



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 PM GMT

PDB ID : 3S17  
Title : RNA Polymerase II Initiation Complex with a 9-nt RNA  
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.  
Deposited on : 2011-05-14  
Resolution : 3.20 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

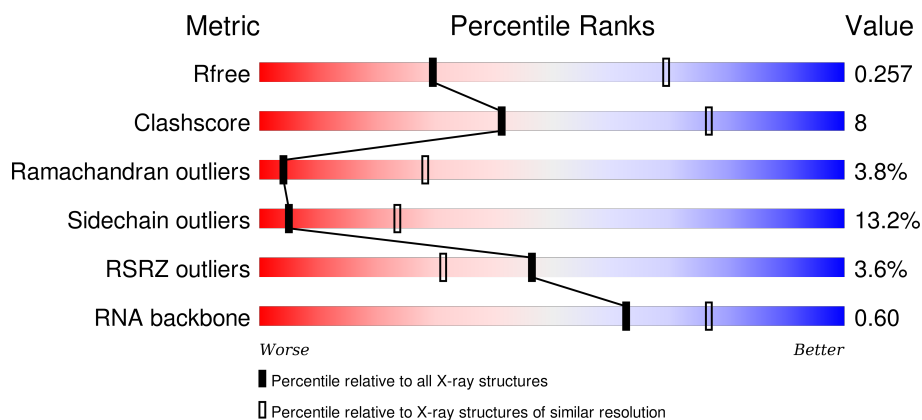
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>4%</div> <div>57%</div> <div>20%</div> <div>•</div> <div>19%</div> </div>
2	B	1224	<div> <div>2%</div> <div>62%</div> <div>24%</div> <div>•</div> <div>9%</div> </div>
3	C	318	<div> <div>%</div> <div>58%</div> <div>23%</div> <div>•</div> <div>16%</div> </div>
4	E	215	<div> <div>4%</div> <div>73%</div> <div>24%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	<div><div></div><div>39%13%45%</div></div>
6	H	146	<div><div>5%</div><div>58%24%8%9%</div></div>
7	I	122	<div><div>2%</div><div>74%18%6%</div></div>
8	J	70	<div><div></div><div>61%27%7%</div></div>
9	K	120	<div><div></div><div>66%27%5%</div></div>
10	L	70	<div><div>%</div><div>29%26%10%34%</div></div>
11	R	9	<div><div></div><div>44%44%11%</div></div>
12	T	29	<div><div></div><div>14%21%10%55%</div></div>

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	9	Total	C	N	O	P	0	0	0
			195	88	40	59	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

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

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

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

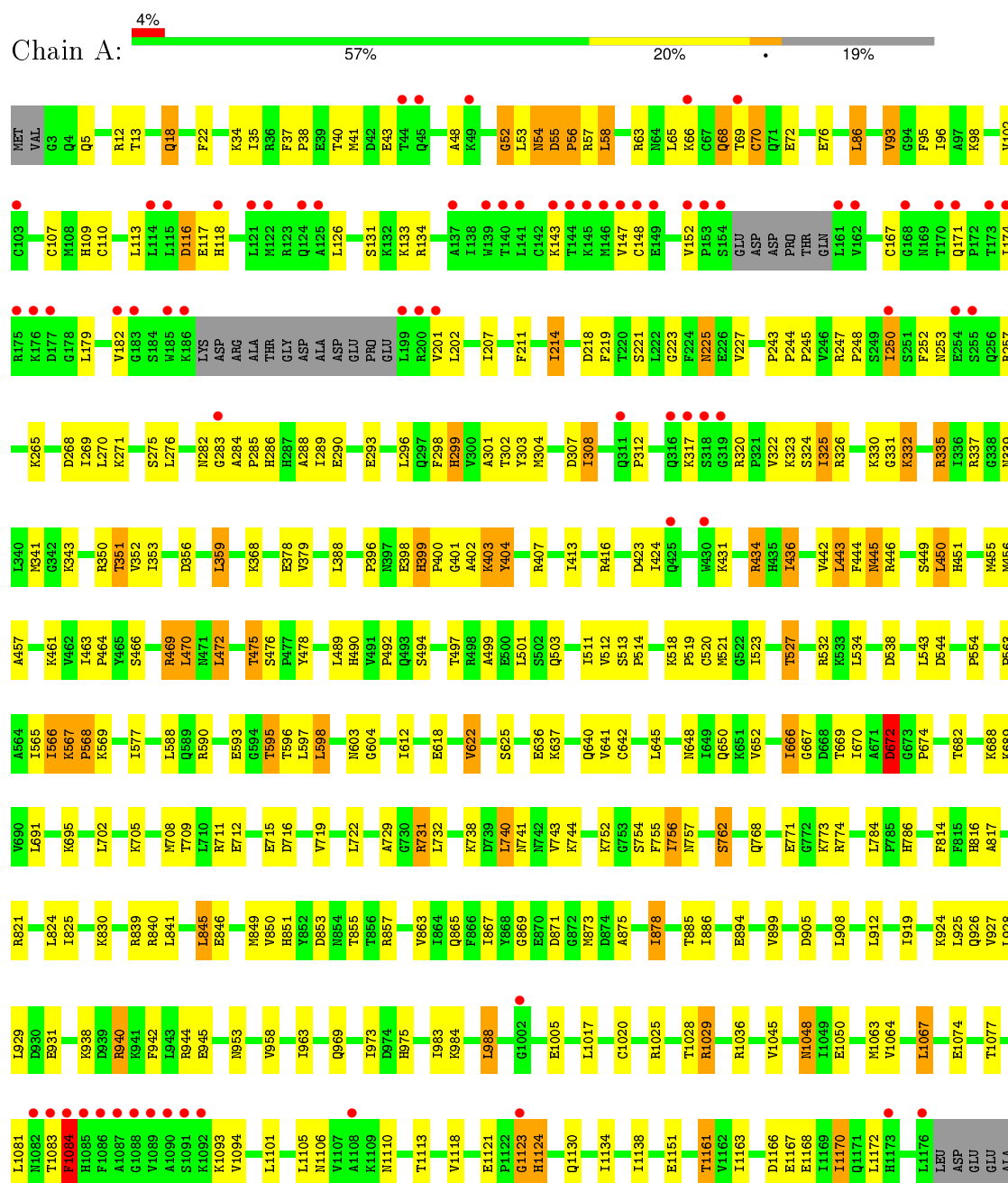
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 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.

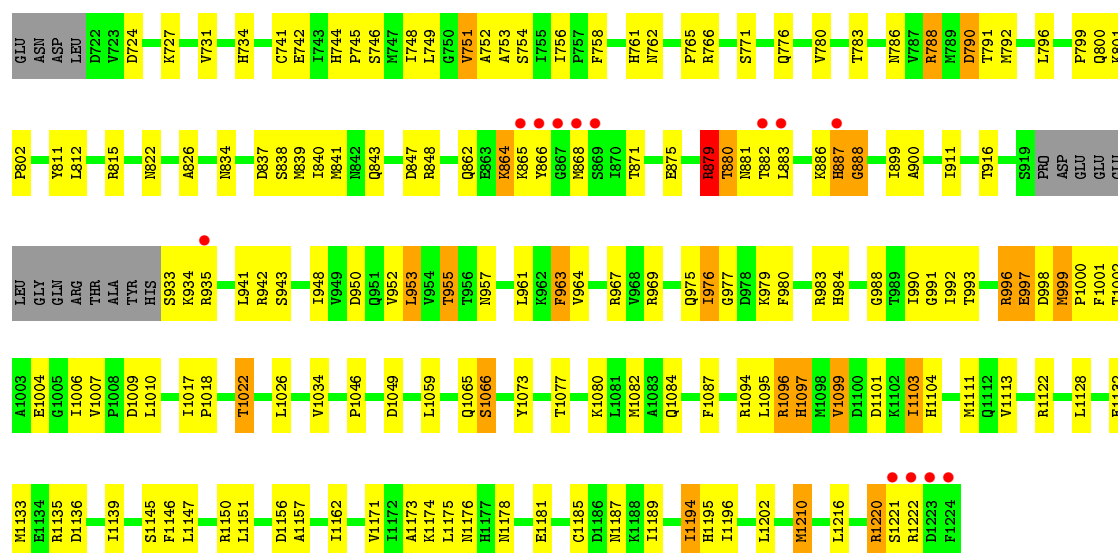
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



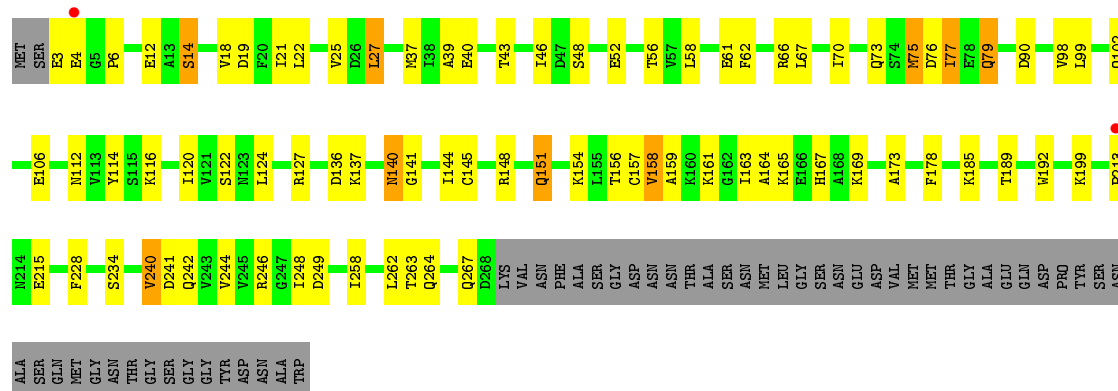


E612	ARG	A409	I284	G188	SER	MET
ASP	G410	I285	R169	ASN	SER	ASP
LVS	K418	D294	R175	ILE	LEU	LEU
K625	LVS	G295	G295	SER	ALA	ASN
T628	A509	F421	N178	ARG	ASN	ASN
	R512	L424	L181	LVS	SER	GLU
G631	H515	T425	E299	E89	LVS	LVS
Y634	H516	I428	M313	E194	TRR	TRR
	T517	F429	V323	M199	ASP	GLU
F638	H518	V323	I204	T98	ASP	ASP
V640	H519	Q325	I205	M101	PRQ	PRQ
	E526	M432	N206	V102	TRR	TRR
S645	GLU	G207	G207	S105	GLY	GLY
L646	ALA	F333	I334	D106	PHE	PHE
G647	HIS	G335	V211	P114	GLU	GLU
H648	ASP	ARG	L212	E21	E21	E21
K649	PHE	ARG	I213	R120	I25	I25
E650	ASN	GLY	I222	R120	E28	E28
L651	GLY	THR	V223	N121	D29	D29
K652	GLY	ALA	LEU	L122	S35	S35
F653	LVS	ILE	A229	T123	F38	F38
V654	L446	ILE	S232	K134	R39	R39
H654	A447	K345	P233	R135	E40	E40
K655	I448	E346	I234	T136	K41	K41
G656	M449	K347	V237	E138	G42	G42
H657	LVS	I349	A238	A139	L43	L43
L658	LVS	Q357	R241	D141	Q46	Q46
	T454	K345	R249	VAL	F54	F54
E659	H465	H363	L244	PRQ	T58	T58
L660	GLU	I364	E245	GLY	D61	D61
GLU	Q468	T365	R249	ARG	I62	I62
GLY	Q469	G366	K249	GLU	I63	I63
GLY	K470	I367	T250	LEU	S67	S67
PHE	K471	E368	G369	LVS	T68	T68
ASP	A477	S474	F370	TRR	L69	L69
VAL	A577	S475	E371	GLU	I70	I70
GLU	T576	R476	Q255	LEU	I63	I63
E678	H579	A477	V256	ILE	S67	S67
E687	F581	V482	K257	ALA	T68	T68
V690	V585	L483	G260	GLU	L69	L69
A704	H586	H484	R261	GLU	I70	I70
M705	H587	Q588	E262	SER	GLY	GLY
Q706	G588	R485	L386	GLU	LEU	LEU
P707	V589	R485	K393	ASP	GLU	GLU
E708	H590	Y486	R267	ASP	GLU	GLU
D709	H591	T487	T272	ASP	LEU	LEU
L710	E598	L492	K404	SER	GLU	GLU
P712	K606	R497	R405	GLU	ALA	ALA
A715	G607	R497	I276	GLY	HIS	HIS
ASN	D608	L502	K277	K164	TRR	TRR
TRR	GLY	GLY	V282	T487	TRR	TRR
GLU	GLY	L408	V282	T487	GLU	GLU

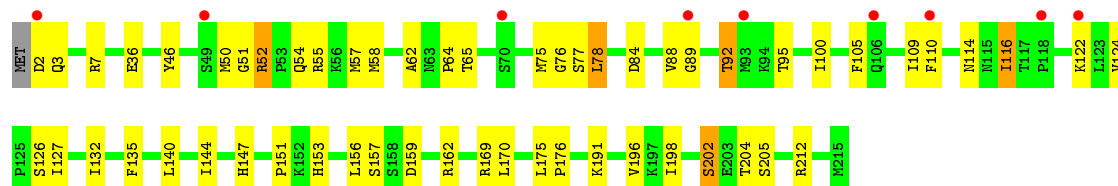
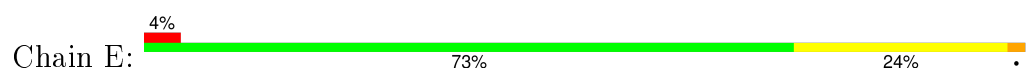




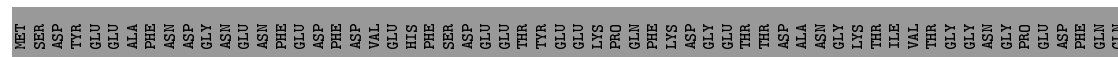
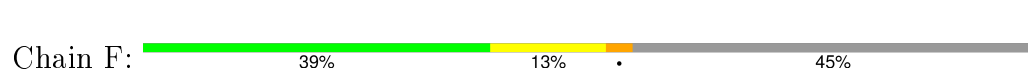
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



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

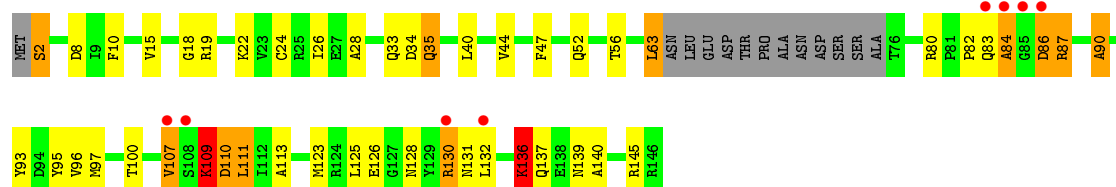


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2





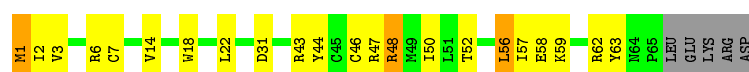
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



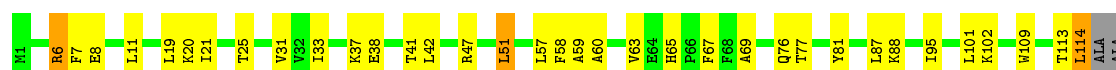
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



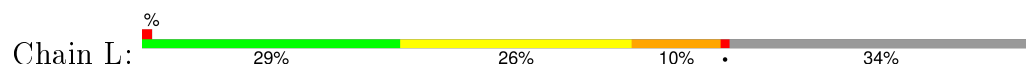
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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

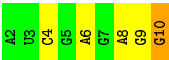


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

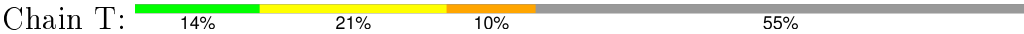


- Molecule 11: RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*G)-3')





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.97Å 220.90Å 192.03Å 90.00° 98.16° 90.00°	Depositor
Resolution (Å)	43.65 – 3.20 43.65 – 3.17	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.65-3.20) 98.8 (43.65-3.17)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.188 , 0.236 0.208 , 0.257	Depositor DCC
$R_{free}$ test set	5438 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.9	Xtriage
Anisotropy	0.836	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 69.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 109832 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.46	0/11241	0.76	1/15199 (0.0%)
2	B	0.49	0/9033	0.78	3/12181 (0.0%)
3	C	0.45	0/2133	0.77	0/2891
4	E	0.43	0/1788	0.68	0/2406
5	F	0.46	0/700	0.69	0/945
6	H	0.46	0/1086	0.80	1/1470 (0.1%)
7	I	0.48	0/989	0.79	0/1331
8	J	0.49	0/541	0.85	1/727 (0.1%)
9	K	0.43	0/937	0.70	0/1265
10	L	0.50	0/365	0.90	0/485
11	R	0.97	0/219	1.56	3/341 (0.9%)
12	T	1.02	0/290	2.07	18/444 (4.1%)
All	All	0.48	0/29322	0.80	27/39685 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	24	DT	O4'-C1'-N1	11.49	116.04	108.00
12	T	23	DC	O4'-C1'-N1	9.60	114.72	108.00
12	T	16	DC	P-O3'-C3'	9.57	131.18	119.70
12	T	17	DG	O4'-C4'-C3'	-8.45	100.93	106.00
2	B	647	GLY	C-N-CA	8.03	141.78	121.70
1	A	116	ASP	C-N-CA	6.96	139.09	121.70
12	T	17	DG	O4'-C1'-N9	6.84	112.79	108.00
12	T	22	DT	C4'-C3'-C2'	-6.62	97.14	103.10
12	T	21	DC	C4'-C3'-C2'	-6.59	97.17	103.10
12	T	21	DC	O4'-C4'-C3'	-6.55	101.88	104.50
12	T	22	DT	O4'-C4'-C3'	-6.54	101.89	104.50
11	R	4	C	O4'-C1'-N1	6.46	113.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	19	DT	C4-C5-C7	6.28	122.77	119.00
2	B	648	HIS	N-CA-CB	6.20	121.77	110.60
11	R	6	A	O4'-C1'-N9	5.82	112.86	108.20
12	T	25	DC	O4'-C1'-N1	5.55	111.88	108.00
12	T	19	DT	C4'-C3'-C2'	-5.47	98.18	103.10
12	T	22	DT	C4-C5-C7	5.31	122.19	119.00
8	J	1	MET	C-N-CA	5.28	134.89	121.70
12	T	19	DT	O4'-C1'-N1	5.23	111.66	108.00
12	T	19	DT	P-O3'-C3'	5.22	125.96	119.70
12	T	20	DC	O4'-C1'-N1	5.21	111.64	108.00
12	T	19	DT	C6-C5-C7	-5.11	119.84	122.90
2	B	140	ILE	C-N-CA	5.03	134.27	121.70
11	R	8	A	O4'-C4'-C3'	-5.02	98.98	104.00
6	H	2	SER	C-N-CA	5.02	134.25	121.70
12	T	17	DG	C1'-O4'-C4'	-5.01	105.09	110.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	199	0
2	B	8861	0	8884	189	0
3	C	2095	0	2051	45	0
4	E	1752	0	1776	20	0
5	F	688	0	707	11	0
6	H	1068	0	1040	18	0
7	I	971	0	927	12	0
8	J	532	0	542	18	0
9	K	919	0	929	23	0
10	L	363	0	386	12	0
11	R	195	0	99	1	0
12	T	261	0	148	2	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28757	0	28622	487	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (487) 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:HD2	1.44	1.00
4:E:77:SER:HB3	4:E:105:PHE:HA	1.53	0.89
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.52	0.89
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.39	0.87
1:A:567:LYS:HB3	6:H:96:VAL:H	1.41	0.85
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.65	0.78
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.66	0.77
2:B:706:GLN:O	2:B:710:LEU:HB2	1.85	0.77
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.67	0.76
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.68	0.76
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.14	0.75
2:B:363:HIS:O	2:B:364:ILE:HB	1.85	0.75
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.50	0.75
1:A:741:ASN:HD22	1:A:744:LYS:H	1.35	0.74
3:C:56:THR:HG21	3:C:145:CYS:SG	2.28	0.73
2:B:862:GLN:HG2	2:B:963:PHE:HB2	1.69	0.73
2:B:801:LYS:O	8:J:52:THR:HG23	1.88	0.73
8:J:48:ARG:O	8:J:52:THR:HB	1.88	0.73
1:A:399:HIS:O	1:A:401:GLY:N	2.23	0.72
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.71	0.71
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.06	0.70
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.56	0.70
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.25	0.69
1:A:855:THR:HG21	1:A:857:ARG:HE	1.58	0.69
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.74	0.69
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.75	0.68
2:B:975:GLN:HG2	2:B:976:ILE:H	1.57	0.68
1:A:1323:ASP:OD1	1:A:1325:THR:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.75	0.68
2:B:563:MET:HE2	2:B:587:HIS:HB2	1.76	0.68
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.20	0.67
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.76	0.67
2:B:654:ARG:H	2:B:657:HIS:HD2	1.42	0.67
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.59	0.67
1:A:885:THR:O	1:A:940:ARG:HD3	1.95	0.67
1:A:669:THR:O	1:A:762:SER:HB3	1.96	0.66
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.78	0.66
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.78	0.65
2:B:879:ARG:O	2:B:882:THR:HG22	1.96	0.65
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.27	0.65
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.77	0.65
1:A:511:ILE:HA	1:A:521:MET:HE3	1.79	0.65
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.78	0.65
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.77	0.64
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.27	0.64
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.79	0.64
2:B:515:HIS:HD2	2:B:517:THR:H	1.45	0.64
2:B:465:ASN:HA	2:B:476:ARG:HA	1.80	0.64
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.33	0.64
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.79	0.64
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.80	0.64
2:B:638:PHE:CD2	2:B:653:VAL:HG21	2.33	0.63
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.80	0.63
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.64	0.63
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.97	0.63
2:B:744:HIS:HD2	2:B:746:SER:H	1.46	0.63
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.46	0.62
1:A:756:ILE:H	1:A:756:ILE:HD13	1.63	0.62
1:A:1325:THR:HA	4:E:147:HIS:HA	1.82	0.62
2:B:38:PHE:H	2:B:41:LYS:HB2	1.64	0.62
6:H:137:GLN:HB3	6:H:139:ASN:HB2	1.82	0.61
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.81	0.61
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	1.83	0.61
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.82	0.60
1:A:456:MET:HB2	1:A:478:TYR:OH	2.01	0.60
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.82	0.60
1:A:869:GLY:O	4:E:204:THR:HG21	2.02	0.60
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.83	0.60
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:HB2	1:A:57:ARG:HH21	1.66	0.60
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.85	0.60
3:C:73:GLN:HE21	3:C:75:MET:H	1.50	0.59
2:B:283:VAL:HG12	2:B:297:ILE:HG21	1.83	0.59
1:A:378:GLU:OE2	1:A:434:ARG:HD3	2.01	0.59
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.66	0.59
1:A:68:GLN:NE2	1:A:70:CYS:HB3	2.17	0.59
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.37	0.59
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.85	0.59
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.84	0.59
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.66	0.59
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.84	0.59
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.84	0.59
1:A:899:VAL:HB	1:A:929:LEU:HD22	1.85	0.58
7:I:116:ASN:HD22	7:I:118:ARG:HH12	1.49	0.58
2:B:43:LEU:HD11	2:B:811:TYR:O	2.03	0.58
3:C:46:ILE:HA	3:C:159:ALA:HA	1.84	0.58
1:A:754:SER:H	1:A:757:ASN:HD22	1.51	0.58
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.04	0.58
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.86	0.58
1:A:554:PRO:HD2	1:A:648:ASN:ND2	2.18	0.58
1:A:1161:THR:OG1	1:A:1170:ILE:HG13	2.03	0.58
2:B:515:HIS:H	2:B:518:HIS:HD2	1.52	0.58
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.69	0.58
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.85	0.58
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.34	0.57
7:I:111:THR:HG23	7:I:113:ASP:H	1.68	0.57
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.19	0.57
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.86	0.57
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.86	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.86	0.57
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.38	0.57
3:C:76:ASP:HB3	3:C:79:GLN:HG3	1.85	0.57
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.35	0.57
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.86	0.57
7:I:28:GLU:HB3	7:I:35:VAL:HG13	1.87	0.57
3:C:167:HIS:HD2	3:C:169:LYS:H	1.51	0.57
2:B:843:GLN:HB2	2:B:993:THR:HB	1.87	0.57
1:A:596:THR:C	1:A:598:LEU:H	2.07	0.57
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.88	0.56
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.35	0.56
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.87	0.56
1:A:95:PHE:CE2	1:A:1414:ALA:HB2	2.41	0.56
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.87	0.56
1:A:404:TYR:HA	1:A:413:ILE:O	2.05	0.56
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.53	0.56
1:A:34:LYS:HE2	1:A:57:ARG:HH12	1.71	0.56
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.87	0.56
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.06	0.56
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.87	0.56
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.88	0.56
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.86	0.56
12:T:19:DT:H2'	12:T:20:DC:C6	2.41	0.56
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.54	0.56
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.87	0.56
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.88	0.56
2:B:241:ARG:HA	2:B:253:THR:HG22	1.87	0.55
2:B:834:ASN:HA	2:B:838:SER:HB2	1.88	0.55
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.89	0.55
2:B:976:ILE:O	2:B:990:ILE:HB	2.06	0.55
3:C:6:PRO:HB3	3:C:25:VAL:HG22	1.89	0.55
9:K:21:ILE:HG13	9:K:33:ILE:HG12	1.87	0.55
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.89	0.55
2:B:260:GLY:O	2:B:267:ARG:HD3	2.06	0.55
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.88	0.55
2:B:516:ASN:HD22	2:B:516:ASN:H	1.55	0.55
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.72	0.55
1:A:709:THR:HG22	1:A:711:ARG:H	1.72	0.55
1:A:1084:PHE:HZ	1:A:1093:LYS:HA	1.72	0.55
1:A:709:THR:HB	1:A:712:GLU:HB2	1.89	0.55
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.42	0.55
2:B:975:GLN:O	2:B:990:ILE:HD12	2.07	0.54
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.89	0.54
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.90	0.54
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.39	0.54
1:A:554:PRO:HD2	1:A:648:ASN:HD22	1.72	0.54
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.87	0.54
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.90	0.54
3:C:14:SER:HA	9:K:114:LEU:HD22	1.88	0.54
1:A:55:ASP:O	1:A:57:ARG:N	2.40	0.54
2:B:486:TYR:CZ	2:B:1096:ARG:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.90	0.53
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.31	0.53
2:B:953:LEU:O	2:B:964:VAL:HG23	2.08	0.53
8:J:3:VAL:CG1	8:J:18:TRP:HB2	2.36	0.53
1:A:472:LEU:O	1:A:475:THR:HB	2.09	0.53
2:B:370:PHE:O	2:B:372:SER:N	2.36	0.53
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.91	0.53
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.74	0.53
4:E:64:PRO:HD3	4:E:76:GLY:HA2	1.91	0.53
2:B:724:ASP:HB3	2:B:727:LYS:HD2	1.91	0.53
2:B:35:SER:O	2:B:39:ARG:HB2	2.09	0.53
5:F:128:LYS:HG2	5:F:149:GLU:HA	1.91	0.53
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.44	0.52
2:B:762:ASN:HD21	2:B:984:HIS:HD2	1.56	0.52
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.91	0.52
4:E:202:SER:HB3	4:E:205:SER:H	1.75	0.52
1:A:666:ILE:HG12	2:B:1026:LEU:HB2	1.91	0.52
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.90	0.52
2:B:483:LEU:HG	2:B:484:ASN:H	1.74	0.52
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.89	0.52
2:B:255:GLN:H	2:B:272:THR:HB	1.73	0.52
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.90	0.52
2:B:515:HIS:H	2:B:518:HIS:CD2	2.26	0.52
1:A:68:GLN:O	1:A:68:GLN:NE2	2.42	0.52
2:B:887:HIS:HA	2:B:888:GLY:C	2.29	0.52
7:I:88:SER:C	7:I:90:GLN:H	2.13	0.52
2:B:428:ILE:HD12	2:B:448:ILE:HD12	1.91	0.52
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.44	0.52
5:F:93:ILE:HD13	5:F:134:ILE:HD11	1.91	0.52
1:A:116:ASP:HB3	1:A:117:GLU:HB2	1.90	0.52
1:A:494:SER:HB3	1:A:497:THR:OG1	2.09	0.52
1:A:863:VAL:HG23	4:E:170:LEU:HD21	1.90	0.52
1:A:731:ARG:HD3	1:A:755:PHE:CZ	2.45	0.52
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.91	0.52
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.74	0.52
1:A:672:ASP:HB3	1:A:674:PRO:HD2	1.92	0.52
2:B:976:ILE:HG23	2:B:977:GLY:H	1.75	0.52
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.91	0.52
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.52
9:K:65:HIS:HD2	9:K:67:PHE:H	1.58	0.52
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LYS:O	1:A:988:LEU:HB2	2.10	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.91	0.51
4:E:50:MET:HB3	4:E:52:ARG:HH12	1.75	0.51
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.92	0.51
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.46	0.51
4:E:198:ILE:HD13	4:E:212:ARG:HG3	1.92	0.51
1:A:1130:GLN:HE21	1:A:1134:ILE:HD11	1.75	0.51
9:K:38:GLU:O	9:K:69:ALA:O	2.28	0.51
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.42	0.51
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.92	0.51
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.58	0.51
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.92	0.51
3:C:98:VAL:HG22	3:C:158:VAL:HG13	1.92	0.51
2:B:1082:MET:HA	3:C:189:THR:HA	1.93	0.51
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.92	0.50
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.46	0.50
6:H:125:LEU:HG	6:H:130:ARG:NH1	2.25	0.50
2:B:276:ILE:HG13	2:B:334:ILE:HG23	1.93	0.50
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.94	0.50
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.93	0.50
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.91	0.50
1:A:290:GLU:HA	1:A:293:GLU:HB2	1.93	0.50
1:A:1017:LEU:O	1:A:1020:CYS:HB2	2.12	0.50
1:A:899:VAL:CG2	1:A:1029:ARG:HG3	2.41	0.50
2:B:516:ASN:ND2	2:B:516:ASN:H	2.09	0.50
1:A:1259:MET:HA	1:A:1262:LYS:HE2	1.93	0.50
4:E:88:VAL:HG13	4:E:92:THR:HB	1.93	0.50
1:A:499:ALA:HB2	5:F:118:LEU:HD11	1.94	0.50
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.93	0.50
1:A:265:LYS:HD3	1:A:322:VAL:HG21	1.93	0.50
6:H:113:ALA:HB2	6:H:126:GLU:HG3	1.92	0.50
9:K:65:HIS:CD2	9:K:67:PHE:H	2.30	0.49
2:B:58:THR:O	2:B:62:ILE:HG12	2.12	0.49
2:B:63:ILE:O	2:B:67:SER:HB3	2.11	0.49
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.94	0.49
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.92	0.49
2:B:706:GLN:H	2:B:710:LEU:HG	1.78	0.49
2:B:744:HIS:CD2	2:B:746:SER:OG	2.65	0.49
2:B:549:THR:HB	2:B:628:THR:HB	1.95	0.49
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.94	0.49
1:A:86:LEU:HD11	1:A:296:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.95	0.49
2:B:140:ILE:HB	2:B:141:ASP:HB2	1.93	0.49
1:A:512:VAL:HA	1:A:519:PRO:HA	1.94	0.49
1:A:642:CYS:O	1:A:645:LEU:HB3	2.12	0.49
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.60	0.49
2:B:837:ASP:O	2:B:988:GLY:HA2	2.12	0.49
1:A:490:HIS:HB3	2:B:1150:ARG:HH21	1.78	0.49
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.95	0.49
2:B:864:LYS:HG2	2:B:871:THR:HA	1.94	0.49
2:B:519:TRP:HZ2	2:B:705:MET:CE	2.26	0.48
3:C:58:LEU:HD21	8:J:57:ILE:HD12	1.95	0.48
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.94	0.48
1:A:444:PHE:CE2	1:A:470:LEU:HD22	2.49	0.48
5:F:110:ASP:O	5:F:123:LYS:HE2	2.14	0.48
10:L:28:LYS:HB2	10:L:39:SER:HA	1.95	0.48
2:B:705:MET:HG3	2:B:745:PRO:HG3	1.95	0.48
2:B:237:VAL:HG22	2:B:257:LYS:HB3	1.94	0.48
2:B:123:THR:HA	2:B:204:ILE:O	2.14	0.48
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.96	0.48
2:B:25:ILE:HD13	2:B:653:VAL:HB	1.95	0.48
3:C:262:LEU:HD13	9:K:88:LYS:HG3	1.96	0.48
1:A:469:ARG:NH2	2:B:991:GLY:O	2.45	0.48
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.96	0.48
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.95	0.48
2:B:887:HIS:HA	2:B:888:GLY:O	2.13	0.48
3:C:165:LYS:O	9:K:6:ARG:NH1	2.47	0.47
10:L:49:LYS:O	10:L:50:ASP:HB2	2.14	0.47
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.44	0.47
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.43	0.47
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.96	0.47
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.29	0.47
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.96	0.47
1:A:341:MET:HB2	2:B:1132:GLU:HG2	1.96	0.47
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.96	0.47
2:B:515:HIS:N	2:B:518:HIS:HD2	2.13	0.47
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.14	0.47
3:C:248:ILE:HD13	9:K:102:LYS:HA	1.94	0.47
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.79	0.47
3:C:234:SER:HB3	3:C:240:VAL:HG13	1.97	0.47
1:A:1166:ASP:O	1:A:1168:GLU:N	2.48	0.47
1:A:975:HIS:CG	1:A:1036:ARG:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:HA	1:A:521:MET:CE	2.43	0.47
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.14	0.47
2:B:565:PRO:HD2	2:B:568:ASP:HB2	1.96	0.47
1:A:325:ILE:HB	2:B:1210:MET:SD	2.55	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.68	0.47
4:E:78:LEU:HD21	4:E:109:ILE:HG12	1.97	0.47
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.50	0.47
2:B:745:PRO:O	2:B:748:ILE:HG12	2.16	0.46
1:A:1422:ARG:HG3	2:B:1220:ARG:HH12	1.80	0.46
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.80	0.46
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.80	0.46
1:A:942:PHE:O	1:A:945:GLU:HG2	2.15	0.46
1:A:886:ILE:HG13	1:A:944:ARG:HG3	1.96	0.46
2:B:822:ASN:HD22	8:J:52:THR:CG2	2.27	0.46
2:B:563:MET:HA	2:B:589:VAL:O	2.15	0.46
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.97	0.46
1:A:225:ASN:HD22	1:A:227:VAL:H	1.63	0.46
6:H:63:LEU:HB2	6:H:90:ALA:H	1.80	0.46
8:J:1:MET:HB2	8:J:56:LEU:HD12	1.97	0.46
1:A:523:ILE:HG23	1:A:527:THR:HB	1.98	0.46
1:A:396:PRO:HG2	1:A:416:ARG:HB3	1.98	0.46
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.36	0.46
2:B:727:LYS:HE2	2:B:1049:ASP:HB3	1.98	0.46
2:B:492:LEU:HB3	2:B:751:VAL:HG21	1.98	0.46
1:A:738:LYS:HD2	1:A:740:LEU:HD21	1.97	0.46
1:A:752:LYS:HB3	2:B:1018:PRO:HG2	1.98	0.46
2:B:38:PHE:HA	2:B:42:GLY:H	1.81	0.46
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.96	0.46
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.81	0.46
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.98	0.46
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.97	0.46
2:B:997:GLU:CD	2:B:997:GLU:H	2.19	0.46
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.98	0.46
1:A:756:ILE:CD1	1:A:756:ILE:H	2.29	0.45
3:C:173:ALA:HA	3:C:234:SER:HA	1.97	0.45
3:C:258:ILE:HG23	9:K:19:LEU:HD11	1.97	0.45
1:A:68:GLN:HE22	1:A:70:CYS:HB3	1.82	0.45
1:A:343:LYS:HE3	2:B:1151:LEU:HG	1.99	0.45
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.98	0.45
2:B:839:MET:CE	2:B:980:PHE:HB2	2.47	0.45
1:A:5:GLN:HB3	2:B:1175:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.80	0.45
1:A:1404:GLU:O	1:A:1408:ILE:HG12	2.16	0.45
3:C:98:VAL:H	3:C:122:SER:CB	2.30	0.45
1:A:743:VAL:HG13	2:B:1018:PRO:HB3	1.98	0.45
2:B:367:LEU:HB3	2:B:368:GLU:H	1.68	0.45
4:E:55:ARG:HG2	4:E:58:MET:HE1	1.99	0.45
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.98	0.45
1:A:919:ILE:HD11	1:A:925:LEU:HG	1.98	0.45
1:A:116:ASP:CB	1:A:117:GLU:HB2	2.46	0.45
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.52	0.45
2:B:563:MET:HE2	2:B:587:HIS:CB	2.45	0.45
1:A:57:ARG:O	1:A:68:GLN:HG2	2.16	0.45
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.98	0.45
1:A:567:LYS:O	1:A:569:LYS:N	2.50	0.44
1:A:851:HIS:HB2	1:A:855:THR:HG22	2.00	0.44
1:A:924:LYS:O	1:A:927:VAL:HG12	2.16	0.44
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.99	0.44
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.99	0.44
5:F:72:LYS:HG2	5:F:142:SER:HA	1.98	0.44
1:A:814:PHE:O	1:A:817:ALA:HB3	2.18	0.44
12:T:20:DC:H2'	12:T:21:DC:O4'	2.17	0.44
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.99	0.44
1:A:98:LYS:O	1:A:102:VAL:HG23	2.17	0.44
1:A:595:THR:HG21	1:A:604:GLY:HA3	1.99	0.44
3:C:99:LEU:HD13	3:C:120:ILE:HG12	2.00	0.44
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.99	0.44
1:A:351:THR:HG21	1:A:466:SER:O	2.18	0.44
1:A:449:SER:O	2:B:1133:MET:HG2	2.18	0.44
7:I:65:ASP:HB3	7:I:68:LEU:HD12	1.99	0.44
2:B:277:LYS:HZ1	2:B:335:GLY:H	1.66	0.44
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.99	0.44
2:B:563:MET:HE3	2:B:580:VAL:HB	2.00	0.44
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.52	0.44
3:C:98:VAL:H	3:C:122:SER:HB2	1.83	0.44
5:F:133:VAL:HG22	5:F:147:SER:HA	2.00	0.44
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.98	0.44
3:C:12:GLU:HB2	3:C:19:ASP:HB3	1.99	0.44
4:E:176:PRO:O	4:E:212:ARG:HA	2.17	0.43
1:A:57:ARG:HA	1:A:68:GLN:HB3	2.00	0.43
2:B:140:ILE:H	2:B:141:ASP:C	2.22	0.43
2:B:54:PHE:HB2	2:B:410:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:CD2	2:B:517:THR:H	2.29	0.43
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.18	0.43
2:B:295:GLY:O	2:B:299:GLU:HB2	2.18	0.43
1:A:738:LYS:HA	6:H:19:ARG:HH22	1.83	0.43
1:A:1084:PHE:HE2	1:A:1094:VAL:H	1.66	0.43
1:A:304:MET:O	1:A:326:ARG:HB2	2.18	0.43
2:B:841:MET:O	2:B:993:THR:HA	2.19	0.43
1:A:1411:GLU:HA	1:A:1414:ALA:HB3	2.01	0.43
7:I:73:ARG:O	7:I:81:ARG:HA	2.18	0.43
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.83	0.43
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.01	0.43
4:E:124:VAL:HG22	4:E:132:ILE:HD11	2.01	0.43
1:A:824:LEU:HD21	2:B:765:PRO:HB3	2.00	0.43
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.00	0.43
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.00	0.43
1:A:983:ILE:HD12	1:A:1028:THR:HG21	2.01	0.43
3:C:22:LEU:HG	3:C:25:VAL:HG21	2.01	0.43
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.54	0.43
1:A:250:ILE:HD11	2:B:1113:VAL:HG21	2.01	0.43
2:B:421:PHE:O	2:B:425:THR:HB	2.18	0.43
1:A:182:VAL:HG22	1:A:201:VAL:HG12	2.01	0.43
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.48	0.43
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.99	0.43
2:B:62:ILE:HG23	2:B:418:LYS:HG3	2.01	0.43
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	2.01	0.43
2:B:839:MET:HE2	2:B:980:PHE:HB2	2.00	0.43
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.83	0.43
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.16	0.43
9:K:113:THR:O	9:K:114:LEU:HB2	2.19	0.42
3:C:77:ILE:HD12	3:C:161:LYS:HG3	2.00	0.42
4:E:151:PRO:HD2	4:E:153:HIS:HE1	1.84	0.42
3:C:70:ILE:CD1	3:C:144:ILE:HD12	2.48	0.42
4:E:110:PHE:HE2	4:E:116:ILE:HD11	1.84	0.42
4:E:62:ALA:HB3	4:E:78:LEU:HB3	2.01	0.42
7:I:69:PRO:HD2	7:I:85:PHE:O	2.19	0.42
1:A:855:THR:HG21	1:A:857:ARG:NE	2.29	0.42
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.54	0.42
7:I:62:ILE:HG12	7:I:84:VAL:HG11	2.00	0.42
1:A:849:MET:HB3	1:A:1063:MET:SD	2.59	0.42
2:B:21:GLU:HB2	2:B:656:GLY:HA3	2.00	0.42
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:9:G:H2'	11:R:10:G:C8	2.55	0.42
1:A:1151:GLU:HG2	7:I:45:ARG:HG3	2.02	0.42
2:B:800:GLN:CB	8:J:52:THR:HG22	2.48	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.20	0.42
3:C:148:ARG:HB3	3:C:151:GLN:HG3	2.01	0.42
1:A:563:PRO:HG2	1:A:566:ILE:HG12	2.00	0.42
1:A:107:CYS:HA	1:A:171:GLN:HE21	1.83	0.42
9:K:8:GLU:O	9:K:37:LYS:HD2	2.19	0.42
1:A:514:PRO:HG2	1:A:1067:LEU:HD21	2.01	0.42
1:A:284:ALA:HB1	1:A:289:ILE:HD11	2.01	0.42
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.90	0.42
3:C:40:GLU:HG2	3:C:163:ILE:HD12	2.01	0.42
2:B:563:MET:CE	2:B:587:HIS:HB2	2.47	0.42
2:B:654:ARG:H	2:B:657:HIS:CD2	2.29	0.42
1:A:839:ARG:HH21	1:A:1402:PHE:HA	1.85	0.42
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.20	0.42
1:A:715:GLU:O	1:A:719:VAL:HG23	2.19	0.42
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.42
1:A:928:LEU:HA	1:A:931:GLU:HG2	2.01	0.42
2:B:754:SER:HB2	2:B:812:LEU:CD1	2.48	0.42
5:F:109:VAL:HG22	5:F:123:LYS:HE3	2.01	0.42
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.55	0.42
2:B:840:ILE:HG12	2:B:992:ILE:HG22	2.02	0.42
7:I:14:LEU:HB3	7:I:27:PHE:HB3	2.02	0.42
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.54	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.01	0.42
1:A:1293:SER:HB3	1:A:1299:VAL:HG23	2.01	0.42
1:A:648:ASN:O	1:A:652:VAL:HG23	2.19	0.42
3:C:99:LEU:HB2	3:C:157:CYS:HB2	2.02	0.42
6:H:80:ARG:HG2	9:K:57:LEU:HD22	2.01	0.41
1:A:356:ASP:HB3	1:A:359:LEU:HB2	2.01	0.41
2:B:1162:ILE:HG12	2:B:1194:ILE:HD12	2.01	0.41
1:A:1426:GLU:HG2	1:A:1426:GLU:H	1.49	0.41
1:A:298:PHE:O	1:A:298:PHE:CD1	2.73	0.41
2:B:424:LEU:O	2:B:428:ILE:HG12	2.20	0.41
2:B:708:GLU:H	2:B:708:GLU:HG3	1.57	0.41
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.95	0.41
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.56	0.41
6:H:109:LYS:HZ3	6:H:111:LEU:HB2	1.85	0.41
10:L:68:GLU:C	10:L:70:ARG:H	2.23	0.41
1:A:403:LYS:HG2	1:A:403:LYS:H	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ILE:HD12	1:A:436:ILE:HA	1.87	0.41
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	2.01	0.41
9:K:7:PHE:O	9:K:11:LEU:HB2	2.20	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.41
1:A:527:THR:HG21	1:A:650:GLN:HA	2.02	0.41
2:B:796:LEU:HD23	2:B:799:PRO:HA	2.03	0.41
1:A:332:LYS:HD2	1:A:332:LYS:HA	1.89	0.41
2:B:704:ALA:HB1	2:B:710:LEU:HB3	2.02	0.41
2:B:483:LEU:CG	2:B:484:ASN:H	2.33	0.41
1:A:351:THR:HG22	1:A:352:VAL:H	1.85	0.41
2:B:244:LEU:HD12	2:B:250:PHE:HB2	2.02	0.41
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.85	0.41
2:B:46:GLN:HG3	2:B:46:GLN:H	1.73	0.41
1:A:1084:PHE:CZ	1:A:1093:LYS:HA	2.54	0.41
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.03	0.41
6:H:40:LEU:HD13	6:H:123:MET:HG3	2.02	0.41
4:E:196:VAL:HG13	4:E:198:ILE:HD11	2.03	0.41
6:H:109:LYS:HD2	6:H:110:ASP:H	1.86	0.41
1:A:148:CYS:HB3	1:A:167:CYS:O	2.20	0.41
10:L:27:LEU:HB3	10:L:37:LYS:HD2	2.02	0.41
1:A:567:LYS:HZ1	6:H:97:MET:HG2	1.86	0.41
2:B:640:VAL:CG2	2:B:651:LEU:HD23	2.50	0.41
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.86	0.41
2:B:749:LEU:HD22	2:B:753:ALA:HB1	2.01	0.41
2:B:98:THR:O	2:B:178:ASN:ND2	2.53	0.41
1:A:118:HIS:CD2	1:A:152:VAL:HG21	2.55	0.41
1:A:37:PHE:HA	1:A:38:PRO:HD3	2.00	0.41
2:B:900:ALA:HA	10:L:58:LYS:HD3	2.03	0.41
2:B:294:ASP:H	7:I:12:ASN:ND2	2.19	0.41
3:C:185:LYS:HG2	3:C:213:PRO:HG3	2.03	0.41
9:K:47:ARG:HD2	9:K:60:ALA:HA	2.03	0.40
2:B:1185:CYS:C	2:B:1187:ASN:H	2.25	0.40
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.61	0.40
1:A:565:ILE:HG22	1:A:569:LYS:O	2.22	0.40
2:B:957:ASN:HB3	2:B:961:LEU:HB2	2.03	0.40
10:L:27:LEU:HD23	10:L:37:LYS:HZ3	1.86	0.40
2:B:880:THR:HG22	2:B:933:SER:HB2	2.03	0.40
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.03	0.40
2:B:345:LYS:HA	2:B:347:LYS:H	1.87	0.40
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.54	0.40
1:A:134:ARG:HD2	1:A:221:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.54	0.40
2:B:955:THR:OG1	10:L:54:ARG:O	2.32	0.40
4:E:88:VAL:HB	4:E:116:ILE:HG13	2.04	0.40
2:B:569:TYR:HE1	2:B:574:SER:HB2	1.87	0.40
6:H:136:LYS:H	6:H:136:LYS:HD3	1.86	0.40
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.54	0.40
2:B:346:GLU:HA	2:B:349:ILE:HD12	2.04	0.40
1:A:442:VAL:O	1:A:457:ALA:HA	2.22	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	1395/1733 (80%)	1221 (88%)	131 (9%)	43 (3%)	5	34
2	B	1096/1224 (90%)	952 (87%)	91 (8%)	53 (5%)	3	22
3	C	264/318 (83%)	238 (90%)	22 (8%)	4 (2%)	13	55
4	E	212/215 (99%)	199 (94%)	8 (4%)	5 (2%)	7	43
5	F	83/155 (54%)	73 (88%)	7 (8%)	3 (4%)	4	30
6	H	129/146 (88%)	100 (78%)	16 (12%)	13 (10%)	1	4
7	I	117/122 (96%)	101 (86%)	14 (12%)	2 (2%)	11	52
8	J	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	5	33
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100	100
10	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	0
All	All	3515/4173 (84%)	3075 (88%)	307 (9%)	133 (4%)	4	28

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	ASP
1	A	66	LYS
1	A	250	ILE
1	A	283	GLY
1	A	399	HIS
1	A	567	LYS
1	A	1167	GLU
2	B	67	SER
2	B	137	TYR
2	B	250	PHE
2	B	371	GLU
2	B	449	ASN
2	B	469	GLN
2	B	477	ALA
2	B	482	VAL
2	B	648	HIS
2	B	712	PRO
2	B	751	VAL
2	B	943	SER
2	B	976	ILE
2	B	1046	PRO
2	B	1156	ASP
3	C	141	GLY
3	C	267	GLN
6	H	131	ASN
8	J	2	ILE
8	J	6	ARG
10	L	50	ASP
10	L	56	LEU
10	L	64	LEU
1	A	56	PRO
1	A	312	PRO
1	A	331	GLY
1	A	404	TYR
1	A	423	ASP
1	A	1123	GLY
1	A	1234	GLU
1	A	1437	GLY
2	B	139	ALA
2	B	229	ALA
2	B	465	ASN
2	B	483	LEU

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Mol	Chain	Res	Type
2	B	526	GLU
2	B	879	ARG
2	B	883	LEU
2	B	887	HIS
2	B	888	GLY
2	B	1096	ARG
2	B	1220	ARG
4	E	126	SER
5	F	111	LEU
6	H	18	GLY
6	H	90	ALA
6	H	109	LYS
6	H	140	ALA
1	A	275	SER
1	A	286	HIS
1	A	332	LYS
1	A	543	LEU
1	A	846	GLU
1	A	1221	LYS
2	B	249	ARG
2	B	364	ILE
2	B	471	LYS
2	B	708	GLU
2	B	734	HIS
2	B	881	ASN
2	B	1066	SER
2	B	1157	ALA
2	B	1221	SER
3	C	4	GLU
4	E	114	ASN
6	H	35	GLN
6	H	132	LEU
10	L	39	SER
10	L	59	ALA
1	A	48	ALA
1	A	214	ILE
1	A	257	ARG
1	A	597	LEU
1	A	672	ASP
1	A	1084	PHE
2	B	367	LEU
2	B	619	ILE

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Mol	Chain	Res	Type
2	B	709	ASP
2	B	792	MET
2	B	942	ARG
2	B	1099	VAL
2	B	1171	VAL
2	B	1173	ALA
2	B	1181	GLU
4	E	36	GLU
5	F	154	ASP
6	H	84	ALA
6	H	128	ASN
7	I	115	LYS
10	L	42	ARG
10	L	47	ARG
1	A	35	ILE
1	A	54	ASN
1	A	109	HIS
1	A	324	SER
1	A	424	ILE
1	A	1081	LEU
1	A	1083	THR
1	A	1124	HIS
1	A	1377	THR
2	B	476	ARG
2	B	531	GLN
2	B	563	MET
2	B	707	PRO
2	B	1017	ILE
2	B	1097	HIS
3	C	90	ASP
6	H	86	ASP
6	H	136	LYS
10	L	46	VAL
1	A	248	PRO
1	A	400	PRO
1	A	958	VAL
2	B	346	GLU
2	B	468	GLU
2	B	647	GLY
5	F	73	ALA
1	A	568	PRO
4	E	51	GLY

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Mol	Chain	Res	Type
1	A	52	GLY
6	H	82	PRO
6	H	107	VAL
4	E	89	GLY
7	I	52	ILE
1	A	308	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1225/1520 (81%)	1056 (86%)	169 (14%)	4	21
2	B	967/1061 (91%)	850 (88%)	117 (12%)	6	28
3	C	234/274 (85%)	207 (88%)	27 (12%)	7	30
4	E	196/197 (100%)	172 (88%)	24 (12%)	6	27
5	F	75/137 (55%)	67 (89%)	8 (11%)	8	34
6	H	117/128 (91%)	94 (80%)	23 (20%)	1	8
7	I	113/116 (97%)	99 (88%)	14 (12%)	6	27
8	J	60/65 (92%)	52 (87%)	8 (13%)	5	23
9	K	99/102 (97%)	86 (87%)	13 (13%)	5	24
10	L	40/57 (70%)	29 (72%)	11 (28%)	0	1
All	All	3126/3657 (86%)	2712 (87%)	414 (13%)	5	23

All (414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	22	PHE
1	A	41	MET
1	A	43	GLU
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	63	ARG
1	A	65	LEU
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	86	LEU
1	A	93	VAL
1	A	96	ILE
1	A	110	CYS
1	A	113	LEU
1	A	126	LEU
1	A	133	LYS
1	A	143	LYS
1	A	147	VAL
1	A	174	ILE
1	A	179	LEU
1	A	218	ASP
1	A	219	PHE
1	A	225	ASN
1	A	247	ARG
1	A	252	PHE
1	A	253	ASN
1	A	270	LEU
1	A	271	LYS
1	A	276	LEU
1	A	282	ASN
1	A	299	HIS
1	A	302	THR
1	A	303	TYR
1	A	307	ASP
1	A	308	ILE
1	A	317	LYS
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	368	LYS

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Mol	Chain	Res	Type
1	A	398	GLU
1	A	403	LYS
1	A	407	ARG
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	518	LYS
1	A	527	THR
1	A	532	ARG
1	A	538	ASP
1	A	544	ASP
1	A	566	ILE
1	A	588	LEU
1	A	590	ARG
1	A	593	GLU
1	A	595	THR
1	A	598	LEU
1	A	603	ASN
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	636	GLU
1	A	640	GLN
1	A	666	ILE
1	A	672	ASP
1	A	682	THR
1	A	688	LYS
1	A	689	LYS
1	A	691	LEU
1	A	695	LYS

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	705	LYS
1	A	708	MET
1	A	716	ASP
1	A	722	LEU
1	A	731	ARG
1	A	740	LEU
1	A	756	ILE
1	A	762	SER
1	A	771	GLU
1	A	773	LYS
1	A	774	ARG
1	A	821	ARG
1	A	830	LYS
1	A	845	LEU
1	A	865	GLN
1	A	867	ILE
1	A	878	ILE
1	A	894	GLU
1	A	905	ASP
1	A	908	LEU
1	A	912	LEU
1	A	926	GLN
1	A	938	LYS
1	A	940	ARG
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE
1	A	988	LEU
1	A	1005	GLU
1	A	1025	ARG
1	A	1029	ARG
1	A	1048	ASN
1	A	1050	GLU
1	A	1067	LEU
1	A	1077	THR
1	A	1084	PHE
1	A	1110	ASN
1	A	1121	GLU
1	A	1138	ILE
1	A	1161	THR
1	A	1170	ILE

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Mol	Chain	Res	Type
1	A	1172	LEU
1	A	1195	LEU
1	A	1221	LYS
1	A	1223	ASP
1	A	1231	ASP
1	A	1233	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1264	GLU
1	A	1266	THR
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1293	SER
1	A	1297	GLU
1	A	1307	GLU
1	A	1309	ASP
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1345	ARG
1	A	1350	LYS
1	A	1351	GLU
1	A	1361	SER
1	A	1366	ARG
1	A	1378	GLN
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1425	SER
1	A	1426	GLU
1	A	1433	MET
1	A	1442	ASP
2	B	25	ILE
2	B	28	GLU
2	B	46	GLN
2	B	61	ASP
2	B	63	ILE
2	B	68	THR

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Mol	Chain	Res	Type
2	B	89	GLU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	105	SER
2	B	134	LYS
2	B	135	ARG
2	B	175	ARG
2	B	178	ASN
2	B	194	GLU
2	B	199	MET
2	B	222	ILE
2	B	223	VAL
2	B	232	SER
2	B	234	ILE
2	B	245	GLU
2	B	250	PHE
2	B	254	LEU
2	B	257	LYS
2	B	262	GLU
2	B	267	ARG
2	B	276	ILE
2	B	277	LYS
2	B	285	ILE
2	B	323	VAL
2	B	325	GLN
2	B	333	PHE
2	B	357	GLN
2	B	365	THR
2	B	367	LEU
2	B	376	PHE
2	B	393	LYS
2	B	398	ARG
2	B	404	LYS
2	B	425	THR
2	B	437	GLU
2	B	458	LYS
2	B	468	GLU
2	B	469	GLN
2	B	471	LYS
2	B	482	VAL
2	B	485	ARG

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Mol	Chain	Res	Type
2	B	487	THR
2	B	526	GLU
2	B	531	GLN
2	B	537	LYS
2	B	547	VAL
2	B	554	ILE
2	B	579	ARG
2	B	591	ARG
2	B	598	GLU
2	B	612	GLU
2	B	645	SER
2	B	649	LYS
2	B	653	VAL
2	B	658	ILE
2	B	687	GLU
2	B	690	VAL
2	B	708	GLU
2	B	710	LEU
2	B	731	VAL
2	B	766	ARG
2	B	776	GLN
2	B	780	VAL
2	B	786	ASN
2	B	788	ARG
2	B	790	ASP
2	B	791	THR
2	B	815	ARG
2	B	864	LYS
2	B	865	LYS
2	B	866	TYR
2	B	868	MET
2	B	875	GLU
2	B	879	ARG
2	B	880	THR
2	B	886	LYS
2	B	934	LYS
2	B	941	LEU
2	B	948	ILE
2	B	953	LEU
2	B	955	THR
2	B	963	PHE
2	B	983	ARG

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Mol	Chain	Res	Type
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1022	THR
2	B	1065	GLN
2	B	1066	SER
2	B	1077	THR
2	B	1097	HIS
2	B	1099	VAL
2	B	1101	ASP
2	B	1103	ILE
2	B	1111	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1176	ASN
2	B	1178	ASN
2	B	1189	ILE
2	B	1194	ILE
2	B	1195	HIS
2	B	1196	ILE
2	B	1202	LEU
2	B	1210	MET
2	B	1216	LEU
2	B	1222	ARG
3	C	3	GLU
3	C	14	SER
3	C	21	ILE
3	C	27	LEU
3	C	37	MET
3	C	43	THR
3	C	48	SER
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	106	GLU
3	C	112	ASN
3	C	124	LEU
3	C	127	ARG
3	C	136	ASP

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Mol	Chain	Res	Type
3	C	137	LYS
3	C	140	ASN
3	C	151	GLN
3	C	156	THR
3	C	158	VAL
3	C	199	LYS
3	C	215	GLU
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	263	THR
3	C	264	GLN
4	E	2	ASP
4	E	3	GLN
4	E	7	ARG
4	E	52	ARG
4	E	54	GLN
4	E	65	THR
4	E	75	MET
4	E	78	LEU
4	E	84	ASP
4	E	92	THR
4	E	95	THR
4	E	100	ILE
4	E	116	ILE
4	E	122	LYS
4	E	127	ILE
4	E	144	ILE
4	E	156	LEU
4	E	157	SER
4	E	159	ASP
4	E	162	ARG
4	E	169	ARG
4	E	175	LEU
4	E	191	LYS
4	E	202	SER
5	F	76	LYS
5	F	82	THR
5	F	93	ILE
5	F	99	LEU
5	F	111	LEU
5	F	118	LEU

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Mol	Chain	Res	Type
5	F	124	GLU
5	F	128	LYS
6	H	2	SER
6	H	8	ASP
6	H	15	VAL
6	H	22	LYS
6	H	24	CYS
6	H	26	ILE
6	H	33	GLN
6	H	34	ASP
6	H	35	GLN
6	H	44	VAL
6	H	52	GLN
6	H	56	THR
6	H	63	LEU
6	H	83	GLN
6	H	86	ASP
6	H	87	ARG
6	H	100	THR
6	H	107	VAL
6	H	109	LYS
6	H	110	ASP
6	H	111	LEU
6	H	130	ARG
6	H	136	LYS
7	I	17	ARG
7	I	30	ARG
7	I	35	VAL
7	I	52	ILE
7	I	61	ASP
7	I	77	LYS
7	I	83	ASN
7	I	84	VAL
7	I	88	SER
7	I	90	GLN
7	I	97	MET
7	I	111	THR
7	I	116	ASN
7	I	119	THR
8	J	7	CYS
8	J	22	LEU
8	J	31	ASP

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Mol	Chain	Res	Type
8	J	48	ARG
8	J	56	LEU
8	J	58	GLU
8	J	59	LYS
8	J	62	ARG
9	K	6	ARG
9	K	20	LYS
9	K	25	THR
9	K	31	VAL
9	K	41	THR
9	K	42	LEU
9	K	51	LEU
9	K	63	VAL
9	K	77	THR
9	K	81	TYR
9	K	95	ILE
9	K	101	LEU
9	K	114	LEU
10	L	27	LEU
10	L	35	SER
10	L	47	ARG
10	L	50	ASP
10	L	51	CYS
10	L	53	HIS
10	L	55	ILE
10	L	58	LYS
10	L	61	THR
10	L	65	VAL
10	L	66	GLN

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	18	GLN
1	A	54	ASN
1	A	68	GLN
1	A	92	HIS
1	A	118	HIS
1	A	171	GLN
1	A	225	ASN
1	A	256	GLN
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	339	ASN
1	A	503	GLN
1	A	517	ASN
1	A	611	GLN
1	A	626	ASN
1	A	648	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	935	GLN
1	A	1040	GLN
1	A	1048	ASN
1	A	1052	GLN
1	A	1130	GLN
1	A	1140	HIS
1	A	1171	GLN
1	A	1211	GLN
1	A	1364	ASN
2	B	46	GLN
2	B	121	ASN
2	B	215	GLN
2	B	325	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	590	HIS
2	B	657	HIS
2	B	744	HIS
2	B	822	ASN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1025	HIS
2	B	1074	ASN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN

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Mol	Chain	Res	Type
2	B	1177	HIS
2	B	1178	ASN
2	B	1179	GLN
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
4	E	5	ASN
5	F	100	GLN
6	H	11	GLN
7	I	12	ASN
9	K	65	HIS
9	K	89	ASN

### 5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	10	G

There are no RNA pucker outliers to report.

## 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	1405/1733 (81%)	0.05	77 (5%)	29	16	52, 98, 181, 233	0
2	B	1114/1224 (91%)	-0.08	29 (2%)	59	45	53, 88, 148, 200	0
3	C	266/318 (83%)	-0.25	2 (0%)	87	80	62, 86, 123, 171	0
4	E	214/215 (99%)	0.11	9 (4%)	40	26	72, 128, 183, 201	0
5	F	85/155 (54%)	-0.20	0	100	100	73, 100, 144, 162	0
6	H	133/146 (91%)	0.17	8 (6%)	25	14	94, 138, 168, 181	0
7	I	119/122 (97%)	-0.22	2 (1%)	73	60	68, 101, 140, 152	0
8	J	65/70 (92%)	-0.35	0	100	100	57, 77, 111, 127	0
9	K	114/120 (95%)	-0.26	0	100	100	61, 89, 116, 131	0
10	L	46/70 (65%)	-0.07	1 (2%)	65	50	80, 124, 153, 164	0
11	R	9/9 (100%)	-0.54	0	100	100	79, 103, 145, 148	0
12	T	13/29 (44%)	-0.22	0	100	100	85, 110, 168, 175	0
All	All	3583/4211 (85%)	-0.04	128 (3%)	46	31	52, 96, 167, 233	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	10.3
1	A	1082	ASN	6.8
1	A	161	LEU	6.5
2	B	883	LEU	6.2
6	H	85	GLY	6.1
1	A	318	SER	6.0
2	B	1224	PHE	5.7
1	A	255	SER	5.7
1	A	144	THR	5.6
1	A	317	LYS	5.4
1	A	182	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	5.3
1	A	1087	ALA	5.2
1	A	319	GLY	5.2
4	E	93	MET	5.2
6	H	86	ASP	4.9
1	A	49	LYS	4.9
1	A	141	LEU	4.8
1	A	1091	SER	4.7
1	A	250	ILE	4.6
2	B	136	THR	4.6
1	A	66	LYS	4.6
1	A	153	PRO	4.6
2	B	645	SER	4.5
1	A	1083	THR	4.4
2	B	1223	ASP	4.3
1	A	152	VAL	4.2
1	A	44	THR	4.2
1	A	183	GLY	4.2
1	A	1090	ALA	4.2
1	A	254	GLU	4.1
1	A	69	THR	4.0
1	A	1085	HIS	4.0
2	B	1222	ARG	4.0
1	A	168	GLY	4.0
2	B	647	GLY	3.9
1	A	1086	PHE	3.8
2	B	474	SER	3.7
10	L	27	LEU	3.7
1	A	199	LEU	3.6
1	A	174	ILE	3.6
4	E	2	ASP	3.5
1	A	1088	GLY	3.5
1	A	114	LEU	3.5
1	A	45	GLN	3.5
1	A	176	LYS	3.4
4	E	110	PHE	3.4
2	B	882	THR	3.4
1	A	140	THR	3.4
1	A	154	SER	3.4
1	A	175	ARG	3.4
1	A	145	LYS	3.3
1	A	430	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	122	MET	3.1
1	A	316	GLN	3.1
2	B	865	LYS	3.1
1	A	1254	ALA	3.1
1	A	115	LEU	3.0
1	A	103	CYS	3.0
1	A	139	TRP	3.0
1	A	147	VAL	2.9
1	A	171	GLN	2.9
1	A	1092	LYS	2.8
6	H	108	SER	2.8
1	A	283	GLY	2.8
1	A	137	ALA	2.8
1	A	124	GLN	2.8
1	A	1255	GLU	2.8
2	B	477	ALA	2.8
2	B	709	ASP	2.7
1	A	1256	GLU	2.7
4	E	106	GLN	2.7
2	B	866	TYR	2.7
2	B	250	PHE	2.7
1	A	186	LYS	2.7
2	B	867	GLY	2.7
4	E	122	LYS	2.6
1	A	1123	GLY	2.6
1	A	148	CYS	2.6
6	H	130	ARG	2.6
1	A	201	VAL	2.5
2	B	708	GLU	2.5
1	A	170	THR	2.5
4	E	118	PRO	2.5
2	B	646	LEU	2.5
7	I	105	SER	2.5
4	E	89	GLY	2.5
2	B	432	MET	2.4
1	A	1089	VAL	2.4
6	H	84	ALA	2.4
2	B	935	ARG	2.4
6	H	132	LEU	2.4
4	E	49	SER	2.3
1	A	1002	GLY	2.3
1	A	200	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1173	HIS	2.3
2	B	135	ARG	2.3
2	B	429	PHE	2.3
1	A	125	ALA	2.3
1	A	1390	ASN	2.3
7	I	104	LEU	2.3
1	A	173	THR	2.3
2	B	106	ASP	2.2
4	E	70	SER	2.2
6	H	83	GLN	2.2
1	A	121	LEU	2.2
1	A	143	LYS	2.2
1	A	146	MET	2.2
2	B	138	GLU	2.2
3	C	4	GLU	2.1
1	A	1084	PHE	2.1
1	A	1236	LEU	2.1
6	H	107	VAL	2.1
2	B	1221	SER	2.1
1	A	185	TRP	2.1
3	C	213	PRO	2.1
1	A	311	GLN	2.1
1	A	1220	PHE	2.1
2	B	869	SER	2.1
2	B	887	HIS	2.1
1	A	177	ASP	2.1
2	B	167	ILE	2.1
2	B	139	ALA	2.1
1	A	118	HIS	2.0
1	A	1108	ALA	2.1
1	A	162	VAL	2.0
1	A	425	GLN	2.0
2	B	868	MET	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, 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
13	ZN	B	1307	1/1	0.98	0.13	-0.33	144,144,144,144	0
13	ZN	I	203	1/1	0.98	0.12	-0.69	104,104,104,104	0
13	ZN	A	1735	1/1	0.98	0.13	-0.91	128,128,128,128	0
13	ZN	L	105	1/1	0.99	0.09	-1.03	117,117,117,117	0
13	ZN	C	319	1/1	0.97	0.10	-1.15	88,88,88,88	0
13	ZN	J	101	1/1	1.00	0.19	-1.24	71,71,71,71	0
13	ZN	A	1734	1/1	0.93	0.13	-1.24	230,230,230,230	0
13	ZN	I	204	1/1	1.00	0.07	-1.55	78,78,78,78	0
14	MG	A	2001	1/1	0.98	0.13	-	45,45,45,45	0

## 6.5 Other polymers

There are no such residues in this entry.