



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

PDB ID : 3S1Q  
Title : RNA Polymerase II Initiation Complex with a 5-nt 3'-deoxy RNA soaked with ATP  
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.  
Deposited on : 2011-05-16  
Resolution : 3.30 Å(reported)

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

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

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

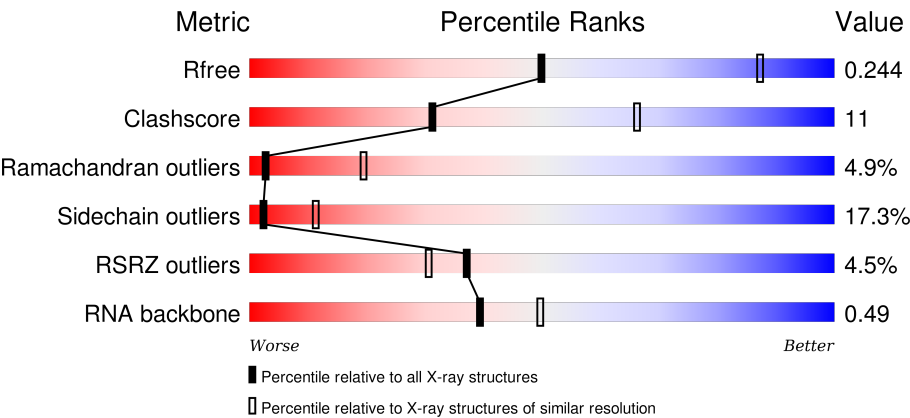
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



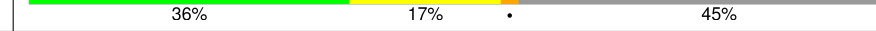



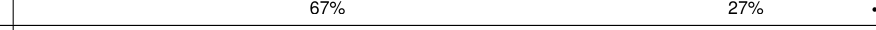

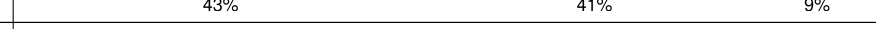

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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>5%</div><div><div></div><div>50%</div><div>25%</div><div>5%</div><div>19%</div></div><div>5%</div></div>
2	B	1224	<div><div>4%</div><div><div></div><div>57%</div><div>28%</div><div>5%</div><div>9%</div></div><div>4%</div></div>
3	C	318	<div><div></div><div><div></div><div>52%</div><div>25%</div><div>6%</div><div>16%</div></div><div></div></div>
4	E	215	<div><div>2%</div><div><div></div><div>69%</div><div>28%</div><div></div></div><div>2%</div></div>

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

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 28703 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\*GP\*AP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			109	50	25	30	4			

- 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			

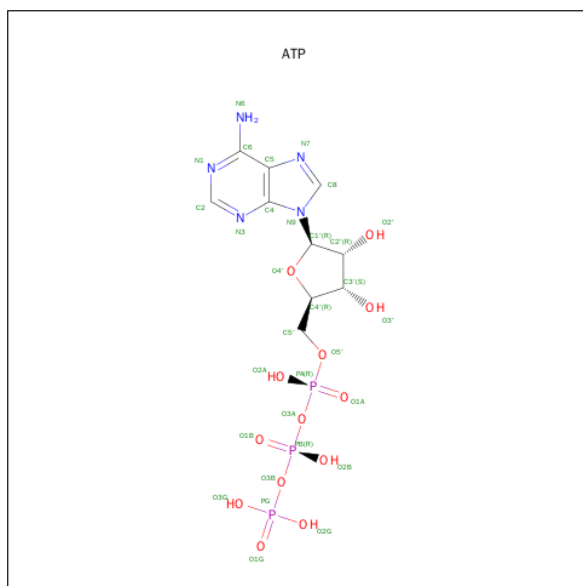
- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Mg	0	0
			2	2		

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

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

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

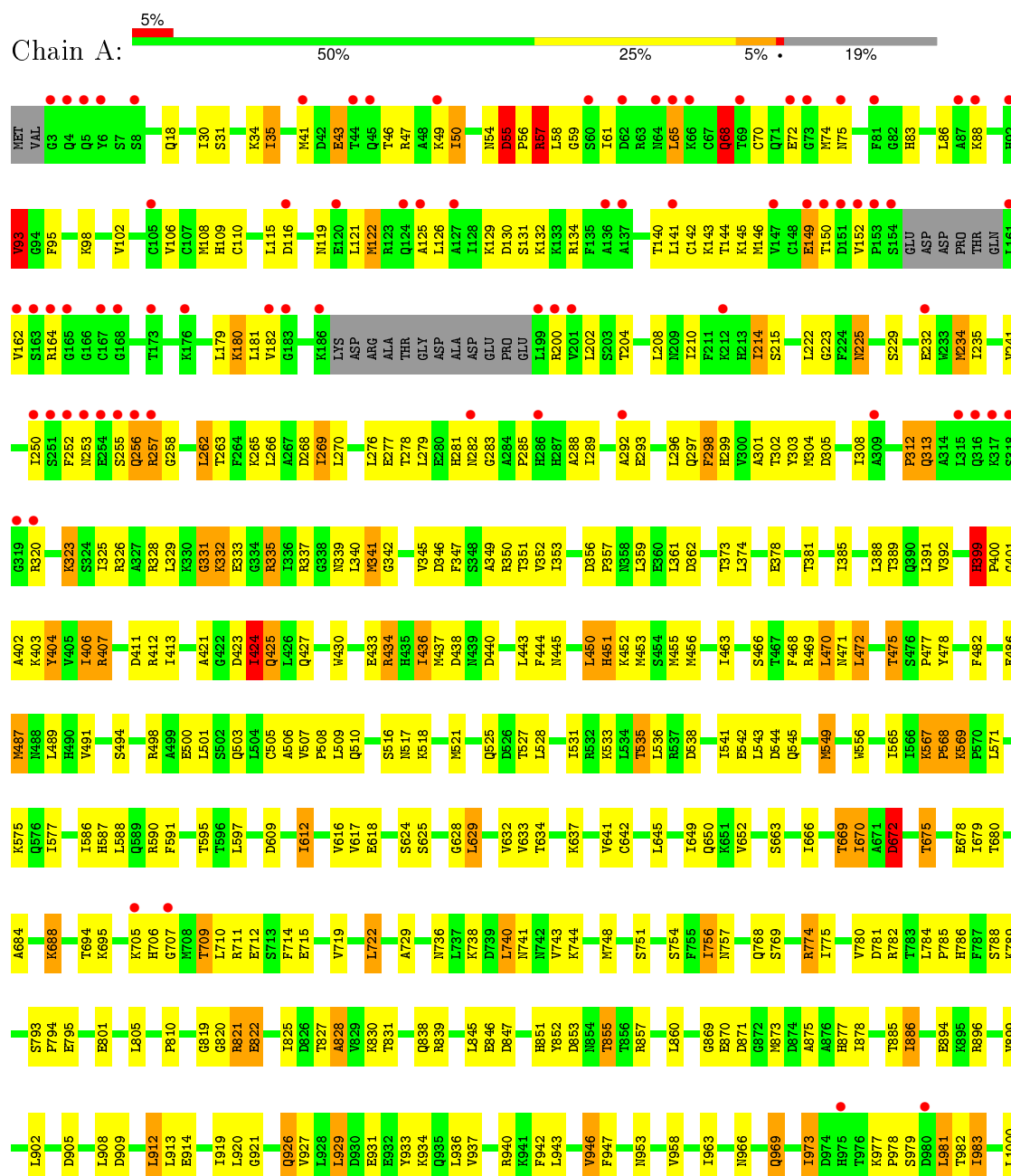


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

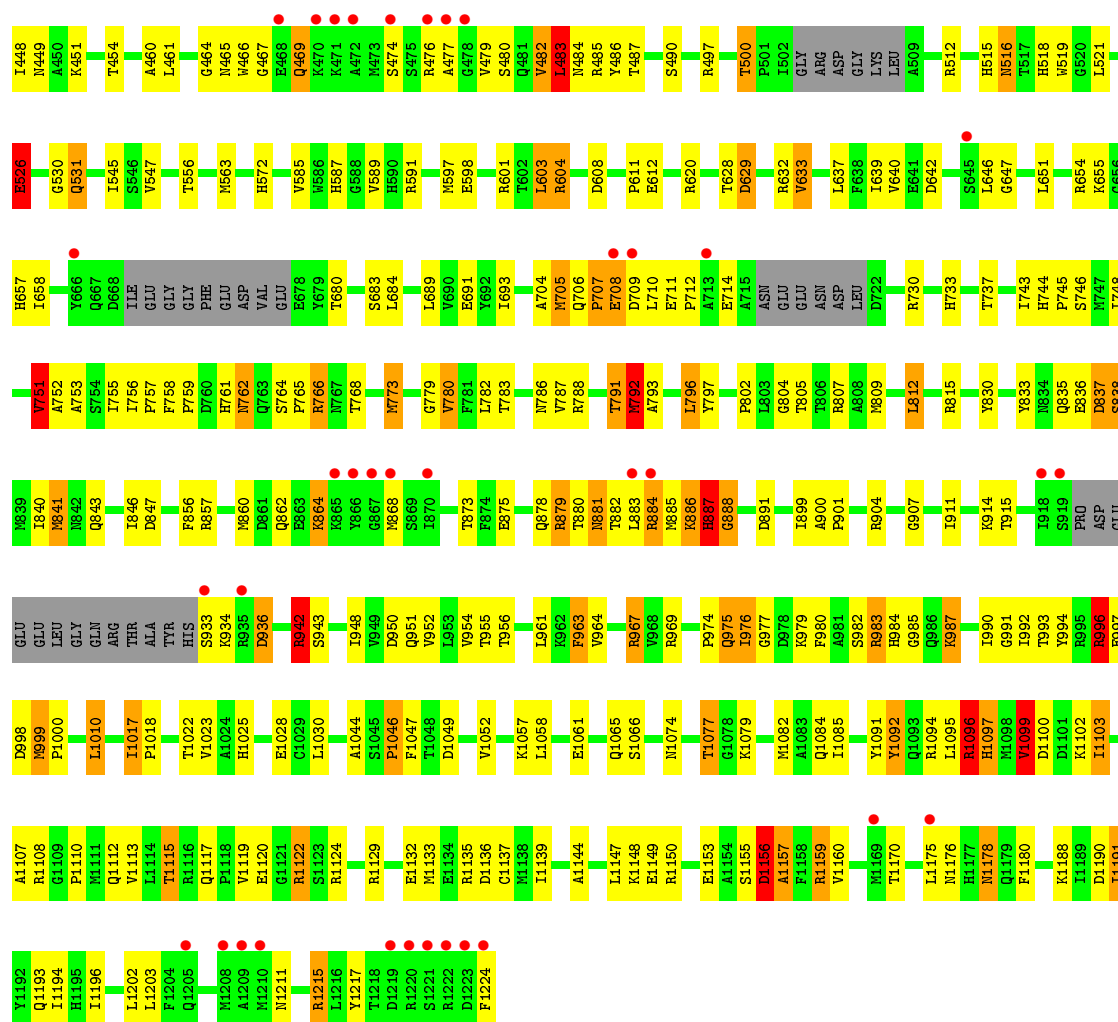
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





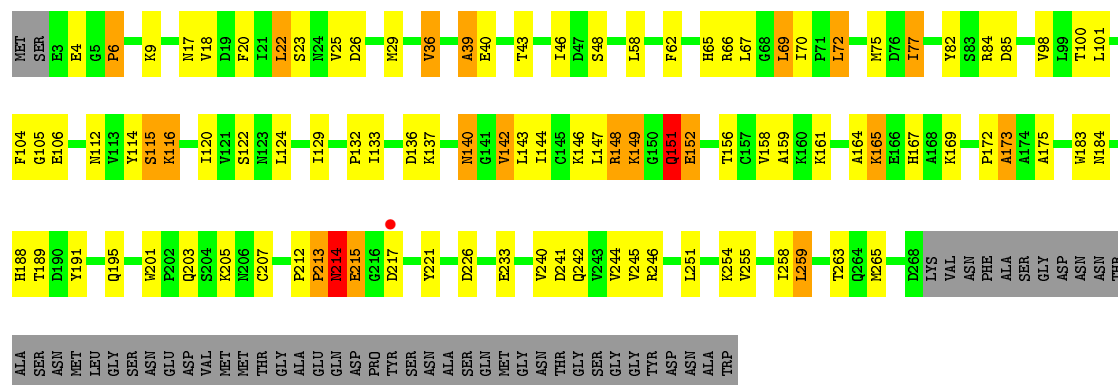
K345	G247	SER	THR	MET
E346	S248	GLU	GLU	SER
K347	R249	SER	ASP	ASP
	F250	GLY	ASP	LEU
D354		GLY	ASN	ALA
	L254	V165	ILE	ASN
Q357	Q255	F166	SER	SER
K358	V256	I167	ARG	GLU
E359	R257	G168	LYS	LYS
			TYR	TYR
H363	G260	P171	E89	
I364	R261	I172	I90	ASP
I365	E262	M173	S91	GLU
Q366		L174		ASP
L367	S265	R175	K94	PRQ
E368	A266	G179	M101	TYR
G369	R267	Y180	V102	GLY
F370	T268	L181		PHE
E371	I269		L112	GLU
			V113	D20
F376	T272	T185	P114	
	L273			T26
I382	P274	L189	R120	A27
K383	V275		M121	E28
R384	I276	K193	L122	D29
L385	R277	E194	T123	
L386	Q278	C195	Y124	S35
		P196	S125	
D396	P281	F197		F38
D397		D198	R39	R39
R398		M199	E40	E40
	T284		K41	K41
R405	T292	I205	K133	G42
	P293	L206	L143	L43
L408	D294	G207	K134	V44
G295	D295	S208	R135	V44
G410	E296		T136	S45
P411		V211	Y137	Q46
L416	L311	L212	E138	Q47
F417	K312	I213	I139	L48
K418	K313	A214	I140	Q53
	L314	Q215	D141	F54
	K315	E216	VAL	
I428		R217	PRO	T58
F429	F322	S218	GLY	
			ARG	I63
Q433	Q325	E227	GLU	
			LEU	I63
V436	F333	A230	LYS	D66
E437	T334	P231	TYR	S67
GLU	G335	S232	GLU	T68
ALA	ARG	P233	LEU	L69
HIS	ARG	T234	ILE	I70
ASP	GLY	S235	ALA	LEU
PHE	THR	R236	GLN	GLU
ASN	ALA	V237	GLU	LEU
MET	LEU		SER	ALA
	GLY	L244	GLU	GLU
L446	T15	E245	HIS	HIS
L447	V15	E246	ASP	THR





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

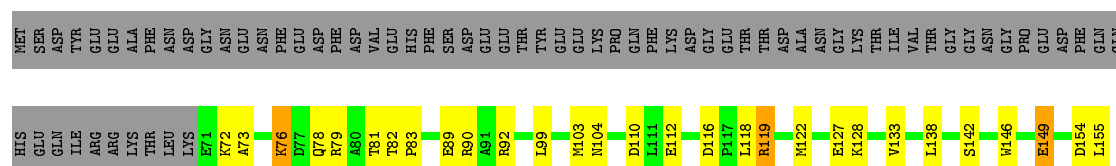
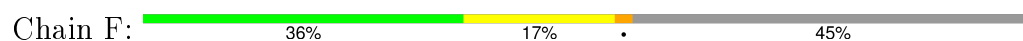
Chain C: 52% 25% 6% 16%



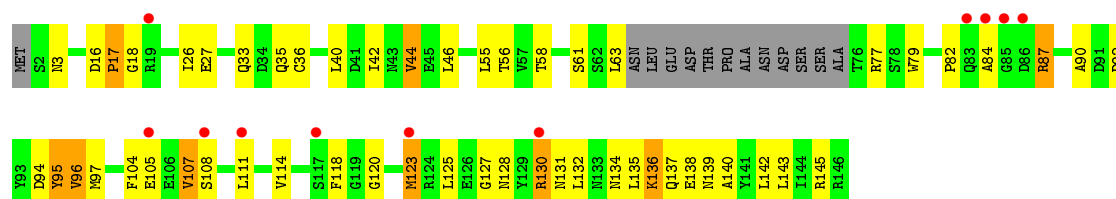
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 2% 69% 28%

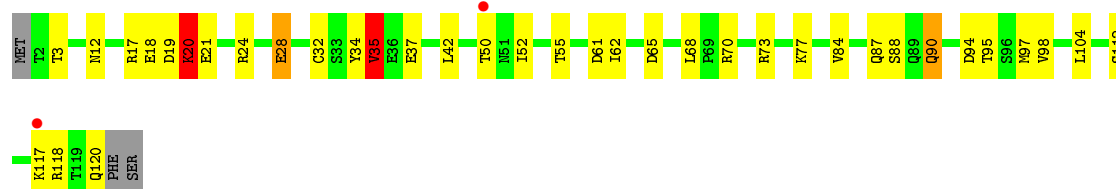
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



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

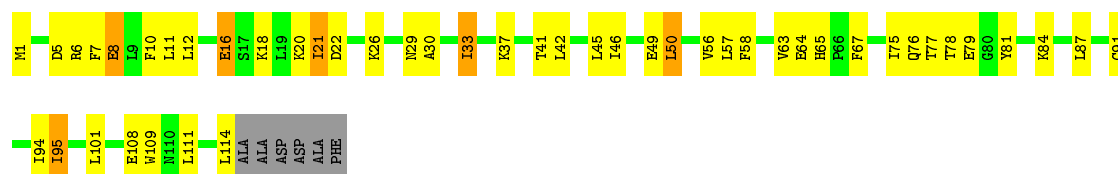


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

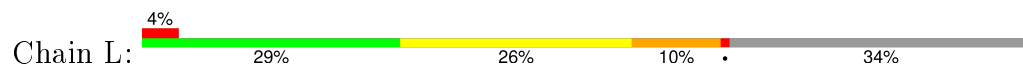


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11





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



- Molecule 11: RNA (5'-R(\*AP\*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, $\alpha$ , $\beta$ , $\gamma$	161.94Å 220.53Å 193.72Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	29.67 – 3.30 29.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.67-3.30) 99.3 (29.67-3.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.31Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.176 , 0.229 0.192 , 0.244	Depositor DCC
$R_{free}$ test set	4989 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 110.9	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	0 of 99956 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, ATP

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	0.51	0/11241	0.83	6/15199 (0.0%)
2	B	0.54	0/9033	0.83	3/12181 (0.0%)
3	C	0.49	0/2133	0.84	1/2891 (0.0%)
4	E	0.46	0/1788	0.72	0/2406
5	F	0.49	0/700	0.74	0/945
6	H	0.49	0/1086	0.82	0/1470
7	I	0.50	0/989	0.81	0/1331
8	J	0.59	0/541	0.93	0/727
9	K	0.46	0/937	0.74	0/1265
10	L	0.58	0/365	1.05	0/485
11	R	0.93	0/123	1.42	0/191
12	T	1.14	0/290	2.13	17/444 (3.8%)
All	All	0.53	0/29226	0.85	27/39535 (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	16	DC	P-O3'-C3'	10.52	132.32	119.70
12	T	25	DC	O4'-C1'-N1	9.54	114.68	108.00
12	T	23	DC	O4'-C1'-N1	8.20	113.74	108.00
12	T	22	DT	C4'-C3'-C2'	-8.13	95.78	103.10
12	T	24	DT	O4'-C1'-N1	8.12	113.69	108.00
12	T	18	DA	O4'-C4'-C3'	-7.73	101.36	106.00
12	T	26	DG	O4'-C1'-N9	7.11	112.97	108.00
3	C	172	PRO	C-N-CA	6.83	138.77	121.70
12	T	20	DC	O4'-C1'-N1	6.58	112.60	108.00
12	T	27	DA	P-O3'-C3'	6.43	127.41	119.70
2	B	628	THR	C-N-CA	6.19	137.17	121.70
1	A	451	HIS	N-CA-CB	-5.75	100.24	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	C4-C5-C7	5.66	122.39	119.00
1	A	1123	GLY	C-N-CA	5.63	135.78	121.70
1	A	399	HIS	N-CA-CB	5.58	120.65	110.60
12	T	19	DT	O4'-C4'-C3'	-5.40	102.34	104.50
1	A	1082	ASN	C-N-CA	5.35	135.07	121.70
2	B	140	ILE	C-N-CA	5.31	134.97	121.70
12	T	24	DT	C6-C5-C7	-5.20	119.78	122.90
1	A	1093	LYS	C-N-CA	5.19	134.67	121.70
2	B	887	HIS	C-N-CA	5.17	133.16	122.30
12	T	22	DT	C6-C5-C7	-5.12	119.83	122.90
12	T	25	DC	P-O3'-C3'	5.11	125.83	119.70
12	T	22	DT	P-O3'-C3'	5.07	125.78	119.70
12	T	26	DG	C4'-C3'-C2'	5.07	107.66	103.10
1	A	1083	THR	C-N-CA	5.06	134.35	121.70
12	T	24	DT	C4-C5-C7	5.02	122.01	119.00

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	11043	0	11133	280	0
2	B	8861	0	8884	215	0
3	C	2095	0	2051	56	0
4	E	1752	0	1776	36	0
5	F	688	0	707	9	0
6	H	1068	0	1040	20	0
7	I	971	0	927	11	0
8	J	532	0	542	23	0
9	K	919	0	929	27	0
10	L	363	0	386	14	0
11	R	109	0	55	2	0
12	T	261	0	148	0	0
13	A	2	0	0	0	0
14	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	31	0	12	5	0
All	All	28703	0	28590	619	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 11.

All (619) 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)
15:A:1736:ATP:H8	15:A:1736:ATP:H5'1	1.25	1.01
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.45	0.99
1:A:855:THR:HG21	1:A:857:ARG:HE	1.37	0.88
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.55	0.87
1:A:525:GLN:HB2	2:B:835:GLN:HE21	1.43	0.84
15:A:1736:ATP:C8	15:A:1736:ATP:H5'1	2.13	0.83
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.41	0.83
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.58	0.83
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.62	0.81
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.60	0.81
1:A:869:GLY:O	4:E:204:THR:HG21	1.83	0.80
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.64	0.79
1:A:741:ASN:HD22	1:A:744:LYS:H	1.32	0.78
1:A:421:ALA:HA	1:A:424:ILE:HD11	1.68	0.75
2:B:797:TYR:O	8:J:1:MET:HG2	1.87	0.75
10:L:32:ALA:HB3	10:L:55:ILE:HG13	1.67	0.75
1:A:1004:ASN:HD21	1:A:1007:ILE:HD12	1.52	0.74
2:B:232:SER:HB3	2:B:261:ARG:HH22	1.52	0.73
2:B:744:HIS:CD2	2:B:746:SER:OG	2.41	0.73
1:A:756:ILE:HD12	1:A:756:ILE:H	1.53	0.73
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.69	0.73
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.19	0.72
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.72	0.71
2:B:244:LEU:HD12	2:B:250:PHE:HB2	1.73	0.71
2:B:516:ASN:H	2:B:516:ASN:HD22	1.39	0.70
2:B:54:PHE:HA	2:B:58:THR:HB	1.72	0.70
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG11	1:A:214:ILE:HD12	1.73	0.70
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.72	0.70
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.73	0.69
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.73	0.69
3:C:214:ASN:HB3	3:C:217:ASP:HB2	1.73	0.69
1:A:469:ARG:NH2	2:B:991:GLY:O	2.27	0.68
2:B:38:PHE:HA	2:B:42:GLY:H	1.59	0.67
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.74	0.67
7:I:28:GLU:HB3	7:I:35:VAL:HG13	1.76	0.67
2:B:38:PHE:H	2:B:41:LYS:HB2	1.60	0.67
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.60	0.67
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.10	0.66
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.76	0.66
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.77	0.66
2:B:887:HIS:HA	2:B:888:GLY:O	1.96	0.65
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.43	0.65
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.78	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.77	0.65
1:A:709:THR:HB	1:A:712:GLU:H	1.61	0.65
2:B:63:ILE:O	2:B:67:SER:HB3	1.97	0.65
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.78	0.65
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.77	0.65
2:B:363:HIS:O	2:B:364:ILE:HB	1.96	0.65
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.78	0.64
1:A:399:HIS:O	1:A:401:GLY:N	2.30	0.64
1:A:466:SER:HB3	2:B:1103:ILE:HD13	1.79	0.64
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.79	0.64
2:B:1180:PHE:HB3	2:B:1191:ILE:HG21	1.79	0.64
2:B:843:GLN:HB2	2:B:993:THR:HB	1.79	0.64
1:A:57:ARG:HB3	1:A:68:GLN:H	1.63	0.64
8:J:28:ASP:HB3	8:J:30:LEU:HD12	1.79	0.63
1:A:378:GLU:OE2	1:A:434:ARG:HD3	1.97	0.63
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.80	0.63
2:B:762:ASN:HD21	2:B:1022:THR:HA	1.62	0.63
1:A:827:THR:OG1	1:A:1083:THR:HG21	1.99	0.63
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.81	0.63
1:A:140:THR:HA	1:A:143:LYS:HE3	1.80	0.63
1:A:855:THR:CG2	1:A:857:ARG:HE	2.10	0.63
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.13	0.63
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.81	0.63
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:HB2	1:A:675:THR:HB	1.81	0.62
2:B:744:HIS:HD2	2:B:746:SER:H	1.47	0.62
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.82	0.62
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.81	0.62
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.80	0.62
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.80	0.62
1:A:853:ASP:OD2	1:A:855:THR:HG22	2.00	0.62
1:A:1154:TYR:CE2	1:A:1156:PRO:HG3	2.34	0.62
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.64	0.62
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.82	0.62
1:A:1083:THR:N	1:A:1084:PHE:O	2.33	0.61
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.65	0.61
1:A:349:ALA:HB3	1:A:489:LEU:HB3	1.82	0.61
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.41	0.61
1:A:567:LYS:HB3	6:H:96:VAL:H	1.64	0.61
1:A:1083:THR:HG23	1:A:1084:PHE:HB3	1.82	0.60
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.83	0.60
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.36	0.60
2:B:976:ILE:O	2:B:990:ILE:HB	2.00	0.60
2:B:887:HIS:HA	2:B:888:GLY:C	2.21	0.60
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.84	0.60
1:A:278:THR:O	1:A:282:ASN:HB3	2.00	0.60
1:A:885:THR:O	1:A:940:ARG:HD3	2.01	0.60
5:F:90:ARG:HD2	5:F:155:LEU:HD13	1.84	0.60
2:B:976:ILE:HG23	2:B:977:GLY:H	1.67	0.60
2:B:873:THR:O	2:B:914:LYS:HA	2.01	0.60
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.84	0.60
2:B:486:TYR:CZ	2:B:1096:ARG:HG2	2.36	0.59
1:A:388:LEU:O	1:A:392:VAL:HG23	2.02	0.59
1:A:304:MET:HG2	1:A:325:ILE:HD12	1.83	0.59
9:K:21:ILE:HG23	9:K:33:ILE:HG12	1.84	0.59
2:B:654:ARG:H	2:B:657:HIS:HD2	1.48	0.59
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.85	0.59
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.67	0.59
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.50	0.59
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.85	0.59
1:A:331:GLY:HA2	1:A:337:ARG:HG3	1.84	0.59
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.84	0.59
3:C:115:SER:HB3	3:C:142:VAL:H	1.67	0.59
3:C:36:VAL:HG23	9:K:41:THR:HG21	1.85	0.59
2:B:975:GLN:O	2:B:990:ILE:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:TYR:HB3	3:C:84:ARG:HG2	1.85	0.58
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.85	0.58
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.33	0.58
1:A:709:THR:HG23	7:I:94:ASP:HA	1.84	0.58
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.85	0.58
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.84	0.58
1:A:587:HIS:HD2	1:A:966:ASN:HA	1.69	0.58
1:A:830:LYS:HD3	1:A:1080:THR:HB	1.85	0.58
1:A:119:ASN:HB2	1:A:122:MET:HB2	1.83	0.58
1:A:1325:THR:HA	4:E:147:HIS:HA	1.86	0.58
1:A:1080:THR:C	1:A:1082:ASN:H	2.06	0.58
1:A:913:LEU:HD11	1:A:981:LEU:O	2.04	0.58
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.86	0.58
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.85	0.58
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.34	0.58
1:A:628:GLY:O	1:A:632:VAL:HG23	2.04	0.57
3:C:147:LEU:HD23	3:C:151:GLN:HB2	1.85	0.57
2:B:345:LYS:HA	2:B:347:LYS:H	1.69	0.57
1:A:152:VAL:HG23	1:A:162:VAL:HG23	1.85	0.57
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.69	0.57
2:B:885:MET:HA	2:B:936:ASP:HB2	1.87	0.57
2:B:516:ASN:H	2:B:516:ASN:ND2	2.02	0.57
1:A:179:LEU:HB3	1:A:297:GLN:HG2	1.87	0.57
10:L:53:HIS:HB3	10:L:55:ILE:CD1	2.35	0.57
1:A:347:PHE:H	2:B:1107:ALA:HA	1.69	0.57
1:A:1354:ASN:O	1:A:1358:SER:HB2	2.05	0.57
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.86	0.57
1:A:567:LYS:HE3	6:H:46:LEU:HB2	1.87	0.56
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.87	0.56
3:C:167:HIS:HD2	3:C:169:LYS:H	1.51	0.56
15:A:1736:ATP:H5'2	11:R:10:G:H2'	1.87	0.56
1:A:885:THR:HG23	1:A:1024:SER:HB2	1.86	0.56
2:B:950:ASP:HB3	2:B:967:ARG:HG3	1.87	0.56
1:A:1081:LEU:HD11	15:A:1736:ATP:C5	2.41	0.56
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.88	0.56
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.87	0.56
2:B:862:GLN:HB3	2:B:963:PHE:HB2	1.88	0.56
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.41	0.56
3:C:251:LEU:O	3:C:255:VAL:HG23	2.06	0.56
1:A:323:LYS:HE2	1:A:328:ARG:HE	1.70	0.56
2:B:955:THR:HG22	2:B:956:THR:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.88	0.56
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.38	0.56
10:L:55:ILE:HD13	10:L:55:ILE:H	1.69	0.56
4:E:19:VAL:O	4:E:23:VAL:HG23	2.04	0.56
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.87	0.55
1:A:1364:ASN:C	1:A:1364:ASN:HD22	2.10	0.55
2:B:915:THR:HA	2:B:936:ASP:O	2.06	0.55
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.86	0.55
1:A:1264:GLU:HA	1:A:1267:MET:HE2	1.87	0.55
2:B:879:ARG:NH1	2:B:879:ARG:HA	2.21	0.55
2:B:654:ARG:H	2:B:657:HIS:CD2	2.24	0.55
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.21	0.55
1:A:256:GLN:HG2	1:A:257:ARG:HD2	1.89	0.55
5:F:72:LYS:HB3	5:F:142:SER:HA	1.89	0.55
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.88	0.55
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.39	0.55
2:B:1074:ASN:HB3	2:B:1077:THR:HG22	1.89	0.55
1:A:831:THR:HG21	1:A:1081:LEU:HD13	1.87	0.55
4:E:10:SER:O	4:E:14:ARG:HG3	2.06	0.55
3:C:148:ARG:H	3:C:151:GLN:HG3	1.72	0.55
3:C:98:VAL:H	3:C:122:SER:HB2	1.71	0.54
3:C:105:GLY:O	3:C:149:LYS:O	2.26	0.54
1:A:1092:LYS:HB2	1:A:1096:SER:HB3	1.89	0.54
1:A:55:ASP:O	1:A:57:ARG:N	2.32	0.54
1:A:1030:ARG:O	1:A:1034:GLU:HB2	2.07	0.54
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.89	0.54
2:B:791:THR:HG22	2:B:792:MET:HE3	1.89	0.54
2:B:706:GLN:H	2:B:710:LEU:HG	1.72	0.54
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.88	0.54
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.88	0.54
2:B:787:VAL:O	2:B:787:VAL:HG12	2.08	0.54
1:A:756:ILE:CD1	1:A:756:ILE:H	2.21	0.53
2:B:1097:HIS:HB2	2:B:1102:LYS:HE3	1.90	0.53
2:B:904:ARG:HG2	2:B:948:ILE:HG12	1.90	0.53
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.89	0.53
2:B:755:ILE:HD13	2:B:809:MET:HG2	1.90	0.53
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.38	0.53
1:A:743:VAL:HG13	2:B:1018:PRO:HB3	1.91	0.53
1:A:332:LYS:O	1:A:333:GLU:HG2	2.08	0.53
2:B:237:VAL:HG22	2:B:257:LYS:HB3	1.90	0.53
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD12	1:A:296:LEU:HD21	1.90	0.53
5:F:76:LYS:HA	5:F:79:ARG:HH11	1.74	0.53
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.90	0.53
1:A:587:HIS:CD2	1:A:966:ASN:HA	2.43	0.52
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.91	0.52
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.91	0.52
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.91	0.52
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.91	0.52
1:A:518:LYS:HD2	1:A:624:SER:O	2.08	0.52
1:A:31:SER:HB2	1:A:83:HIS:HD2	1.73	0.52
4:E:94:LYS:HA	4:E:97:VAL:HG22	1.92	0.52
1:A:95:PHE:HB3	1:A:234:MET:HE3	1.92	0.52
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.90	0.52
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.92	0.52
1:A:549:MET:HB3	1:A:577:ILE:HD13	1.91	0.52
1:A:351:THR:O	1:A:486:GLU:O	2.28	0.52
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.92	0.52
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.91	0.52
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.74	0.52
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.90	0.52
2:B:597:MET:HG3	2:B:601:ARG:HH12	1.75	0.52
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.58	0.52
1:A:1035:TYR:HB3	1:A:1037:LEU:HD23	1.92	0.52
1:A:886:ILE:HG13	1:A:943:LEU:HB3	1.90	0.52
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.45	0.52
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.40	0.52
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.44	0.52
1:A:1075:PRO:O	1:A:1079:MET:HG2	2.10	0.52
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.31	0.52
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.25	0.51
3:C:175:ALA:HB3	8:J:43:ARG:HE	1.75	0.51
2:B:1115:THR:HG23	2:B:1117:GLN:HB2	1.92	0.51
2:B:70:ILE:H	2:B:429:PHE:HE1	1.57	0.51
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.92	0.51
2:B:792:MET:HE2	2:B:857:ARG:HG3	1.91	0.51
1:A:1016:THR:HB	4:E:205:SER:O	2.11	0.51
6:H:104:PHE:CE1	6:H:136:LYS:HA	2.45	0.51
1:A:341:MET:HB3	2:B:1132:GLU:HG2	1.93	0.51
2:B:563:MET:HA	2:B:589:VAL:O	2.10	0.51
2:B:766:ARG:HG2	2:B:1022:THR:HG22	1.91	0.51
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:804:GLY:O	2:B:983:ARG:NH2	2.43	0.51
1:A:225:ASN:HB3	1:A:229:SER:H	1.75	0.51
2:B:1215:ARG:HB2	2:B:1217:TYR:CE1	2.46	0.51
2:B:955:THR:HG23	10:L:54:ARG:O	2.10	0.51
2:B:857:ARG:NH2	2:B:942:ARG:HE	2.09	0.51
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.76	0.51
1:A:1035:TYR:CB	1:A:1037:LEU:HD23	2.41	0.51
1:A:820:GLY:HA3	2:B:764:SER:OG	2.11	0.51
1:A:179:LEU:HB2	1:A:180:LYS:HE2	1.92	0.51
1:A:361:LEU:HD12	1:A:471:ASN:HD22	1.75	0.51
6:H:58:THR:HB	6:H:143:LEU:HB2	1.93	0.51
1:A:406:ILE:HD11	1:A:433:GLU:HG3	1.92	0.51
1:A:528:LEU:HD23	1:A:751:SER:HA	1.93	0.50
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.46	0.50
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.94	0.50
5:F:128:LYS:HD3	5:F:149:GLU:HA	1.93	0.50
1:A:402:ALA:CB	1:A:434:ARG:HA	2.42	0.50
3:C:39:ALA:HB1	3:C:165:LYS:HB2	1.92	0.50
1:A:1284:MET:HG3	1:A:1306:LEU:CD2	2.41	0.50
4:E:66:GLU:HA	4:E:69:ILE:HD12	1.93	0.50
1:A:830:LYS:HE3	1:A:1098:VAL:HB	1.94	0.50
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.46	0.50
1:A:423:ASP:CG	1:A:424:ILE:H	2.14	0.50
3:C:98:VAL:H	3:C:122:SER:CB	2.25	0.50
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.94	0.50
8:J:8:PHE:H	8:J:49:MET:HE3	1.77	0.50
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.94	0.50
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.49
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.94	0.49
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.93	0.49
8:J:36:LEU:HD11	8:J:51:LEU:HD13	1.94	0.49
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.93	0.49
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.94	0.49
3:C:242:GLN:HG3	3:C:246:ARG:HH21	1.77	0.49
2:B:1112:GLN:HB3	2:B:1115:THR:HG22	1.94	0.49
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.93	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.49
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.77	0.49
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.27	0.49
2:B:357:GLN:HG3	2:B:368:GLU:HA	1.95	0.49
1:A:981:LEU:H	1:A:981:LEU:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:N	3:C:151:GLN:HG3	2.27	0.49
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.94	0.49
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.42	0.49
1:A:252:PHE:HD1	1:A:253:ASN:H	1.60	0.49
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.95	0.49
3:C:184:ASN:ND2	3:C:189:THR:O	2.45	0.49
9:K:63:VAL:HG23	9:K:63:VAL:O	2.13	0.49
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.94	0.49
6:H:33:GLN:HB2	6:H:36:CYS:HB3	1.95	0.49
1:A:666:ILE:HG21	2:B:1030:LEU:HD22	1.95	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.49
3:C:18:VAL:CG2	9:K:109:TRP:HZ3	2.26	0.49
1:A:781:ASP:HB2	1:A:789:LYS:HD3	1.95	0.49
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.95	0.48
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.46	0.48
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.95	0.48
1:A:456:MET:HE2	1:A:510:GLN:HB2	1.95	0.48
3:C:66:ARG:NH2	8:J:3:VAL:O	2.43	0.48
2:B:840:ILE:O	2:B:1010:LEU:HA	2.14	0.48
9:K:5:ASP:HB2	9:K:8:GLU:OE2	2.12	0.48
2:B:847:ASP:O	3:C:65:HIS:HE1	1.96	0.48
1:A:810:PRO:HB2	2:B:519:TRP:HH2	1.78	0.48
11:R:6:A:H2'	11:R:7:G:H8	1.78	0.48
1:A:942:PHE:O	1:A:946:VAL:HG12	2.13	0.48
1:A:684:ALA:O	1:A:688:LYS:HG2	2.13	0.48
1:A:567:LYS:CE	6:H:46:LEU:HB2	2.43	0.48
2:B:515:HIS:H	2:B:518:HIS:CD2	2.31	0.48
1:A:586:ILE:N	1:A:609:ASP:O	2.47	0.48
2:B:707:PRO:HG2	2:B:708:GLU:HG3	1.95	0.48
1:A:297:GLN:C	1:A:299:HIS:H	2.17	0.48
2:B:884:ARG:O	2:B:936:ASP:HB2	2.13	0.48
2:B:879:ARG:CZ	2:B:879:ARG:HA	2.43	0.48
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.96	0.48
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.94	0.48
10:L:61:THR:HB	10:L:63:ARG:H	1.78	0.48
1:A:825:ILE:CD1	2:B:512:ARG:HB3	2.44	0.48
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.28	0.48
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.48	0.48
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.95	0.48
1:A:276:LEU:HD11	1:A:292:ALA:HB1	1.96	0.48
2:B:35:SER:O	2:B:39:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:THR:HG23	2:B:490:SER:H	1.78	0.48
2:B:1110:PRO:HG2	2:B:1124:ARG:O	2.14	0.48
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.96	0.48
4:E:118:PRO:HA	4:E:121:MET:HB2	1.96	0.47
1:A:715:GLU:O	1:A:719:VAL:HG23	2.14	0.47
3:C:213:PRO:O	3:C:214:ASN:HB2	2.14	0.47
8:J:1:MET:HB2	8:J:56:LEU:HD12	1.96	0.47
1:A:709:THR:CG2	7:I:94:ASP:HA	2.43	0.47
2:B:68:THR:HA	2:B:90:ILE:O	2.14	0.47
1:A:1088:GLY:HA2	1:A:1089:VAL:HA	1.71	0.47
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.31	0.47
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.96	0.47
2:B:994:TYR:HD1	2:B:999:MET:HE3	1.80	0.47
3:C:191:TYR:HD2	3:C:201:TRP:CE2	2.32	0.47
2:B:358:LYS:HA	2:B:366:GLN:HG2	1.97	0.47
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.54	0.47
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.96	0.47
8:J:36:LEU:HD13	8:J:47:ARG:HD2	1.95	0.47
9:K:65:HIS:CD2	9:K:67:PHE:H	2.32	0.47
2:B:881:ASN:HB3	2:B:933:SER:OG	2.15	0.47
6:H:130:ARG:HB3	6:H:134:ASN:HD21	1.80	0.47
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.97	0.47
1:A:642:CYS:O	1:A:645:LEU:HB3	2.15	0.47
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.50	0.47
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.44	0.47
7:I:73:ARG:HH12	7:I:112:SER:HA	1.80	0.47
2:B:545:ILE:HG13	2:B:633:VAL:HG13	1.96	0.47
1:A:494:SER:O	1:A:498:ARG:HG3	2.14	0.47
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.80	0.47
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.97	0.46
1:A:262:LEU:HD11	1:A:325:ILE:HG12	1.97	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.56	0.46
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.96	0.46
6:H:137:GLN:C	6:H:139:ASN:H	2.19	0.46
1:A:1368:MET:O	1:A:1372:VAL:HG23	2.15	0.46
1:A:830:LYS:HG3	1:A:1098:VAL:CG1	2.37	0.46
4:E:101:GLN:HG3	4:E:102:GLU:HG3	1.96	0.46
2:B:1110:PRO:HB2	2:B:1119:VAL:HG21	1.98	0.46
2:B:563:MET:HE1	2:B:587:HIS:CB	2.45	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.98	0.46
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:50:LEU:O	9:K:56:VAL:HG11	2.15	0.46
1:A:116:ASP:HB3	1:A:164:ARG:HH12	1.80	0.46
3:C:66:ARG:HH21	8:J:4:PRO:HA	1.81	0.46
1:A:352:VAL:HB	2:B:1099:VAL:HG13	1.96	0.46
1:A:109:HIS:H	1:A:210:ILE:HD12	1.80	0.46
2:B:979:LYS:HD3	2:B:1095:LEU:HD12	1.97	0.46
1:A:780:VAL:HG12	1:A:789:LYS:HE2	1.97	0.46
2:B:408:LEU:H	2:B:411:PRO:HG2	1.79	0.46
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.98	0.46
1:A:353:ILE:HG22	1:A:468:PHE:CB	2.45	0.46
1:A:181:LEU:O	1:A:202:LEU:HB3	2.16	0.46
2:B:680:THR:O	2:B:683:SER:HB2	2.16	0.46
2:B:955:THR:HG22	2:B:956:THR:N	2.31	0.46
1:A:535:THR:HG22	1:A:575:LYS:HG2	1.98	0.46
4:E:94:LYS:O	4:E:98:ILE:HB	2.16	0.46
2:B:1120:GLU:H	2:B:1124:ARG:HH21	1.64	0.46
8:J:43:ARG:HG2	8:J:43:ARG:HH11	1.81	0.46
2:B:212:LEU:HD13	2:B:409:ALA:HA	1.98	0.46
1:A:1205:LYS:O	1:A:1207:LEU:N	2.45	0.46
1:A:695:LYS:HA	1:A:695:LYS:HD2	1.88	0.46
1:A:983:ILE:HD12	1:A:1028:THR:HG21	1.97	0.46
2:B:1058:LEU:O	2:B:1061:GLU:HB2	2.15	0.46
1:A:43:GLU:HG3	1:A:50:ILE:HG12	1.97	0.46
1:A:41:MET:HA	1:A:49:LYS:HA	1.97	0.46
1:A:1080:THR:O	1:A:1082:ASN:N	2.46	0.45
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.98	0.45
3:C:65:HIS:O	3:C:69:LEU:HD12	2.16	0.45
4:E:98:ILE:HA	4:E:101:GLN:HG2	1.97	0.45
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.29	0.45
9:K:12:LEU:HD21	9:K:18:LYS:HG2	1.98	0.45
3:C:173:ALA:O	3:C:233:GLU:O	2.34	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.52	0.45
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.97	0.45
1:A:694:THR:HA	1:A:714:PHE:HE1	1.80	0.45
1:A:1093:LYS:HG3	1:A:1359:ASP:HB2	1.98	0.45
6:H:118:PHE:HE1	6:H:123:MET:HB2	1.80	0.45
2:B:835:GLN:O	2:B:838:SER:HB2	2.17	0.45
8:J:4:PRO:O	8:J:14:VAL:HG23	2.15	0.45
1:A:131:SER:HB3	1:A:223:GLY:CA	2.45	0.45
3:C:151:GLN:H	3:C:151:GLN:HG2	1.25	0.45
1:A:947:PHE:HE2	1:A:1017:LEU:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:LEU:HG	15:A:1736:ATP:H2'	1.99	0.45
2:B:1099:VAL:O	2:B:1103:ILE:HG12	2.17	0.45
2:B:841:MET:HG2	2:B:1010:LEU:HD12	1.99	0.45
7:I:18:GLU:HG2	7:I:20:LYS:H	1.82	0.45
2:B:114:PRO:HB3	2:B:174:LEU:HD21	1.99	0.45
3:C:6:PRO:HB2	9:K:101:LEU:HD13	1.99	0.45
1:A:279:LEU:HD22	1:A:289:ILE:HA	1.98	0.45
10:L:34:CYS:SG	10:L:34:CYS:O	2.75	0.45
2:B:744:HIS:HD2	2:B:746:SER:OG	1.96	0.45
2:B:900:ALA:HA	10:L:58:LYS:HD3	1.98	0.45
3:C:255:VAL:O	3:C:258:ILE:HG22	2.16	0.45
1:A:1317:MET:HG3	4:E:142:VAL:HG21	1.99	0.45
1:A:744:LYS:O	1:A:748:MET:HG3	2.17	0.45
1:A:946:VAL:HB	4:E:201:LYS:HD2	1.98	0.45
8:J:6:ARG:HG3	8:J:13:VAL:HG13	1.99	0.45
4:E:61:GLN:HG3	4:E:105:PHE:CE2	2.51	0.45
2:B:44:VAL:HA	2:B:46:GLN:HE21	1.82	0.45
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.17	0.44
9:K:65:HIS:HD2	9:K:67:PHE:H	1.65	0.44
1:A:1318:THR:HG22	4:E:142:VAL:HG22	1.99	0.44
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.99	0.44
1:A:129:LYS:HA	1:A:134:ARG:HH21	1.82	0.44
2:B:125:SER:HB3	2:B:171:PRO:HA	1.98	0.44
8:J:24:LEU:HA	8:J:28:ASP:HB2	2.00	0.44
4:E:147:HIS:HD2	4:E:149:LEU:HB2	1.82	0.44
2:B:751:VAL:HG22	2:B:812:LEU:HD22	1.98	0.44
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.99	0.44
3:C:259:LEU:HD13	9:K:91:CYS:HB2	1.99	0.44
10:L:61:THR:HB	10:L:63:ARG:HB2	2.00	0.44
1:A:55:ASP:C	1:A:57:ARG:H	2.19	0.44
3:C:165:LYS:O	9:K:6:ARG:NH1	2.51	0.44
1:A:795:GLU:H	1:A:795:GLU:CD	2.21	0.44
8:J:53:HIS:CE1	8:J:55:ASP:HB2	2.53	0.44
1:A:711:ARG:HA	7:I:97:MET:HE1	2.00	0.44
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.52	0.44
2:B:765:PRO:O	2:B:768:THR:N	2.50	0.44
1:A:115:LEU:HD21	1:A:145:LYS:HG3	1.99	0.44
2:B:773:MET:SD	2:B:987:LYS:HG3	2.58	0.44
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.99	0.44
2:B:446:LEU:O	2:B:448:ILE:HD12	2.18	0.44
2:B:745:PRO:O	2:B:748:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:O	1:A:569:LYS:N	2.41	0.44
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.53	0.44
2:B:213:ILE:O	2:B:215:GLN:HG2	2.18	0.44
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.92	0.44
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.99	0.44
2:B:597:MET:HG3	2:B:601:ARG:NH1	2.32	0.43
2:B:757:PRO:CB	2:B:1044:ALA:HB1	2.48	0.43
2:B:637:LEU:HD12	2:B:693:ILE:HG13	2.00	0.43
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.99	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.99	0.43
1:A:98:LYS:O	1:A:102:VAL:HG23	2.18	0.43
2:B:211:VAL:CG2	2:B:483:LEU:HA	2.47	0.43
1:A:456:MET:HB2	1:A:478:TYR:OH	2.18	0.43
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	2.00	0.43
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.18	0.43
2:B:836:GLU:O	2:B:837:ASP:HB2	2.18	0.43
1:A:877:HIS:HB3	1:A:1056:SER:HA	2.00	0.43
6:H:96:VAL:HG13	6:H:143:LEU:HG	1.99	0.43
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.51	0.43
1:A:471:ASN:HD21	1:A:650:GLN:HE22	1.65	0.43
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.43
2:B:48:LEU:HD23	2:B:173:MET:SD	2.58	0.43
6:H:79:TRP:CH2	6:H:82:PRO:HD3	2.54	0.43
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.49	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.18	0.43
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.33	0.43
2:B:365:THR:HG21	2:B:370:PHE:HD1	1.83	0.43
1:A:1376:THR:HG22	1:A:1377:THR:N	2.34	0.43
9:K:30:ALA:HA	9:K:75:ILE:O	2.19	0.43
1:A:1316:VAL:O	1:A:1319:VAL:HB	2.18	0.43
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.54	0.43
4:E:20:LYS:HE3	4:E:35:VAL:HA	2.00	0.43
1:A:587:HIS:CE1	1:A:969:GLN:HE21	2.37	0.43
4:E:176:PRO:O	4:E:212:ARG:HA	2.19	0.43
2:B:640:VAL:HG22	2:B:651:LEU:HG	2.01	0.43
1:A:933:TYR:O	1:A:937:VAL:HG13	2.19	0.43
1:A:208:LEU:HG	1:A:235:ILE:HD11	2.01	0.43
1:A:852:TYR:O	5:F:81:THR:HG22	2.18	0.43
1:A:830:LYS:HD2	1:A:1094:VAL:HG23	2.01	0.43
1:A:361:LEU:HD11	1:A:521:MET:HE2	2.00	0.43
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.47	0.43
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.54	0.43
1:A:35:ILE:HG13	1:A:241:VAL:HG21	2.01	0.43
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	2.01	0.43
1:A:851:HIS:HB2	1:A:855:THR:HG22	2.01	0.43
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	2.01	0.43
6:H:40:LEU:HD21	6:H:142:LEU:HD21	2.00	0.43
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.52	0.43
1:A:754:SER:H	1:A:757:ASN:HD22	1.67	0.43
1:A:710:LEU:H	1:A:710:LEU:HD22	1.83	0.43
2:B:753:ALA:HA	2:B:756:ILE:HD12	2.01	0.42
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.01	0.42
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.54	0.42
7:I:19:ASP:HB3	7:I:24:ARG:H	1.84	0.42
9:K:79:GLU:CD	9:K:79:GLU:H	2.23	0.42
8:J:1:MET:N	8:J:56:LEU:N	2.67	0.42
2:B:956:THR:HB	10:L:46:VAL:HG21	2.01	0.42
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.23	0.42
1:A:588:LEU:HD12	1:A:632:VAL:HG21	2.01	0.42
4:E:65:THR:O	4:E:69:ILE:HG13	2.20	0.42
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	2.00	0.42
1:A:738:LYS:HD2	1:A:740:LEU:HD21	2.01	0.42
1:A:1390:ASN:O	1:A:1399:ARG:HD2	2.19	0.42
3:C:148:ARG:HD3	8:J:61:LEU:O	2.18	0.42
2:B:123:THR:HG23	2:B:205:ILE:HA	2.01	0.42
4:E:97:VAL:HG23	4:E:98:ILE:HD12	2.01	0.42
2:B:764:SER:HB3	2:B:765:PRO:HD3	2.01	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.55	0.42
2:B:487:THR:HG22	2:B:490:SER:HB3	2.01	0.42
2:B:54:PHE:HA	2:B:58:THR:CB	2.45	0.42
1:A:774:ARG:HH21	1:A:794:PRO:HA	1.83	0.42
1:A:353:ILE:HG21	1:A:487:MET:HB2	2.02	0.42
2:B:857:ARG:HH21	2:B:942:ARG:HE	1.66	0.42
2:B:91:SER:HB3	2:B:133:LYS:HB2	2.01	0.42
1:A:404:TYR:HA	1:A:413:ILE:O	2.19	0.42
1:A:516:SER:C	1:A:518:LYS:H	2.23	0.42
1:A:694:THR:HA	1:A:714:PHE:CE1	2.55	0.42
1:A:819:GLY:O	1:A:822:GLU:HB2	2.20	0.42
1:A:131:SER:CB	1:A:223:GLY:HA2	2.49	0.42
8:J:44:TYR:HA	8:J:47:ARG:HB2	2.00	0.42
1:A:182:VAL:HG22	1:A:202:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:H	1:A:56:PRO:HD3	1.85	0.42
2:B:428:ILE:HG12	2:B:448:ILE:HG13	2.01	0.42
1:A:877:HIS:CB	1:A:1056:SER:HA	2.50	0.42
1:A:670:ILE:HD12	2:B:1052:VAL:HG11	2.01	0.42
1:A:860:LEU:HD21	1:A:1394:THR:HA	2.02	0.42
1:A:1128:GLN:HG2	1:A:1304:TRP:NE1	2.35	0.42
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	2.00	0.42
1:A:506:ALA:HB3	1:A:509:LEU:HD12	2.01	0.42
1:A:121:LEU:HB3	1:A:141:LEU:HD22	2.00	0.42
1:A:1366:ARG:HA	1:A:1369:ALA:HB3	2.02	0.42
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.31	0.42
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.55	0.42
3:C:77:ILE:CD1	3:C:161:LYS:HG3	2.50	0.42
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	2.02	0.42
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.02	0.42
9:K:91:CYS:O	9:K:95:ILE:HG12	2.20	0.42
3:C:241:ASP:O	3:C:245:VAL:HG23	2.20	0.42
1:A:453:MET:HB3	1:A:477:PRO:HB2	2.02	0.42
10:L:68:GLU:C	10:L:70:ARG:H	2.23	0.42
7:I:32:CYS:SG	7:I:34:TYR:HB2	2.60	0.42
1:A:568:PRO:O	1:A:569:LYS:HB2	2.19	0.42
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.55	0.42
1:A:793:SER:HB2	1:A:795:GLU:OE2	2.19	0.41
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.84	0.41
2:B:293:PRO:HB2	2:B:296:GLU:HB2	2.02	0.41
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.54	0.41
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.56	0.41
2:B:260:GLY:O	2:B:267:ARG:HD3	2.20	0.41
4:E:124:VAL:HA	4:E:132:ILE:HD11	2.01	0.41
1:A:342:GLY:HA3	2:B:1129:ARG:NH2	2.35	0.41
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.01	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.55	0.41
4:E:47:CYS:HB3	4:E:51:GLY:HA2	2.03	0.41
6:H:87:ARG:HH11	6:H:87:ARG:HA	1.84	0.41
10:L:55:ILE:HG12	10:L:56:LEU:H	1.85	0.41
1:A:456:MET:CE	1:A:510:GLN:HB2	2.50	0.41
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.85	0.41
1:A:302:THR:HA	1:A:305:ASP:O	2.21	0.41
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.65	0.41
2:B:29:ASP:HB3	2:B:658:ILE:HG13	2.03	0.41
2:B:364:ILE:HD13	2:B:585:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:791:THR:HG22	2:B:792:MET:CE	2.50	0.41
2:B:899:ILE:HD11	2:B:911:ILE:HA	2.02	0.41
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.99	0.41
1:A:870:GLU:HG2	4:E:208:TYR:CD1	2.56	0.41
3:C:58:LEU:HD21	8:J:57:ILE:HD12	2.02	0.41
2:B:193:LYS:HB3	2:B:787:VAL:HG11	2.02	0.41
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.02	0.41
3:C:29:MET:HE2	9:K:45:LEU:HD11	2.02	0.41
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.50	0.41
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.02	0.41
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.85	0.41
1:A:407:ARG:HD2	1:A:413:ILE:HD11	2.03	0.41
1:A:345:VAL:HA	2:B:1155:SER:HB2	2.02	0.41
3:C:46:ILE:HA	3:C:159:ALA:HA	2.02	0.41
2:B:189:LEU:HB3	2:B:194:GLU:O	2.21	0.41
9:K:16:GLU:OE2	9:K:37:LYS:NZ	2.53	0.41
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.56	0.41
2:B:46:GLN:HG3	2:B:46:GLN:H	1.71	0.41
6:H:56:THR:HB	6:H:145:ARG:HB3	2.02	0.41
1:A:1426:GLU:HG2	1:A:1426:GLU:H	1.73	0.41
2:B:1100:ASP:OD1	2:B:1103:ILE:HD11	2.21	0.41
2:B:843:GLN:HA	2:B:846:ILE:HD12	2.01	0.41
2:B:976:ILE:HG23	2:B:977:GLY:N	2.32	0.41
1:A:456:MET:HE2	1:A:507:VAL:HA	2.03	0.41
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.01	0.41
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.56	0.41
1:A:41:MET:HB3	1:A:49:LYS:HE3	2.03	0.41
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.01	0.41
2:B:982:SER:HB3	2:B:1092:TYR:CZ	2.56	0.41
1:A:1086:PHE:HB2	1:A:1087:ALA:H	1.73	0.41
1:A:912:LEU:HB3	1:A:1036:ARG:HH22	1.86	0.41
2:B:684:LEU:HA	2:B:689:LEU:HD12	2.01	0.41
1:A:1364:ASN:C	1:A:1364:ASN:ND2	2.74	0.41
3:C:67:LEU:HA	3:C:70:ILE:HD12	2.02	0.41
3:C:72:LEU:HB3	3:C:132:PRO:HA	2.03	0.41
1:A:312:PRO:HB2	1:A:313:GLN:H	1.74	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.21	0.40
2:B:780:VAL:HG11	8:J:56:LEU:HD13	2.03	0.40
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.04	0.40
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.22	0.40
2:B:745:PRO:HB2	2:B:1047:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	2.02	0.40
9:K:42:LEU:HG	9:K:46:ILE:HD12	2.01	0.40
1:A:425:GLN:NE2	1:A:425:GLN:H	2.19	0.40
9:K:5:ASP:HB3	9:K:7:PHE:CE2	2.57	0.40
4:E:147:HIS:CD2	4:E:149:LEU:H	2.39	0.40
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.51	0.40
1:A:669:THR:HB	1:A:805:LEU:HD13	2.02	0.40
2:B:275:TYR:CD1	2:B:275:TYR:N	2.89	0.40
1:A:535:THR:HB	1:A:616:VAL:HG13	2.02	0.40
9:K:57:LEU:HD12	9:K:76:GLN:HG2	2.02	0.40
7:I:88:SER:C	7:I:90:GLN:H	2.25	0.40
9:K:33:ILE:HD13	9:K:87:LEU:HD22	2.04	0.40
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	2.03	0.40
2:B:1149:GLU:HG2	2:B:1153:GLU:HB2	2.04	0.40
1:A:31:SER:HB2	1:A:83:HIS:CD2	2.53	0.40
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.86	0.40
2:B:53:GLN:HG2	2:B:547:VAL:HB	2.04	0.40
7:I:65:ASP:HB3	7:I:68:LEU:HD12	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	1395/1733 (80%)	1177 (84%)	149 (11%)	69 (5%)	3	19
2	B	1096/1224 (90%)	927 (85%)	110 (10%)	59 (5%)	2	17
3	C	264/318 (83%)	235 (89%)	19 (7%)	10 (4%)	4	26
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	21	60
5	F	83/155 (54%)	73 (88%)	7 (8%)	3 (4%)	4	28
6	H	129/146 (88%)	93 (72%)	24 (19%)	12 (9%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	117/122 (96%)	103 (88%)	10 (8%)	4 (3%)	5	29
8	J	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	5	31
9	K	112/120 (93%)	101 (90%)	8 (7%)	3 (3%)	6	35
10	L	44/70 (63%)	28 (64%)	7 (16%)	9 (20%)	0	1
All	All	3515/4173 (84%)	2991 (85%)	351 (10%)	173 (5%)	3	19

All (173) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	215	SER
1	A	250	ILE
1	A	312	PRO
1	A	556	TRP
1	A	569	LYS
1	A	672	ASP
1	A	978	PRO
1	A	1206	ASP
1	A	1377	THR
1	A	1394	THR
2	B	67	SER
2	B	168	GLY
2	B	230	ALA
2	B	265	SER
2	B	451	LYS
2	B	474	SER
2	B	477	ALA
2	B	479	VAL
2	B	712	PRO
2	B	880	THR
2	B	883	LEU
2	B	888	GLY
2	B	936	ASP
2	B	976	ILE
2	B	1156	ASP
2	B	1178	ASN
3	C	4	GLU
3	C	40	GLU
3	C	173	ALA
3	C	213	PRO
3	C	214	ASN

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Mol	Chain	Res	Type
3	C	215	GLU
8	J	2	ILE
8	J	6	ARG
9	K	16	GLU
10	L	53	HIS
10	L	55	ILE
1	A	54	ASN
1	A	65	LEU
1	A	200	ARG
1	A	214	ILE
1	A	255	SER
1	A	331	GLY
1	A	385	ILE
1	A	399	HIS
1	A	411	ASP
1	A	487	MET
1	A	775	ILE
1	A	1005	GLU
1	A	1094	VAL
1	A	1123	GLY
1	A	1124	HIS
1	A	1221	LYS
1	A	1359	ASP
1	A	1378	GLN
1	A	1393	ASN
1	A	1437	GLY
2	B	137	TYR
2	B	277	LYS
2	B	371	GLU
2	B	449	ASN
2	B	629	ASP
2	B	647	GLY
2	B	707	PRO
2	B	751	VAL
2	B	864	LYS
2	B	881	ASN
2	B	884	ARG
2	B	887	HIS
2	B	907	GLY
2	B	943	SER
2	B	996	ARG
2	B	1099	VAL

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Mol	Chain	Res	Type
2	B	1176	ASN
5	F	73	ALA
6	H	61	SER
6	H	90	ALA
6	H	131	ASN
6	H	135	LEU
10	L	35	SER
10	L	39	SER
10	L	50	ASP
10	L	51	CYS
1	A	110	CYS
1	A	258	GLY
1	A	298	PHE
1	A	517	ASN
1	A	707	GLY
1	A	846	GLU
1	A	1064	VAL
1	A	1081	LEU
2	B	467	GLY
2	B	484	ASN
2	B	705	MET
2	B	792	MET
2	B	837	ASP
2	B	886	LYS
2	B	891	ASP
2	B	934	LYS
3	C	165	LYS
4	E	3	GLN
4	E	36	GLU
6	H	44	VAL
7	I	77	LYS
9	K	26	LYS
1	A	57	ARG
1	A	72	GLU
1	A	125	ALA
1	A	149	GLU
1	A	404	TYR
1	A	567	LYS
1	A	591	PHE
1	A	706	HIS
1	A	828	ALA
1	A	1084	PHE

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Mol	Chain	Res	Type
1	A	1175	SER
1	A	1376	THR
2	B	139	ALA
2	B	365	THR
2	B	469	GLN
2	B	483	LEU
2	B	531	GLN
2	B	974	PRO
2	B	1017	ILE
2	B	1046	PRO
2	B	1096	ARG
2	B	1097	HIS
2	B	1157	ALA
3	C	151	GLN
5	F	154	ASP
6	H	77	ARG
6	H	84	ALA
6	H	107	VAL
7	I	3	THR
7	I	20	LYS
10	L	64	LEU
1	A	35	ILE
1	A	55	ASP
1	A	130	ASP
1	A	132	LYS
1	A	283	GLY
1	A	350	ARG
1	A	424	ILE
1	A	958	VAL
1	A	973	ILE
1	A	1255	GLU
1	A	1388	GLY
2	B	526	GLU
2	B	704	ALA
2	B	942	ARG
3	C	39	ALA
5	F	78	GLN
6	H	17	PRO
6	H	18	GLY
6	H	140	ALA
7	I	35	VAL
9	K	64	GLU

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Mol	Chain	Res	Type
10	L	33	GLU
10	L	59	ALA
1	A	400	PRO
1	A	1093	LYS
1	A	1395	GLY
2	B	737	THR
6	H	128	ASN
2	B	482	VAL
1	A	93	VAL
1	A	568	PRO
1	A	1384	VAL
2	B	1023	VAL
1	A	59	GLY
2	B	364	ILE
3	C	6	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	1225/1520 (81%)	1008 (82%)	217 (18%)	2	10
2	B	967/1061 (91%)	811 (84%)	156 (16%)	3	14
3	C	234/274 (85%)	191 (82%)	43 (18%)	2	9
4	E	196/197 (100%)	173 (88%)	23 (12%)	7	28
5	F	75/137 (55%)	60 (80%)	15 (20%)	1	6
6	H	117/128 (91%)	96 (82%)	21 (18%)	2	10
7	I	113/116 (97%)	91 (80%)	22 (20%)	2	7
8	J	60/65 (92%)	46 (77%)	14 (23%)	1	4
9	K	99/102 (97%)	83 (84%)	16 (16%)	3	14
10	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
All	All	3126/3657 (86%)	2585 (83%)	541 (17%)	2	11

All (541) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	30	ILE
1	A	34	LYS
1	A	43	GLU
1	A	46	THR
1	A	47	ARG
1	A	50	ILE
1	A	55	ASP
1	A	57	ARG
1	A	58	LEU
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	74	MET
1	A	75	ASN
1	A	88	LYS
1	A	93	VAL
1	A	108	MET
1	A	122	MET
1	A	126	LEU
1	A	142	CYS
1	A	144	THR
1	A	146	MET
1	A	149	GLU
1	A	150	THR
1	A	180	LYS
1	A	204	THR
1	A	222	LEU
1	A	225	ASN
1	A	232	GLU
1	A	234	MET
1	A	256	GLN
1	A	257	ARG
1	A	262	LEU
1	A	263	THR
1	A	265	LYS
1	A	266	LEU
1	A	268	ASP
1	A	269	ILE
1	A	270	LEU
1	A	277	GLU
1	A	281	HIS

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Mol	Chain	Res	Type
1	A	293	GLU
1	A	298	PHE
1	A	303	TYR
1	A	308	ILE
1	A	313	GLN
1	A	320	ARG
1	A	323	LYS
1	A	326	ARG
1	A	332	LYS
1	A	335	ARG
1	A	341	MET
1	A	373	THR
1	A	381	THR
1	A	389	THR
1	A	391	LEU
1	A	403	LYS
1	A	406	ILE
1	A	407	ARG
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	437	MET
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	455	MET
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	500	GLU
1	A	501	LEU
1	A	505	CYS
1	A	527	THR
1	A	533	LYS
1	A	535	THR
1	A	536	LEU
1	A	538	ASP

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Mol	Chain	Res	Type
1	A	541	ILE
1	A	542	GLU
1	A	543	LEU
1	A	544	ASP
1	A	545	GLN
1	A	549	MET
1	A	571	LEU
1	A	590	ARG
1	A	595	THR
1	A	597	LEU
1	A	612	ILE
1	A	618	GLU
1	A	625	SER
1	A	629	LEU
1	A	634	THR
1	A	652	VAL
1	A	669	THR
1	A	670	ILE
1	A	672	ASP
1	A	675	THR
1	A	678	GLU
1	A	680	THR
1	A	688	LYS
1	A	705	LYS
1	A	709	THR
1	A	722	LEU
1	A	740	LEU
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	774	ARG
1	A	788	SER
1	A	801	GLU
1	A	821	ARG
1	A	822	GLU
1	A	838	GLN
1	A	839	ARG
1	A	847	ASP
1	A	855	THR
1	A	886	ILE
1	A	894	GLU
1	A	896	ARG

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Mol	Chain	Res	Type
1	A	905	ASP
1	A	908	LEU
1	A	909	ASP
1	A	912	LEU
1	A	914	GLU
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	927	VAL
1	A	929	LEU
1	A	931	GLU
1	A	934	LYS
1	A	936	LEU
1	A	946	VAL
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE
1	A	977	LYS
1	A	979	SER
1	A	981	LEU
1	A	982	THR
1	A	983	ILE
1	A	1000	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1009	ASN
1	A	1024	SER
1	A	1025	ARG
1	A	1030	ARG
1	A	1033	GLN
1	A	1037	LEU
1	A	1048	ASN
1	A	1052	GLN
1	A	1062	GLU
1	A	1067	LEU
1	A	1077	THR
1	A	1078	GLN
1	A	1081	LEU
1	A	1084	PHE
1	A	1086	PHE
1	A	1093	LYS
1	A	1124	HIS

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Mol	Chain	Res	Type
1	A	1128	GLN
1	A	1129	GLU
1	A	1130	GLN
1	A	1143	LEU
1	A	1147	THR
1	A	1170	ILE
1	A	1176	LEU
1	A	1188	GLN
1	A	1205	LYS
1	A	1215	ARG
1	A	1221	LYS
1	A	1224	LEU
1	A	1231	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1257	ASP
1	A	1261	LYS
1	A	1264	GLU
1	A	1271	ILE
1	A	1280	GLU
1	A	1283	VAL
1	A	1284	MET
1	A	1288	ASP
1	A	1299	VAL
1	A	1308	THR
1	A	1322	ILE
1	A	1327	ILE
1	A	1333	ILE
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1381	LEU
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET

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Mol	Chain	Res	Type
1	A	1403	GLU
1	A	1406	VAL
1	A	1411	GLU
1	A	1422	ARG
1	A	1425	SER
1	A	1438	THR
2	B	26	THR
2	B	28	GLU
2	B	44	VAL
2	B	46	GLN
2	B	66	ASP
2	B	70	ILE
2	B	89	GLU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	128	LEU
2	B	135	ARG
2	B	136	THR
2	B	175	ARG
2	B	185	THR
2	B	194	GLU
2	B	199	MET
2	B	208	SER
2	B	217	ARG
2	B	218	SER
2	B	234	ILE
2	B	246	LYS
2	B	249	ARG
2	B	254	LEU
2	B	257	LYS
2	B	262	GLU
2	B	272	THR
2	B	273	LEU
2	B	277	LYS
2	B	278	GLN
2	B	292	ILE
2	B	296	GLU
2	B	311	LEU
2	B	315	LYS
2	B	322	PHE
2	B	325	GLN

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Mol	Chain	Res	Type
2	B	333	PHE
2	B	345	LYS
2	B	354	ASP
2	B	359	GLU
2	B	365	THR
2	B	366	GLN
2	B	367	LEU
2	B	371	GLU
2	B	376	PHE
2	B	382	ILE
2	B	384	ARG
2	B	396	ASP
2	B	398	ARG
2	B	405	ARG
2	B	408	LEU
2	B	416	LEU
2	B	418	LYS
2	B	436	VAL
2	B	437	GLU
2	B	454	THR
2	B	465	ASN
2	B	469	GLN
2	B	476	ARG
2	B	482	VAL
2	B	483	LEU
2	B	485	ARG
2	B	500	THR
2	B	516	ASN
2	B	521	LEU
2	B	526	GLU
2	B	531	GLN
2	B	556	THR
2	B	572	HIS
2	B	591	ARG
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	612	GLU
2	B	620	ARG
2	B	633	VAL
2	B	642	ASP
2	B	646	LEU

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Mol	Chain	Res	Type
2	B	655	LYS
2	B	708	GLU
2	B	709	ASP
2	B	711	GLU
2	B	714	GLU
2	B	730	ARG
2	B	733	HIS
2	B	743	ILE
2	B	751	VAL
2	B	762	ASN
2	B	766	ARG
2	B	773	MET
2	B	780	VAL
2	B	786	ASN
2	B	788	ARG
2	B	791	THR
2	B	792	MET
2	B	796	LEU
2	B	807	ARG
2	B	812	LEU
2	B	815	ARG
2	B	838	SER
2	B	841	MET
2	B	860	MET
2	B	864	LYS
2	B	868	MET
2	B	875	GLU
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	886	LYS
2	B	942	ARG
2	B	951	GLN
2	B	954	VAL
2	B	961	LEU
2	B	963	PHE
2	B	964	VAL
2	B	967	ARG
2	B	975	GLN
2	B	983	ARG
2	B	987	LYS
2	B	996	ARG

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Mol	Chain	Res	Type
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1010	LEU
2	B	1028	GLU
2	B	1049	ASP
2	B	1057	LYS
2	B	1065	GLN
2	B	1066	SER
2	B	1077	THR
2	B	1092	TYR
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1122	ARG
2	B	1133	MET
2	B	1137	CYS
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1170	THR
2	B	1175	LEU
2	B	1178	ASN
2	B	1188	LYS
2	B	1190	ASP
2	B	1191	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1215	ARG
2	B	1224	PHE
3	C	9	LYS
3	C	17	ASN
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP

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Mol	Chain	Res	Type
3	C	36	VAL
3	C	43	THR
3	C	48	SER
3	C	69	LEU
3	C	72	LEU
3	C	75	MET
3	C	77	ILE
3	C	85	ASP
3	C	100	THR
3	C	101	LEU
3	C	106	GLU
3	C	115	SER
3	C	116	LYS
3	C	129	ILE
3	C	133	ILE
3	C	136	ASP
3	C	137	LYS
3	C	140	ASN
3	C	142	VAL
3	C	148	ARG
3	C	149	LYS
3	C	151	GLN
3	C	152	GLU
3	C	156	THR
3	C	188	HIS
3	C	195	GLN
3	C	203	GLN
3	C	205	LYS
3	C	214	ASN
3	C	215	GLU
3	C	226	ASP
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	263	THR
3	C	265	MET
4	E	3	GLN
4	E	8	ASN
4	E	52	ARG
4	E	54	GLN
4	E	57	MET

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Mol	Chain	Res	Type
4	E	75	MET
4	E	77	SER
4	E	78	LEU
4	E	80	VAL
4	E	84	ASP
4	E	85	GLU
4	E	92	THR
4	E	98	ILE
4	E	107	THR
4	E	115	ASN
4	E	137	GLU
4	E	142	VAL
4	E	146	HIS
4	E	156	LEU
4	E	159	ASP
4	E	165	LEU
4	E	169	ARG
4	E	200	ARG
5	F	76	LYS
5	F	82	THR
5	F	92	ARG
5	F	99	LEU
5	F	103	MET
5	F	104	ASN
5	F	110	ASP
5	F	112	GLU
5	F	118	LEU
5	F	119	ARG
5	F	122	MET
5	F	127	GLU
5	F	133	VAL
5	F	138	LEU
5	F	149	GLU
6	H	3	ASN
6	H	26	ILE
6	H	27	GLU
6	H	35	GLN
6	H	44	VAL
6	H	55	LEU
6	H	63	LEU
6	H	87	ARG
6	H	92	ASP

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Mol	Chain	Res	Type
6	H	94	ASP
6	H	95	TYR
6	H	96	VAL
6	H	105	GLU
6	H	107	VAL
6	H	108	SER
6	H	111	LEU
6	H	123	MET
6	H	130	ARG
6	H	132	LEU
6	H	136	LYS
6	H	138	GLU
7	I	17	ARG
7	I	20	LYS
7	I	21	GLU
7	I	28	GLU
7	I	35	VAL
7	I	37	GLU
7	I	42	LEU
7	I	50	THR
7	I	52	ILE
7	I	55	THR
7	I	61	ASP
7	I	62	ILE
7	I	70	ARG
7	I	84	VAL
7	I	87	GLN
7	I	90	GLN
7	I	95	THR
7	I	98	VAL
7	I	104	LEU
7	I	117	LYS
7	I	118	ARG
7	I	120	GLN
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	26	GLN
8	J	28	ASP

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Mol	Chain	Res	Type
8	J	30	LEU
8	J	31	ASP
8	J	43	ARG
8	J	48	ARG
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	8	GLU
9	K	20	LYS
9	K	21	ILE
9	K	22	ASP
9	K	29	ASN
9	K	33	ILE
9	K	50	LEU
9	K	77	THR
9	K	78	THR
9	K	81	TYR
9	K	84	LYS
9	K	95	ILE
9	K	108	GLU
9	K	111	LEU
9	K	114	LEU
10	L	27	LEU
10	L	33	GLU
10	L	38	LEU
10	L	39	SER
10	L	42	ARG
10	L	44	ASP
10	L	50	ASP
10	L	55	ILE
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
10	L	64	LEU
10	L	65	VAL
10	L	66	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN

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Mol	Chain	Res	Type
1	A	18	GLN
1	A	83	HIS
1	A	225	ASN
1	A	297	GLN
1	A	339	ASN
1	A	425	GLN
1	A	451	HIS
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN
1	A	587	HIS
1	A	626	ASN
1	A	631	HIS
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	877	HIS
1	A	906	HIS
1	A	965	GLN
1	A	969	GLN
1	A	1004	ASN
1	A	1009	ASN
1	A	1033	GLN
1	A	1140	HIS
1	A	1203	ASN
1	A	1265	ASN
1	A	1364	ASN
2	B	46	GLN
2	B	53	GLN
2	B	103	ASN
2	B	366	GLN
2	B	383	ASN
2	B	499	ASN
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN

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Mol	Chain	Res	Type
2	B	763	GLN
2	B	776	GLN
2	B	835	GLN
2	B	887	HIS
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1025	HIS
2	B	1097	HIS
2	B	1161	HIS
2	B	1195	HIS
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
4	E	147	HIS
6	H	11	GLN
6	H	83	GLN
6	H	133	ASN
6	H	134	ASN
7	I	60	GLN
7	I	108	HIS
8	J	23	ASN
9	K	65	HIS
9	K	76	GLN
9	K	89	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/5 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	ATP	A	1736	13	24,33,33	1.20	3 (12%)	31,52,52	1.54	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ATP	A	1736	13	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1736	ATP	PB-O1B	2.16	1.59	1.51
15	A	1736	ATP	C2-N1	2.28	1.38	1.33
15	A	1736	ATP	C2-N3	3.13	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1736	ATP	N3-C2-N1	-3.22	126.42	128.89
15	A	1736	ATP	C1'-N9-C4	-2.60	123.01	126.94
15	A	1736	ATP	PA-O3A-PB	2.31	139.23	132.73
15	A	1736	ATP	O3'-C3'-C4'	2.38	118.19	111.05
15	A	1736	ATP	C4-C5-N7	2.61	111.88	109.48
15	A	1736	ATP	O4'-C1'-N9	2.92	114.22	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1736	ATP	O3'-C3'-C2'	3.26	122.43	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1736	ATP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	0.09	86 (6%) 25 20	78, 133, 223, 254	0
2	B	1114/1224 (91%)	-0.03	49 (4%) 38 31	71, 115, 183, 241	0
3	C	266/318 (83%)	-0.21	1 (0%) 93 92	87, 113, 153, 215	0
4	E	214/215 (99%)	-0.04	5 (2%) 64 57	102, 159, 206, 216	0
5	F	85/155 (54%)	-0.13	0 100 100	109, 139, 178, 196	0
6	H	133/146 (91%)	0.38	11 (8%) 14 11	131, 172, 202, 222	0
7	I	119/122 (97%)	-0.14	2 (1%) 73 67	93, 138, 185, 200	0
8	J	65/70 (92%)	-0.16	0 100 100	81, 104, 136, 151	0
9	K	114/120 (95%)	-0.21	0 100 100	87, 123, 150, 175	0
10	L	46/70 (65%)	0.27	3 (6%) 22 18	99, 155, 188, 214	0
11	R	5/5 (100%)	0.30	0 100 100	148, 153, 180, 183	0
12	T	13/29 (44%)	1.44	5 (38%) 0 1	150, 170, 237, 245	0
All	All	3579/4207 (85%)	0.01	162 (4%) 37 30	71, 128, 208, 254	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	8.9
2	B	1222	ARG	7.1
2	B	1224	PHE	6.9
1	A	1176	LEU	6.5
1	A	66	LYS	6.3
1	A	72	GLU	5.8
6	H	84	ALA	5.4
1	A	45	GLN	5.3
2	B	1221	SER	5.2
12	T	28	DT	5.1
2	B	866	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	1086	PHE	5.0
2	B	477	ALA	4.7
6	H	83	GLN	4.7
1	A	44	THR	4.7
2	B	1223	ASP	4.7
1	A	251	SER	4.5
1	A	253	ASN	4.4
2	B	231	PRO	4.4
1	A	319	GLY	4.4
1	A	250	ILE	4.3
1	A	256	GLN	4.2
6	H	86	ASP	4.2
2	B	919	SER	4.2
1	A	87	ALA	4.2
1	A	182	VAL	4.2
1	A	318	SER	4.2
2	B	250	PHE	4.2
2	B	470	LYS	4.1
2	B	884	ARG	4.1
1	A	124	GLN	4.1
1	A	252	PHE	4.1
2	B	935	ARG	4.1
1	A	65	LEU	4.0
1	A	73	GLY	4.0
2	B	471	LYS	3.9
1	A	152	VAL	3.9
1	A	255	SER	3.8
10	L	50	ASP	3.8
6	H	85	GLY	3.8
1	A	316	GLN	3.8
2	B	135	ARG	3.8
2	B	1205	GLN	3.8
2	B	1169	MET	3.7
1	A	141	LEU	3.6
1	A	151	ASP	3.6
12	T	25	DC	3.6
1	A	125	ALA	3.5
4	E	119	SER	3.5
1	A	168	GLY	3.5
2	B	645	SER	3.5
10	L	27	LEU	3.5
1	A	317	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1085	HIS	3.4
1	A	1302	PRO	3.4
2	B	136	THR	3.4
2	B	867	GLY	3.4
1	A	161	LEU	3.4
1	A	232	GLU	3.4
1	A	88	LYS	3.3
2	B	883	LEU	3.3
1	A	149	GLU	3.3
1	A	137	ALA	3.3
1	A	6	TYR	3.2
1	A	1093	LYS	3.2
1	A	257	ARG	3.2
2	B	1209	ALA	3.1
1	A	282	ASN	3.1
1	A	176	LYS	3.1
1	A	1002	GLY	3.1
4	E	90	VAL	3.1
12	T	27	DA	3.0
2	B	230	ALA	3.0
2	B	1208	MET	2.9
2	B	474	SER	2.9
1	A	199	LEU	2.9
2	B	140	ILE	2.9
1	A	254	GLU	2.9
2	B	472	ALA	2.9
1	A	183	GLY	2.9
2	B	865	LYS	2.9
10	L	38	LEU	2.8
2	B	708	GLU	2.8
6	H	130	ARG	2.8
2	B	868	MET	2.8
1	A	1391	ARG	2.8
2	B	478	GLY	2.8
1	A	41	MET	2.8
1	A	320	ARG	2.8
12	T	24	DT	2.8
1	A	8	SER	2.7
4	E	2	ASP	2.7
2	B	1219	ASP	2.7
2	B	918	ILE	2.6
3	C	217	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	286	HIS	2.6
2	B	249	ARG	2.6
2	B	1220	ARG	2.6
2	B	476	ARG	2.6
1	A	3	GLY	2.6
6	H	108	SER	2.6
2	B	933	SER	2.6
4	E	118	PRO	2.6
1	A	62	ASP	2.6
1	A	60	SER	2.6
6	H	105	GLU	2.5
1	A	116	ASP	2.5
2	B	141	ASP	2.5
1	A	136	ALA	2.5
2	B	709	ASP	2.5
1	A	163	SER	2.5
1	A	1300	LYS	2.5
2	B	247	GLY	2.5
2	B	1175	LEU	2.5
2	B	870	ILE	2.5
1	A	147	VAL	2.5
1	A	201	VAL	2.5
6	H	117	SER	2.4
1	A	975	HIS	2.4
2	B	666	TYR	2.4
1	A	167	CYS	2.4
6	H	111	LEU	2.4
1	A	980	ASP	2.4
1	A	81	PHE	2.4
2	B	1210	MET	2.4
1	A	120	GLU	2.4
1	A	200	ARG	2.4
1	A	1123	GLY	2.4
2	B	89	GLU	2.4
1	A	186	LYS	2.4
1	A	153	PRO	2.3
1	A	5	GLN	2.3
1	A	705	LYS	2.3
2	B	139	ALA	2.3
1	A	164	ARG	2.3
2	B	433	GLN	2.3
1	A	212	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	173	THR	2.3
1	A	162	VAL	2.2
1	A	150	THR	2.2
2	B	713	ALA	2.2
1	A	75	ASN	2.2
1	A	64	ASN	2.2
1	A	127	ALA	2.2
2	B	248	SER	2.2
1	A	92	HIS	2.1
1	A	4	GLN	2.1
1	A	292	ALA	2.1
1	A	315	LEU	2.1
6	H	19	ARG	2.1
6	H	123	MET	2.1
2	B	468	GLU	2.1
1	A	707	GLY	2.1
4	E	121	MET	2.1
7	I	50	THR	2.1
7	I	117	LYS	2.1
1	A	105	CYS	2.1
1	A	165	GLY	2.1
1	A	154	SER	2.0
1	A	49	LYS	2.0
1	A	309	ALA	2.0
12	T	16	DC	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	ATP	A	1736	31/31	0.88	0.23	-0.07	162,165,195,197	0
14	ZN	J	101	1/1	0.98	0.20	-0.59	102,102,102,102	0
14	ZN	I	203	1/1	0.98	0.08	-0.88	134,134,134,134	0
14	ZN	A	1735	1/1	0.95	0.15	-1.02	198,198,198,198	0
14	ZN	C	319	1/1	0.99	0.09	-1.18	113,113,113,113	0
14	ZN	I	204	1/1	0.99	0.07	-1.30	112,112,112,112	0
14	ZN	L	105	1/1	0.97	0.03	-1.53	142,142,142,142	0
13	MG	A	2002	1/1	0.92	0.14	-1.67	131,131,131,131	0
14	ZN	B	1307	1/1	0.82	0.10	-1.72	221,221,221,221	0
14	ZN	A	1734	1/1	0.24	0.15	-1.78	300,300,300,300	0
13	MG	A	2001	1/1	0.90	0.04	-4.05	102,102,102,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.