



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:05 AM UTC

PDB ID : 3S2H / pdb_00003s2h
Title : RNA Polymerase II Initiation Complex with a 6-nt RNA containing a 2[prime]-iodo 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

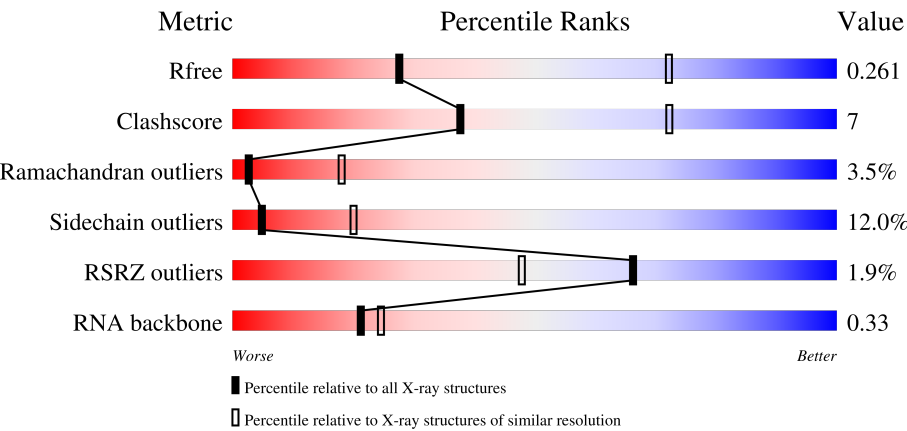
1 Overall quality at a glance i

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 _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	2% 58% 20% • 19%
2	B	1224	2% 61% 26% • 9%
3	C	318	% 57% 25% • 16%
4	E	215	% 79% 19% •

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Mol	Chain	Length	Quality of chain
5	F	155	39%13%45%
6	H	146	3% 66%23%9%
7	I	122	2% 70%25%
8	J	70	% 49%33%10%7%
9	K	120	% 70%22%5%
10	L	70	6% 44%13%9%34%
11	R	6	33%50%17%
12	T	29	3% 34%7%59%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28674 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*GP*(2IA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	6	Total	C	I	N	O	P	0	0
			132	60	1	30	36	5		

- 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	12	Total	C	N	O	P	0	0	0
			241	115	41	73	12			

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

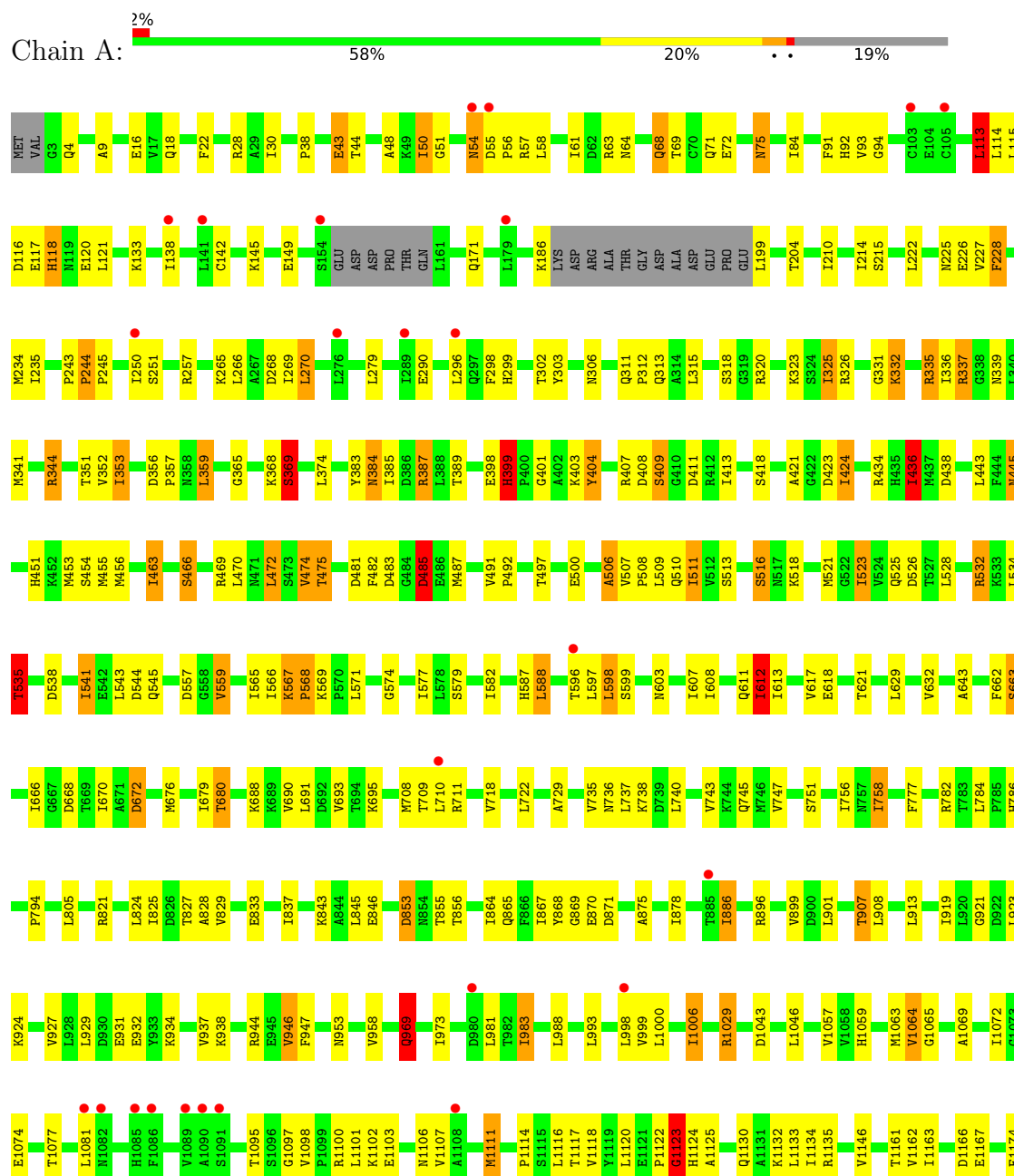
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

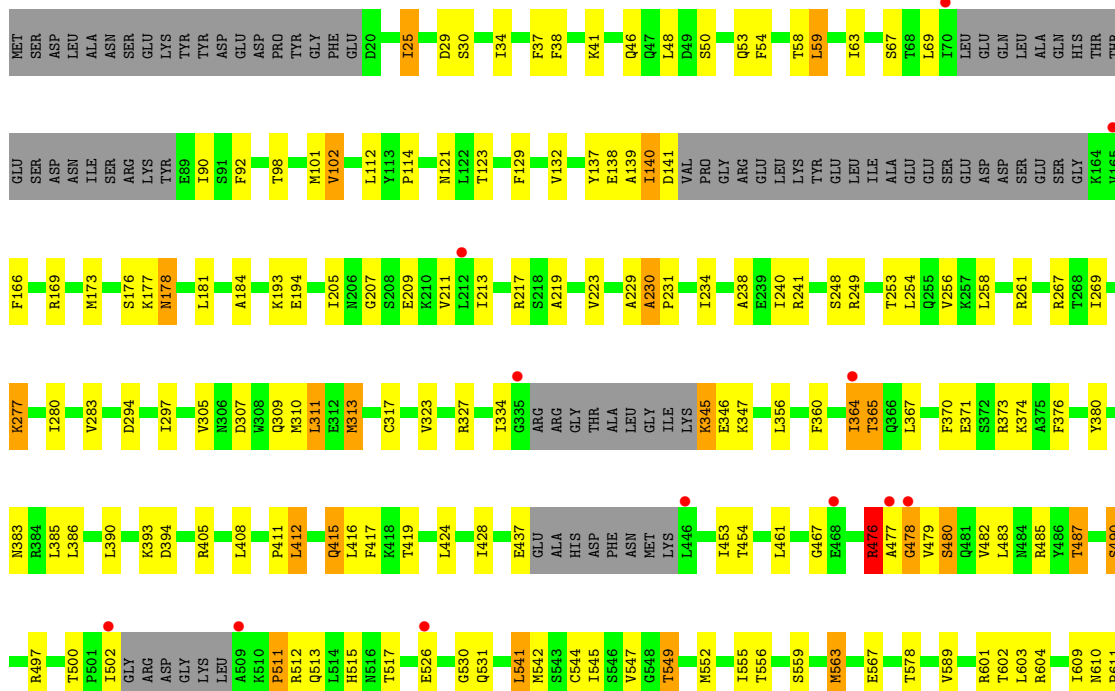
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

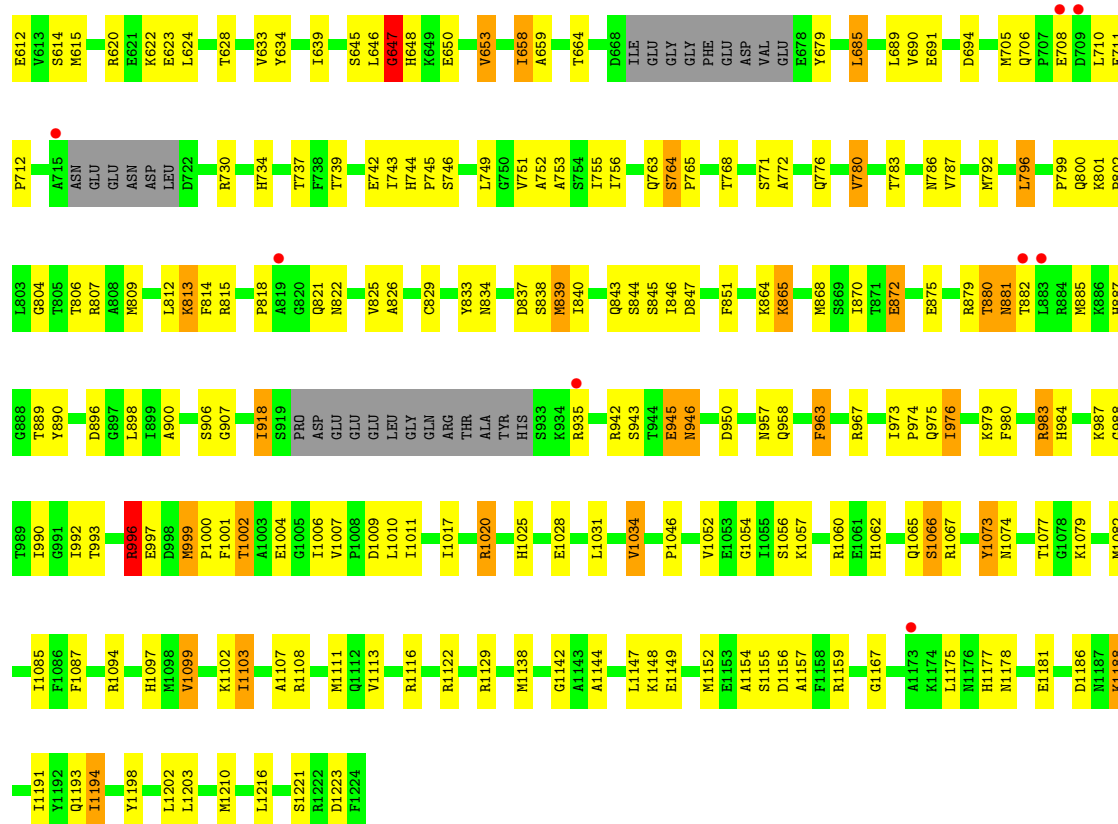
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

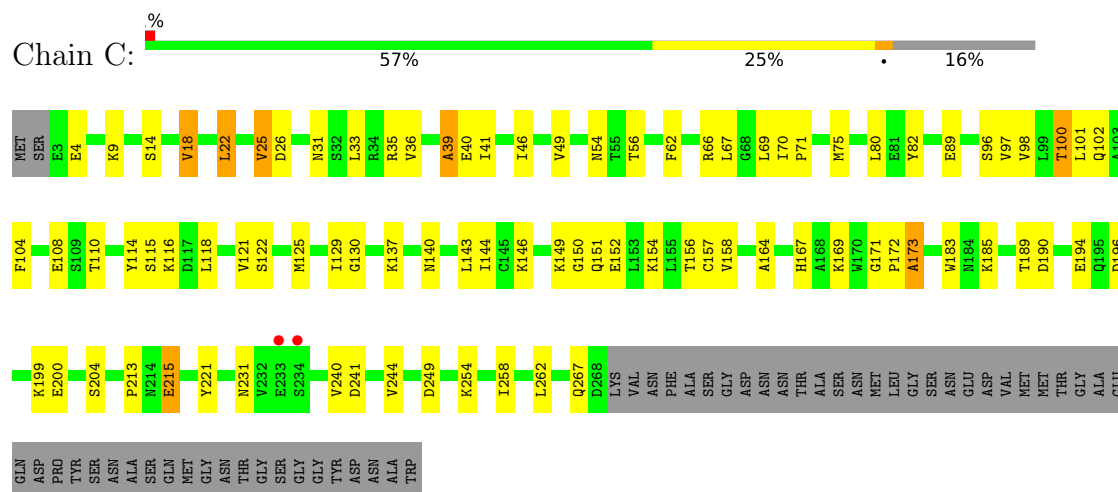
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



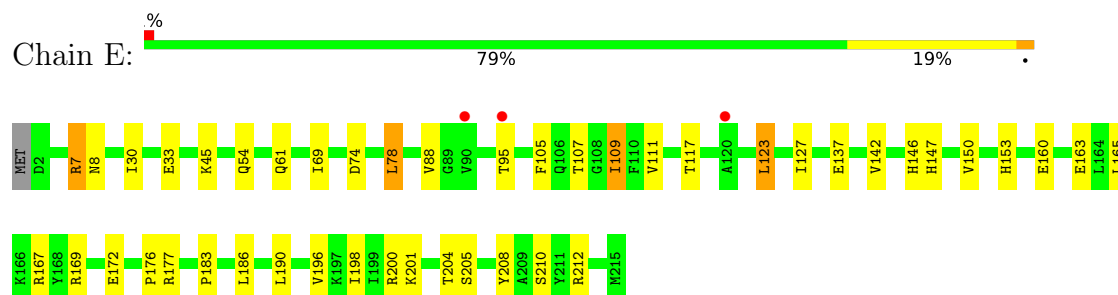




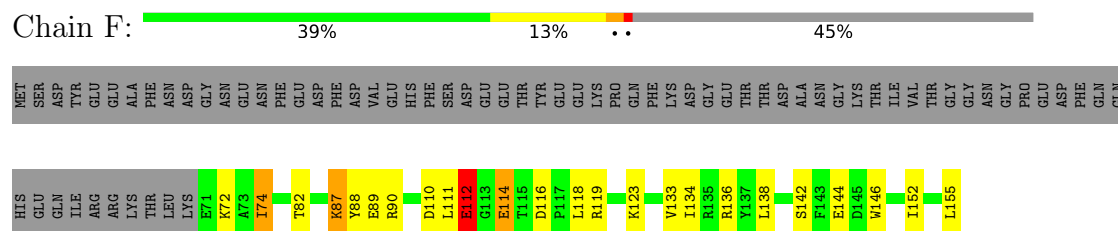
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



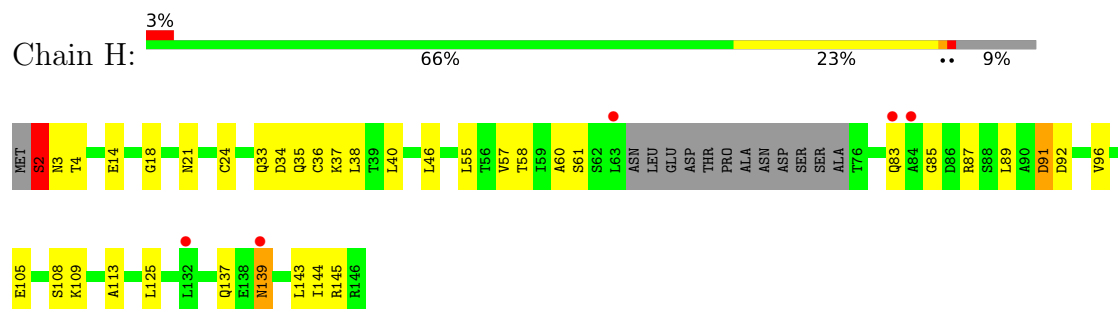
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



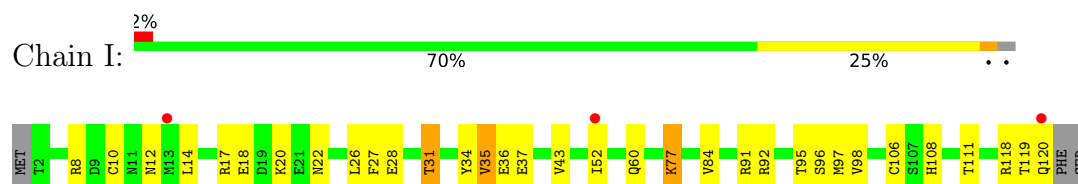
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



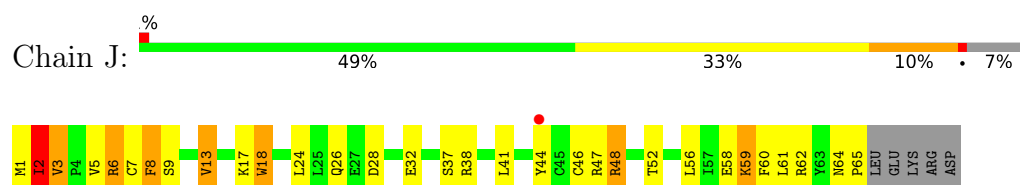
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



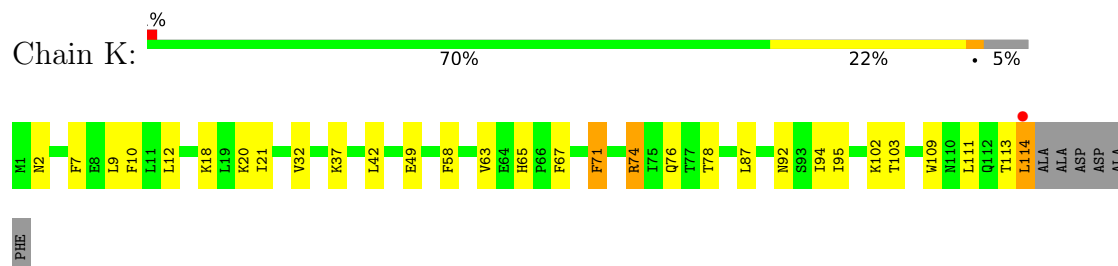
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



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

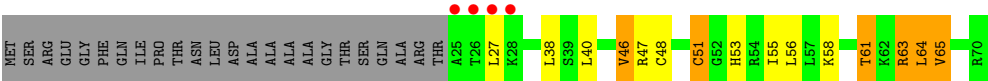


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

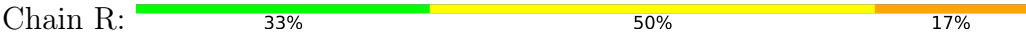


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

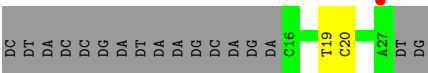




● Molecule 11: RNA (5'-R(*AP*GP*AP*GP*GP*(2IA))-3')



● 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, α , β , γ	165.53Å 221.61Å 194.06Å 90.00° 99.67° 90.00°	Depositor
Resolution (Å)	49.81 – 3.30 49.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.81-3.30) 96.5 (49.81-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.33Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.191 , 0.240 0.210 , 0.261	Depositor DCC
R_{free} test set	4987 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 109.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28674	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: ZN, MG, 2IA

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	0.79	1/11241 (0.0%)	1.44	77/15199 (0.5%)
2	B	0.79	0/9033	1.42	51/12181 (0.4%)
3	C	0.72	0/2133	1.35	12/2891 (0.4%)
4	E	0.78	0/1788	1.38	7/2406 (0.3%)
5	F	0.79	0/700	1.32	2/945 (0.2%)
6	H	0.72	0/1086	1.19	10/1470 (0.7%)
7	I	0.73	0/989	1.29	1/1331 (0.1%)
8	J	0.80	0/541	1.55	6/727 (0.8%)
9	K	0.68	0/937	1.39	5/1265 (0.4%)
10	L	0.80	0/365	1.39	2/485 (0.4%)
11	R	0.41	0/124	0.93	0/193
12	T	0.40	0/268	1.12	0/410
All	All	0.77	1/29205 (0.0%)	1.40	173/39503 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1074	GLU	CA-C	5.32	1.58	1.52

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	827	THR	N-CA-C	-10.45	100.26	113.43
2	B	890	TYR	N-CA-C	-9.11	102.17	113.28
2	B	1009	ASP	N-CA-C	-8.29	103.30	113.50
3	C	172	PRO	CA-C-N	8.27	137.34	121.54
3	C	172	PRO	C-N-CA	8.27	137.34	121.54
1	A	921	GLY	N-CA-C	-8.22	104.11	111.67
6	H	92	ASP	N-CA-C	-8.20	100.94	113.89
9	K	71	PHE	CA-CB-CG	8.04	121.84	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	18	TRP	N-CA-C	7.57	120.25	111.02
2	B	140	ILE	CA-C-N	7.13	134.53	121.70
2	B	140	ILE	C-N-CA	7.13	134.53	121.70
1	A	466	SER	N-CA-C	7.10	121.53	113.01
1	A	864	ILE	N-CA-C	-6.87	105.14	111.67
2	B	647	GLY	CA-C-N	6.86	134.06	121.70
2	B	647	GLY	C-N-CA	6.86	134.06	121.70
2	B	541	LEU	N-CA-C	6.65	119.09	111.11
1	A	485	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	506	ALA	CA-C-N	6.59	126.76	120.43
1	A	506	ALA	C-N-CA	6.59	126.76	120.43
2	B	847	ASP	CA-CB-CG	6.54	119.14	112.60
2	B	786	ASN	CA-C-N	6.53	130.83	121.55
2	B	786	ASN	C-N-CA	6.53	130.83	121.55
1	A	244	PRO	N-CA-C	6.53	118.66	110.70
2	B	345	LYS	CA-C-N	6.50	133.41	121.70
2	B	345	LYS	C-N-CA	6.50	133.41	121.70
1	A	1291	VAL	CB-CA-C	6.49	115.69	109.33
2	B	37	PHE	N-CA-C	-6.49	102.43	110.41
2	B	711	GLU	N-CA-C	6.28	117.81	108.76
1	A	1064	VAL	N-CA-C	6.22	116.96	110.62
1	A	947	PHE	CA-C-N	6.22	129.30	120.53
1	A	947	PHE	C-N-CA	6.22	129.30	120.53
1	A	481	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	1258	HIS	CA-C-N	6.14	129.13	120.28
1	A	1258	HIS	C-N-CA	6.14	129.13	120.28
1	A	663	SER	CA-C-N	6.12	129.90	121.33
1	A	663	SER	C-N-CA	6.12	129.90	121.33
1	A	983	ILE	N-CA-C	-6.10	104.56	110.72
2	B	602	THR	CA-C-N	6.09	128.36	120.44
2	B	602	THR	C-N-CA	6.09	128.36	120.44
8	J	5	VAL	N-CA-C	-6.05	101.74	109.30
1	A	1072	ILE	N-CA-C	-6.04	105.93	111.67
3	C	172	PRO	N-CA-C	-6.03	106.82	114.35
3	C	39	ALA	N-CA-C	6.01	121.98	113.02
1	A	511	ILE	N-CA-CB	6.00	116.92	110.62
1	A	445	ASN	CA-CB-CG	6.00	118.59	112.60
2	B	865	LYS	N-CA-C	-5.98	106.62	114.04
8	J	8	PHE	CA-CB-CG	5.96	119.76	113.80
4	E	33	GLU	N-CA-C	-5.95	104.71	111.14
6	H	91	ASP	CA-C-N	5.93	131.25	121.99
6	H	91	ASP	C-N-CA	5.93	131.25	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	63	VAL	CA-C-N	5.93	129.03	120.38
9	K	63	VAL	C-N-CA	5.93	129.03	120.38
6	H	92	ASP	CA-C-N	5.89	131.58	121.86
6	H	92	ASP	C-N-CA	5.89	131.58	121.86
1	A	541	ILE	N-CA-C	5.86	116.92	108.48
1	A	120	GLU	CA-C-N	5.82	132.66	121.54
1	A	120	GLU	C-N-CA	5.82	132.66	121.54
1	A	1123	GLY	CA-C-N	5.82	132.17	121.70
1	A	1123	GLY	C-N-CA	5.82	132.17	121.70
2	B	1223	ASP	N-CA-C	5.81	117.90	108.08
1	A	1388	GLY	N-CA-C	5.80	115.49	110.21
1	A	526	ASP	CA-CB-CG	5.78	118.38	112.60
2	B	834	ASN	CA-CB-CG	5.77	118.37	112.60
3	C	194	GLU	N-CA-C	-5.75	104.41	112.12
1	A	436	ILE	CB-CA-C	5.72	117.59	111.35
2	B	609	ILE	N-CA-C	-5.69	100.29	108.48
1	A	318	SER	CA-C-N	5.68	125.37	119.92
1	A	318	SER	C-N-CA	5.68	125.37	119.92
1	A	574	GLY	CA-C-N	5.66	128.14	120.38
1	A	574	GLY	C-N-CA	5.66	128.14	120.38
1	A	794	PRO	CA-C-N	5.66	128.43	120.28
1	A	794	PRO	C-N-CA	5.66	128.43	120.28
2	B	851	PHE	N-CA-C	5.65	119.48	112.47
1	A	603	ASN	CA-CB-CG	5.65	118.25	112.60
8	J	17	LYS	N-CA-C	5.64	119.26	112.38
4	E	160	GLU	CA-C-N	5.62	128.08	120.44
4	E	160	GLU	C-N-CA	5.62	128.08	120.44
1	A	708	MET	N-CA-C	5.61	118.63	109.59
2	B	140	ILE	N-CA-C	5.61	116.26	110.82
1	A	1103	GLU	CA-C-N	5.60	127.70	120.70
1	A	1103	GLU	C-N-CA	5.60	127.70	120.70
2	B	957	ASN	CA-C-N	5.60	127.78	120.28
2	B	957	ASN	C-N-CA	5.60	127.78	120.28
1	A	1228	TRP	N-CA-C	5.58	116.75	108.60
9	K	113	THR	CA-C-N	5.56	131.71	121.70
9	K	113	THR	C-N-CA	5.56	131.71	121.70
2	B	1103	ILE	N-CA-CB	5.54	117.36	110.05
4	E	88	VAL	N-CA-C	5.54	115.55	108.12
2	B	818	PRO	N-CA-C	5.53	119.24	111.33
6	H	139	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	474	VAL	N-CA-C	-5.51	107.90	113.47
1	A	1354	ASN	N-CA-C	5.51	118.05	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	772	ALA	CA-C-N	5.49	128.42	120.79
2	B	772	ALA	C-N-CA	5.49	128.42	120.79
7	I	119	THR	CB-CA-C	5.49	116.24	109.16
1	A	463	ILE	N-CA-C	5.49	115.03	108.45
1	A	228	PHE	N-CA-C	5.48	118.08	111.40
2	B	963	PHE	CA-CB-CG	5.47	119.28	113.80
1	A	369	SER	CA-C-N	5.47	127.45	120.56
1	A	369	SER	C-N-CA	5.47	127.45	120.56
2	B	1154	ALA	N-CA-C	-5.46	100.78	109.96
1	A	853	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	708	MET	CA-C-N	5.46	128.59	120.90
1	A	708	MET	C-N-CA	5.46	128.59	120.90
1	A	523	ILE	CB-CA-C	5.45	117.55	110.96
1	A	470	LEU	N-CA-C	5.43	117.52	108.99
1	A	1043	ASP	CA-C-N	5.42	127.55	120.28
1	A	1043	ASP	C-N-CA	5.42	127.55	120.28
1	A	525	GLN	N-CA-C	5.42	116.55	108.31
3	C	213	PRO	N-CA-C	5.40	120.94	113.65
3	C	96	SER	N-CA-C	5.40	117.27	109.07
3	C	150	GLY	CA-C-N	5.39	128.53	120.87
3	C	150	GLY	C-N-CA	5.39	128.53	120.87
2	B	1066	SER	N-CA-C	5.37	119.32	112.87
2	B	184	ALA	N-CA-C	5.36	118.12	110.24
6	H	2	SER	CA-C-N	5.33	131.29	121.70
6	H	2	SER	C-N-CA	5.33	131.29	121.70
2	B	881	ASN	CA-C-N	5.31	127.66	120.65
2	B	881	ASN	C-N-CA	5.31	127.66	120.65
1	A	875	ALA	N-CA-C	5.27	118.49	111.75
6	H	145	ARG	CA-C-N	5.27	131.18	121.70
6	H	145	ARG	C-N-CA	5.27	131.18	121.70
1	A	535	THR	CB-CA-C	5.26	120.10	110.11
2	B	628	THR	CA-C-N	5.26	128.69	120.75
2	B	628	THR	C-N-CA	5.26	128.69	120.75
2	B	1052	VAL	CA-C-N	5.25	127.32	120.28
2	B	1052	VAL	C-N-CA	5.25	127.32	120.28
3	C	108	GLU	N-CA-C	-5.25	105.73	111.82
1	A	1097	GLY	CA-C-N	5.24	125.46	120.43
1	A	1097	GLY	C-N-CA	5.24	125.46	120.43
1	A	969	GLN	CA-C-N	5.23	127.29	120.28
1	A	969	GLN	C-N-CA	5.23	127.29	120.28
3	C	82	TYR	N-CA-C	-5.21	100.81	109.46
10	L	65	VAL	N-CA-C	5.19	115.44	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	317	CYS	CA-C-N	5.18	127.84	120.53
2	B	317	CYS	C-N-CA	5.18	127.84	120.53
1	A	718	VAL	CA-C-N	5.18	127.28	120.60
1	A	718	VAL	C-N-CA	5.18	127.28	120.60
1	A	93	VAL	N-CA-C	5.17	115.79	110.36
10	L	40	LEU	N-CA-C	5.17	117.10	108.99
4	E	186	LEU	CA-C-N	5.16	127.15	120.44
4	E	186	LEU	C-N-CA	5.16	127.15	120.44
2	B	882	THR	N-CA-C	5.15	116.59	110.97
2	B	482	VAL	N-CA-CB	5.14	116.84	110.05
1	A	384	ASN	CA-CB-CG	5.13	117.73	112.60
2	B	1167	GLY	N-CA-C	-5.13	107.98	115.72
1	A	612	ILE	N-CA-CB	5.12	116.68	110.95
1	A	532	ARG	CA-C-N	5.11	127.40	120.65
1	A	532	ARG	C-N-CA	5.11	127.40	120.65
2	B	807	ARG	CA-C-N	5.10	127.62	120.28
2	B	807	ARG	C-N-CA	5.10	127.62	120.28
2	B	1194	ILE	N-CA-C	5.09	116.05	108.46
2	B	659	ALA	CA-C-N	5.08	127.09	120.28
2	B	659	ALA	C-N-CA	5.08	127.09	120.28
1	A	64	ASN	CA-C-N	5.07	127.78	120.38
1	A	64	ASN	C-N-CA	5.07	127.78	120.38
1	A	399	HIS	N-CA-CB	5.07	119.39	110.37
8	J	2	ILE	CA-C-N	5.06	131.50	122.13
8	J	2	ILE	C-N-CA	5.06	131.50	122.13
1	A	946	VAL	N-CA-CB	5.06	116.71	110.64
1	A	1135	ARG	CA-C-N	5.05	127.32	120.65
1	A	1135	ARG	C-N-CA	5.05	127.32	120.65
5	F	87	LYS	CA-C-N	5.04	127.45	120.29
5	F	87	LYS	C-N-CA	5.04	127.45	120.29
1	A	938	LYS	CA-C-N	5.04	127.00	120.44
1	A	938	LYS	C-N-CA	5.04	127.00	120.44
2	B	1186	ASP	CA-C-N	5.04	128.36	120.75
2	B	1186	ASP	C-N-CA	5.04	128.36	120.75
1	A	680	THR	CB-CA-C	5.03	119.14	110.79
2	B	1085	ILE	N-CA-C	5.03	116.20	108.71
3	C	89	GLU	N-CA-C	-5.03	102.20	109.59
1	A	1098	VAL	N-CA-CB	5.02	113.88	110.52
4	E	7	ARG	N-CA-C	-5.01	105.72	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	162	0
2	B	8861	0	8884	155	0
3	C	2095	0	2051	35	0
4	E	1752	0	1776	20	0
5	F	688	0	707	14	0
6	H	1068	0	1040	14	0
7	I	971	0	927	15	0
8	J	532	0	542	19	0
9	K	919	0	929	17	0
10	L	363	0	386	4	0
11	R	132	0	67	6	0
12	T	241	0	136	2	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28674	0	28578	403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (403) 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)
2:B:664:THR:HG21	2:B:679:TYR:H	1.37	0.87
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.10	0.87
8:J:48:ARG:O	8:J:52:THR:HB	1.75	0.86
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.58	0.86
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.43	0.84
1:A:511:ILE:HA	1:A:521:MET:HE3	1.63	0.81
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.63	0.80
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ILE:HG23	1:A:567:LYS:HD2	1.66	0.76
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.68	0.75
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.69	0.74
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.03	0.73
1:A:466:SER:HB3	2:B:1103:ILE:HD11	1.71	0.73
11:R:5:A:H2'	11:R:6:G:H8	1.52	0.73
1:A:1107:VAL:HG12	1:A:1383:SER:HB3	1.70	0.72
1:A:567:LYS:HB3	6:H:96:VAL:H	1.54	0.72
1:A:1118:VAL:HG13	1:A:1306:LEU:HB2	1.72	0.71
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.75	0.69
2:B:801:LYS:O	8:J:52:THR:HG23	1.93	0.68
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.74	0.68
3:C:167:HIS:HD2	3:C:169:LYS:H	1.39	0.68
1:A:1111:MET:HB3	1:A:1114:PRO:HG3	1.76	0.67
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.77	0.67
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.76	0.66
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.76	0.66
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.61	0.66
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.60	0.66
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.79	0.65
1:A:901:LEU:HA	1:A:907:THR:HG23	1.79	0.65
1:A:472:LEU:O	1:A:475:THR:HB	1.97	0.65
3:C:54:ASN:OD1	3:C:56:THR:HG22	1.97	0.64
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.78	0.64
2:B:313:MET:HE2	2:B:390:LEU:HG	1.79	0.64
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	1.79	0.64
2:B:783:THR:HG21	8:J:59:LYS:HB3	1.79	0.64
3:C:104:PHE:HD1	3:C:152:GLU:HB3	1.63	0.64
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.79	0.64
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.80	0.64
1:A:456:MET:HE2	1:A:507:VAL:HA	1.79	0.63
1:A:711:ARG:HH12	7:I:95:THR:HB	1.64	0.63
1:A:946:VAL:HG12	4:E:201:LYS:HB3	1.81	0.63
1:A:596:THR:C	1:A:598:LEU:H	2.06	0.63
2:B:408:LEU:H	2:B:411:PRO:HG2	1.63	0.62
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.80	0.62
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.81	0.62
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.65	0.61
6:H:89:LEU:C	6:H:91:ASP:H	2.06	0.61
8:J:1:MET:H1	8:J:56:LEU:H	1.47	0.61
2:B:230:ALA:H	2:B:231:PRO:HD2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLY:O	4:E:204:THR:HG21	2.01	0.61
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.66	0.61
1:A:399:HIS:O	1:A:401:GLY:N	2.32	0.60
1:A:899:VAL:HG23	1:A:1029:ARG:HG2	1.83	0.60
2:B:706:GLN:O	2:B:710:LEU:HB2	2.01	0.60
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.84	0.60
1:A:535:THR:HG21	1:A:617:VAL:H	1.66	0.60
1:A:924:LYS:O	1:A:927:VAL:HG12	2.02	0.60
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.84	0.59
2:B:1082:MET:HA	3:C:189:THR:HA	1.84	0.59
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.17	0.59
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.84	0.59
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.67	0.59
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.83	0.59
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.03	0.59
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.66	0.59
1:A:332:LYS:H	1:A:337:ARG:HB2	1.68	0.58
2:B:511:PRO:O	2:B:513:GLN:N	2.36	0.58
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.69	0.58
3:C:196:ASP:O	3:C:200:GLU:HG2	2.04	0.58
1:A:485:ASP:HA	11:R:10:2IA:I	2.74	0.58
2:B:98:THR:O	2:B:178:ASN:ND2	2.36	0.57
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.85	0.57
2:B:345:LYS:HA	2:B:347:LYS:H	1.69	0.57
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.86	0.57
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.51	0.57
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.86	0.57
2:B:744:HIS:CD2	2:B:746:SER:OG	2.57	0.57
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.84	0.57
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.87	0.57
2:B:578:THR:HG22	2:B:622:LYS:HA	1.87	0.57
2:B:976:ILE:O	2:B:990:ILE:HB	2.05	0.57
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.86	0.57
7:I:8:ARG:HB3	7:I:34:TYR:HE1	1.70	0.56
6:H:57:VAL:HG22	6:H:144:ILE:HG12	1.85	0.56
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.87	0.56
3:C:183:TRP:HB2	3:C:185:LYS:HG3	1.88	0.56
8:J:41:LEU:HD23	8:J:46:CYS:HB3	1.87	0.56
1:A:351:THR:HG21	1:A:466:SER:O	2.05	0.56
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.71	0.56
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:MET:HE3	1:A:510:GLN:HB2	1.89	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.88	0.55
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.71	0.55
1:A:1329:THR:HG22	1:A:1331:SER:H	1.72	0.55
2:B:54:PHE:HA	2:B:58:THR:HB	1.87	0.55
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.89	0.54
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.88	0.54
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.89	0.54
2:B:906:SER:HA	2:B:946:ASN:HB3	1.90	0.54
1:A:535:THR:CG2	1:A:617:VAL:H	2.21	0.54
2:B:744:HIS:HD2	2:B:746:SER:OG	1.91	0.54
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.90	0.54
1:A:482:PHE:HB2	2:B:838:SER:OG	2.08	0.53
2:B:800:GLN:CB	8:J:52:THR:HG22	2.35	0.53
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.90	0.53
6:H:105:GLU:HB3	6:H:113:ALA:HB3	1.90	0.53
10:L:61:THR:HG21	10:L:63:ARG:HD3	1.90	0.53
2:B:69:LEU:HD12	2:B:90:ILE:HB	1.91	0.53
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.90	0.53
2:B:38:PHE:H	2:B:41:LYS:HB2	1.72	0.53
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.91	0.53
1:A:871:ASP:OD2	4:E:204:THR:HG23	2.09	0.53
1:A:43:GLU:HG3	1:A:50:ILE:HG12	1.91	0.52
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.91	0.52
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.39	0.52
2:B:999:MET:HE3	2:B:999:MET:HA	1.90	0.52
1:A:1059:HIS:CE1	5:F:87:LYS:H	2.27	0.52
3:C:167:HIS:CD2	3:C:169:LYS:H	2.25	0.52
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.90	0.52
8:J:24:LEU:O	8:J:28:ASP:HB2	2.10	0.52
2:B:310:MET:HE3	2:B:386:LEU:HB2	1.92	0.52
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.74	0.52
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.92	0.52
1:A:225:ASN:HD22	1:A:228:PHE:H	1.56	0.52
1:A:825:ILE:O	1:A:829:VAL:HG23	2.10	0.52
2:B:864:LYS:H	2:B:872:GLU:HB2	1.75	0.52
1:A:265:LYS:HZ1	1:A:302:THR:HG23	1.75	0.51
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.68	0.51
1:A:1318:THR:HG22	4:E:142:VAL:HG12	1.92	0.51
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.93	0.51
1:A:418:SER:HB3	1:A:421:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.75	0.51
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.93	0.51
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.75	0.51
2:B:241:ARG:HA	2:B:253:THR:HG22	1.93	0.51
4:E:198:ILE:HD13	4:E:212:ARG:HG3	1.92	0.51
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.75	0.51
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.93	0.51
1:A:351:THR:HG22	1:A:352:VAL:N	2.26	0.51
1:A:84:ILE:HD11	1:A:270:LEU:HG	1.92	0.50
1:A:1444:MET:HB2	5:F:133:VAL:HB	1.93	0.50
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.93	0.50
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.94	0.50
2:B:1054:GLY:HA2	2:B:1057:LYS:HE2	1.94	0.50
4:E:61:GLN:HG3	4:E:105:PHE:HE2	1.77	0.50
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.93	0.50
1:A:114:LEU:HB3	1:A:115:LEU:HD12	1.94	0.50
2:B:307:ASP:O	2:B:311:LEU:HD12	2.12	0.50
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.46	0.50
1:A:445:ASN:HB2	1:A:455:MET:HG3	1.94	0.49
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.94	0.49
4:E:204:THR:HG22	4:E:205:SER:N	2.26	0.49
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.93	0.49
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.93	0.49
2:B:563:MET:HA	2:B:589:VAL:O	2.11	0.49
2:B:843:GLN:HB2	2:B:993:THR:HB	1.93	0.49
5:F:72:LYS:HG2	5:F:142:SER:HA	1.94	0.49
2:B:1082:MET:HE3	3:C:190:ASP:HB2	1.95	0.49
3:C:18:VAL:O	3:C:231:ASN:HA	2.13	0.49
6:H:2:SER:HA	6:H:3:ASN:HB2	1.94	0.49
1:A:113:LEU:HD12	1:A:116:ASP:HB2	1.95	0.49
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.28	0.49
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.78	0.49
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.79	0.48
9:K:12:LEU:HA	9:K:37:LYS:HE3	1.95	0.48
9:K:65:HIS:HD2	9:K:67:PHE:H	1.61	0.48
1:A:114:LEU:HD21	1:A:171:GLN:HE22	1.77	0.48
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.43	0.48
2:B:845:SER:HA	8:J:8:PHE:O	2.12	0.48
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.94	0.48
1:A:886:ILE:HG12	1:A:944:ARG:HG3	1.96	0.48
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.94	0.48
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.49	0.48
2:B:230:ALA:H	2:B:231:PRO:CD	2.26	0.48
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.77	0.48
3:C:46:ILE:HG23	3:C:157:CYS:HB2	1.95	0.48
1:A:68:GLN:HG3	1:A:69:THR:H	1.77	0.48
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.96	0.48
8:J:32:GLU:CD	8:J:32:GLU:H	2.22	0.48
4:E:196:VAL:HG13	4:E:198:ILE:HD11	1.96	0.48
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.95	0.48
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.95	0.47
1:A:747:VAL:HG21	1:A:758:ILE:HD11	1.97	0.47
1:A:91:PHE:HA	1:A:235:ILE:HG22	1.96	0.47
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.95	0.47
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.96	0.47
1:A:325:ILE:HB	2:B:1210:MET:HE3	1.97	0.47
1:A:670:ILE:HD12	2:B:1067:ARG:HD2	1.96	0.47
2:B:1020:ARG:H	2:B:1020:ARG:HG2	1.52	0.47
4:E:78:LEU:HD12	4:E:107:THR:HB	1.97	0.47
2:B:53:GLN:HG2	2:B:547:VAL:HB	1.95	0.47
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.96	0.47
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.44	0.47
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.96	0.47
11:R:6:G:H2'	11:R:7:A:C8	2.50	0.47
2:B:813:LYS:O	2:B:815:ARG:N	2.47	0.47
4:E:111:VAL:HG12	4:E:137:GLU:HG2	1.97	0.47
7:I:34:TYR:HE2	7:I:36:GLU:HB3	1.80	0.47
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.50	0.47
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.45	0.47
2:B:768:THR:O	2:B:771:SER:HB2	2.15	0.47
3:C:14:SER:HA	9:K:114:LEU:HD22	1.96	0.47
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.97	0.46
1:A:777:PHE:CD1	1:A:782:ARG:HA	2.49	0.46
1:A:1436:ILE:HB	2:B:1144:ALA:HB2	1.97	0.46
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.97	0.46
12:T:19:DT:H2'	12:T:20:DC:O4'	2.15	0.46
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.98	0.46
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.96	0.46
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.98	0.46
3:C:31:ASN:O	3:C:35:ARG:HG3	2.16	0.46
5:F:110:ASP:O	5:F:123:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.97	0.46
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.98	0.46
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.81	0.46
1:A:369:SER:HB3	9:K:2:ASN:HD21	1.81	0.46
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.98	0.46
9:K:32:VAL:HG22	9:K:74:ARG:HG3	1.97	0.46
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.81	0.46
2:B:896:ASP:OD2	10:L:58:LYS:HE2	2.15	0.46
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.98	0.46
1:A:1220:PHE:CD1	1:A:1224:LEU:HD22	2.51	0.46
1:A:690:VAL:HA	1:A:693:VAL:HG12	1.98	0.45
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.98	0.45
1:A:1006:ILE:HD12	4:E:167:ARG:HB2	1.98	0.45
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.98	0.45
2:B:424:LEU:O	2:B:428:ILE:HG12	2.16	0.45
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.51	0.45
2:B:601:ARG:HA	2:B:615:MET:HE1	1.98	0.45
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.98	0.45
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.98	0.45
7:I:17:ARG:HE	7:I:28:GLU:HG2	1.82	0.45
1:A:587:HIS:HE1	1:A:969:GLN:HE21	1.64	0.45
2:B:1156:ASP:HB2	2:B:1198:TYR:H	1.81	0.45
3:C:33:LEU:HA	3:C:36:VAL:HG12	1.98	0.45
1:A:670:ILE:HG12	1:A:805:LEU:HD11	1.97	0.45
1:A:9:ALA:HB3	2:B:1193:GLN:HE21	1.80	0.45
1:A:408:ASP:O	1:A:409:SER:HB2	2.15	0.45
1:A:344:ARG:O	2:B:1155:SER:OG	2.35	0.45
1:A:404:TYR:HA	1:A:413:ILE:O	2.17	0.45
2:B:647:GLY:HA2	2:B:648:HIS:C	2.41	0.45
1:A:907:THR:HG22	1:A:908:LEU:H	1.82	0.45
2:B:223:VAL:HG11	2:B:380:TYR:HE2	1.82	0.45
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.99	0.45
1:A:786:HIS:HE1	2:B:742:GLU:OE1	2.00	0.45
2:B:283:VAL:HG12	2:B:297:ILE:HG21	1.98	0.45
1:A:567:LYS:O	1:A:568:PRO:C	2.59	0.45
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.98	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.52	0.45
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.51	0.45
3:C:49:VAL:HG22	3:C:157:CYS:HB3	1.98	0.45
3:C:101:LEU:HD13	3:C:118:LEU:HG	1.99	0.45
2:B:48:LEU:HD23	2:B:173:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.32	0.44
2:B:476:ARG:O	2:B:478:GLY:N	2.50	0.44
2:B:864:LYS:N	2:B:872:GLU:HB2	2.32	0.44
3:C:262:LEU:HD11	9:K:87:LEU:HD12	1.98	0.44
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.99	0.44
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.00	0.44
3:C:100:THR:HB	3:C:121:VAL:HG21	1.99	0.44
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.17	0.44
2:B:1031:LEU:O	2:B:1034:VAL:HG12	2.17	0.44
1:A:913:LEU:HD11	1:A:981:LEU:O	2.17	0.44
3:C:18:VAL:CG1	9:K:109:TRP:HZ3	2.30	0.44
4:E:153:HIS:HB3	4:E:196:VAL:HG21	2.00	0.44
5:F:114:GLU:CD	5:F:119:ARG:HE	2.26	0.44
1:A:528:LEU:HD23	1:A:751:SER:HA	2.00	0.44
2:B:211:VAL:HG21	2:B:483:LEU:HD13	2.00	0.44
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.82	0.44
6:H:4:THR:HA	6:H:60:ALA:HA	2.00	0.44
7:I:26:LEU:HD23	7:I:37:GLU:HA	2.00	0.44
8:J:64:ASN:N	8:J:65:PRO:HD2	2.33	0.44
1:A:567:LYS:HE3	6:H:96:VAL:O	2.17	0.44
7:I:34:TYR:CD2	7:I:35:VAL:N	2.86	0.44
1:A:516:SER:HB3	1:A:518:LYS:HG2	2.00	0.44
1:A:1325:THR:HA	4:E:147:HIS:HA	2.00	0.44
2:B:975:GLN:O	2:B:990:ILE:HD12	2.17	0.44
6:H:89:LEU:C	6:H:91:ASP:N	2.74	0.44
7:I:92:ARG:HB3	7:I:95:THR:OG1	2.18	0.44
11:R:5:A:H2'	11:R:6:G:C8	2.43	0.44
1:A:1107:VAL:HG23	1:A:1332:PHE:HE1	1.83	0.44
1:A:1117:THR:HG22	1:A:1307:GLU:HG2	2.00	0.44
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.66	0.44
2:B:59:LEU:HD13	2:B:417:PHE:HE1	1.83	0.44
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.99	0.44
7:I:10:CYS:SG	7:I:31:THR:HB	2.58	0.44
2:B:487:THR:HG22	2:B:490:SER:H	1.83	0.44
2:B:763:GLN:NE2	2:B:765:PRO:HD2	2.33	0.44
2:B:764:SER:HB3	2:B:765:PRO:HD3	1.99	0.44
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.52	0.44
9:K:7:PHE:C	9:K:9:LEU:H	2.26	0.44
2:B:749:LEU:HB3	2:B:753:ALA:HB3	2.00	0.43
11:R:6:G:H2'	11:R:7:A:H8	1.81	0.43
1:A:298:PHE:HZ	1:A:311:GLN:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:THR:HB	1:A:865:GLN:HB2	1.99	0.43
6:H:137:GLN:C	6:H:139:ASN:H	2.27	0.43
4:E:198:ILE:HB	4:E:210:SER:HB3	2.00	0.43
1:A:269:ILE:HG22	1:A:299:HIS:HB3	2.01	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG21	2.00	0.43
2:B:783:THR:CG2	8:J:59:LYS:HB3	2.46	0.43
2:B:840:ILE:HG12	2:B:992:ILE:HG22	2.01	0.43
2:B:942:ARG:HB3	2:B:945:GLU:HB2	2.01	0.43
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.18	0.43
1:A:92:HIS:HD2	1:A:94:GLY:H	1.65	0.43
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.66	0.43
1:A:579:SER:HA	1:A:582:ILE:HD12	1.99	0.43
1:A:1195:LEU:HD11	1:A:1267:MET:SD	2.59	0.43
6:H:33:GLN:HB2	6:H:36:CYS:HB3	2.01	0.43
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.00	0.43
1:A:588:LEU:HD12	1:A:632:VAL:HG21	2.01	0.43
1:A:837:ILE:HD11	1:A:1102:LYS:HG3	2.01	0.43
1:A:353:ILE:HG21	1:A:487:MET:HB2	2.01	0.43
3:C:36:VAL:HG23	3:C:40:GLU:HB2	2.00	0.43
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.59	0.43
1:A:934:LYS:HA	1:A:937:VAL:HG22	2.01	0.42
2:B:67:SER:HB2	2:B:92:PHE:H	1.84	0.42
2:B:552:MET:HA	2:B:555:ILE:HD12	2.01	0.42
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.01	0.42
2:B:211:VAL:HG23	2:B:483:LEU:HB2	2.00	0.42
2:B:280:ILE:HD13	2:B:334:ILE:HG12	2.00	0.42
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.32	0.42
1:A:993:LEU:HD22	1:A:1046:LEU:HG	2.01	0.42
1:A:1107:VAL:HG21	1:A:1381:LEU:HB3	2.01	0.42
2:B:140:ILE:HB	2:B:141:ASP:HB2	2.02	0.42
2:B:364:ILE:HG22	2:B:365:THR:HG22	2.01	0.42
2:B:839:MET:HG2	2:B:990:ILE:HA	2.01	0.42
3:C:71:PRO:HG3	8:J:13:VAL:HG11	2.00	0.42
1:A:51:GLY:HA2	1:A:56:PRO:HB3	2.01	0.42
1:A:116:ASP:HA	1:A:117:GLU:HA	1.85	0.42
4:E:78:LEU:HD11	4:E:109:ILE:HD13	2.00	0.42
7:I:18:GLU:HG2	7:I:20:LYS:H	1.84	0.42
7:I:96:SER:HB2	7:I:98:VAL:HG23	2.02	0.42
1:A:1122:PRO:HA	1:A:1125:ALA:HB2	2.02	0.42
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.66	0.42
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HG23	1:A:1029:ARG:CG	2.48	0.42
2:B:30:SER:O	2:B:34:ILE:HG12	2.19	0.42
2:B:412:LEU:HA	2:B:415:GLN:HB2	2.00	0.42
2:B:755:ILE:HA	2:B:809:MET:HE2	2.01	0.42
2:B:541:LEU:HD21	2:B:812:LEU:HD21	2.02	0.42
2:B:804:GLY:O	2:B:983:ARG:NH2	2.53	0.42
1:A:483:ASP:HB3	2:B:837:ASP:HB3	2.00	0.42
1:A:571:LEU:HD22	6:H:46:LEU:HD11	2.01	0.42
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.02	0.42
2:B:706:GLN:H	2:B:710:LEU:HD23	1.85	0.42
2:B:900:ALA:HA	10:L:58:LYS:HD3	2.01	0.42
3:C:115:SER:HA	3:C:144:ILE:HD11	2.02	0.42
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.85	0.42
1:A:901:LEU:HD22	1:A:919:ILE:HG22	2.01	0.41
2:B:50:SER:OG	2:B:411:PRO:HD2	2.20	0.41
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.85	0.41
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.54	0.41
6:H:85:GLY:C	6:H:87:ARG:H	2.27	0.41
1:A:325:ILE:H	1:A:325:ILE:HG13	1.75	0.41
1:A:1107:VAL:HG23	1:A:1332:PHE:CE1	2.56	0.41
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.01	0.41
3:C:18:VAL:HG11	9:K:109:TRP:HZ3	1.85	0.41
11:R:10:2IA:C2	12:T:19:DT:H3	2.33	0.41
1:A:709:THR:HG22	1:A:711:ARG:H	1.86	0.41
2:B:310:MET:HE1	2:B:383:ASN:HA	2.02	0.41
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.56	0.41
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.55	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.41
1:A:1290:LYS:HE2	1:A:1298:TYR:HB3	2.01	0.41
2:B:705:MET:HG3	2:B:745:PRO:HG3	2.02	0.41
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.86	0.41
1:A:1293:SER:HB3	1:A:1299:VAL:HG23	2.01	0.41
1:A:1436:ILE:HG22	2:B:1142:GLY:HA2	2.03	0.41
2:B:542:MET:HE1	2:B:743:ILE:HD12	2.03	0.41
8:J:44:TYR:HA	8:J:47:ARG:HB2	2.03	0.41
10:L:48:CYS:SG	10:L:51:CYS:HB3	2.60	0.41
1:A:306:ASN:HD21	1:A:313:GLN:HB2	1.85	0.41
2:B:846:ILE:HG23	2:B:974:PRO:HD2	2.03	0.41
5:F:72:LYS:HE2	5:F:142:SER:HB3	2.02	0.41
5:F:87:LYS:HE2	5:F:88:TYR:CZ	2.55	0.41
2:B:123:THR:H	2:B:958:GLN:HE22	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:58:THR:HG23	6:H:143:LEU:HB2	2.03	0.41
1:A:353:ILE:HG13	1:A:487:MET:HE3	2.03	0.41
1:A:579:SER:HB3	1:A:611:GLN:HA	2.02	0.41
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.56	0.41
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.54	0.41
2:B:114:PRO:HG2	2:B:181:LEU:HD11	2.03	0.41
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.56	0.41
4:E:176:PRO:O	4:E:212:ARG:HA	2.21	0.41
5:F:90:ARG:HD3	5:F:155:LEU:HD11	2.02	0.41
1:A:384:ASN:HB2	1:A:387:ARG:HH21	1.86	0.41
2:B:424:LEU:HD22	2:B:453:ILE:HD11	2.03	0.41
2:B:1074:ASN:HD22	2:B:1077:THR:H	1.69	0.41
3:C:171:GLY:C	3:C:173:ALA:H	2.28	0.41
1:A:608:ILE:HD12	1:A:613:ILE:HG13	2.02	0.40
2:B:408:LEU:HD11	2:B:545:ILE:HD13	2.02	0.40
7:I:34:TYR:HD2	7:I:35:VAL:N	2.18	0.40
1:A:55:ASP:N	1:A:56:PRO:HD3	2.37	0.40
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.04	0.40
2:B:1175:LEU:C	2:B:1177:HIS:H	2.28	0.40
1:A:71:GLN:HB3	1:A:72:GLU:H	1.77	0.40
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	2.03	0.40
2:B:345:LYS:HA	2:B:347:LYS:N	2.34	0.40
2:B:515:HIS:CD2	2:B:517:THR:H	2.40	0.40
2:B:549:THR:HG21	2:B:610:ASN:HD22	1.86	0.40
4:E:167:ARG:HA	4:E:167:ARG:HD3	1.93	0.40
5:F:112:GLU:H	5:F:112:GLU:HG3	1.69	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%)	1181 (85%)	165 (12%)	49 (4%)	3	18
2	B	1096/1224 (90%)	936 (85%)	112 (10%)	48 (4%)	2	13
3	C	264/318 (83%)	242 (92%)	18 (7%)	4 (2%)	8	32
4	E	212/215 (99%)	194 (92%)	15 (7%)	3 (1%)	9	33
5	F	83/155 (54%)	68 (82%)	13 (16%)	2 (2%)	4	24
6	H	129/146 (88%)	99 (77%)	26 (20%)	4 (3%)	3	20
7	I	117/122 (96%)	100 (86%)	15 (13%)	2 (2%)	7	30
8	J	63/70 (90%)	56 (89%)	4 (6%)	3 (5%)	2	12
9	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
10	L	44/70 (63%)	30 (68%)	7 (16%)	7 (16%)	0	1
All	All	3515/4173 (84%)	3013 (86%)	380 (11%)	122 (4%)	3	18

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ARG
1	A	853	ASP
1	A	1437	GLY
2	B	137	TYR
2	B	229	ALA
2	B	230	ALA
2	B	249	ARG
2	B	477	ALA
2	B	512	ARG
2	B	531	GLN
2	B	646	LEU
2	B	712	PRO
2	B	734	HIS
2	B	751	VAL
2	B	814	PHE
2	B	880	THR
2	B	889	THR
2	B	976	ILE
2	B	1221	SER
3	C	4	GLU
3	C	173	ALA
8	J	2	ILE
10	L	64	LEU
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	57	ARG
1	A	68	GLN
1	A	113	LEU
1	A	121	LEU
1	A	214	ILE
1	A	251	SER
1	A	331	GLY
1	A	385	ILE
1	A	423	ASP
1	A	424	ILE
1	A	662	PHE
1	A	672	ASP
1	A	846	GLU
1	A	923	LEU
1	A	1081	LEU
1	A	1123	GLY
1	A	1405	THR
2	B	138	GLU
2	B	176	SER
2	B	277	LYS
2	B	480	SER
2	B	511	PRO
2	B	647	GLY
2	B	792	MET
2	B	943	SER
2	B	1046	PRO
2	B	1099	VAL
6	H	83	GLN
7	I	77	LYS
8	J	6	ARG
8	J	13	VAL
10	L	56	LEU
10	L	63	ARG
1	A	118	HIS
1	A	145	LYS
1	A	907	THR
1	A	1167	GLU
1	A	1377	THR
1	A	1416	ALA
2	B	248	SER
2	B	526	GLU
2	B	881	ASN

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Mol	Chain	Res	Type
2	B	1017	ILE
2	B	1097	HIS
3	C	215	GLU
3	C	267	GLN
4	E	123	LEU
5	F	112	GLU
10	L	51	CYS
1	A	48	ALA
1	A	215	SER
1	A	399	HIS
1	A	404	TYR
1	A	569	LYS
1	A	597	LEU
1	A	599	SER
1	A	736	ASN
1	A	1255	GLU
2	B	139	ALA
2	B	476	ARG
2	B	478	GLY
2	B	563	MET
2	B	764	SER
2	B	907	GLY
2	B	918	ILE
2	B	1108	ARG
4	E	45	LYS
4	E	172	GLU
6	H	109	LYS
7	I	60	GLN
1	A	63	ARG
1	A	149	GLU
1	A	226	GLU
1	A	250	ILE
1	A	332	LYS
1	A	958	VAL
1	A	1166	ASP
2	B	177	LYS
2	B	752	ALA
2	B	996	ARG
2	B	1181	GLU
5	F	114	GLU
6	H	108	SER
10	L	47	ARG

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Mol	Chain	Res	Type
1	A	312	PRO
1	A	409	SER
2	B	346	GLU
2	B	467	GLY
2	B	1188	LYS
1	A	568	PRO
1	A	735	VAL
1	A	1360	GLY
2	B	364	ILE
6	H	18	GLY
10	L	46	VAL
2	B	780	VAL
10	L	55	ILE
1	A	210	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%)	1070 (87%)	155 (13%)	4	18
2	B	967/1061 (91%)	850 (88%)	117 (12%)	5	20
3	C	234/274 (85%)	207 (88%)	27 (12%)	5	21
4	E	196/197 (100%)	177 (90%)	19 (10%)	8	28
5	F	75/137 (55%)	68 (91%)	7 (9%)	8	30
6	H	117/128 (91%)	107 (92%)	10 (8%)	10	33
7	I	113/116 (97%)	102 (90%)	11 (10%)	8	28
8	J	60/65 (92%)	50 (83%)	10 (17%)	2	11
9	K	99/102 (97%)	88 (89%)	11 (11%)	6	22
10	L	40/57 (70%)	33 (82%)	7 (18%)	2	9
All	All	3126/3657 (86%)	2752 (88%)	374 (12%)	5	20

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	18	GLN
1	A	22	PHE
1	A	28	ARG
1	A	30	ILE
1	A	43	GLU
1	A	44	THR
1	A	50	ILE
1	A	54	ASN
1	A	61	ILE
1	A	75	ASN
1	A	113	LEU
1	A	118	HIS
1	A	133	LYS
1	A	138	ILE
1	A	142	CYS
1	A	186	LYS
1	A	199	LEU
1	A	204	THR
1	A	222	LEU
1	A	227	VAL
1	A	234	MET
1	A	266	LEU
1	A	268	ASP
1	A	270	LEU
1	A	279	LEU
1	A	290	GLU
1	A	296	LEU
1	A	303	TYR
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	359	LEU
1	A	368	LYS
1	A	369	SER
1	A	383	TYR
1	A	387	ARG
1	A	389	THR

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Mol	Chain	Res	Type
1	A	398	GLU
1	A	403	LYS
1	A	411	ASP
1	A	424	ILE
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	451	HIS
1	A	453	MET
1	A	454	SER
1	A	463	ILE
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	485	ASP
1	A	500	GLU
1	A	513	SER
1	A	516	SER
1	A	523	ILE
1	A	534	LEU
1	A	535	THR
1	A	538	ASP
1	A	541	ILE
1	A	543	LEU
1	A	544	ASP
1	A	545	GLN
1	A	559	VAL
1	A	566	ILE
1	A	567	LYS
1	A	577	ILE
1	A	588	LEU
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	621	THR
1	A	629	LEU
1	A	663	SER
1	A	666	ILE
1	A	672	ASP
1	A	676	MET
1	A	680	THR

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Mol	Chain	Res	Type
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	710	LEU
1	A	722	LEU
1	A	737	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	758	ILE
1	A	821	ARG
1	A	833	GLU
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	886	ILE
1	A	896	ARG
1	A	929	LEU
1	A	931	GLU
1	A	932	GLU
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE
1	A	983	ILE
1	A	988	LEU
1	A	998	LEU
1	A	999	VAL
1	A	1000	LEU
1	A	1006	ILE
1	A	1029	ARG
1	A	1057	VAL
1	A	1077	THR
1	A	1095	THR
1	A	1111	MET
1	A	1116	LEU
1	A	1120	LEU
1	A	1132	LYS
1	A	1134	ILE
1	A	1146	VAL
1	A	1162	VAL
1	A	1174	PHE
1	A	1176	LEU

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Mol	Chain	Res	Type
1	A	1209	MET
1	A	1217	LYS
1	A	1230	GLU
1	A	1237	ILE
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1293	SER
1	A	1299	VAL
1	A	1309	ASP
1	A	1314	SER
1	A	1316	VAL
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1354	ASN
1	A	1359	ASP
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1403	GLU
1	A	1407	GLU
1	A	1424	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
2	B	25	ILE
2	B	46	GLN
2	B	59	LEU
2	B	63	ILE
2	B	101	MET
2	B	102	VAL
2	B	132	VAL
2	B	178	ASN
2	B	194	GLU
2	B	209	GLU
2	B	217	ARG
2	B	234	ILE
2	B	240	ILE
2	B	254	LEU

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	267	ARG
2	B	277	LYS
2	B	305	VAL
2	B	309	GLN
2	B	311	LEU
2	B	313	MET
2	B	323	VAL
2	B	365	THR
2	B	367	LEU
2	B	376	PHE
2	B	393	LYS
2	B	394	ASP
2	B	412	LEU
2	B	415	GLN
2	B	416	LEU
2	B	419	THR
2	B	437	GLU
2	B	476	ARG
2	B	479	VAL
2	B	480	SER
2	B	485	ARG
2	B	487	THR
2	B	490	SER
2	B	500	THR
2	B	502	ILE
2	B	549	THR
2	B	556	THR
2	B	559	SER
2	B	567	GLU
2	B	603	LEU
2	B	604	ARG
2	B	612	GLU
2	B	614	SER
2	B	620	ARG
2	B	623	GLU
2	B	624	LEU
2	B	633	VAL
2	B	645	SER
2	B	650	GLU
2	B	653	VAL
2	B	658	ILE

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Mol	Chain	Res	Type
2	B	685	LEU
2	B	690	VAL
2	B	694	ASP
2	B	708	GLU
2	B	730	ARG
2	B	737	THR
2	B	739	THR
2	B	776	GLN
2	B	780	VAL
2	B	796	LEU
2	B	806	THR
2	B	813	LYS
2	B	825	VAL
2	B	829	CYS
2	B	839	MET
2	B	844	SER
2	B	865	LYS
2	B	868	MET
2	B	870	ILE
2	B	872	GLU
2	B	875	GLU
2	B	879	ARG
2	B	880	THR
2	B	885	MET
2	B	887	HIS
2	B	898	LEU
2	B	918	ILE
2	B	935	ARG
2	B	945	GLU
2	B	946	ASN
2	B	963	PHE
2	B	973	ILE
2	B	979	LYS
2	B	983	ARG
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1020	ARG
2	B	1028	GLU

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Mol	Chain	Res	Type
2	B	1034	VAL
2	B	1060	ARG
2	B	1062	HIS
2	B	1065	GLN
2	B	1073	TYR
2	B	1099	VAL
2	B	1102	LYS
2	B	1111	MET
2	B	1113	VAL
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1149	GLU
2	B	1178	ASN
2	B	1188	LYS
2	B	1191	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1216	LEU
3	C	9	LYS
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	41	ILE
3	C	75	MET
3	C	80	LEU
3	C	100	THR
3	C	110	THR
3	C	116	LYS
3	C	122	SER
3	C	125	MET
3	C	129	ILE
3	C	137	LYS
3	C	149	LYS
3	C	151	GLN
3	C	156	THR
3	C	199	LYS
3	C	204	SER
3	C	215	GLU
3	C	221	TYR
3	C	240	VAL

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Mol	Chain	Res	Type
3	C	244	VAL
3	C	249	ASP
3	C	254	LYS
3	C	258	ILE
4	E	7	ARG
4	E	8	ASN
4	E	30	ILE
4	E	54	GLN
4	E	69	ILE
4	E	74	ASP
4	E	78	LEU
4	E	95	THR
4	E	109	ILE
4	E	117	THR
4	E	123	LEU
4	E	127	ILE
4	E	146	HIS
4	E	150	VAL
4	E	165	LEU
4	E	169	ARG
4	E	177	ARG
4	E	190	LEU
4	E	200	ARG
5	F	74	ILE
5	F	82	THR
5	F	111	LEU
5	F	112	GLU
5	F	118	LEU
5	F	138	LEU
5	F	152	ILE
6	H	2	SER
6	H	14	GLU
6	H	21	ASN
6	H	24	CYS
6	H	34	ASP
6	H	35	GLN
6	H	37	LYS
6	H	40	LEU
6	H	55	LEU
6	H	61	SER
7	I	22	ASN
7	I	31	THR

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Mol	Chain	Res	Type
7	I	35	VAL
7	I	52	ILE
7	I	77	LYS
7	I	84	VAL
7	I	91	ARG
7	I	97	MET
7	I	111	THR
7	I	118	ARG
7	I	120	GLN
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	26	GLN
8	J	37	SER
8	J	38	ARG
8	J	48	ARG
8	J	59	LYS
8	J	62	ARG
9	K	18	LYS
9	K	20	LYS
9	K	21	ILE
9	K	42	LEU
9	K	71	PHE
9	K	74	ARG
9	K	78	THR
9	K	102	LYS
9	K	103	THR
9	K	111	LEU
9	K	114	LEU
10	L	27	LEU
10	L	38	LEU
10	L	46	VAL
10	L	53	HIS
10	L	61	THR
10	L	64	LEU
10	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN

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Mol	Chain	Res	Type
1	A	5	GLN
1	A	54	ASN
1	A	83	HIS
1	A	118	HIS
1	A	119	ASN
1	A	171	GLN
1	A	225	ASN
1	A	306	ASN
1	A	339	ASN
1	A	439	ASN
1	A	445	ASN
1	A	451	HIS
1	A	517	ASN
1	A	640	GLN
1	A	650	GLN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	935	GLN
1	A	966	ASN
1	A	969	GLN
1	A	1070	GLN
1	A	1171	GLN
1	A	1265	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1393	ASN
2	B	121	ASN
2	B	178	ASN
2	B	224	GLN
2	B	255	GLN
2	B	325	GLN
2	B	357	GLN
2	B	363	HIS
2	B	383	ASN
2	B	415	GLN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS

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Mol	Chain	Res	Type
2	B	587	HIS
2	B	686	ASN
2	B	744	HIS
2	B	763	GLN
2	B	794	ASN
2	B	822	ASN
2	B	842	ASN
2	B	958	GLN
2	B	984	HIS
2	B	1013	ASN
2	B	1025	HIS
2	B	1074	ASN
2	B	1117	GLN
2	B	1178	ASN
2	B	1187	ASN
2	B	1193	GLN
3	C	17	ASN
3	C	65	HIS
3	C	112	ASN
3	C	123	ASN
3	C	131	HIS
3	C	151	GLN
3	C	167	HIS
3	C	231	ASN
3	C	267	GLN
4	E	99	HIS
4	E	106	GLN
4	E	113	GLN
4	E	179	GLN
5	F	100	GLN
6	H	133	ASN
6	H	134	ASN
7	I	12	ASN
7	I	60	GLN
7	I	87	GLN
7	I	90	GLN
8	J	26	GLN
9	K	29	ASN
9	K	52	ASN
9	K	65	HIS
9	K	89	ASN
10	L	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	4/6 (66%)	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 ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
11	2IA	R	10	11,14	19,24,25	1.06	1 (5%)	28,35,38	2.16	8 (28%)

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
11	2IA	R	10	11,14	-	1/7/25/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	10	2IA	C8-N7	2.21	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	10	2IA	C5-C4-N3	-5.31	119.40	126.72
11	R	10	2IA	N3-C2-N1	-5.13	120.82	128.58
11	R	10	2IA	C2-N3-C4	3.67	120.78	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	10	2IA	N9-C8-N7	-3.27	109.30	113.94
11	R	10	2IA	N3-C4-N9	3.18	132.58	127.17
11	R	10	2IA	C4-C5-N7	-2.95	107.21	110.58
11	R	10	2IA	C5-N7-C8	2.76	107.78	103.45
11	R	10	2IA	C5-C4-N9	2.03	108.02	105.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	10	2IA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	R	10	2IA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	1405/1733 (81%)	0.09	28 (1%) 65 46	72, 120, 213, 242	0
2	B	1114/1224 (91%)	0.06	20 (1%) 67 49	67, 110, 181, 232	0
3	C	266/318 (83%)	-0.09	2 (0%) 82 68	83, 111, 153, 201	0
4	E	214/215 (99%)	0.07	3 (1%) 73 55	85, 153, 214, 225	0
5	F	85/155 (54%)	-0.09	0 100 100	88, 126, 166, 188	0
6	H	133/146 (91%)	0.22	5 (3%) 44 30	128, 170, 186, 196	0
7	I	119/122 (97%)	0.14	3 (2%) 58 39	89, 129, 162, 181	0
8	J	65/70 (92%)	-0.22	1 (1%) 72 53	67, 101, 131, 145	0
9	K	114/120 (95%)	-0.20	1 (0%) 81 65	84, 121, 148, 155	0
10	L	46/70 (65%)	0.46	4 (8%) 16 12	98, 139, 169, 173	0
11	R	5/6 (83%)	-0.36	0 100 100	152, 160, 171, 177	0
12	T	12/29 (41%)	1.02	1 (8%) 17 13	184, 198, 229, 229	0
All	All	3578/4208 (85%)	0.06	68 (1%) 66 48	67, 119, 201, 242	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	715	ALA	4.1
1	A	1108	ALA	4.0
2	B	1173	ALA	3.5
2	B	478	GLY	3.5
4	E	95	THR	3.3
1	A	154	SER	3.3
1	A	1085	HIS	3.3
2	B	882	THR	3.3
2	B	477	ALA	3.2
2	B	709	ASP	3.2
1	A	1081	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
10	L	27	LEU	3.1
1	A	1086	PHE	3.0
2	B	502	ILE	3.0
10	L	28	LYS	3.0
1	A	1273	LEU	3.0
7	I	52	ILE	2.9
1	A	1091	SER	2.9
1	A	980	ASP	2.8
1	A	179	LEU	2.8
2	B	883	LEU	2.8
8	J	44	TYR	2.7
1	A	105	CYS	2.7
2	B	335	GLY	2.7
2	B	212	LEU	2.7
4	E	90	VAL	2.7
6	H	139	ASN	2.6
1	A	1090	ALA	2.6
1	A	141	LEU	2.5
1	A	998	LEU	2.5
3	C	234	SER	2.5
6	H	84	ALA	2.5
1	A	296	LEU	2.5
6	H	63	LEU	2.5
1	A	289	ILE	2.4
2	B	819	ALA	2.4
1	A	250	ILE	2.4
2	B	708	GLU	2.4
1	A	55	ASP	2.4
1	A	276	LEU	2.4
3	C	233	GLU	2.4
1	A	138	ILE	2.4
4	E	120	ALA	2.3
2	B	446	LEU	2.3
1	A	1306	LEU	2.3
2	B	165	VAL	2.3
6	H	83	GLN	2.3
1	A	1089	VAL	2.3
2	B	70	ILE	2.2
12	T	27	DA	2.2
1	A	885	THR	2.2
7	I	120	GLN	2.2
2	B	468	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	364	ILE	2.2
1	A	54	ASN	2.2
10	L	26	THR	2.2
2	B	526	GLU	2.2
1	A	1332	PHE	2.2
1	A	103	CYS	2.1
1	A	1082	ASN	2.1
6	H	132	LEU	2.1
2	B	509	ALA	2.1
1	A	710	LEU	2.1
2	B	935	ARG	2.1
7	I	13	MET	2.1
10	L	25	ALA	2.1
1	A	596	THR	2.0
9	K	114	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
11	2IA	R	10	22/23	0.79	0.11	147,150,152,152	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
13	ZN	A	1734	1/1	0.82	0.13	300,300,300,300	0
13	ZN	A	1735	1/1	0.93	0.08	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	B	1307	1/1	0.97	0.04	226,226,226,226	0
14	MG	A	2001	1/1	0.97	0.07	47,47,47,47	0
13	ZN	I	203	1/1	0.99	0.04	129,129,129,129	0
13	ZN	L	105	1/1	0.99	0.03	169,169,169,169	0
13	ZN	C	319	1/1	0.99	0.03	126,126,126,126	0
13	ZN	I	204	1/1	1.00	0.03	118,118,118,118	0
13	ZN	J	101	1/1	1.00	0.02	112,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.