



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

PDB ID : 3K1F  
Title : Crystal structure of RNA Polymerase II in complex with TFIIB  
Authors : Kostrewa, D.; Zeller, M.E.; Armache, K.-J.; Seizl, M.; Leike, K.; Thomm, M.; Cramer, P.  
Deposited on : 2009-09-27  
Resolution : 4.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

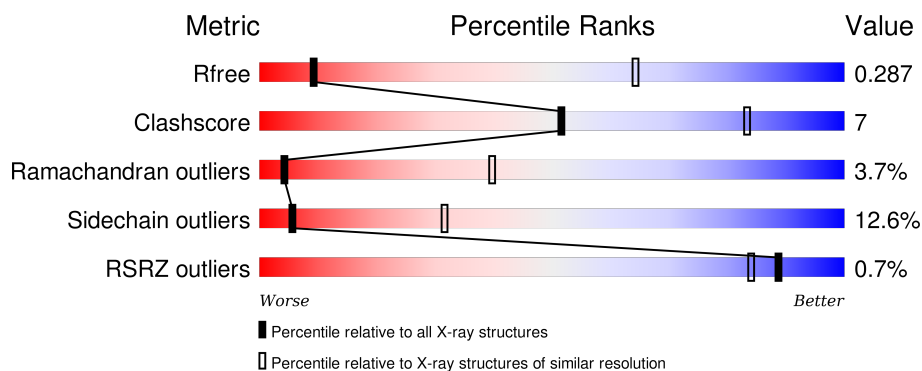
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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))
$R_{free}$	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>59%</div> <div>19%</div> <div>•</div> <div>18%</div> </div>
2	B	1224	<div> <div>64%</div> <div>24%</div> <div>•</div> <div>8%</div> </div>
3	C	318	<div> <div>63%</div> <div>19%</div> <div>•</div> <div>16%</div> </div>
4	D	221	<div> <div>2%</div> <div>58%</div> <div>21%</div> <div>•</div> <div>19%</div> </div>
5	E	215	<div> <div>•</div> <div>74%</div> <div>23%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	197	

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 32332 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	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1120	Total	C	N	O	S	0	0	0
			8910	5639	1560	1656	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 polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	185	Total	C	N	O	S	0	0	0
			1083	662	207	210	4			

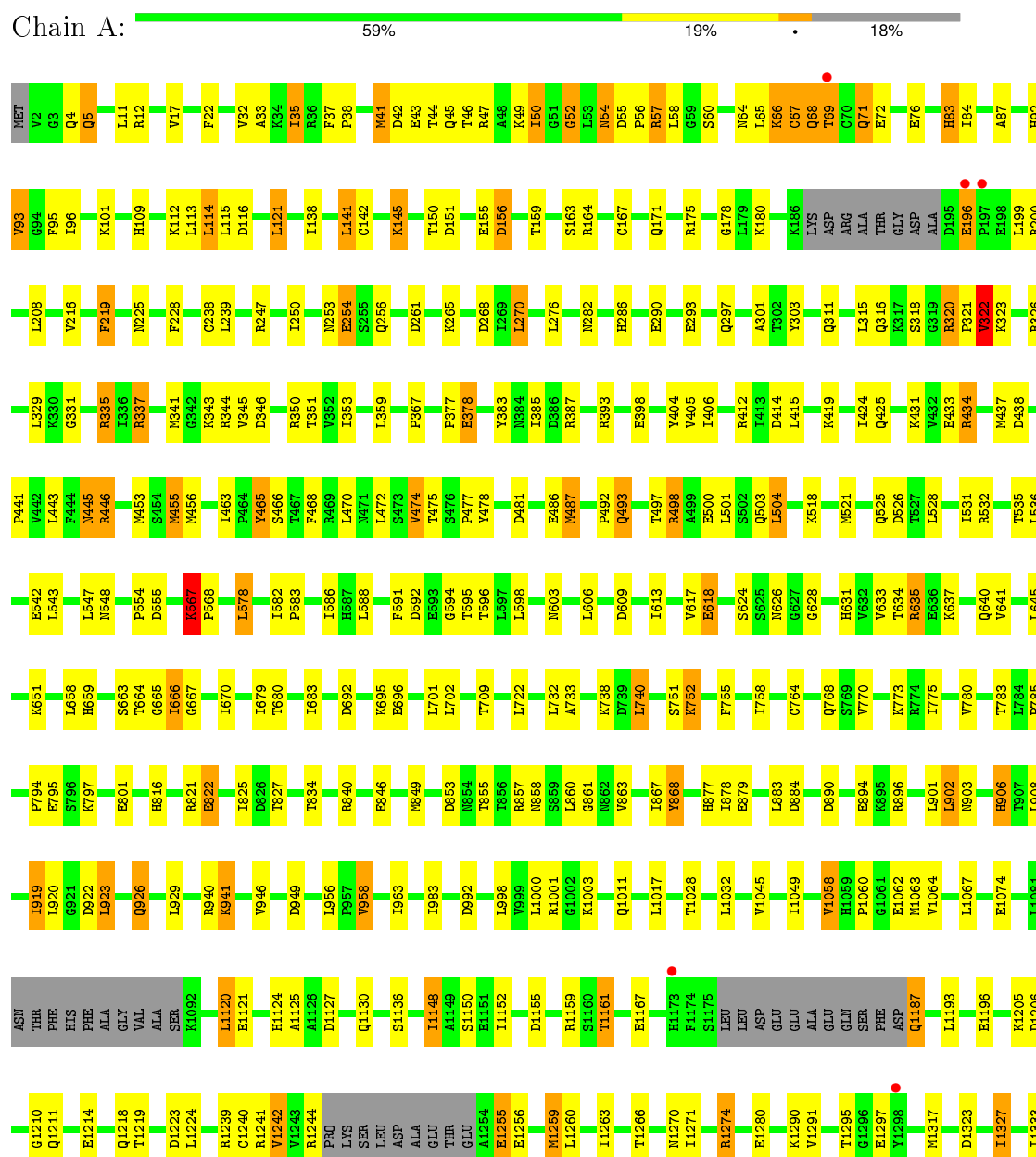
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

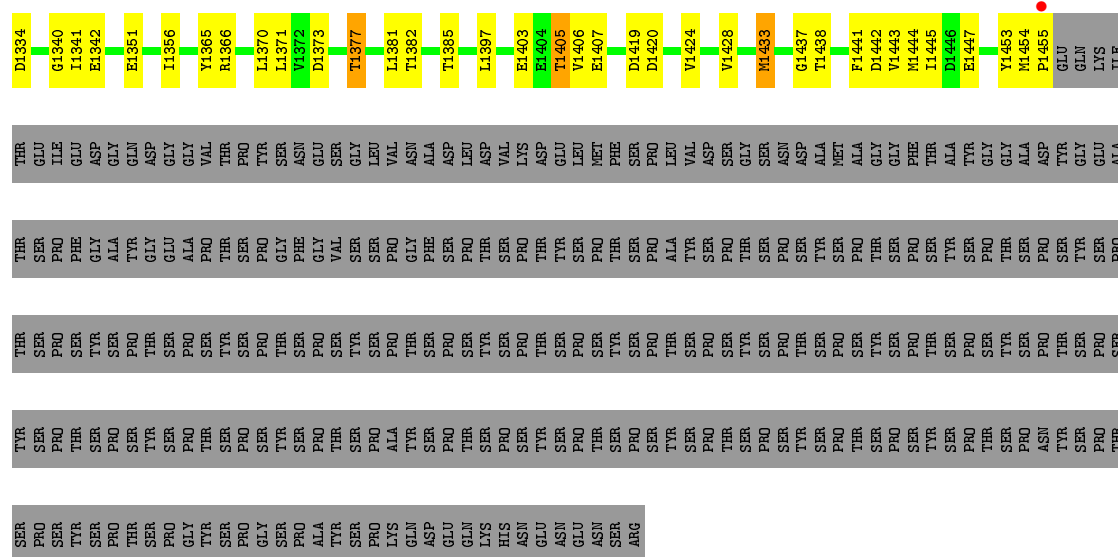
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total 1	Zn 1	0	0
14	B	1	Total 1	Zn 1	0	0
14	I	2	Total 2	Zn 2	0	0
14	C	1	Total 1	Zn 1	0	0
14	A	2	Total 2	Zn 2	0	0
14	L	1	Total 1	Zn 1	0	0
14	M	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

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

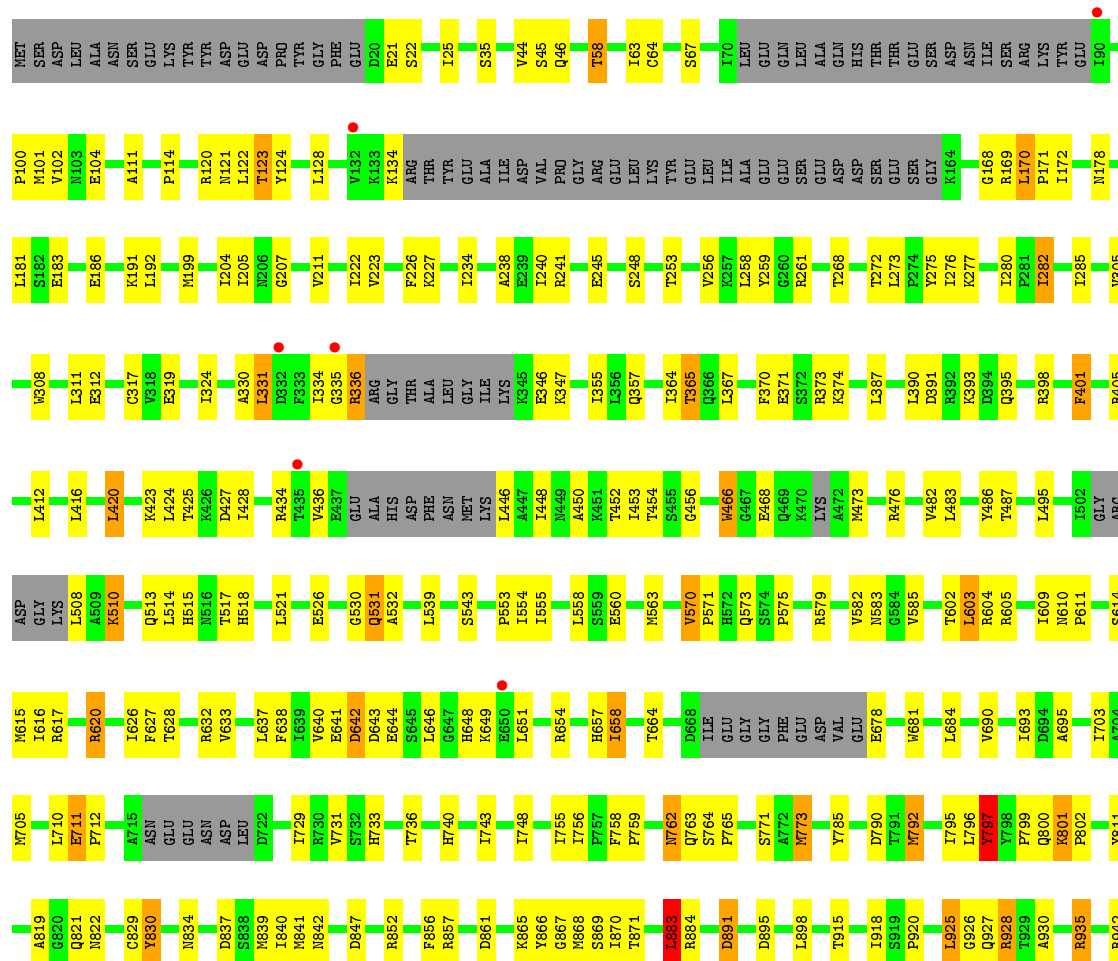
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



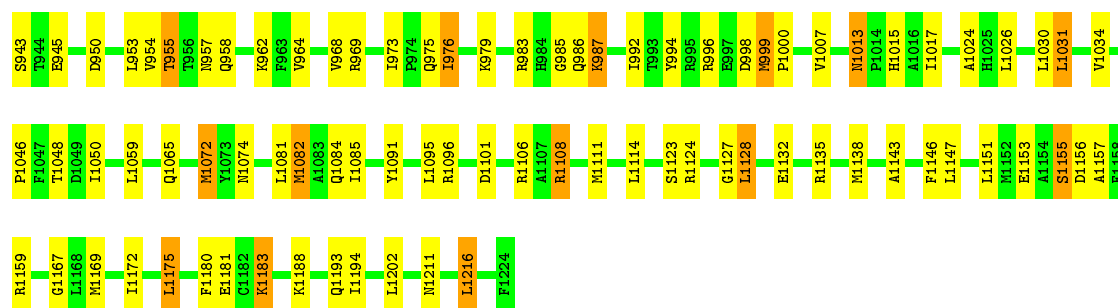


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

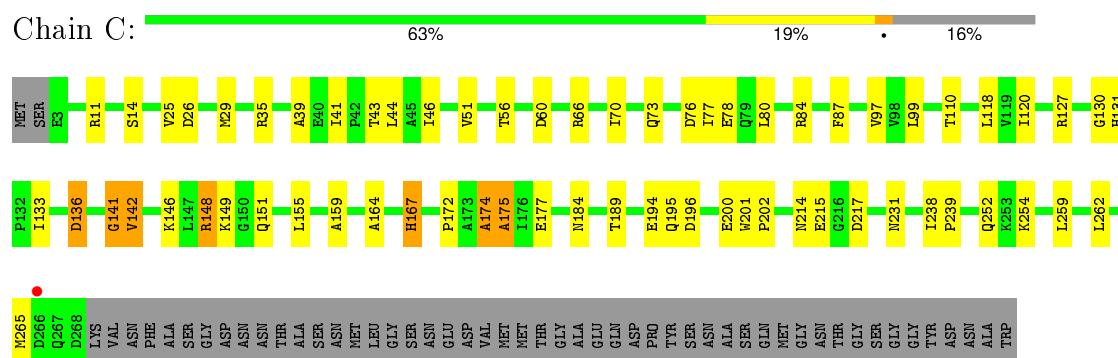
Chain B:  64% 24% • 8%



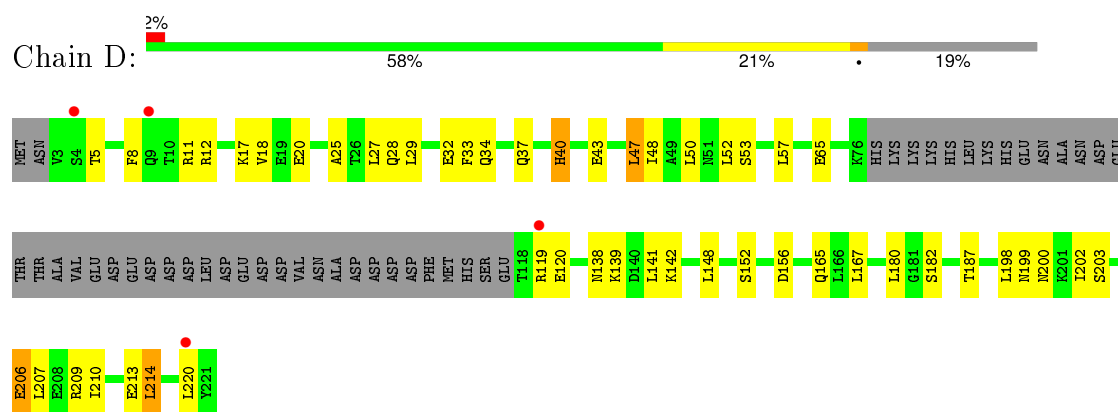




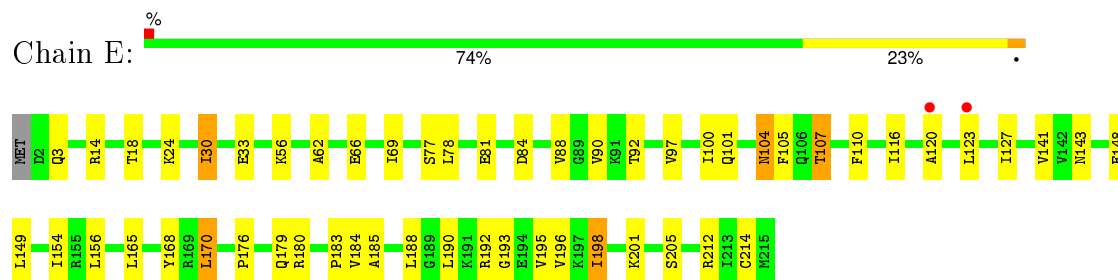
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

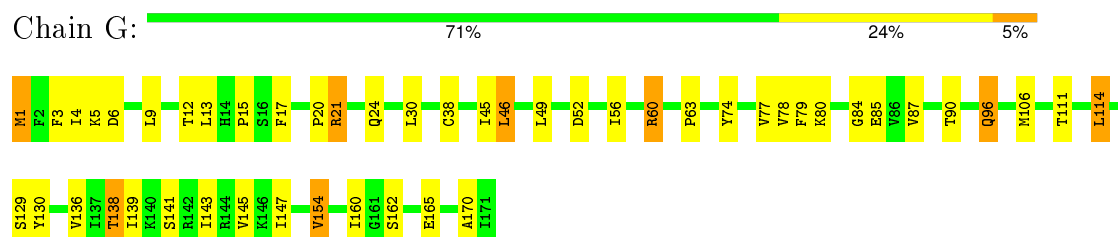


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

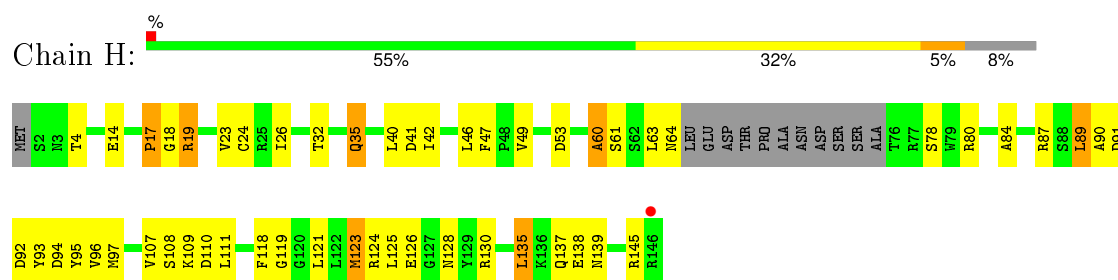




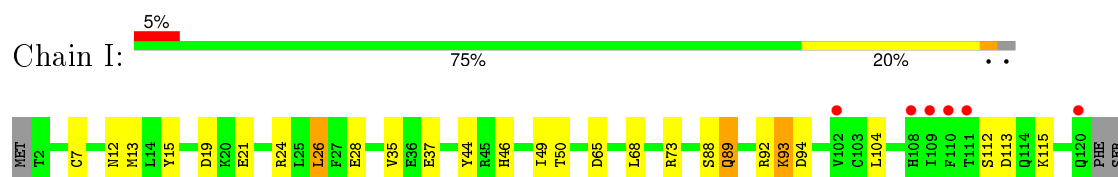
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



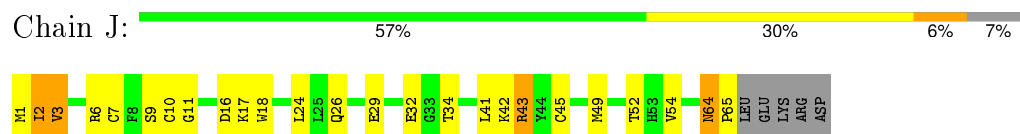
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



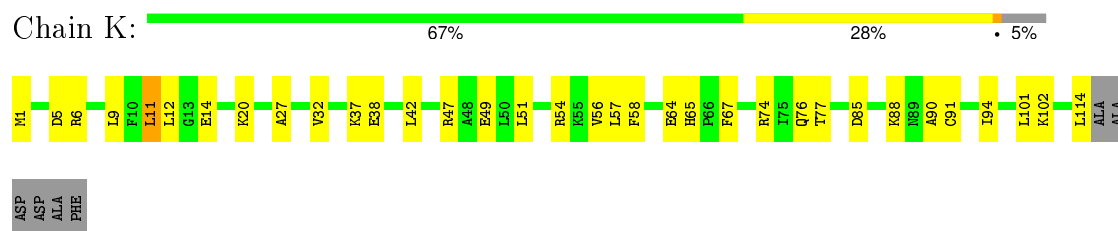
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



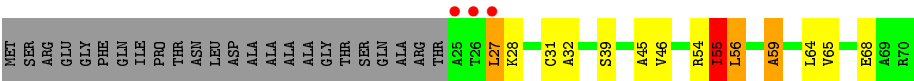
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



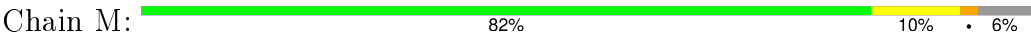
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



● Molecule 13: Transcription initiation factor IIB



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.97Å 408.27Å 275.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.69 – 4.30 39.69 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.69-4.30) 99.4 (39.69-4.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 4.28Å)	Xtriage
Refinement program	BUSTER 2.7.0	Depositor
R, $R_{free}$	0.220 , 0.255 0.250 , 0.287	Depositor DCC
$R_{free}$ test set	2055 reflections (2.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.9	Xtriage
Anisotropy	0.780	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 111.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 83919 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	32332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.44	0/11342	0.72	0/15337
2	B	0.44	0/9084	0.69	0/12251
3	C	0.43	0/2133	0.71	0/2891
4	D	0.42	0/1444	0.68	0/1935
5	E	0.43	0/1788	0.66	0/2406
6	F	0.46	0/717	0.75	0/967
7	G	0.41	0/1368	0.74	0/1844
8	H	0.45	0/1094	0.74	0/1481
9	I	0.41	0/989	0.73	0/1331
10	J	0.45	0/541	0.74	0/727
11	K	0.44	0/937	0.64	0/1265
12	L	0.49	0/365	0.78	0/485
13	M	0.43	0/449	0.72	0/609
All	All	0.44	0/32251	0.71	0/43529

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11143	0	11217	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8910	0	8926	135	0
3	C	2095	0	2051	31	0
4	D	1434	0	1460	18	0
5	E	1752	0	1776	27	0
6	F	705	0	731	15	0
7	G	1340	0	1357	28	0
8	H	1076	0	1046	21	0
9	I	971	0	927	12	0
10	J	532	0	542	13	0
11	K	919	0	929	15	0
12	L	363	0	386	5	0
13	M	1083	0	578	12	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
14	M	1	0	0	0	0
All	All	32332	0	31926	434	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 7.

All (434) 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:567:LYS:HB2	1:A:568:PRO:HD3	1.48	0.94
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.60	0.83
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.62	0.82
1:A:225:ASN:HD22	1:A:228:PHE:H	1.28	0.81
3:C:142:VAL:H	10:J:16:ASP:HB3	1.46	0.79
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.67	0.75
11:K:38:GLU:HG3	11:K:42:LEU:HD22	1.69	0.75
1:A:250:ILE:HD13	13:M:62:GLU:HG2	1.68	0.74
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.70	0.72
6:F:99:LEU:O	6:F:103:MET:HG2	1.88	0.72
1:A:853:ASP:OD1	1:A:855:THR:HG22	1.90	0.72
1:A:343:LYS:HE3	2:B:1151:LEU:HD23	1.72	0.71
12:L:27:LEU:HD12	12:L:59:ALA:HB1	1.73	0.70
7:G:1:MET:HE3	7:G:80:LYS:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.57	0.70
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.73	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.75	0.68
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.76	0.68
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.76	0.67
2:B:865:LYS:HE2	2:B:869:SER:H	1.58	0.67
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	1.77	0.67
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.78	0.66
1:A:567:LYS:HB3	8:H:96:VAL:H	1.61	0.65
1:A:855:THR:CG2	1:A:857:ARG:HE	2.09	0.65
1:A:640:GLN:HE21	1:A:641:VAL:HG23	1.61	0.65
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.78	0.65
3:C:254:LYS:HB3	11:K:42:LEU:HD11	1.78	0.65
3:C:66:ARG:NH2	10:J:3:VAL:O	2.30	0.65
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.77	0.65
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.62	0.64
2:B:25:ILE:HG21	2:B:658:ILE:HD13	1.77	0.64
6:F:124:GLU:HB3	6:F:130:ILE:HG13	1.79	0.64
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.79	0.64
2:B:1111:MET:HG3	13:M:55:LYS:HG2	1.78	0.64
1:A:121:LEU:HB3	1:A:141:LEU:HD21	1.80	0.64
1:A:740:LEU:HD23	8:H:19:ARG:HH12	1.63	0.63
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.81	0.63
3:C:136:ASP:HB2	3:C:141:GLY:H	1.64	0.63
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.79	0.63
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.81	0.62
1:A:225:ASN:ND2	1:A:228:PHE:H	1.98	0.62
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.82	0.62
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.82	0.61
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.27	0.61
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.83	0.61
1:A:855:THR:HG21	1:A:857:ARG:HE	1.65	0.61
1:A:41:MET:HA	1:A:49:LYS:HA	1.82	0.60
9:I:7:CYS:HB3	9:I:12:ASN:H	1.65	0.60
1:A:1120:LEU:HD13	1:A:1125:ALA:HA	1.84	0.60
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.82	0.60
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.83	0.59
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.84	0.59
1:A:350:ARG:HE	1:A:486:GLU:HB3	1.67	0.59
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.82	0.59
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:HG2	2:B:111:ALA:HA	1.84	0.59
2:B:925:LEU:HG	13:M:22:LEU:HD12	1.85	0.59
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.85	0.59
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.67	0.59
7:G:9:LEU:HD23	7:G:30:LEU:HD12	1.85	0.58
1:A:755:PHE:HA	1:A:758:ILE:HD12	1.85	0.58
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.84	0.58
2:B:319:GLU:HG2	9:I:15:TYR:HE2	1.69	0.58
2:B:925:LEU:HB3	2:B:928:ARG:HB3	1.85	0.58
4:D:37:GLN:HE21	4:D:47:LEU:HD22	1.68	0.58
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.84	0.58
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.86	0.58
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.39	0.57
1:A:692:ASP:HA	1:A:695:LYS:HD2	1.86	0.57
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.86	0.57
1:A:150:THR:O	1:A:163:SER:HA	2.05	0.57
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.86	0.56
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.86	0.56
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.85	0.56
2:B:705:MET:H	2:B:710:LEU:HD12	1.71	0.56
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.40	0.56
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.30	0.56
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.87	0.56
2:B:1124:ARG:HH12	13:M:60:ARG:HB2	1.71	0.56
1:A:446:ARG:HG3	1:A:487:MET:HG2	1.87	0.56
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.88	0.55
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.89	0.55
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.89	0.55
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.89	0.55
11:K:12:LEU:HA	11:K:37:LYS:HG3	1.88	0.55
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.88	0.55
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.88	0.55
2:B:530:GLY:O	2:B:532:ALA:N	2.40	0.55
10:J:32:GLU:CD	10:J:32:GLU:H	2.10	0.55
1:A:567:LYS:H	8:H:96:VAL:HB	1.72	0.55
2:B:428:ILE:HG12	2:B:448:ILE:HG23	1.88	0.55
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.89	0.55
2:B:227:LYS:HE2	2:B:395:GLN:H	1.73	0.54
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.89	0.54
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.89	0.54
5:E:88:VAL:HG11	5:E:110:PHE:HZ	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:55:ILE:HG12	12:L:56:LEU:H	1.72	0.54
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.72	0.54
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.89	0.54
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.91	0.54
1:A:532:ARG:HG3	1:A:618:GLU:HB3	1.90	0.53
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.90	0.53
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.90	0.53
5:E:24:LYS:HD2	5:E:30:ILE:HG22	1.91	0.53
2:B:521:LEU:HA	2:B:543:SER:HB3	1.89	0.53
1:A:387:ARG:HH12	1:A:434:ARG:HH11	1.57	0.53
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.91	0.53
6:F:138:LEU:HD23	6:F:139:PRO:HD2	1.90	0.53
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.91	0.53
6:F:74:ILE:HD11	6:F:142:SER:HB3	1.90	0.52
2:B:792:MET:HE2	2:B:857:ARG:HE	1.74	0.52
1:A:1433:MET:HG3	7:G:63:PRO:HB2	1.92	0.52
1:A:320:ARG:HE	1:A:323:LYS:HE3	1.74	0.52
7:G:111:THR:HG22	7:G:114:LEU:HD22	1.91	0.52
1:A:583:PRO:O	1:A:586:ILE:HG12	2.10	0.52
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.92	0.52
2:B:241:ARG:HA	2:B:253:THR:HG22	1.92	0.52
1:A:1211:GLN:HE22	1:A:1274:ARG:HD2	1.74	0.52
1:A:1187:GLN:HA	1:A:1244:ARG:HE	1.73	0.52
1:A:949:ASP:HB2	1:A:1290:LYS:HD3	1.91	0.52
10:J:7:CYS:HA	10:J:49:MET:HG2	1.92	0.52
7:G:114:LEU:HG	7:G:162:SER:HB3	1.92	0.52
1:A:42:ASP:HA	1:A:46:THR:O	2.09	0.52
1:A:337:ARG:HA	1:A:341:MET:HB2	1.93	0.52
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.75	0.52
1:A:680:THR:HA	1:A:683:ILE:HD12	1.92	0.51
1:A:315:LEU:HA	1:A:321:PRO:HA	1.92	0.51
2:B:637:LEU:HB2	2:B:693:ILE:HD13	1.92	0.51
4:D:202:ILE:HG21	4:D:207:LEU:HD13	1.92	0.51
3:C:51:VAL:HA	3:C:155:LEU:HD23	1.92	0.51
11:K:27:ALA:HB3	11:K:74:ARG:HH12	1.74	0.51
1:A:378:GLU:O	1:A:431:LYS:HA	2.11	0.51
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.91	0.51
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.13	0.51
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.92	0.51
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.93	0.51
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:HA	2:B:811:TYR:HE2	1.75	0.50
2:B:412:LEU:HB3	2:B:466:TRP:HZ2	1.77	0.50
1:A:1161:THR:HG23	1:A:1239:ARG:HH21	1.76	0.50
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.92	0.50
13:M:63:TRP:HA	13:M:66:PHE:HD2	1.76	0.50
2:B:1106:ARG:HG2	2:B:1127:GLY:HA2	1.94	0.50
1:A:351:THR:HG22	1:A:468:PHE:CD1	2.45	0.50
1:A:696:GLU:HB3	1:A:702:LEU:HB2	1.94	0.50
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.75	0.50
6:F:103:MET:HG3	7:G:15:PRO:HG2	1.94	0.50
1:A:216:VAL:HA	1:A:219:PHE:HB2	1.92	0.50
1:A:770:VAL:HG13	1:A:822:GLU:HG3	1.93	0.50
4:D:180:LEU:HD11	4:D:198:LEU:HD21	1.94	0.50
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.93	0.50
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.94	0.49
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.94	0.49
2:B:420:LEU:HD21	2:B:456:GLY:HA3	1.93	0.49
1:A:528:LEU:HD23	1:A:751:SER:HA	1.94	0.49
2:B:979:LYS:HB3	2:B:1095:LEU:HB2	1.92	0.49
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.93	0.49
2:B:405:ARG:CZ	2:B:632:ARG:HG2	2.43	0.49
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.95	0.49
3:C:142:VAL:N	10:J:16:ASP:HB3	2.23	0.49
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.94	0.49
1:A:472:LEU:O	1:A:475:THR:HG22	2.12	0.49
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.94	0.49
3:C:196:ASP:O	3:C:200:GLU:HB2	2.12	0.49
9:I:19:ASP:HB3	9:I:24:ARG:HG3	1.95	0.49
2:B:644:GLU:HB3	2:B:648:HIS:O	2.12	0.49
2:B:64:CYS:HA	2:B:67:SER:HB3	1.95	0.49
2:B:703:ILE:HA	2:B:740:HIS:O	2.13	0.48
4:D:32:GLU:HB3	7:G:5:LYS:HE2	1.96	0.48
12:L:28:LYS:HB3	12:L:39:SER:HA	1.95	0.48
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.94	0.48
2:B:664:THR:HG1	2:B:678:GLU:N	2.12	0.48
1:A:406:ILE:HG13	1:A:412:ARG:HG3	1.95	0.48
9:I:73:ARG:HH12	9:I:112:SER:HA	1.79	0.48
5:E:101:GLN:HG3	5:E:127:ILE:HD13	1.95	0.48
1:A:1121:GLU:HB3	1:A:1124:HIS:HD2	1.78	0.48
2:B:487:THR:HG21	2:B:819:ALA:HB2	1.94	0.48
2:B:602:THR:HA	2:B:605:ARG:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD12	5:E:107:THR:HB	1.94	0.48
4:D:139:LYS:HA	4:D:142:LYS:HD2	1.95	0.48
4:D:25:ALA:HB2	7:G:84:GLY:HA3	1.96	0.48
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.78	0.48
5:E:77:SER:HB2	5:E:105:PHE:HA	1.96	0.48
1:A:596:THR:C	1:A:598:LEU:H	2.17	0.48
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.96	0.48
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.96	0.47
1:A:923:LEU:HA	1:A:926:GLN:HB2	1.96	0.47
2:B:842:ASN:HD21	2:B:996:ARG:HG3	1.78	0.47
5:E:193:GLY:H	5:E:214:CYS:HB3	1.79	0.47
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.97	0.47
2:B:603:LEU:HD12	2:B:609:ILE:HG12	1.95	0.47
6:F:72:LYS:HB2	6:F:142:SER:HA	1.96	0.47
1:A:71:GLN:HE21	13:M:18:LEU:HD23	1.80	0.47
1:A:594:GLY:H	1:A:603:ASN:HD22	1.62	0.47
7:G:96:GLN:HE21	7:G:96:GLN:H	1.63	0.47
2:B:762:ASN:HD22	2:B:1024:ALA:HB3	1.79	0.47
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.54	0.47
5:E:56:LYS:HE2	5:E:84:ASP:H	1.79	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.47
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.96	0.47
3:C:174:ALA:HB1	10:J:11:GLY:HA3	1.96	0.47
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.33	0.47
2:B:883:LEU:HD23	2:B:884:ARG:H	1.79	0.47
10:J:17:LYS:HG2	10:J:41:LEU:HD21	1.97	0.47
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.97	0.46
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.79	0.46
2:B:555:ILE:HA	2:B:558:LEU:HD12	1.96	0.46
1:A:775:ILE:O	1:A:797:LYS:HD2	2.15	0.46
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.97	0.46
8:H:4:THR:HA	8:H:60:ALA:HB2	1.97	0.46
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.98	0.46
1:A:32:VAL:O	1:A:57:ARG:HD2	2.15	0.46
4:D:52:LEU:H	4:D:182:SER:HB3	1.80	0.46
4:D:206:GLU:HA	4:D:209:ARG:HD2	1.98	0.46
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.98	0.46
8:H:91:ASP:C	8:H:93:TYR:H	2.17	0.46
3:C:148:ARG:HB3	3:C:151:GLN:NE2	2.31	0.46
2:B:640:VAL:HA	2:B:651:LEU:HA	1.96	0.46
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:PRO:HD2	6:F:86:THR:HG21	1.96	0.46
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	1.98	0.46
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.97	0.46
1:A:857:ARG:HD3	1:A:861:GLY:O	2.16	0.46
2:B:979:LYS:HE2	2:B:987:LYS:HB2	1.96	0.46
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.99	0.46
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.97	0.46
2:B:553:PRO:HG2	2:B:554:ILE:HD12	1.96	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.46
1:A:83:HIS:HB2	1:A:238:CYS:SG	2.55	0.46
11:K:90:ALA:O	11:K:94:ILE:HG13	2.16	0.46
2:B:234:ILE:HG23	2:B:258:LEU:H	1.81	0.46
2:B:796:LEU:HD23	2:B:799:PRO:HA	1.97	0.46
2:B:1180:PHE:H	2:B:1188:LYS:HE3	1.81	0.46
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.96	0.46
2:B:927:GLN:HA	2:B:930:ALA:HB3	1.98	0.46
2:B:122:LEU:HD22	2:B:958:GLN:HG3	1.98	0.46
1:A:1152:ILE:HB	9:I:44:TYR:HB3	1.97	0.46
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.96	0.46
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.80	0.46
1:A:445:ASN:HB2	1:A:455:MET:HA	1.98	0.46
2:B:614:SER:HB3	2:B:627:PHE:HB2	1.97	0.46
5:E:168:TYR:HB3	5:E:170:LEU:HD21	1.98	0.46
5:E:100:ILE:HA	5:E:105:PHE:HD1	1.80	0.46
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.97	0.46
2:B:620:ARG:HH21	9:I:89:GLN:HG2	1.81	0.46
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.80	0.46
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.98	0.46
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	1.97	0.46
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.16	0.45
2:B:276:ILE:HG23	2:B:336:ARG:HB2	1.98	0.45
2:B:123:THR:HG23	2:B:205:ILE:HA	1.98	0.45
4:D:40:HIS:ND1	7:G:6:ASP:HB3	2.30	0.45
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.16	0.45
8:H:125:LEU:HG	8:H:126:GLU:H	1.80	0.45
1:A:633:VAL:HG11	1:A:645:LEU:HD22	1.97	0.45
1:A:456:MET:HB2	1:A:478:TYR:OH	2.16	0.45
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.99	0.45
8:H:41:ASP:HB3	8:H:121:LEU:HD22	1.98	0.45
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.97	0.45
1:A:55:ASP:N	1:A:56:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ILE:HG21	1:A:801:GLU:HB2	1.98	0.45
2:B:170:LEU:HG	2:B:171:PRO:HD2	1.98	0.45
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.99	0.45
8:H:42:ILE:HD13	8:H:49:VAL:HG21	1.99	0.45
1:A:446:ARG:HH11	1:A:446:ARG:HB3	1.82	0.45
1:A:329:LEU:HA	1:A:335:ARG:HB3	1.97	0.45
7:G:130:TYR:O	7:G:136:VAL:HA	2.17	0.45
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.98	0.45
2:B:801:LYS:O	10:J:52:THR:HG23	2.17	0.45
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.99	0.45
3:C:252:GLN:HE22	11:K:102:LYS:HE3	1.82	0.45
4:D:167:LEU:HD21	4:D:214:LEU:HD21	1.99	0.45
1:A:1260:LEU:HA	1:A:1263:ILE:HD12	1.98	0.45
1:A:855:THR:HG23	1:A:857:ARG:HE	1.82	0.44
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.99	0.44
1:A:858:ASN:HD21	1:A:860:LEU:HD12	1.82	0.44
13:M:37:ARG:HA	13:M:37:ARG:HD3	1.89	0.44
2:B:950:ASP:HB2	2:B:969:ARG:HG3	1.98	0.44
1:A:1148:ILE:HG23	9:I:49:ILE:HB	1.99	0.44
13:M:62:GLU:HA	13:M:65:THR:HG22	1.98	0.44
5:E:198:ILE:HD11	5:E:212:ARG:HB2	1.99	0.44
5:E:97:VAL:HG21	5:E:123:LEU:HB3	1.98	0.44
5:E:62:ALA:HB3	5:E:78:LEU:HD23	1.98	0.44
1:A:261:ASP:HB3	1:A:322:VAL:HG22	1.99	0.44
7:G:96:GLN:NE2	7:G:96:GLN:H	2.15	0.44
1:A:1444:MET:HG3	7:G:60:ARG:HA	2.00	0.44
7:G:46:LEU:HD11	7:G:79:PHE:HB2	2.00	0.44
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.52	0.44
1:A:1210:GLY:O	1:A:1214:GLU:HG2	2.18	0.44
2:B:797:TYR:HB2	2:B:852:ARG:O	2.17	0.44
11:K:85:ASP:HA	11:K:88:LYS:HD2	1.99	0.44
2:B:168:GLY:H	2:B:450:ALA:HB1	1.83	0.44
5:E:154:ILE:O	5:E:196:VAL:HA	2.18	0.44
2:B:124:TYR:HB2	2:B:204:ILE:HB	2.00	0.44
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.99	0.44
10:J:1:MET:N	10:J:54:VAL:O	2.51	0.44
2:B:898:LEU:HD21	2:B:964:VAL:HG21	1.98	0.44
1:A:658:LEU:HD23	1:A:659:HIS:CD2	2.52	0.44
2:B:711:GLU:H	2:B:712:PRO:HD2	1.83	0.43
2:B:918:ILE:HB	2:B:935:ARG:HG2	1.99	0.43
1:A:849:MET:HB3	1:A:1063:MET:SD	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:29:VAL:HG23	13:M:32:PRO:HB3	2.00	0.43
1:A:180:LYS:HE2	1:A:297:GLN:HG2	1.99	0.43
13:M:30:TYR:O	13:M:32:PRO:HD3	2.18	0.43
8:H:135:LEU:HD22	8:H:137:GLN:HE21	1.83	0.43
1:A:940:ARG:HG2	1:A:941:LYS:HE3	2.00	0.43
1:A:84:ILE:HB	1:A:239:LEU:HB3	1.99	0.43
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.99	0.43
3:C:51:VAL:HG21	3:C:60:ASP:HB3	2.00	0.43
3:C:238:ILE:HG13	3:C:239:PRO:HD2	2.00	0.43
1:A:1447:GLU:HG3	7:G:56:ILE:HG12	2.01	0.43
2:B:642:ASP:HA	2:B:649:LYS:HA	2.00	0.43
1:A:631:HIS:HE1	1:A:879:GLU:HG2	1.83	0.43
1:A:254:GLU:HB2	2:B:918:ILE:HG21	2.01	0.43
1:A:554:PRO:HG3	1:A:651:LYS:HE3	2.00	0.43
1:A:592:ASP:H	1:A:595:THR:HG21	1.83	0.43
8:H:87:ARG:HB2	8:H:89:LEU:HD11	2.00	0.43
1:A:453:MET:HB3	1:A:477:PRO:CB	2.49	0.43
3:C:194:GLU:HB3	3:C:195:GLN:HE21	1.84	0.43
1:A:114:LEU:HD11	1:A:171:GLN:HG3	2.01	0.43
2:B:1138:MET:HB2	2:B:1147:LEU:HD13	2.00	0.43
1:A:497:THR:HG23	2:B:1146:PHE:HA	2.00	0.43
1:A:500:GLU:O	1:A:504:LEU:HB2	2.19	0.43
2:B:925:LEU:HB3	2:B:928:ARG:CB	2.48	0.43
2:B:365:THR:HG22	2:B:374:LYS:HE3	2.00	0.43
8:H:118:PHE:HE1	8:H:123:MET:HB2	1.84	0.43
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.99	0.43
2:B:756:ILE:O	2:B:759:PRO:HD3	2.19	0.43
9:I:26:LEU:HG	9:I:37:GLU:HA	2.00	0.43
1:A:709:THR:HG23	9:I:94:ASP:HA	2.01	0.43
7:G:129:SER:HB3	7:G:138:THR:HG23	2.01	0.43
4:D:37:GLN:NE2	4:D:48:ILE:HG12	2.34	0.42
1:A:346:ASP:CG	2:B:1108:ARG:HA	2.39	0.42
1:A:998:LEU:HA	1:A:1011:GLN:HE22	1.84	0.42
12:L:31:CYS:SG	12:L:55:ILE:HD11	2.58	0.42
2:B:420:LEU:HD22	2:B:453:ILE:HA	2.01	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HH11	1.66	0.42
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.20	0.42
2:B:331:LEU:HA	2:B:334:ILE:HD12	2.00	0.42
2:B:120:ARG:HG2	2:B:955:THR:HG21	2.01	0.42
3:C:84:ARG:HD2	11:K:11:LEU:HD11	2.01	0.42
1:A:867:ILE:HG12	1:A:1000:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:ILE:HG13	7:G:170:ALA:HA	2.01	0.42
2:B:308:TRP:HA	2:B:311:LEU:HB2	2.01	0.42
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	2.02	0.42
2:B:515:HIS:CD2	2:B:517:THR:H	2.37	0.42
8:H:23:VAL:HG21	8:H:121:LEU:HD21	2.02	0.42
1:A:679:ILE:HD11	1:A:733:ALA:HB2	2.01	0.42
1:A:663:SER:CB	2:B:1085:ILE:HA	2.50	0.42
1:A:50:ILE:H	1:A:50:ILE:HG13	1.74	0.42
1:A:635:ARG:NH2	1:A:877:HIS:HA	2.34	0.42
2:B:22:SER:HB3	2:B:654:ARG:HH11	1.85	0.42
1:A:92:HIS:CG	1:A:95:PHE:HD1	2.38	0.42
6:F:103:MET:HB2	7:G:15:PRO:HB2	2.01	0.42
3:C:164:ALA:HA	3:C:167:HIS:O	2.20	0.42
2:B:1167:GLY:HA3	2:B:1216:LEU:N	2.35	0.42
1:A:1428:VAL:HG11	2:B:1135:ARG:HD2	2.02	0.42
1:A:567:LYS:CB	1:A:568:PRO:CD	2.95	0.42
7:G:13:LEU:HD22	7:G:17:PHE:HB2	2.02	0.42
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.42
1:A:1438:THR:HG23	6:F:92:ARG:HB2	2.02	0.42
2:B:758:PHE:HZ	2:B:1031:LEU:HD13	1.83	0.42
4:D:29:LEU:HB3	4:D:33:PHE:HB2	2.01	0.42
7:G:30:LEU:HD11	7:G:74:TYR:CD2	2.53	0.42
13:M:63:TRP:HA	13:M:66:PHE:CD2	2.55	0.42
1:A:114:LEU:HD22	1:A:145:LYS:HB3	2.01	0.42
1:A:606:LEU:HG	1:A:613:ILE:HD13	2.02	0.42
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.01	0.42
1:A:956:LEU:HD11	1:A:1017:LEU:HG	2.02	0.42
3:C:87:PHE:N	3:C:87:PHE:CD1	2.88	0.42
1:A:42:ASP:HB3	1:A:45:GLN:HA	2.02	0.41
8:H:93:TYR:HA	8:H:145:ARG:HB3	2.02	0.41
2:B:324:ILE:HD13	2:B:330:ALA:HA	2.02	0.41
1:A:1256:GLU:HA	1:A:1259:MET:HB3	2.02	0.41
8:H:80:ARG:HG2	11:K:57:LEU:HD22	2.02	0.41
1:A:543:LEU:O	1:A:547:LEU:HG	2.20	0.41
6:F:94:LEU:HD22	6:F:122:MET:HE2	2.02	0.41
3:C:70:ILE:HG23	3:C:142:VAL:HG21	2.01	0.41
8:H:63:LEU:HB3	8:H:90:ALA:H	1.85	0.41
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.92	0.41
2:B:1172:ILE:HG12	2:B:1183:LYS:HE2	2.02	0.41
2:B:856:PHE:HA	2:B:968:VAL:O	2.20	0.41
1:A:35:ILE:HA	1:A:52:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.53	0.41
4:D:8:PHE:HZ	7:G:5:LYS:HZ1	1.68	0.41
5:E:165:LEU:HD23	5:E:170:LEU:HD12	2.02	0.41
2:B:401:PHE:HB3	2:B:695:ALA:HB1	2.02	0.41
1:A:701:LEU:HA	9:I:115:LYS:HE3	2.02	0.41
2:B:259:TYR:HB2	2:B:268:THR:HG23	2.02	0.41
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.02	0.41
5:E:97:VAL:HG13	5:E:127:ILE:HG12	2.02	0.41
1:A:1193:LEU:HB2	1:A:1260:LEU:HD23	2.02	0.41
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.92	0.41
2:B:638:PHE:HA	2:B:690:VAL:HG12	2.02	0.41
1:A:825:ILE:HD13	2:B:513:GLN:HE21	1.85	0.41
2:B:275:TYR:HD2	2:B:355:ILE:HD11	1.84	0.41
5:E:77:SER:HB3	5:E:105:PHE:HD2	1.85	0.41
2:B:637:LEU:HA	2:B:743:ILE:HD11	2.02	0.41
2:B:211:VAL:HG11	2:B:495:LEU:HA	2.01	0.41
1:A:254:GLU:HG2	2:B:920:PRO:HG2	2.03	0.41
1:A:518:LYS:HB3	1:A:626:ASN:HD22	1.84	0.41
5:E:66:GLU:HA	5:E:69:ILE:HD12	2.01	0.41
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	2.02	0.41
2:B:425:THR:HA	2:B:428:ILE:HD12	2.02	0.41
1:A:503:GLN:NE2	6:F:90:ARG:HH21	2.19	0.41
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.60	0.41
1:A:55:ASP:C	1:A:57:ARG:H	2.25	0.41
1:A:66:LYS:HG2	13:M:18:LEU:HD22	2.03	0.41
9:I:92:ARG:HG2	9:I:93:LYS:HD3	2.03	0.41
3:C:73:GLN:HB2	3:C:131:HIS:HB2	2.03	0.41
3:C:41:ILE:HB	3:C:172:PRO:HG2	2.02	0.41
2:B:172:ILE:HG12	2:B:178:ASN:HD22	1.86	0.41
1:A:474:VAL:HG23	1:A:521:MET:SD	2.61	0.41
2:B:654:ARG:H	2:B:657:HIS:HD2	1.68	0.41
3:C:46:ILE:HA	3:C:159:ALA:HA	2.03	0.41
5:E:18:THR:HG23	5:E:143:ASN:HD22	1.86	0.41
1:A:665:GLY:HA2	2:B:1026:LEU:HD22	2.03	0.41
1:A:43:GLU:HB3	1:A:50:ILE:HG23	2.02	0.40
7:G:49:LEU:HD21	7:G:77:VAL:HG23	2.02	0.40
7:G:3:PHE:HB2	7:G:78:VAL:HG23	2.03	0.40
1:A:567:LYS:HB3	8:H:96:VAL:N	2.33	0.40
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.56	0.40
1:A:1224:LEU:HD12	1:A:1242:VAL:H	1.86	0.40
4:D:37:GLN:HE21	4:D:47:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:HB3	3:C:131:HIS:H	1.87	0.40
1:A:367:PRO:HA	1:A:463:ILE:O	2.21	0.40
6:F:82:THR:HG22	6:F:84:TYR:H	1.87	0.40
9:I:65:ASP:HB3	9:I:68:LEU:HD12	2.02	0.40
1:A:901:LEU:HD22	1:A:919:ILE:HG12	2.03	0.40
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.36	0.40
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.36	0.40
1:A:49:LYS:HB3	1:A:54:ASN:O	2.21	0.40
2:B:1138:MET:CE	2:B:1143:ALA:HB3	2.52	0.40
1:A:404:TYR:HD2	1:A:414:ASP:HA	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	1215 (86%)	137 (10%)	54 (4%)	4	39
2	B	1102/1224 (90%)	938 (85%)	126 (11%)	38 (3%)	5	42
3	C	264/318 (83%)	219 (83%)	37 (14%)	8 (3%)	5	44
4	D	174/221 (79%)	147 (84%)	20 (12%)	7 (4%)	4	37
5	E	212/215 (99%)	192 (91%)	16 (8%)	4 (2%)	10	54
6	F	85/155 (55%)	74 (87%)	11 (13%)	0	100	100
7	G	169/171 (99%)	145 (86%)	21 (12%)	3 (2%)	11	55
8	H	130/146 (89%)	97 (75%)	18 (14%)	15 (12%)	0	9
9	I	117/122 (96%)	96 (82%)	19 (16%)	2 (2%)	11	56
10	J	63/70 (90%)	51 (81%)	7 (11%)	5 (8%)	1	19
11	K	112/120 (93%)	101 (90%)	10 (9%)	1 (1%)	21	67
12	L	44/70 (63%)	34 (77%)	5 (11%)	5 (11%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	54/197 (27%)	43 (80%)	8 (15%)	3 (6%)	2	29
All	All	3932/4762 (83%)	3352 (85%)	435 (11%)	145 (4%)	4	40

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	65	LEU
1	A	66	LYS
1	A	167	CYS
1	A	311	GLN
1	A	567	LYS
1	A	780	VAL
1	A	846	GLU
1	A	1206	ASP
1	A	1405	THR
2	B	282	ILE
2	B	531	GLN
2	B	731	VAL
2	B	785	TYR
2	B	891	ASP
2	B	895	ASP
3	C	149	LYS
4	D	18	VAL
4	D	27	LEU
7	G	20	PRO
7	G	139	ILE
7	G	154	VAL
8	H	128	ASN
10	J	64	ASN
12	L	55	ILE
1	A	5	GLN
1	A	52	GLY
1	A	54	ASN
1	A	68	GLN
1	A	72	GLU
1	A	178	GLY
1	A	282	ASN
1	A	322	VAL
1	A	331	GLY
1	A	624	SER
1	A	903	ASN

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Mol	Chain	Res	Type
1	A	1242	VAL
1	A	1280	GLU
1	A	1365	TYR
1	A	1403	GLU
2	B	45	SER
2	B	245	GLU
2	B	367	LEU
2	B	468	GLU
2	B	476	ARG
2	B	575	PRO
2	B	797	TYR
2	B	926	GLY
2	B	1046	PRO
2	B	1153	GLU
2	B	1155	SER
2	B	1157	ALA
2	B	1175	LEU
3	C	142	VAL
3	C	175	ALA
3	C	184	ASN
4	D	20	GLU
4	D	53	SER
4	D	199	ASN
5	E	3	GLN
5	E	141	VAL
8	H	92	ASP
10	J	2	ILE
12	L	46	VAL
12	L	56	LEU
13	M	17	ASN
1	A	4	GLN
1	A	67	CYS
1	A	71	GLN
1	A	286	HIS
1	A	318	SER
1	A	466	SER
1	A	525	GLN
1	A	591	PHE
1	A	628	GLY
1	A	868	TYR
1	A	906	HIS
1	A	920	LEU

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Mol	Chain	Res	Type
2	B	248	SER
2	B	335	GLY
2	B	641	GLU
2	B	711	GLU
2	B	883	LEU
8	H	18	GLY
8	H	78	SER
8	H	108	SER
8	H	109	LYS
8	H	110	ASP
9	I	21	GLU
9	I	88	SER
10	J	42	LYS
12	L	45	ALA
13	M	28	LYS
1	A	47	ARG
1	A	69	THR
1	A	156	ASP
1	A	196	GLU
1	A	253	ASN
1	A	290	GLU
1	A	465	TYR
1	A	922	ASP
1	A	1255	GLU
2	B	58	THR
2	B	962	LYS
2	B	1017	ILE
2	B	1082	MET
2	B	1108	ARG
3	C	110	THR
3	C	141	GLY
5	E	104	ASN
8	H	35	GLN
8	H	84	ALA
8	H	139	ASN
10	J	6	ARG
10	J	9	SER
11	K	64	GLU
12	L	59	ALA
13	M	15	GLY
1	A	35	ILE
1	A	958	VAL

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Mol	Chain	Res	Type
1	A	1377	THR
2	B	642	ASP
2	B	792	MET
2	B	1156	ASP
2	B	1181	GLU
3	C	167	HIS
3	C	174	ALA
4	D	5	THR
4	D	119	ARG
5	E	148	GLU
8	H	60	ALA
8	H	61	SER
2	B	100	PRO
1	A	1327	ILE
2	B	510	LYS
2	B	867	GLY
8	H	107	VAL
1	A	1437	GLY
8	H	17	PRO
1	A	424	ILE
8	H	119	GLY
1	A	1454	MET
1	A	1064	VAL
2	B	571	PRO
2	B	764	SER

### 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	1239/1520 (82%)	1071 (86%)	168 (14%)	5	29
2	B	972/1061 (92%)	847 (87%)	125 (13%)	5	31
3	C	234/274 (85%)	210 (90%)	24 (10%)	9	40
4	D	160/200 (80%)	138 (86%)	22 (14%)	4	29
5	E	196/197 (100%)	181 (92%)	15 (8%)	16	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	77/137 (56%)	68 (88%)	9 (12%)	7	35
7	G	152/152 (100%)	135 (89%)	17 (11%)	7	37
8	H	118/128 (92%)	102 (86%)	16 (14%)	5	29
9	I	113/116 (97%)	103 (91%)	10 (9%)	12	48
10	J	60/65 (92%)	53 (88%)	7 (12%)	7	35
11	K	99/102 (97%)	87 (88%)	12 (12%)	6	33
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	25
13	M	52/62 (84%)	40 (77%)	12 (23%)	1	8
All	All	3512/4071 (86%)	3069 (87%)	443 (13%)	5	31

All (443) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	11	LEU
1	A	22	PHE
1	A	41	MET
1	A	44	THR
1	A	50	ILE
1	A	64	ASN
1	A	67	CYS
1	A	68	GLN
1	A	69	THR
1	A	76	GLU
1	A	83	HIS
1	A	93	VAL
1	A	96	ILE
1	A	101	LYS
1	A	109	HIS
1	A	112	LYS
1	A	113	LEU
1	A	114	LEU
1	A	116	ASP
1	A	121	LEU
1	A	138	ILE
1	A	141	LEU
1	A	145	LYS
1	A	151	ASP
1	A	155	GLU

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Mol	Chain	Res	Type
1	A	156	ASP
1	A	159	THR
1	A	164	ARG
1	A	175	ARG
1	A	196	GLU
1	A	199	LEU
1	A	200	ARG
1	A	208	LEU
1	A	219	PHE
1	A	254	GLU
1	A	256	GLN
1	A	265	LYS
1	A	268	ASP
1	A	270	LEU
1	A	293	GLU
1	A	303	TYR
1	A	316	GLN
1	A	320	ARG
1	A	322	VAL
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	359	LEU
1	A	378	GLU
1	A	383	TYR
1	A	385	ILE
1	A	393	ARG
1	A	398	GLU
1	A	419	LYS
1	A	425	GLN
1	A	433	GLU
1	A	434	ARG
1	A	437	MET
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
1	A	455	MET
1	A	470	LEU
1	A	474	VAL
1	A	481	ASP
1	A	487	MET

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Mol	Chain	Res	Type
1	A	493	GLN
1	A	498	ARG
1	A	504	LEU
1	A	526	ASP
1	A	536	LEU
1	A	542	GLU
1	A	548	ASN
1	A	555	ASP
1	A	567	LYS
1	A	578	LEU
1	A	582	ILE
1	A	588	LEU
1	A	609	ASP
1	A	618	GLU
1	A	634	THR
1	A	635	ARG
1	A	664	THR
1	A	666	ILE
1	A	732	LEU
1	A	738	LYS
1	A	740	LEU
1	A	752	LYS
1	A	764	CYS
1	A	773	LYS
1	A	783	THR
1	A	795	GLU
1	A	821	ARG
1	A	822	GLU
1	A	827	THR
1	A	834	THR
1	A	840	ARG
1	A	878	ILE
1	A	883	LEU
1	A	884	ASP
1	A	890	ASP
1	A	894	GLU
1	A	896	ARG
1	A	902	LEU
1	A	906	HIS
1	A	908	LEU
1	A	919	ILE
1	A	923	LEU

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Mol	Chain	Res	Type
1	A	926	GLN
1	A	929	LEU
1	A	941	LYS
1	A	983	ILE
1	A	992	ASP
1	A	1001	ARG
1	A	1003	LYS
1	A	1028	THR
1	A	1032	LEU
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1074	GLU
1	A	1120	LEU
1	A	1136	SER
1	A	1148	ILE
1	A	1150	SER
1	A	1155	ASP
1	A	1159	ARG
1	A	1161	THR
1	A	1167	GLU
1	A	1187	GLN
1	A	1196	GLU
1	A	1205	LYS
1	A	1218	GLN
1	A	1223	ASP
1	A	1241	ARG
1	A	1255	GLU
1	A	1259	MET
1	A	1266	THR
1	A	1270	ASN
1	A	1274	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1323	ASP
1	A	1333	ILE
1	A	1334	ASP
1	A	1341	ILE
1	A	1351	GLU
1	A	1356	ILE
1	A	1366	ARG

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Mol	Chain	Res	Type
1	A	1370	LEU
1	A	1371	LEU
1	A	1373	ASP
1	A	1381	LEU
1	A	1382	THR
1	A	1385	THR
1	A	1397	LEU
1	A	1405	THR
1	A	1420	ASP
1	A	1424	VAL
1	A	1433	MET
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE
1	A	1453	TYR
1	A	1455	PRO
2	B	21	GLU
2	B	44	VAL
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	102	VAL
2	B	104	GLU
2	B	123	THR
2	B	128	LEU
2	B	134	LYS
2	B	170	LEU
2	B	183	GLU
2	B	186	GLU
2	B	191	LYS
2	B	192	LEU
2	B	199	MET
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE
2	B	261	ARG
2	B	272	THR
2	B	273	LEU
2	B	277	LYS
2	B	280	ILE
2	B	305	VAL
2	B	312	GLU

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Mol	Chain	Res	Type
2	B	317	CYS
2	B	331	LEU
2	B	336	ARG
2	B	346	GLU
2	B	347	LYS
2	B	357	GLN
2	B	365	THR
2	B	371	GLU
2	B	373	ARG
2	B	387	LEU
2	B	390	LEU
2	B	391	ASP
2	B	393	LYS
2	B	398	ARG
2	B	401	PHE
2	B	416	LEU
2	B	420	LEU
2	B	423	LYS
2	B	424	LEU
2	B	427	ASP
2	B	434	ARG
2	B	436	VAL
2	B	446	LEU
2	B	452	THR
2	B	466	TRP
2	B	473	MET
2	B	482	VAL
2	B	508	LEU
2	B	510	LYS
2	B	531	GLN
2	B	539	LEU
2	B	560	GLU
2	B	563	MET
2	B	570	VAL
2	B	579	ARG
2	B	603	LEU
2	B	604	ARG
2	B	615	MET
2	B	616	ILE
2	B	617	ARG
2	B	620	ARG
2	B	643	ASP

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Mol	Chain	Res	Type
2	B	646	LEU
2	B	658	ILE
2	B	729	ILE
2	B	736	THR
2	B	748	ILE
2	B	755	ILE
2	B	762	ASN
2	B	773	MET
2	B	790	ASP
2	B	795	ILE
2	B	797	TYR
2	B	801	LYS
2	B	829	CYS
2	B	830	TYR
2	B	837	ASP
2	B	839	MET
2	B	841	MET
2	B	861	ASP
2	B	868	MET
2	B	871	THR
2	B	883	LEU
2	B	891	ASP
2	B	915	THR
2	B	925	LEU
2	B	928	ARG
2	B	935	ARG
2	B	943	SER
2	B	953	LEU
2	B	954	VAL
2	B	955	THR
2	B	957	ASN
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	994	TYR
2	B	998	ASP
2	B	999	MET
2	B	1013	ASN
2	B	1031	LEU
2	B	1048	THR

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Mol	Chain	Res	Type
2	B	1050	ILE
2	B	1065	GLN
2	B	1072	MET
2	B	1074	ASN
2	B	1101	ASP
2	B	1114	LEU
2	B	1123	SER
2	B	1128	LEU
2	B	1132	GLU
2	B	1169	MET
2	B	1175	LEU
2	B	1183	LYS
2	B	1202	LEU
2	B	1211	ASN
2	B	1216	LEU
3	C	11	ARG
3	C	14	SER
3	C	25	VAL
3	C	26	ASP
3	C	29	MET
3	C	35	ARG
3	C	43	THR
3	C	44	LEU
3	C	56	THR
3	C	76	ASP
3	C	77	ILE
3	C	78	GLU
3	C	80	LEU
3	C	120	ILE
3	C	127	ARG
3	C	133	ILE
3	C	136	ASP
3	C	146	LYS
3	C	148	ARG
3	C	214	ASN
3	C	215	GLU
3	C	217	ASP
3	C	262	LEU
3	C	265	MET
4	D	11	ARG
4	D	12	ARG
4	D	17	LYS

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Mol	Chain	Res	Type
4	D	28	GLN
4	D	34	GLN
4	D	40	HIS
4	D	43	GLU
4	D	47	LEU
4	D	50	LEU
4	D	57	LEU
4	D	65	GLU
4	D	120	GLU
4	D	148	LEU
4	D	152	SER
4	D	156	ASP
4	D	165	GLN
4	D	187	THR
4	D	200	ASN
4	D	206	GLU
4	D	213	GLU
4	D	214	LEU
4	D	220	LEU
5	E	14	ARG
5	E	30	ILE
5	E	33	GLU
5	E	81	GLU
5	E	92	THR
5	E	104	ASN
5	E	107	THR
5	E	116	ILE
5	E	149	LEU
5	E	170	LEU
5	E	179	GLN
5	E	184	VAL
5	E	188	LEU
5	E	198	ILE
5	E	205	SER
6	F	70	LYS
6	F	78	GLN
6	F	79	ARG
6	F	112	GLU
6	F	118	LEU
6	F	119	ARG
6	F	122	MET
6	F	154	ASP

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Mol	Chain	Res	Type
6	F	155	LEU
7	G	1	MET
7	G	12	THR
7	G	21	ARG
7	G	38	CYS
7	G	46	LEU
7	G	52	ASP
7	G	60	ARG
7	G	87	VAL
7	G	90	THR
7	G	96	GLN
7	G	106	MET
7	G	114	LEU
7	G	138	THR
7	G	141	SER
7	G	154	VAL
7	G	160	ILE
7	G	165	GLU
8	H	14	GLU
8	H	19	ARG
8	H	26	ILE
8	H	32	THR
8	H	35	GLN
8	H	46	LEU
8	H	53	ASP
8	H	64	ASN
8	H	89	LEU
8	H	94	ASP
8	H	111	LEU
8	H	123	MET
8	H	124	ARG
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
9	I	13	MET
9	I	26	LEU
9	I	28	GLU
9	I	35	VAL
9	I	46	HIS
9	I	50	THR
9	I	89	GLN
9	I	93	LYS

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Mol	Chain	Res	Type
9	I	104	LEU
9	I	113	ASP
10	J	2	ILE
10	J	3	VAL
10	J	24	LEU
10	J	26	GLN
10	J	29	GLU
10	J	34	THR
10	J	43	ARG
11	K	1	MET
11	K	5	ASP
11	K	9	LEU
11	K	11	LEU
11	K	14	GLU
11	K	20	LYS
11	K	32	VAL
11	K	47	ARG
11	K	51	LEU
11	K	54	ARG
11	K	101	LEU
11	K	114	LEU
12	L	27	LEU
12	L	54	ARG
12	L	55	ILE
12	L	64	LEU
12	L	65	VAL
12	L	68	GLU
13	M	18	LEU
13	M	20	ILE
13	M	26	GLU
13	M	29	VAL
13	M	38	PHE
13	M	39	SER
13	M	44	VAL
13	M	45	CYS
13	M	50	LEU
13	M	59	THR
13	M	63	TRP
13	M	66	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	54	ASN
1	A	64	ASN
1	A	71	GLN
1	A	118	HIS
1	A	225	ASN
1	A	256	GLN
1	A	339	ASN
1	A	425	GLN
1	A	445	ASN
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN
1	A	603	ASN
1	A	626	ASN
1	A	631	HIS
1	A	640	GLN
1	A	650	GLN
1	A	659	HIS
1	A	736	ASN
1	A	741	ASN
1	A	926	GLN
1	A	965	GLN
1	A	969	GLN
1	A	1124	HIS
1	A	1128	GLN
1	A	1211	GLN
2	B	121	ASN
2	B	178	ASN
2	B	206	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	744	HIS
2	B	878	GLN
2	B	957	ASN
2	B	986	GLN
2	B	1013	ASN
2	B	1015	HIS
2	B	1025	HIS
2	B	1062	HIS
2	B	1074	ASN

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Mol	Chain	Res	Type
2	B	1076	HIS
2	B	1097	HIS
2	B	1161	HIS
2	B	1193	GLN
2	B	1195	HIS
2	B	1211	ASN
3	C	7	GLN
3	C	123	ASN
3	C	131	HIS
3	C	195	GLN
4	D	9	GLN
4	D	37	GLN
5	E	101	GLN
5	E	113	GLN
5	E	115	ASN
7	G	14	HIS
7	G	71	ASN
7	G	96	GLN
7	G	97	HIS
7	G	122	ASN
7	G	126	ASN
8	H	33	GLN
8	H	137	GLN
9	I	83	ASN
10	J	53	HIS
11	K	2	ASN
11	K	44	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1416/1733 (81%)	-0.24	6 (0%) 93 90	53, 106, 168, 238	0
2	B	1120/1224 (91%)	-0.18	6 (0%) 91 88	53, 122, 192, 238	0
3	C	266/318 (83%)	-0.27	1 (0%) 93 90	63, 117, 167, 202	0
4	D	178/221 (80%)	0.02	4 (2%) 65 56	65, 132, 190, 228	0
5	E	214/215 (99%)	-0.04	2 (0%) 85 80	74, 138, 210, 245	0
6	F	87/155 (56%)	-0.38	0 100 100	56, 88, 114, 128	0
7	G	171/171 (100%)	-0.28	0 100 100	64, 108, 146, 188	0
8	H	134/146 (91%)	-0.04	1 (0%) 89 84	101, 144, 209, 224	0
9	I	119/122 (97%)	0.29	6 (5%) 32 25	103, 170, 220, 232	0
10	J	65/70 (92%)	-0.29	0 100 100	78, 114, 152, 177	0
11	K	114/120 (95%)	-0.19	0 100 100	74, 120, 143, 198	0
12	L	46/70 (65%)	0.23	3 (6%) 22 16	81, 152, 165, 202	0
13	M	56/197 (28%)	-0.22	0 100 100	89, 117, 157, 174	0
All	All	3986/4762 (83%)	-0.18	29 (0%) 89 84	53, 118, 192, 245	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1455	PRO	3.8
12	L	26	THR	3.4
4	D	9	GLN	3.0
1	A	1173	HIS	2.9
1	A	69	THR	2.9
1	A	196	GLU	2.8
2	B	332	ASP	2.7
12	L	27	LEU	2.7
4	D	4	SER	2.7

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Mol	Chain	Res	Type	RSRZ
9	I	108	HIS	2.6
9	I	110	PHE	2.5
2	B	335	GLY	2.5
3	C	266	ASP	2.4
9	I	120	GLN	2.4
9	I	111	THR	2.4
4	D	220	LEU	2.2
9	I	102	VAL	2.2
1	A	197	PRO	2.2
2	B	132	VAL	2.2
5	E	123	LEU	2.1
12	L	25	ALA	2.1
4	D	119	ARG	2.1
1	A	1298	TYR	2.1
2	B	90	ILE	2.1
8	H	146	ARG	2.1
5	E	120	ALA	2.1
2	B	650	GLU	2.0
2	B	435	THR	2.0
9	I	109	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	ZN	I	3004	1/1	0.98	0.16	-1.64	196,196,196,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
14	ZN	A	3008	1/1	0.97	0.07	-1.70	65,65,65,65	0
14	ZN	C	3002	1/1	0.98	0.06	-1.76	62,62,62,62	0
14	ZN	I	3003	1/1	0.97	0.07	-1.80	151,151,151,151	0
14	ZN	M	3009	1/1	0.98	0.06	-2.01	71,71,71,71	0
14	ZN	J	3001	1/1	0.94	0.16	-2.06	124,124,124,124	0
14	ZN	L	3005	1/1	0.96	0.07	-2.17	190,190,190,190	0
14	ZN	A	3006	1/1	0.95	0.05	-3.22	130,130,130,130	0
14	ZN	B	3007	1/1	0.97	0.06	-	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.