



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:20 PM GMT

PDB ID : 4C3J
Title : Structure of 14-subunit RNA polymerase I at 3.35 Å resolution, crystal form C2-90
Authors : Fernandez-Tornero, C.; Moreno-Morcillo, M.; Rashid, U.J.; Taylor, N.M.I.; Ruiz, F.M.; Gruene, T.; Legrand, P.; Steuerwald, U.; Muller, C.W.
Deposited on : 2013-08-24
Resolution : 3.35 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

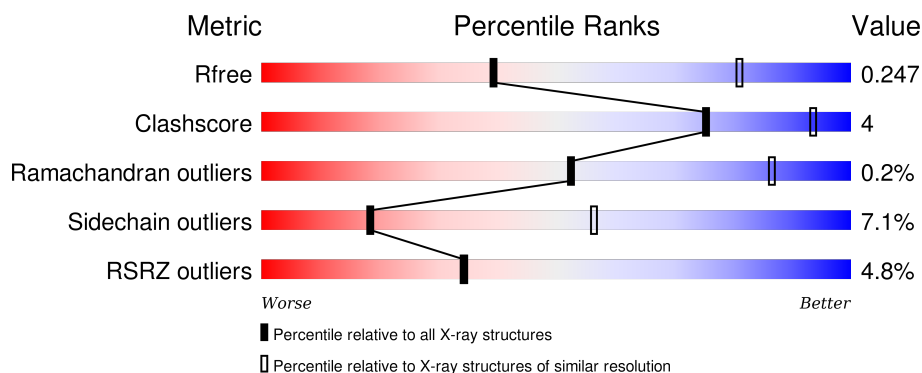
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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. 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	1664	<div> <div>3%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>
2	B	1203	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
3	C	335	<div> <div>2%</div> <div>74%</div> <div>16%</div> <div>• 9%</div> </div>
4	D	137	<div> <div>2%</div> <div>35%</div> <div>8%</div> <div>57%</div> </div>
5	E	215	<div> <div>3%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	155	<div><div></div><div>56%8%35%</div></div>
7	G	326	<div><div>5%</div><div></div><div>68%11%21%</div></div>
8	H	146	<div><div>8%</div><div></div><div>79%12%8%</div></div>
9	I	125	<div><div>14%</div><div></div><div>77%22%</div></div>
10	J	70	<div><div>%</div><div></div><div>77%13%9%</div></div>
11	K	142	<div><div>%</div><div></div><div>58%12%27%</div></div>
12	L	70	<div><div>3%</div><div></div><div>56%9%36%</div></div>
13	M	415	<div><div>5%</div><div></div><div>21%75%</div></div>
14	N	233	<div><div>14%</div><div></div><div>53%6%40%</div></div>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 34552 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 I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1523	Total	C	N	O	S	0	0	0
			12019	7577	2086	2292	64			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1176	Total	C	N	O	S	0	0	0
			9322	5898	1629	1745	50			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	304	Total	C	N	O	S	0	0	0
			2418	1536	414	460	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	59	Total	C	N	O	0	0	0
			466	292	80	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	12	SER	THR	CONFLICT	UNP P50106

- 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	215	Total	C	N	O	S	0	0	0
			1759	1116	310	321	12			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	259	Total	C	N	O	S	0	0	0
			2052	1301	348	398	5			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1072	676	181	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	124	Total	C	N	O	S	0	0	0
			942	584	160	189	9			

- 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	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUB-UNIT RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	103	Total	C	N	O	S	0	0	0
			810	506	132	167	5			

- 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	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	105	Total	C	N	O	0	0	0
			831	528	137	166			

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	139	Total	C	N	O	S	0	0	0
			1103	706	179	214	4			

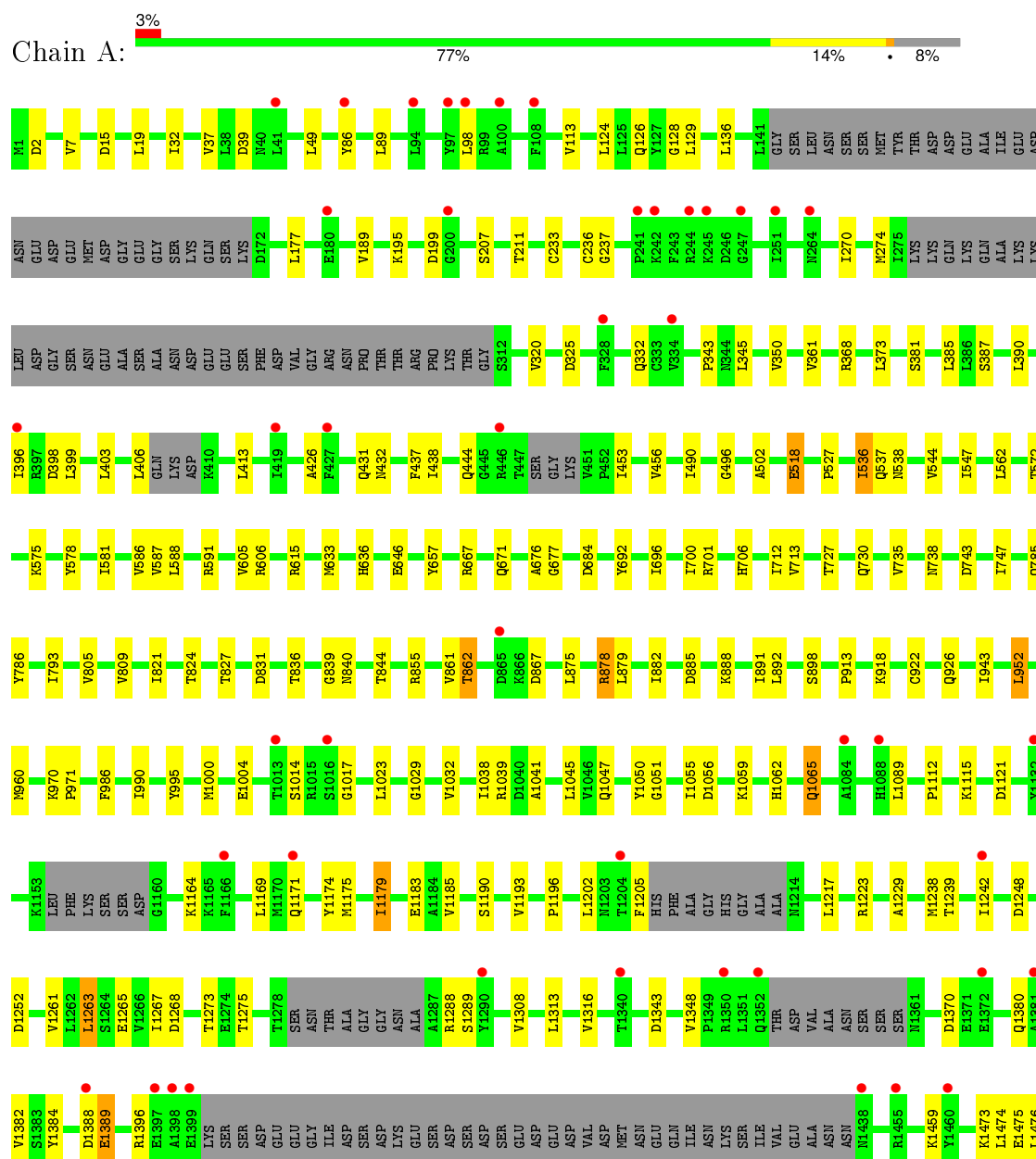
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

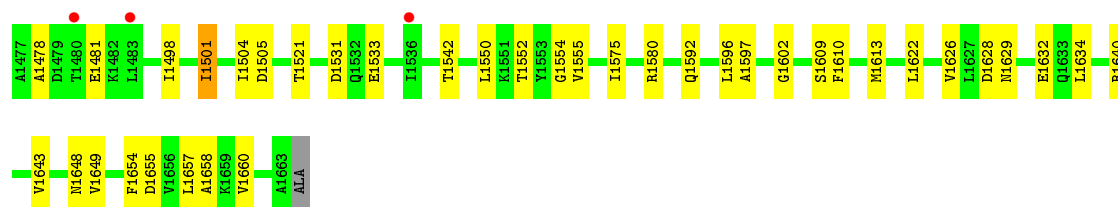
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	1	Total	Zn	0	0
			1	1		
15	A	2	Total	Zn	0	0
			2	2		
15	L	1	Total	Zn	0	0
			1	1		
15	J	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		

3 Residue-property plots

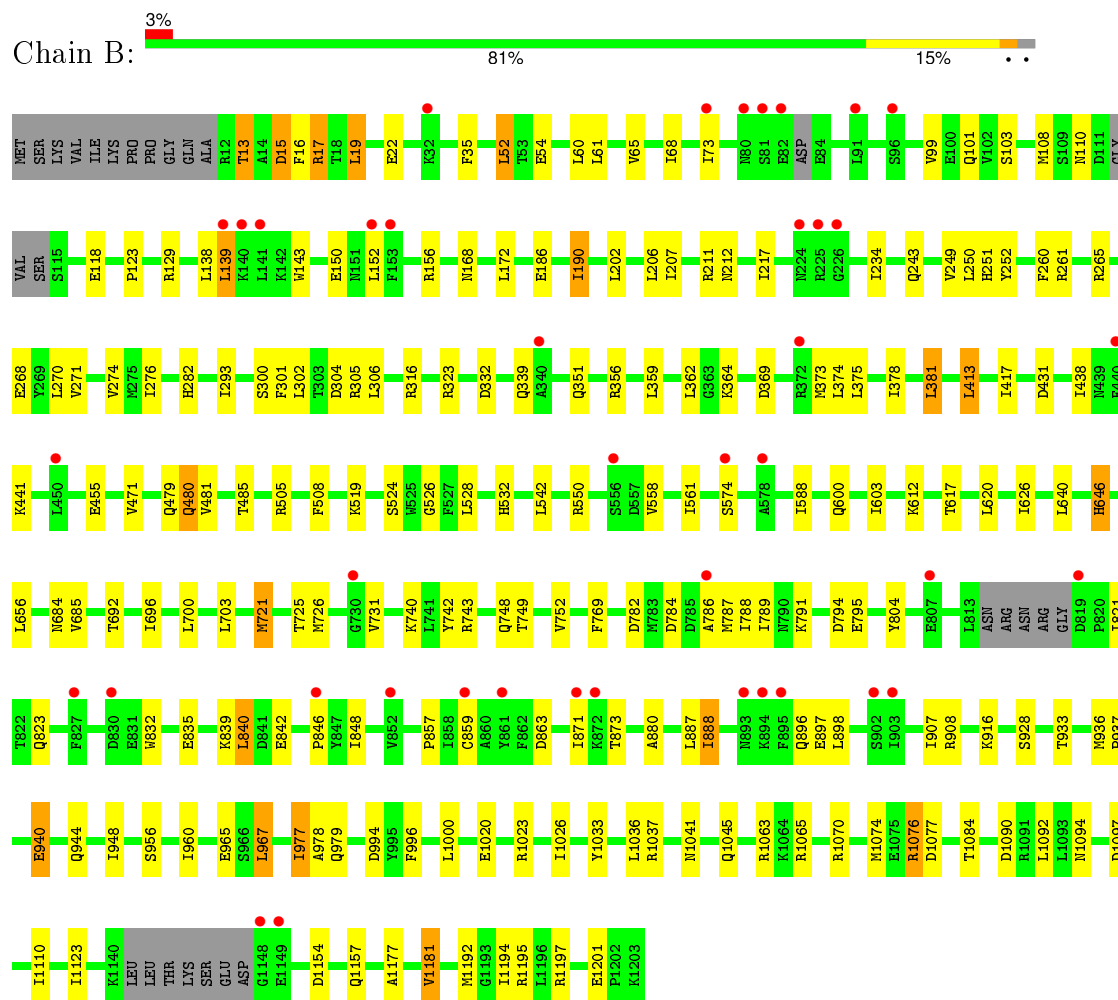
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 I SUBUNIT RPA190

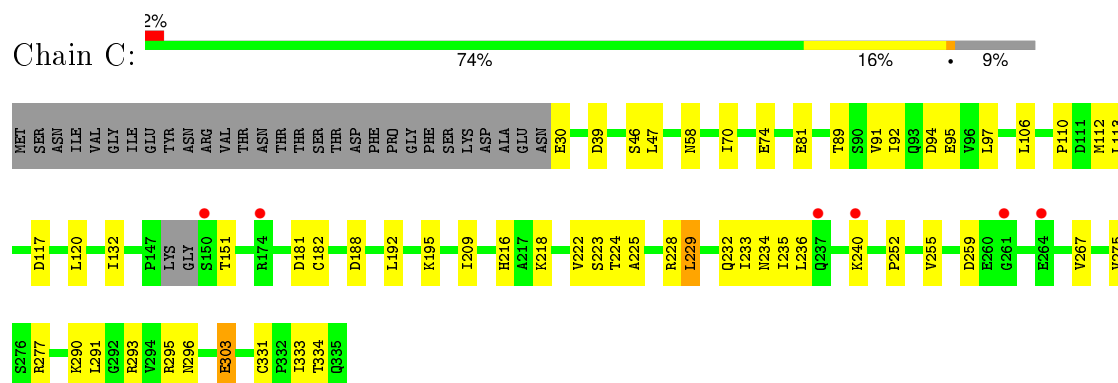




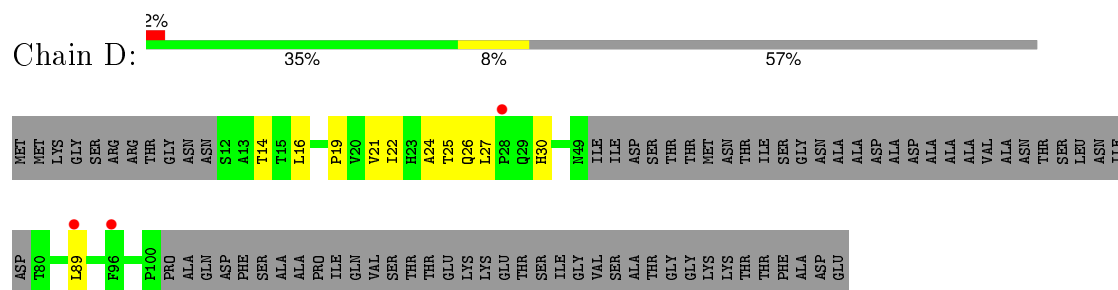
• Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135



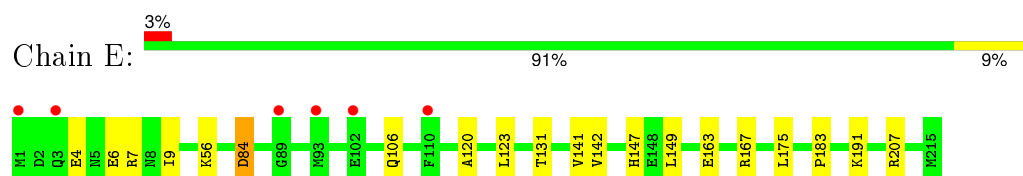
• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1



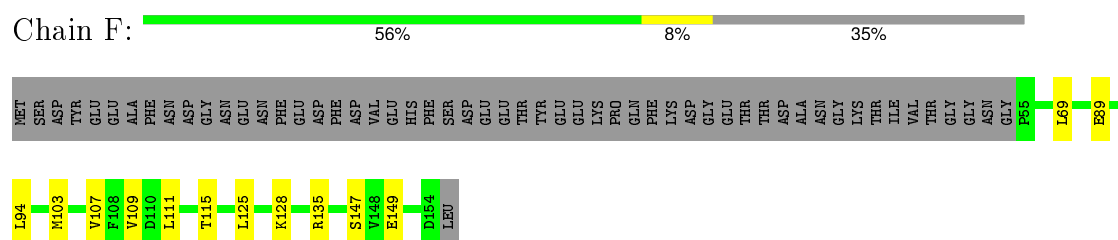
- Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14



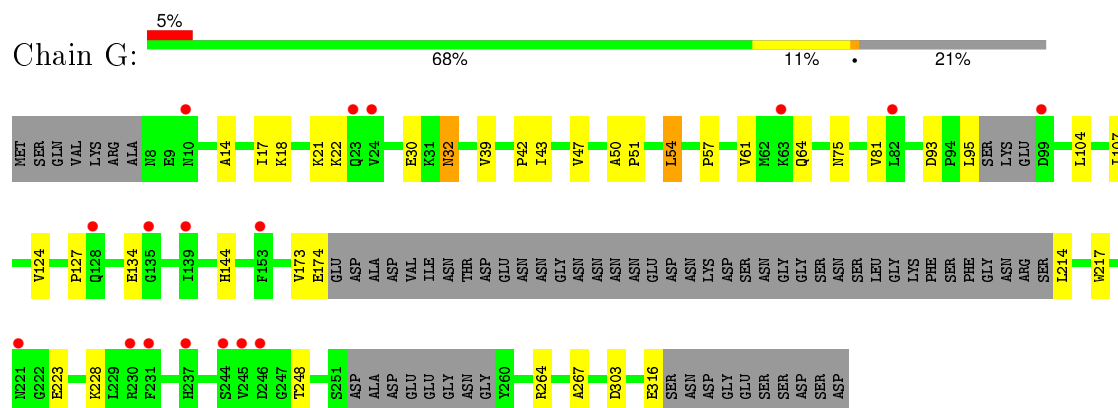
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1



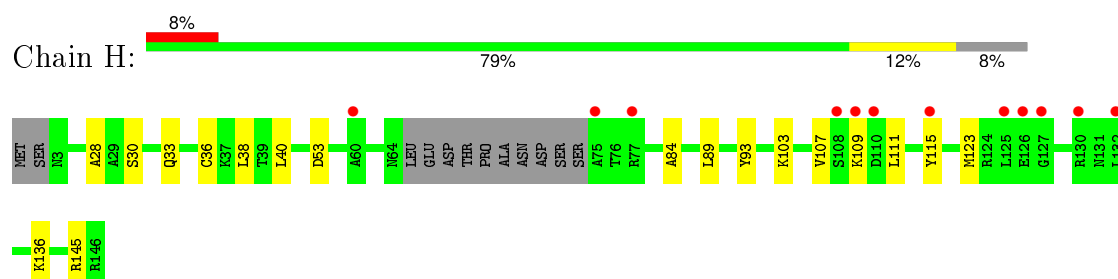
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



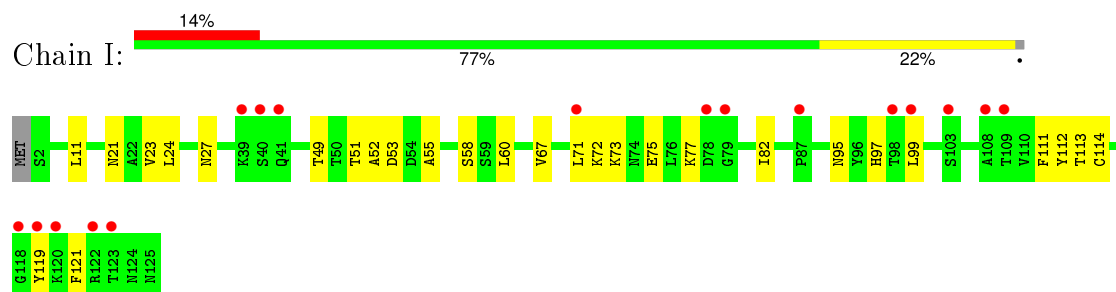
- Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43



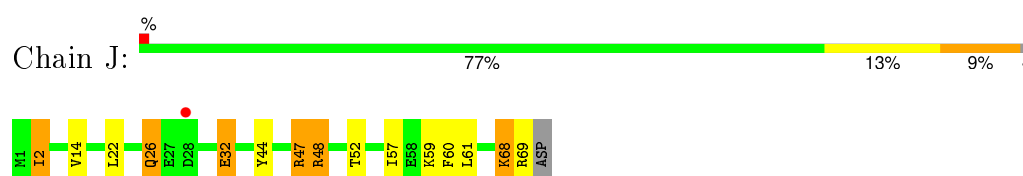
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3



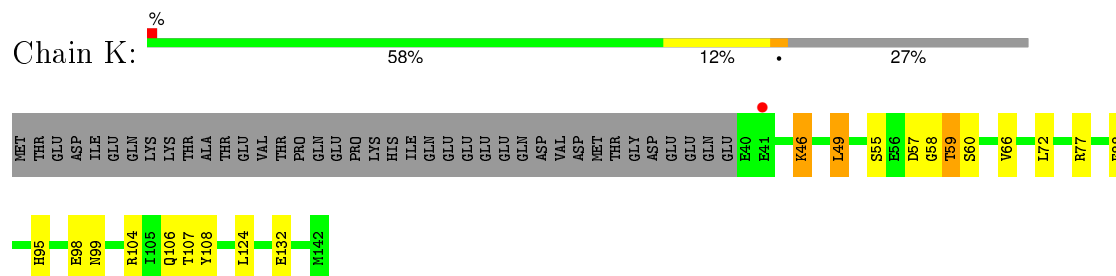
- Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12



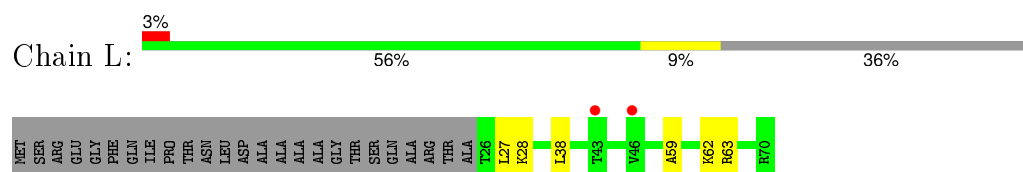
● Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



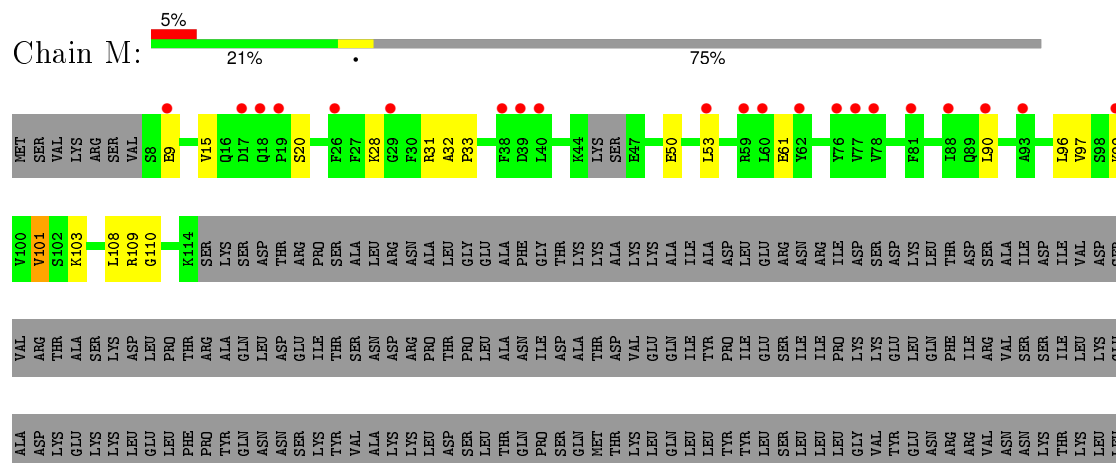
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



● Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4



- Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



GLU ARG
LEU LEU
ASN SER
PRO LEU
PRO PRO
GLU PRO
ILE ILE
LEU LEU
VAL VAL
ASP ASP
GLY GLY
ILE ILE
LEU LEU
SER SER
VAL VAL
ARG ARG
PHE PHE
THR THR
VAL VAL
ILE ILE
LYS LYS
PRO PRO
GLY GLY
GLN GLN
PHE PHE

GLU ILE
MET THR
ARG ARG
LEU LEU
ALA HIS
GLU GLU
LEU LEU
ASN ASN
SER SER
LYS LYS
PRO PRO
SER SER
LYS LYS
VAL VAL
VAL VAL
SER SER
PHE PHE
THR THR
ILE ILE
ARG ARG
VAL VAL
LYS LYS
LEU LEU
GLY GLY
ALA ILE
PHE PHE
VAL VAL
LYS LYS
GLY GLY
ALA ILE
THR THR
VAL VAL
ALA ILE
GLN GLN
PHE PHE
ILE ILE
ASP ASP
PRO PRO
GLN GLN
ASN ASN
LYS LYS
ASP ASP
LYS LYS
SER SER
THR THR
ALA ILE
CYS CYS
TYR TYR
SER SER
TYR TYR
LYS LYS
LEU LEU
ALA ILE
ILE ILE
ALA ILE
THR THR
MET MET
HIS HIS
LEU LEU
ASP ASP
ASN ASN
PHE PHE
LYS LYS
ILE ILE
PRO PRO

GLU MET
THR THR
ARG ARG
GLY GLY
ARG ARG
GLY GLY
PRO PRO
ARG ARG

● Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34



MET SER
LYS LYS
LEU LEU
SER SER
LYS LYS
ASP ASP
TYR TYR
VAL VAL
SER SER
SER SER
SER SER
SER SER
SER SER
ASP ASP
ASP ASP
GLU GLU
VAL VAL
SER SER
ILE ILE
SER SER
ASN ASN
F23 F23
D27 D27
K30 K30
K31 K31
H34 H34
L35 L35
K36 K36
N37 N37
F38 F38
P39 P39
L40 L40
N41 N41
G42 G42
D43 D43
N44 N44
LYS LYS
LYS LYS
LYS LYS
ALA ILE
K49 K49
Q50 Q50
Q51 Q51
Q52 Q52
V53 V53
W54 W54
L55 L55
I56 I56
N61 N61
L67 L67
K68 K68
S69 S69
L70 L70
P71 P71

V72 V72
D73 D73
F74 F74
E75 E75
S76 S76
D94 D94
ILE ILE
GLU GLU
VAL VAL
SER SER
SER SER
SER SER
THR THR
THR THR
GLN GLN
ASN ASN
ASP ASP
SER SER
M106 M106
L109 L109
L110 L110
V111 V111
P112 P112
S113 S113
E114 E114
S115 S115
K116 K116
E117 E117
K120 K120
I121 I121
A125 A125
LYS LYS
ASP ASP
ASN ASN
ALA ILE
P130 P130
L131 L131
Q132 Q132
F133 F133
I148 I148
V163 V163
E164 E164
G165 G165
L166 L166
K167 K167
L168 L168
E178 E178
D179 D179
F180 F180
HIS HIS
VAL VAL
ALA ILE
GLU GLU
GLU GLU

VAL LYS
LYS GLU
ASN ASN
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LYS LYS
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PRO PRO
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ARG ARG
GLU GLU
LYS LYS
LYS LYS
LYS LYS
ASP ASP
LYS LYS
LYS LYS
ASP ASP
LYS LYS
LYS LYS
LYS LYS
HIS HIS
ARG ARG
ASP ASP

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	401.02Å 139.84Å 140.94Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	49.05 – 3.35 48.66 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.05-3.35) 99.6 (48.66-3.35)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.213 , 0.220 0.235 , 0.247	Depositor DCC
R_{free} test set	5607 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.1	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 111523 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34552	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.375 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	0.39	0/12233	0.58	0/16523
2	B	0.39	0/9527	0.59	0/12879
3	C	0.39	0/2469	0.60	0/3347
4	D	0.40	0/472	0.52	0/639
5	E	0.39	0/1795	0.55	0/2416
6	F	0.38	0/838	0.54	0/1129
7	G	0.38	0/2094	0.57	0/2843
8	H	0.38	0/1090	0.57	0/1476
9	I	0.39	0/954	0.57	0/1285
10	J	0.41	0/578	0.61	0/775
11	K	0.39	0/821	0.59	0/1108
12	L	0.38	0/361	0.60	0/478
13	M	0.38	0/846	0.53	0/1136
14	N	0.38	0/1124	0.52	0/1512
All	All	0.39	0/35202	0.58	0/47546

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	12019	0	12051	118	0
2	B	9322	0	9187	90	0
3	C	2418	0	2401	22	0
4	D	466	0	466	4	0
5	E	1759	0	1788	9	0
6	F	823	0	841	7	0
7	G	2052	0	2016	14	0
8	H	1072	0	1042	6	0
9	I	942	0	933	13	0
10	J	569	0	585	13	0
11	K	810	0	801	12	0
12	L	359	0	381	1	0
13	M	831	0	820	12	0
14	N	1103	0	1106	6	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	34552	0	34418	269	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 4.

All (269) 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)
11:K:59:THR:HG22	11:K:107:THR:OG1	1.46	1.13
11:K:60:SER:OG	11:K:106:GLN:HG2	1.63	0.97
2:B:99:VAL:HG21	2:B:417:ILE:HD11	1.58	0.84
1:A:1382:VAL:HA	2:B:1070:ARG:NH1	1.94	0.81
3:C:222:VAL:HG21	3:C:225:ALA:HB2	1.68	0.75
1:A:824:THR:HG23	2:B:1023:ARG:HB2	1.71	0.73
1:A:86:TYR:H	1:A:431:GLN:HE22	1.36	0.72
2:B:16:PHE:HD2	2:B:978:ALA:HB2	1.53	0.72
1:A:432:ASN:HD21	1:A:444:GLN:H	1.37	0.72
1:A:712:ILE:H	11:K:106:GLN:HE22	1.39	0.70
1:A:1023:LEU:HB3	1:A:1190:SER:HB3	1.74	0.69
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.77	0.67
3:C:229:LEU:HB3	3:C:293:ARG:HG2	1.78	0.66
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.77	0.65
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:HIS:HD2	5:E:149:LEU:H	1.46	0.63
2:B:749:THR:O	10:J:52:THR:HG23	1.99	0.62
2:B:558:VAL:HA	2:B:561:ILE:HD12	1.81	0.62
3:C:275:VAL:HG21	3:C:293:ARG:HH21	1.64	0.62
2:B:748:GLN:HB3	10:J:52:THR:HG22	1.82	0.62
1:A:713:VAL:H	1:A:738:ASN:HD21	1.49	0.61
13:M:61:GLU:HB3	13:M:101:VAL:HG23	1.82	0.60
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.83	0.60
1:A:1038:ILE:HB	1:A:1047:GLN:HB2	1.83	0.60
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.84	0.59
1:A:332:GLN:HE22	1:A:350:VAL:H	1.50	0.59
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.83	0.59
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.84	0.59
2:B:190:ILE:HD13	2:B:190:ILE:H	1.68	0.59
2:B:211:ARG:HH22	2:B:243:GLN:HE22	1.51	0.58
1:A:701:ARG:H	1:A:706:HIS:HD2	1.50	0.58
2:B:839:LYS:HG3	2:B:857:PRO:HD2	1.86	0.58
1:A:943:ILE:HG12	2:B:960:ILE:HD11	1.85	0.58
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.87	0.57
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.86	0.56
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.86	0.56
2:B:840:LEU:HD21	2:B:857:PRO:HB2	1.87	0.56
3:C:232:GLN:HE21	3:C:234:ASN:HD21	1.54	0.56
1:A:438:ILE:HA	1:A:456:VAL:HG22	1.87	0.55
2:B:721:MET:HG3	2:B:1036:LEU:HD21	1.88	0.55
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.87	0.55
2:B:300:SER:HB3	9:I:49:THR:HG22	1.89	0.55
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.88	0.55
1:A:970:LYS:HE2	2:B:685:VAL:HG21	1.89	0.55
10:J:48:ARG:O	10:J:52:THR:HB	2.06	0.55
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.88	0.55
1:A:1017:GLY:O	1:A:1384:TYR:HB3	2.05	0.55
2:B:791:LYS:O	2:B:795:GLU:HG2	2.07	0.55
1:A:952:LEU:HD21	1:A:1000:MET:HB3	1.87	0.54
1:A:438:ILE:HG23	2:B:1192:MET:HG2	1.89	0.54
3:C:92:ILE:HG12	10:J:2:ILE:HD11	1.89	0.54
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.89	0.54
1:A:1501:ILE:HG23	1:A:1504:ILE:HB	1.90	0.54
2:B:323:ARG:HH22	2:B:351:GLN:HE22	1.55	0.54
1:A:727:THR:HG22	1:A:730:GLN:HG3	1.88	0.54
1:A:701:ARG:H	1:A:706:HIS:CD2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:PRO:HB3	2:B:871:ILE:HD13	1.89	0.53
13:M:9:GLU:HG2	14:N:71:PRO:HB3	1.89	0.53
2:B:282:HIS:HD2	13:M:99:LYS:HD2	1.73	0.53
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.91	0.53
1:A:1062:HIS:HA	1:A:1065:GLN:HB2	1.89	0.53
11:K:46:LYS:HA	11:K:66:VAL:HG22	1.90	0.53
10:J:2:ILE:HG23	10:J:57:ILE:HG21	1.91	0.53
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.90	0.53
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.90	0.53
2:B:52:LEU:HG	2:B:61:LEU:HD13	1.90	0.53
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.91	0.52
7:G:134:GLU:HB3	7:G:228:LYS:HE2	1.90	0.52
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.09	0.52
1:A:891:ILE:HG23	9:I:71:LEU:HG	1.89	0.52
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.91	0.52
1:A:1239:THR:HB	1:A:1542:THR:HB	1.91	0.52
13:M:28:LYS:HD2	14:N:106:ASN:HB2	1.91	0.52
1:A:1478:ALA:HB1	9:I:21:ASN:HB3	1.92	0.52
2:B:574:SER:HB2	13:M:97:VAL:HG11	1.92	0.52
1:A:1056:ASP:HB3	1:A:1059:LYS:HD3	1.92	0.52
7:G:51:PRO:HA	7:G:54:LEU:HD13	1.92	0.51
7:G:81:VAL:HA	7:G:124:VAL:HG12	1.91	0.51
2:B:646:HIS:H	2:B:646:HIS:CD2	2.29	0.51
3:C:333:ILE:HG22	11:K:49:LEU:HB2	1.92	0.51
11:K:104:ARG:HD2	11:K:106:GLN:HG3	1.92	0.51
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.75	0.51
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.92	0.51
13:M:53:LEU:HB2	13:M:96:LEU:HD22	1.92	0.51
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.92	0.51
5:E:131:THR:HG21	5:E:191:LYS:HE2	1.93	0.50
1:A:918:LYS:HE2	1:A:922:CYS:HB3	1.92	0.50
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.92	0.50
1:A:1265:GLU:HA	9:I:58:SER:HB3	1.94	0.50
2:B:293:ILE:HG12	2:B:302:LEU:HD23	1.93	0.50
7:G:50:ALA:H	7:G:64:GLN:HE22	1.58	0.50
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.91	0.50
1:A:1039:ARG:HD2	1:A:1045:LEU:HA	1.94	0.50
1:A:1038:ILE:HD12	1:A:1185:VAL:HG21	1.94	0.50
9:I:97:HIS:HB3	9:I:111:PHE:HB2	1.94	0.50
1:A:1382:VAL:HA	2:B:1070:ARG:HH11	1.74	0.50
13:M:109:ARG:HG3	13:M:110:GLY:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:LYS:HA	7:G:21:LYS:HD2	1.94	0.49
1:A:588:LEU:HB2	1:A:636:HIS:HB2	1.93	0.49
11:K:95:HIS:HB3	11:K:98:GLU:HG2	1.95	0.49
1:A:518:GLU:HG3	6:F:115:THR:HG21	1.94	0.49
1:A:381:SER:HB2	1:A:453:ILE:HG23	1.94	0.49
3:C:216:HIS:HD2	3:C:218:LYS:H	1.61	0.49
2:B:700:LEU:HA	2:B:703:LEU:HD12	1.94	0.49
1:A:1112:PRO:HD2	1:A:1115:LYS:HB2	1.94	0.49
10:J:68:LYS:HD3	10:J:69:ARG:HD2	1.94	0.49
1:A:1263:LEU:HD22	1:A:1267:ILE:HD11	1.95	0.49
1:A:19:LEU:HG	2:B:1195:ARG:HB2	1.95	0.49
11:K:55:SER:HB2	11:K:60:SER:HB2	1.95	0.48
1:A:1348:VAL:HG11	2:B:270:LEU:HD12	1.94	0.48
1:A:986:PHE:HB2	2:B:960:ILE:HD12	1.95	0.48
2:B:908:ARG:HD2	3:C:95:GLU:HG2	1.94	0.48
8:H:103:LYS:HB3	8:H:115:TYR:HB2	1.96	0.48
2:B:656:LEU:HB3	14:N:148:ILE:HG12	1.95	0.48
7:G:14:ALA:HA	7:G:17:ILE:HD12	1.96	0.48
1:A:952:LEU:HD23	1:A:1004:GLU:HG3	1.95	0.48
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.95	0.48
1:A:538:ASN:HA	1:A:575:LYS:HG2	1.96	0.48
1:A:536:ILE:HD11	1:A:575:LYS:HD3	1.96	0.47
2:B:110:ASN:HB3	2:B:118:GLU:HG2	1.95	0.47
9:I:52:ALA:HB3	9:I:55:ALA:HB2	1.96	0.47
2:B:740:LYS:HA	2:B:804:TYR:O	2.14	0.47
2:B:129:ARG:HA	2:B:888:ILE:HG21	1.96	0.47
1:A:836:THR:HG23	1:A:839:GLY:H	1.80	0.47
1:A:727:THR:H	1:A:730:GLN:HE21	1.63	0.47
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.97	0.47
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.45	0.47
2:B:123:PRO:HG2	2:B:172:LEU:HD11	1.97	0.47
2:B:375:LEU:HA	2:B:378:ILE:HD12	1.97	0.47
2:B:362:LEU:HD22	2:B:369:ASP:HB3	1.97	0.47
2:B:823:GLN:HG2	2:B:863:ASP:HB3	1.96	0.47
1:A:879:LEU:HA	1:A:882:ILE:HD12	1.97	0.47
1:A:898:SER:HB2	9:I:77:LYS:HB2	1.95	0.47
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.97	0.47
1:A:862:THR:OG1	1:A:878:ARG:HB3	2.14	0.47
8:H:107:VAL:O	8:H:111:LEU:HB2	2.15	0.46
1:A:1288:ARG:HB2	1:A:1476:LEU:HB2	1.97	0.46
1:A:502:ALA:HA	1:A:581:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1610:PHE:CD2	1:A:1632:GLU:HG2	2.50	0.46
7:G:47:VAL:HG21	7:G:61:VAL:HG13	1.98	0.46
5:E:4:GLU:HG2	5:E:7:ARG:HH12	1.81	0.46
5:E:56:LYS:HE2	5:E:84:ASP:H	1.81	0.46
1:A:1640:ARG:HH11	1:A:1648:ASN:HB3	1.80	0.46
1:A:986:PHE:CB	2:B:960:ILE:HD12	2.45	0.46
1:A:1196:PRO:HB2	1:A:1575:ILE:HG21	1.98	0.46
2:B:103:SER:HB3	2:B:138:LEU:HB2	1.97	0.46
1:A:700:ILE:HD11	1:A:735:VAL:HA	1.98	0.46
2:B:480:GLN:HE21	2:B:508:PHE:H	1.63	0.46
2:B:977:ILE:HD13	14:N:163:VAL:HG21	1.98	0.46
1:A:862:THR:HG21	1:A:875:LEU:HD12	1.98	0.46
9:I:114:CYS:HB3	9:I:119:TYR:H	1.81	0.46
2:B:748:GLN:HB3	10:J:52:THR:CG2	2.45	0.46
2:B:916:LYS:HB3	2:B:1036:LEU:HD12	1.97	0.46
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.96	0.45
1:A:1658:ALA:HB2	7:G:107:ILE:HD11	1.97	0.45
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.97	0.45
3:C:110:PRO:C	3:C:112:MET:H	2.20	0.45
2:B:721:MET:O	2:B:725:THR:HG23	2.16	0.45
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.97	0.45
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.52	0.45
1:A:438:ILE:HD12	2:B:1192:MET:HA	1.99	0.45
1:A:1029:GLY:HA3	1:A:1041:ALA:HB2	1.98	0.45
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.98	0.45
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.99	0.45
1:A:1275:THR:HG23	1:A:1289:SER:HB2	1.98	0.45
11:K:59:THR:CG2	11:K:108:TYR:O	2.65	0.45
1:A:1032:VAL:HG21	1:A:1179:ILE:HG12	1.99	0.45
1:A:1038:ILE:HD11	1:A:1050:TYR:HB2	1.98	0.45
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	1.99	0.45
1:A:1613:MET:HE3	1:A:1622:LEU:HD13	1.98	0.45
1:A:1014:SER:HA	1:A:1223:ARG:HH22	1.82	0.45
9:I:72:LYS:HB2	9:I:75:GLU:HB2	1.98	0.45
1:A:657:TYR:HA	1:A:667:ARG:HG3	1.99	0.44
1:A:537:GLN:HB2	1:A:578:TYR:HE1	1.82	0.44
2:B:940:GLU:OE2	3:C:228:ARG:HB2	2.17	0.44
1:A:32:ILE:HG21	1:A:49:LEU:HD13	1.98	0.44
5:E:120:ALA:HA	5:E:123:LEU:HD12	2.00	0.44
1:A:1384:TYR:HE2	2:B:1077:ASP:OD2	2.00	0.44
3:C:195:LYS:HB3	10:J:61:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:VAL:HA	2:B:68:ILE:HG12	1.98	0.44
3:C:113:LEU:HD11	3:C:132:ILE:HD12	1.99	0.44
5:E:141:VAL:HG12	5:E:142:VAL:HG23	1.99	0.44
7:G:30:GLU:HG2	7:G:32:ASN:HB2	1.99	0.44
1:A:126:GLN:HB3	1:A:343:PRO:HD3	1.99	0.44
2:B:13:THR:HG21	2:B:977:ILE:HB	2.00	0.44
1:A:671:GLN:HE22	2:B:784:ASP:HB2	1.83	0.44
6:F:107:VAL:HG12	6:F:109:VAL:H	1.83	0.44
1:A:128:GLY:H	1:A:207:SER:HB3	1.82	0.44
1:A:1238:MET:HB2	1:A:1521:THR:HB	2.00	0.44
1:A:862:THR:HA	9:I:67:VAL:HG12	1.99	0.43
1:A:124:LEU:HD21	1:A:189:VAL:HA	1.98	0.43
2:B:788:ILE:HB	2:B:948:ILE:HB	2.00	0.43
4:D:19:PRO:HG2	4:D:22:ILE:HD11	2.00	0.43
1:A:1626:VAL:HG21	2:B:1194:ILE:HG12	1.99	0.43
1:A:1634:LEU:HD13	1:A:1643:VAL:HG11	2.00	0.43
2:B:1097:ASP:OD2	2:B:1181:VAL:HG22	2.18	0.43
2:B:61:LEU:HD21	2:B:413:LEU:HD13	1.99	0.43
6:F:94:LEU:HD21	6:F:125:LEU:HD22	2.00	0.43
1:A:885:ASP:HB3	1:A:888:LYS:HB2	2.01	0.43
2:B:936:MET:HG3	2:B:937:PRO:HD2	2.00	0.43
3:C:229:LEU:HD23	3:C:293:ARG:HB3	2.00	0.43
3:C:229:LEU:HD21	3:C:295:ARG:HA	2.01	0.43
10:J:32:GLU:H	10:J:32:GLU:HG2	1.52	0.43
11:K:57:ASP:HA	11:K:58:GLY:HA2	1.82	0.43
2:B:301:PHE:O	2:B:305:ARG:HG2	2.18	0.43
1:A:396:ILE:HG12	1:A:426:ALA:HB1	2.01	0.43
1:A:1261:VAL:HG11	1:A:1308:VAL:HG21	2.00	0.43
1:A:970:LYS:HG2	1:A:971:PRO:HD2	2.00	0.43
2:B:526:GLY:HA2	2:B:696:ILE:HA	2.01	0.43
13:M:9:GLU:HA	14:N:71:PRO:HA	2.01	0.42
1:A:1459:LYS:HB2	1:A:1473:LYS:HB2	2.01	0.42
1:A:387:SER:HA	1:A:390:LEU:HD12	2.01	0.42
1:A:490:ILE:HG22	1:A:606:ARG:HD3	2.01	0.42
1:A:456:VAL:HG21	2:B:1192:MET:HG3	2.01	0.42
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	2.01	0.42
2:B:612:LYS:HD3	2:B:626:ILE:HD11	2.01	0.42
1:A:692:TYR:O	1:A:696:ILE:HG12	2.19	0.42
1:A:98:LEU:HD13	1:A:320:VAL:HG13	2.01	0.42
2:B:561:ILE:HG12	2:B:620:LEU:HD12	2.00	0.42
1:A:591:ARG:HB2	1:A:633:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:VAL:HB	2:B:261:ARG:HB3	2.01	0.42
1:A:385:LEU:HD13	1:A:437:PHE:HA	2.01	0.42
11:K:59:THR:HG21	11:K:108:TYR:O	2.20	0.42
2:B:15:ASP:HA	2:B:978:ALA:HB3	2.01	0.42
2:B:251:HIS:HE1	2:B:261:ARG:HD2	1.85	0.42
2:B:19:LEU:HD11	10:J:26:GLN:HG2	2.01	0.42
1:A:646:GLU:HB3	2:B:1084:THR:OG1	2.20	0.42
12:L:28:LYS:HB2	12:L:59:ALA:HB3	2.02	0.42
4:D:24:ALA:HA	7:G:43:ILE:HG22	2.02	0.42
2:B:139:LEU:HD22	2:B:417:ILE:HD13	2.02	0.41
3:C:233:ILE:HB	3:C:267:VAL:HG11	2.01	0.41
13:M:20:SER:HB3	14:N:36:LYS:HB2	2.01	0.41
2:B:207:ILE:HB	2:B:505:ARG:HA	2.02	0.41
2:B:840:LEU:HA	2:B:846:PRO:HA	2.03	0.41
1:A:805:VAL:O	1:A:809:VAL:HG23	2.20	0.41
1:A:827:THR:HG21	2:B:1026:ILE:HA	2.03	0.41
2:B:880:ALA:HB2	2:B:907:ILE:HG13	2.01	0.41
7:G:264:ARG:H	7:G:267:ALA:HB3	1.85	0.41
13:M:32:ALA:HB1	13:M:33:PRO:HD2	2.03	0.41
2:B:260:PHE:HB3	2:B:271:VAL:HG23	2.03	0.41
9:I:95:ASN:HB2	9:I:113:THR:HB	2.02	0.41
5:E:6:GLU:HA	5:E:9:ILE:HD12	2.03	0.41
8:H:93:TYR:HA	8:H:145:ARG:HG3	2.03	0.41
1:A:502:ALA:HA	1:A:581:ILE:HG22	2.02	0.41
2:B:211:ARG:HH22	2:B:243:GLN:NE2	2.18	0.41
1:A:1384:TYR:CE2	2:B:1074:MET:HG2	2.56	0.41
1:A:1654:PHE:CZ	6:F:89:GLU:HA	2.56	0.41
1:A:855:ARG:HH21	1:A:867:ASP:HB3	1.84	0.41
2:B:600:GLN:HA	2:B:603:ILE:HD12	2.03	0.41
1:A:1550:LEU:HD12	1:A:1555:VAL:HA	2.02	0.41
9:I:112:TYR:HB2	9:I:121:PHE:HB3	2.03	0.41
2:B:967:LEU:HD13	2:B:996:PHE:HB2	2.03	0.41
3:C:252:PRO:HD2	3:C:255:VAL:HG21	2.03	0.41
2:B:1076:ARG:HG3	2:B:1092:LEU:HD11	2.03	0.41
3:C:223:SER:HB2	3:C:303:GLU:HB2	2.03	0.41
13:M:15:VAL:HG12	13:M:90:LEU:HB2	2.03	0.41
8:H:40:LEU:HB2	8:H:123:MET:HG3	2.02	0.40
2:B:17:ARG:HG2	2:B:17:ARG:H	1.64	0.40
1:A:233:CYS:HB3	1:A:236:CYS:O	2.21	0.40
1:A:536:ILE:HG23	1:A:544:VAL:HB	2.03	0.40
9:I:11:LEU:HD22	13:M:31:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1554:GLY:HA2	5:E:183:PRO:HD2	2.03	0.40
8:H:28:ALA:HB3	8:H:38:LEU:HB3	2.03	0.40
1:A:49:LEU:HD12	1:A:368:ARG:HH21	1.85	0.40
4:D:26:GLN:HB2	7:G:42:PRO:HG2	2.02	0.40
8:H:30:SER:HB3	8:H:36:CYS:HB3	2.04	0.40
1:A:990:ILE:HD12	1:A:995:TYR:HA	2.04	0.40
1:A:1121:ASP:HA	5:E:207:ARG:HH22	1.85	0.40
4:D:30:HIS:HA	7:G:39:VAL:HG23	2.02	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	1503/1664 (90%)	1422 (95%)	79 (5%)	2 (0%)	56	89
2	B	1166/1203 (97%)	1094 (94%)	68 (6%)	4 (0%)	46	82
3	C	300/335 (90%)	283 (94%)	17 (6%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	95 (97%)	3 (3%)	0	100	100
7	G	251/326 (77%)	232 (92%)	17 (7%)	2 (1%)	24	65
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	24	65
9	I	120/125 (96%)	108 (90%)	12 (10%)	0	100	100
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	101/142 (71%)	95 (94%)	5 (5%)	1 (1%)	19	60
12	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
13	M	101/415 (24%)	94 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	131/233 (56%)	122 (93%)	9 (7%)	0	100	100
All	All	4279/5236 (82%)	4020 (94%)	249 (6%)	10 (0%)	52	86

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1389	GLU
1	A	237	GLY
2	B	532	HIS
2	B	1154	ASP
11	K	46	LYS
2	B	339	GLN
2	B	359	LEU
8	H	84	ALA
7	G	173	VAL
7	G	127	PRO

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	1343/1465 (92%)	1268 (94%)	75 (6%)	26	65
2	B	1024/1053 (97%)	928 (91%)	96 (9%)	11	39
3	C	269/296 (91%)	243 (90%)	26 (10%)	10	38
4	D	56/116 (48%)	50 (89%)	6 (11%)	8	32
5	E	197/197 (100%)	192 (98%)	5 (2%)	55	83
6	F	90/137 (66%)	86 (96%)	4 (4%)	35	72
7	G	234/291 (80%)	219 (94%)	15 (6%)	22	60
8	H	116/128 (91%)	111 (96%)	5 (4%)	35	73
9	I	109/110 (99%)	100 (92%)	9 (8%)	14	48
10	J	64/65 (98%)	56 (88%)	8 (12%)	6	24
11	K	93/130 (72%)	86 (92%)	7 (8%)	17	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	40/57 (70%)	36 (90%)	4 (10%)	9	36
13	M	94/371 (25%)	90 (96%)	4 (4%)	35	73
14	N	128/220 (58%)	117 (91%)	11 (9%)	13	46
All	All	3857/4636 (83%)	3582 (93%)	275 (7%)	18	56

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	39	ASP
1	A	89	LEU
1	A	113	VAL
1	A	129	LEU
1	A	136	LEU
1	A	177	LEU
1	A	195	LYS
1	A	199	ASP
1	A	211	THR
1	A	270	ILE
1	A	274	MET
1	A	325	ASP
1	A	345	LEU
1	A	361	VAL
1	A	373	LEU
1	A	398	ASP
1	A	399	LEU
1	A	403	LEU
1	A	406	LEU
1	A	413	LEU
1	A	518	GLU
1	A	536	ILE
1	A	562	LEU
1	A	572	THR
1	A	586	VAL
1	A	587	VAL
1	A	684	ASP
1	A	743	ASP
1	A	747	ILE
1	A	831	ASP
1	A	840	ASN
1	A	844	THR

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Mol	Chain	Res	Type
1	A	862	THR
1	A	878	ARG
1	A	952	LEU
1	A	960	MET
1	A	1065	GLN
1	A	1089	LEU
1	A	1164	LYS
1	A	1169	LEU
1	A	1171	GLN
1	A	1175	MET
1	A	1179	ILE
1	A	1183	GLU
1	A	1193	VAL
1	A	1202	LEU
1	A	1205	PHE
1	A	1217	LEU
1	A	1242	ILE
1	A	1248	ASP
1	A	1252	ASP
1	A	1263	LEU
1	A	1268	ASP
1	A	1273	THR
1	A	1313	LEU
1	A	1343	ASP
1	A	1370	ASP
1	A	1380	GLN
1	A	1388	ASP
1	A	1389	GLU
1	A	1396	ARG
1	A	1474	LEU
1	A	1475	GLU
1	A	1481	GLU
1	A	1501	ILE
1	A	1505	ASP
1	A	1531	ASP
1	A	1533	GLU
1	A	1552	THR
1	A	1592	GLN
1	A	1609	SER
1	A	1628	ASP
1	A	1629	ASN
1	A	1649	VAL

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Mol	Chain	Res	Type
2	B	13	THR
2	B	15	ASP
2	B	17	ARG
2	B	19	LEU
2	B	22	GLU
2	B	35	PHE
2	B	52	LEU
2	B	54	GLU
2	B	60	LEU
2	B	73	ILE
2	B	101	GLN
2	B	108	MET
2	B	139	LEU
2	B	150	GLU
2	B	156	ARG
2	B	168	ASN
2	B	186	GLU
2	B	190	ILE
2	B	202	LEU
2	B	206	LEU
2	B	212	ASN
2	B	217	ILE
2	B	234	ILE
2	B	250	LEU
2	B	265	ARG
2	B	268	GLU
2	B	274	VAL
2	B	276	ILE
2	B	304	ASP
2	B	306	LEU
2	B	316	ARG
2	B	332	ASP
2	B	356	ARG
2	B	364	LYS
2	B	373	MET
2	B	374	LEU
2	B	381	LEU
2	B	413	LEU
2	B	431	ASP
2	B	438	ILE
2	B	441	LYS
2	B	455	GLU

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Mol	Chain	Res	Type
2	B	471	VAL
2	B	479	GLN
2	B	480	GLN
2	B	481	VAL
2	B	485	THR
2	B	519	LYS
2	B	542	LEU
2	B	550	ARG
2	B	588	ILE
2	B	617	THR
2	B	640	LEU
2	B	646	HIS
2	B	684	ASN
2	B	692	THR
2	B	721	MET
2	B	743	ARG
2	B	752	VAL
2	B	782	ASP
2	B	787	MET
2	B	789	ILE
2	B	794	ASP
2	B	821	ILE
2	B	832	TRP
2	B	835	GLU
2	B	840	LEU
2	B	842	GLU
2	B	848	ILE
2	B	859	CYS
2	B	873	THR
2	B	887	LEU
2	B	888	ILE
2	B	896	GLN
2	B	897	GLU
2	B	898	LEU
2	B	933	THR
2	B	940	GLU
2	B	944	GLN
2	B	956	SER
2	B	965	GLU
2	B	967	LEU
2	B	977	ILE
2	B	994	ASP

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Mol	Chain	Res	Type
2	B	1000	LEU
2	B	1020	GLU
2	B	1033	TYR
2	B	1037	ARG
2	B	1041	ASN
2	B	1065	ARG
2	B	1076	ARG
2	B	1110	ILE
2	B	1123	ILE
2	B	1157	GLN
2	B	1181	VAL
2	B	1201	GLU
3	C	30	GLU
3	C	39	ASP
3	C	46	SER
3	C	47	LEU
3	C	81	GLU
3	C	89	THR
3	C	94	ASP
3	C	97	LEU
3	C	106	LEU
3	C	117	ASP
3	C	120	LEU
3	C	151	THR
3	C	181	ASP
3	C	182	CYS
3	C	188	ASP
3	C	209	ILE
3	C	224	THR
3	C	229	LEU
3	C	235	ILE
3	C	240	LYS
3	C	259	ASP
3	C	277	ARG
3	C	291	LEU
3	C	303	GLU
3	C	331	CYS
3	C	334	THR
4	D	14	THR
4	D	16	LEU
4	D	21	VAL
4	D	25	THR

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Mol	Chain	Res	Type
4	D	27	LEU
4	D	89	LEU
5	E	84	ASP
5	E	106	GLN
5	E	163	GLU
5	E	167	ARG
5	E	175	LEU
6	F	69	LEU
6	F	103	MET
6	F	111	LEU
6	F	147	SER
7	G	22	LYS
7	G	32	ASN
7	G	54	LEU
7	G	75	ASN
7	G	93	ASP
7	G	95	LEU
7	G	104	LEU
7	G	144	HIS
7	G	174	GLU
7	G	214	LEU
7	G	217	TRP
7	G	223	GLU
7	G	248	THR
7	G	303	ASP
7	G	316	GLU
8	H	33	GLN
8	H	53	ASP
8	H	89	LEU
8	H	109	LYS
8	H	136	LYS
9	I	23	VAL
9	I	24	LEU
9	I	27	ASN
9	I	51	THR
9	I	53	ASP
9	I	60	LEU
9	I	73	LYS
9	I	82	ILE
9	I	99	LEU
10	J	2	ILE
10	J	14	VAL

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Mol	Chain	Res	Type
10	J	22	LEU
10	J	26	GLN
10	J	32	GLU
10	J	47	ARG
10	J	48	ARG
10	J	68	LYS
11	K	49	LEU
11	K	59	THR
11	K	72	LEU
11	K	77	ARG
11	K	99	ASN
11	K	124	LEU
11	K	132	GLU
12	L	27	LEU
12	L	38	LEU
12	L	62	LYS
12	L	63	ARG
13	M	50	GLU
13	M	101	VAL
13	M	103	LYS
13	M	108	LEU
14	N	36	LYS
14	N	67	LEU
14	N	74	PHE
14	N	94	ASP
14	N	114	GLU
14	N	117	GLU
14	N	131	LEU
14	N	164	GLU
14	N	166	LEU
14	N	168	LEU
14	N	178	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	332	GLN
1	A	431	GLN
1	A	432	ASN
1	A	580	HIS
1	A	590	ASN

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Mol	Chain	Res	Type
1	A	592	GLN
1	A	636	HIS
1	A	671	GLN
1	A	693	GLN
1	A	706	HIS
1	A	730	GLN
1	A	738	ASN
1	A	901	ASN
1	A	926	GLN
1	A	1026	GLN
1	A	1036	ASN
1	A	1113	HIS
1	A	1128	ASN
1	A	1380	GLN
1	A	1599	ASN
1	A	1620	GLN
2	B	146	ASN
2	B	151	ASN
2	B	212	ASN
2	B	243	GLN
2	B	251	HIS
2	B	282	HIS
2	B	351	GLN
2	B	361	HIS
2	B	400	GLN
2	B	480	GLN
2	B	646	HIS
2	B	686	HIS
2	B	695	ASN
2	B	724	GLN
2	B	755	ASN
2	B	896	GLN
2	B	975	HIS
2	B	987	ASN
2	B	999	GLN
2	B	1041	ASN
2	B	1053	ASN
2	B	1114	GLN
3	C	130	ASN
3	C	232	GLN
4	D	30	HIS
5	E	147	HIS

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Mol	Chain	Res	Type
5	E	179	GLN
7	G	20	HIS
7	G	26	ASN
7	G	32	ASN
7	G	64	GLN
7	G	65	HIS
7	G	128	GLN
7	G	140	GLN
7	G	150	HIS
8	H	35	GLN
9	I	21	ASN
9	I	100	GLN
10	J	64	ASN
11	K	106	GLN
13	M	16	GLN
14	N	132	GLN

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 7 ligands modelled in this entry, 7 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, 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	1523/1664 (91%)	0.22	48 (3%)	51	51	82, 114, 166, 248	0
2	B	1176/1203 (97%)	0.35	41 (3%)	48	47	80, 119, 170, 238	0
3	C	304/335 (90%)	0.18	6 (1%)	68	68	108, 134, 171, 191	0
4	D	59/137 (43%)	0.39	3 (5%)	32	31	114, 157, 188, 193	0
5	E	215/215 (100%)	0.12	6 (2%)	56	57	95, 143, 193, 201	0
6	F	100/155 (64%)	-0.08	0	100	100	88, 115, 156, 167	0
7	G	259/326 (79%)	0.49	17 (6%)	22	22	102, 167, 256, 274	0
8	H	134/146 (91%)	0.55	12 (8%)	12	12	114, 141, 173, 184	0
9	I	124/125 (99%)	0.62	17 (13%)	4	3	105, 177, 215, 229	0
10	J	69/70 (98%)	0.32	1 (1%)	78	79	105, 124, 150, 176	0
11	K	103/142 (72%)	0.01	1 (0%)	84	85	101, 125, 165, 206	0
12	L	45/70 (64%)	0.21	2 (4%)	38	37	130, 156, 183, 191	0
13	M	105/415 (25%)	1.16	21 (20%)	1	1	161, 209, 254, 264	0
14	N	139/233 (59%)	1.10	32 (23%)	1	1	113, 211, 252, 271	0
All	All	4355/5236 (83%)	0.33	207 (4%)	34	34	80, 126, 209, 274	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1340	THR	7.5
13	M	39	ASP	5.5
13	M	17	ASP	5.4
9	I	41	GLN	5.3
14	N	54	TRP	5.2
13	M	38	PHE	5.2
14	N	113	SER	5.0
7	G	23	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
14	N	70	LEU	4.8
14	N	41	ASN	4.7
1	A	1388	ASP	4.7
5	E	1	MET	4.7
2	B	894	LYS	4.6
2	B	81	SER	4.5
14	N	106	ASN	4.4
3	C	261	GLY	4.4
3	C	150	SER	4.3
1	A	264	ASN	4.3
9	I	122	ARG	4.3
2	B	440	PHE	4.3
8	H	77	ARG	4.3
2	B	141	LEU	4.3
14	N	34	HIS	4.2
2	B	225	ARG	4.2
7	G	24	VAL	4.1
1	A	1399	GLU	4.1
9	I	103	SER	4.0
9	I	120	LYS	4.0
2	B	152	LEU	4.0
1	A	1438	ASN	3.9
7	G	99	ASP	3.9
7	G	245	VAL	3.8
14	N	31	LYS	3.7
5	E	110	PHE	3.7
8	H	126	GLU	3.7
2	B	893	ASN	3.7
1	A	1013	THR	3.6
13	M	77	VAL	3.6
14	N	94	ASP	3.6
1	A	1398	ALA	3.6
14	N	40	LEU	3.5
14	N	121	ILE	3.5
8	H	127	GLY	3.5
2	B	1148	GLY	3.5
2	B	895	PHE	3.5
2	B	903	ILE	3.5
2	B	830	ASP	3.4
9	I	87	PRO	3.4
13	M	59	ARG	3.4
7	G	128	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
9	I	79	GLY	3.4
14	N	111	VAL	3.3
13	M	9	GLU	3.3
1	A	1171	GLN	3.3
1	A	1290	TYR	3.3
1	A	251	ILE	3.3
1	A	1166	PHE	3.3
14	N	76	SER	3.3
14	N	44	ASN	3.2
14	N	43	ASP	3.2
2	B	224	ASN	3.2
1	A	1480	THR	3.1
1	A	245	LYS	3.1
2	B	859	CYS	3.1
1	A	1483	LEU	3.1
9	I	99	LEU	3.1
7	G	139	ILE	3.1
14	N	56	ILE	3.1
8	H	110	ASP	3.0
8	H	132	LEU	3.0
13	M	26	PHE	3.0
2	B	340	ALA	3.0
14	N	112	PRO	3.0
13	M	60	LEU	3.0
14	N	27	ASP	3.0
7	G	221	ASN	2.9
1	A	1204	THR	2.9
2	B	846	PRO	2.9
8	H	75	ALA	2.9
14	N	109	LEU	2.9
1	A	41	LEU	2.9
2	B	139	LEU	2.9
2	B	82	GLU	2.9
9	I	39	LYS	2.9
1	A	1455	ARG	2.9
3	C	174	ARG	2.8
9	I	40	SER	2.8
2	B	226	GLY	2.8
9	I	118	GLY	2.8
2	B	450	LEU	2.8
14	N	120	LYS	2.8
14	N	55	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
7	G	135	GLY	2.8
13	M	78	VAL	2.8
1	A	1088	HIS	2.8
14	N	51	GLN	2.8
14	N	52	GLN	2.7
14	N	117	GLU	2.7
1	A	97	TYR	2.7
2	B	872	LYS	2.7
8	H	60	ALA	2.7
9	I	123	THR	2.7
7	G	237	HIS	2.7
1	A	328	PHE	2.7
1	A	1242	ILE	2.7
14	N	71	PRO	2.7
9	I	98	THR	2.7
2	B	80	ASN	2.7
1	A	180	GLU	2.6
11	K	41	GLU	2.6
7	G	230	ARG	2.6
9	I	109	THR	2.6
1	A	396	ILE	2.6
1	A	419	ILE	2.6
1	A	1397	GLU	2.6
13	M	19	PRO	2.5
8	H	108	SER	2.5
2	B	556	SER	2.5
2	B	574	SER	2.5
13	M	18	GLN	2.5
2	B	852	VAL	2.5
7	G	63	LYS	2.5
2	B	861	TYR	2.5
5	E	93	MET	2.5
7	G	82	LEU	2.4
1	A	241	PRO	2.4
1	A	1132	TYR	2.4
2	B	91	LEU	2.4
13	M	53	LEU	2.4
2	B	140	LYS	2.4
3	C	264	GLU	2.4
1	A	334	VAL	2.4
14	N	30	LYS	2.4
14	N	67	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
14	N	72	VAL	2.4
2	B	730	GLY	2.4
12	L	46	VAL	2.4
1	A	1016	SER	2.3
1	A	1372	GLU	2.3
2	B	902	SER	2.3
3	C	240	LYS	2.3
8	H	130	ARG	2.3
9	I	119	TYR	2.3
7	G	231	PHE	2.3
1	A	94	LEU	2.3
1	A	244	ARG	2.3
2	B	871	ILE	2.3
5	E	102	GLU	2.3
7	G	244	SER	2.3
13	M	29	GLY	2.3
13	M	99	LYS	2.3
1	A	1352	GLN	2.3
5	E	89	GLY	2.3
14	N	133	PHE	2.3
1	A	200	GLY	2.2
9	I	71	LEU	2.2
14	N	61	ASN	2.2
2	B	819	ASP	2.2
1	A	1381	ALA	2.2
1	A	86	TYR	2.2
2	B	1149	GLU	2.2
3	C	237	GLN	2.2
13	M	90	LEU	2.2
14	N	68	LYS	2.2
4	D	96	PHE	2.2
5	E	3	GLN	2.2
2	B	578	ALA	2.2
1	A	427	PHE	2.2
8	H	125	LEU	2.2
2	B	73	ILE	2.2
8	H	115	TYR	2.2
9	I	108	ALA	2.2
1	A	1350	ARG	2.2
1	A	100	ALA	2.2
1	A	242	LYS	2.2
13	M	62	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1536	ILE	2.1
2	B	32	LYS	2.1
14	N	38	PHE	2.1
2	B	372	ARG	2.1
2	B	153	PHE	2.1
2	B	827	PHE	2.1
2	B	807	GLU	2.1
1	A	1460	TYR	2.1
13	M	76	TYR	2.1
13	M	88	ILE	2.1
12	L	43	THR	2.1
4	D	28	PRO	2.1
1	A	1084	ALA	2.1
7	G	10	ASN	2.1
1	A	98	LEU	2.1
7	G	153	PHE	2.1
2	B	96	SER	2.1
1	A	865	ASP	2.1
1	A	446	ARG	2.1
7	G	246	ASP	2.0
9	I	78	ASP	2.0
13	M	81	PHE	2.0
14	N	116	LYS	2.0
2	B	786	ALA	2.0
4	D	89	LEU	2.0
13	M	40	LEU	2.0
1	A	247	GLY	2.0
13	M	93	ALA	2.0
8	H	109	LYS	2.0
10	J	28	ASP	2.0
1	A	108	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	LLDF	B-factors(Å ²)	Q<0.9
15	ZN	B	2204	1/1	0.99	0.18	-0.29	109,109,109,109	0
15	ZN	I	1126	1/1	0.98	0.14	-0.62	151,151,151,151	0
15	ZN	A	2665	1/1	0.99	0.13	-0.68	111,111,111,111	0
15	ZN	L	1071	1/1	0.99	0.11	-0.91	136,136,136,136	0
15	ZN	A	2664	1/1	0.99	0.09	-1.33	122,122,122,122	0
15	ZN	J	1070	1/1	0.99	0.24	-1.47	111,111,111,111	0
15	ZN	I	1127	1/1	0.93	0.09	-2.15	156,156,156,156	0

6.5 Other polymers

There are no such residues in this entry.