



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 01:58 AM EDT

PDB ID : 1SFO / pdb_00001sfo
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COMPLEX
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-02-20
Resolution : 3.61 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

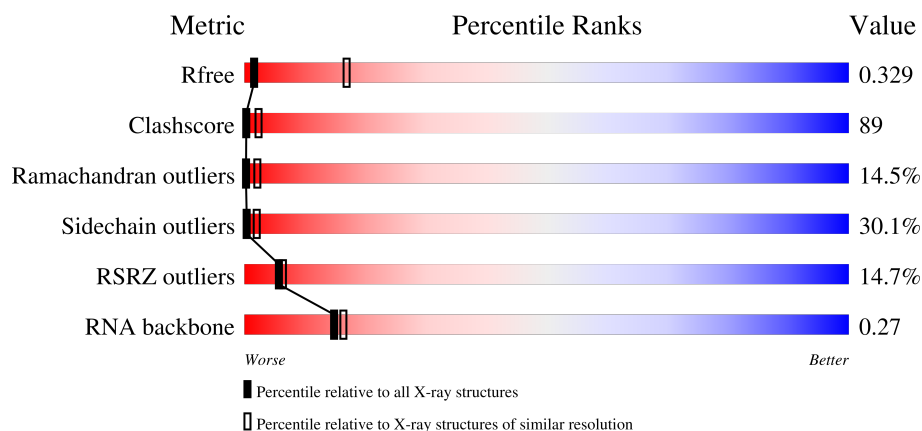
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)
RNA backbone	3983	1018 (4.18-3.06)

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	R	10	100% 40% 40% 20%
2	T	14	93% 21% 64% 14%
3	A	1733	12% 9% 34% 27% 11% 20%
4	B	1224	12% 12% 39% 29% 10% 10%

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Mol	Chain	Length	Quality of chain
5	C	318	4% 15% 34% 28% 6% 16%
6	E	215	30% 11% 40% 38% 11%
7	F	155	6% 8% 27% 18% 46%
8	H	146	17% 9% 30% 34% 18% 9%
9	I	122	14% 16% 30% 39% 12%
10	J	70	6% 13% 41% 24% 14% 7%
11	K	120	2% 10% 53% 25% 7% 5%
12	L	70	10% 26% 20% 17% 34%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28647 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 RNA chain called RNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called DNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	14	Total	C	N	O	P	0	0	0
			279	135	48	83	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1106	Total	C	N	O	S	0	0	0
			8793	5568	1538	1632	55			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

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

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

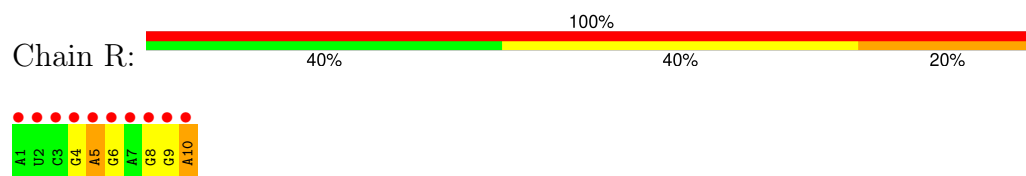
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

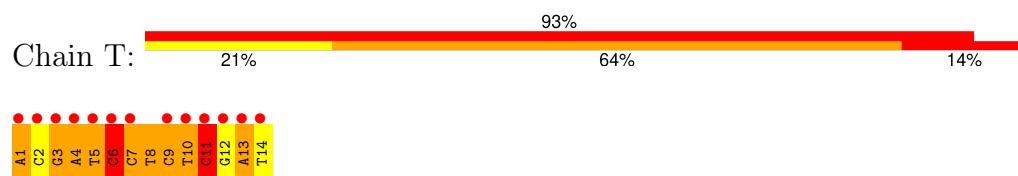
3 Residue-property plots

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.

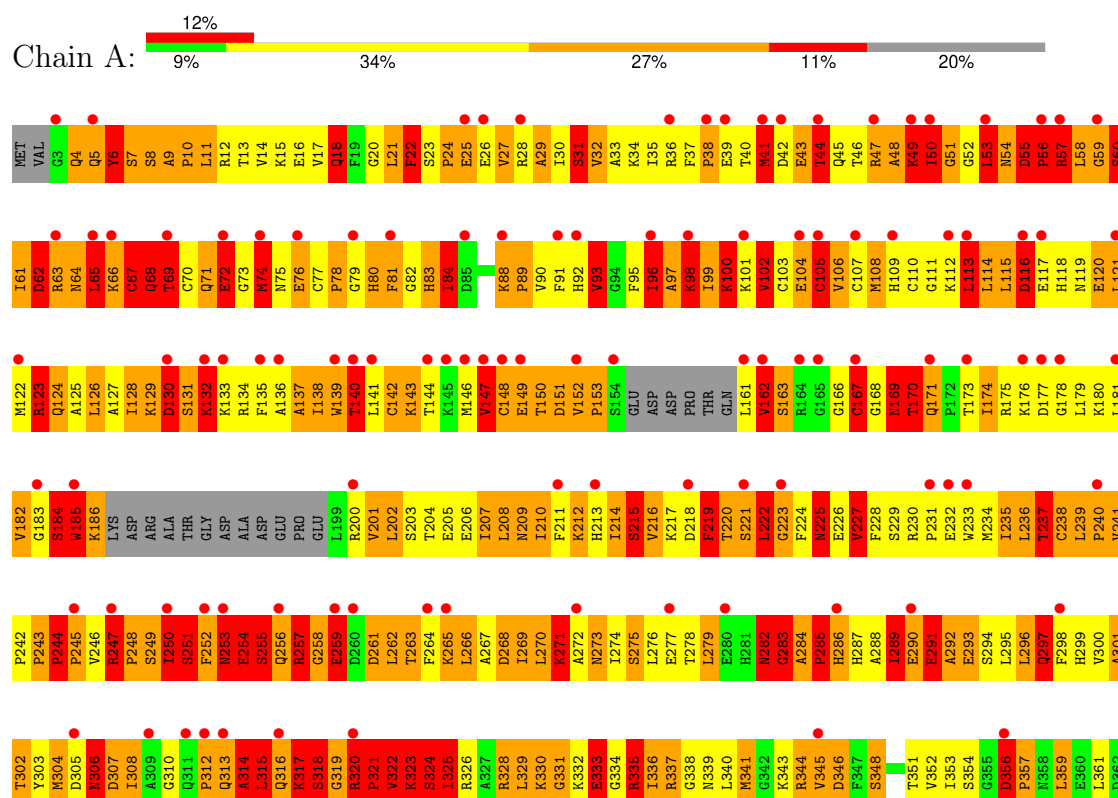
• Molecule 1: RNA STRAND



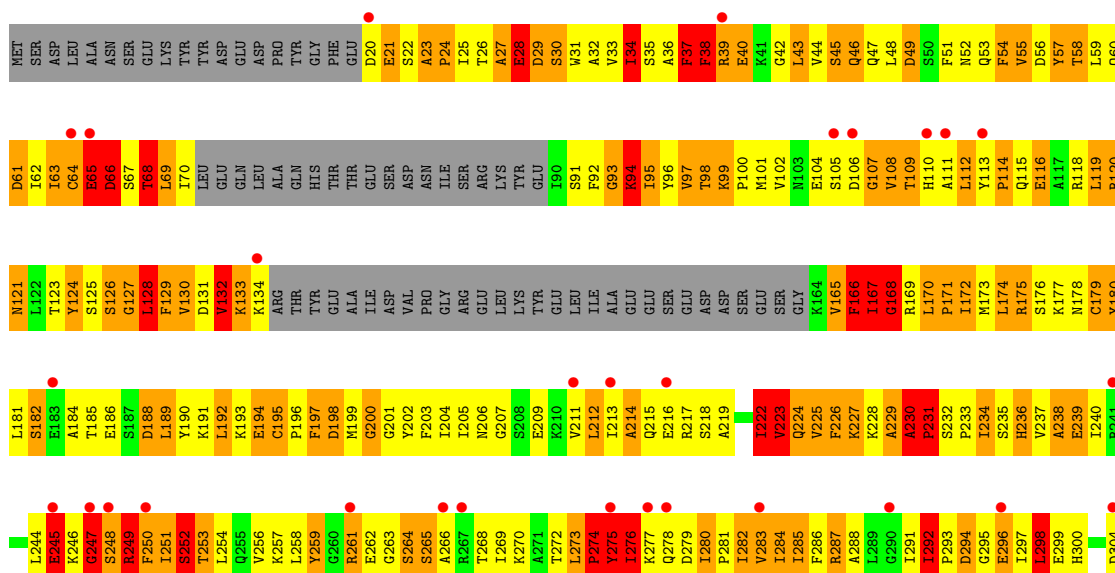
• Molecule 2: DNA STRAND

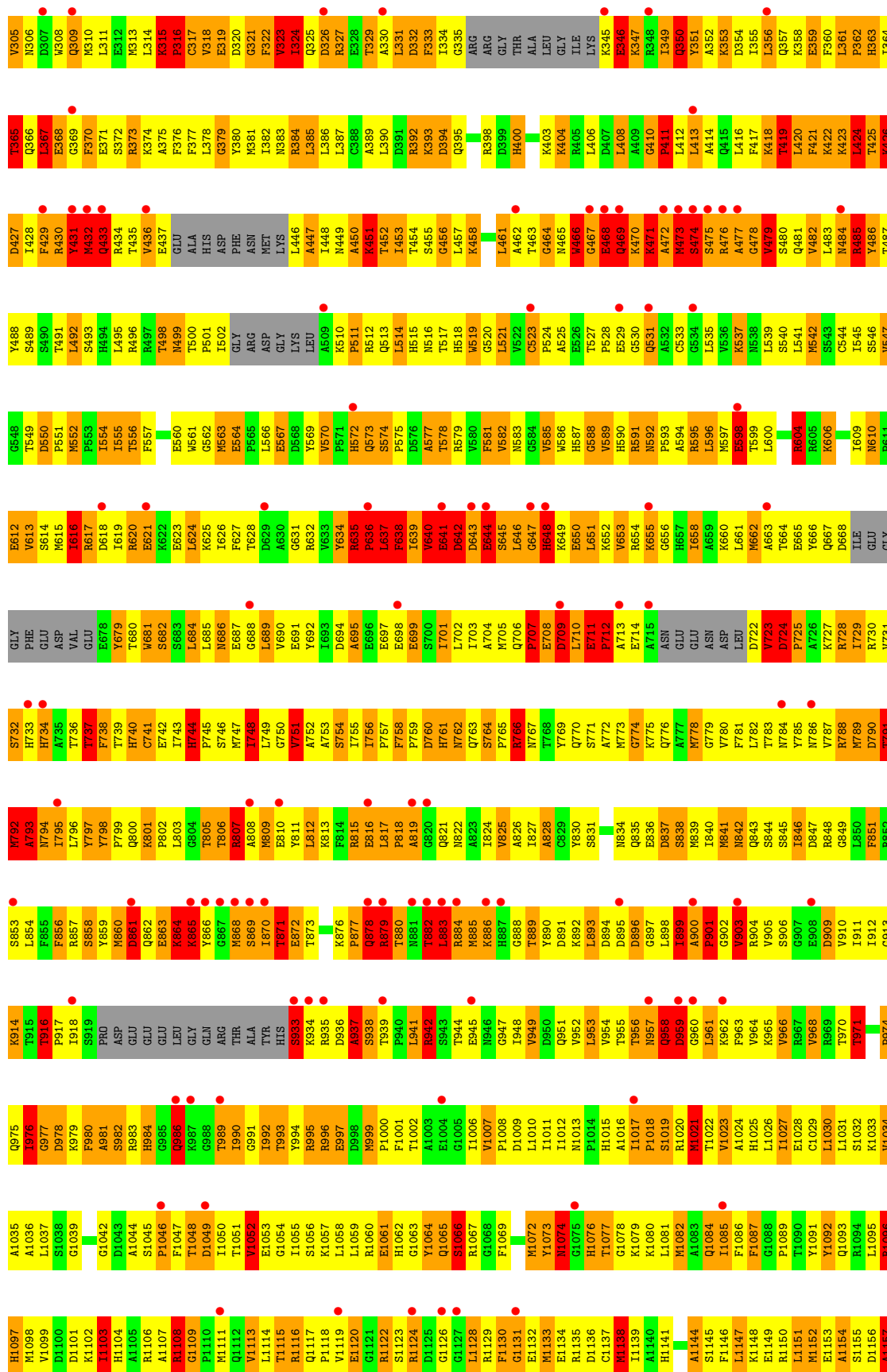


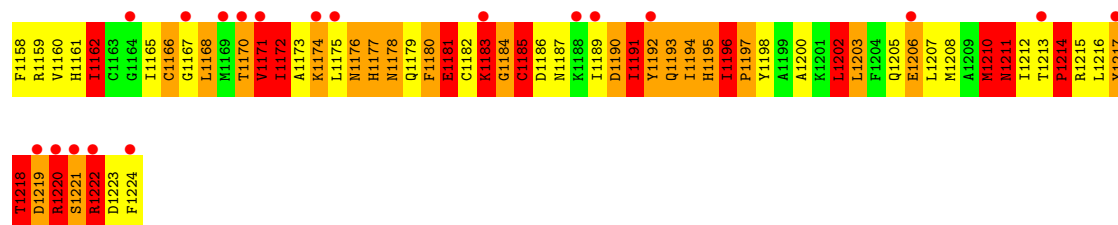
• Molecule 3: DNA-directed RNA polymerase II largest subunit



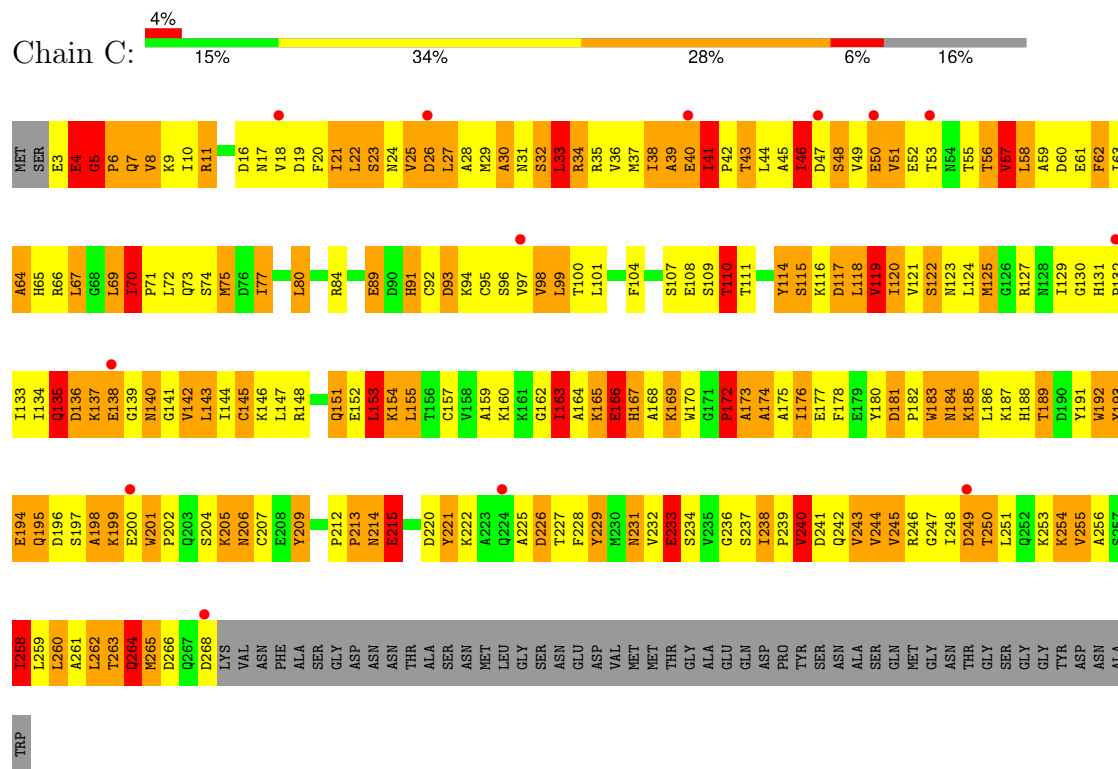
D1157	P1156	G1097	L1037	K977	S917	R857	E795	A733	G673	Q611	Y551	M487	Q425	Q363
P1158	P1159	V1095	T1038	P978	E918	N858	S796	E734	P674	I612	W551	M487	L426	V364
S1160	R1100	R1099	K1039	S979	I919	S859	K797	N735	T675	I613	W553	H490	Q427	G365
T1161	R1101	P1099	Q1040	D980	L920	N860		N736	M676	F614	P554	H491	Y428	V366
V1162	F1042	T982	G821	N981	G921	G861	E800	K738	R677	G615	W555	Q493	G429	P367
I1163	D1043	T982	D922	N862	D922	N862	N802	K738	E678	V616	W556	Q493	M430	K368
P1164	W1044	I983	L923	V863	L923	V863	N802	K738	T679	V617	D557	S494	K431	S369
E1165	V1045	K984	K924	I864	L925	I864	S803	L740	T680	E618	G558	E496	V432	I370
L1105	D985	D985	L925	Q865	L925	Q865	Y804	N741	E681	K619	V559	E496	E433	T373
D1106	L1046	I986	Q926	F866	Q926	F866	L805	N742	T682	I620	I560	T497	R435	L374
E1167	V1047	V987	V927	I867	V927	I867	R806	V743	T683	T621	R434	T497	R435	L374
N1108	N1048	L988	L928	Y868	L928	Y868	G807	K744	A684	G623	T562	A499	I436	T375
K1109	T1049	G989	L929	G869	L929	G869	L808	K744	A684	G623	T562	A499	I436	T375
N1110	E1050	E870	T809	E870	D930	E870	T809	N746	A686	S624	A564	E500	M437	Y376
M1111	K991	D871	P810	D871	E931	D871	P810	N747	K687	S625	I565	E500	M437	Y376
K1112	Q1052	G872	Q811	G872	E932	G872	Q811	N748	K688	S625	I565	E500	M437	Y376
T1113	F1053	M873	E812	M873	K934	M873	E812	A749	K689	G627	K567	A506	P441	T381
F1174	L1054	D874	F813	D874	K934	D874	F813	G750	V690	G628	K568	A506	P441	T381
S1115	Q994	Q935	F814	Q935	Q935	F814	F814	S751	V690	G628	K568	A506	P441	T381
L1116	E995	L936	F815	L936	L936	F815	F815	S751	V690	G628	K568	A506	P441	T381
T1117	N996	V937	H816	V937	V937	H816	H816	G753	D692	I630	P570	E507	L443	Y382
V1118	K938	K938	A817	K938	K938	A817	A817	S754	T694	V633	L571	V512	Q447	T385
Y1119	V1058	E879	M818	E879	D939	E879	M818	F755	K695	T634	S573	S513	Q447	T385
L1120	P1060	K880	G819	K880	R940	K880	G819	I758	E696	R635	K574	P514	P448	R387
G1061	G1061	K941	G820	K941	R940	K941	G820	N757	E697		K575	P514	P448	R387
E1062	E1062	F942	S882	F942	G1002	S882	S882	I758	Q698	G638	Q576	S516	L450	T389
F1063	F1063	L943	E822	L943	K1003	E822	E822	A759	A699	P639	L577	S517	H451	Q390
V1064	V1064	R944	G823	R944	N004	G823	G823	Q760	A699	Q640	L577	S517	R452	Q390
G1065	G1065	E945	L824	E945	E1005	L824	L824	L701	K695	Q641	S579	P519	R446	T392
V1066	V1066	I886	I825	I886	I1006	I886	I825	G764	L702	C642	V580	C520	S454	R393
L1067	L1067	F947	D826	F947	I1007	D826	D826	V765	L703	N643	A581	N521	M455	K394
A1068	A1068	V948	T827	V948	Q1068	T827	T827	G766	A704	K644	I582	G522	M456	C395
E1069	E1069	D949	T829	D949	R1009	T829	T829	Q767	A704	L645	I582	G522	M456	C395
Q1070	Q1070	G950	V829	G950	E951	V829	V829	Q768	H706	F646	N584	V524	H458	P396
S1071	S1071	E951	K830	E951	K830	S769	K830	S769	H706	G647	N584	V524	H458	N397
I1072	I1072	A952	T831	A952	R1012	T831	T831	V770	M708	N648	I586	D526	V462	E398
G1073	G1073	N953	A832	N953	D1013	A832	A832	E771	T709	I649	H587	T527	T463	H399
E1074	E1074	W954	E894	W954	A1014	E894	E894	G772	L710	Q650	L588	L528	P464	P400
F1075	F1075	P955	K895	P955	V1015	K895	T834	K773	R711	K651	Q589	C529	P464	G401
A1076	A1076	L956	R896	L956	T1016	R896	G836	R774	E712	V652	R590	G530	Y465	A402
T1077	T1077	P957	Y897	P957	L1017	Y897	Y836	I775	S713	V653	F591	S531	S466	K403
Q1078	Q1078	V958	R898	V958	F1018	R898	I837	A776	F714	N654	D592	R532	T467	V404
M1079	M1079	N959	V899	N959	C1019	V899	Q838	F777	E715	F655	E593	K833	F468	I406
T1080	T1080	D900	D900	D900	C1020	D900	R839	G778	D716	W656	G594	L534	R469	R407
L1081	L1081	L901	L901	L901	L1021	L901	R840	F779	N717	L857	T595	T635	L471	D408
ASN	ASN	R962	L902	R962	L1022	R962	L841	W780	V718	L688	T596	L536	L472	S409
THR	THR	I963	N903	I963	R1023	N903	V842	D781	V719	L688	T596	L536	L472	R412
PHE	PHE	I964	T904	I964	S1024	T904	K843	R782	W659	N660	L597	R537	S473	R416
HIS	HIS	Q965	D905	Q965	R1025	D905	A844	F783	R720	D599	L598	D538	V474	Y417
PHE	PHE	N966	H906	N966	L1026	H906	L845	T784	F721	G661	M605	D544	T475	S418
ALA	ALA	A967	T807	A967	A1027	T807	E846	F785	L722	F662	P600	F540	S478	K419
GLY	GLY	Q968	L908	Q968	T1028	L908	D847	W786	N723	S663	K601	E541	P477	R420
VAL	VAL	Q969	D909	Q969	R1029	D909	T848	F787	E724	T664	D602	E542	Y478	R416
ALA	ALA	T970	P910	T970	R1030	P910	M849	S788	A725	G665	N603	L543	P477	R416
SER	SER	F971	S911	F971	V1031	S911	H872	K789	R726	G666	G804	D544	T478	Y417
K1032	K1032	H972	L912	H972	L1032	L912	V852	W790	K728	G667	M605	Q545	F482	S418
Q1033	Q1033	I973	L913	I973	Q1033	L913	D853	D791	A729	D668	L606	V546	D483	K419
E1034	E1034	R974	E914	R974	E1034	E914	N854	Y792	G730	T669	I607	L547	D483	R420
H975	H975	D975	S855	D975	T855	D975	T855	S793	R731	I670	I608	N548	G484	A421
S1096	S1096	T976	T976	T976	R1036	T976	T856	P794	L732	D672	G610	L550	E496	G422



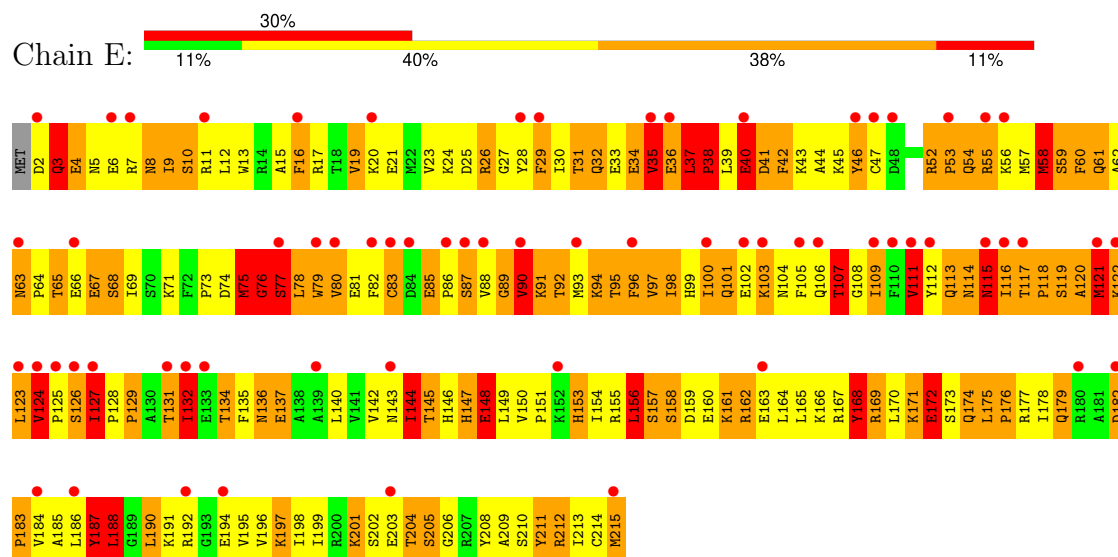




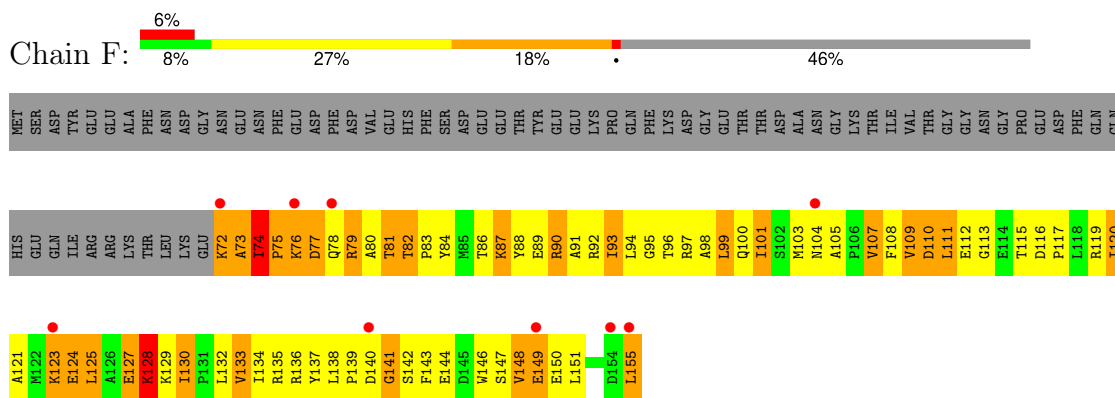
• Molecule 5: DNA-directed RNA polymerase II 45 kDa polypeptide



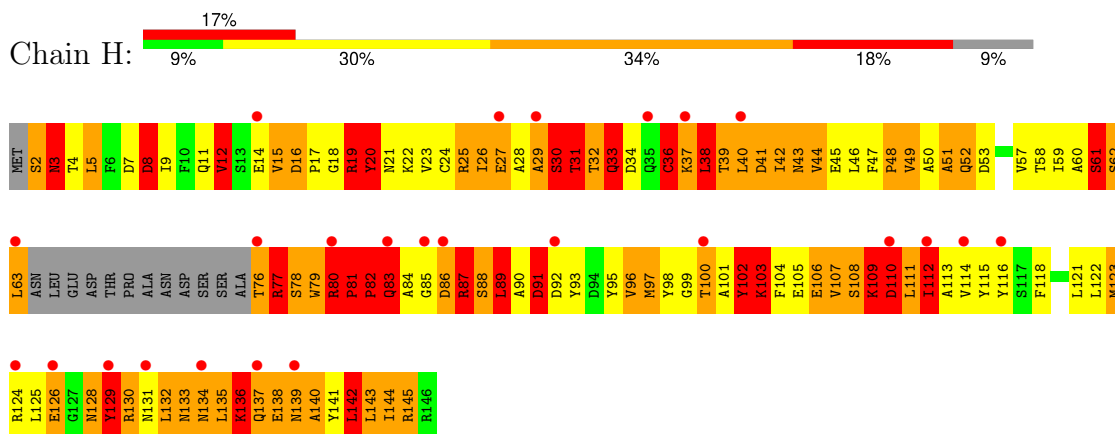
• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



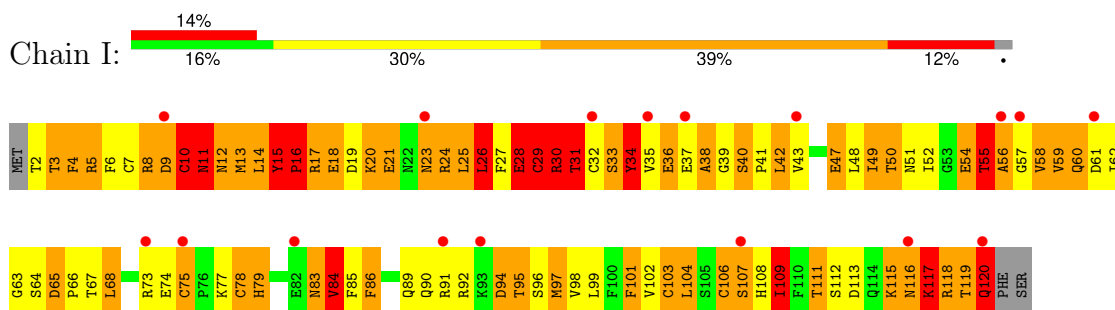
• Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



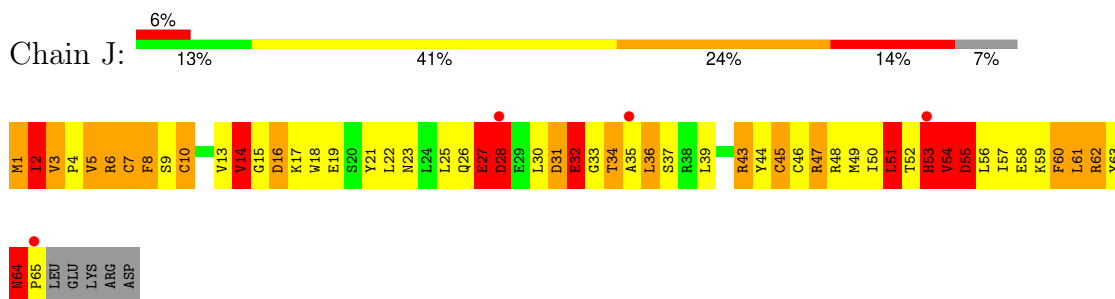
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



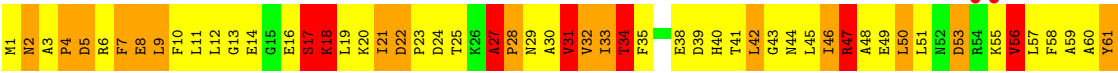
- Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide



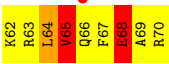
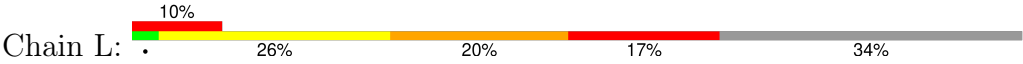
- Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



● Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.08Å 221.26Å 193.69Å 90.00° 100.10° 90.00°	Depositor
Resolution (Å)	39.86 – 3.61 39.86 – 3.61	Depositor EDS
% Data completeness (in resolution range)	92.7 (39.86-3.61) 92.6 (39.86-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.315 , 0.343 0.309 , 0.329	Depositor DCC
R_{free} test set	8031 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 18.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	28647	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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

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	R	0.56	0/244	0.91	0/380
2	T	0.49	0/311	1.62	9/477 (1.9%)
3	A	1.14	45/11163 (0.4%)	2.10	539/15091 (3.6%)
4	B	1.09	31/8964 (0.3%)	1.96	353/12086 (2.9%)
5	C	0.96	0/2133	1.85	77/2891 (2.7%)
6	E	1.10	4/1788 (0.2%)	2.08	74/2406 (3.1%)
7	F	1.06	0/691	2.06	18/933 (1.9%)
8	H	1.12	3/1086 (0.3%)	2.15	60/1470 (4.1%)
9	I	1.28	6/989 (0.6%)	2.24	59/1331 (4.4%)
10	J	0.94	0/541	2.02	18/727 (2.5%)
11	K	0.89	0/937	1.71	29/1265 (2.3%)
12	L	1.16	0/366	2.38	23/485 (4.7%)
All	All	1.09	89/29213 (0.3%)	2.02	1259/39542 (3.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	5
3	A	1	6
4	B	0	7
5	C	0	2
6	E	0	1
9	I	0	1
All	All	1	22

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	319	GLY	C-O	12.81	1.41	1.23
3	A	320	ARG	CA-CB	12.00	1.72	1.53
3	A	323	LYS	N-CA	9.82	1.58	1.46
4	B	981	ALA	CA-C	-9.07	1.40	1.52
3	A	531	ILE	CA-CB	8.73	1.66	1.54

The worst 5 of 1259 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	821	ARG	N-CA-C	-26.04	79.39	112.72
4	B	479	VAL	N-CA-C	-22.98	84.24	110.21
7	F	74	ILE	CA-C-N	20.19	140.48	119.89
7	F	74	ILE	C-N-CA	20.19	140.48	119.89
3	A	322	VAL	N-CA-C	19.68	150.26	109.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	322	VAL	CA

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	T	10	DT	Sidechain
2	T	11	DC	Sidechain
2	T	13	DA	Sidechain
2	T	6	DC	Sidechain
2	T	8	DT	Sidechain

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	R	217	0	110	19	0
2	T	279	0	160	43	0
3	A	10969	0	11070	2196	0
4	B	8793	0	8823	1668	0
5	C	2095	0	2051	355	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1752	0	1776	310	0
7	F	679	0	701	133	0
8	H	1068	0	1040	204	0
9	I	971	0	929	173	0
10	J	532	0	542	127	0
11	K	919	0	929	181	0
12	L	364	0	387	66	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	28647	0	28518	5075	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 89.

The worst 5 of 5075 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:A:853:ASP:OD1	3:A:855:THR:HB	1.32	1.25
3:A:90:VAL:HG12	3:A:297:GLN:NE2	1.49	1.24
4:B:635:ARG:HB2	4:B:636:PRO:CD	1.65	1.21
3:A:321:PRO:O	3:A:322:VAL:HG22	1.41	1.18
3:A:351:THR:HG23	4:B:1103:ILE:HD12	1.23	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1383/1733 (80%)	851 (62%)	315 (23%)	217 (16%)	0	2
4	B	1088/1224 (89%)	730 (67%)	214 (20%)	144 (13%)	0	3
5	C	264/318 (83%)	187 (71%)	49 (19%)	28 (11%)	0	4
6	E	212/215 (99%)	142 (67%)	41 (19%)	29 (14%)	0	2
7	F	82/155 (53%)	49 (60%)	26 (32%)	7 (8%)	0	6
8	H	129/146 (88%)	87 (67%)	16 (12%)	26 (20%)	0	1
9	I	117/122 (96%)	74 (63%)	24 (20%)	19 (16%)	0	2
10	J	63/70 (90%)	42 (67%)	11 (18%)	10 (16%)	0	2
11	K	112/120 (93%)	81 (72%)	20 (18%)	11 (10%)	0	5
12	L	44/70 (63%)	20 (46%)	10 (23%)	14 (32%)	0	0
All	All	3494/4173 (84%)	2263 (65%)	726 (21%)	505 (14%)	0	2

5 of 505 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	44	THR
3	A	50	ILE
3	A	55	ASP
3	A	56	PRO
3	A	57	ARG

5.3.2 Protein sidechains [i](#)

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	
3	A	1218/1520 (80%)	834 (68%)	384 (32%)	0	2
4	B	960/1061 (90%)	684 (71%)	276 (29%)	0	2
5	C	234/274 (85%)	168 (72%)	66 (28%)	0	2
6	E	196/197 (100%)	134 (68%)	62 (32%)	0	2
7	F	74/137 (54%)	53 (72%)	21 (28%)	0	2
8	H	117/128 (91%)	76 (65%)	41 (35%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	113/116 (97%)	85 (75%)	28 (25%)	1	4
10	J	60/65 (92%)	42 (70%)	18 (30%)	0	2
11	K	99/102 (97%)	74 (75%)	25 (25%)	0	4
12	L	40/57 (70%)	25 (62%)	15 (38%)	0	0
All	All	3111/3657 (85%)	2175 (70%)	936 (30%)	0	2

5 of 936 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	408	LEU
10	J	31	ASP
4	B	886	LYS
9	I	120	GLN
7	F	115	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	255	GLN
9	I	12	ASN
4	B	657	HIS
8	H	137	GLN
11	K	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	5	A
1	R	10	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 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	R	10/10 (100%)	4.80	10 (100%) 0 0	30, 82, 200, 200	0
2	T	14/14 (100%)	3.48	13 (92%) 0 0	30, 106, 200, 200	0
3	A	1395/1733 (80%)	1.07	207 (14%) 5 6	30, 32, 134, 200	0
4	B	1106/1224 (90%)	1.06	151 (13%) 6 7	30, 30, 118, 198	0
5	C	266/318 (83%)	0.81	13 (4%) 35 21	30, 30, 84, 140	0
6	E	214/215 (99%)	1.60	65 (30%) 1 1	30, 67, 153, 200	0
7	F	84/155 (54%)	0.78	9 (10%) 11 11	30, 31, 93, 141	0
8	H	133/146 (91%)	1.25	25 (18%) 3 4	30, 47, 138, 190	0
9	I	119/122 (97%)	1.23	17 (14%) 6 7	30, 32, 114, 163	0
10	J	65/70 (92%)	0.75	4 (6%) 26 17	30, 30, 96, 141	0
11	K	114/120 (95%)	0.66	3 (2%) 57 35	30, 30, 73, 107	0
12	L	46/70 (65%)	1.18	7 (15%) 5 6	30, 45, 132, 158	0
All	All	3566/4197 (84%)	1.09	524 (14%) 6 6	30, 31, 130, 200	0

The worst 5 of 524 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	183	GLY	7.9
1	R	4	G	7.4
1	R	3	C	6.7
4	B	475	SER	6.6
6	E	93	MET	6.1

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 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($\text{\AA}^2$)	Q<0.9
13	ZN	A	1734	1/1	0.91	0.28	22,22,22,22	0
13	ZN	B	1307	1/1	0.93	0.18	22,22,22,22	0
14	MG	A	2000	1/1	0.93	0.10	22,22,22,22	0
13	ZN	I	204	1/1	0.94	0.18	22,22,22,22	0
13	ZN	I	203	1/1	0.94	0.23	22,22,22,22	0
13	ZN	A	1735	1/1	0.96	0.15	22,22,22,22	0
13	ZN	L	105	1/1	0.99	0.07	22,22,22,22	0
13	ZN	J	101	1/1	0.99	0.04	22,22,22,22	0
13	ZN	C	319	1/1	1.00	0.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.