Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 07:03 PM EDT

PDB ID	:	6UQ1
Title	:	RNA polymerase II elongation complex with 5-guanidinohydantoin lesion in state 6
Authors	:	Oh, J.; Wang, D.
Deposited on	:	2019-10-18
Resolution	:	3.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

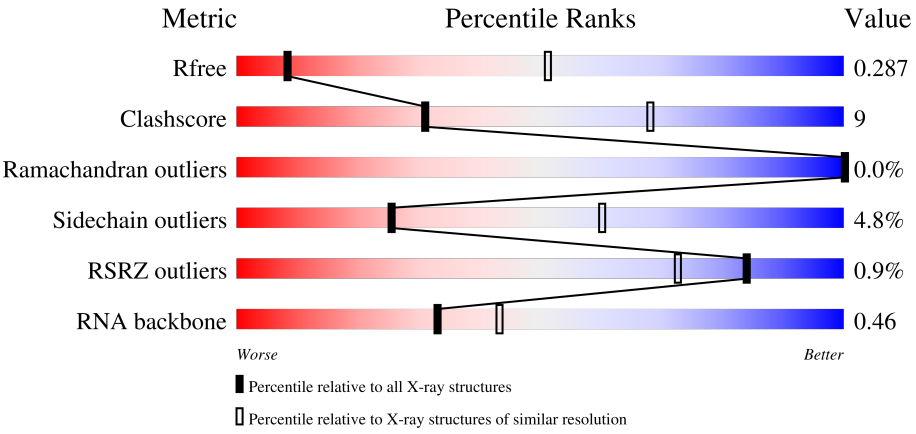
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 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 <=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	12	42% 50% 8%
2	T	29	52% 38% 10%
3	N	18	61% 28% 11%
4	A	1733	% 61% 18% . 20%

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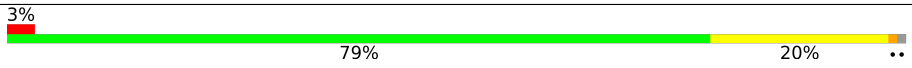
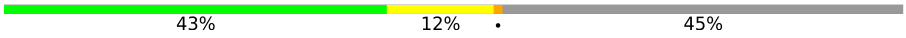
Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29097 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	11	Total	C	N	O	P	0	0	0
			238	106	44	77	11			

- 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
			519	248	81	164	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	16	Total	C	N	O	P	0	0	0
			339	158	76	89	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1382	Total	C	N	O	S	0	0	0
			10812	6820	1894	2038	60			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	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	213	Total	C	N	O	S	0	0	0
			1740	1105	307	317	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	85	Total	C	N	O	S	0	0	0
			676	431	114	128	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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

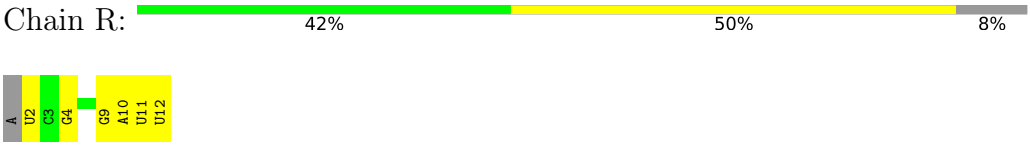
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0

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

Chain R:



• Molecule 2: Template strand DNA

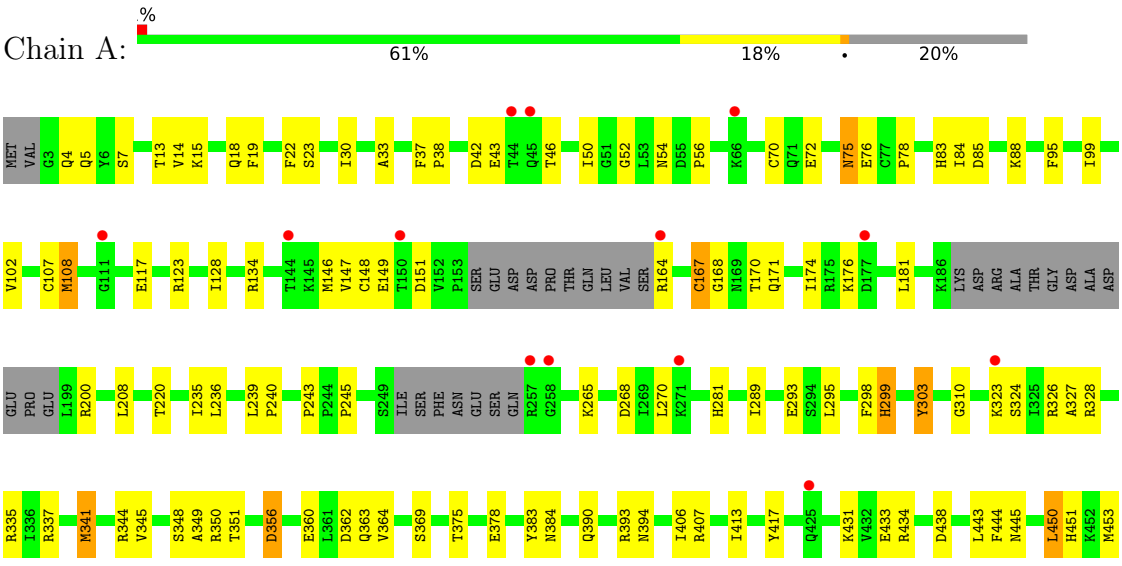
Chain T:

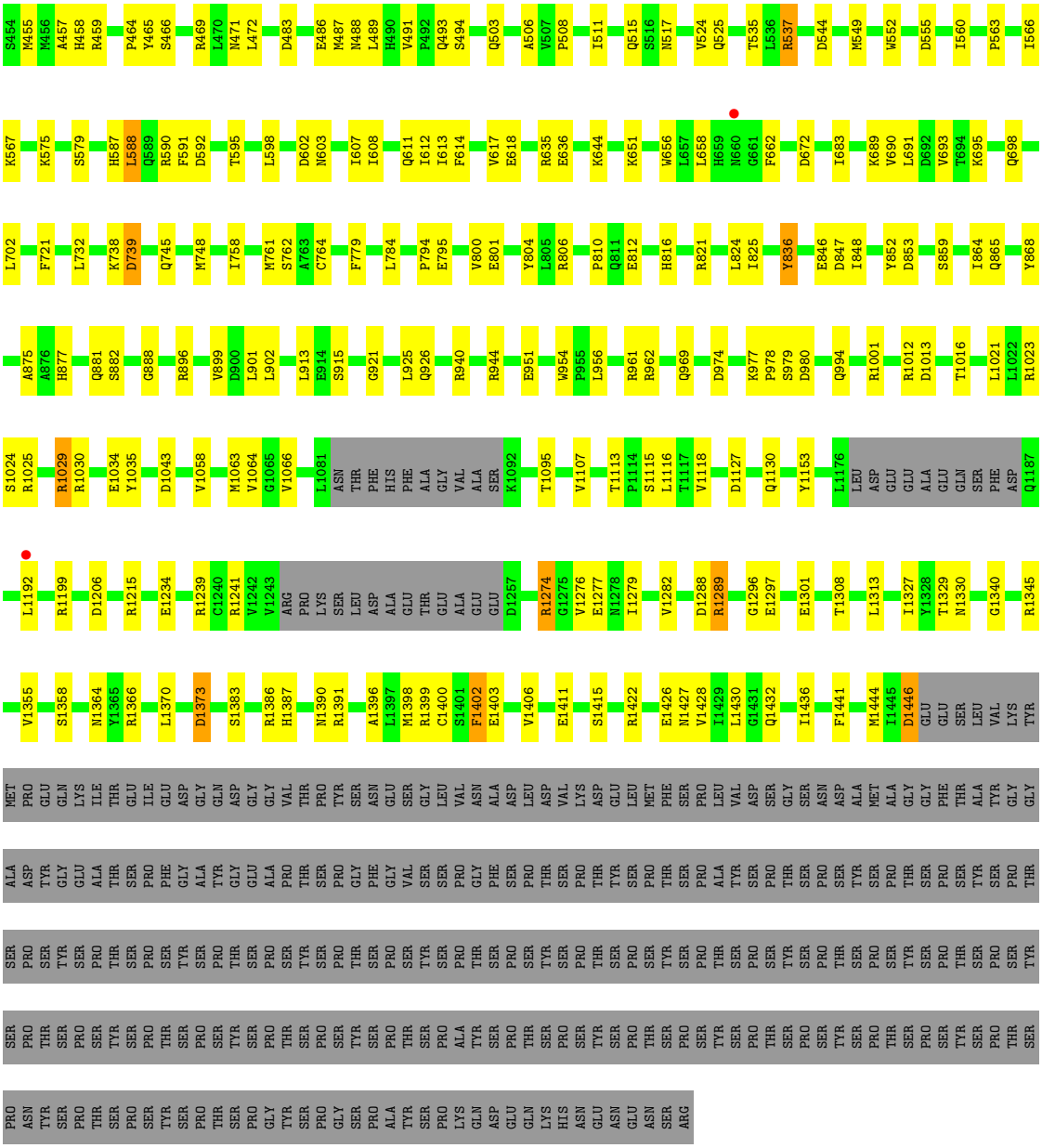
• Molecule 3: Non-template strand DNA

Chain N:

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

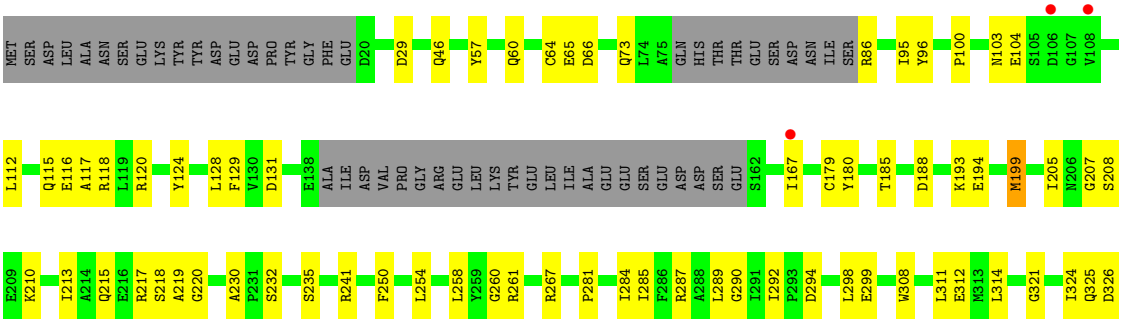
Chain A:

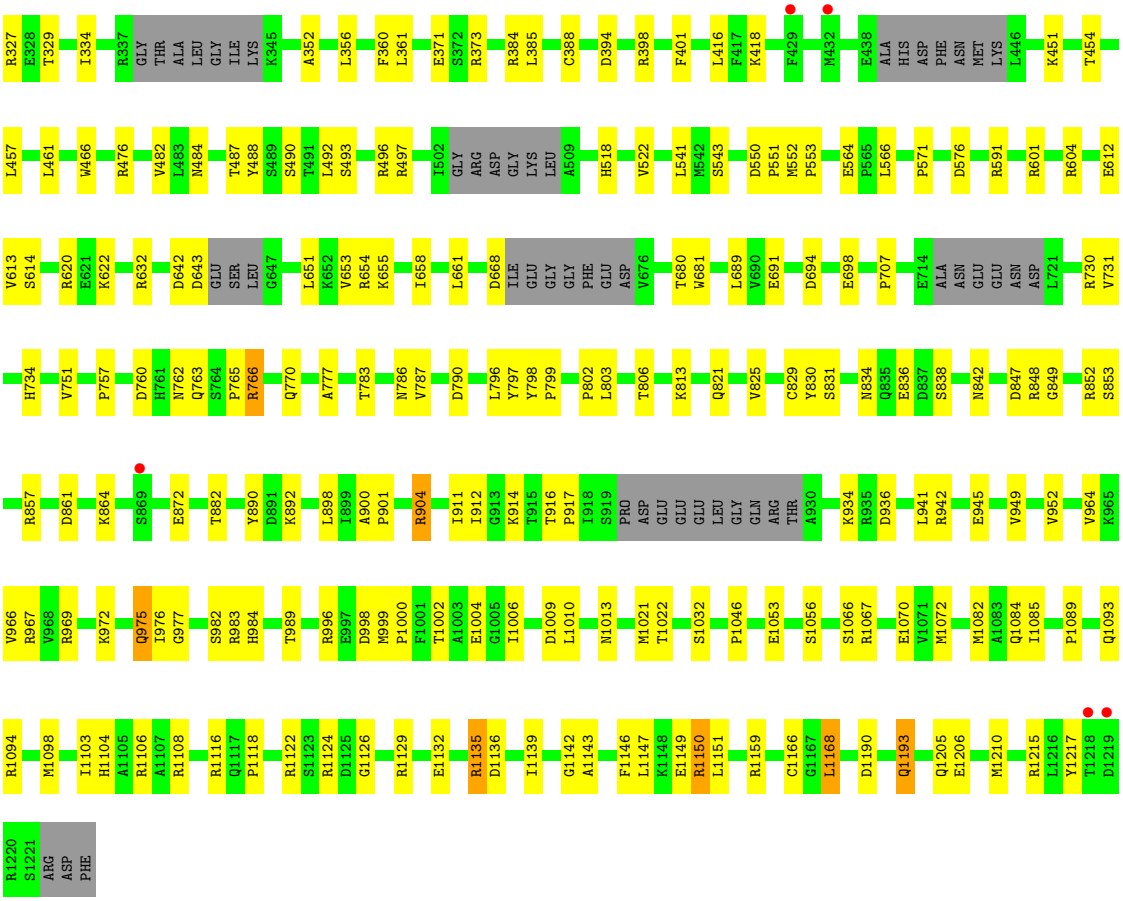




• Molecule 5: DNA-directed RNA polymerase II subunit RPB2

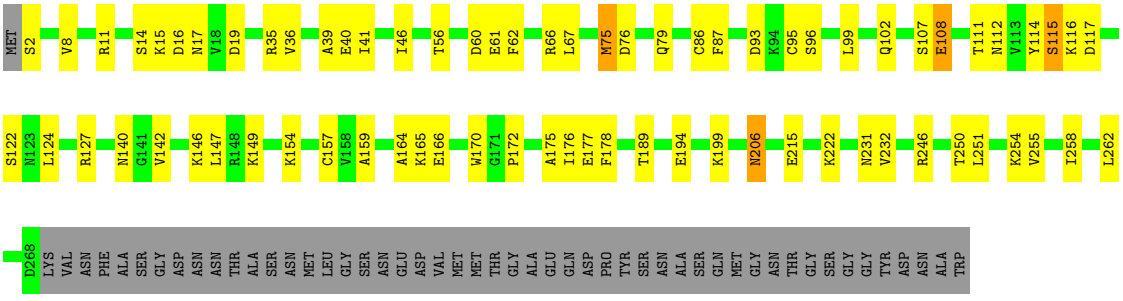
Chain B:





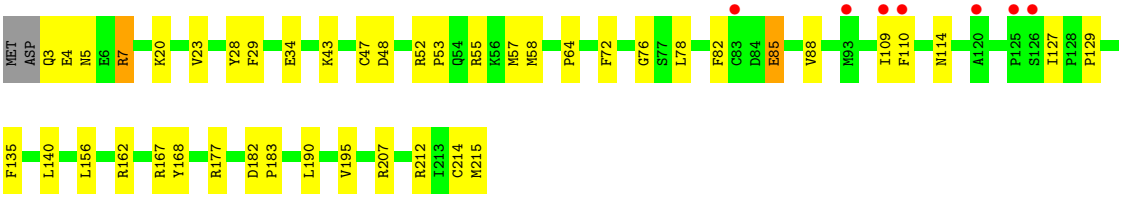
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C:



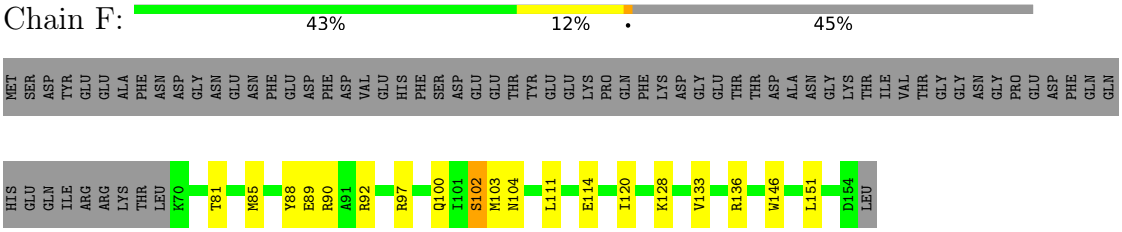
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



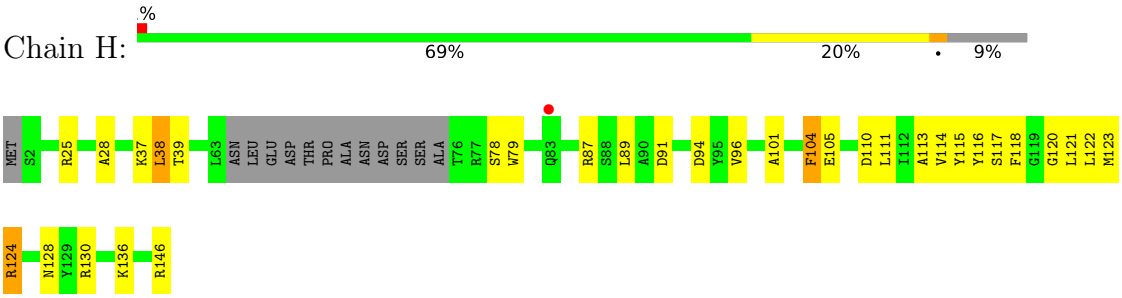
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



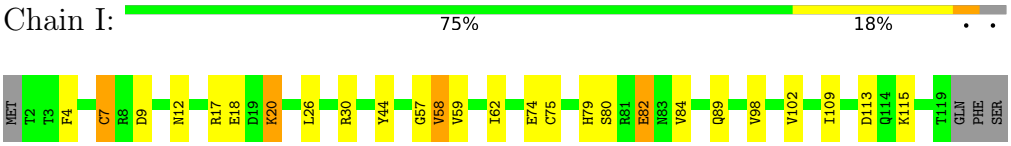
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



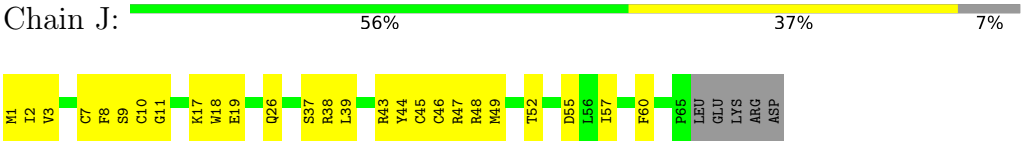
• Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I:



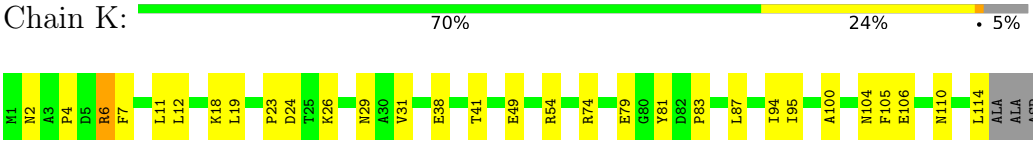
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



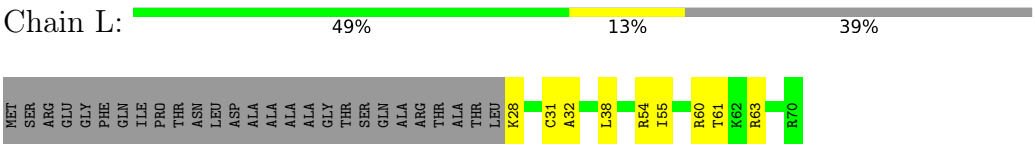
• Molecule 12: DNA-directed RNA polymerase II subunit RPB11

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.50Å 223.51Å 194.94Å 90.00° 101.58° 90.00°	Depositor
Resolution (Å)	49.52 – 3.60 49.52 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.52-3.60) 99.9 (49.52-3.60)	Depositor EDS
R_{merge}	0.49	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.240 , 0.287 0.240 , 0.287	Depositor DCC
R_{free} test set	1900 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å^2)	93.2	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 65.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29097	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: MG, ZN, G35

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	0.23	0/266	0.84	0/413
2	T	0.58	0/550	1.05	0/841
3	N	0.59	0/384	0.85	0/592
4	A	0.25	0/11004	0.48	0/14885
5	B	0.25	0/9030	0.47	0/12186
6	C	0.25	0/2139	0.46	0/2899
7	E	0.26	0/1776	0.48	0/2390
8	F	0.24	0/688	0.45	0/932
9	H	0.26	0/1082	0.53	0/1466
10	I	0.31	0/970	0.60	2/1308 (0.2%)
11	J	0.24	0/541	0.46	0/727
12	K	0.23	0/937	0.44	0/1265
13	L	0.26	0/339	0.51	0/450
All	All	0.27	0/29706	0.51	2/40354 (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	2
10	I	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	82	GLU	OE1-CD-OE2	-7.12	114.76	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	82	GLU	CG-CD-OE2	6.21	130.73	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	310	GLY	Peptide
4	A	524	VAL	Peptide
10	I	57	GLY	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	238	0	119	3	0
2	T	519	0	298	13	0
3	N	339	0	177	4	0
4	A	10812	0	10850	222	0
5	B	8859	0	8818	179	0
6	C	2101	0	2056	50	0
7	E	1740	0	1766	27	0
8	F	676	0	681	14	0
9	H	1064	0	1029	26	0
10	I	952	0	898	13	2
11	J	532	0	543	22	0
12	K	919	0	929	21	0
13	L	337	0	352	6	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	29097	0	28516	518	2

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 9.

All (518) 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)
7:E:4:GLU:CA	7:E:7:ARG:HH22	1.35	1.40
7:E:4:GLU:HA	7:E:7:ARG:NH2	1.40	1.34
4:A:899:VAL:HG22	4:A:1029:ARG:NH2	1.51	1.25
5:B:218:SER:O	5:B:241:ARG:NH2	1.76	1.18
4:A:899:VAL:HA	4:A:1029:ARG:HH22	1.04	1.16
9:H:115:TYR:HE2	9:H:124:ARG:HD3	1.05	1.15
4:A:899:VAL:HG22	4:A:1029:ARG:CZ	1.80	1.11
5:B:220:GLY:N	5:B:241:ARG:HH21	1.52	1.07
4:A:567:LYS:HB2	9:H:96:VAL:HG12	1.41	1.02
9:H:115:TYR:CE2	9:H:124:ARG:HD3	1.97	1.00
5:B:219:ALA:C	5:B:241:ARG:HH21	1.68	0.96
4:A:899:VAL:HA	4:A:1029:ARG:NH2	1.80	0.95
4:A:899:VAL:CG2	4:A:1029:ARG:NH2	2.31	0.92
5:B:219:ALA:C	5:B:241:ARG:NH2	2.26	0.89
4:A:50:ILE:CD1	4:A:52:GLY:H	1.84	0.89
4:A:913:LEU:HD23	4:A:915:SER:H	1.40	0.86
13:L:55:ILE:HD12	13:L:55:ILE:O	1.75	0.86
5:B:219:ALA:O	5:B:241:ARG:NE	2.10	0.83
4:A:50:ILE:HD13	4:A:52:GLY:H	1.45	0.80
12:K:7:PHE:HB2	12:K:11:LEU:HD13	1.64	0.79
2:T:17:DG:H5'	4:A:1403:GLU:OE2	1.83	0.78
4:A:836:TYR:OH	4:A:1403:GLU:OE1	2.01	0.78
5:B:218:SER:O	5:B:241:ARG:CZ	2.30	0.78
4:A:899:VAL:CA	4:A:1029:ARG:HH22	1.92	0.77
5:B:218:SER:OG	5:B:241:ARG:NH1	2.18	0.77
4:A:899:VAL:CG2	4:A:1029:ARG:CZ	2.63	0.75
4:A:913:LEU:HD23	4:A:915:SER:N	2.02	0.73
9:H:110:ASP:O	9:H:111:LEU:HD12	1.88	0.73
7:E:4:GLU:HB3	7:E:7:ARG:HH12	1.53	0.73
4:A:567:LYS:CB	9:H:96:VAL:HG12	2.16	0.73
4:A:323:LYS:HE3	4:A:328:ARG:HE	1.53	0.72
7:E:4:GLU:CA	7:E:7:ARG:NH2	2.19	0.71
4:A:445:ASN:ND2	4:A:455:MET:SD	2.64	0.71
6:C:36:VAL:HG23	6:C:40:GLU:HB2	1.74	0.70
7:E:4:GLU:C	7:E:7:ARG:NH2	2.46	0.69
4:A:899:VAL:CA	4:A:1029:ARG:NH2	2.54	0.69
4:A:899:VAL:HG22	4:A:1029:ARG:HH21	1.56	0.69
7:E:4:GLU:O	7:E:7:ARG:NH1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:4:GLU:HA	7:E:7:ARG:HH22	0.58	0.69
2:T:17:DG:OP1	4:A:1403:GLU:OE2	2.11	0.68
7:E:4:GLU:C	7:E:7:ARG:HH22	1.97	0.68
4:A:50:ILE:HD13	4:A:52:GLY:N	2.08	0.68
9:H:115:TYR:HE2	9:H:124:ARG:CD	1.96	0.67
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.77	0.66
4:A:444:PHE:CZ	4:A:487:MET:SD	2.88	0.66
4:A:50:ILE:HD12	4:A:52:GLY:H	1.58	0.66
4:A:351:THR:HG22	5:B:1103:ILE:HG12	1.77	0.65
4:A:994:GLN:HE22	4:A:1023:ARG:HH21	1.44	0.65
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.30	0.65
4:A:174:ILE:HD11	4:A:181:LEU:HB3	1.78	0.64
5:B:213:ILE:HD11	5:B:497:ARG:HB3	1.80	0.64
5:B:757:PRO:HD3	5:B:983:ARG:HE	1.61	0.64
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.80	0.64
5:B:853:SER:HB3	5:B:972:LYS:HB2	1.80	0.64
11:J:10:CYS:SG	11:J:43:ARG:NH2	2.70	0.64
4:A:899:VAL:CB	4:A:1029:ARG:NH2	2.62	0.63
6:C:254:LYS:NZ	12:K:38:GLU:OE1	2.32	0.63
5:B:112:LEU:HD21	5:B:117:ALA:HB2	1.80	0.63
4:A:1116:LEU:HD13	4:A:1329:THR:HG22	1.81	0.63
9:H:110:ASP:O	9:H:128:ASN:ND2	2.32	0.62
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.82	0.62
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.80	0.62
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.33	0.62
4:A:961:ARG:HH11	4:A:1025:ARG:HH22	1.48	0.61
4:A:7:SER:OG	5:B:1193:GLN:NE2	2.33	0.61
2:T:25:DC:H5"	5:B:482:VAL:HG21	1.82	0.61
4:A:328:ARG:NH1	5:B:1206:GLU:OE1	2.32	0.61
6:C:165:LYS:O	12:K:6:ARG:NH1	2.34	0.61
4:A:1013:ASP:OD1	7:E:207:ARG:NH1	2.33	0.61
7:E:177:ARG:NH1	7:E:215:MET:SD	2.73	0.61
5:B:287:ARG:NH1	5:B:324:ILE:O	2.33	0.60
4:A:326:ARG:HE	4:A:1406:VAL:HG11	1.66	0.60
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.34	0.60
6:C:8:VAL:HG11	12:K:105:PHE:HD1	1.66	0.60
6:C:86:CYS:SG	6:C:87:PHE:N	2.74	0.60
4:A:38:PRO:HB3	4:A:270:LEU:HB3	1.83	0.60
4:A:464:PRO:O	12:K:2:ASN:ND2	2.34	0.60
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.81	0.60
8:F:85:MET:HG3	8:F:89:GLU:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.35	0.60
4:A:134:ARG:NH2	4:A:220:THR:O	2.34	0.60
5:B:653:VAL:HG12	5:B:689:LEU:HB3	1.83	0.60
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.84	0.60
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.83	0.59
13:L:32:ALA:H	13:L:55:ILE:CD1	2.15	0.59
2:T:25:DC:H2"	2:T:26:DG:H5"	1.83	0.59
4:A:882:SER:H	4:A:961:ARG:HH12	1.49	0.59
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.84	0.59
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.34	0.59
11:J:10:CYS:SG	11:J:11:GLY:N	2.75	0.59
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.35	0.59
5:B:334:ILE:HG21	5:B:352:ALA:HB2	1.84	0.59
5:B:882:THR:HG23	5:B:934:LYS:HG3	1.84	0.59
6:C:60:ASP:OD2	13:L:60:ARG:NH1	2.36	0.59
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.84	0.59
4:A:590:ARG:NH1	4:A:592:ASP:OD2	2.36	0.59
12:K:100:ALA:O	12:K:104:ASN:ND2	2.35	0.59
12:K:106:GLU:O	12:K:110:ASN:ND2	2.35	0.59
2:T:7:DC:O2	3:N:12:DG:N2	2.36	0.58
11:J:37:SER:OG	11:J:47:ARG:NH2	2.36	0.58
4:A:761:MET:HG3	5:B:1021:MET:HG2	1.84	0.58
5:B:118:ARG:HA	5:B:207:GLY:HA2	1.86	0.58
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.85	0.58
4:A:107:CYS:SG	4:A:171:GLN:NE2	2.75	0.58
4:A:491:VAL:O	5:B:1150:ARG:NH2	2.36	0.58
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.85	0.58
4:A:579:SER:HB3	4:A:611:GLN:HA	1.86	0.58
4:A:75:ASN:OD1	5:B:1116:ARG:NH1	2.37	0.58
5:B:232:SER:O	5:B:261:ARG:NH2	2.36	0.58
4:A:349:ALA:HB3	4:A:489:LEU:HB3	1.86	0.57
5:B:260:GLY:O	5:B:267:ARG:NH1	2.37	0.57
4:A:37:PHE:CE1	4:A:50:ILE:HD13	2.39	0.57
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.85	0.57
5:B:552:MET:HG3	5:B:553:PRO:HD3	1.85	0.57
4:A:563:PRO:HG2	4:A:566:ILE:HG12	1.85	0.57
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.37	0.57
7:E:28:TYR:HA	7:E:64:PRO:HA	1.86	0.57
4:A:378:GLU:OE2	4:A:384:ASN:ND2	2.34	0.57
4:A:575:LYS:NZ	4:A:602:ASP:OD2	2.38	0.57
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1427:ASN:OD1	4:A:1432:GLN:NE2	2.38	0.57
5:B:287:ARG:NH1	5:B:321:GLY:O	2.37	0.57
5:B:496:ARG:HH12	5:B:541:LEU:HA	1.70	0.57
9:H:94:ASP:N	9:H:94:ASP:OD1	2.38	0.57
4:A:588:LEU:HB3	4:A:607:ILE:HB	1.87	0.57
4:A:636:GLU:OE1	4:A:962:ARG:NH1	2.38	0.56
5:B:1142:GLY:HA3	8:F:88:TYR:HE2	1.70	0.56
6:C:2:SER:N	12:K:104:ASN:OD1	2.38	0.56
6:C:258:ILE:HG23	12:K:19:LEU:HD11	1.87	0.56
7:E:85:GLU:OE1	7:E:88:VAL:HG12	2.04	0.56
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.86	0.56
10:I:58:VAL:HA	10:I:62:ILE:HD12	1.86	0.56
4:A:738:LYS:NZ	6:C:194:GLU:O	2.38	0.56
4:A:902:LEU:HB3	4:A:921:GLY:HA2	1.88	0.56
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.88	0.56
6:C:11:ARG:NH1	6:C:19:ASP:OD2	2.38	0.56
6:C:115:SER:HB3	6:C:142:VAL:HG12	1.87	0.56
4:A:375:THR:HG21	5:B:1108:ARG:HH11	1.70	0.56
5:B:802:PRO:HB3	5:B:983:ARG:HH12	1.71	0.56
4:A:72:GLU:HB3	4:A:76:GLU:HB3	1.87	0.56
5:B:73:GLN:O	5:B:86:ARG:N	2.39	0.56
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.88	0.56
8:F:81:THR:HG1	8:F:146:TRP:HE1	1.52	0.56
4:A:378:GLU:OE1	4:A:434:ARG:NH1	2.39	0.56
5:B:29:ASP:OD2	5:B:655:LYS:NZ	2.38	0.56
5:B:892:LYS:NZ	5:B:904:ARG:O	2.35	0.56
4:A:108:MET:SD	4:A:108:MET:N	2.78	0.55
4:A:560:ILE:HG23	9:H:79:TRP:H	1.72	0.55
4:A:50:ILE:CD1	4:A:52:GLY:N	2.62	0.55
4:A:1390:ASN:HD21	4:A:1402:PHE:HB3	1.71	0.55
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.87	0.55
4:A:614:PHE:HB3	9:H:122:LEU:HD21	1.88	0.55
5:B:643:ASP:OD2	5:B:654:ARG:NH2	2.36	0.55
5:B:762:ASN:HD21	5:B:984:HIS:HD2	1.55	0.55
5:B:798:TYR:O	5:B:821:GLN:NE2	2.39	0.55
10:I:58:VAL:HG21	10:I:109:ILE:HD11	1.89	0.55
5:B:46:GLN:HE22	5:B:496:ARG:HA	1.72	0.55
5:B:766:ARG:HG2	5:B:1022:THR:HG22	1.87	0.55
10:I:18:GLU:OE1	10:I:20:LYS:NZ	2.39	0.55
4:A:555:ASP:OD2	4:A:644:LYS:NZ	2.35	0.55
5:B:299:GLU:HB3	5:B:571:PRO:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:325:GLN:OE1	10:I:12:ASN:ND2	2.39	0.55
6:C:176:ILE:HG22	6:C:232:VAL:HA	1.88	0.54
5:B:254:LEU:HD22	5:B:361:LEU:CD1	2.37	0.54
6:C:102:GLN:HG2	6:C:154:LYS:HG3	1.89	0.54
4:A:356:ASP:OD2	4:A:469:ARG:NH2	2.36	0.54
4:A:1396:ALA:HA	4:A:1399:ARG:HH21	1.71	0.54
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.39	0.54
12:K:29:ASN:HD21	12:K:79:GLU:HA	1.73	0.54
4:A:95:PHE:O	4:A:99:ILE:N	2.40	0.54
5:B:911:ILE:HG22	5:B:912:ILE:HG13	1.89	0.54
6:C:175:ALA:HB2	11:J:10:CYS:HB2	1.89	0.54
4:A:1276:VAL:HB	4:A:1279:ILE:HD13	1.90	0.54
5:B:118:ARG:NH2	5:B:194:GLU:OE2	2.41	0.53
9:H:101:ALA:HB1	9:H:104:PHE:HE2	1.73	0.53
2:T:16:DT:H2'	2:T:17:DG:C8	2.43	0.53
5:B:612:GLU:O	5:B:632:ARG:NH2	2.30	0.53
4:A:18:GLN:NE2	4:A:19:PHE:O	2.33	0.53
4:A:43:GLU:O	4:A:46:THR:OG1	2.27	0.53
5:B:116:GLU:OE2	5:B:120:ARG:NH1	2.42	0.53
6:C:41:ILE:HB	6:C:172:PRO:HG2	1.90	0.53
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.90	0.53
5:B:326:ASP:OD1	5:B:329:THR:OG1	2.24	0.53
5:B:564:GLU:OE2	5:B:591:ARG:NH2	2.42	0.53
5:B:898:LEU:HD21	5:B:964:VAL:HG11	1.90	0.53
4:A:980:ASP:OD1	4:A:980:ASP:N	2.41	0.53
7:E:48:ASP:OD2	7:E:52:ARG:N	2.42	0.53
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.91	0.53
5:B:230:ALA:O	5:B:261:ARG:NH2	2.42	0.52
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.43	0.52
6:C:14:SER:HA	12:K:114:LEU:HD12	1.91	0.52
4:A:128:ILE:HG23	4:A:134:ARG:HB2	1.89	0.52
4:A:457:ALA:O	4:A:458:HIS:CD2	2.62	0.52
4:A:824:LEU:HD21	5:B:765:PRO:HB3	1.91	0.52
5:B:760:ASP:OD1	5:B:760:ASP:N	2.42	0.52
2:T:16:DT:O2	4:A:1386:ARG:NH2	2.43	0.52
5:B:917:PRO:HA	5:B:934:LYS:HA	1.90	0.52
4:A:951:GLU:HB3	4:A:954:TRP:HE1	1.74	0.52
5:B:604:ARG:NH2	5:B:613:VAL:O	2.42	0.52
7:E:23:VAL:HG12	7:E:28:TYR:HB2	1.91	0.52
5:B:620:ARG:NH2	10:I:89:GLN:OE1	2.43	0.52
6:C:56:THR:HG22	6:C:147:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:105:GLU:N	9:H:113:ALA:O	2.42	0.52
4:A:268:ASP:HB3	4:A:299:HIS:HD2	1.74	0.52
4:A:1095:THR:HG22	4:A:1113:THR:HB	1.91	0.52
4:A:926:GLN:O	4:A:926:GLN:NE2	2.43	0.52
6:C:107:SER:OG	6:C:111:THR:OG1	2.28	0.52
5:B:848:ARG:NH1	11:J:8:PHE:O	2.43	0.51
6:C:46:ILE:HD13	6:C:157:CYS:HB3	1.91	0.51
4:A:78:PRO:O	5:B:1205:GLN:NE2	2.44	0.51
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.91	0.51
5:B:219:ALA:O	5:B:241:ARG:CZ	2.59	0.51
12:K:23:PRO:HA	12:K:31:VAL:HA	1.92	0.51
4:A:739:ASP:O	4:A:745:GLN:NE2	2.38	0.51
9:H:39:THR:HB	9:H:124:ARG:HB3	1.93	0.51
4:A:117:GLU:O	4:A:123:ARG:NE	2.44	0.51
4:A:1030:ARG:HA	4:A:1034:GLU:HG3	1.92	0.51
4:A:341:MET:HB3	5:B:1132:GLU:HB3	1.91	0.51
5:B:220:GLY:HA2	5:B:241:ARG:HE	1.75	0.51
6:C:146:LYS:NZ	11:J:55:ASP:OD2	2.44	0.51
11:J:9:SER:OG	11:J:48:ARG:NH2	2.44	0.51
12:K:12:LEU:HD21	12:K:18:LYS:HG2	1.92	0.51
4:A:1116:LEU:HD22	4:A:1329:THR:HG22	1.93	0.51
11:J:3:VAL:HG11	11:J:18:TRP:HB2	1.92	0.51
9:H:118:PHE:N	9:H:121:LEU:O	2.41	0.51
4:A:295:LEU:HA	4:A:298:PHE:HB3	1.91	0.51
4:A:635:ARG:HH11	4:A:635:ARG:HA	1.76	0.50
4:A:390:GLN:NE2	4:A:394:ASN:OD1	2.37	0.50
5:B:1006:ILE:HG23	11:J:45:CYS:HB3	1.92	0.50
6:C:116:LYS:NZ	6:C:117:ASP:OD1	2.43	0.50
4:A:85:ASP:OD1	4:A:85:ASP:N	2.41	0.50
4:A:567:LYS:HB2	9:H:96:VAL:CG1	2.30	0.50
8:F:97:ARG:NH1	8:F:100:GLN:OE1	2.40	0.50
4:A:1115:SER:N	4:A:1330:ASN:OD1	2.44	0.50
5:B:806:THR:HG23	5:B:1046:PRO:HD3	1.93	0.50
5:B:1082:MET:O	5:B:1084:GLN:NE2	2.44	0.50
11:J:1:MET:HB2	11:J:60:PHE:HE2	1.76	0.50
4:A:1116:LEU:HD11	4:A:1313:LEU:HD23	1.94	0.50
4:A:1436:ILE:HD13	5:B:1139:ILE:HG12	1.92	0.50
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.44	0.50
5:B:371:GLU:OE1	5:B:371:GLU:N	2.45	0.50
4:A:901:LEU:HD11	4:A:925:LEU:HD22	1.93	0.50
4:A:662:PHE:HB3	5:B:829:CYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.93	0.50
5:B:60:GLN:NE2	5:B:64:CYS:SG	2.85	0.49
6:C:14:SER:OG	6:C:15:LYS:N	2.45	0.49
4:A:326:ARG:HG3	4:A:1406:VAL:HG21	1.93	0.49
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.95	0.49
4:A:690:VAL:HG11	4:A:794:PRO:HD3	1.95	0.49
4:A:864:ILE:HG22	4:A:865:GLN:HG3	1.95	0.49
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.94	0.49
5:B:208:SER:OG	5:B:210:LYS:NZ	2.45	0.49
4:A:471:ASN:OD1	4:A:472:LEU:N	2.45	0.49
4:A:881:GLN:HG3	4:A:956:LEU:HD12	1.93	0.49
5:B:651:LEU:HD11	5:B:707:PRO:HB3	1.94	0.49
5:B:694:ASP:OD1	5:B:694:ASP:N	2.44	0.49
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.12	0.49
7:E:177:ARG:O	7:E:212:ARG:NH2	2.46	0.49
2:T:24:DT:OP1	5:B:857:ARG:NH2	2.46	0.49
5:B:1166:CYS:SG	5:B:1168:LEU:HD21	2.53	0.49
7:E:78:LEU:HD21	7:E:109:ILE:HD13	1.93	0.49
4:A:658:LEU:HD13	5:B:831:SER:H	1.78	0.49
4:A:1199:ARG:NH1	4:A:1234:GLU:OE1	2.46	0.49
5:B:115:GLN:NE2	5:B:193:LYS:O	2.44	0.49
8:F:128:LYS:NZ	8:F:151:LEU:O	2.46	0.49
2:T:3:DT:O2	3:N:17:DG:N1	2.46	0.49
6:C:93:ASP:O	6:C:127:ARG:NH2	2.46	0.49
4:A:344:ARG:HB2	5:B:1118:PRO:HG2	1.95	0.48
4:A:84:ILE:HG23	4:A:239:LEU:HB3	1.95	0.48
4:A:695:LYS:HA	4:A:698:GLN:HE21	1.78	0.48
4:A:149:GLU:O	4:A:164:ARG:NH1	2.36	0.48
4:A:804:TYR:HH	4:A:816:HIS:HE2	1.55	0.48
5:B:890:TYR:OH	5:B:936:ASP:OD2	2.30	0.48
4:A:944:ARG:NH2	4:A:1296:GLY:O	2.32	0.48
4:A:1116:LEU:CD1	4:A:1329:THR:HG22	2.42	0.48
5:B:218:SER:C	5:B:241:ARG:NH2	2.62	0.48
5:B:1104:HIS:NE2	5:B:1126:GLY:O	2.46	0.48
5:B:1053:GLU:OE2	5:B:1067:ARG:NH1	2.47	0.48
4:A:268:ASP:HB3	4:A:299:HIS:CD2	2.48	0.48
5:B:326:ASP:OD1	5:B:326:ASP:N	2.45	0.48
5:B:487:THR:OG1	5:B:777:ALA:O	2.32	0.48
4:A:575:LYS:HB3	4:A:612:ILE:HD11	1.95	0.48
4:A:859:SER:O	4:A:1422:ARG:NH1	2.46	0.48
5:B:220:GLY:N	5:B:241:ARG:NH2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:517:ASN:OD1	4:A:1364:ASN:ND2	2.46	0.48
4:A:555:ASP:OD1	4:A:555:ASP:N	2.44	0.48
4:A:804:TYR:OH	4:A:816:HIS:NE2	2.36	0.48
4:A:1206:ASP:HB2	4:A:1274:ARG:HH12	1.77	0.48
7:E:190:LEU:HD12	7:E:214:CYS:HB2	1.96	0.48
4:A:603:ASN:OD1	4:A:603:ASN:N	2.40	0.48
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.95	0.48
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.96	0.47
6:C:166:GLU:HB3	6:C:170:TRP:HZ3	1.78	0.47
4:A:868:TYR:CD2	4:A:1058:VAL:HG21	2.49	0.47
4:A:901:LEU:N	4:A:926:GLN:OE1	2.44	0.47
5:B:100:PRO:O	5:B:180:TYR:OH	2.31	0.47
5:B:312:GLU:O	10:I:44:TYR:OH	2.31	0.47
4:A:848:ILE:HG22	4:A:1064:VAL:HG23	1.96	0.47
5:B:857:ARG:NH1	5:B:945:GLU:OE2	2.48	0.47
9:H:136:LYS:H	9:H:136:LYS:HG2	1.51	0.47
8:F:103:MET:SD	8:F:103:MET:N	2.88	0.47
8:F:104:ASN:OD1	8:F:104:ASN:N	2.45	0.47
4:A:450:LEU:O	4:A:450:LEU:CD1	2.62	0.47
4:A:1289:ARG:O	4:A:1301:GLU:N	2.44	0.47
5:B:185:THR:OG1	5:B:188:ASP:OD1	2.33	0.47
4:A:1025:ARG:O	4:A:1035:TYR:OH	2.33	0.47
5:B:218:SER:O	5:B:241:ARG:NH1	2.48	0.47
5:B:680:THR:OG1	5:B:681:TRP:N	2.47	0.47
5:B:952:VAL:HG22	5:B:966:VAL:HG22	1.97	0.47
4:A:888:GLY:O	4:A:940:ARG:NH2	2.46	0.47
4:A:974:ASP:OD2	4:A:977:LYS:NZ	2.45	0.47
4:A:683:ILE:HG21	4:A:801:GLU:HG3	1.96	0.47
5:B:790:ASP:OD2	5:B:790:ASP:N	2.46	0.47
9:H:105:GLU:OE1	9:H:115:TYR:OH	2.25	0.47
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.97	0.46
5:B:215:GLN:HG2	5:B:476:ARG:HD2	1.97	0.46
5:B:770:GLN:NE2	5:B:1093:GLN:OE1	2.45	0.46
4:A:537:ARG:H	4:A:537:ARG:HG2	1.48	0.46
5:B:451:LYS:HA	5:B:454:THR:HB	1.97	0.46
5:B:1143:ALA:HB1	5:B:1146:PHE:HB3	1.97	0.46
6:C:108:GLU:HA	6:C:149:LYS:HE2	1.98	0.46
5:B:825:VAL:HG22	5:B:1010:LEU:HB3	1.97	0.46
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.32	0.46
4:A:1153:TYR:HB2	4:A:1192:LEU:HD23	1.97	0.46
4:A:148:CYS:HB2	4:A:164:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:830:TYR:OH	5:B:998:ASP:O	2.31	0.46
6:C:75:MET:O	6:C:246:ARG:NH2	2.48	0.46
8:F:89:GLU:OE2	8:F:136:ARG:NH2	2.45	0.46
4:A:33:ALA:HB1	4:A:56:PRO:HG2	1.98	0.46
4:A:899:VAL:HG22	4:A:1029:ARG:NE	2.26	0.46
5:B:1094:ARG:NH1	5:B:1098:MET:SD	2.86	0.46
6:C:16:ASP:OD2	6:C:16:ASP:N	2.46	0.46
6:C:46:ILE:HD12	6:C:67:LEU:HB3	1.97	0.46
5:B:199:MET:SD	5:B:199:MET:N	2.80	0.46
11:J:8:PHE:H	11:J:49:MET:HE3	1.81	0.46
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	1.99	0.46
5:B:219:ALA:C	5:B:241:ARG:CZ	2.83	0.46
5:B:1072:MET:HG3	5:B:1085:ILE:HB	1.97	0.46
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.98	0.46
10:I:17:ARG:N	10:I:26:LEU:O	2.45	0.45
4:A:689:LYS:HE3	4:A:689:LYS:HB2	1.87	0.45
5:B:1106:ARG:CZ	5:B:1118:PRO:HB3	2.46	0.45
4:A:364:VAL:N	4:A:459:ARG:O	2.49	0.45
5:B:1082:MET:HA	6:C:189:THR:HA	1.97	0.45
6:C:199:LYS:HE3	6:C:199:LYS:HB2	1.84	0.45
6:C:46:ILE:HA	6:C:159:ALA:HA	1.98	0.45
4:A:881:GLN:HA	4:A:961:ARG:HH22	1.80	0.45
5:B:982:SER:OG	5:B:983:ARG:N	2.49	0.45
4:A:54:ASN:OD1	4:A:54:ASN:N	2.50	0.45
4:A:464:PRO:HB2	12:K:4:PRO:HD3	1.99	0.45
4:A:493:GLN:N	5:B:1149:GLU:OE2	2.44	0.45
4:A:853:ASP:OD1	4:A:853:ASP:N	2.48	0.45
4:A:979:SER:OG	4:A:980:ASP:N	2.48	0.45
5:B:898:LEU:HD23	5:B:898:LEU:HA	1.79	0.45
6:C:66:ARG:HH21	11:J:2:ILE:HG23	1.82	0.45
4:A:360:GLU:OE2	4:A:651:LYS:NZ	2.40	0.45
5:B:872:GLU:HG2	5:B:916:THR:HB	1.99	0.45
7:E:20:LYS:NZ	7:E:34:GLU:O	2.47	0.45
4:A:13:THR:OG1	4:A:14:VAL:N	2.50	0.45
4:A:433:GLU:OE1	5:B:1108:ARG:NH1	2.50	0.45
4:A:1398:MET:N	4:A:1426:GLU:OE2	2.49	0.45
4:A:852:TYR:CZ	8:F:136:ARG:HG2	2.51	0.45
5:B:285:ILE:O	5:B:289:LEU:N	2.47	0.45
7:E:4:GLU:CB	7:E:7:ARG:HH12	2.26	0.45
4:A:364:VAL:HB	4:A:458:HIS:HB3	1.98	0.44
4:A:443:LEU:HD21	4:A:455:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:591:PHE:HA	4:A:595:THR:HG21	1.98	0.44
4:A:1282:VAL:HG22	4:A:1308:THR:HG22	1.98	0.44
5:B:416:LEU:HD23	5:B:457:LEU:HD23	1.99	0.44
5:B:803:LEU:HD13	11:J:52:THR:HG22	1.99	0.44
5:B:1009:ASP:OD2	11:J:9:SER:OG	2.32	0.44
4:A:899:VAL:HG13	4:A:1029:ARG:NH2	2.32	0.44
5:B:104:GLU:OE1	13:L:54:ARG:NH1	2.50	0.44
5:B:658:ILE:HA	5:B:661:LEU:HD12	1.98	0.44
6:C:222:LYS:HD2	6:C:222:LYS:HA	1.74	0.44
4:A:1427:ASN:HA	4:A:1430:LEU:HB2	1.98	0.44
7:E:47:CYS:HA	7:E:53:PRO:HB3	1.98	0.44
4:A:575:LYS:HE3	9:H:120:GLY:HA3	1.99	0.44
4:A:1428:VAL:HG13	5:B:1151:LEU:HD21	2.00	0.44
5:B:96:TYR:HB2	5:B:129:PHE:HB2	1.98	0.44
1:R:9:G:H1	2:T:20:DC:H42	1.66	0.44
4:A:1276:VAL:HG12	4:A:1277:GLU:H	1.83	0.44
4:A:745:GLN:HA	4:A:748:MET:HB2	1.99	0.44
4:A:779:PHE:HE2	5:B:698:GLU:HG3	1.82	0.44
5:B:813:LYS:HA	5:B:813:LYS:HD3	1.86	0.44
8:F:102:SER:OG	8:F:103:MET:SD	2.76	0.44
4:A:465:TYR:HB3	5:B:976:ILE:HG21	1.98	0.44
4:A:1355:VAL:O	4:A:1358:SER:OG	2.31	0.44
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.81	0.44
4:A:239:LEU:HD12	4:A:240:PRO:HD2	2.00	0.44
5:B:849:GLY:HA2	5:B:852:ARG:HG3	2.00	0.44
6:C:177:GLU:HB2	6:C:231:ASN:HB3	2.00	0.44
7:E:3:GLN:HG3	7:E:5:ASN:H	1.82	0.44
4:A:167:CYS:SG	4:A:168:GLY:N	2.91	0.44
4:A:575:LYS:O	4:A:579:SER:OG	2.36	0.44
4:A:896:ARG:HH22	4:A:1030:ARG:HE	1.65	0.44
5:B:384:ARG:HA	5:B:384:ARG:HD3	1.85	0.44
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.53	0.43
5:B:842:ASN:HA	5:B:999:MET:HE1	2.00	0.43
13:L:28:LYS:N	13:L:38:LEU:O	2.51	0.43
2:T:10:DT:O2	3:N:10:DG:N2	2.50	0.43
4:A:457:ALA:HB3	4:A:506:ALA:HA	2.00	0.43
5:B:124:TYR:OH	5:B:179:CYS:SG	2.66	0.43
9:H:25:ARG:HD2	9:H:39:THR:HG22	2.01	0.43
10:I:75:CYS:HB3	10:I:80:SER:H	1.83	0.43
5:B:622:LYS:HD2	10:I:59:VAL:HG11	2.00	0.43
4:A:324:SER:H	4:A:327:ALA:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:350:ARG:NE	4:A:486:GLU:OE2	2.49	0.43
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.66	0.43
5:B:604:ARG:HD3	5:B:691:GLU:HG2	2.00	0.43
4:A:4:GLN:NE2	4:A:76:GLU:OE1	2.51	0.43
4:A:369:SER:OG	12:K:2:ASN:OD1	2.27	0.43
4:A:508:PRO:HA	4:A:511:ILE:HG13	2.01	0.43
5:B:861:ASP:OD1	5:B:914:LYS:NZ	2.46	0.43
4:A:483:ASP:OD2	4:A:483:ASP:N	2.51	0.43
5:B:290:GLY:HA2	5:B:327:ARG:HD2	2.00	0.43
5:B:418:LYS:HB3	5:B:418:LYS:HE3	1.75	0.43
5:B:484:ASN:OD1	5:B:490:SER:OG	2.28	0.43
6:C:93:ASP:OD1	6:C:122:SER:OG	2.28	0.43
6:C:114:TYR:OH	11:J:19:GLU:OE2	2.37	0.43
4:A:453:MET:HE2	4:A:453:MET:HB2	1.85	0.43
4:A:1192:LEU:HD22	4:A:1239:ARG:HH21	1.83	0.43
12:K:49:GLU:HG3	12:K:94:ILE:HG12	2.00	0.43
4:A:147:VAL:HG12	4:A:170:THR:HA	2.00	0.43
4:A:345:VAL:O	4:A:348:SER:OG	2.37	0.43
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.99	0.43
4:A:30:ILE:HD12	4:A:30:ILE:HA	1.75	0.43
5:B:115:GLN:HG3	5:B:193:LYS:HB2	2.00	0.43
6:C:124:LEU:HD23	6:C:124:LEU:HA	1.88	0.43
4:A:758:ILE:O	4:A:762:SER:OG	2.34	0.43
5:B:901:PRO:HA	5:B:949:VAL:HB	1.99	0.43
4:A:362:ASP:OD1	4:A:459:ARG:NH1	2.40	0.42
6:C:36:VAL:HG11	6:C:251:LEU:HB2	2.00	0.42
6:C:206:ASN:OD1	6:C:206:ASN:N	2.52	0.42
1:R:9:G:H1	2:T:20:DC:N4	2.17	0.42
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.84	0.42
4:A:1411:GLU:OE2	4:A:1415:SER:OG	2.37	0.42
5:B:373:ARG:HA	5:B:566:LEU:HD23	2.00	0.42
9:H:117:SER:O	9:H:117:SER:OG	2.37	0.42
4:A:466:SER:OG	5:B:975:GLN:NE2	2.52	0.42
5:B:518:HIS:HB3	5:B:522:VAL:HG12	2.01	0.42
4:A:265:LYS:HD3	4:A:265:LYS:HA	1.81	0.42
5:B:60:GLN:HG2	5:B:95:ILE:HG22	2.01	0.42
6:C:95:CYS:SG	6:C:96:SER:N	2.92	0.42
11:J:2:ILE:HD12	11:J:57:ILE:HD12	2.02	0.42
5:B:128:LEU:HB3	5:B:167:ILE:HB	2.01	0.42
5:B:210:LYS:HZ2	5:B:482:VAL:HG22	1.84	0.42
9:H:104:PHE:HD2	9:H:114:VAL:HG13	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:795:GLU:HG2	5:B:731:VAL:HG11	2.01	0.42
4:A:977:LYS:HA	4:A:978:PRO:HD3	1.92	0.42
4:A:1446:ASP:OD1	4:A:1446:ASP:N	2.52	0.42
5:B:298:LEU:HD22	5:B:314:LEU:HD13	2.01	0.42
5:B:1070:GLU:OE1	11:J:44:TYR:OH	2.36	0.42
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.55	0.42
4:A:88:LYS:HA	4:A:88:LYS:HD3	1.83	0.42
4:A:1444:MET:HB2	8:F:133:VAL:HB	2.00	0.42
7:E:64:PRO:HD3	7:E:76:GLY:HA2	2.02	0.42
5:B:493:SER:O	5:B:497:ARG:NH2	2.53	0.42
5:B:942:ARG:HA	5:B:942:ARG:HD3	1.82	0.42
6:C:14:SER:N	6:C:17:ASN:O	2.53	0.42
2:T:6:DT:H6	2:T:6:DT:H2'	1.70	0.42
4:A:881:GLN:HE21	4:A:956:LEU:HB2	1.84	0.42
5:B:281:PRO:HD2	5:B:284:ILE:HD12	2.02	0.42
6:C:246:ARG:O	6:C:250:THR:OG1	2.32	0.42
8:F:120:ILE:HD13	8:F:120:ILE:HA	1.89	0.42
5:B:550:ASP:HA	5:B:551:PRO:HD3	1.91	0.41
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.53	0.41
4:A:289:ILE:O	4:A:293:GLU:N	2.50	0.41
4:A:360:GLU:HB2	4:A:363:GLN:HG3	2.03	0.41
4:A:810:PRO:HD3	5:B:730:ARG:HH21	1.85	0.41
1:R:2:U:OP2	5:B:1124:ARG:NH1	2.53	0.41
4:A:1118:VAL:HG13	4:A:1327:ILE:HD11	2.01	0.41
4:A:1444:MET:O	8:F:133:VAL:N	2.52	0.41
5:B:213:ILE:HD12	5:B:213:ILE:HA	1.94	0.41
9:H:116:TYR:HB2	9:H:123:MET:HB3	2.03	0.41
4:A:99:ILE:HA	4:A:102:VAL:HG12	2.02	0.41
4:A:265:LYS:HB3	4:A:303:TYR:HB2	2.02	0.41
5:B:356:LEU:HA	5:B:360:PHE:HB3	2.02	0.41
5:B:783:THR:H	5:B:783:THR:HG1	1.60	0.41
11:J:17:LYS:HB3	11:J:39:LEU:HD13	2.02	0.41
4:A:445:ASN:HB3	4:A:488:ASN:HB2	2.02	0.41
4:A:587:HIS:NE2	4:A:969:GLN:HG3	2.35	0.41
4:A:825:ILE:HD13	4:A:825:ILE:HA	1.90	0.41
5:B:218:SER:C	5:B:241:ARG:CZ	2.87	0.41
6:C:61:GLU:H	6:C:61:GLU:HG3	1.68	0.41
7:E:167:ARG:HA	7:E:167:ARG:HD3	1.78	0.41
10:I:84:VAL:HG12	10:I:102:VAL:HB	2.03	0.41
4:A:451:HIS:NE2	4:A:515:GLN:OE1	2.47	0.41
4:A:784:LEU:HD23	4:A:784:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1021:LEU:O	4:A:1024:SER:OG	2.32	0.41
5:B:977:GLY:HA2	5:B:989:THR:HB	2.03	0.41
5:B:999:MET:HE2	5:B:999:MET:HB2	1.97	0.41
5:B:1147:LEU:HD23	5:B:1147:LEU:HA	1.93	0.41
6:C:255:VAL:HB	12:K:95:ILE:HD11	2.03	0.41
7:E:135:PHE:HB3	7:E:140:LEU:HD11	2.01	0.41
4:A:693:VAL:HG21	4:A:721:PHE:HE1	1.86	0.41
7:E:156:LEU:HD12	7:E:195:VAL:HB	2.03	0.41
10:I:74:GLU:OE2	10:I:79:HIS:ND1	2.39	0.41
4:A:1116:LEU:CD2	4:A:1329:THR:HG22	2.51	0.40
5:B:492:LEU:HB3	5:B:751:VAL:HG21	2.02	0.40
6:C:76:ASP:HB3	6:C:79:GLN:NE2	2.36	0.40
7:E:127:ILE:HG22	7:E:129:PRO:HD2	2.02	0.40
9:H:28:ALA:HB3	9:H:38:LEU:CD2	2.51	0.40
9:H:136:LYS:HE2	9:H:136:LYS:HB3	1.85	0.40
12:K:83:PRO:O	12:K:87:LEU:N	2.52	0.40
4:A:702:LEU:HD23	4:A:702:LEU:HA	1.95	0.40
5:B:786:ASN:OD1	5:B:967:ARG:NH2	2.55	0.40
5:B:1032:SER:HB2	5:B:1089:PRO:HG2	2.03	0.40
9:H:89:LEU:H	9:H:89:LEU:HG	1.77	0.40
4:A:146:MET:N	4:A:146:MET:SD	2.94	0.40
4:A:525:GLN:NE2	5:B:836:GLU:OE2	2.53	0.40
9:H:110:ASP:C	9:H:111:LEU:HD12	2.41	0.40
3:N:5:DC:H2'	3:N:6:DG:C8	2.57	0.40
4:A:1288:ASP:OD1	4:A:1288:ASP:N	2.55	0.40
5:B:261:ARG:HE	5:B:261:ARG:HB2	1.77	0.40
4:A:407:ARG:HD3	4:A:413:ILE:HD11	2.03	0.40
5:B:941:LEU:HD13	5:B:942:ARG:N	2.37	0.40
10:I:7:CYS:SG	10:I:9:ASP:N	2.94	0.40

All (2) 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)
10:I:82:GLU:CD	10:I:82:GLU:OE2[2_556]	1.22	0.98
10:I:82:GLU:OE1	10:I:82:GLU:OE2[2_556]	2.06	0.14

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	1368/1733 (79%)	1292 (94%)	76 (6%)	0	100	100
5	B	1103/1224 (90%)	1059 (96%)	44 (4%)	0	100	100
6	C	265/318 (83%)	254 (96%)	11 (4%)	0	100	100
7	E	211/215 (98%)	198 (94%)	13 (6%)	0	100	100
8	F	83/155 (54%)	80 (96%)	3 (4%)	0	100	100
9	H	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
10	I	116/122 (95%)	107 (92%)	8 (7%)	1 (1%)	17	57
11	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
12	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3491/4173 (84%)	3320 (95%)	170 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	I	58	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	
4	A	1191/1520 (78%)	1133 (95%)	58 (5%)	25	59
5	B	955/1061 (90%)	918 (96%)	37 (4%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	C	235/274 (86%)	225 (96%)	10 (4%)	29 63
7	E	194/197 (98%)	180 (93%)	14 (7%)	14 47
8	F	72/137 (53%)	68 (94%)	4 (6%)	21 56
9	H	116/128 (91%)	107 (92%)	9 (8%)	12 44
10	I	110/116 (95%)	105 (96%)	5 (4%)	27 62
11	J	60/65 (92%)	56 (93%)	4 (7%)	16 50
12	K	99/102 (97%)	95 (96%)	4 (4%)	31 65
13	L	37/57 (65%)	35 (95%)	2 (5%)	22 57
All	All	3069/3657 (84%)	2922 (95%)	147 (5%)	25 60

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	15	LYS
4	A	22	PHE
4	A	23	SER
4	A	42	ASP
4	A	70	CYS
4	A	75	ASN
4	A	83	HIS
4	A	108	MET
4	A	151	ASP
4	A	167	CYS
4	A	176	LYS
4	A	200	ARG
4	A	236	LEU
4	A	281	HIS
4	A	299	HIS
4	A	303	TYR
4	A	335	ARG
4	A	337	ARG
4	A	341	MET
4	A	356	ASP
4	A	383	TYR
4	A	393	ARG
4	A	417	TYR
4	A	438	ASP
4	A	450	LEU
4	A	494	SER

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Mol	Chain	Res	Type
4	A	537	ARG
4	A	544	ASP
4	A	552	TRP
4	A	588	LEU
4	A	598	LEU
4	A	618	GLU
4	A	672	ASP
4	A	691	LEU
4	A	732	LEU
4	A	739	ASP
4	A	764	CYS
4	A	806	ARG
4	A	821	ARG
4	A	836	TYR
4	A	847	ASP
4	A	877	HIS
4	A	1001	ARG
4	A	1029	ARG
4	A	1043	ASP
4	A	1063	MET
4	A	1215	ARG
4	A	1274	ARG
4	A	1289	ARG
4	A	1297	GLU
4	A	1370	LEU
4	A	1373	ASP
4	A	1387	HIS
4	A	1391	ARG
4	A	1400	CYS
4	A	1402	PHE
4	A	1441	PHE
4	A	1446	ASP
5	B	57	TYR
5	B	65	GLU
5	B	66	ASP
5	B	103	ASN
5	B	131	ASP
5	B	199	MET
5	B	217	ARG
5	B	235	SER
5	B	250	PHE
5	B	388	CYS

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Mol	Chain	Res	Type
5	B	394	ASP
5	B	398	ARG
5	B	401	PHE
5	B	466	TRP
5	B	488	TYR
5	B	543	SER
5	B	576	ASP
5	B	601	ARG
5	B	614	SER
5	B	642	ASP
5	B	668	ASP
5	B	734	HIS
5	B	766	ARG
5	B	797	TYR
5	B	838	SER
5	B	864	LYS
5	B	904	ARG
5	B	975	GLN
5	B	996	ARG
5	B	1135	ARG
5	B	1150	ARG
5	B	1168	LEU
5	B	1190	ASP
5	B	1193	GLN
5	B	1210	MET
5	B	1215	ARG
5	B	1217	TYR
6	C	62	PHE
6	C	75	MET
6	C	108	GLU
6	C	112	ASN
6	C	115	SER
6	C	140	ASN
6	C	178	PHE
6	C	206	ASN
6	C	215	GLU
6	C	262	LEU
7	E	7	ARG
7	E	29	PHE
7	E	43	LYS
7	E	55	ARG
7	E	57	MET

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Mol	Chain	Res	Type
7	E	58	MET
7	E	72	PHE
7	E	82	PHE
7	E	85	GLU
7	E	110	PHE
7	E	114	ASN
7	E	162	ARG
7	E	168	TYR
7	E	182	ASP
8	F	92	ARG
8	F	102	SER
8	F	111	LEU
8	F	114	GLU
9	H	37	LYS
9	H	38	LEU
9	H	78	SER
9	H	87	ARG
9	H	91	ASP
9	H	104	PHE
9	H	124	ARG
9	H	130	ARG
9	H	146	ARG
10	I	4	PHE
10	I	7	CYS
10	I	20	LYS
10	I	30	ARG
10	I	115	LYS
11	J	7	CYS
11	J	26	GLN
11	J	38	ARG
11	J	46	CYS
12	K	6	ARG
12	K	26	LYS
12	K	54	ARG
12	K	81	TYR
13	L	31	CYS
13	L	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	45	GLN

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Mol	Chain	Res	Type
4	A	299	HIS
4	A	445	ASN
4	A	458	HIS
4	A	654	ASN
4	A	698	GLN
4	A	1390	ASN
5	B	46	GLN
5	B	60	GLN
5	B	103	ASN
5	B	481	GLN
5	B	499	ASN
5	B	763	GLN
5	B	975	GLN
5	B	984	HIS
5	B	1193	GLN
5	B	1195	HIS
6	C	79	GLN
7	E	99	HIS
7	E	114	ASN
7	E	146	HIS
9	H	128	ASN
12	K	29	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/12 (83%)	4 (40%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	4	G
1	R	10	A
1	R	11	U
1	R	12	U

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	G35	T	19	2	18,23,24	4.66	14 (77%)	20,33,36	1.48	3 (15%)

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
2	G35	T	19	2	-	4/10/41/42	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	G35	C2-N3	9.24	1.49	1.33
2	T	19	G35	O4'-C4'	7.75	1.62	1.45
2	T	19	G35	C3'-C4'	-6.87	1.34	1.53
2	T	19	G35	C5-N7	6.41	1.45	1.37
2	T	19	G35	C8-N9	6.08	1.46	1.37
2	T	19	G35	O4'-C1'	-5.22	1.30	1.42
2	T	19	G35	C8-N7	4.71	1.47	1.38
2	T	19	G35	C2-N12	4.14	1.48	1.32
2	T	19	G35	C4-N3	3.31	1.48	1.44
2	T	19	G35	O3'-C3'	3.15	1.50	1.43
2	T	19	G35	O8-C8	-2.90	1.17	1.23
2	T	19	G35	O5-C5	-2.62	1.18	1.23
2	T	19	G35	C1'-N9	2.52	1.49	1.45
2	T	19	G35	C2-N11	-2.28	1.25	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	19	G35	C5-C4-N9	4.42	108.14	102.28
2	T	19	G35	C5-C4-N3	-2.57	107.30	112.76
2	T	19	G35	C2'-C1'-N9	-2.14	112.70	115.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	G35	O4'-C1'-N9-C4
2	T	19	G35	O4'-C4'-C5'-O5'
2	T	19	G35	C3'-C4'-C5'-O5'
2	T	19	G35	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	R	11/12 (91%)	-0.02	0 100 100	120, 133, 197, 200	0
2	T	25/29 (86%)	-0.26	0 100 100	120, 191, 237, 249	0
3	N	16/18 (88%)	-0.17	0 100 100	180, 209, 248, 270	0
4	A	1382/1733 (79%)	-0.17	15 (1%) 80 68	53, 105, 171, 311	0
5	B	1123/1224 (91%)	-0.18	8 (0%) 87 78	37, 95, 157, 274	0
6	C	267/318 (83%)	-0.29	0 100 100	58, 98, 142, 184	0
7	E	213/215 (99%)	-0.14	7 (3%) 46 31	69, 133, 224, 276	0
8	F	85/155 (54%)	-0.33	0 100 100	62, 108, 146, 175	0
9	H	133/146 (91%)	-0.14	1 (0%) 86 75	78, 116, 182, 250	0
10	I	118/122 (96%)	-0.41	0 100 100	69, 108, 142, 179	0
11	J	65/70 (92%)	-0.33	0 100 100	46, 89, 131, 150	0
12	K	114/120 (95%)	-0.28	0 100 100	47, 96, 127, 165	0
13	L	43/70 (61%)	-0.26	0 100 100	60, 134, 174, 191	0
All	All	3595/4232 (84%)	-0.20	31 (0%) 84 73	37, 103, 177, 311	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	93	MET	5.1
4	A	111	GLY	4.4
5	B	1218	THR	4.2
5	B	1219	ASP	4.2
4	A	44	THR	4.0
7	E	83	CYS	3.8
4	A	258	GLY	3.6
7	E	126	SER	3.2
4	A	271	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
5	B	429	PHE	3.1
5	B	869	SER	3.1
5	B	106	ASP	3.0
4	A	45	GLN	2.9
9	H	83	GLN	2.9
4	A	164	ARG	2.7
7	E	110	PHE	2.6
4	A	323	LYS	2.5
4	A	144	THR	2.4
7	E	120	ALA	2.3
4	A	1192	LEU	2.3
4	A	257	ARG	2.2
4	A	660	ASN	2.2
4	A	150	THR	2.2
4	A	425	GLN	2.2
7	E	125	PRO	2.2
5	B	167	ILE	2.2
5	B	432	MET	2.1
5	B	108	VAL	2.1
4	A	66	LYS	2.1
7	E	109	ILE	2.0
4	A	177	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	G35	T	19	22/23	0.86	0.20	136,151,189,197	0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	ZN	A	1801	1/1	0.79	0.07	319,319,319,319	0
14	ZN	B	1301	1/1	0.88	0.12	149,149,149,149	0
14	ZN	L	101	1/1	0.90	0.04	149,149,149,149	0
14	ZN	J	101	1/1	0.91	0.39	218,218,218,218	0
15	MG	A	1803	1/1	0.91	0.11	89,89,89,89	0
14	ZN	A	1802	1/1	0.95	0.07	117,117,117,117	0
14	ZN	C	401	1/1	0.96	0.24	223,223,223,223	0
14	ZN	I	202	1/1	0.97	0.12	108,108,108,108	0
14	ZN	I	201	1/1	0.98	0.15	101,101,101,101	0

6.5 Other polymers (i)

There are no such residues in this entry.