



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2017 – 03:30 PM EDT

PDB ID : 2PMZ
Title : Archaeal RNA polymerase from *Sulfolobus solfataricus*
Authors : Murakami, K.S.
Deposited on : unknown
Resolution : 3.40 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

<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 : rb-20030345
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) : rb-20030345

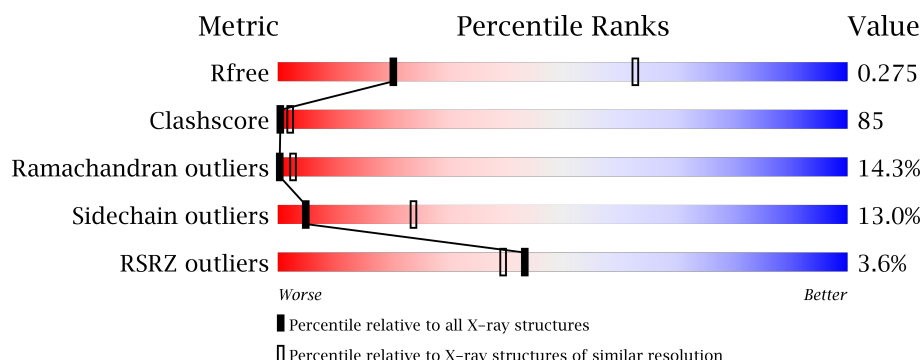
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	880	<div> <div>2%</div> <div>16% 52% 18% 12%</div> </div>
1	Q	880	<div> <div>3%</div> <div>16% 54% 17% 12%</div> </div>
2	C	392	<div> <div>3%</div> <div>11% 42% 15% 29%</div> </div>
2	G	392	<div> <div>3%</div> <div>11% 41% 16% 29%</div> </div>
3	B	1124	<div> <div>2%</div> <div>17% 60% 18% ..</div> </div>

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Mol	Chain	Length	Quality of chain
3	R	1124	
4	D	265	
4	S	265	
5	E	180	
5	T	180	
6	F	113	
6	U	113	
7	H	84	
7	V	84	
8	K	95	
8	W	95	
9	L	92	
9	X	92	
10	N	66	
10	Y	66	
11	P	48	
11	Z	48	

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
14	F3S	D	1001	-	-	X	-
14	F3S	S	1001	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 48122 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 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	776	Total	C	N	O	S	0	0	0
			6173	3936	1081	1135	21			
1	Q	776	Total	C	N	O	S	0	0	0
			6173	3936	1081	1135	21			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit A".

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	279	Total	C	N	O	S	0	0	0
			2169	1376	375	412	6			
2	G	279	Total	C	N	O	S	0	0	0
			2169	1376	375	412	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1090	Total	C	N	O	S	0	0	0
			8645	5483	1529	1602	31			
3	R	1090	Total	C	N	O	S	0	0	0
			8645	5483	1529	1602	31			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	264	Total	C	N	O	S	0	0	0
			2114	1355	342	403	14			
4	S	264	Total	C	N	O	S	0	0	0
			2114	1355	342	403	14			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	176	Total	C	N	O	S	0	0	0
			1402	903	236	259	4			
5	T	176	Total	C	N	O	S	0	0	0
			1402	903	236	259	4			

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	89	Total	C	N	O	S	0	0	0
			694	433	115	142	4			
6	U	89	Total	C	N	O	S	0	0	0
			694	433	115	142	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	74	Total	C	N	O		0	0	0
			611	397	109	105				
7	V	74	Total	C	N	O		0	0	0
			611	397	109	105				

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			
8	W	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	92	Total	C	N	O	S	0	0	0
			723	459	121	141	2			
9	X	92	Total	C	N	O	S	0	0	0
			723	459	121	141	2			

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	64	Total	C	N	O	S	0	0	0
			514	326	94	88	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Y	64	Total	C	N	O	S	0	0	0
			514	326	94	88	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			
11	Z	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			

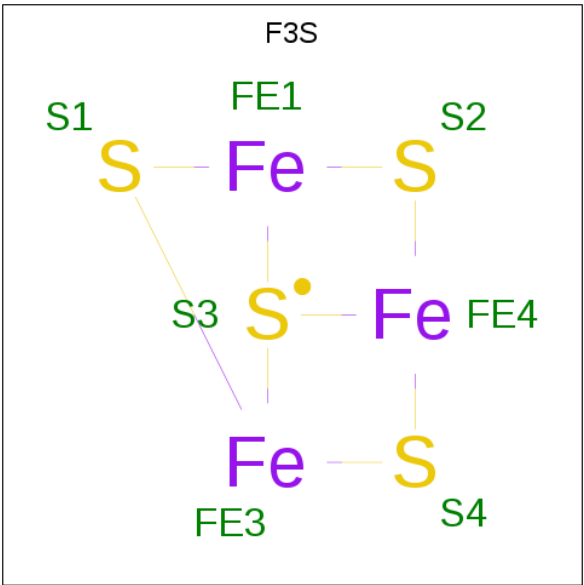
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	P	1	Total	Zn	0	0
			1	1		
12	Q	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		
12	Z	1	Total	Zn	0	0
			1	1		
12	A	1	Total	Zn	0	0
			1	1		
12	N	1	Total	Zn	0	0
			1	1		
12	R	1	Total	Zn	0	0
			1	1		
12	Y	1	Total	Zn	0	0
			1	1		

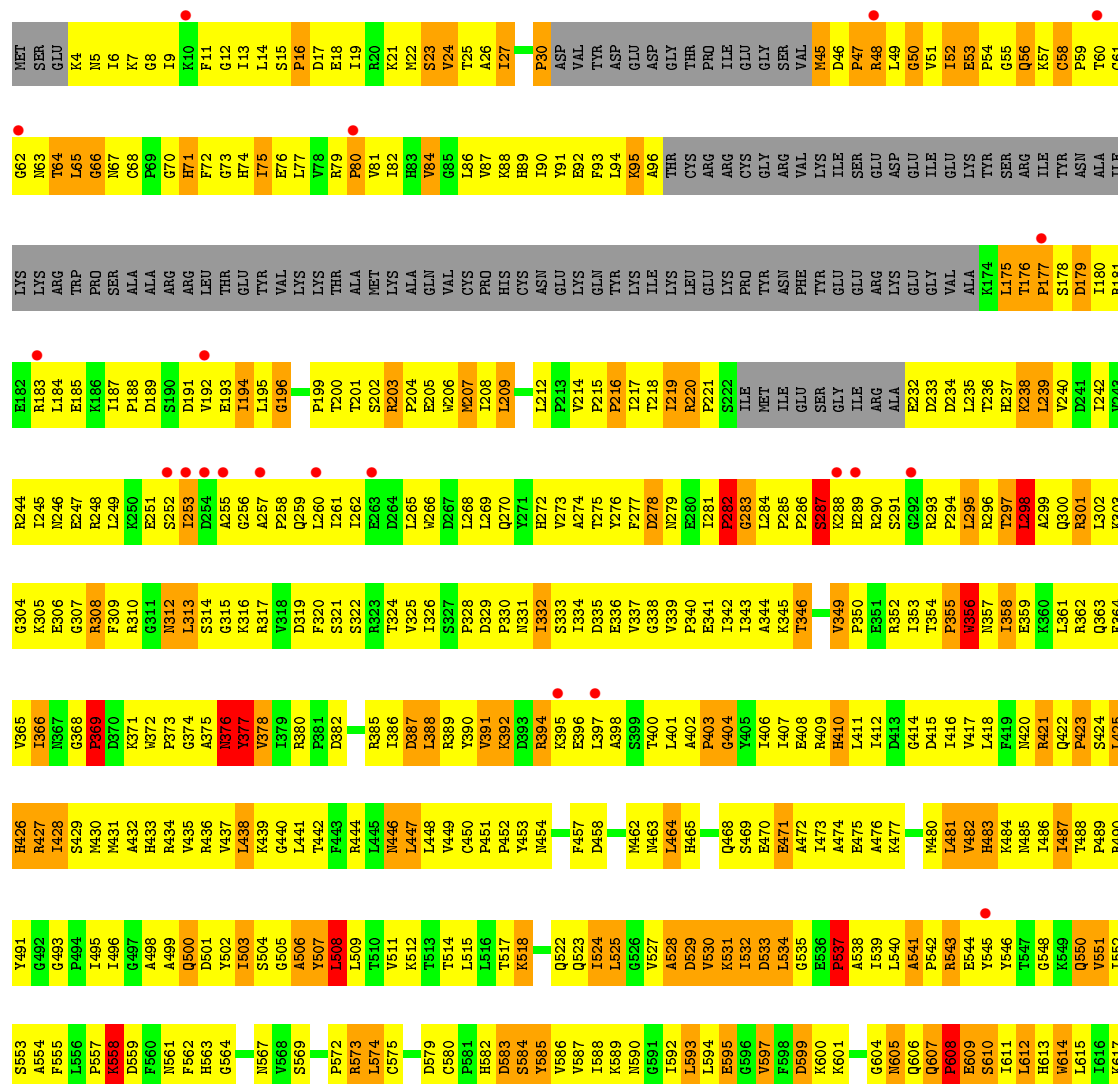
- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

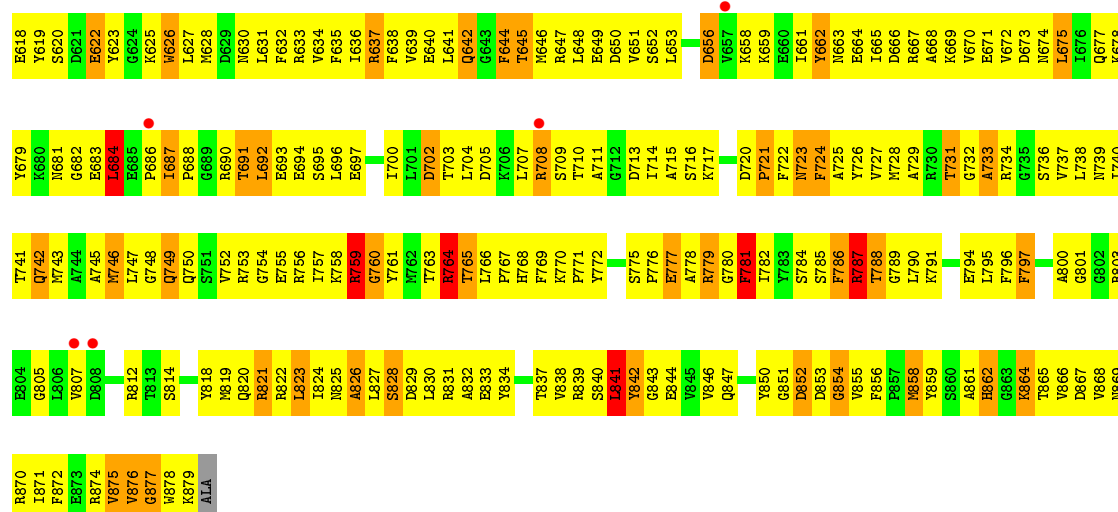
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	Q	1	Total	Mg	0	0
			1	1		
13	A	1	Total	Mg	0	0
			1	1		

- Molecule 14 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).

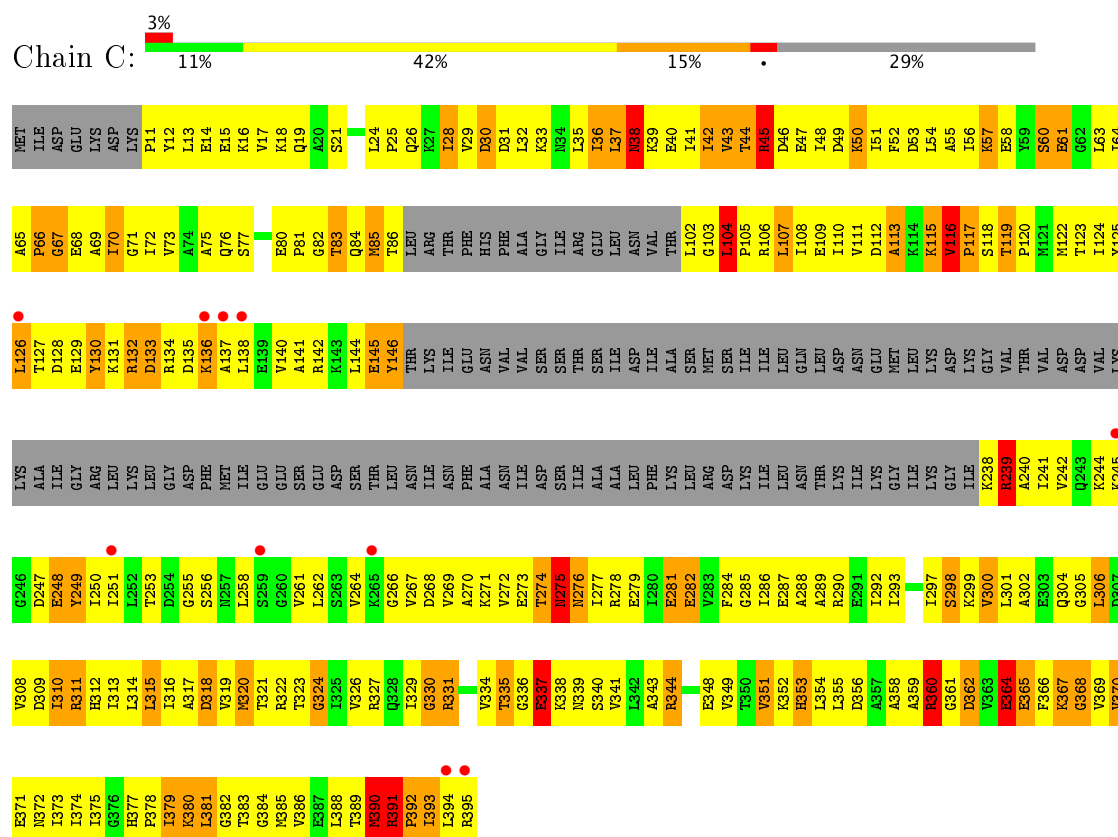


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	Fe	S	0	0
			7	3	4		
14	S	1	Total	Fe	S	0	0
			7	3	4		

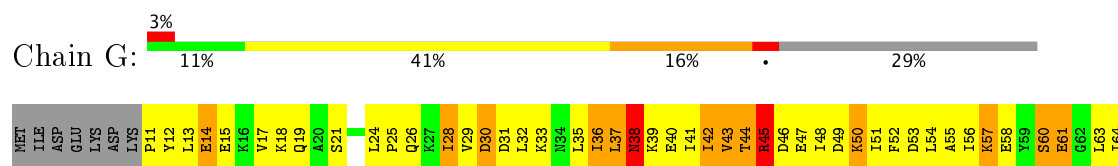


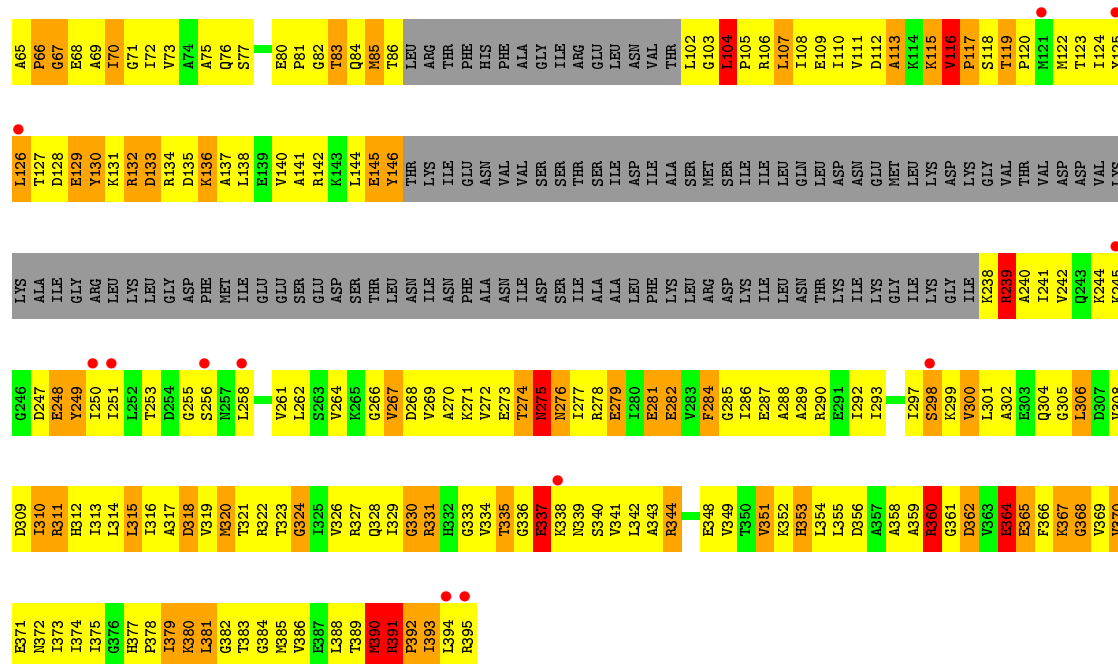


• Molecule 2: DNA-directed RNA polymerase subunit A"

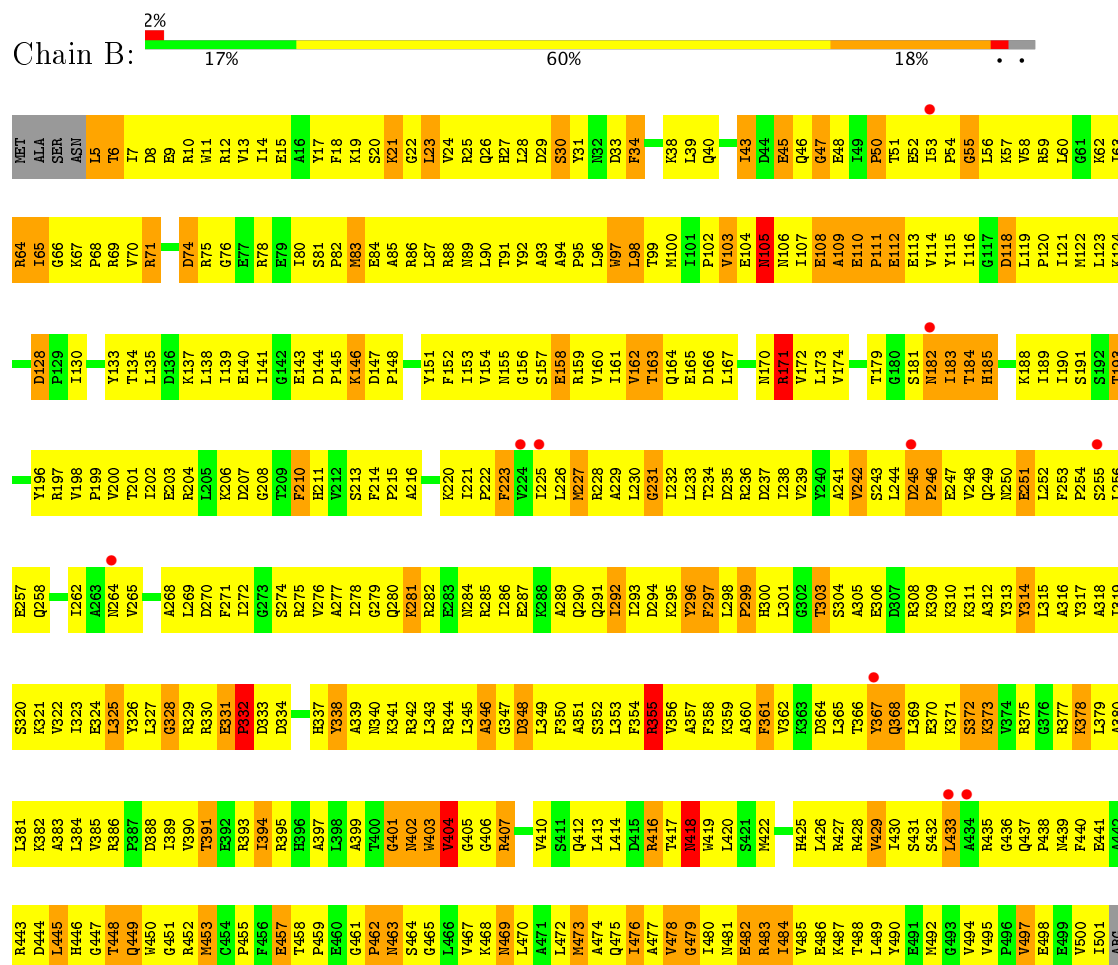


• Molecule 2: DNA-directed RNA polymerase subunit A"





• Molecule 3: DNA-directed RNA polymerase subunit B



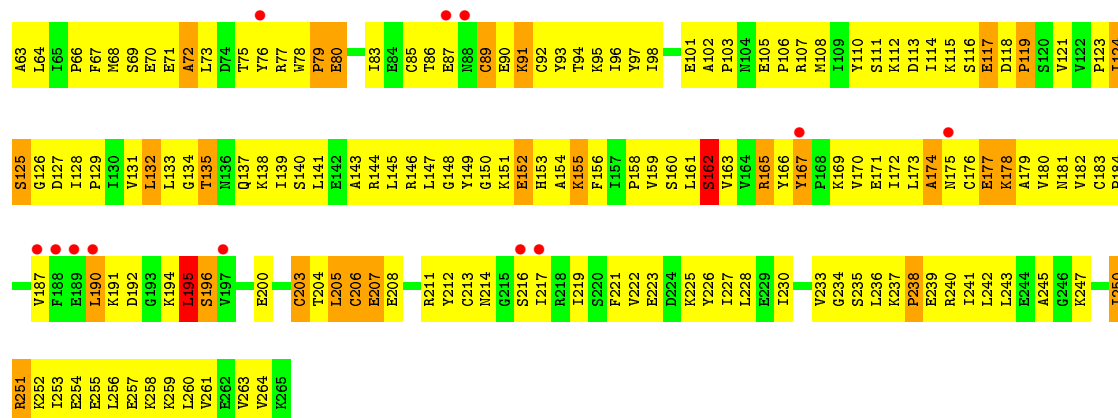


SER	G1061	L1001	S936	I874	K813	R751	R691	V636	I563	I501	E441	L379	V317
GLY	D1062	H1002	I939	G875	V814	S752	A692	A627	N064	ARG	A442	A380	A318
GLY	C1063	A1003	V940	K877	S815	T753	R693	E628	E565	ARG	R443	L381	L319
	G1064	R1004	V940	K877	P816	F754	R693	E529	V566	VAL	D444	K382	S320
	G1065	A1005	D941	F878	P817	F755	L695	P630	H567	THR	L445	K383	K321
	G1066	R1006	A942	A879	R818	R756	H696		V568	GLU	H446	L384	V322
	I1067	G1007	T943	S880	PHE	R757	H697		V569	GLY	G447	V385	I323
	G1068	F1008	P944	R881	LEU	L758	P698		K570	GLY	T448	K386	E324
	W1069	V1009	F945	H882	GLN	S759	Q699	P635	D571	GLU	Q449	P387	L325
	Y1070	Q1010	Y946	Q883	GLU		Q699		G572	ASP	H450	L388	V326
	D1071	I1011	K947	Q884	PHE	E762	P701		G573	GLN	G451	L389	L327
	K1072	L1012	T948	K885	LYS	V763	L702		R574	ASN	R452	V390	G328
	N1073	T1013	P949	G886	GLU	K764	V703		V575	GLU	H453	R329	R329
	K1074	A1014	I850	V887	LEU	V765	Q704		R576	TYR	C454	R330	R330
	N1075	Q1015	E951	I888	SER	R766	T705		R577	LEU	P455	E331	E331
	K1076	P1016	Q952	G889	PRO	G767	R706		R578	GLU	F456	P332	P332
	Y1077	I1017	L953	M890	GLN	G768	A707		L579	ASN	T457	R395	R395
	V1078	E1018	Q954	L891	GLN	G769	L708		L580	GLY	H458	R396	R396
	C1079	G1019	N955	I892	GLN	E770	D709		L581	GLY	P459	A397	A397
	P1080	R1020	E956	P893	K832	D771	I710		L582	GLY	E460	L398	L398
	I1081	A1021	I957	Q894	R833	K772	I711		N586	GLY	G461	A399	A399
	H1082	R1022	L958	V895	D834	L773	G712		P587	GLY	P462	T400	N340
	G1083	E1023	R959	D896	T835	V774	G713		L591	GLY	H463	G401	K341
	D1084	G1024	R959	D896	T835	V774	G713		L592	GLY	H463	G401	K341
	K1085	G1025	Y962	M897	S836	M775	G714		L593	GLY	H463	G401	K341
	S1086	L1026	L963	P898	V838	A778	R716		L594	GLY	H463	G401	K341
	N1087	R1027	P964	T899	T839	G779	P717		L595	GLY	H463	G401	K341
	L1088	F1028	D965	V901	R840	G780	P718		L596	GLY	H463	G401	K341
	F1089	G1029	A966	K902	D834	G781	P719		L597	GLY	H463	G401	K341
	P1090	E1030	G973	G903	R843	G782	V726		L598	GLY	H463	G401	K341
	V1091	M1031	E968	V904	K844	G783	V727		L599	GLY	H463	G401	K341
	S1094	E1032	Y969	V905	G845	G784	T723		L600	GLY	H463	G401	K341
	Y1095	R1033	V970	P906	L846	G785	I724		L601	GLY	H463	G401	K341
	A1096	D1034	Y971	D907	V847	G786	L724		L602	GLY	H463	G401	K341
	F1097	C1035	G972	I908	D848	G787	A725		L603	GLY	H463	G401	K341
	K1098	L1036	G973	I909	L849	G788	V726		L604	GLY	H463	G401	K341
	L1099	I1037	R974	I910	V850	G789	T727		L605	GLY	H463	G401	K341
	L1100	G1038	T975	N911	L851	R790	S728		L606	GLY	H463	G401	K341
	I1101	F1039	G976	P912	L852	L791	F729		L607	GLY	H463	G401	K341
	Q1102	G1040	Q977	H913	T853	L792	T730		L608	GLY	H463	G401	K341
	E1103	T1041	K978	A914	E854	G793	G731		L609	GLY	H463	G401	K341
	L1104	A1042	I979	L915	T855	D794	Y732		L610	GLY	H463	G401	K341
	M1105	M1043	P916	P916	A856	N795	N733		L611	GLY	H463	G401	K341
	S1106	L1044	R882	S917	E857	G796	N734		L612	GLY	H463	G401	K341
	M1107	L1045	I983	R918	G858	V797	E735		L613	GLY	H463	G401	K341
	I1108	K1046	Y984	M919	N859	V798	D736		L614	GLY	H463	G401	K341
	I1109	D1047	F985	T920	R860	S799	S737		L615	GLY	H463	G401	K341
	S1110	R1048	G986	G922	L861	P800	I738		L616	GLY	H463	G401	K341
	P1111	L1049	V987	G922	V862	E801	I739		L617	GLY	H463	G401	K341
	R1112	D1051	Y988	Q923	K863	V802	N740		L618	GLY	H463	G401	K341
	L1113	D1052	Y989	I924	V864	E803	N741		L619	GLY	H463	G401	K341
	V1114	R1053	Y990	M925	R865	R742	G682		L620	GLY	H463	G401	K341
	L1115	D1054	Q991	E926	V866	S743	N683		L621	GLY	H463	G401	K341
	E1116	R1055	K992	G992	R867	S744	G684		L622	GLY	H463	G401	K341
	I1117	T1056	L993	I993	D868	V745	D685		L623	GLY	H463	G401	K341
	K1118	M1057	H994	K931	L869	G807	E746		L624	GLY	H463	G401	K341
	V1119	I1058	H995	Y932	R870	R747	L686		L625	GLY	H463	G401	K341
	LEU	P1059	H996	A933	L871	G748	T688		L626	GLY	H463	G401	K341
				A934	P872	M749	D689		L627	GLY	H463	G401	K341
				L935	T873	V750	T690		L628	GLY	H463	G401	K341

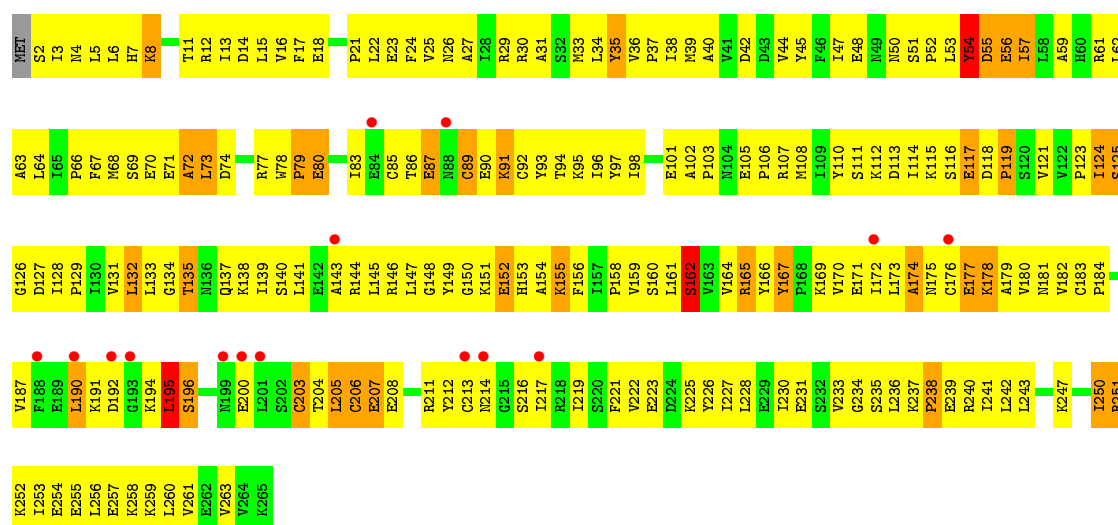
• Molecule 4: DNA-directed RNA polymerase subunit D



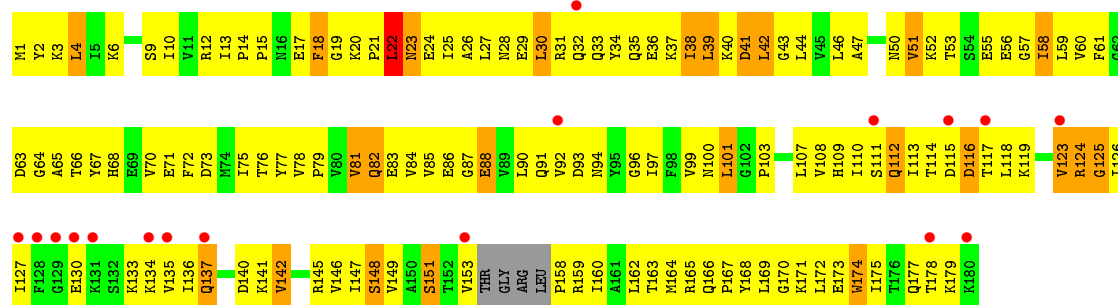
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• Molecule 4: DNA-directed RNA polymerase subunit D

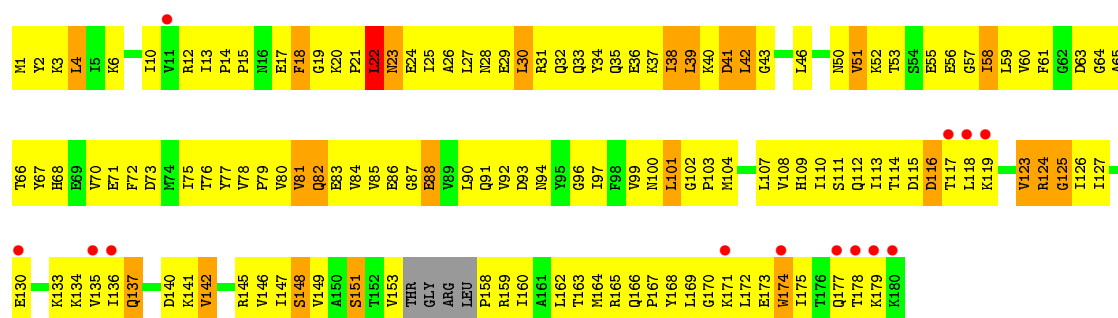


• Molecule 5: DNA-directed RNA polymerase subunit E

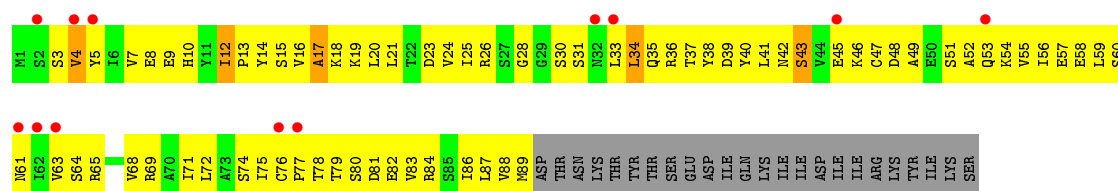
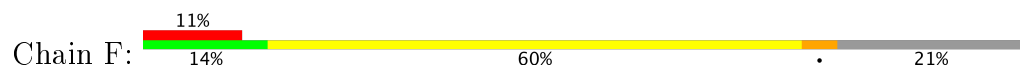


• Molecule 5: DNA-directed RNA polymerase subunit E

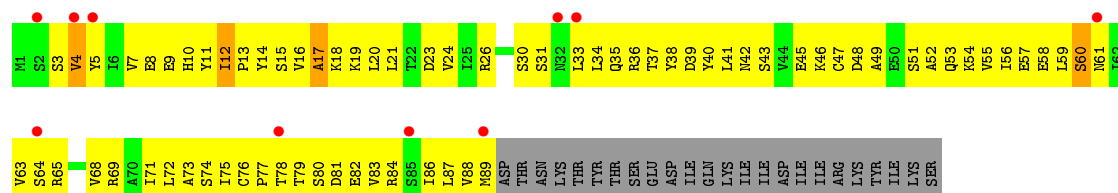
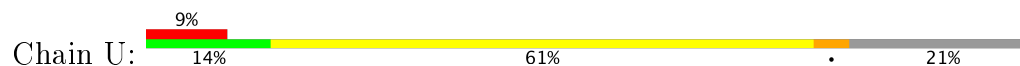




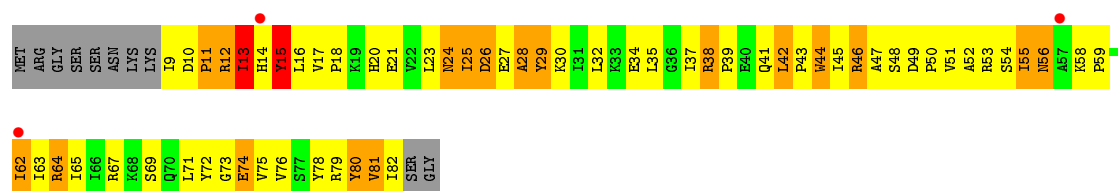
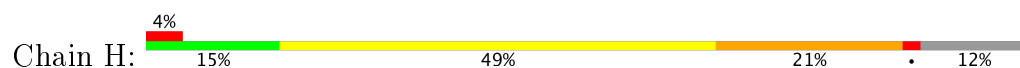
• Molecule 6: DNA-directed RNA polymerase subunit F



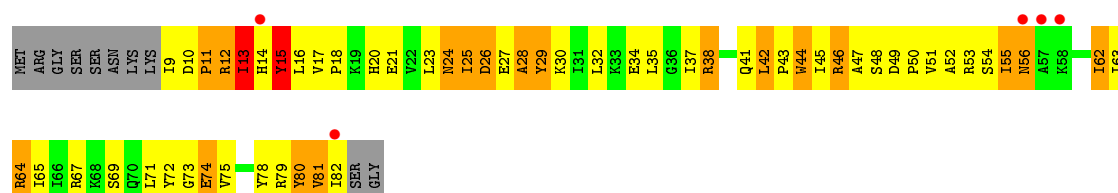
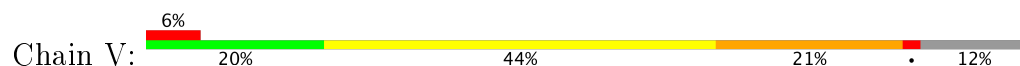
• Molecule 6: DNA-directed RNA polymerase subunit F

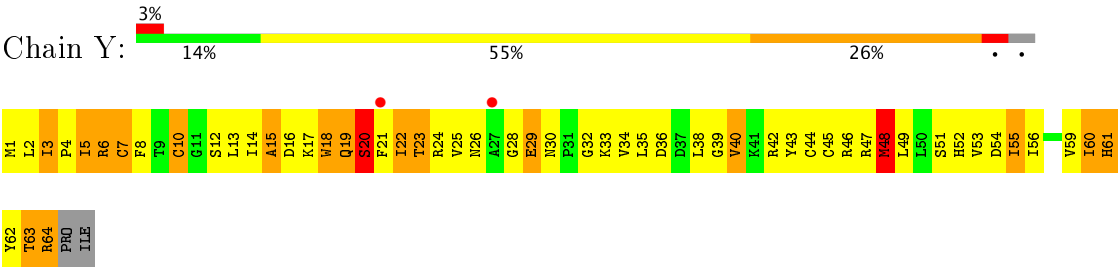


• Molecule 7: DNA-directed RNA polymerase subunit H

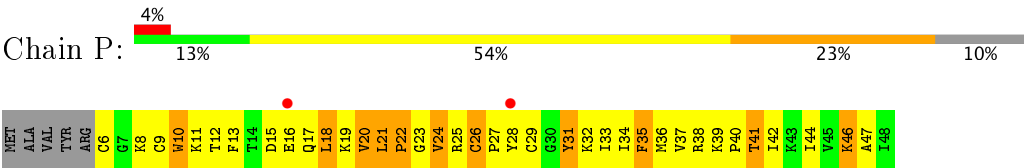


• Molecule 7: DNA-directed RNA polymerase subunit H

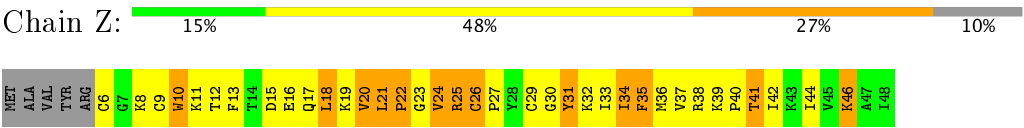




• Molecule 11: DNA-directed RNA polymerase subunit P



• Molecule 11: DNA-directed RNA polymerase subunit P



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.82Å 201.24Å 196.05Å 90.00° 100.92° 90.00°	Depositor
Resolution (Å)	39.79 – 3.40 39.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	80.4 (39.79-3.40) 80.3 (39.79-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.274 , 0.343 0.271 , 0.275	Depositor DCC
R_{free} test set	5323 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	48122	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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, F3S, 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	0.48	0/6306	0.80	4/8539 (0.0%)
1	Q	0.46	0/6306	0.79	4/8539 (0.0%)
2	C	0.46	0/2189	0.81	0/2947
2	G	0.43	0/2189	0.80	0/2947
3	B	0.46	0/8810	0.79	5/11921 (0.0%)
3	R	0.45	0/8810	0.79	3/11921 (0.0%)
4	D	0.40	0/2152	0.68	0/2911
4	S	0.37	0/2152	0.67	0/2911
5	E	0.38	0/1423	0.69	0/1919
5	T	0.37	0/1423	0.69	0/1919
6	F	0.35	0/701	0.63	0/949
6	U	0.35	0/701	0.62	0/949
7	H	0.44	0/625	0.76	0/848
7	V	0.41	0/625	0.76	0/848
8	K	0.50	0/667	0.82	0/903
8	W	0.49	0/667	0.81	0/903
9	L	0.39	0/733	0.72	0/986
9	X	0.38	0/733	0.72	0/986
10	N	0.38	0/523	0.75	0/705
10	Y	0.37	0/523	0.74	0/705
11	P	0.45	0/354	0.68	0/475
11	Z	0.46	0/354	0.67	0/475
All	All	0.44	0/48966	0.77	16/66206 (0.0%)

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
3	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	R	0	1
4	D	0	1
4	S	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	LEU	CA-CB-CG	7.67	132.93	115.30
1	Q	841	LEU	CA-CB-CG	7.56	132.69	115.30
3	B	436	GLY	N-CA-C	-6.16	97.70	113.10
3	R	436	GLY	N-CA-C	-5.97	98.17	113.10
1	A	508	LEU	N-CA-C	-5.89	95.11	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	314	TYR	Sidechain
4	D	54	TYR	Sidechain
3	R	314	TYR	Sidechain
4	S	54	TYR	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	A	6173	0	6243	1147	0
1	Q	6173	0	6243	1128	0
2	C	2169	0	2288	501	0
2	G	2169	0	2288	526	0
3	B	8645	0	8782	1656	0
3	R	8645	0	8780	1698	0
4	D	2114	0	2145	357	0
4	S	2114	0	2145	348	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1402	0	1467	222	0
5	T	1402	0	1467	246	0
6	F	694	0	705	129	0
6	U	694	0	705	139	0
7	H	611	0	641	117	0
7	V	611	0	641	125	0
8	K	658	0	692	161	0
8	W	658	0	692	174	0
9	L	723	0	749	94	0
9	X	723	0	749	91	0
10	N	514	0	528	159	0
10	Y	514	0	529	151	0
11	P	346	0	376	63	0
11	Z	346	0	375	58	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
12	Q	1	0	0	0	0
12	R	1	0	0	0	0
12	Y	1	0	0	0	0
12	Z	1	0	0	0	0
13	A	1	0	0	0	0
13	Q	1	0	0	0	0
14	D	7	0	0	4	0
14	S	7	0	0	3	0
All	All	48122	0	49230	8272	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 85.

The worst 5 of 8272 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:NZ	1:A:297:THR:HB	1.42	1.31
1:Q:238:LYS:NZ	1:Q:297:THR:HB	1.43	1.31
1:A:803:ARG:HG2	3:B:444:ASP:HA	1.20	1.17
1:A:308:ARG:HH21	3:B:1099:LEU:HD13	1.10	1.16
3:R:329:ARG:HD2	3:R:562:PHE:HB3	1.24	1.15

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	768/880 (87%)	513 (67%)	136 (18%)	119 (16%)	0	2
1	Q	768/880 (87%)	509 (66%)	141 (18%)	118 (15%)	0	2
2	C	273/392 (70%)	158 (58%)	66 (24%)	49 (18%)	0	1
2	G	273/392 (70%)	161 (59%)	61 (22%)	51 (19%)	0	1
3	B	1084/1124 (96%)	698 (64%)	238 (22%)	148 (14%)	0	3
3	R	1084/1124 (96%)	698 (64%)	237 (22%)	149 (14%)	0	3
4	D	262/265 (99%)	166 (63%)	69 (26%)	27 (10%)	0	6
4	S	262/265 (99%)	167 (64%)	66 (25%)	29 (11%)	0	5
5	E	172/180 (96%)	123 (72%)	31 (18%)	18 (10%)	0	6
5	T	172/180 (96%)	122 (71%)	32 (19%)	18 (10%)	0	6
6	F	87/113 (77%)	56 (64%)	22 (25%)	9 (10%)	0	6
6	U	87/113 (77%)	56 (64%)	23 (26%)	8 (9%)	1	8
7	H	72/84 (86%)	46 (64%)	13 (18%)	13 (18%)	0	1
7	V	72/84 (86%)	44 (61%)	15 (21%)	13 (18%)	0	1
8	K	80/95 (84%)	44 (55%)	19 (24%)	17 (21%)	0	1
8	W	80/95 (84%)	44 (55%)	20 (25%)	16 (20%)	0	1
9	L	90/92 (98%)	64 (71%)	19 (21%)	7 (8%)	1	11
9	X	90/92 (98%)	66 (73%)	17 (19%)	7 (8%)	1	11
10	N	62/66 (94%)	30 (48%)	18 (29%)	14 (23%)	0	1
10	Y	62/66 (94%)	31 (50%)	18 (29%)	13 (21%)	0	1
11	P	41/48 (85%)	24 (58%)	10 (24%)	7 (17%)	0	2
11	Z	41/48 (85%)	23 (56%)	11 (27%)	7 (17%)	0	2
All	All	5982/6678 (90%)	3843 (64%)	1282 (21%)	857 (14%)	0	3

5 of 857 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	58	CYS
1	A	64	THR
1	A	65	LEU
1	A	194	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	675/766 (88%)	580 (86%)	95 (14%)	4	21
1	Q	675/766 (88%)	583 (86%)	92 (14%)	4	22
2	C	237/338 (70%)	201 (85%)	36 (15%)	3	18
2	G	237/338 (70%)	199 (84%)	38 (16%)	3	15
3	B	937/965 (97%)	807 (86%)	130 (14%)	4	21
3	R	937/965 (97%)	810 (86%)	127 (14%)	4	22
4	D	241/242 (100%)	224 (93%)	17 (7%)	17	54
4	S	241/242 (100%)	223 (92%)	18 (8%)	16	51
5	E	156/159 (98%)	142 (91%)	14 (9%)	11	41
5	T	156/159 (98%)	142 (91%)	14 (9%)	11	41
6	F	82/106 (77%)	79 (96%)	3 (4%)	39	73
6	U	82/106 (77%)	79 (96%)	3 (4%)	39	73
7	H	67/75 (89%)	54 (81%)	13 (19%)	1	8
7	V	67/75 (89%)	55 (82%)	12 (18%)	2	10
8	K	72/84 (86%)	57 (79%)	15 (21%)	1	6
8	W	72/84 (86%)	57 (79%)	15 (21%)	1	6
9	L	81/81 (100%)	75 (93%)	6 (7%)	16	51
9	X	81/81 (100%)	75 (93%)	6 (7%)	16	51
10	N	58/60 (97%)	50 (86%)	8 (14%)	4	22
10	Y	58/60 (97%)	49 (84%)	9 (16%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	P	39/43 (91%)	31 (80%)	8 (20%)	1	6
11	Z	39/43 (91%)	31 (80%)	8 (20%)	1	6
All	All	5290/5838 (91%)	4603 (87%)	687 (13%)	5	24

5 of 687 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	K	23	TRP
1	Q	425	LEU
6	U	5	TYR
8	K	74	LEU
1	Q	52	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
7	H	41	GLN
1	Q	376	ASN
5	T	109	HIS
8	K	42	GLN
1	Q	56	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	$\# Z > 2$
14	F3S	D	1001	4	0,9,9	0.00	-	0,15,15	0.00	-
14	F3S	S	1001	4	0,9,9	0.00	-	0,15,15	0.00	-

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
14	F3S	D	1001	4	-	0/0/24/24	0/0/3/3
14	F3S	S	1001	4	-	0/0/24/24	0/0/3/3

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.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	1001	F3S	4	0
14	S	1001	F3S	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	776/880 (88%)	-0.17	17 (2%) 62 57	23, 75, 132, 186	0
1	Q	776/880 (88%)	-0.03	26 (3%) 46 41	29, 87, 145, 202	0
2	C	279/392 (71%)	-0.05	10 (3%) 43 39	29, 81, 153, 190	0
2	G	279/392 (71%)	0.00	12 (4%) 36 33	42, 97, 153, 181	0
3	B	1090/1124 (96%)	-0.19	17 (1%) 72 67	24, 78, 145, 196	0
3	R	1090/1124 (96%)	-0.10	33 (3%) 51 47	36, 84, 149, 196	0
4	D	264/265 (99%)	0.09	12 (4%) 34 31	44, 94, 144, 179	0
4	S	264/265 (99%)	0.22	15 (5%) 24 23	61, 111, 157, 192	0
5	E	176/180 (97%)	0.38	17 (9%) 8 9	39, 112, 189, 202	0
5	T	176/180 (97%)	0.36	13 (7%) 15 16	57, 113, 176, 202	0
6	F	89/113 (78%)	0.35	12 (13%) 3 4	73, 142, 182, 196	0
6	U	89/113 (78%)	0.59	10 (11%) 6 6	93, 141, 184, 201	0
7	H	74/84 (88%)	0.22	3 (4%) 38 34	46, 90, 137, 165	0
7	V	74/84 (88%)	0.21	5 (6%) 18 18	70, 101, 159, 198	0
8	K	82/95 (86%)	-0.25	1 (1%) 79 75	30, 72, 118, 154	0
8	W	82/95 (86%)	0.03	3 (3%) 42 38	47, 82, 139, 189	0
9	L	92/92 (100%)	0.01	2 (2%) 62 57	42, 81, 125, 200	0
9	X	92/92 (100%)	0.31	9 (9%) 8 9	52, 102, 140, 159	0
10	N	64/66 (96%)	-0.23	0 100 100	60, 90, 124, 174	0
10	Y	64/66 (96%)	-0.02	2 (3%) 49 46	61, 98, 145, 185	0
11	P	43/48 (89%)	-0.03	2 (4%) 32 30	48, 101, 137, 155	0
11	Z	43/48 (89%)	-0.13	0 100 100	64, 100, 144, 180	0
All	All	6058/6678 (90%)	-0.03	221 (3%) 43 39	23, 88, 153, 202	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	434	ALA	8.5
5	T	135	VAL	6.6
6	U	33	LEU	6.1
4	D	217	ILE	5.8
6	U	2	SER	5.7

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(\AA^2)	Q<0.9
12	ZN	N	1001	1/1	0.99	0.17	-0.45	93,93,93,93	0
12	ZN	Z	1001	1/1	0.99	0.12	-0.69	106,106,106,106	0
12	ZN	B	2001	1/1	0.97	0.12	-0.92	91,91,91,91	0
12	ZN	P	1001	1/1	0.99	0.10	-0.95	103,103,103,103	0
14	F3S	D	1001	7/7	0.97	0.12	-1.25	79,80,80,80	0
14	F3S	S	1001	7/7	0.98	0.11	-1.65	111,111,112,113	0
12	ZN	A	1002	1/1	0.99	0.06	-1.75	87,87,87,87	0
12	ZN	R	2001	1/1	0.97	0.06	-1.94	101,101,101,101	0
12	ZN	Q	1002	1/1	0.99	0.05	-2.20	89,89,89,89	0
12	ZN	Y	1001	1/1	0.99	0.17	-3.81	93,93,93,93	0
13	MG	A	1003	1/1	0.92	0.18	-	57,57,57,57	0
13	MG	Q	1003	1/1	0.97	0.25	-	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.