.47
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	1.95	0.47
5:B:893:LEU:HD11	5:B:910:VAL:HG12	1.95	0.47
4:A:180:LYS:NZ	4:A:294:SER:HB2	2.29	0.47
4:A:450:LEU:HD13	4:A:1077:THR:HG21	1.95	0.47
4:A:857:ARG:HD3	4:A:861:GLY:O	2.14	0.47
4:A:1102:LYS:HG2	4:A:1106:ASN:ND2	2.29	0.47
4:A:1120:LEU:CD2	4:A:1125:ALA:HA	2.45	0.47
5:B:211:VAL:O	5:B:480:SER:HA	2.14	0.47
5:B:877:PRO:CB	5:B:882:THR:HG21	2.44	0.47
6:C:254:LYS:HD3	12:K:38:GLU:OE2	2.14	0.47
7:E:29:PHE:O	7:E:30:ILE:HD12	2.15	0.47
9:H:12:VAL:HG22	9:H:53:ASP:N	2.29	0.47
9:H:38:LEU:HD12	9:H:39:THR:N	2.29	0.47
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.97	0.47
3:N:9:DC:H1'	3:N:10:DA:H5'	1.96	0.47
4:A:120:GLU:HA	4:A:123:ARG:HG2	1.96	0.47
4:A:406:ILE:HD13	4:A:412:ARG:HG3	1.96	0.47
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.15	0.47
4:A:1140:HIS:HB2	4:A:1276:VAL:O	2.14	0.47
5:B:416:LEU:O	5:B:420:LEU:HG	2.14	0.47
2:T:21:DC:H2'	2:T:22:DT:O4'	2.15	0.47
4:A:569:LYS:NZ	6:C:221:TYR:O	2.46	0.47
4:A:806:ARG:NH1	5:B:725:PRO:O	2.40	0.47
4:A:1100:ARG:O	4:A:1104:ILE:HG13	2.14	0.47
4:A:1287:TYR:O	4:A:1302:PRO:HA	2.15	0.47
5:B:35:SER:HA	5:B:811:TYR:CE2	2.50	0.47
7:E:31:THR:CG2	7:E:33:GLU:HG3	2.44	0.47
7:E:147:HIS:CE1	7:E:149:LEU:HG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:177:ARG:HG2	7:E:215:MET:HG3	1.96	0.47
4:A:451:HIS:HB3	4:A:453:MET:H	1.80	0.47
4:A:595:THR:CG2	4:A:603:ASN:HB2	2.45	0.47
6:C:32:SER:O	6:C:36:VAL:HG23	2.14	0.47
4:A:244:PRO:HA	4:A:247:ARG:CG	2.45	0.46
4:A:1258:HIS:HA	4:A:1261:LYS:NZ	2.30	0.46
6:C:101:LEU:HB2	6:C:118:LEU:HD23	1.97	0.46
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.97	0.46
8:F:97:ARG:HH21	8:F:101:ILE:HD11	1.80	0.46
4:A:1073:GLY:O	4:A:1077:THR:HG23	2.14	0.46
4:A:1167:GLU:OE2	4:A:1170:ILE:HD11	2.15	0.46
5:B:114:PRO:HG2	5:B:181:LEU:HD11	1.97	0.46
4:A:153:PRO:HA	4:A:161:LEU:HB2	1.97	0.46
4:A:209:ASN:HA	4:A:212:LYS:HG3	1.98	0.46
4:A:265:LYS:HG3	4:A:303:TYR:HB2	1.97	0.46
4:A:524:VAL:HG12	4:A:525:GLN:N	2.23	0.46
4:A:556:TRP:O	12:K:26:LYS:NZ	2.48	0.46
4:A:738:LYS:NZ	6:C:194:GLU:O	2.37	0.46
4:A:1221:LYS:O	4:A:1223:ASP:N	2.49	0.46
10:I:5:ARG:NH2	10:I:36:GLU:OE2	2.46	0.46
13:L:43:THR:HG22	13:L:43:THR:O	2.15	0.46
4:A:856:THR:HB	4:A:865:GLN:HB2	1.97	0.46
5:B:257:LYS:HE2	5:B:272:THR:CG2	2.45	0.46
5:B:997:GLU:HG2	6:C:39:ALA:HB2	1.97	0.46
7:E:64:PRO:CG	7:E:76:GLY:HA2	2.46	0.46
4:A:550:LEU:HD12	4:A:577:ILE:CD1	2.46	0.46
5:B:63:ILE:HG13	5:B:95:ILE:HD12	1.98	0.46
6:C:33:LEU:O	6:C:37:MET:HG3	2.15	0.46
12:K:51:LEU:CD1	12:K:59:ALA:HB3	2.45	0.46
4:A:682:THR:O	4:A:685:GLU:HG2	2.15	0.46
4:A:1217:LYS:HZ2	4:A:1217:LYS:HG3	1.48	0.46
5:B:566:LEU:HD11	5:B:586:TRP:CE2	2.50	0.46
6:C:7:GLN:HB2	6:C:23:SER:HB2	1.97	0.46
7:E:9:ILE:HD13	7:E:53:PRO:HG3	1.98	0.46
9:H:47:PHE:CZ	9:H:146:ARG:HD2	2.51	0.46
4:A:356:ASP:CB	4:A:359:LEU:HD12	2.44	0.46
4:A:830:LYS:O	4:A:834:THR:HG23	2.16	0.46
4:A:1258:HIS:HA	4:A:1261:LYS:HZ3	1.81	0.46
7:E:108:GLY:O	7:E:132:ILE:HA	2.15	0.46
4:A:11:LEU:HD12	5:B:1193:GLN:O	2.15	0.46
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1364:ASN:OD1	4:A:1366:ARG:HG2	2.16	0.46
6:C:248:ILE:HG21	12:K:102:LYS:HB2	1.97	0.46
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.97	0.46
4:A:596:THR:HB	4:A:599:SER:H	1.80	0.46
4:A:618:GLU:OE2	4:A:620:LYS:HB2	2.15	0.46
4:A:806:ARG:NH2	5:B:729:ILE:HD11	2.31	0.46
4:A:1224:LEU:HG	4:A:1241:ARG:O	2.16	0.46
5:B:824:ILE:HD13	11:J:48:ARG:NH1	2.31	0.46
7:E:127:ILE:CG2	7:E:130:ALA:HB3	2.46	0.46
10:I:4:PHE:HD1	10:I:4:PHE:HA	1.54	0.46
11:J:1:MET:HB2	11:J:57:ILE:HG23	1.97	0.46
4:A:570:PRO:O	4:A:571:LEU:HD23	2.16	0.46
4:A:1402:PHE:CD2	4:A:1403:GLU:HB2	2.51	0.46
5:B:117:ALA:HA	5:B:122:LEU:HB2	1.98	0.46
7:E:61:GLN:HA	7:E:79:TRP:HD1	1.81	0.46
8:F:86:THR:OG1	8:F:89:GLU:HG2	2.16	0.46
4:A:944:ARG:HG2	4:A:1298:TYR:OH	2.15	0.45
4:A:1267:MET:O	4:A:1271:ILE:HG13	2.17	0.45
5:B:987:LYS:H	5:B:987:LYS:HG2	1.36	0.45
5:B:1001:PHE:CZ	5:B:1073:TYR:HB2	2.50	0.45
6:C:256:ALA:O	6:C:260:LEU:HG	2.15	0.45
4:A:100:LYS:HZ2	4:A:174:ILE:HB	1.80	0.45
4:A:123:ARG:HA	4:A:126:LEU:HD13	1.98	0.45
4:A:666:ILE:HD11	5:B:1030:LEU:HD13	1.98	0.45
4:A:793:SER:HB3	4:A:796:SER:HB3	1.97	0.45
4:A:1107:VAL:O	4:A:1107:VAL:HG23	2.16	0.45
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.98	0.45
5:B:1163:CYS:HB3	5:B:1166:CYS:O	2.15	0.45
9:H:56:THR:O	9:H:144:ILE:HA	2.16	0.45
9:H:108:SER:HB2	9:H:111:LEU:HB2	1.98	0.45
10:I:15:TYR:HD2	10:I:30:ARG:CZ	2.30	0.45
4:A:122:MET:HE3	4:A:126:LEU:HD11	1.97	0.45
4:A:778:GLY:HA3	5:B:516:ASN:HB2	1.97	0.45
4:A:1196:GLU:C	4:A:1197:LEU:HD23	2.36	0.45
5:B:94:LYS:HD3	5:B:96:TYR:CE2	2.52	0.45
5:B:103:ASN:CG	5:B:109:THR:HG22	2.37	0.45
5:B:268:THR:OG1	5:B:270:LYS:NZ	2.49	0.45
5:B:1213:THR:HG21	5:B:1215:ARG:HH22	1.80	0.45
8:F:82:THR:HG22	8:F:84:TYR:H	1.82	0.45
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.51	0.45
12:K:61:TYR:HA	12:K:72:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:436:ILE:HD11	4:A:491:VAL:HG11	1.97	0.45
4:A:873:MET:HG3	4:A:957:PRO:CG	2.47	0.45
4:A:1199:ARG:HE	4:A:1236:LEU:HD21	1.82	0.45
6:C:51:VAL:HG13	13:L:60:ARG:HH22	1.81	0.45
4:A:80:HIS:O	4:A:243:PRO:HB3	2.16	0.45
4:A:351:THR:HB	5:B:1103:ILE:HA	1.99	0.45
4:A:406:ILE:CD1	4:A:412:ARG:HG3	2.46	0.45
4:A:1195:LEU:HD11	4:A:1267:MET:CE	2.45	0.45
5:B:837:ASP:O	5:B:988:GLY:HA3	2.16	0.45
5:B:1174:LYS:NZ	5:B:1179:GLN:OE1	2.49	0.45
9:H:96:VAL:HG23	9:H:142:LEU:O	2.16	0.45
11:J:45:CYS:O	11:J:48:ARG:HG2	2.17	0.45
2:T:19:DG:O4'	4:A:835:GLY:HA3	2.16	0.45
4:A:104:GLU:CB	4:A:139:TRP:HE1	2.29	0.45
4:A:1217:LYS:NZ	4:A:1222:ASN:H	2.15	0.45
7:E:12:LEU:HD12	7:E:42:PHE:HZ	1.80	0.45
4:A:104:GLU:HA	4:A:174:ILE:HD12	1.98	0.45
4:A:446:ARG:HD3	4:A:478:TYR:O	2.17	0.45
4:A:473:SER:O	4:A:521:MET:HB3	2.17	0.45
4:A:1399:ARG:HB3	4:A:1408:ILE:HG21	1.99	0.45
5:B:31:TRP:CZ3	5:B:34:ILE:HD12	2.51	0.45
5:B:35:SER:HA	5:B:811:TYR:HE2	1.82	0.45
5:B:764:SER:OG	5:B:765:PRO:HD3	2.16	0.45
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.52	0.45
7:E:91:LYS:HA	7:E:94:LYS:CB	2.46	0.45
9:H:112:ILE:HG13	9:H:113:ALA:N	2.31	0.45
11:J:57:ILE:HD12	11:J:58:GLU:N	2.32	0.45
4:A:24:PRO:HG3	4:A:237:THR:CG2	2.41	0.45
4:A:687:LYS:O	4:A:690:VAL:HG22	2.17	0.45
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.98	0.45
5:B:908:GLU:OE1	5:B:943:SER:HB3	2.17	0.45
5:B:1164:GLY:HA3	5:B:1190:ASP:CG	2.37	0.45
6:C:70:ILE:HD11	6:C:144:ILE:HG12	1.99	0.45
9:H:24:CYS:HB2	9:H:44:VAL:HG23	1.97	0.45
4:A:12:ARG:HD2	5:B:1218:THR:HG21	1.99	0.45
4:A:91:PHE:HB3	4:A:96:ILE:HD11	1.99	0.45
12:K:63:VAL:HG13	12:K:70:ARG:O	2.17	0.45
4:A:243:PRO:C	4:A:247:ARG:HD3	2.36	0.45
4:A:963:ILE:HD13	4:A:1048:ASN:HB3	1.98	0.45
5:B:1171:VAL:HG21	5:B:1191:ILE:HD12	1.98	0.45
6:C:26:ASP:OD1	6:C:26:ASP:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:72:PHE:HE2	7:E:157:SER:HA	1.82	0.45
7:E:122:LYS:O	7:E:122:LYS:HD3	2.16	0.45
10:I:15:TYR:CD2	10:I:30:ARG:CZ	3.00	0.45
12:K:12:LEU:HD12	12:K:12:LEU:H	1.81	0.45
4:A:130:ASP:CG	4:A:133:LYS:HG3	2.38	0.44
4:A:1387:HIS:HA	4:A:1391:ARG:HD2	1.99	0.44
5:B:882:THR:CG2	5:B:934:LYS:CE	2.74	0.44
7:E:37:LEU:HD23	7:E:38:PRO:O	2.17	0.44
7:E:113:GLN:OE1	7:E:113:GLN:HA	2.17	0.44
13:L:49:LYS:HB3	13:L:49:LYS:HE2	1.72	0.44
9:H:30:SER:HB2	9:H:33:GLN:O	2.17	0.44
9:H:114:VAL:HG22	9:H:115:TYR:H	1.82	0.44
10:I:70:ARG:HG3	10:I:70:ARG:HH11	1.82	0.44
2:T:19:DG:O5'	2:T:19:DG:H8	1.98	0.44
4:A:42:ASP:OD2	4:A:46:THR:HB	2.17	0.44
4:A:658:LEU:CD2	5:B:1074:ASN:HD21	2.29	0.44
4:A:1215:ARG:HE	4:A:1215:ARG:HA	1.82	0.44
4:A:1390:ASN:HD22	4:A:1399:ARG:CG	2.30	0.44
7:E:31:THR:HG21	7:E:33:GLU:HG3	1.98	0.44
12:K:108:GLU:HA	12:K:111:LEU:HD13	1.98	0.44
3:N:4:DA:H1'	3:N:5:DT:C6	2.52	0.44
5:B:210:LYS:HZ2	5:B:482:VAL:HG22	1.82	0.44
5:B:308:TRP:CH2	10:I:45:ARG:HG2	2.52	0.44
13:L:60:ARG:HG2	13:L:61:THR:N	2.33	0.44
3:N:11:DG:C6	3:N:12:DA:N6	2.85	0.44
4:A:1161:THR:HG22	4:A:1170:ILE:HG12	2.00	0.44
5:B:1174:LYS:HD2	5:B:1177:HIS:CG	2.52	0.44
4:A:445:ASN:OD1	4:A:446:ARG:N	2.50	0.44
4:A:683:ILE:HD13	4:A:683:ILE:HA	1.87	0.44
5:B:643:ASP:HB2	5:B:648:HIS:O	2.17	0.44
6:C:58:LEU:HD21	11:J:57:ILE:HG21	1.98	0.44
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.99	0.44
5:B:512:ARG:NH2	5:B:532:ALA:H	2.15	0.44
5:B:906:SER:OG	5:B:907:GLY:N	2.50	0.44
6:C:97:VAL:HG11	6:C:129:ILE:HG22	1.99	0.44
7:E:45:LYS:HB3	7:E:46:TYR:CD1	2.53	0.44
7:E:137:GLU:O	7:E:141:VAL:HG23	2.18	0.44
1:R:6:G:H2'	1:R:7:A:O4'	2.18	0.44
4:A:31:SER:HG	4:A:83:HIS:CG	2.30	0.44
4:A:451:HIS:HB3	4:A:453:MET:N	2.33	0.44
4:A:901:LEU:HD23	4:A:907:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:65:GLU:OE1	5:B:247:GLY:HA2	2.17	0.44
5:B:325:GLN:O	5:B:325:GLN:HG3	2.17	0.44
5:B:1166:CYS:O	5:B:1168:LEU:N	2.46	0.44
6:C:17:ASN:HB3	6:C:233:GLU:CG	2.48	0.44
11:J:1:MET:O	11:J:57:ILE:HG13	2.18	0.44
5:B:622:LYS:NZ	10:I:59:VAL:HG11	2.33	0.44
5:B:890:TYR:OH	5:B:936:ASP:OD2	2.34	0.44
7:E:56:LYS:HZ3	7:E:84:ASP:HB2	1.80	0.44
4:A:86:LEU:HD12	4:A:238:CYS:CA	2.41	0.43
4:A:315:LEU:HA	4:A:321:PRO:HA	1.99	0.43
4:A:884:ASP:HB3	4:A:896:ARG:HH12	1.83	0.43
4:A:1215:ARG:CZ	4:A:1218:GLN:OE1	2.66	0.43
5:B:308:TRP:HH2	10:I:47:GLU:HG3	1.82	0.43
5:B:1000:PRO:HB2	5:B:1072:MET:CE	2.32	0.43
7:E:101:GLN:O	7:E:101:GLN:NE2	2.28	0.43
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.99	0.43
4:A:265:LYS:HD3	4:A:265:LYS:HA	1.74	0.43
4:A:470:LEU:HD21	4:A:487:MET:HE3	2.00	0.43
4:A:635:ARG:NH1	4:A:877:HIS:HB3	2.33	0.43
4:A:979:SER:OG	4:A:980:ASP:N	2.49	0.43
4:A:1300:LYS:HD3	4:A:1300:LYS:N	2.17	0.43
4:A:1390:ASN:OD1	4:A:1402:PHE:HB3	2.18	0.43
6:C:137:LYS:H	6:C:137:LYS:HD2	1.82	0.43
6:C:214:ASN:HB2	6:C:217:ASP:OD2	2.18	0.43
7:E:37:LEU:CD2	7:E:42:PHE:HB2	2.48	0.43
9:H:137:GLN:HG2	9:H:139:ASN:H	1.82	0.43
4:A:761:MET:CG	5:B:1021:MET:HG2	2.48	0.43
5:B:102:VAL:O	5:B:109:THR:HA	2.18	0.43
5:B:234:ILE:HD11	5:B:257:LYS:CB	2.44	0.43
5:B:1194:ILE:CD1	5:B:1196:ILE:CG2	2.92	0.43
9:H:12:VAL:HG21	9:H:50:ALA:O	2.18	0.43
11:J:5:VAL:HG12	11:J:6:ARG:HG2	2.00	0.43
4:A:36:ARG:NE	4:A:274:ILE:HD12	2.33	0.43
4:A:357:PRO:HD2	5:B:833:TYR:CZ	2.52	0.43
4:A:567:LYS:HG2	9:H:94:ASP:O	2.18	0.43
5:B:1165:ILE:HD11	5:B:1185:CYS:SG	2.59	0.43
7:E:127:ILE:HG13	7:E:130:ALA:H	1.84	0.43
7:E:147:HIS:HE1	7:E:149:LEU:HG	1.82	0.43
8:F:123:LYS:HD3	8:F:123:LYS:HA	1.86	0.43
12:K:53:ASP:O	12:K:56:VAL:HG12	2.17	0.43
4:A:437:MET:HB2	4:A:437:MET:HE3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1017:LEU:HD23	4:A:1017:LEU:HA	1.86	0.43
5:B:276:ILE:CG1	5:B:335:GLY:H	2.31	0.43
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.82	0.43
5:B:1135:ARG:O	5:B:1139:ILE:HG12	2.17	0.43
5:B:1204:PHE:O	5:B:1208:MET:HG3	2.17	0.43
6:C:222:LYS:HD3	6:C:222:LYS:HA	1.74	0.43
8:F:69:LEU:HB3	8:F:70:LYS:H	1.62	0.43
9:H:38:LEU:HB2	9:H:125:LEU:CD1	2.47	0.43
4:A:176:LYS:HD2	4:A:176:LYS:C	2.39	0.43
4:A:229:SER:OG	4:A:1414:ALA:O	2.22	0.43
4:A:563:PRO:HB3	4:A:572:TRP:CE2	2.54	0.43
5:B:957:ASN:CG	5:B:958:GLN:N	2.72	0.43
5:B:1213:THR:O	5:B:1213:THR:HG23	2.19	0.43
9:H:104:PHE:HZ	9:H:136:LYS:HA	1.84	0.43
9:H:107:VAL:CG2	9:H:111:LEU:HB3	2.34	0.43
3:N:15:DG:O5'	3:N:15:DG:H8	2.02	0.43
4:A:960:ILE:HG23	4:A:964:ILE:HD13	2.01	0.43
9:H:103:LYS:HB3	9:H:115:TYR:CD1	2.54	0.43
4:A:481:ASP:O	4:A:485:ASP:HB2	2.19	0.43
4:A:1352:VAL:O	4:A:1355:VAL:HG12	2.19	0.43
5:B:680:THR:N	5:B:683:SER:OG	2.51	0.43
9:H:26:ILE:CD1	9:H:40:LEU:HB3	2.41	0.43
4:A:40:THR:HG23	4:A:41:MET:N	2.34	0.43
4:A:1327:ILE:HD12	4:A:1327:ILE:HA	1.74	0.43
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.52	0.43
9:H:22:LYS:HD3	9:H:45:GLU:OE1	2.19	0.43
11:J:13:VAL:O	11:J:17:LYS:NZ	2.52	0.43
13:L:31:CYS:HA	13:L:56:LEU:HD23	2.00	0.43
4:A:42:ASP:CG	4:A:46:THR:HB	2.39	0.43
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.49	0.43
4:A:567:LYS:HB2	9:H:96:VAL:H	1.84	0.43
4:A:684:ALA:O	4:A:688:LYS:HD3	2.19	0.43
4:A:916:GLY:O	4:A:919:ILE:HG22	2.19	0.43
4:A:1420:ASP:CG	4:A:1422:ARG:HG3	2.38	0.43
5:B:468:GLU:O	5:B:468:GLU:HG3	2.18	0.43
5:B:528:PRO:HD2	5:B:536:VAL:HB	2.01	0.43
6:C:59:ALA:O	6:C:63:ILE:HG13	2.19	0.43
4:A:113:LEU:CD1	4:A:218:ASP:HB3	2.49	0.42
5:B:175:ARG:HG3	5:B:200:GLY:HA3	2.00	0.42
6:C:46:ILE:HG23	6:C:157:CYS:HB3	2.01	0.42
11:J:57:ILE:HA	11:J:60:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:50:LEU:CD2	12:K:90:ALA:HB2	2.49	0.42
4:A:1384:VAL:HA	4:A:1389:PHE:HD2	1.84	0.42
5:B:299:GLU:HG3	5:B:571:PRO:HG2	2.01	0.42
5:B:378:LEU:O	5:B:382:ILE:HG13	2.19	0.42
5:B:705:MET:CE	5:B:745:PRO:HB3	2.49	0.42
6:C:80:LEU:HD21	6:C:95:CYS:C	2.40	0.42
6:C:177:GLU:O	6:C:230:MET:HA	2.19	0.42
13:L:65:VAL:HG23	13:L:65:VAL:O	2.18	0.42
1:R:3:C:H2'	1:R:4:G:O4'	2.20	0.42
2:T:20:DC:H6	2:T:20:DC:OP2	2.01	0.42
3:N:12:DA:H4'	3:N:13:DG:OP2	2.18	0.42
4:A:173:THR:O	4:A:183:GLY:HA2	2.19	0.42
5:B:766:ARG:NH2	5:B:1020:ARG:HD2	2.34	0.42
5:B:871:THR:HG23	5:B:872:GLU:O	2.19	0.42
5:B:904:ARG:NH1	13:L:66:GLN:O	2.53	0.42
5:B:1082:MET:HE3	5:B:1082:MET:HB3	1.89	0.42
5:B:129:PHE:HA	5:B:165:VAL:O	2.18	0.42
5:B:357:GLN:HE21	5:B:368:GLU:HA	1.84	0.42
6:C:145:CYS:SG	6:C:146:LYS:N	2.92	0.42
4:A:767:GLN:NE2	4:A:774:ARG:HG2	2.34	0.42
5:B:195:CYS:HB3	5:B:782:LEU:HD22	2.02	0.42
5:B:997:GLU:CG	6:C:39:ALA:HB2	2.50	0.42
6:C:263:THR:O	6:C:266:ASP:HB2	2.19	0.42
4:A:111:GLY:O	4:A:214:ILE:HG23	2.19	0.42
4:A:209:ASN:OD1	4:A:212:LYS:NZ	2.45	0.42
4:A:741:ASN:OD1	4:A:743:VAL:HG22	2.19	0.42
4:A:964:ILE:O	4:A:968:GLN:HG3	2.19	0.42
4:A:1443:VAL:CG1	8:F:132:LEU:HD22	2.49	0.42
7:E:161:LYS:NZ	7:E:172:GLU:OE2	2.44	0.42
8:F:76:LYS:HG3	8:F:79:ARG:CZ	2.49	0.42
13:L:61:THR:HB	13:L:63:ARG:H	1.84	0.42
5:B:272:THR:O	5:B:273:LEU:HD23	2.20	0.42
5:B:417:PHE:HA	5:B:420:LEU:HD11	2.01	0.42
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.20	0.42
6:C:166:GLU:HG3	12:K:10:PHE:HZ	1.84	0.42
8:F:103:MET:O	8:F:105:ALA:N	2.51	0.42
2:T:8:DT:C2'	2:T:9:DC:H5'	2.50	0.42
2:T:27:DA:H8	2:T:27:DA:H5''	1.85	0.42
3:N:7:DA:H2''	3:N:8:DC:C6	2.54	0.42
3:N:8:DC:H2''	3:N:9:DC:C6	2.54	0.42
4:A:266:LEU:HD12	4:A:266:LEU:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:778:MET:O	5:B:796:LEU:HD13	2.18	0.42
7:E:60:PHE:C	7:E:79:TRP:HD1	2.21	0.42
12:K:50:LEU:HD23	12:K:90:ALA:HB2	2.02	0.42
4:A:374:LEU:O	4:A:436:ILE:HD13	2.19	0.42
4:A:549:MET:CE	4:A:656:TRP:HD1	2.33	0.42
4:A:882:SER:HA	4:A:953:ASN:HA	2.02	0.42
4:A:1140:HIS:NE2	4:A:1272:THR:HG22	2.34	0.42
4:A:1322:ILE:O	4:A:1324:PRO:HD3	2.20	0.42
5:B:255:GLN:HB2	5:B:272:THR:OG1	2.20	0.42
5:B:616:ILE:HG13	5:B:625:LYS:HB2	2.02	0.42
5:B:651:LEU:HD23	5:B:651:LEU:H	1.85	0.42
5:B:779:GLY:HA2	5:B:796:LEU:CD1	2.46	0.42
5:B:863:GLU:O	5:B:961:LEU:HD22	2.19	0.42
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.55	0.42
7:E:41:ASP:N	7:E:41:ASP:OD1	2.53	0.42
7:E:144:ILE:HG13	7:E:145:THR:N	2.35	0.42
10:I:4:PHE:CE2	10:I:13:MET:SD	3.13	0.42
11:J:18:TRP:O	11:J:21:TYR:HB3	2.20	0.42
4:A:4:GLN:OE1	5:B:1159:ARG:HD2	2.20	0.41
4:A:605:MET:HE3	4:A:621:THR:HG21	2.02	0.41
5:B:779:GLY:CA	5:B:796:LEU:HD13	2.49	0.41
5:B:832:GLY:O	5:B:835:GLN:HG3	2.19	0.41
9:H:58:THR:O	9:H:142:LEU:HA	2.20	0.41
9:H:99:GLY:HA2	9:H:118:PHE:HA	2.02	0.41
9:H:123:MET:HE1	9:H:142:LEU:CD1	2.50	0.41
4:A:172:PRO:HB3	4:A:185:TRP:CG	2.55	0.41
4:A:404:TYR:HB2	4:A:433:GLU:HG3	2.02	0.41
4:A:494:SER:OG	5:B:1149:GLU:OE2	2.38	0.41
4:A:678:GLU:O	4:A:681:GLU:HG2	2.21	0.41
5:B:221:ASN:O	5:B:222:ILE:HD13	2.20	0.41
5:B:467:GLY:HA3	5:B:474:SER:OG	2.20	0.41
5:B:878:GLN:HB2	5:B:881:ASN:HB3	2.02	0.41
6:C:20:PHE:CE1	6:C:22:LEU:HD21	2.55	0.41
7:E:124:VAL:CG1	7:E:132:ILE:HD12	2.51	0.41
7:E:127:ILE:CD1	7:E:129:PRO:HD2	2.49	0.41
9:H:97:MET:HE3	9:H:118:PHE:CG	2.55	0.41
1:R:5:A:H2'	1:R:6:G:C8	2.55	0.41
2:T:5:DC:H2''	2:T:6:DT:C6	2.55	0.41
3:N:14:DA:H2''	3:N:15:DG:C8	2.55	0.41
4:A:91:PHE:HB2	4:A:297:GLN:NE2	2.35	0.41
4:A:204:THR:CG2	4:A:235:ILE:HD12	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:218:ASP:O	4:A:222:LEU:HB2	2.19	0.41
4:A:1030:ARG:HA	4:A:1034:GLU:HG3	2.02	0.41
4:A:1072:ILE:HD11	4:A:1368:MET:HA	2.03	0.41
4:A:1408:ILE:HG12	4:A:1408:ILE:H	1.73	0.41
5:B:255:GLN:H	5:B:272:THR:HG1	1.65	0.41
5:B:861:ASP:OD1	5:B:862:GLN:N	2.49	0.41
6:C:67:LEU:HA	6:C:70:ILE:HD12	2.02	0.41
9:H:103:LYS:HD3	9:H:103:LYS:HA	1.75	0.41
4:A:69:THR:HB	5:B:1172:ILE:CG2	2.50	0.41
4:A:269:ILE:HG13	4:A:299:HIS:HB3	2.01	0.41
5:B:778:MET:C	5:B:796:LEU:HD11	2.38	0.41
5:B:844:SER:O	5:B:847:ASP:HB2	2.21	0.41
9:H:91:ASP:CB	9:H:143:LEU:HD23	2.51	0.41
9:H:118:PHE:N	9:H:118:PHE:CD1	2.88	0.41
9:H:142:LEU:HD21	9:H:144:ILE:CD1	2.51	0.41
10:I:101:PHE:O	10:I:109:ILE:HA	2.20	0.41
2:T:16:DT:H2'	2:T:17:DG:N9	2.36	0.41
4:A:526:ASP:HB2	5:B:835:GLN:CD	2.40	0.41
4:A:956:LEU:HA	4:A:957:PRO:HD3	1.77	0.41
5:B:283:VAL:CG2	5:B:321:GLY:HA3	2.51	0.41
5:B:408:LEU:HD23	5:B:408:LEU:HA	1.88	0.41
5:B:782:LEU:HB3	5:B:784:ASN:OD1	2.20	0.41
6:C:262:LEU:HD23	6:C:262:LEU:HA	1.89	0.41
7:E:82:PHE:HA	7:E:111:VAL:HG13	2.01	0.41
4:A:767:GLN:HB2	4:A:799:PHE:HD1	1.86	0.41
4:A:890:ASP:OD1	4:A:1296:GLY:HA3	2.20	0.41
4:A:1004:ASN:ND2	4:A:1007:ILE:HD12	2.31	0.41
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.51	0.41
4:A:1106:ASN:O	4:A:1107:VAL:C	2.59	0.41
4:A:1436:ILE:HG22	4:A:1437:GLY:N	2.35	0.41
5:B:879:ARG:HA	5:B:885:MET:HE2	2.02	0.41
6:C:146:LYS:HE3	11:J:57:ILE:CD1	2.48	0.41
7:E:55:ARG:NH2	7:E:113:GLN:HE21	2.08	0.41
7:E:175:LEU:HD12	7:E:176:PRO:CD	2.48	0.41
4:A:567:LYS:CB	9:H:96:VAL:H	2.33	0.41
4:A:1118:VAL:HA	4:A:1327:ILE:CD1	2.51	0.41
4:A:1390:ASN:OD1	4:A:1402:PHE:HD2	2.03	0.41
5:B:386:LEU:O	5:B:390:LEU:HG	2.20	0.41
5:B:387:LEU:HD23	5:B:392:ARG:HD2	2.02	0.41
5:B:570:VAL:HG23	5:B:573:GLN:HB3	2.03	0.41
6:C:80:LEU:HD23	6:C:81:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:97:ARG:HD2	8:F:97:ARG:HA	1.91	0.41
4:A:29:ALA:HB1	5:B:1184:GLY:HA3	2.01	0.41
4:A:528:LEU:O	4:A:531:ILE:HG22	2.20	0.41
4:A:1154:TYR:CE1	10:I:18:GLU:HG3	2.56	0.41
4:A:1425:SER:O	4:A:1429:ILE:HG13	2.21	0.41
5:B:43:LEU:HD11	5:B:811:TYR:O	2.20	0.41
5:B:50:SER:OG	5:B:410:GLY:N	2.42	0.41
5:B:358:LYS:HE2	5:B:359:GLU:OE1	2.20	0.41
5:B:576:ASP:OD1	5:B:576:ASP:N	2.43	0.41
5:B:835:GLN:HE21	5:B:835:GLN:HB3	1.57	0.41
8:F:97:ARG:O	8:F:101:ILE:HD12	2.20	0.41
8:F:116:ASP:O	8:F:120:ILE:HD13	2.20	0.41
9:H:112:ILE:HG22	9:H:127:GLY:O	2.21	0.41
3:N:9:DC:OP1	3:N:9:DC:H4'	2.21	0.41
4:A:290:GLU:O	4:A:294:SER:HB3	2.20	0.41
4:A:483:ASP:HA	5:B:988:GLY:HA2	2.02	0.41
4:A:560:ILE:CG2	9:H:79:TRP:HB3	2.51	0.41
5:B:210:LYS:NZ	5:B:482:VAL:HG22	2.35	0.41
5:B:404:LYS:O	5:B:405:ARG:HD2	2.20	0.41
5:B:420:LEU:HD12	5:B:421:PHE:N	2.36	0.41
5:B:565:PRO:HB2	5:B:567:GLU:OE2	2.20	0.41
5:B:705:MET:HE2	5:B:745:PRO:HB3	2.03	0.41
5:B:884:ARG:NH1	5:B:884:ARG:HG3	2.36	0.41
5:B:1202:LEU:HD23	5:B:1202:LEU:HA	1.85	0.41
9:H:114:VAL:HG22	9:H:115:TYR:N	2.36	0.41
9:H:139:ASN:N	9:H:139:ASN:ND2	2.69	0.41
10:I:68:LEU:HD13	10:I:84:VAL:HG11	2.03	0.41
4:A:305:ASP:CG	4:A:326:ARG:HD3	2.41	0.41
4:A:368:LYS:O	4:A:372:LYS:HG3	2.20	0.41
4:A:925:LEU:HD23	4:A:925:LEU:HA	1.83	0.41
4:A:1436:ILE:HG22	5:B:1142:GLY:HA2	2.03	0.41
5:B:164:LYS:H	5:B:164:LYS:HG3	1.71	0.41
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.36	0.41
7:E:153:HIS:HB3	7:E:196:VAL:CG2	2.47	0.41
10:I:4:PHE:CD1	10:I:5:ARG:N	2.89	0.41
4:A:376:TYR:CZ	4:A:498:ARG:HD2	2.57	0.40
5:B:345:LYS:O	5:B:348:ARG:HB2	2.21	0.40
6:C:69:LEU:HD13	6:C:69:LEU:HA	1.93	0.40
6:C:92:CYS:SG	6:C:94:LYS:HG3	2.61	0.40
9:H:46:LEU:HD23	9:H:46:LEU:HA	1.80	0.40
4:A:1215:ARG:NE	4:A:1218:GLN:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:276:ILE:HA	5:B:276:ILE:HD12	1.75	0.40
7:E:37:LEU:HD21	7:E:42:PHE:N	2.35	0.40
9:H:137:GLN:HG2	9:H:139:ASN:CB	2.51	0.40
9:H:137:GLN:HG2	9:H:139:ASN:CG	2.42	0.40
1:R:5:A:H2'	1:R:6:G:H8	1.86	0.40
4:A:335:ARG:HH11	4:A:339:ASN:HD22	1.68	0.40
4:A:353:ILE:HG22	4:A:468:PHE:HB2	2.04	0.40
4:A:714:PHE:O	4:A:718:VAL:HG23	2.22	0.40
4:A:839:ARG:NH2	4:A:1402:PHE:HA	2.35	0.40
4:A:849:MET:HE3	4:A:849:MET:HB3	1.76	0.40
5:B:405:ARG:HH21	5:B:629:ASP:CB	2.34	0.40
5:B:876:LYS:NZ	5:B:891:ASP:HA	2.36	0.40
12:K:91:CYS:O	12:K:95:ILE:HG13	2.21	0.40
4:A:111:GLY:HA3	4:A:213:HIS:O	2.22	0.40
4:A:1393:ASN:OD1	4:A:1393:ASN:N	2.45	0.40
4:A:1409:LEU:HD23	5:B:1207:LEU:HD21	2.03	0.40
7:E:94:LYS:O	7:E:98:ILE:HD12	2.21	0.40
9:H:55:LEU:HB3	9:H:144:ILE:HG23	2.03	0.40
14:T:101:5N0:N23	3:N:11:DG:H1'	2.36	0.40
4:A:108:MET:HA	4:A:210:ILE:HD13	2.04	0.40
4:A:270:LEU:C	4:A:270:LEU:HD23	2.42	0.40
4:A:1101:LEU:O	4:A:1105:LEU:HD12	2.22	0.40
5:B:44:VAL:HG11	5:B:495:LEU:HD13	2.04	0.40
5:B:63:ILE:HD13	5:B:63:ILE:HA	1.89	0.40
7:E:31:THR:O	7:E:35:VAL:HG13	2.21	0.40
7:E:112:TYR:HE2	7:E:134:THR:OG1	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:419:LYS:NZ	6:C:90:ASP:O[2_555]	2.14	0.06

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	
4	A	1370/1733 (79%)	1299 (95%)	68 (5%)	3 (0%)	47	78
5	B	1111/1224 (91%)	1068 (96%)	43 (4%)	0	100	100
6	C	265/318 (83%)	256 (97%)	7 (3%)	2 (1%)	19	51
7	E	210/215 (98%)	201 (96%)	9 (4%)	0	100	100
8	F	84/155 (54%)	79 (94%)	5 (6%)	0	100	100
9	H	129/146 (88%)	118 (92%)	11 (8%)	0	100	100
10	I	116/122 (95%)	111 (96%)	5 (4%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3501/4173 (84%)	3343 (96%)	153 (4%)	5 (0%)	51	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
6	C	173	ALA
6	C	174	ALA
4	A	1107	VAL
4	A	567	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1194/1520 (79%)	1137 (95%)	57 (5%)	25	58
5	B	958/1061 (90%)	925 (97%)	33 (3%)	37	71
6	C	235/274 (86%)	225 (96%)	10 (4%)	29	62
7	E	193/197 (98%)	180 (93%)	13 (7%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	73/137 (53%)	69 (94%)	4 (6%)	21	53
9	H	116/128 (91%)	110 (95%)	6 (5%)	23	55
10	I	110/116 (95%)	103 (94%)	7 (6%)	17	45
11	J	60/65 (92%)	56 (93%)	4 (7%)	16	43
12	K	99/102 (97%)	98 (99%)	1 (1%)	76	92
13	L	37/57 (65%)	34 (92%)	3 (8%)	11	33
All	All	3075/3657 (84%)	2937 (96%)	138 (4%)	27	61

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	6	TYR
4	A	22	PHE
4	A	42	ASP
4	A	43	GLU
4	A	74	MET
4	A	83	HIS
4	A	85	ASP
4	A	176	LYS
4	A	180	LYS
4	A	184	SER
4	A	185	TRP
4	A	203	SER
4	A	238	CYS
4	A	261	ASP
4	A	265	LYS
4	A	279	LEU
4	A	326	ARG
4	A	343	LYS
4	A	361	LEU
4	A	383	TYR
4	A	444	PHE
4	A	525	GLN
4	A	555	ASP
4	A	618	GLU
4	A	635	ARG
4	A	688	LYS
4	A	752	LYS
4	A	764	CYS
4	A	769	SER

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Mol	Chain	Res	Type
4	A	796	SER
4	A	816	HIS
4	A	821	ARG
4	A	830	LYS
4	A	847	ASP
4	A	849	MET
4	A	877	HIS
4	A	911	SER
4	A	941	LYS
4	A	975	HIS
4	A	1000	LEU
4	A	1025	ARG
4	A	1035	TYR
4	A	1062	GLU
4	A	1079	MET
4	A	1124	HIS
4	A	1167	GLU
4	A	1215	ARG
4	A	1224	LEU
4	A	1262	LYS
4	A	1289	ARG
4	A	1300	LYS
4	A	1366	ARG
4	A	1368	MET
4	A	1390	ASN
4	A	1398	MET
4	A	1418	LEU
4	A	1444	MET
5	B	69	LEU
5	B	103	ASN
5	B	106	ASP
5	B	164	LYS
5	B	215	GLN
5	B	217	ARG
5	B	261	ARG
5	B	277	LYS
5	B	347	LYS
5	B	394	ASP
5	B	401	PHE
5	B	404	LYS
5	B	483	LEU
5	B	489	SER

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Mol	Chain	Res	Type
5	B	493	SER
5	B	568	ASP
5	B	592	ASN
5	B	606	LYS
5	B	629	ASP
5	B	642	ASP
5	B	643	ASP
5	B	666	TYR
5	B	668	ASP
5	B	906	SER
5	B	934	LYS
5	B	963	PHE
5	B	996	ARG
5	B	999	MET
5	B	1089	PRO
5	B	1096	ARG
5	B	1122	ARG
5	B	1186	ASP
5	B	1210	MET
6	C	17	ASN
6	C	32	SER
6	C	34	ARG
6	C	116	LYS
6	C	137	LYS
6	C	140	ASN
6	C	148	ARG
6	C	187	LYS
6	C	188	HIS
6	C	254	LYS
7	E	10	SER
7	E	11	ARG
7	E	22	MET
7	E	29	PHE
7	E	33	GLU
7	E	52	ARG
7	E	66	GLU
7	E	72	PHE
7	E	83	CYS
7	E	84	ASP
7	E	122	LYS
7	E	177	ARG
7	E	214	CYS

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Mol	Chain	Res	Type
8	F	90	ARG
8	F	111	LEU
8	F	114	GLU
8	F	123	LYS
9	H	21	ASN
9	H	36	CYS
9	H	94	ASP
9	H	110	ASP
9	H	117	SER
9	H	124	ARG
10	I	4	PHE
10	I	7	CYS
10	I	8	ARG
10	I	13	MET
10	I	37	GLU
10	I	45	ARG
10	I	115	LYS
11	J	7	CYS
11	J	38	ARG
11	J	55	ASP
11	J	64	ASN
12	K	81	TYR
13	L	36	SER
13	L	48	CYS
13	L	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	287	HIS
4	A	311	GLN
4	A	339	ASN
4	A	659	HIS
4	A	660	ASN
4	A	854	ASN
4	A	877	HIS
5	B	224	GLN
5	B	357	GLN
5	B	433	GLN
5	B	513	GLN
5	B	531	GLN
5	B	587	HIS

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Mol	Chain	Res	Type
5	B	734	HIS
5	B	822	ASN
5	B	835	GLN
5	B	951	GLN
5	B	1177	HIS
7	E	174	GLN
8	F	104	ASN
9	H	139	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	9	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, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	5N0	T	101	-	91,107,107	2.55	28 (30%)	91,153,153	1.57	10 (10%)

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
14	5N0	T	101	-	-	13/47/92/92	0/9/9/9

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	101	5N0	C59-C63	7.28	1.54	1.47
14	T	101	5N0	C49-N23	6.65	1.48	1.33
14	T	101	5N0	C56-N25	6.18	1.47	1.33
14	T	101	5N0	C30-C31	6.02	1.58	1.53
14	T	101	5N0	C22-N10	5.95	1.46	1.33
14	T	101	5N0	C26-N14	5.74	1.48	1.35
14	T	101	5N0	C6-C10	5.12	1.57	1.53
14	T	101	5N0	C10-N6	4.89	1.48	1.35
14	T	101	5N0	C5-N3	4.62	1.48	1.35
14	T	101	5N0	C43-N21	4.54	1.47	1.35
14	T	101	5N0	C31-N17	4.39	1.47	1.35
14	T	101	5N0	C37-N19	4.38	1.47	1.35
14	T	101	5N0	C16-N8	4.25	1.47	1.35
14	T	101	5N0	C4-C5	3.82	1.56	1.53
14	T	101	5N0	C36-N17	3.73	1.49	1.41
14	T	101	5N0	C14-N6	3.72	1.49	1.41
14	T	101	5N0	C9-N3	3.56	1.48	1.40
14	T	101	5N0	C29-N14	3.55	1.48	1.40
14	T	101	5N0	C21-N8	3.48	1.48	1.41
14	T	101	5N0	C42-N19	3.38	1.48	1.41
14	T	101	5N0	C48-N21	3.26	1.48	1.41
14	T	101	5N0	C2-N1	-2.59	1.33	1.37
14	T	101	5N0	C57-C56	2.45	1.55	1.50
14	T	101	5N0	O5-C26	-2.13	1.19	1.23
14	T	101	5N0	O2-C10	-2.05	1.19	1.23
14	T	101	5N0	O6-C31	-2.05	1.19	1.23
14	T	101	5N0	O9-C49	-2.05	1.19	1.23
14	T	101	5N0	O8-C43	-2.05	1.19	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	101	5N0	C30-C31-N17	7.45	121.78	113.69
14	T	101	5N0	C6-C10-N6	6.59	120.85	113.69
14	T	101	5N0	C4-C5-N3	3.76	117.78	113.69
14	T	101	5N0	C29-N14-C26	-3.24	122.96	127.55
14	T	101	5N0	O3-C16-N8	-2.51	117.98	123.71
14	T	101	5N0	O6-C31-N17	-2.35	118.34	123.71
14	T	101	5N0	C19-N9-C17	2.17	110.96	108.65
14	T	101	5N0	C24-C25-C26	-2.16	106.18	110.85
14	T	101	5N0	C36-N17-C31	-2.12	121.08	126.58
14	T	101	5N0	C3-N2-C4	2.08	109.10	104.01

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	101	5N0	C23-C24-C25-N11
14	T	101	5N0	C23-C24-C25-C26
14	T	101	5N0	C47-C44-C49-O9
14	T	101	5N0	C51-C52-N24-C64
14	T	101	5N0	N23-C50-C51-C52
14	T	101	5N0	C50-C51-C52-N24
14	T	101	5N0	C53-C54-C55-N25
14	T	101	5N0	O10-C56-C57-C58
14	T	101	5N0	N25-C56-C57-C58
14	T	101	5N0	N24-C53-C54-C55
14	T	101	5N0	O10-C56-C57-C62
14	T	101	5N0	N25-C56-C57-C62
14	T	101	5N0	C51-C52-N24-C53

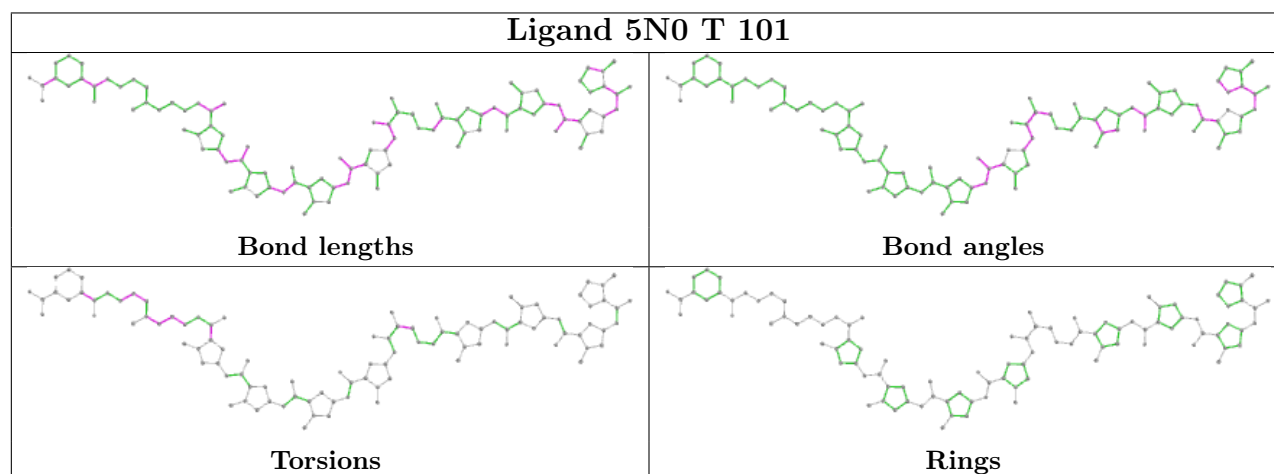
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	101	5N0	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	0.55	0 100 100	83, 93, 159, 175	0
2	T	26/30 (86%)	-0.06	0 100 100	109, 168, 239, 254	0
3	N	15/20 (75%)	-0.24	0 100 100	144, 193, 223, 233	0
4	A	1384/1733 (79%)	0.16	45 (3%) 46 41	41, 92, 176, 245	0
5	B	1129/1224 (92%)	0.08	19 (1%) 70 69	33, 76, 148, 223	0
6	C	267/318 (83%)	-0.08	0 100 100	48, 80, 120, 170	0
7	E	212/215 (98%)	0.31	16 (7%) 14 11	66, 122, 185, 231	0
8	F	86/155 (55%)	-0.00	1 (1%) 79 79	61, 93, 145, 204	0
9	H	133/146 (91%)	0.62	11 (8%) 11 8	84, 127, 186, 223	0
10	I	118/122 (96%)	-0.27	0 100 100	58, 93, 138, 203	0
11	J	65/70 (92%)	-0.08	0 100 100	50, 71, 115, 146	0
12	K	114/120 (95%)	0.02	0 100 100	53, 87, 125, 163	0
13	L	43/70 (61%)	0.14	1 (2%) 60 58	67, 113, 175, 206	0
All	All	3601/4232 (85%)	0.11	93 (2%) 56 52	33, 88, 170, 254	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	286	HIS	8.2
5	B	250	PHE	5.6
4	A	141	LEU	5.5
4	A	182	VAL	5.4
4	A	183	GLY	5.2
4	A	274	ILE	4.8
4	A	276	LEU	4.7
4	A	292	ALA	4.7
4	A	114	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
4	A	200	ARG	4.5
7	E	93	MET	4.5
4	A	103	CYS	4.4
5	B	248	SER	4.3
5	B	869	SER	4.3
5	B	106	ASP	4.3
4	A	163	SER	4.0
4	A	44	THR	3.9
9	H	132	LEU	3.8
8	F	69	LEU	3.8
4	A	69	THR	3.8
4	A	287	HIS	3.8
7	E	128	PRO	3.7
4	A	201	VAL	3.7
7	E	123	LEU	3.6
5	B	475	SER	3.5
7	E	83	CYS	3.5
4	A	199	LEU	3.5
9	H	84	ALA	3.3
9	H	133	ASN	3.3
4	A	288	ALA	3.3
5	B	356	LEU	3.3
4	A	1081	LEU	3.3
4	A	144	THR	3.2
4	A	1002	GLY	3.2
7	E	110	PHE	3.1
4	A	280	GLU	3.1
4	A	181	LEU	3.1
5	B	666	TYR	3.1
7	E	90	VAL	3.0
5	B	433	GLN	3.0
4	A	111	GLY	3.0
7	E	85	GLU	3.0
4	A	998	LEU	2.9
4	A	290	GLU	2.8
7	E	84	ASP	2.8
7	E	122	LYS	2.8
5	B	1184	GLY	2.8
4	A	36	ARG	2.8
5	B	931	TYR	2.8
4	A	113	LEU	2.8
7	E	121	MET	2.7

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Mol	Chain	Res	Type	RSRZ
4	A	289	ILE	2.7
4	A	278	THR	2.7
4	A	997	LEU	2.7
4	A	238	CYS	2.7
4	A	219	PHE	2.6
4	A	149	GLU	2.6
4	A	68	GLN	2.6
7	E	82	PHE	2.6
5	B	92	PHE	2.5
7	E	105	PHE	2.5
9	H	146	ARG	2.5
9	H	86	ASP	2.5
5	B	163	GLY	2.5
9	H	83	GLN	2.5
7	E	102	GLU	2.5
4	A	1126	ALA	2.4
4	A	150	THR	2.4
9	H	139	ASN	2.4
5	B	429	PHE	2.3
4	A	106	VAL	2.3
4	A	108	MET	2.3
7	E	109	ILE	2.3
5	B	434	ARG	2.3
5	B	420	LEU	2.3
4	A	176	LYS	2.3
13	L	45	ALA	2.2
7	E	125	PRO	2.2
9	H	113	ALA	2.2
5	B	249	ARG	2.2
4	A	1232	ASN	2.1
9	H	129	TYR	2.1
4	A	235	ILE	2.1
4	A	164	ARG	2.1
4	A	43	GLU	2.1
4	A	184	SER	2.1
9	H	137	GLN	2.1
4	A	1313	LEU	2.1
7	E	116	ILE	2.1
9	H	127	GLY	2.0
5	B	431	TYR	2.0
5	B	244	LEU	2.0
5	B	430	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

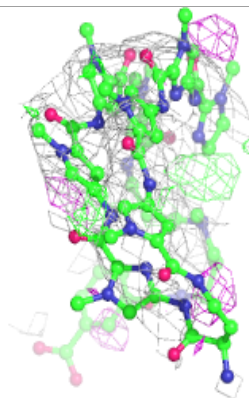
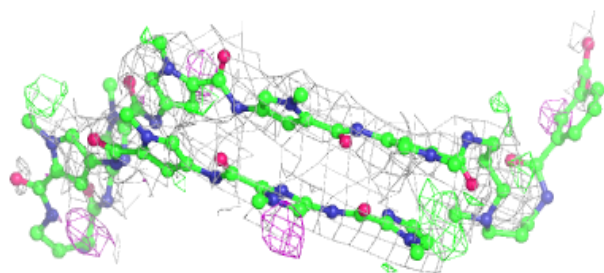
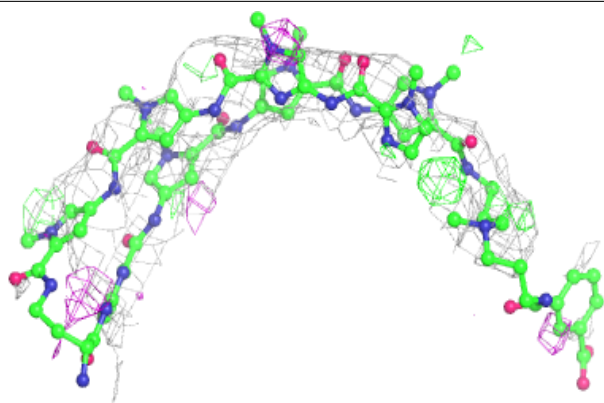
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	5N0	T	101	99/99	0.73	0.33	142,171,236,249	0
15	ZN	A	1801	1/1	0.84	0.05	179,179,179,179	0
15	ZN	B	1301	1/1	0.93	0.14	134,134,134,134	0
15	ZN	I	202	1/1	0.93	0.26	106,106,106,106	0
15	ZN	J	101	1/1	0.93	0.23	86,86,86,86	0
15	ZN	L	101	1/1	0.95	0.09	110,110,110,110	0
15	ZN	A	1802	1/1	0.96	0.15	95,95,95,95	0
16	MG	A	1803	1/1	0.96	0.11	79,79,79,79	0
15	ZN	C	401	1/1	0.99	0.23	81,81,81,81	0
15	ZN	I	201	1/1	0.99	0.16	90,90,90,90	0

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

Electron density around 5N0 T 101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.