



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:58 am GMT

PDB ID : 3S1R
Title : RNA Polymerase II Initiation Complex with a 5-nt 3'-deoxy RNA soaked with GTP
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-16
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

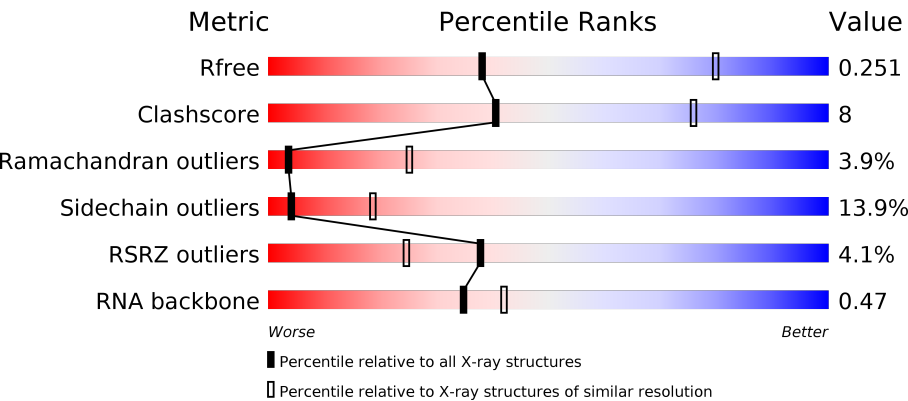
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



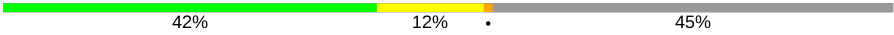





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div><div>5%</div><div><div></div><div>56%</div><div>21%</div><div>• •</div><div>19%</div></div></div>
2	B	1224	<div><div>3%</div><div><div></div><div>62%</div><div>25%</div><div>•</div><div>9%</div></div></div>
3	C	318	<div><div></div><div><div></div><div>56%</div><div>24%</div><div>•</div><div>16%</div></div></div>
4	E	215	<div><div>3%</div><div><div></div><div>70%</div><div>26%</div><div>•</div></div></div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	GTP	R	100	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 28601 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			

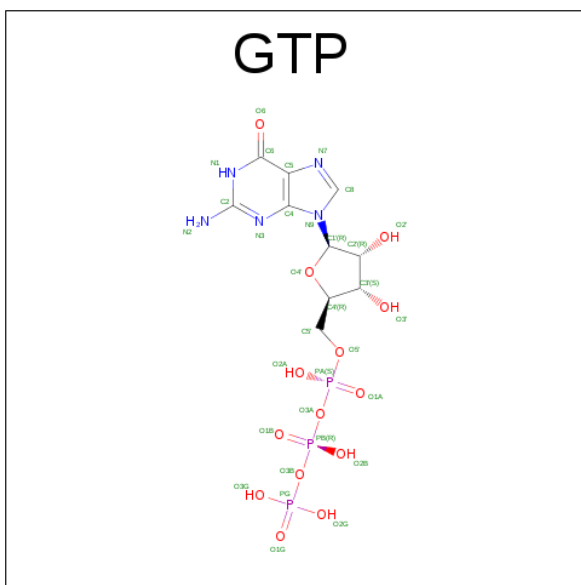
- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*G*)-3').

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	8	Total	C	N	O	P	0	0	0
			159	76	26	49	8			

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	R	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- 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		

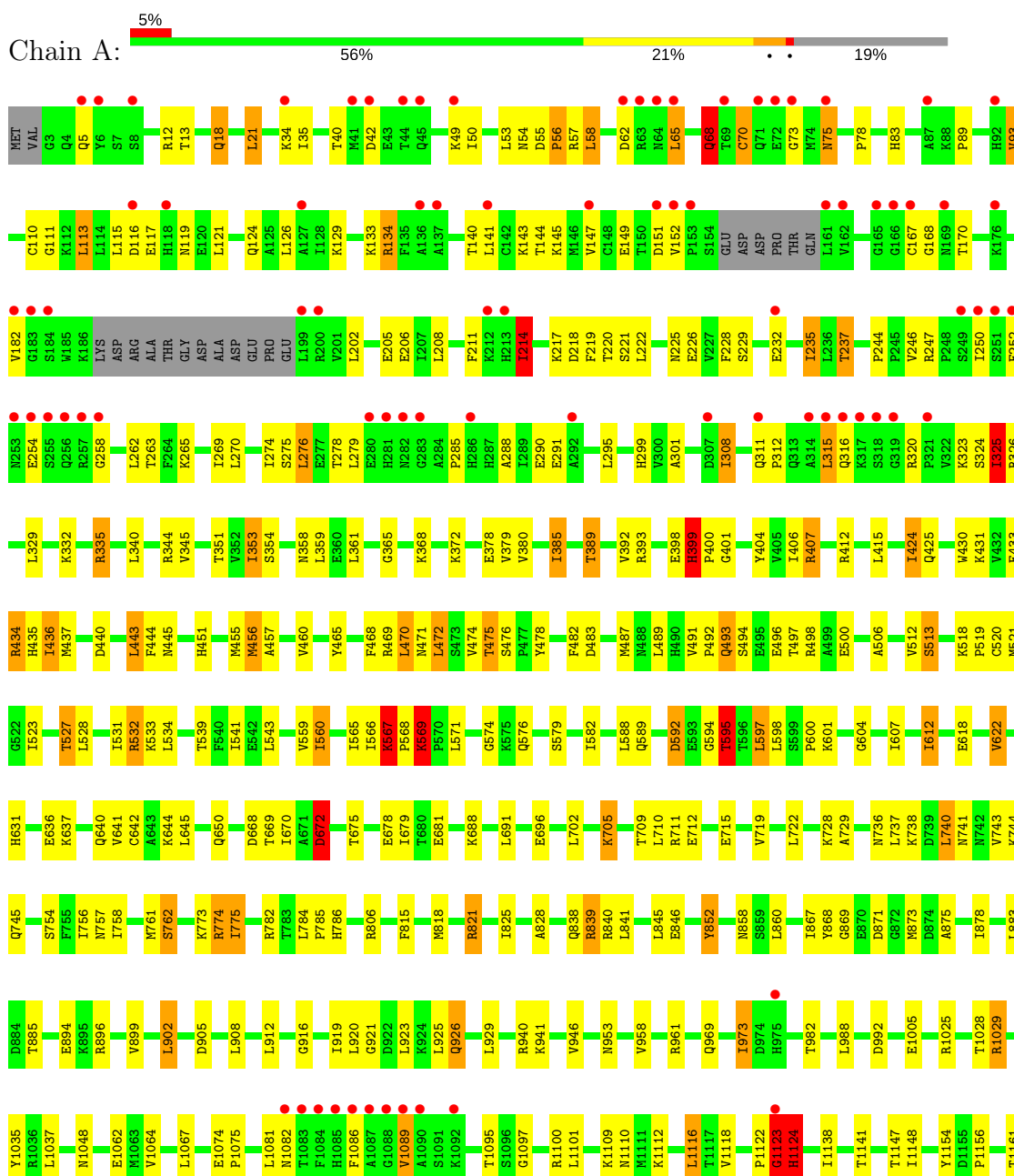
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

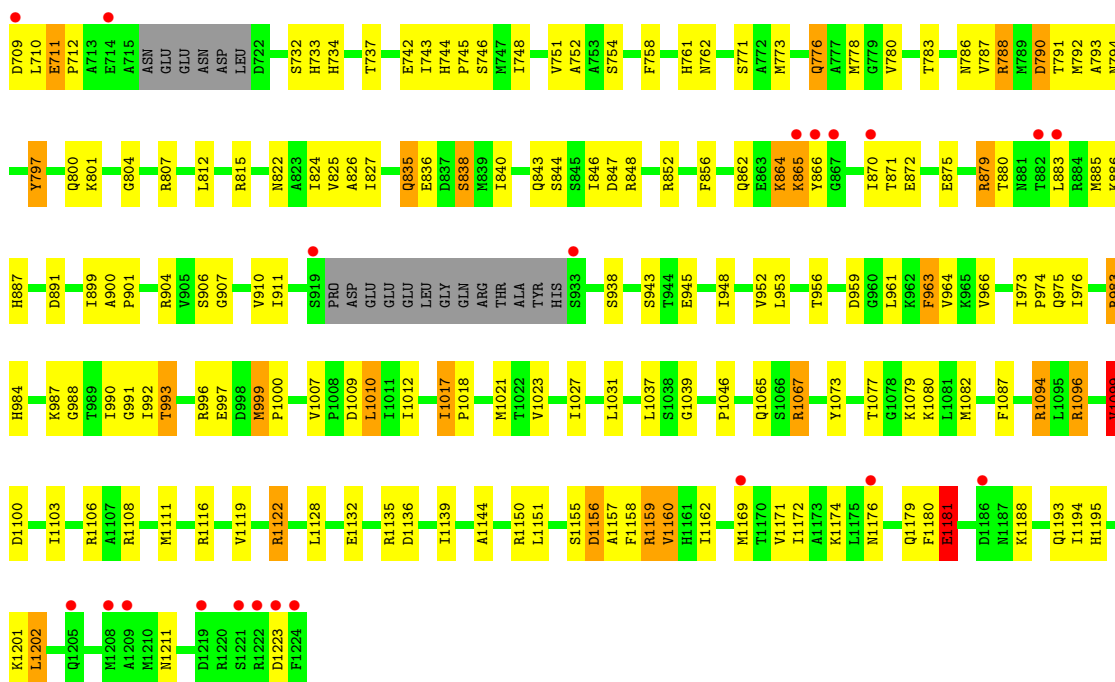
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

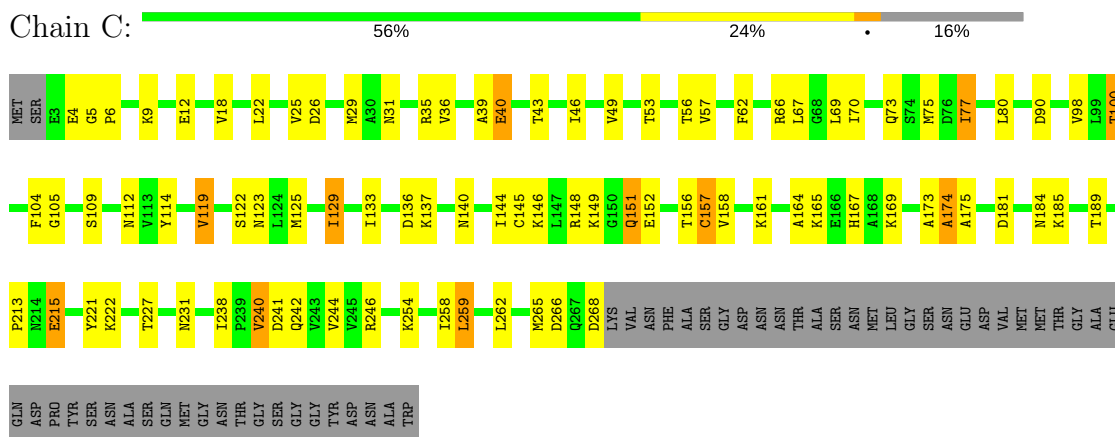




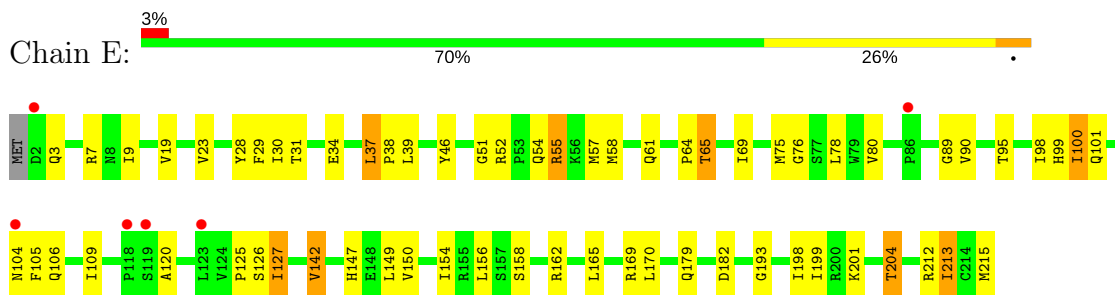
R604	A477	R383	T288	R175	ARG	MET
N610	G478	R384	I269	S176	LYS	SER
V613	S480	L386	L273	E89	TYR	ASP
I616	R485	C388	I276	N178	I90	LEU
R617	Y486	A389	K277	L181	I95	ASN
D618	T487	R392	I280	S187	M101	GLU
R620	S490	K393	P281	L281	Y102	LYS
E621	R497	D394	I282	Y190	ASP	TYR
D629	I502	R398	V283	L193	B196	ASP
F638	GLY	F401	I284	C195	L112	GLU
D642	ASP	L416	I285	F196	Y113	ASP
D643	GLY	F417	R287	F197	P114	PRO
E644	LYS	K418	I282	I204	R118	GLY
S645	LEU	I428	P283	I205	T123	PHE
L646	A509	I428	D294	S208	L128	GLU
G647	K510	M432	E299	I213	F129	D20
H648	L514	Q433	R306	R217	V130	I25
K649	H515	N516	B307	N221	R134	E28
V653	T517	ALA	V323	I222	R135	D29
R654	H518	HIS	I324	V223	T136	S35
K655	H519	ASP	Q325	A139	Y137	R39
G656	PHE	ASN	F333	K227	E138	E40
H657	E526	GLY	I334	A228	A139	K41
D668	I530	MET	G335	A230	I140	ASP
GLU	Q531	LYS	ARG	P231	VAL	Q46
GLY	K537	L446	ARG	P231	PRO	S45
PHE	V547	A447	GLY	I234	GLY	F54
GLU	I554	I448	THR	S235	LEU	T58
ASP	V563	K451	ALA	H236	LYS	I63
VAL	E563	T454	GLY	V237	TYR	S67
E578	L566	K458	ILE	A238	GLU	T68
S683	P571	Y459	LYS	A243	LEU	L69
E687	S574	A460	R348	L244	ALA	I70
V690	A577	L461	I349	E245	GLU	LEU
D694	V585	Q464	Q350	K246	GLU	GLU
A695	G467	R465	H363	F250	SER	GLN
E696	G467	W466	I364	I251	GLY	LEU
E696	G467	Q468	L367	L254	ASP	ALA
I703	V589	K470	R373	V256	ASP	GLN
A704	H590	K471	F376	R261	SER	GLY
M705	N592	A472	F376	S265	THR	THR
Q706	E598	M473	R373	F166	GLY	THR
P707	E598	S474	K381	I167	K184	GLU
T708	E598	S475	I282	P627	V165	SER
		R476		S627	F166	ASN
					I167	ASN
					C189	ILE
						SER



• 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



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

HIS GLU GLN ILE ARG LYS THR LEU LYS E71 K72 A73 Q78 T81 T82 P83 Y84 E89 L99 D110 L111 E112 D116 R119 E127 I130 L138 W146 S147 V148 I152 L155

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

Chain H: 7% 58% 29% 9%

MET S2 Q11 Q12 S13 D16 P17 G18 C24 R25 I26 E27 Q33 D34 Q35 C36 K37 L38 T39 L40 V44 F47 P48 V49 T56 L63 ASN LEU GLU ASP THR PRO ALA ASN ASP SER SER ALA T76 S77 S78 W79 P82 Q83 Q84 G85 D86 R87 A90

D91 D92 Y95 Y96 Y97 Y98 V107 S108 K109 D110 L111 S117 M123 R130 N131 L132 M133 L135 K136 N139 A140 R145 R146

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

Chain I: 75% 17% 5%

MET T2 C10 H11 M12 R17 E18 D19 R24 E28 T31 V35 E36 E37 R45 V58 D61 E62 R70 C75 C78 V84 Q87 S88 Q89 Q90 R91 M97 V102 I109 K115 R118 T119 Q120 PHE SER

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

Chain J: 61% 23% 9% 7%

M1 T2 V3 R6 R7 C7 V13 V14 W18 E19 L22 E32 S37 R43 R47 R48 M49 I50 L51 T52 K59 F60 L61 R62 N64 F65 LEU GLU LYS ARG ASP

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

Chain K: 67% 24% 5%

M1 R6 F7 F10 L11 L12 G13 E14 G15 K20 K26 V31 D39 H40 L42 R54 K55 V56 L57 F58 V63 F64 H65 R74 T75 Q76 T77 T78 Y81 D85 A86 L87 K88 C91 K97 L101 W109 T113 L114 ALA ALA ASP

ALA PHE

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

Chain L: 3% 34% 17% 10% 34%

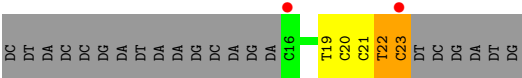
MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN ASP ALA ALA ALA GLY THR SER GLN ARG THR T26 L27 K28 E33 L38 S39 L40 D44 A45 V46 R47 C48 R49 P50 C51 T55 L56 L57 K58 A59 R60 T61 K62 R63 L64 V65 R70

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

Chain R: 60% 80% 20%



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.67Å 221.32Å 193.21Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	29.97 – 3.20 29.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.97-3.20) 99.4 (29.97-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.177 , 0.226 0.201 , 0.251	Depositor DCC
R_{free} test set	5429 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28601	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	0.50	0/11241	0.77	3/15199 (0.0%)
2	B	0.52	0/9033	0.80	2/12181 (0.0%)
3	C	0.49	0/2133	0.81	0/2891
4	E	0.45	0/1788	0.73	0/2406
5	F	0.51	0/700	0.76	0/945
6	H	0.50	0/1086	0.83	1/1470 (0.1%)
7	I	0.51	0/989	0.82	0/1331
8	J	0.55	0/541	0.88	0/727
9	K	0.45	0/937	0.71	0/1265
10	L	0.57	0/365	1.13	2/485 (0.4%)
11	R	0.93	0/123	1.64	0/191
12	T	1.29	0/176	1.87	5/268 (1.9%)
All	All	0.51	0/29112	0.81	13/39359 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	O4'-C1'-N1	8.14	113.70	108.00
2	B	647	GLY	C-N-CA	7.65	140.83	121.70
10	L	50	ASP	C-N-CA	7.62	140.74	121.70
12	T	23	DC	O4'-C1'-N1	6.07	112.25	108.00
1	A	1123	GLY	C-N-CA	6.02	136.75	121.70
10	L	51	CYS	N-CA-C	-5.90	95.06	111.00
12	T	19	DT	O4'-C1'-N1	5.90	112.13	108.00
12	T	21	DC	O4'-C1'-N1	5.69	111.98	108.00
1	A	399	HIS	N-CA-CB	5.40	120.32	110.60
2	B	140	ILE	C-N-CA	5.33	135.04	121.70
12	T	20	DC	O4'-C1'-N1	5.29	111.70	108.00
1	A	451	HIS	CB-CA-C	-5.11	100.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	91	ASP	C-N-CA	5.02	134.25	121.70

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	208	0
2	B	8861	0	8884	169	0
3	C	2095	0	2051	46	0
4	E	1752	0	1776	32	0
5	F	688	0	707	6	0
6	H	1068	0	1040	18	0
7	I	971	0	927	14	0
8	J	532	0	542	23	0
9	K	919	0	929	19	0
10	L	363	0	386	11	0
11	R	109	0	55	0	0
12	T	159	0	91	2	0
13	R	32	0	12	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	28601	0	28533	468	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 (468) 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)
3:C:57:VAL:HG21	8:J:60:PHE:HB3	1.27	1.11
2:B:800:GLN:HB2	8:J:52:THR:HG22	1.19	1.08
2:B:862:GLN:HB3	2:B:963:PHE:HB2	1.43	1.01
2:B:1094:ARG:HG2	2:B:1094:ARG:HH11	1.26	1.00
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.47	0.96
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.06	0.91
1:A:869:GLY:O	4:E:204:THR:HG21	1.70	0.91
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.51	0.90
1:A:567:LYS:HB3	6:H:96:VAL:H	1.35	0.90
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.53	0.89
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.63	0.79
1:A:741:ASN:HD22	1:A:744:LYS:H	1.26	0.79
2:B:848:ARG:HH22	2:B:996:ARG:NH1	1.80	0.79
2:B:54:PHE:HA	2:B:58:THR:HB	1.64	0.79
2:B:801:LYS:O	8:J:52:THR:HG23	1.83	0.79
2:B:654:ARG:H	2:B:657:HIS:HD2	1.29	0.77
2:B:1094:ARG:HG2	2:B:1094:ARG:NH1	1.99	0.76
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.34	0.74
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.69	0.74
2:B:451:LYS:HA	2:B:454:THR:HB	1.70	0.73
2:B:744:HIS:HD2	2:B:746:SER:H	1.35	0.73
7:I:28:GLU:HB3	7:I:35:VAL:HG13	1.72	0.72
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.54	0.72
3:C:56:THR:HG21	3:C:145:CYS:SG	2.30	0.72
2:B:1094:ARG:CG	2:B:1094:ARG:HH11	2.01	0.72
3:C:57:VAL:HG21	8:J:60:PHE:CB	2.14	0.71
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.71	0.70
1:A:1082:ASN:HB2	1:A:1097:GLY:HA3	1.74	0.70
2:B:1100:ASP:HA	2:B:1103:ILE:HG12	1.74	0.69
2:B:762:ASN:HD21	2:B:984:HIS:HD2	1.39	0.69
2:B:363:HIS:O	2:B:364:ILE:HB	1.91	0.69
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.58	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.75	0.68
8:J:48:ARG:O	8:J:52:THR:HB	1.93	0.68
1:A:709:THR:HB	1:A:712:GLU:HB2	1.75	0.68
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.75	0.68
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.75	0.68
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.75	0.68
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.77	0.67
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.75	0.67
3:C:98:VAL:H	3:C:122:SER:HB2	1.60	0.67
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.40	0.67
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.77	0.67
2:B:25:ILE:HG13	2:B:29:ASP:HB2	1.75	0.67
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.76	0.67
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.79	0.66
2:B:800:GLN:HB2	8:J:52:THR:CG2	2.11	0.66
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.24	0.65
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.77	0.65
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.11	0.65
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.78	0.65
2:B:515:HIS:HD2	2:B:517:THR:H	1.44	0.65
2:B:864:LYS:HG2	2:B:865:LYS:H	1.63	0.64
1:A:469:ARG:NH2	2:B:991:GLY:O	2.31	0.64
6:H:33:GLN:HB2	6:H:36:CYS:HB3	1.79	0.63
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.31	0.63
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.80	0.63
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.82	0.62
2:B:428:ILE:HG12	2:B:448:ILE:HG12	1.82	0.62
1:A:399:HIS:O	1:A:401:GLY:N	2.32	0.62
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.81	0.62
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.28	0.62
1:A:899:VAL:HB	1:A:929:LEU:HD22	1.81	0.62
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.35	0.61
1:A:705:LYS:HE2	1:A:705:LYS:H	1.65	0.61
4:E:55:ARG:HA	4:E:58:MET:HG3	1.82	0.61
1:A:57:ARG:HA	1:A:68:GLN:HB3	1.83	0.61
1:A:1173:HIS:HB2	1:A:1227:ILE:HG23	1.82	0.61
1:A:378:GLU:OE2	1:A:434:ARG:HD3	2.00	0.61
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.81	0.61
1:A:754:SER:H	1:A:757:ASN:HD22	1.46	0.61
2:B:516:ASN:HD22	2:B:516:ASN:H	1.49	0.61
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.84	0.60
1:A:566:ILE:HD11	6:H:98:TYR:HB2	1.82	0.60
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.28	0.60
1:A:56:PRO:HB2	1:A:57:ARG:HH21	1.67	0.60
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.84	0.60
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.83	0.60
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.83	0.60
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.84	0.59
2:B:835:GLN:O	2:B:838:SER:HB2	2.01	0.59
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:711:ARG:H	1.67	0.59
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.83	0.59
8:J:3:VAL:CG1	8:J:18:TRP:HB2	2.29	0.59
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.66	0.59
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.84	0.59
1:A:669:THR:O	1:A:762:SER:HB3	2.03	0.59
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.68	0.59
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.03	0.59
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.85	0.59
2:B:953:LEU:O	2:B:964:VAL:HG23	2.03	0.58
2:B:783:THR:HG21	8:J:59:LYS:HB3	1.83	0.58
1:A:1154:TYR:CE2	1:A:1156:PRO:HG3	2.38	0.58
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.86	0.58
1:A:1377:THR:HA	4:E:212:ARG:NH2	2.19	0.58
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.17	0.57
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.86	0.57
1:A:818:MET:HG3	2:B:514:LEU:HD23	1.85	0.57
1:A:434:ARG:HH21	1:A:437:MET:HB2	1.68	0.57
3:C:173:ALA:O	3:C:174:ALA:HB3	2.04	0.57
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.87	0.57
6:H:47:PHE:HB2	6:H:95:TYR:HD1	1.70	0.57
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.04	0.57
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.38	0.57
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.40	0.57
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.87	0.57
1:A:839:ARG:HH21	1:A:1402:PHE:HA	1.70	0.56
2:B:618:ASP:OD2	2:B:621:GLU:HB2	2.05	0.56
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.87	0.56
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.87	0.56
2:B:223:VAL:HG21	2:B:381:MET:HG2	1.88	0.56
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.87	0.56
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.85	0.56
1:A:670:ILE:HG13	2:B:1067:ARG:HH11	1.70	0.56
6:H:47:PHE:HB2	6:H:95:TYR:CD1	2.40	0.56
1:A:595:THR:HG21	1:A:604:GLY:HA3	1.87	0.56
1:A:208:LEU:HD12	1:A:235:ILE:HD13	1.86	0.56
3:C:31:ASN:O	3:C:35:ARG:HG3	2.06	0.56
12:T:22:DT:H2''	12:T:23:DC:H5'	1.88	0.56
2:B:705:MET:H	2:B:710:LEU:HG	1.71	0.55
1:A:494:SER:O	1:A:498:ARG:HG3	2.06	0.55
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:HD22	1:A:228:PHE:H	1.53	0.55
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.88	0.55
2:B:900:ALA:CB	10:L:61:THR:HG23	2.32	0.55
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.87	0.55
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.89	0.55
7:I:88:SER:HB2	7:I:90:GLN:HB2	1.89	0.55
10:L:38:LEU:HD22	10:L:56:LEU:HD21	1.88	0.55
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.42	0.54
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.42	0.54
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.42	0.54
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.21	0.54
2:B:35:SER:O	2:B:39:ARG:HB2	2.08	0.54
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.89	0.54
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.38	0.54
1:A:40:THR:HG22	1:A:49:LYS:HD2	1.90	0.54
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.90	0.54
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.90	0.54
2:B:243:ALA:HB2	2:B:251:ILE:HD13	1.89	0.53
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.43	0.53
1:A:1325:THR:HA	4:E:147:HIS:HA	1.90	0.53
1:A:1148:ILE:HB	1:A:1196:GLU:HG3	1.91	0.53
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.91	0.53
2:B:843:GLN:HB2	2:B:993:THR:HB	1.90	0.53
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.74	0.53
4:E:154:ILE:HD13	4:E:199:ILE:HD12	1.92	0.52
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.92	0.52
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.74	0.52
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.89	0.52
2:B:848:ARG:NH2	2:B:996:ARG:NH1	2.54	0.52
1:A:406:ILE:HG12	1:A:412:ARG:HG2	1.92	0.52
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.10	0.52
4:E:19:VAL:O	4:E:23:VAL:HG23	2.10	0.52
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.74	0.52
3:C:148:ARG:H	3:C:151:GLN:HG3	1.75	0.52
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.45	0.52
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.91	0.52
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.45	0.52
4:E:147:HIS:CD2	4:E:149:LEU:H	2.27	0.52
2:B:1122:ARG:HG2	12:T:23:DC:OP1	2.10	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.92	0.51
2:B:563:MET:HA	2:B:589:VAL:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.92	0.51
4:E:179:GLN:O	4:E:182:ASP:HB2	2.11	0.51
2:B:864:LYS:HB2	2:B:871:THR:HG23	1.92	0.51
3:C:167:HIS:HD2	3:C:169:LYS:H	1.58	0.51
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.93	0.51
7:I:10:CYS:SG	7:I:31:THR:HB	2.50	0.51
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.45	0.51
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	1.92	0.51
9:K:40:HIS:CE1	9:K:63:VAL:HG11	2.45	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
1:A:775:ILE:HG21	1:A:815:PHE:CE2	2.46	0.51
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.75	0.51
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.14	0.51
2:B:345:LYS:HG2	2:B:348:ARG:HD3	1.92	0.51
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.46	0.51
2:B:1181:GLU:HB2	2:B:1188:LYS:HG2	1.93	0.50
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.92	0.50
3:C:175:ALA:HB3	8:J:43:ARG:HH21	1.76	0.50
7:I:88:SER:C	7:I:90:GLN:H	2.14	0.50
1:A:741:ASN:ND2	1:A:744:LYS:H	2.03	0.50
4:E:31:THR:OG1	4:E:34:GLU:HB2	2.11	0.50
3:C:69:LEU:O	8:J:6:ARG:HD2	2.10	0.50
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.50
1:A:113:LEU:HD23	1:A:218:ASP:HB3	1.94	0.50
2:B:904:ARG:HG2	2:B:948:ILE:HG12	1.94	0.50
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.94	0.50
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.94	0.50
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.77	0.50
2:B:516:ASN:ND2	2:B:516:ASN:H	2.08	0.50
1:A:78:PRO:HB3	2:B:1201:LYS:HD2	1.92	0.50
1:A:821:ARG:HG3	1:A:825:ILE:CD1	2.41	0.49
1:A:738:LYS:HD3	1:A:740:LEU:HD21	1.93	0.49
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.94	0.49
1:A:5:GLN:HE22	2:B:1176:ASN:HD22	1.60	0.49
1:A:372:LYS:HG2	1:A:435:HIS:CD2	2.48	0.49
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.95	0.49
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.46	0.49
9:K:85:ASP:HA	9:K:88:LYS:HG2	1.94	0.49
1:A:121:LEU:HA	1:A:124:GLN:HB2	1.94	0.49
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.47	0.49
2:B:620:ARG:HH21	7:I:89:GLN:HE22	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:VAL:HG11	2:B:938:SER:HB3	1.95	0.48
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.60	0.48
1:A:1035:TYR:HB3	1:A:1037:LEU:HD13	1.95	0.48
3:C:39:ALA:HB1	3:C:165:LYS:HB2	1.96	0.48
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.96	0.48
2:B:797:TYR:HB2	2:B:852:ARG:O	2.14	0.48
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.95	0.48
6:H:28:ALA:HB3	6:H:38:LEU:HB3	1.95	0.48
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.95	0.48
1:A:140:THR:HA	1:A:143:LYS:HE3	1.94	0.48
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.48
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.96	0.48
10:L:61:THR:HB	10:L:63:ARG:H	1.78	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.13	0.48
3:C:46:ILE:HG23	3:C:157:CYS:HB2	1.94	0.48
10:L:40:LEU:HB3	10:L:44:ASP:HB2	1.96	0.48
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.95	0.48
1:A:335:ARG:HD3	2:B:1202:LEU:HD12	1.94	0.48
1:A:885:THR:O	1:A:940:ARG:HD2	2.12	0.48
7:I:19:ASP:HB2	7:I:24:ARG:HG3	1.95	0.48
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.95	0.48
1:A:1318:THR:HG22	4:E:142:VAL:HG22	1.95	0.48
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.95	0.48
1:A:567:LYS:HZ1	6:H:97:MET:HG2	1.80	0.47
2:B:879:ARG:HH12	2:B:885:MET:HG3	1.78	0.47
4:E:80:VAL:HG22	4:E:109:ILE:HD12	1.95	0.47
1:A:89:PRO:HB3	1:A:237:THR:HG23	1.96	0.47
4:E:147:HIS:HD2	4:E:149:LEU:H	1.62	0.47
1:A:775:ILE:HG21	1:A:815:PHE:CD2	2.50	0.47
1:A:858:ASN:HD21	1:A:860:LEU:HD12	1.78	0.47
1:A:761:MET:HG3	2:B:1021:MET:HG3	1.95	0.47
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.97	0.47
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.97	0.47
2:B:190:TYR:CD1	8:J:62:ARG:HG2	2.50	0.47
1:A:404:TYR:HB2	1:A:433:GLU:HG3	1.97	0.47
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.96	0.47
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.96	0.47
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.45	0.47
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.45	0.47
1:A:456:MET:HB2	1:A:478:TYR:OH	2.15	0.47
2:B:822:ASN:HD22	8:J:52:THR:CG2	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:TRP:HZ2	2:B:705:MET:CE	2.28	0.46
2:B:910:VAL:CG1	2:B:938:SER:HB3	2.44	0.46
3:C:104:PHE:CD1	3:C:152:GLU:HG3	2.46	0.46
5:F:83:PRO:HG2	5:F:84:TYR:CD1	2.50	0.46
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.81	0.46
1:A:1116:LEU:HD13	1:A:1329:THR:HB	1.97	0.46
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.97	0.46
2:B:273:LEU:HD12	2:B:280:ILE:HG13	1.97	0.46
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.45	0.46
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.96	0.46
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.97	0.46
4:E:125:PRO:O	4:E:127:ILE:N	2.47	0.46
2:B:387:LEU:HD23	2:B:393:LYS:HD3	1.97	0.46
2:B:308:TRP:CH2	7:I:45:ARG:HD3	2.50	0.46
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.80	0.46
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.36	0.46
4:E:98:ILE:HA	4:E:101:GLN:HG2	1.98	0.46
3:C:22:LEU:HD11	9:K:101:LEU:HD21	1.98	0.46
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.96	0.46
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.97	0.46
2:B:487:THR:H	2:B:490:SER:HB3	1.81	0.46
6:H:56:THR:HB	6:H:145:ARG:HB3	1.97	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.51	0.46
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.97	0.46
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.98	0.46
1:A:672:ASP:HB2	1:A:675:THR:OG1	2.16	0.46
2:B:1099:VAL:HB	2:B:1103:ILE:HD11	1.98	0.46
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.98	0.46
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.96	0.46
2:B:864:LYS:H	2:B:872:GLU:HB2	1.80	0.46
4:E:65:THR:O	4:E:69:ILE:HG12	2.16	0.46
1:A:528:LEU:O	1:A:531:ILE:HG22	2.16	0.46
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.97	0.46
1:A:89:PRO:HG2	1:A:205:GLU:HG2	1.98	0.46
1:A:512:VAL:HA	1:A:519:PRO:HA	1.98	0.45
2:B:704:ALA:HB1	2:B:710:LEU:HB3	1.98	0.45
1:A:1116:LEU:HB2	1:A:1308:THR:CG2	2.47	0.45
1:A:761:MET:CG	2:B:1021:MET:HG3	2.46	0.45
4:E:165:LEU:HD23	4:E:170:LEU:HB2	1.98	0.45
1:A:116:ASP:HA	1:A:117:GLU:HA	1.77	0.45
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:NH2	7:I:87:GLN:OE1	2.49	0.45
4:E:89:GLY:O	4:E:120:ALA:HB2	2.17	0.45
1:A:559:VAL:HG13	6:H:78:SER:HA	1.97	0.45
1:A:523:ILE:HG23	1:A:527:THR:HB	1.98	0.45
1:A:34:LYS:HE2	1:A:57:ARG:HH22	1.81	0.45
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.80	0.45
2:B:68:THR:HA	2:B:90:ILE:O	2.17	0.45
2:B:654:ARG:H	2:B:657:HIS:CD2	2.20	0.45
3:C:181:ASP:OD2	3:C:184:ASN:HA	2.17	0.45
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.97	0.45
2:B:683:SER:O	2:B:687:GLU:HB2	2.17	0.45
3:C:258:ILE:HG13	9:K:42:LEU:HD21	1.99	0.45
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.80	0.45
2:B:758:PHE:CZ	2:B:1031:LEU:HD22	2.51	0.45
2:B:1037:LEU:O	8:J:47:ARG:NH1	2.50	0.45
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.52	0.45
3:C:173:ALA:O	3:C:174:ALA:CB	2.65	0.45
9:K:113:THR:O	9:K:114:LEU:HB2	2.17	0.45
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.98	0.44
1:A:560:ILE:HB	6:H:79:TRP:HB3	1.99	0.44
1:A:75:ASN:HA	2:B:1116:ARG:NH1	2.31	0.44
2:B:137:TYR:HB3	2:B:140:ILE:HD11	1.99	0.44
2:B:732:SER:O	2:B:734:HIS:N	2.50	0.44
4:E:28:TYR:HA	4:E:64:PRO:HA	1.99	0.44
1:A:579:SER:HA	1:A:582:ILE:HD12	1.98	0.44
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.92	0.44
3:C:6:PRO:HB3	3:C:25:VAL:HG22	1.99	0.44
7:I:102:VAL:HG22	7:I:109:ILE:HG12	1.99	0.44
1:A:1116:LEU:HB2	1:A:1308:THR:HG21	1.99	0.44
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.82	0.44
2:B:254:LEU:CD2	2:B:381:MET:HE3	2.47	0.44
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.52	0.44
1:A:115:LEU:HD11	1:A:145:LYS:HG3	2.00	0.44
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.99	0.44
1:A:358:ASN:HB2	9:K:65:HIS:HD2	1.82	0.44
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.97	0.44
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.32	0.44
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.99	0.44
1:A:696:GLU:HG2	1:A:702:LEU:HD23	1.99	0.44
2:B:1082:MET:HA	3:C:189:THR:HA	1.99	0.44
2:B:804:GLY:O	2:B:983:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:193:GLY:HA2	4:E:213:ILE:HD11	2.00	0.44
6:H:130:ARG:HA	6:H:133:ASN:HD21	1.83	0.44
6:H:82:PRO:O	6:H:84:ALA:N	2.51	0.44
1:A:1328:TYR:OH	1:A:1351:GLU:OE1	2.31	0.44
2:B:256:VAL:HG12	2:B:385:LEU:HD22	1.99	0.44
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.53	0.44
1:A:167:CYS:SG	1:A:168:GLY:N	2.91	0.44
1:A:325:ILE:HG13	1:A:325:ILE:H	1.69	0.44
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.99	0.44
1:A:246:VAL:HA	2:B:1202:LEU:HD21	1.99	0.44
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.18	0.44
2:B:900:ALA:HA	10:L:58:LYS:HD3	1.99	0.44
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	2.00	0.44
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.47	0.44
2:B:824:ILE:HG12	8:J:48:ARG:NH2	2.33	0.44
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.51	0.43
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.58	0.43
2:B:773:MET:O	2:B:776:GLN:HB2	2.17	0.43
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.00	0.43
3:C:49:VAL:HG22	3:C:157:CYS:HB3	1.99	0.43
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.00	0.43
1:A:567:LYS:CB	1:A:568:PRO:CD	2.93	0.43
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.53	0.43
1:A:925:LEU:HA	1:A:925:LEU:HD23	1.90	0.43
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.83	0.43
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.58	0.43
2:B:282:ILE:HA	2:B:285:ILE:HD12	2.00	0.43
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.83	0.43
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.99	0.43
6:H:44:VAL:HG23	6:H:49:VAL:H	1.82	0.43
8:J:1:MET:SD	8:J:60:PHE:HE2	2.42	0.43
1:A:642:CYS:O	1:A:645:LEU:HB3	2.18	0.43
3:C:26:ASP:OD2	3:C:29:MET:HB2	2.18	0.43
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.67	0.43
1:A:534:LEU:HA	1:A:539:THR:HG21	2.00	0.43
2:B:976:ILE:O	2:B:990:ILE:O	2.36	0.43
8:J:48:ARG:HD2	8:J:49:MET:HE2	2.01	0.43
1:A:361:LEU:HD21	1:A:521:MET:HE1	2.00	0.43
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.83	0.43
1:A:365:GLY:HA3	1:A:469:ARG:HB2	2.01	0.43
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:55:ILE:HG12	10:L:55:ILE:H	1.65	0.43
2:B:526:GLU:HG3	2:B:771:SER:HB3	2.01	0.42
4:E:29:PHE:HB2	4:E:65:THR:HG23	2.00	0.42
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.96	0.42
1:A:1271:ILE:HA	1:A:1271:ILE:HD13	1.97	0.42
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.93	0.42
1:A:274:ILE:C	1:A:276:LEU:H	2.23	0.42
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.73	0.42
1:A:182:VAL:HA	1:A:202:LEU:HB3	2.00	0.42
1:A:247:ARG:HB3	1:A:262:LEU:HB3	2.02	0.42
1:A:440:ASP:O	1:A:460:VAL:HG23	2.19	0.42
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.85	0.42
2:B:254:LEU:HD23	2:B:381:MET:HE3	2.01	0.42
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.54	0.42
2:B:745:PRO:O	2:B:748:ILE:HG12	2.19	0.42
4:E:37:LEU:HA	4:E:38:PRO:HD3	1.96	0.42
7:I:58:VAL:HG11	7:I:109:ILE:HD11	2.02	0.42
1:A:589:GLN:HB3	1:A:961:ARG:HH22	1.85	0.42
2:B:228:LYS:O	2:B:261:ARG:NH2	2.51	0.42
2:B:1158:PHE:HD2	2:B:1160:VAL:HG22	1.84	0.42
2:B:956:THR:HB	10:L:46:VAL:HG21	2.00	0.42
2:B:975:GLN:O	2:B:990:ILE:HD12	2.19	0.42
2:B:273:LEU:HB2	2:B:276:ILE:HG22	2.01	0.42
3:C:66:ARG:NH2	8:J:3:VAL:O	2.43	0.42
1:A:351:THR:OG1	2:B:1103:ILE:CD1	2.68	0.42
1:A:594:GLY:HA3	1:A:601:LYS:HE2	2.01	0.42
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.20	0.42
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.54	0.42
2:B:459:TYR:CD2	2:B:468:GLU:HA	2.55	0.42
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.85	0.42
9:K:57:LEU:HB2	9:K:76:GLN:HG2	2.01	0.42
9:K:77:THR:HB	9:K:81:TYR:HB3	2.02	0.42
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.20	0.41
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.01	0.41
2:B:827:ILE:HA	2:B:1012:ILE:O	2.20	0.41
3:C:100:THR:HG22	3:C:119:VAL:HG13	2.00	0.41
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.55	0.41
9:K:39:ASP:HB2	9:K:40:HIS:H	1.71	0.41
1:A:345:VAL:HG12	2:B:1155:SER:HB2	2.02	0.41
2:B:620:ARG:NH2	7:I:89:GLN:HE22	2.18	0.41
1:A:134:ARG:HD3	1:A:221:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:VAL:CG1	1:A:385:ILE:HD12	2.50	0.41
1:A:841:LEU:HD12	1:A:1384:VAL:HG11	2.01	0.41
4:E:76:GLY:HA3	4:E:106:GLN:HB2	2.01	0.41
4:E:23:VAL:HG12	4:E:28:TYR:HB2	2.02	0.41
5:F:130:ILE:HB	5:F:148:VAL:HG11	2.03	0.41
7:I:75:CYS:O	7:I:78:CYS:O	2.38	0.41
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.03	0.41
1:A:491:VAL:O	1:A:493:GLN:NE2	2.54	0.41
4:E:198:ILE:HD13	4:E:212:ARG:HG3	2.02	0.41
4:E:9:ILE:HG22	4:E:39:LEU:HD11	2.02	0.41
1:A:600:PRO:HA	6:H:25:ARG:NH1	2.35	0.41
3:C:259:LEU:HD22	9:K:91:CYS:HB3	2.01	0.41
1:A:1216:ILE:HG22	1:A:1226:VAL:HG21	2.02	0.41
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.02	0.41
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.24	0.41
2:B:69:LEU:HD13	2:B:432:MET:HE1	2.03	0.41
1:A:527:THR:HG21	1:A:650:GLN:HA	2.02	0.41
1:A:902:LEU:HG	1:A:926:GLN:HG3	2.03	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.41
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.11	0.41
1:A:361:LEU:HD12	1:A:471:ASN:HD22	1.85	0.41
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.01	0.41
1:A:513:SER:HB3	1:A:520:CYS:HB3	2.03	0.41
1:A:839:ARG:HB2	1:A:839:ARG:HH11	1.85	0.41
2:B:1162:ILE:HG12	2:B:1194:ILE:HG12	2.02	0.41
1:A:786:HIS:CE1	2:B:742:GLU:OE1	2.68	0.41
1:A:315:LEU:HB3	1:A:316:GLN:H	1.79	0.41
1:A:588:LEU:HB3	1:A:607:ILE:HD12	2.02	0.41
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.03	0.41
3:C:105:GLY:O	3:C:149:LYS:O	2.37	0.41
3:C:36:VAL:HG23	3:C:40:GLU:HB2	2.03	0.41
7:I:62:ILE:HG12	7:I:84:VAL:HG21	2.03	0.41
1:A:392:VAL:HG13	1:A:415:LEU:HD11	2.04	0.41
1:A:474:VAL:HG23	1:A:521:MET:HE3	2.03	0.41
2:B:706:GLN:O	2:B:710:LEU:HB2	2.21	0.41
1:A:483:ASP:HA	2:B:988:GLY:HA2	2.03	0.41
1:A:496:GLU:H	1:A:496:GLU:HG2	1.78	0.40
1:A:592:ASP:H	1:A:595:THR:HG21	1.85	0.40
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.57	0.40
6:H:63:LEU:HB2	6:H:90:ALA:H	1.86	0.40
2:B:1039:GLY:O	8:J:32:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.55	0.40
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.40
3:C:73:GLN:O	3:C:129:ILE:HA	2.21	0.40
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.02	0.40
1:A:389:THR:O	1:A:393:ARG:HG2	2.22	0.40
2:B:123:THR:HG23	2:B:205:ILE:HA	2.03	0.40
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.56	0.40
4:E:100:ILE:HG13	4:E:105:PHE:HB2	2.03	0.40
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.03	0.40
1:A:737:LEU:HD11	1:A:758:ILE:HG23	2.03	0.40
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.86	0.40
1:A:852:TYR:O	5:F:81:THR:HG22	2.21	0.40
1:A:113:LEU:HD21	1:A:222:LEU:HD13	2.03	0.40
1:A:351:THR:OG1	2:B:1103:ILE:HD13	2.21	0.40
1:A:358:ASN:HB2	9:K:65:HIS:CD2	2.57	0.40
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1395/1733 (80%)	1205 (86%)	137 (10%)	53 (4%)	4	25
2	B	1096/1224 (90%)	958 (87%)	90 (8%)	48 (4%)	3	22
3	C	264/318 (83%)	238 (90%)	19 (7%)	7 (3%)	6	35
4	E	212/215 (99%)	185 (87%)	22 (10%)	5 (2%)	7	39
5	F	83/155 (54%)	75 (90%)	6 (7%)	2 (2%)	7	39
6	H	129/146 (88%)	102 (79%)	18 (14%)	9 (7%)	1	9
7	I	117/122 (96%)	101 (86%)	14 (12%)	2 (2%)	11	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	63/70 (90%)	55 (87%)	7 (11%)	1 (2%)	11	50
9	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
10	L	44/70 (63%)	27 (61%)	7 (16%)	10 (23%)	0	0
All	All	3515/4173 (84%)	3053 (87%)	325 (9%)	137 (4%)	3	25

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	65	LEU
1	A	119	ASN
1	A	399	HIS
1	A	424	ILE
1	A	567	LYS
1	A	597	LEU
1	A	846	GLU
1	A	1123	GLY
1	A	1221	LYS
1	A	1378	GLN
1	A	1437	GLY
2	B	137	TYR
2	B	476	ARG
2	B	510	LYS
2	B	648	HIS
2	B	709	ASP
2	B	712	PRO
2	B	733	HIS
2	B	751	VAL
2	B	1046	PRO
2	B	1156	ASP
3	C	40	GLU
3	C	215	GLU
3	C	227	THR
4	E	126	SER
5	F	73	ALA
6	H	83	GLN
6	H	131	ASN
7	I	91	ARG
8	J	6	ARG
10	L	50	ASP
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	250	ILE
1	A	312	PRO
1	A	332	LYS
1	A	385	ILE
1	A	672	ASP
1	A	1124	HIS
1	A	1188	GLN
1	A	1377	THR
2	B	67	SER
2	B	138	GLU
2	B	168	GLY
2	B	176	SER
2	B	277	LYS
2	B	364	ILE
2	B	480	SER
2	B	531	GLN
2	B	708	GLU
2	B	891	ASP
2	B	1171	VAL
2	B	1181	GLU
3	C	174	ALA
6	H	90	ALA
7	I	115	LYS
10	L	49	LYS
10	L	51	CYS
10	L	64	LEU
1	A	42	ASP
1	A	308	ILE
1	A	324	SER
1	A	592	ASP
1	A	595	THR
1	A	1089	VAL
2	B	250	PHE
2	B	367	LEU
2	B	468	GLU
2	B	792	MET
2	B	864	LYS
2	B	865	LYS
2	B	879	ARG
2	B	887	HIS
2	B	974	PRO
2	B	1157	ALA

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Mol	Chain	Res	Type
2	B	1180	PHE
2	B	1223	ASP
3	C	4	GLU
4	E	3	GLN
4	E	99	HIS
5	F	112	GLU
6	H	18	GLY
6	H	108	SER
10	L	40	LEU
1	A	53	LEU
1	A	56	PRO
1	A	110	CYS
1	A	111	GLY
1	A	149	GLU
1	A	214	ILE
1	A	275	SER
1	A	569	LYS
1	A	852	TYR
2	B	474	SER
2	B	943	SER
2	B	1017	ILE
3	C	90	ASP
4	E	51	GLY
6	H	109	LYS
6	H	136	LYS
6	H	140	ALA
10	L	47	ARG
10	L	55	ILE
10	L	56	LEU
1	A	217	LYS
1	A	400	PRO
1	A	576	GLN
1	A	916	GLY
1	A	958	VAL
1	A	1376	THR
2	B	139	ALA
2	B	1099	VAL
10	L	46	VAL
10	L	59	ALA
1	A	543	LEU
1	A	1028	THR
2	B	177	LYS

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Mol	Chain	Res	Type
2	B	447	ALA
2	B	471	LYS
4	E	37	LEU
1	A	73	GLY
1	A	258	GLY
1	A	325	ILE
2	B	647	GLY
3	C	5	GLY
1	A	35	ILE
1	A	1122	PRO
1	A	1388	GLY
2	B	592	ASN
2	B	479	VAL
2	B	711	GLU
2	B	907	GLY
2	B	1119	VAL
6	H	107	VAL
1	A	973	ILE
1	A	1384	VAL
1	A	775	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%)	1046 (85%)	179 (15%)	3	17
2	B	967/1061 (91%)	840 (87%)	127 (13%)	5	22
3	C	234/274 (85%)	208 (89%)	26 (11%)	7	30
4	E	196/197 (100%)	174 (89%)	22 (11%)	7	29
5	F	75/137 (55%)	64 (85%)	11 (15%)	3	16
6	H	117/128 (91%)	99 (85%)	18 (15%)	3	15
7	I	113/116 (97%)	101 (89%)	12 (11%)	8	32
8	J	60/65 (92%)	49 (82%)	11 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	K	99/102 (97%)	83 (84%)	16 (16%)	3	13
10	L	40/57 (70%)	27 (68%)	13 (32%)	0	0
All	All	3126/3657 (86%)	2691 (86%)	435 (14%)	4	19

All (435) 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	21	LEU
1	A	50	ILE
1	A	58	LEU
1	A	62	ASP
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	75	ASN
1	A	83	HIS
1	A	93	VAL
1	A	113	LEU
1	A	126	LEU
1	A	129	LYS
1	A	133	LYS
1	A	134	ARG
1	A	141	LEU
1	A	144	THR
1	A	147	VAL
1	A	151	ASP
1	A	152	VAL
1	A	170	THR
1	A	206	GLU
1	A	214	ILE
1	A	219	PHE
1	A	220	THR
1	A	226	GLU
1	A	232	GLU
1	A	235	ILE
1	A	237	THR
1	A	252	PHE
1	A	254	GLU

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Mol	Chain	Res	Type
1	A	263	THR
1	A	265	LYS
1	A	270	LEU
1	A	276	LEU
1	A	278	THR
1	A	279	LEU
1	A	290	GLU
1	A	291	GLU
1	A	295	LEU
1	A	308	ILE
1	A	311	GLN
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	329	LEU
1	A	335	ARG
1	A	344	ARG
1	A	353	ILE
1	A	354	SER
1	A	359	LEU
1	A	368	LYS
1	A	389	THR
1	A	398	GLU
1	A	407	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	455	MET
1	A	456	MET
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	493	GLN
1	A	500	GLU
1	A	513	SER
1	A	518	LYS

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Mol	Chain	Res	Type
1	A	527	THR
1	A	532	ARG
1	A	541	ILE
1	A	560	ILE
1	A	567	LYS
1	A	569	LYS
1	A	595	THR
1	A	597	LEU
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	636	GLU
1	A	640	GLN
1	A	644	LYS
1	A	672	ASP
1	A	678	GLU
1	A	681	GLU
1	A	688	LYS
1	A	691	LEU
1	A	705	LYS
1	A	710	LEU
1	A	719	VAL
1	A	722	LEU
1	A	728	LYS
1	A	740	LEU
1	A	756	ILE
1	A	762	SER
1	A	773	LYS
1	A	774	ARG
1	A	782	ARG
1	A	806	ARG
1	A	821	ARG
1	A	838	GLN
1	A	839	ARG
1	A	867	ILE
1	A	883	LEU
1	A	894	GLU
1	A	896	ARG
1	A	902	LEU
1	A	905	ASP
1	A	908	LEU

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Mol	Chain	Res	Type
1	A	912	LEU
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	926	GLN
1	A	941	LYS
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE
1	A	982	THR
1	A	988	LEU
1	A	992	ASP
1	A	1005	GLU
1	A	1025	ARG
1	A	1029	ARG
1	A	1048	ASN
1	A	1062	GLU
1	A	1067	LEU
1	A	1081	LEU
1	A	1086	PHE
1	A	1089	VAL
1	A	1109	LYS
1	A	1110	ASN
1	A	1116	LEU
1	A	1124	HIS
1	A	1141	THR
1	A	1147	THR
1	A	1165	GLU
1	A	1172	LEU
1	A	1175	SER
1	A	1187	GLN
1	A	1215	ARG
1	A	1227	ILE
1	A	1242	VAL
1	A	1256	GLU
1	A	1261	LYS
1	A	1280	GLU
1	A	1283	VAL
1	A	1284	MET
1	A	1288	ASP
1	A	1293	SER
1	A	1295	THR

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Mol	Chain	Res	Type
1	A	1297	GLU
1	A	1303	GLU
1	A	1308	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1334	ASP
1	A	1350	LYS
1	A	1354	ASN
1	A	1364	ASN
1	A	1366	ARG
1	A	1382	THR
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1432	GLN
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
2	B	28	GLU
2	B	41	LYS
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	89	GLU
2	B	101	MET
2	B	102	VAL
2	B	128	LEU
2	B	130	VAL
2	B	134	LYS
2	B	135	ARG
2	B	165	VAL
2	B	167	ILE
2	B	175	ARG
2	B	178	ASN
2	B	187	SER
2	B	194	GLU
2	B	208	SER
2	B	217	ARG
2	B	221	ASN
2	B	234	ILE
2	B	245	GLU

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	265	SER
2	B	267	ARG
2	B	277	LYS
2	B	292	ILE
2	B	306	ASN
2	B	323	VAL
2	B	325	GLN
2	B	333	PHE
2	B	350	GLN
2	B	367	LEU
2	B	373	ARG
2	B	376	PHE
2	B	384	ARG
2	B	392	ARG
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG
2	B	401	PHE
2	B	418	LYS
2	B	433	GLN
2	B	437	GLU
2	B	448	ILE
2	B	458	LYS
2	B	461	LEU
2	B	466	TRP
2	B	468	GLU
2	B	471	LYS
2	B	479	VAL
2	B	485	ARG
2	B	486	TYR
2	B	537	LYS
2	B	547	VAL
2	B	554	ILE
2	B	574	SER
2	B	591	ARG
2	B	598	GLU
2	B	604	ARG
2	B	616	ILE
2	B	620	ARG
2	B	629	ASP
2	B	642	ASP

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Mol	Chain	Res	Type
2	B	643	ASP
2	B	645	SER
2	B	649	LYS
2	B	653	VAL
2	B	655	LYS
2	B	690	VAL
2	B	694	ASP
2	B	696	GLU
2	B	706	GLN
2	B	711	GLU
2	B	737	THR
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	797	TYR
2	B	807	ARG
2	B	815	ARG
2	B	835	GLN
2	B	838	SER
2	B	844	SER
2	B	866	TYR
2	B	870	ILE
2	B	875	GLU
2	B	880	THR
2	B	883	LEU
2	B	886	LYS
2	B	906	SER
2	B	945	GLU
2	B	959	ASP
2	B	961	LEU
2	B	963	PHE
2	B	973	ILE
2	B	983	ARG
2	B	987	LYS
2	B	993	THR
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU

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Mol	Chain	Res	Type
2	B	1065	GLN
2	B	1067	ARG
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1106	ARG
2	B	1108	ARG
2	B	1111	MET
2	B	1122	ARG
2	B	1128	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1172	ILE
2	B	1181	GLU
2	B	1195	HIS
2	B	1202	LEU
2	B	1211	ASN
3	C	9	LYS
3	C	12	GLU
3	C	43	THR
3	C	53	THR
3	C	75	MET
3	C	77	ILE
3	C	80	LEU
3	C	100	THR
3	C	109	SER
3	C	119	VAL
3	C	129	ILE
3	C	136	ASP
3	C	137	LYS
3	C	151	GLN
3	C	156	THR
3	C	157	CYS
3	C	215	GLU
3	C	222	LYS
3	C	231	ASN
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS

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Mol	Chain	Res	Type
3	C	259	LEU
3	C	265	MET
3	C	266	ASP
3	C	268	ASP
4	E	7	ARG
4	E	30	ILE
4	E	52	ARG
4	E	54	GLN
4	E	55	ARG
4	E	61	GLN
4	E	65	THR
4	E	75	MET
4	E	78	LEU
4	E	90	VAL
4	E	95	THR
4	E	100	ILE
4	E	104	ASN
4	E	127	ILE
4	E	142	VAL
4	E	156	LEU
4	E	158	SER
4	E	162	ARG
4	E	169	ARG
4	E	204	THR
4	E	213	ILE
4	E	215	MET
5	F	71	GLU
5	F	78	GLN
5	F	82	THR
5	F	99	LEU
5	F	110	ASP
5	F	111	LEU
5	F	112	GLU
5	F	119	ARG
5	F	127	GLU
5	F	138	LEU
5	F	152	ILE
6	H	11	GLN
6	H	13	SER
6	H	24	CYS
6	H	26	ILE
6	H	34	ASP

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Mol	Chain	Res	Type
6	H	35	GLN
6	H	56	THR
6	H	63	LEU
6	H	77	ARG
6	H	87	ARG
6	H	92	ASP
6	H	107	VAL
6	H	109	LYS
6	H	111	LEU
6	H	130	ARG
6	H	132	LEU
6	H	135	LEU
6	H	139	ASN
7	I	12	ASN
7	I	17	ARG
7	I	31	THR
7	I	35	VAL
7	I	37	GLU
7	I	61	ASP
7	I	62	ILE
7	I	70	ARG
7	I	88	SER
7	I	90	GLN
7	I	97	MET
7	I	118	ARG
8	J	1	MET
8	J	3	VAL
8	J	7	CYS
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	37	SER
8	J	43	ARG
8	J	48	ARG
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	11	LEU
9	K	12	LEU
9	K	14	GLU
9	K	20	LYS
9	K	26	LYS

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Mol	Chain	Res	Type
9	K	31	VAL
9	K	54	ARG
9	K	63	VAL
9	K	74	ARG
9	K	75	ILE
9	K	78	THR
9	K	81	TYR
9	K	85	ASP
9	K	97	LYS
9	K	101	LEU
10	L	26	THR
10	L	27	LEU
10	L	28	LYS
10	L	33	GLU
10	L	44	ASP
10	L	48	CYS
10	L	50	ASP
10	L	51	CYS
10	L	55	ILE
10	L	58	LYS
10	L	62	LYS
10	L	64	LEU
10	L	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	64	ASN
1	A	225	ASN
1	A	253	ASN
1	A	339	ASN
1	A	445	ASN
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	626	ASN
1	A	631	HIS
1	A	660	ASN
1	A	717	ASN
1	A	741	ASN

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Mol	Chain	Res	Type
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	854	ASN
1	A	877	HIS
1	A	965	GLN
1	A	969	GLN
1	A	1048	ASN
1	A	1052	GLN
1	A	1140	HIS
1	A	1265	ASN
1	A	1278	ASN
1	A	1364	ASN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	395	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	573	GLN
2	B	657	HIS
2	B	744	HIS
2	B	822	ASN
2	B	878	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1112	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1176	ASN
3	C	24	ASN
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	61	GLN
4	E	147	HIS
6	H	11	GLN

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Mol	Chain	Res	Type
6	H	133	ASN
7	I	89	GLN
9	K	89	ASN
9	K	110	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/5 (60%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	8	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	$\# Z > 2$
13	GTP	R	100	-	27,34,34	1.38	4 (14%)	27,54,54	1.88	7 (25%)

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
13	GTP	R	100	-	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	100	GTP	C8-N7	-2.56	1.29	1.34
13	R	100	GTP	C6-N1	2.40	1.37	1.33
13	R	100	GTP	PG-O3B	2.67	1.64	1.60
13	R	100	GTP	O4'-C1'	2.94	1.45	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	100	GTP	N3-C2-N1	-4.10	121.47	127.46
13	R	100	GTP	C5-C6-N1	-3.49	118.52	123.48
13	R	100	GTP	C4-C5-N7	-2.88	106.62	109.41
13	R	100	GTP	C6-C5-C4	-2.68	118.18	120.84
13	R	100	GTP	C4'-O4'-C1'	-2.54	107.06	109.77
13	R	100	GTP	C6-N1-C2	3.03	120.41	116.06
13	R	100	GTP	C2-N3-C4	5.10	121.12	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1405/1733 (81%)	-0.08	85 (6%) 23 13	49, 97, 192, 214	0
2	B	1114/1224 (91%)	-0.25	39 (3%) 44 29	48, 84, 152, 204	0
3	C	266/318 (83%)	-0.43	0 100 100	58, 81, 117, 175	0
4	E	214/215 (99%)	-0.17	6 (2%) 53 39	69, 124, 172, 182	0
5	F	85/155 (54%)	-0.32	0 100 100	73, 103, 140, 156	0
6	H	133/146 (91%)	0.12	10 (7%) 15 8	97, 131, 163, 178	0
7	I	119/122 (97%)	-0.32	0 100 100	61, 101, 141, 156	0
8	J	65/70 (92%)	-0.43	0 100 100	55, 73, 107, 123	0
9	K	114/120 (95%)	-0.42	1 (0%) 84 75	59, 91, 118, 133	0
10	L	46/70 (65%)	0.00	2 (4%) 36 23	70, 116, 147, 156	0
11	R	5/5 (100%)	2.61	3 (60%) 0 0	202, 206, 209, 212	0
12	T	8/29 (27%)	1.52	2 (25%) 1 1	169, 178, 191, 196	0
All	All	3574/4207 (84%)	-0.18	148 (4%) 38 25	48, 94, 180, 214	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	6.8
2	B	883	LEU	5.7
1	A	73	GLY	5.6
1	A	316	GLN	5.5
1	A	161	LEU	5.5
2	B	1222	ARG	5.2
1	A	42	ASP	5.2
1	A	151	ASP	5.2
2	B	1224	PHE	5.0
1	A	72	GLU	5.0
2	B	474	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	318	SER	4.9
1	A	69	THR	4.9
1	A	251	SER	4.9
1	A	1082	ASN	4.6
1	A	1086	PHE	4.6
6	H	86	ASP	4.5
1	A	44	THR	4.4
1	A	45	GLN	4.3
1	A	87	ALA	4.3
1	A	255	SER	4.3
1	A	1087	ALA	4.2
2	B	709	ASP	4.2
2	B	477	ALA	4.2
11	R	6	A	4.2
1	A	317	LYS	4.2
2	B	882	THR	4.1
2	B	1221	SER	4.0
1	A	41	MET	3.8
2	B	1223	ASP	3.8
1	A	250	ILE	3.7
11	R	8	A	3.7
1	A	199	LEU	3.7
1	A	1089	VAL	3.7
1	A	153	PRO	3.6
2	B	250	PHE	3.6
1	A	1085	HIS	3.6
4	E	104	ASN	3.6
2	B	1169	MET	3.6
2	B	865	LYS	3.6
1	A	315	LEU	3.5
1	A	256	GLN	3.4
2	B	468	GLU	3.4
1	A	212	LYS	3.4
1	A	286	HIS	3.4
2	B	866	TYR	3.4
1	A	183	GLY	3.4
1	A	975	HIS	3.4
1	A	65	LEU	3.3
1	A	137	ALA	3.3
1	A	283	GLY	3.3
2	B	471	LYS	3.3
2	B	231	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
6	H	84	ALA	3.3
1	A	62	ASP	3.3
10	L	27	LEU	3.2
1	A	319	GLY	3.2
2	B	136	THR	3.2
6	H	107	VAL	3.2
12	T	23	DC	3.1
2	B	246	LYS	3.1
12	T	16	DC	3.1
1	A	280	GLU	3.1
1	A	162	VAL	3.1
11	R	7	G	3.1
2	B	1205	GLN	3.0
1	A	141	LEU	3.0
1	A	257	ARG	3.0
2	B	478	GLY	2.9
6	H	83	GLN	2.9
1	A	200	ARG	2.9
1	A	253	ASN	2.9
2	B	1209	ALA	2.9
2	B	470	LYS	2.9
1	A	182	VAL	2.9
1	A	176	LYS	2.9
1	A	1090	ALA	2.9
1	A	249	SER	2.9
1	A	165	GLY	2.8
1	A	49	LYS	2.8
1	A	252	PHE	2.8
1	A	64	ASN	2.8
1	A	167	CYS	2.8
1	A	1088	GLY	2.7
2	B	106	ASP	2.7
2	B	1219	ASP	2.7
4	E	2	ASP	2.7
2	B	467	GLY	2.7
2	B	1208	MET	2.7
6	H	132	LEU	2.7
2	B	1186	ASP	2.6
1	A	169	ASN	2.6
1	A	152	VAL	2.6
1	A	1123	GLY	2.6
1	A	311	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	475	SER	2.5
2	B	867	GLY	2.5
4	E	118	PRO	2.5
2	B	919	SER	2.5
1	A	1391	ARG	2.5
1	A	166	GLY	2.4
2	B	139	ALA	2.4
2	B	1176	ASN	2.4
2	B	135	ARG	2.4
1	A	314	ALA	2.4
1	A	1175	SER	2.4
1	A	71	GLN	2.4
1	A	34	LYS	2.4
1	A	1084	PHE	2.4
1	A	254	GLU	2.4
1	A	258	GLY	2.3
6	H	108	SER	2.3
2	B	230	ALA	2.3
1	A	92	HIS	2.3
6	H	139	ASN	2.2
6	H	117	SER	2.2
1	A	307	ASP	2.2
1	A	6	TYR	2.2
1	A	282	ASN	2.2
1	A	321	PRO	2.2
10	L	45	ALA	2.2
1	A	127	ALA	2.2
2	B	714	GLU	2.2
1	A	292	ALA	2.2
1	A	1083	THR	2.2
1	A	213	HIS	2.2
1	A	118	HIS	2.2
1	A	116	ASP	2.2
4	E	119	SER	2.2
1	A	136	ALA	2.1
2	B	933	SER	2.1
1	A	5	GLN	2.1
9	K	15	GLY	2.1
6	H	111	LEU	2.1
1	A	8	SER	2.1
1	A	184	SER	2.1
2	B	870	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	E	123	LEU	2.1
1	A	281	HIS	2.1
1	A	147	VAL	2.1
2	B	645	SER	2.1
4	E	86	PRO	2.0
1	A	63	ARG	2.0
1	A	232	GLU	2.0
6	H	131	ASN	2.0
2	B	473	MET	2.0
1	A	1092	LYS	2.0
1	A	75	ASN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	GTP	R	100	32/32	0.61	0.36	3.72	249,251,254,256	0
14	ZN	C	319	1/1	0.99	0.10	-0.94	89,89,89,89	0
14	ZN	J	101	1/1	0.99	0.17	-1.00	78,78,78,78	0
14	ZN	I	204	1/1	0.98	0.08	-1.29	82,82,82,82	0
14	ZN	B	1307	1/1	0.85	0.09	-1.34	183,183,183,183	0
14	ZN	I	203	1/1	0.98	0.06	-1.39	102,102,102,102	0
14	ZN	A	1735	1/1	0.92	0.16	-1.81	176,176,176,176	0
14	ZN	L	105	1/1	0.99	0.04	-2.33	99,99,99,99	0
14	ZN	A	1734	1/1	0.90	0.05	-	289,289,289,289	0
15	MG	A	2001	1/1	0.98	0.07	-	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.