



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:00 am BST

PDB ID : 3RZO
Title : RNA Polymerase II Initiation Complex with a 4-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-12
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

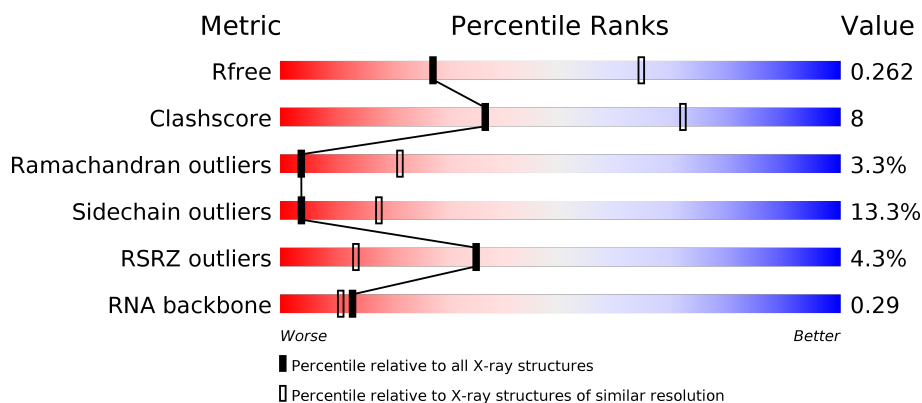
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



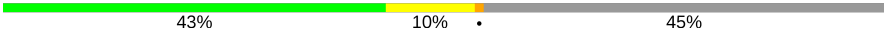







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>20%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	1224	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>57%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
4	E	215	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	4	
12	T	29	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28547 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

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

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

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

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

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

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

- Molecule 11 is a RNA chain called RNA (5'-R(*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	4	Total	C	N	O	P	0	0	0
			88	40	20	25	3			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	8	Total	C	N	O	P	0	0	0
			159	76	26	49	8			

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

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

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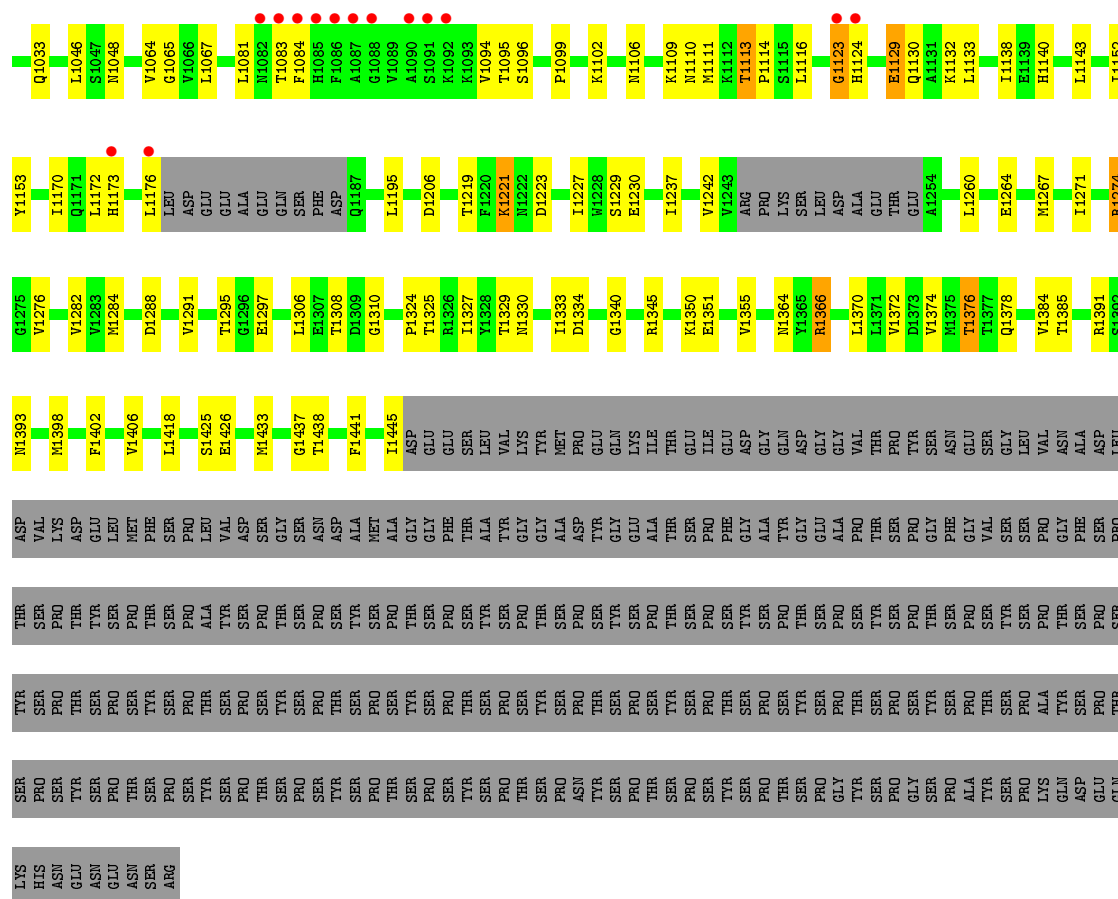
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

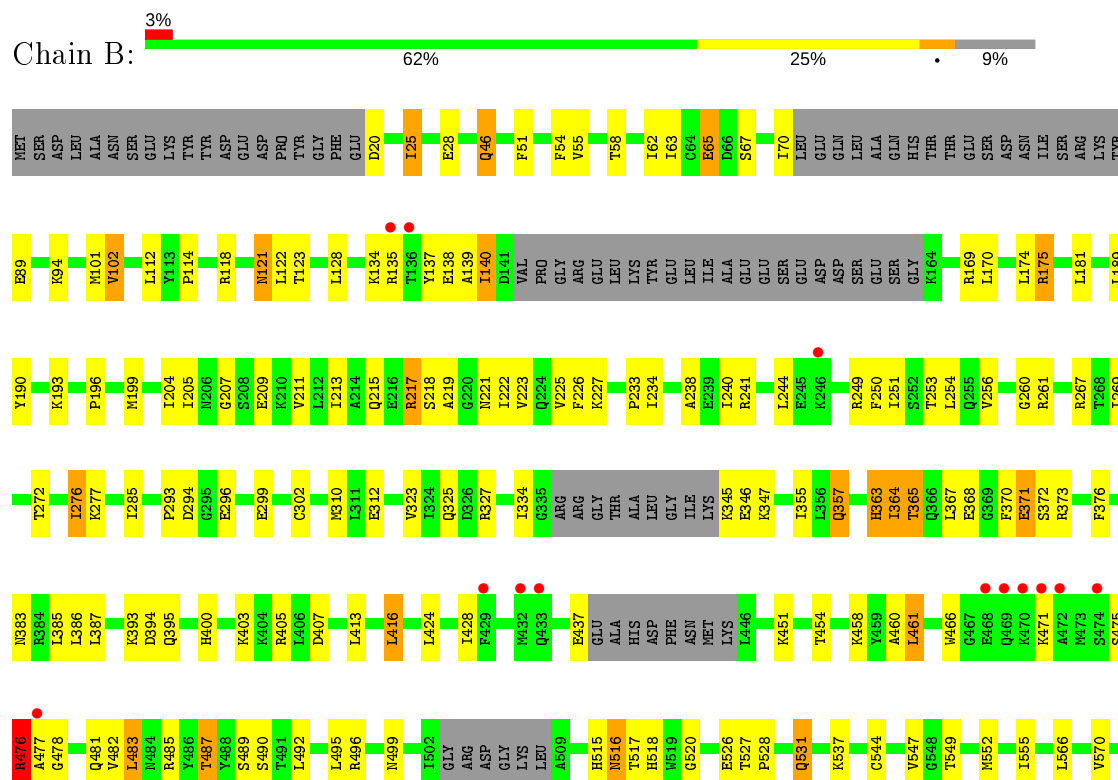
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

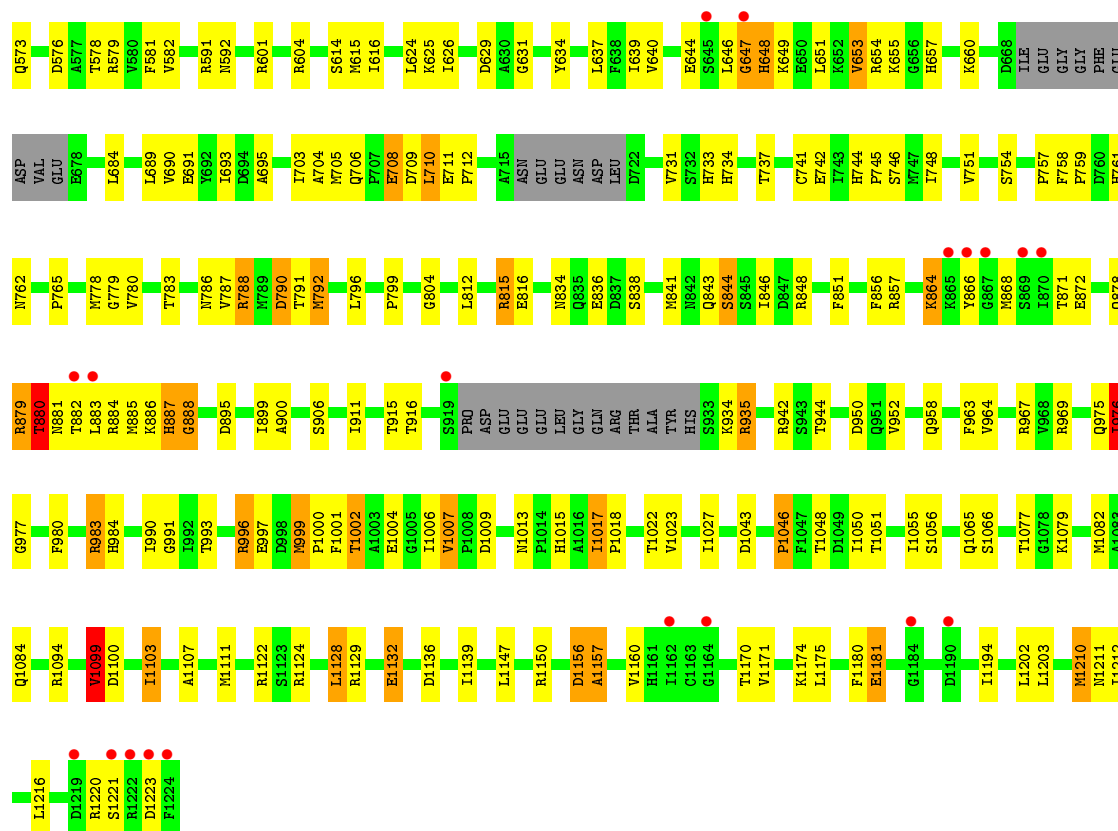
- Chain A:

Sequence logo for Chain A. The y-axis lists amino acids (MET, VAL, P10, L11, R12, K15, Q18, S23, P24, E25, E26, I30, I35, R36, F37, T40, M41, E43, T44, Q45, K49, G52, L53, N54, D55, P56, R57, L58, I61, D62, L65, K66, T69, C70, Q71, G73, E76, L86, A87, F91, H92, V93). The x-axis shows sequence positions (1 to 1000). The logo is a heatmap where color intensity represents the probability of an amino acid at a position. A color scale at the top indicates values from 6% (red) to 19% (grey).

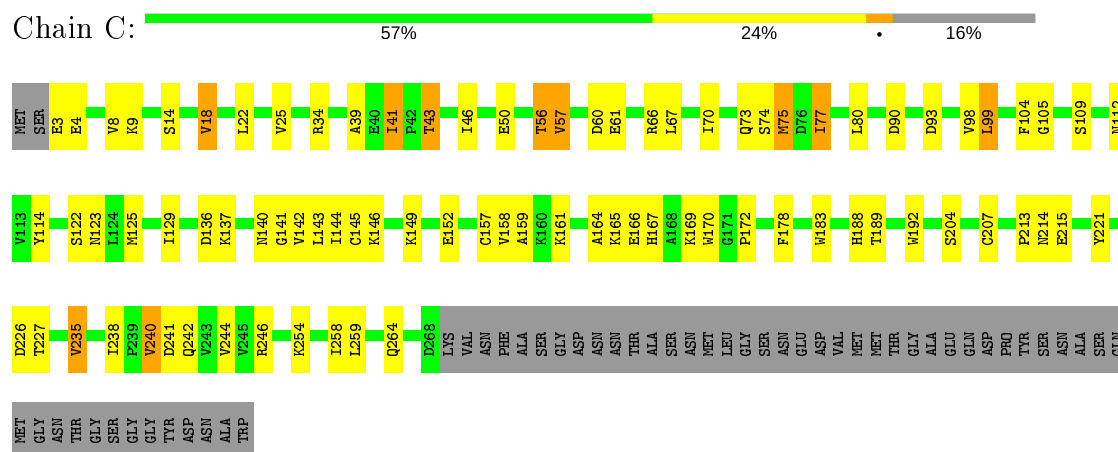


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

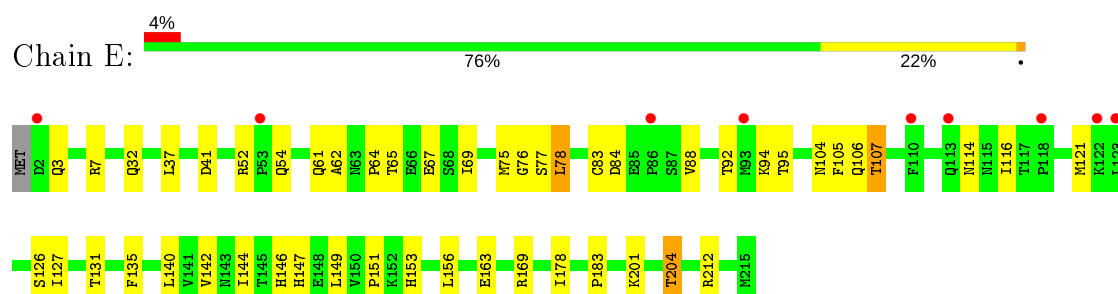




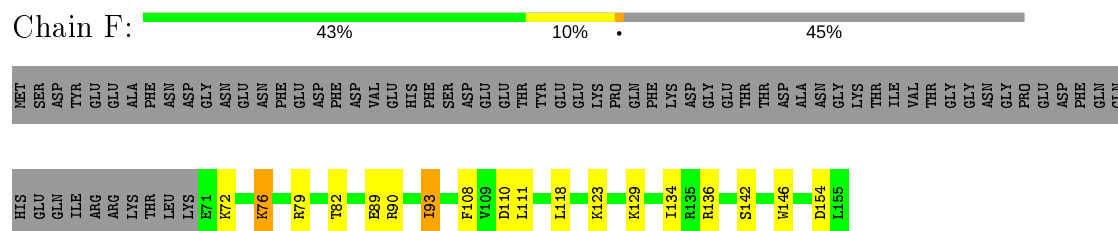
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



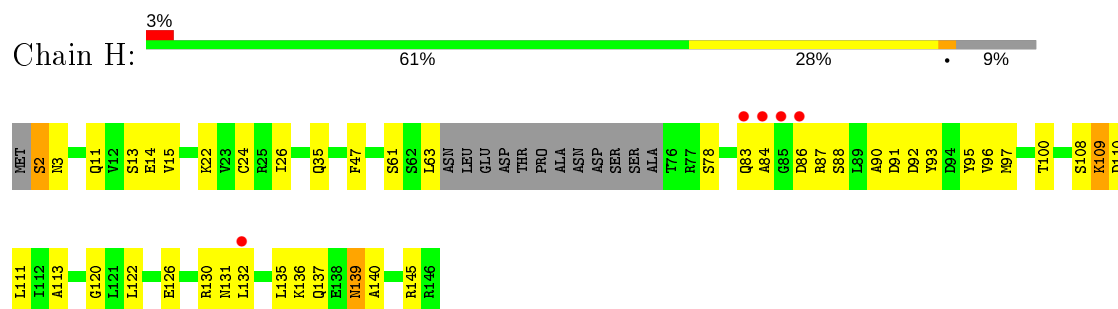
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



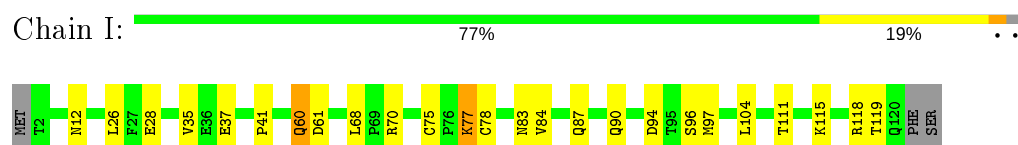
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



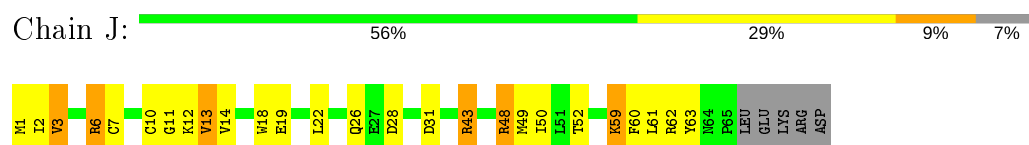
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



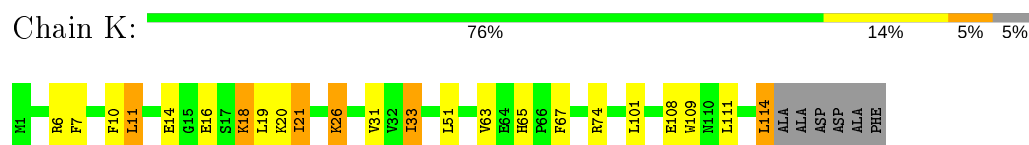
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



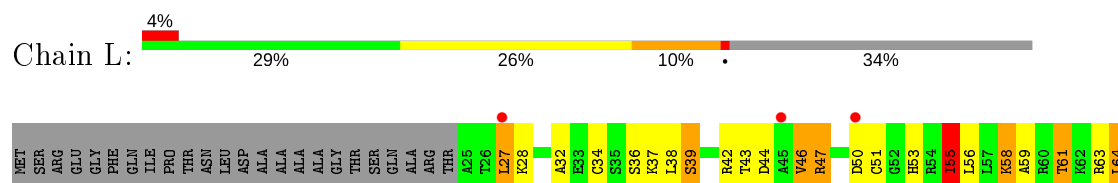
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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

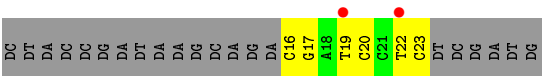




- Molecule 11: RNA (5'-R(*GP*AP*GP*G)-3')



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.04Å 221.15Å 192.88Å 90.00° 98.34° 90.00°	Depositor
Resolution (Å)	40.01 – 3.00 40.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.01-3.00) 99.3 (40.01-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.188 , 0.236 0.213 , 0.262	Depositor DCC
R_{free} test set	6685 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28547	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/11241	0.76	2/15199 (0.0%)
2	B	0.52	0/9033	0.79	4/12181 (0.0%)
3	C	0.47	0/2133	0.80	0/2891
4	E	0.45	0/1788	0.71	0/2406
5	F	0.46	0/700	0.70	0/945
6	H	0.47	0/1086	0.82	1/1470 (0.1%)
7	I	0.48	0/989	0.79	0/1331
8	J	0.55	0/541	0.86	0/727
9	K	0.45	0/937	0.70	0/1265
10	L	0.54	0/365	0.93	1/485 (0.2%)
11	R	0.88	0/99	1.45	0/154
12	T	1.25	0/176	2.19	12/268 (4.5%)
All	All	0.50	0/29088	0.80	20/39322 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	O4'-C1'-N1	8.75	114.12	108.00
2	B	647	GLY	C-N-CA	8.32	142.50	121.70
12	T	22	DT	P-O3'-C3'	7.60	128.82	119.70
12	T	16	DC	C2-N1-C1'	6.96	126.45	118.80
12	T	20	DC	O4'-C1'-N1	6.96	112.87	108.00
12	T	19	DT	O4'-C1'-N1	6.89	112.83	108.00
2	B	648	HIS	N-CA-CB	6.82	122.87	110.60
12	T	16	DC	N1-C2-O2	6.67	122.90	118.90
12	T	23	DC	O4'-C1'-N1	6.36	112.45	108.00
12	T	16	DC	P-O3'-C3'	5.68	126.52	119.70
1	A	451	HIS	CB-CA-C	-5.60	99.19	110.40
12	T	16	DC	C6-N1-C1'	-5.57	114.12	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	N1-C1'-C2'	5.38	122.82	112.60
6	H	2	SER	C-N-CA	5.37	135.13	121.70
2	B	140	ILE	C-N-CA	5.25	134.81	121.70
10	L	50	ASP	C-N-CA	5.18	134.65	121.70
12	T	17	DG	O4'-C4'-C3'	-5.16	102.44	104.50
1	A	399	HIS	N-CA-CB	5.12	119.82	110.60
2	B	476	ARG	C-N-CA	5.07	134.36	121.70
12	T	17	DG	C1'-O4'-C4'	-5.03	105.07	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	182	0
2	B	8861	0	8884	190	0
3	C	2095	0	2051	51	0
4	E	1752	0	1776	18	0
5	F	688	0	707	9	0
6	H	1068	0	1040	12	0
7	I	971	0	927	7	0
8	J	532	0	542	20	0
9	K	919	0	929	16	0
10	L	363	0	386	13	0
11	R	88	0	46	0	0
12	T	159	0	91	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	28547	0	28512	452	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (452) 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)
1:A:756:ILE:CD1	1:A:756:ILE:CG1	1.77	1.56
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.90	1.06
1:A:869:GLY:O	4:E:204:THR:HG21	1.63	0.96
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.89	0.88
6:H:2:SER:HB2	6:H:3:ASN:HB2	1.56	0.88
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.39	0.88
8:J:48:ARG:O	8:J:52:THR:HG22	1.76	0.84
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.22	0.83
3:C:56:THR:HG21	3:C:145:CYS:SG	2.20	0.82
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.61	0.82
1:A:901:LEU:HA	1:A:907:THR:HG23	1.60	0.82
1:A:741:ASN:HD22	1:A:744:LYS:H	1.29	0.81
5:F:110:ASP:O	5:F:123:LYS:HE2	1.81	0.80
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.63	0.79
1:A:754:SER:H	1:A:757:ASN:HD22	1.30	0.77
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.66	0.76
2:B:276:ILE:HG13	2:B:334:ILE:HG23	1.68	0.76
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.69	0.74
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.69	0.74
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.72	0.72
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.54	0.72
3:C:167:HIS:HD2	3:C:169:LYS:H	1.36	0.71
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.74	0.69
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.58	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.38	0.69
1:A:756:ILE:H	1:A:756:ILE:HD13	1.58	0.69
4:E:77:SER:HB3	4:E:105:PHE:HA	1.74	0.68
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.58	0.68
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.76	0.67
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.77	0.67
1:A:399:HIS:O	1:A:401:GLY:N	2.27	0.67
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.43	0.66
2:B:706:GLN:O	2:B:710:LEU:HB2	1.95	0.66
1:A:1364:ASN:HD21	1:A:1366:ARG:HD2	1.61	0.65
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.62	0.65
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.79	0.64
2:B:848:ARG:HH22	2:B:996:ARG:NH1	1.95	0.64
1:A:378:GLU:OE2	1:A:434:ARG:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:ASN:HD22	2:B:516:ASN:H	1.46	0.64
2:B:834:ASN:HA	2:B:838:SER:HB2	1.78	0.64
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.80	0.63
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.12	0.63
1:A:946:VAL:HG13	4:E:201:LYS:HB3	1.81	0.63
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.79	0.63
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.80	0.63
2:B:54:PHE:HA	2:B:58:THR:HB	1.80	0.63
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.81	0.63
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.81	0.63
2:B:864:LYS:HB3	2:B:872:GLU:H	1.61	0.62
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.64	0.62
1:A:469:ARG:NH2	2:B:991:GLY:O	2.32	0.62
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.14	0.62
1:A:567:LYS:HB3	6:H:96:VAL:H	1.63	0.62
1:A:705:LYS:HE3	1:A:705:LYS:H	1.65	0.62
3:C:165:LYS:O	9:K:6:ARG:NH1	2.33	0.62
2:B:260:GLY:O	2:B:267:ARG:HD3	1.99	0.62
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.64	0.61
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.82	0.61
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.81	0.61
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.81	0.61
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.81	0.61
3:C:73:GLN:HE21	3:C:75:MET:H	1.49	0.61
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.54	0.60
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.31	0.60
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.67	0.60
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.84	0.60
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.84	0.60
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.83	0.60
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.84	0.59
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.83	0.59
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.84	0.59
1:A:404:TYR:HA	1:A:413:ILE:O	2.03	0.59
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.48	0.59
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.84	0.59
2:B:345:LYS:HA	2:B:347:LYS:H	1.67	0.59
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.51	0.58
2:B:887:HIS:HA	2:B:888:GLY:O	2.03	0.58
4:E:88:VAL:HB	4:E:116:ILE:HD13	1.84	0.58
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:48:ARG:O	8:J:52:THR:CG2	2.49	0.58
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.03	0.58
3:C:41:ILE:HD12	3:C:246:ARG:HB2	1.86	0.58
9:K:65:HIS:CD2	9:K:67:PHE:H	2.22	0.58
1:A:596:THR:O	1:A:598:LEU:N	2.36	0.58
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.86	0.57
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.85	0.57
2:B:887:HIS:HA	2:B:888:GLY:C	2.24	0.57
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.40	0.57
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.86	0.57
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.85	0.57
8:J:6:ARG:HG3	8:J:13:VAL:HG13	1.87	0.57
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.86	0.57
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.85	0.57
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.86	0.56
2:B:999:MET:HB3	2:B:1007:VAL:HG22	1.87	0.56
2:B:219:ALA:HB3	2:B:222:ILE:HD12	1.87	0.56
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.88	0.56
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.89	0.56
2:B:843:GLN:HB2	2:B:993:THR:HB	1.86	0.56
1:A:924:LYS:O	1:A:927:VAL:HG12	2.06	0.56
2:B:975:GLN:HG2	2:B:976:ILE:H	1.69	0.56
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.88	0.55
1:A:588:LEU:HD23	1:A:605:MET:HG2	1.88	0.55
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.05	0.55
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.89	0.55
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.35	0.55
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.55
2:B:363:HIS:O	2:B:364:ILE:HB	2.07	0.55
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.31	0.54
2:B:705:MET:H	2:B:710:LEU:HG	1.73	0.54
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.88	0.54
1:A:313:GLN:HG2	1:A:322:VAL:HG22	1.88	0.54
1:A:567:LYS:O	1:A:569:LYS:N	2.40	0.54
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.43	0.54
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.54	0.54
2:B:357:GLN:HG2	2:B:368:GLU:HA	1.89	0.54
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.43	0.54
1:A:741:ASN:ND2	1:A:744:LYS:H	2.00	0.54
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.71	0.54
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:7:CYS:HA	8:J:49:MET:HG2	1.89	0.54
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.88	0.54
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.43	0.54
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.72	0.54
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.89	0.54
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.90	0.53
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.89	0.53
2:B:915:THR:HG21	2:B:934:LYS:HD2	1.89	0.53
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.88	0.53
2:B:213:ILE:HG12	2:B:481:GLN:HG3	1.90	0.53
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.90	0.53
2:B:222:ILE:HD13	2:B:403:LYS:HG3	1.90	0.53
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.44	0.53
8:J:6:ARG:HG2	8:J:11:GLY:O	2.09	0.53
2:B:983:ARG:HB2	2:B:983:ARG:HH11	1.74	0.52
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.90	0.52
2:B:999:MET:HA	2:B:999:MET:CE	2.39	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.41	0.52
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.74	0.52
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.92	0.52
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.39	0.52
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.41	0.52
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.44	0.52
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.92	0.52
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.90	0.52
6:H:137:GLN:HB3	6:H:139:ASN:HB2	1.92	0.52
9:K:65:HIS:HD2	9:K:67:PHE:H	1.56	0.52
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.52
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.09	0.51
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.92	0.51
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	1.91	0.51
2:B:516:ASN:ND2	2:B:516:ASN:H	2.08	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:HG12	1.93	0.51
1:A:1096:SER:O	1:A:1099:PRO:HD2	2.11	0.51
2:B:58:THR:O	2:B:62:ILE:HG12	2.10	0.51
1:A:15:LYS:HB3	2:B:1220:ARG:HG2	1.92	0.51
8:J:12:LYS:HD2	8:J:43:ARG:HH12	1.76	0.51
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.93	0.50
3:C:46:ILE:HA	3:C:159:ALA:HA	1.93	0.50
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.93	0.50
2:B:976:ILE:HG23	2:B:977:GLY:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:VAL:HG13	6:H:78:SER:HA	1.93	0.50
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.75	0.50
5:F:111:LEU:H	5:F:111:LEU:HD12	1.77	0.50
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.92	0.50
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.75	0.50
1:A:756:ILE:CD1	1:A:756:ILE:H	2.23	0.50
2:B:705:MET:N	2:B:710:LEU:HG	2.27	0.50
2:B:804:GLY:O	2:B:983:ARG:NH2	2.45	0.50
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.94	0.50
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.93	0.50
1:A:826:ASP:HA	1:A:829:VAL:HB	1.94	0.50
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.93	0.50
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.94	0.49
3:C:235:VAL:HG11	8:J:6:ARG:HH21	1.77	0.49
1:A:315:LEU:HA	1:A:320:ARG:HB3	1.92	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.93	0.49
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.47	0.49
3:C:22:LEU:HD11	9:K:101:LEU:HD11	1.93	0.49
2:B:466:TRP:HB3	2:B:475:SER:HB3	1.93	0.49
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.93	0.49
4:E:65:THR:HG22	4:E:67:GLU:H	1.77	0.49
10:L:27:LEU:HB3	10:L:37:LYS:HG2	1.94	0.49
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.12	0.49
2:B:476:ARG:O	2:B:478:GLY:N	2.45	0.49
2:B:256:VAL:HG12	2:B:385:LEU:HD22	1.93	0.49
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.95	0.49
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.95	0.49
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.44	0.49
2:B:1002:THR:CG2	2:B:1006:ILE:H	2.25	0.49
1:A:371:ALA:HA	1:A:436:ILE:HG22	1.95	0.49
1:A:626:ASN:O	1:A:631:HIS:CD2	2.66	0.49
2:B:1082:MET:HA	3:C:189:THR:HA	1.95	0.49
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.37	0.49
1:A:128:ILE:HG23	1:A:134:ARG:HG3	1.94	0.48
2:B:783:THR:CG2	8:J:59:LYS:HB3	2.43	0.48
1:A:219:PHE:HZ	1:A:226:GLU:HA	1.78	0.48
1:A:396:PRO:HB3	1:A:403:LYS:HB3	1.94	0.48
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.13	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.95	0.48
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.96	0.48
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LYS:O	1:A:748:MET:HG3	2.13	0.48
3:C:167:HIS:CD2	3:C:169:LYS:H	2.24	0.48
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.39	0.48
2:B:640:VAL:HG13	2:B:649:LYS:HB3	1.95	0.48
2:B:708:GLU:O	2:B:710:LEU:N	2.46	0.48
2:B:190:TYR:CD1	8:J:62:ARG:HG2	2.48	0.48
2:B:704:ALA:HB1	2:B:710:LEU:HB3	1.95	0.48
2:B:637:LEU:HD12	2:B:693:ILE:HG13	1.95	0.47
10:L:61:THR:HG21	10:L:63:ARG:HG3	1.96	0.47
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.96	0.47
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	0.47
2:B:492:LEU:O	2:B:496:ARG:HG3	2.14	0.47
2:B:841:MET:O	2:B:993:THR:HA	2.14	0.47
3:C:105:GLY:O	3:C:149:LYS:O	2.32	0.47
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.97	0.47
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.97	0.47
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.96	0.47
1:A:55:ASP:O	1:A:57:ARG:N	2.47	0.47
2:B:880:THR:C	2:B:882:THR:H	2.17	0.47
1:A:323:LYS:HG3	1:A:328:ARG:HG3	1.96	0.47
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.97	0.47
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.96	0.47
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.79	0.47
2:B:705:MET:CE	2:B:742:GLU:HG2	2.45	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.66	0.47
8:J:3:VAL:CG1	8:J:18:TRP:HB2	2.44	0.47
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.97	0.47
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.97	0.47
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.97	0.47
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.97	0.47
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.14	0.47
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.12	0.47
1:A:324:SER:O	1:A:326:ARG:N	2.40	0.47
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.96	0.47
2:B:1048:THR:OG1	2:B:1050:ILE:HD12	2.15	0.47
2:B:792:MET:HA	2:B:856:PHE:O	2.14	0.47
3:C:98:VAL:H	3:C:122:SER:HB2	1.80	0.47
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	1.96	0.46
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.97	0.46
1:A:702:LEU:O	1:A:710:LEU:HD11	2.14	0.46
2:B:370:PHE:O	2:B:372:SER:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:LEU:O	2:B:428:ILE:HG12	2.15	0.46
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.51	0.46
2:B:128:LEU:HD11	2:B:170:LEU:HB2	1.96	0.46
2:B:487:THR:HG22	2:B:490:SER:HB3	1.98	0.46
2:B:601:ARG:HG2	2:B:615:MET:HE3	1.97	0.46
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.97	0.46
1:A:350:ARG:HB2	2:B:1128:LEU:HD21	1.98	0.46
3:C:166:GLU:HG2	9:K:6:ARG:HB2	1.97	0.46
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.97	0.46
1:A:467:THR:HG23	2:B:976:ILE:HG23	1.97	0.46
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.98	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HD12	1.96	0.46
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.97	0.46
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.46	0.46
1:A:704:ALA:H	1:A:710:LEU:HD22	1.81	0.46
1:A:203:SER:HB3	1:A:206:GLU:HB2	1.98	0.45
1:A:23:SER:HB3	1:A:26:GLU:HB2	1.99	0.45
1:A:907:THR:HG22	1:A:908:LEU:H	1.81	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.98	0.45
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.97	0.45
1:A:1102:LYS:HE2	1:A:1106:ASN:HD21	1.81	0.45
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.99	0.45
2:B:654:ARG:H	2:B:657:HIS:HD2	1.63	0.45
2:B:783:THR:HG23	8:J:59:LYS:HB3	1.97	0.45
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.51	0.45
5:F:93:ILE:HD13	5:F:134:ILE:HD11	1.98	0.45
1:A:942:PHE:O	1:A:946:VAL:HG23	2.17	0.45
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.99	0.45
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.98	0.45
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.98	0.45
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.50	0.45
2:B:1103:ILE:O	2:B:1122:ARG:HD2	2.16	0.45
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.99	0.45
3:C:8:VAL:HG12	9:K:108:GLU:HG3	1.97	0.45
5:F:72:LYS:HE2	5:F:142:SER:HB3	1.98	0.45
6:H:135:LEU:C	6:H:137:GLN:H	2.20	0.45
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	1.99	0.45
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.81	0.45
3:C:146:LYS:HB3	8:J:61:LEU:HD11	1.98	0.45
1:A:839:ARG:HH21	1:A:1402:PHE:HA	1.80	0.45
1:A:55:ASP:H	1:A:56:PRO:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:THR:HG22	1:A:983:ILE:H	1.82	0.45
1:A:700:ASN:HD22	7:I:115:LYS:HB2	1.82	0.45
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.50	0.45
2:B:515:HIS:CD2	2:B:517:THR:H	2.35	0.45
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.99	0.45
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.52	0.45
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.99	0.44
1:A:567:LYS:HZ1	6:H:97:MET:HG2	1.82	0.44
4:E:64:PRO:HD3	4:E:76:GLY:CA	2.48	0.44
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.17	0.44
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.47	0.44
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.00	0.44
2:B:778:MET:HB3	2:B:796:LEU:HD13	1.99	0.44
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.99	0.44
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.47	0.44
3:C:258:ILE:HG23	9:K:19:LEU:HD11	1.98	0.44
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.83	0.44
2:B:302:CYS:HA	2:B:310:MET:HE3	1.99	0.44
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.44
2:B:879:ARG:NH1	2:B:879:ARG:HA	2.33	0.44
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.44
1:A:858:ASN:HD21	1:A:860:LEU:HD12	1.83	0.44
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.83	0.44
10:L:61:THR:HB	10:L:63:ARG:H	1.82	0.44
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.99	0.44
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.83	0.44
2:B:815:ARG:HG2	2:B:816:GLU:OE1	2.17	0.44
2:B:976:ILE:O	2:B:990:ILE:HB	2.17	0.44
1:A:642:CYS:O	1:A:645:LEU:HB3	2.17	0.44
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.99	0.44
1:A:702:LEU:HD12	1:A:710:LEU:HD13	2.00	0.44
1:A:341:MET:HB3	2:B:1132:GLU:HB3	2.00	0.44
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.99	0.44
2:B:515:HIS:HD2	2:B:517:THR:H	1.65	0.44
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.15	0.44
2:B:169:ARG:HH22	2:B:958:GLN:HE22	1.64	0.44
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.53	0.44
1:A:729:ALA:O	1:A:732:LEU:HB2	2.17	0.44
5:F:108:PHE:HB3	5:F:129:LYS:HD2	1.99	0.44
1:A:579:SER:HB3	1:A:611:GLN:HA	1.99	0.43
2:B:51:PHE:O	2:B:55:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LYS:HD2	1:A:794:PRO:HG2	2.00	0.43
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.51	0.43
2:B:244:LEU:HD12	2:B:250:PHE:HB2	2.00	0.43
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.18	0.43
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.53	0.43
2:B:123:THR:HA	2:B:204:ILE:O	2.18	0.43
3:C:41:ILE:HG12	3:C:172:PRO:HG3	2.01	0.43
2:B:102:VAL:HG13	2:B:112:LEU:HD22	2.01	0.43
2:B:370:PHE:CD2	2:B:373:ARG:HD2	2.53	0.43
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.99	0.43
5:F:76:LYS:HG2	5:F:79:ARG:HH12	1.82	0.43
7:I:75:CYS:O	7:I:78:CYS:O	2.35	0.43
2:B:848:ARG:NH2	2:B:996:ARG:NH1	2.66	0.43
1:A:709:THR:HG22	1:A:711:ARG:H	1.83	0.43
2:B:20:ASP:N	2:B:655:LYS:HZ3	2.15	0.43
2:B:227:LYS:HG3	2:B:395:GLN:HB2	2.00	0.43
2:B:745:PRO:O	2:B:748:ILE:HG12	2.18	0.43
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.99	0.43
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.54	0.43
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.19	0.43
10:L:28:LYS:HB2	10:L:39:SER:HB2	2.01	0.43
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.71	0.43
1:A:134:ARG:HH11	1:A:221:SER:HA	1.83	0.43
1:A:686:ALA:HB2	1:A:725:ALA:HB2	2.01	0.42
3:C:56:THR:HG22	3:C:57:VAL:H	1.83	0.42
10:L:27:LEU:HD13	10:L:59:ALA:HB1	2.01	0.42
1:A:98:LYS:O	1:A:102:VAL:HG23	2.19	0.42
1:A:181:LEU:HB2	1:A:202:LEU:HB2	2.01	0.42
2:B:1210:MET:HB3	2:B:1212:ILE:HD12	2.00	0.42
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.01	0.42
1:A:786:HIS:HE1	2:B:742:GLU:OE1	2.02	0.42
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.55	0.42
3:C:60:ASP:HB3	10:L:67:PHE:CZ	2.53	0.42
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	2.01	0.42
1:A:792:TYR:HA	1:A:797:LYS:HD2	2.00	0.42
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.72	0.42
4:E:151:PRO:HD2	4:E:153:HIS:HE1	1.84	0.42
1:A:120:GLU:HA	1:A:123:ARG:HH11	1.84	0.42
1:A:1330:ASN:HB2	1:A:1351:GLU:OE2	2.20	0.42
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.42
1:A:667:GLY:HA2	1:A:670:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.49	0.42
1:A:779:PHE:CZ	2:B:517:THR:HA	2.54	0.42
3:C:14:SER:HA	9:K:114:LEU:HD22	2.01	0.42
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.55	0.42
1:A:134:ARG:HD2	1:A:221:SER:O	2.20	0.42
1:A:353:ILE:HD12	1:A:482:PHE:CD2	2.54	0.42
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.55	0.42
1:A:1284:MET:HA	1:A:1306:LEU:HD23	2.02	0.42
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.35	0.42
2:B:759:PRO:HD2	2:B:1046:PRO:HG3	2.02	0.42
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.55	0.42
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.20	0.42
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	2.02	0.42
2:B:241:ARG:HG2	2:B:253:THR:HG22	2.01	0.42
2:B:654:ARG:H	2:B:657:HIS:CD2	2.38	0.42
3:C:183:TRP:HB3	3:C:213:PRO:HD3	2.01	0.42
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	2.01	0.42
1:A:109:HIS:H	1:A:210:ILE:HD12	1.85	0.41
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.02	0.41
2:B:844:SER:HB2	2:B:996:ARG:H	1.85	0.41
2:B:880:THR:HB	2:B:934:LYS:HE2	2.01	0.41
10:L:34:CYS:SG	10:L:36:SER:HB2	2.60	0.41
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.56	0.41
2:B:189:LEU:HD13	2:B:196:PRO:HA	2.02	0.41
2:B:487:THR:HG22	2:B:490:SER:H	1.85	0.41
3:C:50:GLU:HG2	10:L:66:GLN:HG3	2.01	0.41
6:H:113:ALA:HB2	6:H:126:GLU:HG3	2.01	0.41
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.21	0.41
1:A:451:HIS:HB3	1:A:453:MET:H	1.85	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.55	0.41
1:A:577:ILE:H	1:A:577:ILE:HG13	1.76	0.41
2:B:114:PRO:HB3	2:B:174:LEU:HD21	2.01	0.41
2:B:383:ASN:O	2:B:387:LEU:HB2	2.21	0.41
3:C:43:THR:HG22	3:C:170:TRP:HD1	1.85	0.41
9:K:26:LYS:H	9:K:26:LYS:HG2	1.48	0.41
10:L:46:VAL:HG12	10:L:47:ARG:H	1.85	0.41
1:A:403:LYS:HA	1:A:415:LEU:HB2	2.02	0.41
1:A:821:ARG:HG3	1:A:825:ILE:CD1	2.50	0.41
2:B:520:GLY:HA2	2:B:748:ILE:HA	2.03	0.41
2:B:552:MET:HA	2:B:555:ILE:HD12	2.02	0.41
10:L:47:ARG:HA	10:L:53:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HB2	1:A:183:GLY:HA3	2.02	0.41
1:A:251:SER:HB3	1:A:258:GLY:HA3	2.01	0.41
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.00	0.41
4:E:116:ILE:HG22	4:E:121:MET:HG2	2.03	0.41
4:E:64:PRO:HG2	4:E:69:ILE:HD11	2.01	0.41
2:B:1103:ILE:H	2:B:1103:ILE:HG13	1.61	0.41
2:B:345:LYS:N	2:B:346:GLU:HB3	2.36	0.41
2:B:757:PRO:HG3	2:B:983:ARG:NH1	2.36	0.41
2:B:555:ILE:H	2:B:555:ILE:HG13	1.71	0.41
1:A:1004:ASN:HD21	1:A:1007:ILE:HG12	1.86	0.41
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.89	0.41
2:B:950:ASP:HB3	2:B:967:ARG:HG2	2.03	0.41
3:C:98:VAL:HG22	3:C:158:VAL:HG22	2.03	0.41
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	2.02	0.41
1:A:353:ILE:HB	1:A:470:LEU:HD21	2.02	0.41
1:A:760:GLN:HG2	1:A:765:VAL:HA	2.01	0.41
2:B:400:HIS:CD2	2:B:517:THR:HG21	2.55	0.41
2:B:879:ARG:HA	2:B:879:ARG:HD3	1.93	0.41
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.45	0.41
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.02	0.41
2:B:209:GLU:HB3	2:B:483:LEU:HD23	2.02	0.41
2:B:515:HIS:H	2:B:518:HIS:CD2	2.39	0.41
4:E:107:THR:HA	4:E:131:THR:O	2.20	0.41
9:K:108:GLU:HA	9:K:111:LEU:HD12	2.02	0.41
1:A:897:TYR:HB3	1:A:936:LEU:HD13	2.03	0.41
2:B:175:ARG:NH2	2:B:181:LEU:O	2.54	0.41
2:B:706:GLN:H	2:B:710:LEU:HG	1.86	0.41
7:I:60:GLN:HE21	7:I:60:GLN:HA	1.85	0.41
9:K:21:ILE:HG13	9:K:33:ILE:HG12	2.03	0.41
1:A:540:PHE:HB3	1:A:571:LEU:HG	2.03	0.40
1:A:91:PHE:H	1:A:297:GLN:HE22	1.69	0.40
3:C:74:SER:O	3:C:77:ILE:HB	2.21	0.40
1:A:598:LEU:HA	1:A:598:LEU:HD23	1.95	0.40
1:A:601:LYS:HE3	1:A:603:ASN:HD21	1.86	0.40
1:A:910:PRO:HA	1:A:916:GLY:HA3	2.03	0.40
1:A:986:ILE:O	1:A:990:VAL:HG23	2.21	0.40
1:A:964:ILE:HG22	1:A:968:GLN:OE1	2.21	0.40
1:A:965:GLN:HE21	1:A:965:GLN:HB2	1.71	0.40
1:A:587:HIS:HE1	1:A:969:GLN:HE21	1.70	0.40
2:B:950:ASP:OD2	2:B:967:ARG:NH1	2.54	0.40
2:B:952:VAL:HB	10:L:58:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.03	0.40
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.74	0.40
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.54	0.40
1:A:1153:TYR:HD2	7:I:41:PRO:HG2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1395/1733 (80%)	1239 (89%)	110 (8%)	46 (3%)	4	21
2	B	1096/1224 (90%)	962 (88%)	91 (8%)	43 (4%)	3	17
3	C	264/318 (83%)	238 (90%)	22 (8%)	4 (2%)	10	42
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	17	55
5	F	83/155 (54%)	77 (93%)	5 (6%)	1 (1%)	13	48
6	H	129/146 (88%)	101 (78%)	21 (16%)	7 (5%)	2	11
7	I	117/122 (96%)	102 (87%)	13 (11%)	2 (2%)	9	39
8	J	63/70 (90%)	58 (92%)	2 (3%)	3 (5%)	2	13
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	17	55
10	L	44/70 (63%)	31 (70%)	7 (16%)	6 (14%)	0	1
All	All	3515/4173 (84%)	3115 (89%)	285 (8%)	115 (3%)	4	21

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	ASP
1	A	56	PRO

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Mol	Chain	Res	Type
1	A	109	HIS
1	A	260	ASP
1	A	286	HIS
1	A	399	HIS
1	A	418	SER
1	A	424	ILE
1	A	569	LYS
1	A	597	LEU
2	B	67	SER
2	B	137	TYR
2	B	139	ALA
2	B	364	ILE
2	B	367	LEU
2	B	477	ALA
2	B	648	HIS
2	B	709	ASP
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	880	THR
2	B	883	LEU
2	B	976	ILE
2	B	1046	PRO
2	B	1156	ASP
3	C	227	THR
6	H	90	ALA
6	H	109	LYS
6	H	131	ASN
7	I	118	ARG
8	J	2	ILE
8	J	6	ARG
1	A	250	ILE
1	A	283	GLY
1	A	312	PRO
1	A	325	ILE
1	A	556	TRP
1	A	846	GLU
1	A	1083	THR
1	A	1123	GLY
1	A	1221	LYS
1	A	1437	GLY
2	B	138	GLU

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Mol	Chain	Res	Type
2	B	371	GLU
2	B	483	LEU
2	B	531	GLN
2	B	695	ALA
2	B	712	PRO
2	B	881	ASN
2	B	888	GLY
2	B	1124	ARG
2	B	1157	ALA
2	B	1180	PHE
2	B	1181	GLU
3	C	141	GLY
4	E	126	SER
10	L	51	CYS
10	L	64	LEU
1	A	332	LYS
1	A	410	GLY
1	A	662	PHE
1	A	975	HIS
2	B	65	GLU
2	B	737	THR
2	B	887	HIS
2	B	1171	VAL
2	B	1223	ASP
3	C	90	ASP
6	H	140	ALA
7	I	77	LYS
10	L	39	SER
10	L	56	LEU
1	A	35	ILE
1	A	52	GLY
1	A	65	LEU
1	A	214	ILE
1	A	257	ARG
1	A	308	ILE
1	A	310	GLY
1	A	404	TYR
2	B	526	GLU
2	B	644	GLU
2	B	1221	SER
5	F	154	ASP
6	H	84	ALA

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Mol	Chain	Res	Type
8	J	26	GLN
9	K	18	LYS
10	L	46	VAL
10	L	55	ILE
1	A	213	HIS
1	A	299	HIS
1	A	400	PRO
1	A	567	LYS
1	A	958	VAL
2	B	646	LEU
2	B	647	GLY
2	B	792	MET
3	C	142	VAL
6	H	108	SER
1	A	331	GLY
1	A	385	ILE
1	A	543	LEU
1	A	599	SER
4	E	3	GLN
6	H	61	SER
1	A	568	PRO
2	B	592	ASN
2	B	1017	ILE
2	B	711	GLU
2	B	1099	VAL
1	A	178	GLY
1	A	916	GLY
1	A	1384	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1225/1520 (81%)	1066 (87%)	159 (13%)	4	19
2	B	967/1061 (91%)	842 (87%)	125 (13%)	4	19
3	C	234/274 (85%)	205 (88%)	29 (12%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	196/197 (100%)	170 (87%)	26 (13%)	4	17
5	F	75/137 (55%)	71 (95%)	4 (5%)	22	58
6	H	117/128 (91%)	94 (80%)	23 (20%)	1	7
7	I	113/116 (97%)	98 (87%)	15 (13%)	4	17
8	J	60/65 (92%)	49 (82%)	11 (18%)	1	9
9	K	99/102 (97%)	86 (87%)	13 (13%)	4	18
10	L	40/57 (70%)	29 (72%)	11 (28%)	0	2
All	All	3126/3657 (86%)	2710 (87%)	416 (13%)	4	17

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	18	GLN
1	A	25	GLU
1	A	40	THR
1	A	41	MET
1	A	43	GLU
1	A	58	LEU
1	A	61	ILE
1	A	65	LEU
1	A	69	THR
1	A	70	CYS
1	A	86	LEU
1	A	93	VAL
1	A	108	MET
1	A	116	ASP
1	A	122	MET
1	A	126	LEU
1	A	130	ASP
1	A	144	THR
1	A	171	GLN
1	A	177	ASP
1	A	179	LEU
1	A	186	LYS
1	A	204	THR
1	A	205	GLU
1	A	219	PHE
1	A	222	LEU
1	A	252	PHE

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Mol	Chain	Res	Type
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	270	LEU
1	A	295	LEU
1	A	303	TYR
1	A	308	ILE
1	A	320	ARG
1	A	323	LYS
1	A	326	ARG
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	389	THR
1	A	403	LYS
1	A	407	ARG
1	A	408	ASP
1	A	423	ASP
1	A	424	ILE
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	452	LYS
1	A	456	MET
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	476	SER
1	A	489	LEU
1	A	496	GLU
1	A	500	GLU
1	A	501	LEU
1	A	518	LYS
1	A	527	THR
1	A	532	ARG
1	A	541	ILE
1	A	542	GLU

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Mol	Chain	Res	Type
1	A	544	ASP
1	A	555	ASP
1	A	567	LYS
1	A	590	ARG
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	636	GLU
1	A	640	GLN
1	A	672	ASP
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	705	LYS
1	A	708	MET
1	A	710	LEU
1	A	716	ASP
1	A	722	LEU
1	A	756	ILE
1	A	769	SER
1	A	774	ARG
1	A	801	GLU
1	A	821	ARG
1	A	830	LYS
1	A	839	ARG
1	A	867	ILE
1	A	878	ILE
1	A	894	GLU
1	A	896	ARG
1	A	905	ASP
1	A	907	THR
1	A	917	SER
1	A	922	ASP
1	A	927	VAL
1	A	931	GLU
1	A	968	GLN
1	A	969	GLN
1	A	973	ILE
1	A	982	THR

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Mol	Chain	Res	Type
1	A	1006	ILE
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1046	LEU
1	A	1048	ASN
1	A	1067	LEU
1	A	1081	LEU
1	A	1084	PHE
1	A	1095	THR
1	A	1109	LYS
1	A	1110	ASN
1	A	1113	THR
1	A	1129	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1176	LEU
1	A	1195	LEU
1	A	1221	LYS
1	A	1223	ASP
1	A	1229	SER
1	A	1230	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1264	GLU
1	A	1274	ARG
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1350	LYS
1	A	1355	VAL
1	A	1366	ARG
1	A	1376	THR
1	A	1378	GLN
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1406	VAL

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Mol	Chain	Res	Type
1	A	1425	SER
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1445	ILE
2	B	25	ILE
2	B	28	GLU
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	70	ILE
2	B	89	GLU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	121	ASN
2	B	134	LYS
2	B	135	ARG
2	B	140	ILE
2	B	175	ARG
2	B	199	MET
2	B	217	ARG
2	B	218	SER
2	B	221	ASN
2	B	223	VAL
2	B	225	VAL
2	B	233	PRO
2	B	234	ILE
2	B	240	ILE
2	B	249	ARG
2	B	251	ILE
2	B	254	LEU
2	B	261	ARG
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	285	ILE
2	B	299	GLU
2	B	312	GLU
2	B	323	VAL
2	B	325	GLN
2	B	327	ARG

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Mol	Chain	Res	Type
2	B	355	ILE
2	B	357	GLN
2	B	363	HIS
2	B	365	THR
2	B	371	GLU
2	B	376	PHE
2	B	393	LYS
2	B	394	ASP
2	B	413	LEU
2	B	416	LEU
2	B	437	GLU
2	B	451	LYS
2	B	458	LYS
2	B	461	LEU
2	B	471	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	489	SER
2	B	516	ASN
2	B	531	GLN
2	B	537	LYS
2	B	547	VAL
2	B	549	THR
2	B	576	ASP
2	B	578	THR
2	B	579	ARG
2	B	591	ARG
2	B	604	ARG
2	B	614	SER
2	B	616	ILE
2	B	624	LEU
2	B	629	ASP
2	B	653	VAL
2	B	660	LYS
2	B	690	VAL
2	B	708	GLU
2	B	710	LEU
2	B	733	HIS
2	B	762	ASN
2	B	780	VAL

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Mol	Chain	Res	Type
2	B	786	ASN
2	B	788	ARG
2	B	790	ASP
2	B	791	THR
2	B	799	PRO
2	B	815	ARG
2	B	844	SER
2	B	864	LYS
2	B	866	TYR
2	B	868	MET
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	885	MET
2	B	886	LYS
2	B	895	ASP
2	B	906	SER
2	B	935	ARG
2	B	944	THR
2	B	963	PHE
2	B	964	VAL
2	B	976	ILE
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1065	GLN
2	B	1077	THR
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1128	LEU
2	B	1129	ARG
2	B	1132	GLU
2	B	1147	LEU
2	B	1150	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1194	ILE

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Mol	Chain	Res	Type
2	B	1202	LEU
2	B	1210	MET
2	B	1211	ASN
2	B	1216	LEU
3	C	3	GLU
3	C	4	GLU
3	C	9	LYS
3	C	18	VAL
3	C	25	VAL
3	C	34	ARG
3	C	41	ILE
3	C	43	THR
3	C	56	THR
3	C	57	VAL
3	C	66	ARG
3	C	75	MET
3	C	77	ILE
3	C	80	LEU
3	C	93	ASP
3	C	99	LEU
3	C	109	SER
3	C	136	ASP
3	C	137	LYS
3	C	204	SER
3	C	214	ASN
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	264	GLN
4	E	7	ARG
4	E	32	GLN
4	E	37	LEU
4	E	41	ASP
4	E	52	ARG
4	E	54	GLN
4	E	61	GLN
4	E	75	MET
4	E	78	LEU

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Mol	Chain	Res	Type
4	E	83	CYS
4	E	84	ASP
4	E	92	THR
4	E	94	LYS
4	E	95	THR
4	E	104	ASN
4	E	106	GLN
4	E	107	THR
4	E	114	ASN
4	E	127	ILE
4	E	144	ILE
4	E	146	HIS
4	E	149	LEU
4	E	156	LEU
4	E	169	ARG
4	E	178	ILE
4	E	204	THR
5	F	76	LYS
5	F	82	THR
5	F	93	ILE
5	F	118	LEU
6	H	11	GLN
6	H	13	SER
6	H	14	GLU
6	H	15	VAL
6	H	22	LYS
6	H	24	CYS
6	H	26	ILE
6	H	35	GLN
6	H	63	LEU
6	H	83	GLN
6	H	86	ASP
6	H	87	ARG
6	H	88	SER
6	H	91	ASP
6	H	92	ASP
6	H	100	THR
6	H	109	LYS
6	H	110	ASP
6	H	111	LEU
6	H	130	ARG
6	H	132	LEU

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Mol	Chain	Res	Type
6	H	136	LYS
6	H	139	ASN
7	I	28	GLU
7	I	35	VAL
7	I	60	GLN
7	I	61	ASP
7	I	70	ARG
7	I	77	LYS
7	I	83	ASN
7	I	87	GLN
7	I	90	GLN
7	I	94	ASP
7	I	96	SER
7	I	97	MET
7	I	104	LEU
7	I	111	THR
7	I	119	THR
8	J	1	MET
8	J	3	VAL
8	J	10	CYS
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	28	ASP
8	J	31	ASP
8	J	43	ARG
8	J	48	ARG
8	J	59	LYS
9	K	11	LEU
9	K	14	GLU
9	K	16	GLU
9	K	18	LYS
9	K	20	LYS
9	K	21	ILE
9	K	26	LYS
9	K	31	VAL
9	K	33	ILE
9	K	51	LEU
9	K	63	VAL
9	K	74	ARG
9	K	114	LEU
10	L	27	LEU

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Mol	Chain	Res	Type
10	L	38	LEU
10	L	42	ARG
10	L	43	THR
10	L	44	ASP
10	L	47	ARG
10	L	55	ILE
10	L	58	LYS
10	L	61	THR
10	L	64	LEU
10	L	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN
1	A	83	HIS
1	A	225	ASN
1	A	256	GLN
1	A	297	GLN
1	A	339	ASN
1	A	445	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	603	ASN
1	A	631	HIS
1	A	700	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	851	HIS
1	A	906	HIS
1	A	926	GLN
1	A	965	GLN
1	A	969	GLN
1	A	1048	ASN
1	A	1052	GLN
1	A	1110	ASN
1	A	1140	HIS

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Mol	Chain	Res	Type
1	A	1211	GLN
1	A	1258	HIS
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	46	GLN
2	B	53	GLN
2	B	215	GLN
2	B	363	HIS
2	B	395	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	957	ASN
2	B	958	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1074	ASN
2	B	1084	GLN
2	B	1097	HIS
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
4	E	54	GLN
4	E	147	HIS
6	H	11	GLN
7	I	60	GLN
9	K	65	HIS
9	K	89	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/4 (75%)	0	0

There are no RNA backbone outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	A	1405/1733 (81%)	0.06	101 (7%) 15 4	63, 111, 202, 234	0
2	B	1114/1224 (91%)	-0.11	32 (2%) 51 23	62, 96, 166, 219	0
3	C	266/318 (83%)	-0.39	0 100 100	67, 94, 132, 186	0
4	E	214/215 (99%)	-0.00	9 (4%) 36 14	81, 139, 193, 210	0
5	F	85/155 (54%)	-0.18	0 100 100	81, 115, 159, 172	0
6	H	133/146 (91%)	0.10	5 (3%) 40 16	109, 151, 177, 187	0
7	I	119/122 (97%)	-0.30	0 100 100	78, 114, 150, 167	0
8	J	65/70 (92%)	-0.38	0 100 100	65, 83, 114, 130	0
9	K	114/120 (95%)	-0.38	0 100 100	66, 102, 126, 149	0
10	L	46/70 (65%)	-0.07	3 (6%) 18 5	82, 119, 152, 176	0
11	R	4/4 (100%)	2.12	2 (50%) 0 0	210, 216, 218, 219	0
12	T	8/29 (27%)	1.61	2 (25%) 0 0	200, 204, 210, 211	0
All	All	3573/4206 (84%)	-0.06	154 (4%) 35 13	62, 106, 192, 234	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	8.9
1	A	182	VAL	7.6
1	A	1087	ALA	6.7
1	A	318	SER	6.0
1	A	161	LEU	6.0
1	A	250	ILE	5.9
1	A	319	GLY	5.8
2	B	1224	PHE	5.7
1	A	45	GLN	5.5
1	A	1082	ASN	5.3
1	A	171	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	1222	ARG	5.2
1	A	44	THR	5.2
6	H	86	ASP	5.1
1	A	116	ASP	4.9
1	A	183	GLY	4.9
1	A	69	THR	4.9
4	E	93	MET	4.7
1	A	1086	PHE	4.7
1	A	255	SER	4.6
1	A	1090	ALA	4.6
1	A	113	LEU	4.5
6	H	85	GLY	4.5
1	A	199	LEU	4.5
1	A	49	LYS	4.4
1	A	149	GLU	4.4
2	B	865	LYS	4.4
1	A	147	VAL	4.4
1	A	1083	THR	4.4
1	A	141	LEU	4.3
2	B	136	THR	4.2
1	A	314	ALA	4.2
12	T	19	DT	4.2
1	A	1091	SER	4.2
1	A	152	VAL	4.2
11	R	7	G	4.0
1	A	114	LEU	4.0
4	E	2	ASP	4.0
2	B	474	SER	4.0
2	B	647	GLY	3.9
2	B	1223	ASP	3.9
1	A	177	ASP	3.9
2	B	477	ALA	3.9
10	L	50	ASP	3.9
1	A	1085	HIS	3.9
1	A	139	TRP	3.9
1	A	253	ASN	3.7
2	B	883	LEU	3.7
1	A	176	LYS	3.7
1	A	144	THR	3.7
1	A	66	LYS	3.7
1	A	201	VAL	3.7
1	A	87	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	122	MET	3.6
1	A	316	GLN	3.6
1	A	115	LEU	3.6
2	B	471	LYS	3.5
1	A	142	CYS	3.5
1	A	174	ILE	3.5
1	A	173	THR	3.4
1	A	200	ARG	3.3
11	R	8	A	3.3
1	A	168	GLY	3.3
1	A	313	GLN	3.3
1	A	1088	GLY	3.3
1	A	146	MET	3.3
1	A	258	GLY	3.3
1	A	175	ARG	3.2
1	A	1123	GLY	3.2
1	A	125	ALA	3.2
1	A	251	SER	3.1
1	A	62	ASP	3.1
12	T	22	DT	3.1
1	A	254	GLU	3.1
1	A	137	ALA	3.0
1	A	105	CYS	3.0
1	A	214	ILE	3.0
1	A	317	LYS	3.0
1	A	321	PRO	3.0
1	A	169	ASN	3.0
1	A	280	GLU	3.0
10	L	45	ALA	3.0
1	A	72	GLU	3.0
2	B	867	GLY	3.0
1	A	286	HIS	2.9
10	L	27	LEU	2.9
2	B	1184	GLY	2.9
6	H	84	ALA	2.9
2	B	866	TYR	2.8
2	B	870	ILE	2.8
1	A	148	CYS	2.8
2	B	135	ARG	2.8
1	A	12	ARG	2.8
4	E	110	PHE	2.8
4	E	122	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	469	GLN	2.7
2	B	468	GLU	2.7
2	B	869	SER	2.7
1	A	1084	PHE	2.7
1	A	111	GLY	2.6
2	B	470	LYS	2.6
4	E	123	LEU	2.6
1	A	257	ARG	2.5
1	A	124	GLN	2.5
1	A	127	ALA	2.5
1	A	154	SER	2.5
1	A	163	SER	2.5
1	A	315	LEU	2.5
1	A	249	SER	2.5
1	A	172	PRO	2.5
6	H	83	GLN	2.5
1	A	120	GLU	2.5
1	A	162	VAL	2.5
6	H	132	LEU	2.5
1	A	256	GLN	2.5
1	A	153	PRO	2.4
1	A	186	LYS	2.4
1	A	213	HIS	2.4
2	B	882	THR	2.4
2	B	919	SER	2.4
2	B	246	LYS	2.4
1	A	283	GLY	2.4
1	A	121	LEU	2.3
1	A	323	LYS	2.3
2	B	1162	ILE	2.3
1	A	42	ASP	2.3
1	A	295	LEU	2.3
4	E	113	GLN	2.3
1	A	143	LYS	2.3
1	A	165	GLY	2.3
1	A	73	GLY	2.3
2	B	1190	ASP	2.3
1	A	287	HIS	2.3
4	E	53	PRO	2.3
1	A	1002	GLY	2.2
2	B	472	ALA	2.2
1	A	1173	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1124	HIS	2.2
4	E	118	PRO	2.1
1	A	103	CYS	2.1
1	A	164	ARG	2.1
2	B	432	MET	2.1
4	E	86	PRO	2.1
2	B	1221	SER	2.1
1	A	1092	LYS	2.1
1	A	145	LYS	2.1
1	A	320	ARG	2.1
1	A	118	HIS	2.1
2	B	429	PHE	2.1
2	B	1219	ASP	2.1
2	B	1164	GLY	2.0
2	B	433	GLN	2.0
2	B	645	SER	2.0
1	A	71	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
13	ZN	A	1734	1/1	0.15	0.14	300,300,300,300	0
13	ZN	B	1307	1/1	0.75	0.07	206,206,206,206	0
13	ZN	A	1735	1/1	0.80	0.09	177,177,177,177	0
13	ZN	J	101	1/1	0.98	0.20	88,88,88,88	0
13	ZN	L	105	1/1	0.98	0.11	111,111,111,111	0
13	ZN	I	203	1/1	0.98	0.13	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	ZN	I	204	1/1	0.99	0.12	90,90,90,90	0
13	ZN	C	319	1/1	0.99	0.10	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.