



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 03:43 PM EDT

PDB ID : 2PMZ / pdb_00002pmz
Title : Archaeal RNA polymerase from Sulfolobus solfataricus
Authors : Murakami, K.S.
Deposited on : 2007-04-23
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

<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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

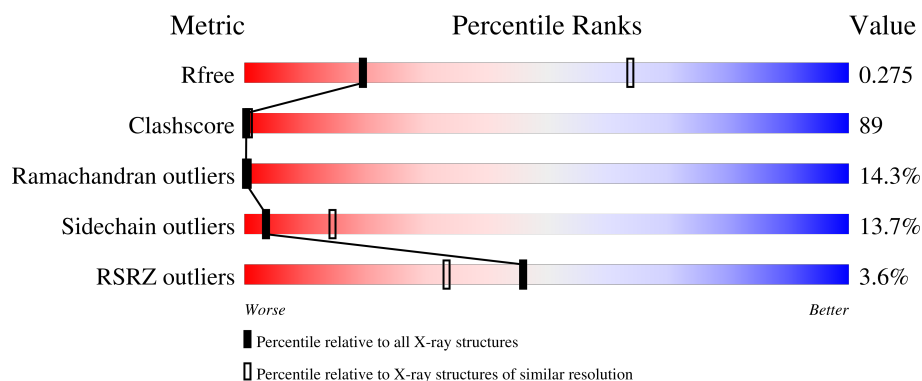
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	880	
1	Q	880	
2	C	392	
2	G	392	
3	B	1124	

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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			

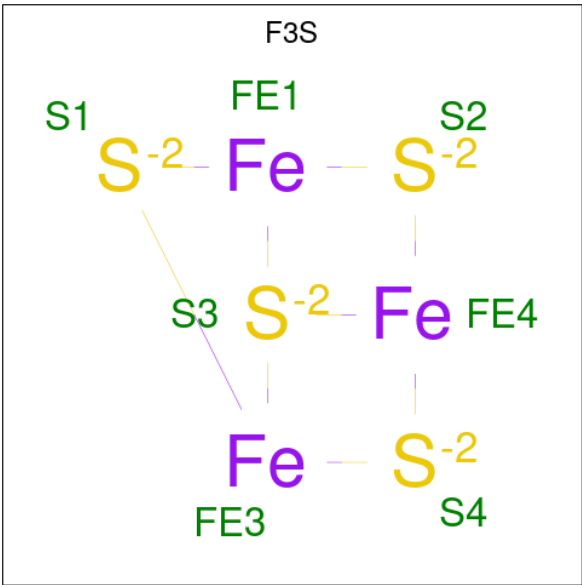
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

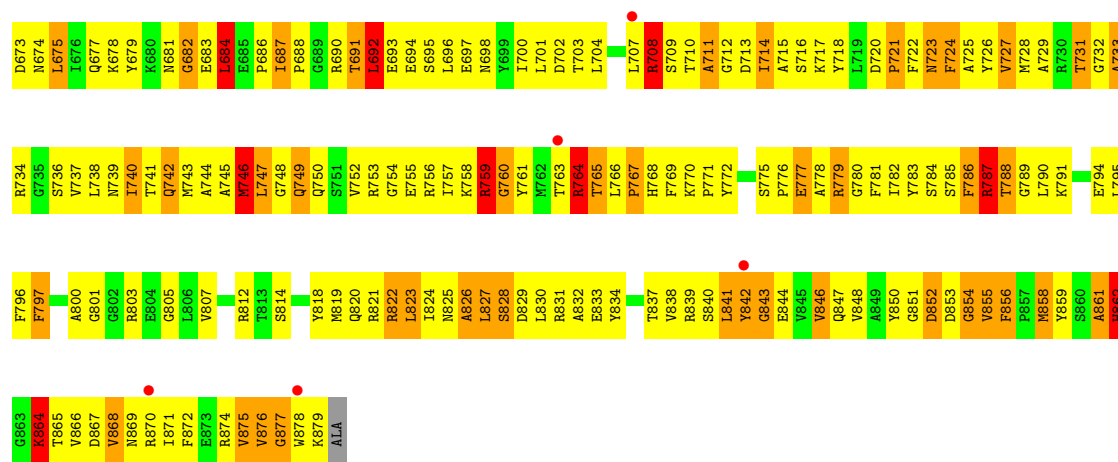
- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

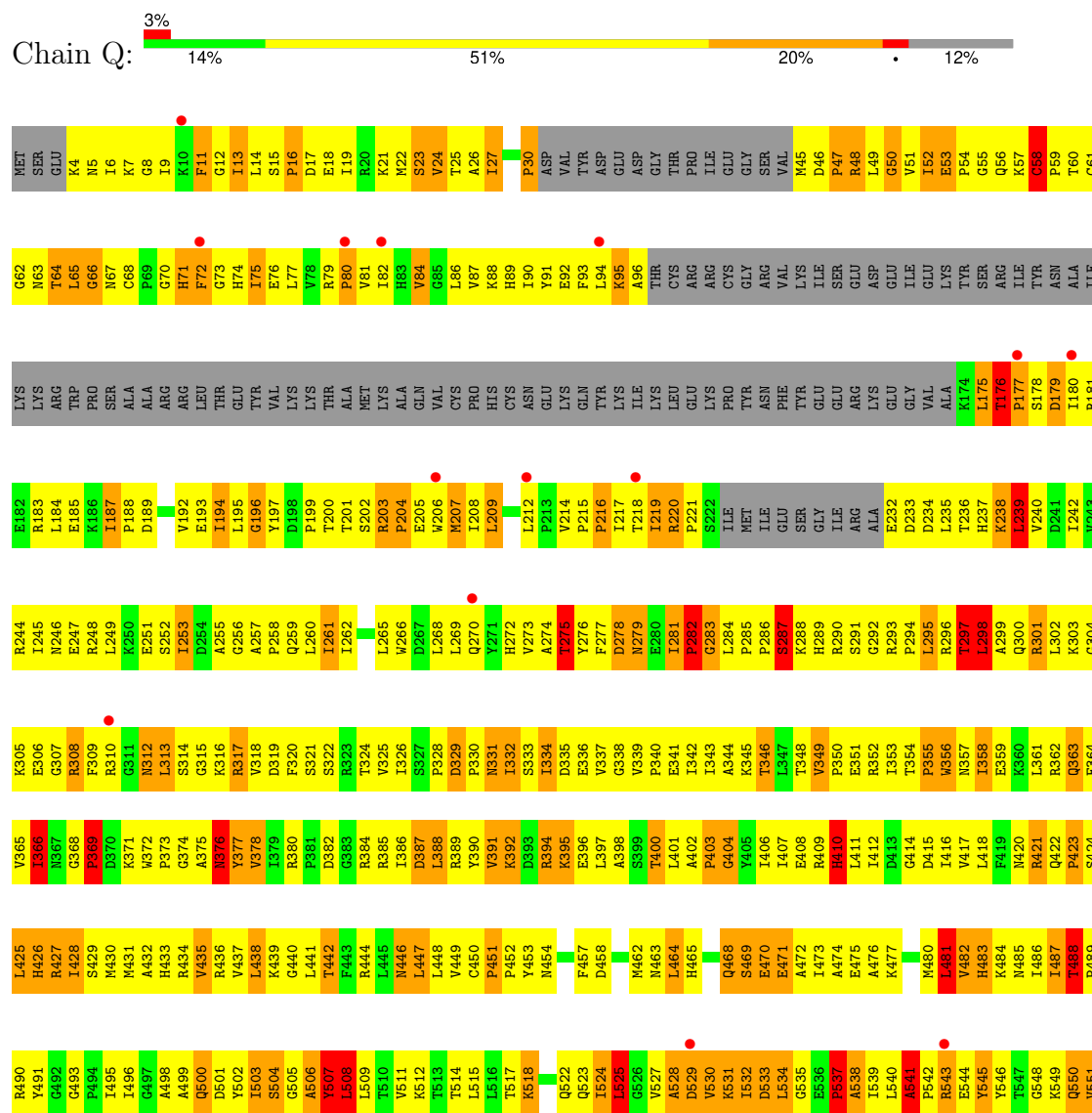
- Molecule 14 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).

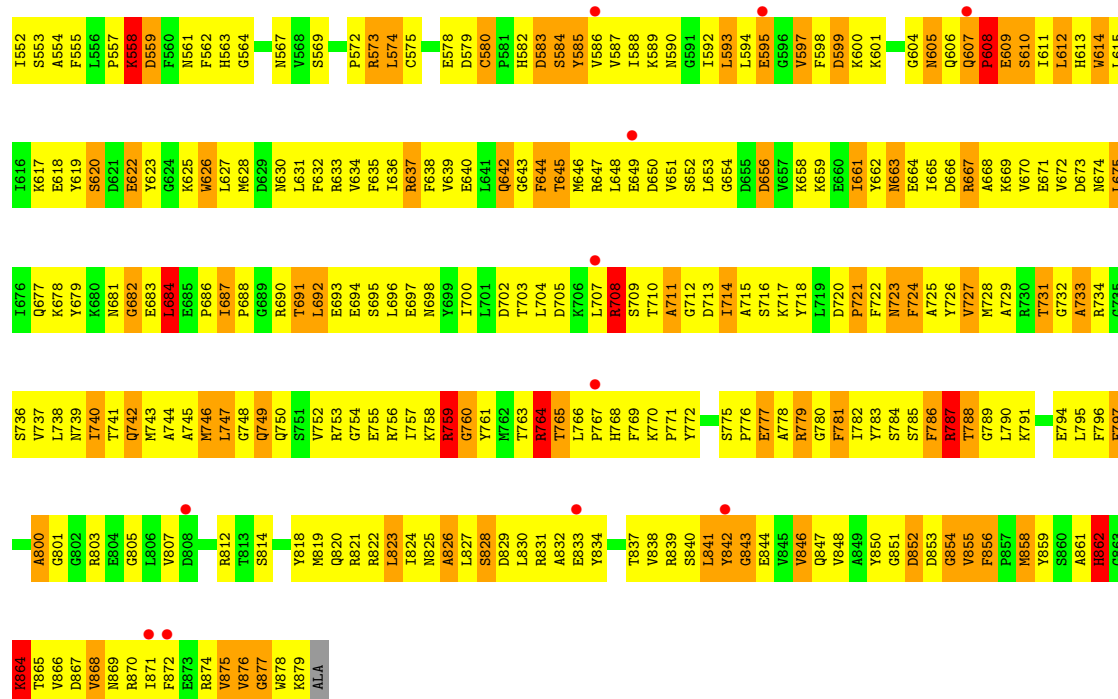


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	Fe	S	0	0
			7	3	4		
14	S	1	Total	Fe	S	0	0
			7	3	4		

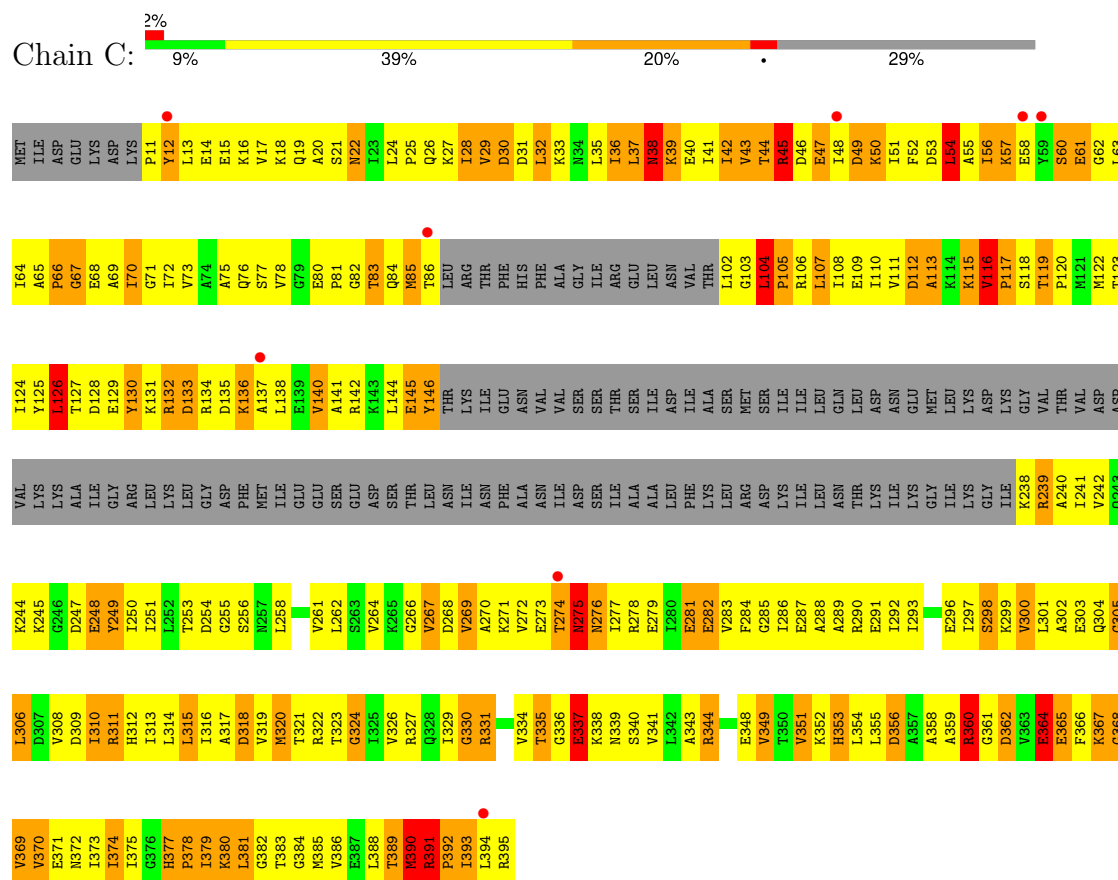


• Molecule 1: DNA-directed RNA polymerase subunit A

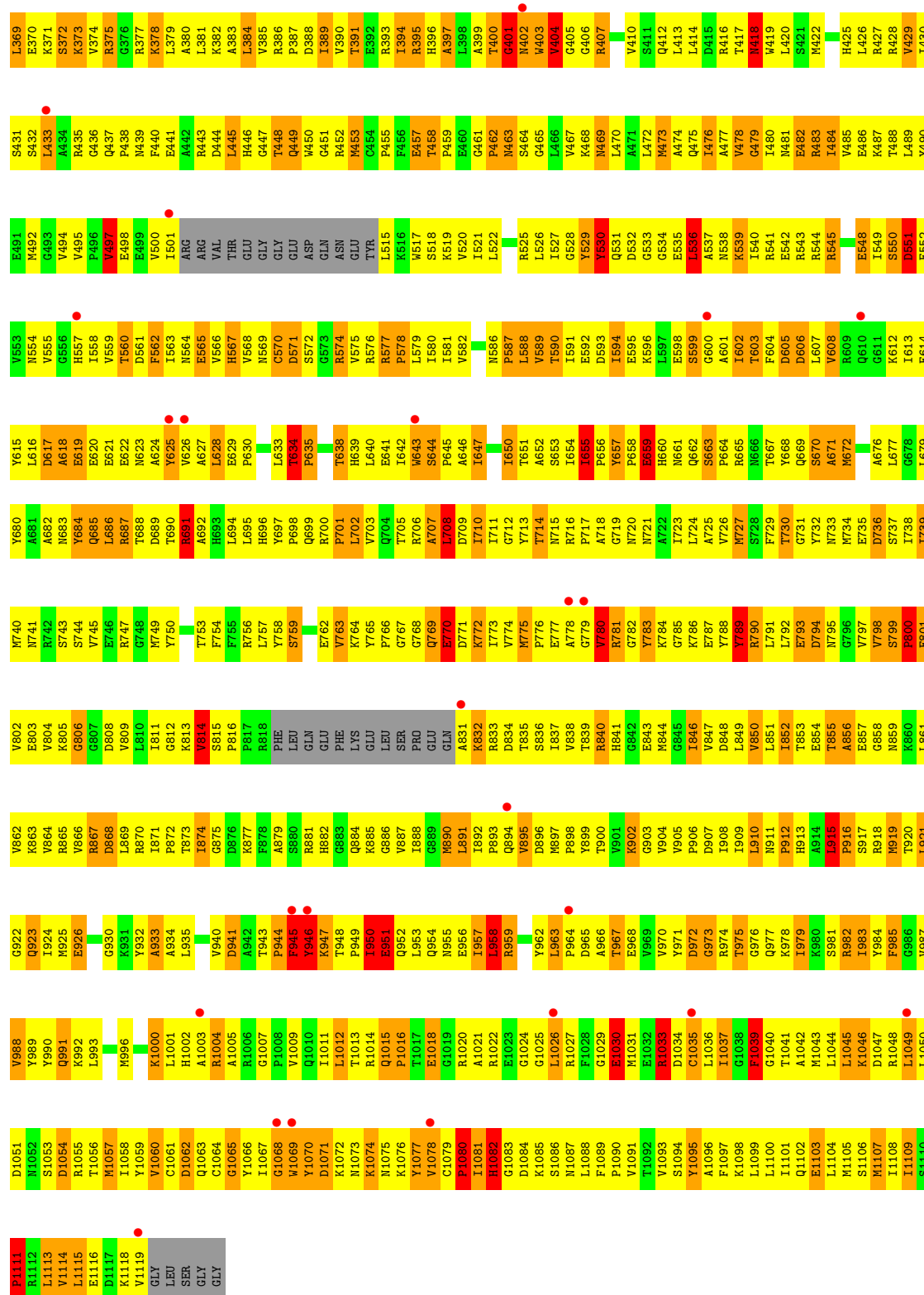




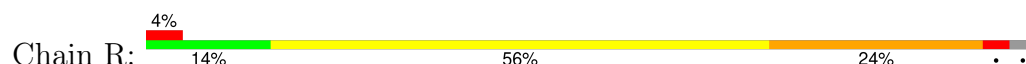
• Molecule 2: DNA-directed RNA polymerase subunit A''



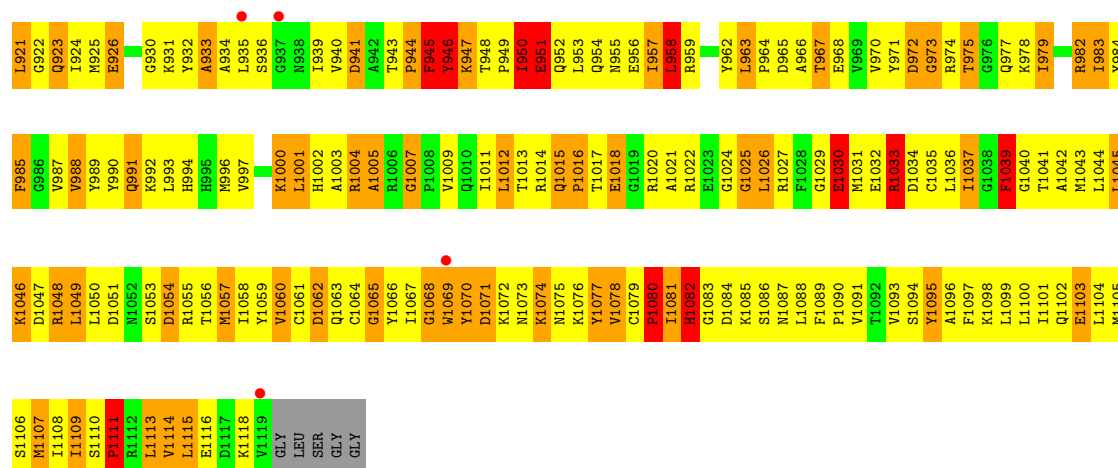
• Molecule 2: DNA-directed RNA polymerase subunit A''



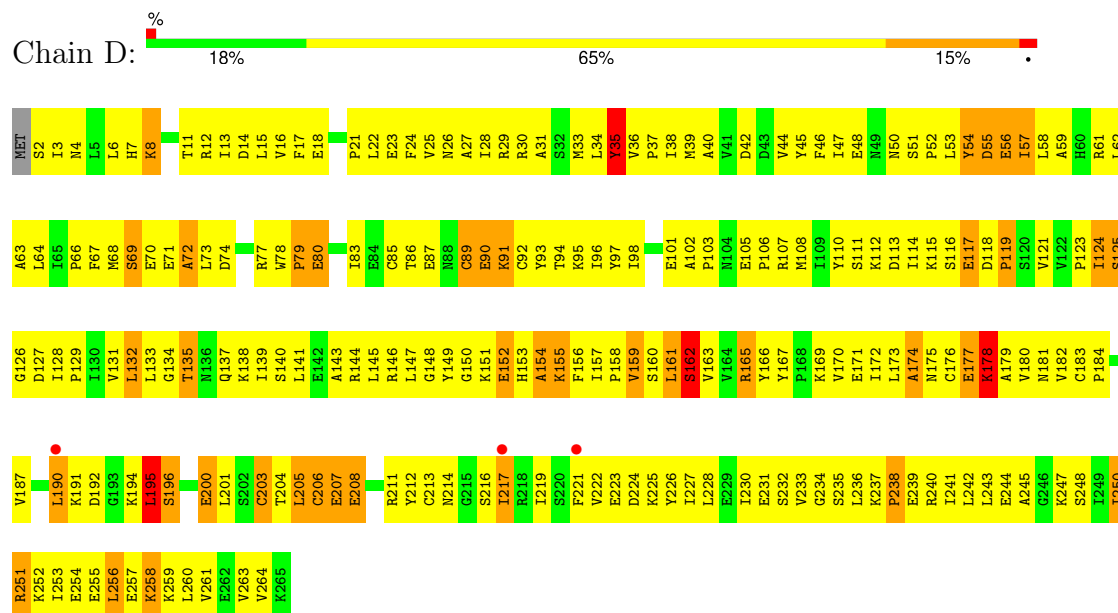
• Molecule 3: DNA-directed RNA polymerase subunit B



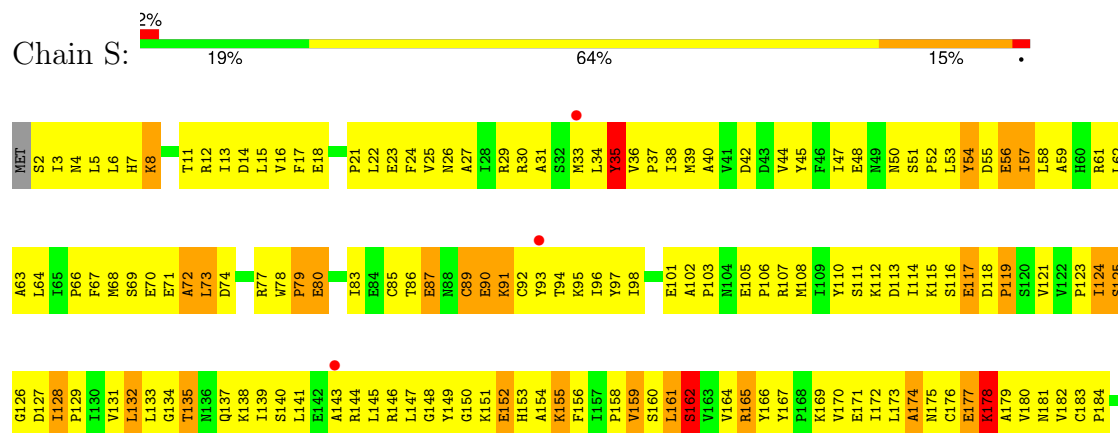


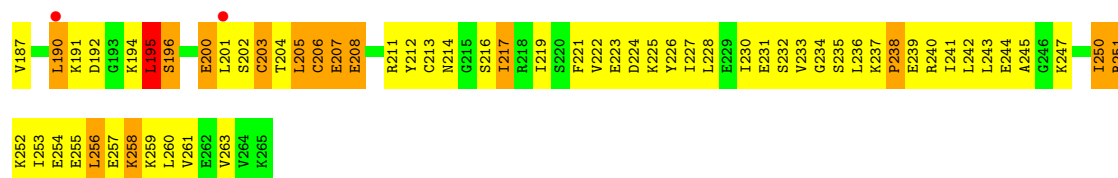


• Molecule 4: DNA-directed RNA polymerase subunit D

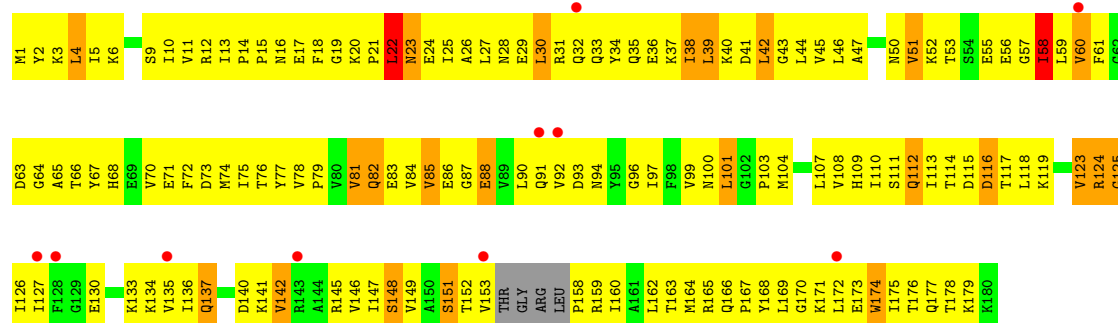


• Molecule 4: DNA-directed RNA polymerase subunit D

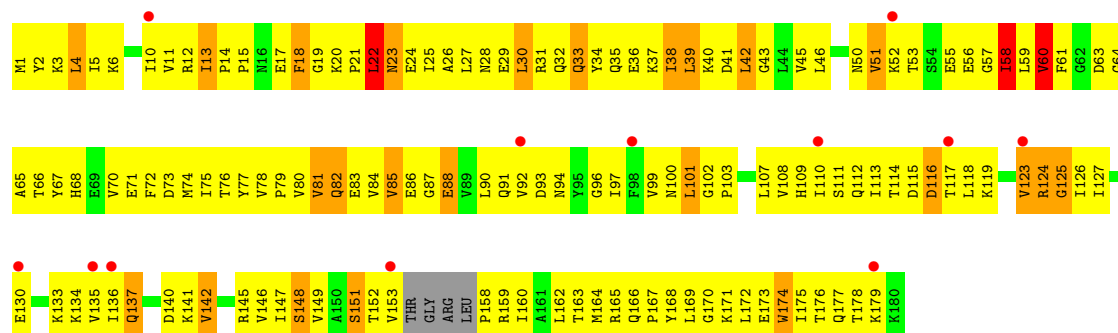




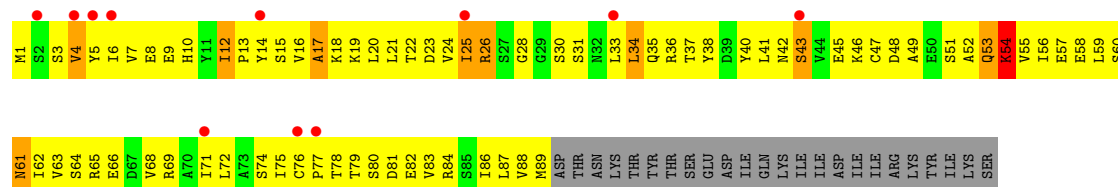
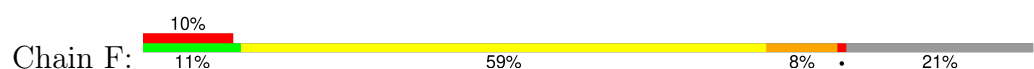
• Molecule 5: DNA-directed RNA polymerase subunit E



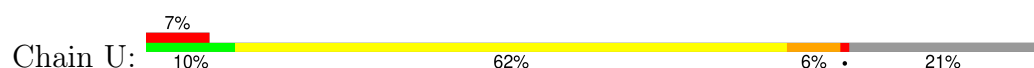
• Molecule 5: DNA-directed RNA polymerase subunit E

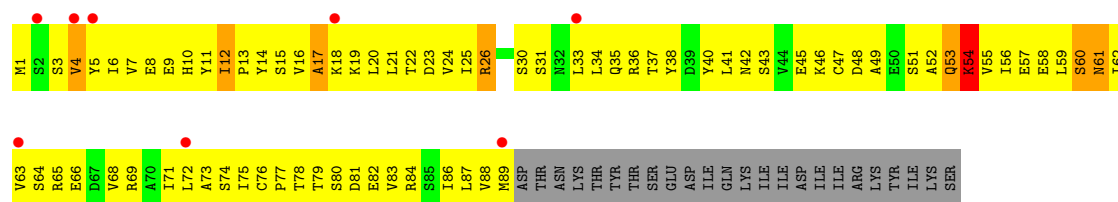


• Molecule 6: DNA-directed RNA polymerase subunit F

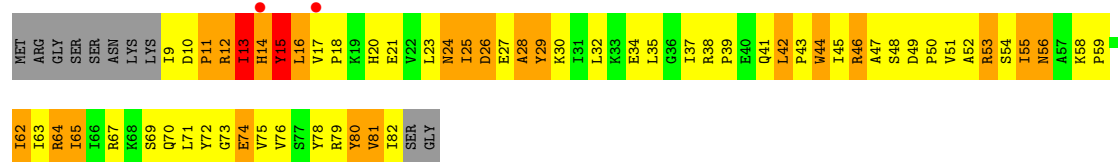
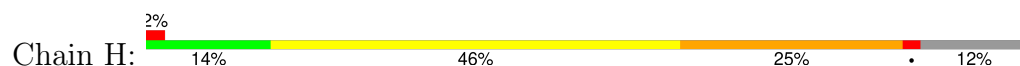


• Molecule 6: DNA-directed RNA polymerase subunit F

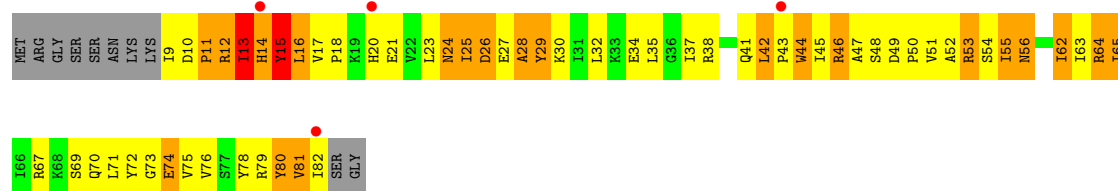
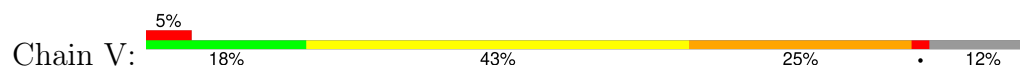




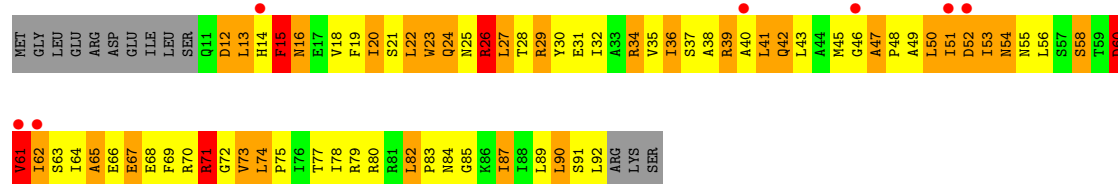
• Molecule 7: DNA-directed RNA polymerase subunit H



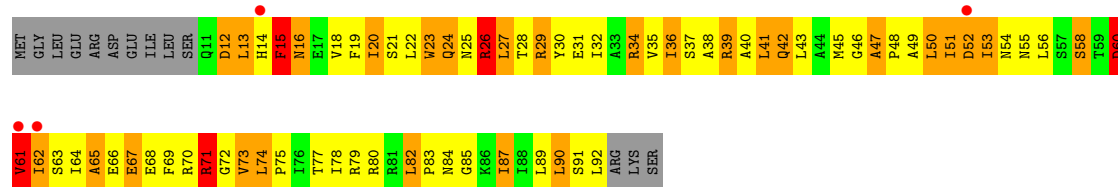
• Molecule 7: DNA-directed RNA polymerase subunit H



• Molecule 8: DNA-directed RNA polymerase subunit K



• Molecule 8: DNA-directed RNA polymerase subunit K



• Molecule 9: DNA-directed RNA polymerase subunit L

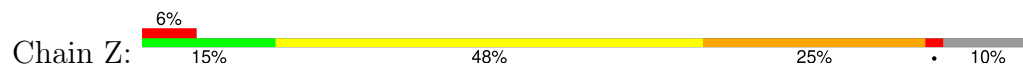
- Molecule 9: DNA-directed RNA polymerase subunit L

- Molecule 10: DNA-directed RNA polymerase subunit N

- Molecule 10: DNA-directed RNA polymerase subunit N

- 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 (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 90.3	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, MG, F3S

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	0.62	1/6306 (0.0%)	1.21	71/8539 (0.8%)
1	Q	0.58	0/6306	1.20	67/8539 (0.8%)
2	C	0.62	0/2189	1.24	25/2947 (0.8%)
2	G	0.59	0/2189	1.22	23/2947 (0.8%)
3	B	0.59	0/8810	1.22	101/11921 (0.8%)
3	R	0.57	0/8810	1.22	104/11921 (0.9%)
4	D	0.49	0/2152	1.02	11/2911 (0.4%)
4	S	0.46	0/2152	1.00	8/2911 (0.3%)
5	E	0.48	0/1423	1.03	5/1919 (0.3%)
5	T	0.47	0/1423	1.02	7/1919 (0.4%)
6	F	0.46	0/701	1.06	7/949 (0.7%)
6	U	0.46	0/701	1.05	7/949 (0.7%)
7	H	0.53	0/625	1.15	5/848 (0.6%)
7	V	0.50	0/625	1.13	5/848 (0.6%)
8	K	0.68	0/667	1.22	10/903 (1.1%)
8	W	0.65	0/667	1.21	10/903 (1.1%)
9	L	0.51	0/733	1.12	4/986 (0.4%)
9	X	0.47	0/733	1.11	4/986 (0.4%)
10	N	0.50	0/523	1.05	4/705 (0.6%)
10	Y	0.49	0/523	1.03	3/705 (0.4%)
11	P	0.55	0/354	1.08	4/475 (0.8%)
11	Z	0.56	0/354	1.04	3/475 (0.6%)
All	All	0.57	1/48966 (0.0%)	1.17	488/66206 (0.7%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	VAL	CA-C	5.04	1.56	1.52

The worst 5 of 488 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	45	GLU	N-CA-C	-12.90	97.46	113.97
3	R	45	GLU	N-CA-C	-12.71	97.70	113.97
2	C	49	ASP	N-CA-C	-11.82	98.11	111.82
1	A	329	ASP	CA-C-N	11.45	130.88	118.97
1	A	329	ASP	C-N-CA	11.45	130.88	118.97

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	1200	0
1	Q	6173	0	6243	1174	0
2	C	2169	0	2288	517	0
2	G	2169	0	2288	549	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8645	0	8782	1751	0
3	R	8645	0	8780	1782	0
4	D	2114	0	2145	373	0
4	S	2114	0	2145	361	0
5	E	1402	0	1467	225	0
5	T	1402	0	1467	251	0
6	F	694	0	705	134	0
6	U	694	0	705	145	0
7	H	611	0	641	119	0
7	V	611	0	641	128	0
8	K	658	0	692	165	0
8	W	658	0	692	177	0
9	L	723	0	749	96	0
9	X	723	0	749	93	0
10	N	514	0	528	165	0
10	Y	514	0	529	159	0
11	P	346	0	376	67	0
11	Z	346	0	375	61	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	8651	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 8651 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:Q:486:ILE:HD11	1:Q:628:MET:HE2	1.19	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	N	62/66 (94%)	30 (48%)	18 (29%)	14 (23%)	0	0
10	Y	62/66 (94%)	31 (50%)	18 (29%)	13 (21%)	0	0
11	P	41/48 (85%)	24 (58%)	10 (24%)	7 (17%)	0	0
11	Z	41/48 (85%)	23 (56%)	11 (27%)	7 (17%)	0	0
All	All	5982/6678 (90%)	3843 (64%)	1282 (21%)	857 (14%)	0	0

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%)	3	13
1	Q	675/766 (88%)	581 (86%)	94 (14%)	3	14
2	C	237/338 (70%)	195 (82%)	42 (18%)	2	8
2	G	237/338 (70%)	195 (82%)	42 (18%)	2	8
3	B	937/965 (97%)	798 (85%)	139 (15%)	3	12
3	R	937/965 (97%)	796 (85%)	141 (15%)	3	11
4	D	241/242 (100%)	221 (92%)	20 (8%)	10	35
4	S	241/242 (100%)	221 (92%)	20 (8%)	10	35
5	E	156/159 (98%)	143 (92%)	13 (8%)	10	35
5	T	156/159 (98%)	141 (90%)	15 (10%)	8	28
6	F	82/106 (77%)	79 (96%)	3 (4%)	30	55
6	U	82/106 (77%)	79 (96%)	3 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	67/75 (89%)	54 (81%)	13 (19%)	1	5
7	V	67/75 (89%)	55 (82%)	12 (18%)	2	7
8	K	72/84 (86%)	55 (76%)	17 (24%)	1	2
8	W	72/84 (86%)	56 (78%)	16 (22%)	1	3
9	L	81/81 (100%)	75 (93%)	6 (7%)	13	38
9	X	81/81 (100%)	73 (90%)	8 (10%)	7	26
10	N	58/60 (97%)	50 (86%)	8 (14%)	3	14
10	Y	58/60 (97%)	50 (86%)	8 (14%)	3	14
11	P	39/43 (91%)	33 (85%)	6 (15%)	2	10
11	Z	39/43 (91%)	33 (85%)	6 (15%)	2	10
All	All	5290/5838 (91%)	4563 (86%)	727 (14%)	3	14

5 of 727 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	57	LYS
3	R	685	GLN
2	G	284	PHE
2	G	54	LEU
3	R	227	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 188 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	582	HIS
3	R	623	ASN
1	Q	742	GLN
3	R	337	HIS
3	R	704	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	-	-	-		
14	F3S	S	1001	4	0,9,9	-	-	-		

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

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%)	0.06	17 (2%) 62 47	23, 75, 132, 186	0
1	Q	776/880 (88%)	0.21	25 (3%) 50 37	29, 87, 145, 202	0
2	C	279/392 (71%)	0.22	8 (2%) 53 39	29, 81, 153, 190	0
2	G	279/392 (71%)	0.31	11 (3%) 43 31	42, 97, 153, 181	0
3	B	1090/1124 (96%)	0.17	35 (3%) 50 37	24, 78, 145, 196	0
3	R	1090/1124 (96%)	0.26	42 (3%) 43 31	36, 84, 149, 196	0
4	D	264/265 (99%)	0.26	3 (1%) 78 65	44, 94, 144, 179	0
4	S	264/265 (99%)	0.39	5 (1%) 66 51	61, 111, 157, 192	0
5	E	176/180 (97%)	0.48	10 (5%) 29 22	39, 112, 189, 202	0
5	T	176/180 (97%)	0.59	12 (6%) 23 19	57, 113, 176, 202	0
6	F	89/113 (78%)	0.89	11 (12%) 8 9	73, 142, 182, 196	0
6	U	89/113 (78%)	0.86	8 (8%) 15 14	93, 141, 184, 201	0
7	H	74/84 (88%)	0.39	2 (2%) 56 42	46, 90, 137, 165	0
7	V	74/84 (88%)	0.40	4 (5%) 31 24	70, 101, 159, 198	0
8	K	82/95 (86%)	0.13	7 (8%) 16 15	30, 72, 118, 154	0
8	W	82/95 (86%)	0.22	4 (4%) 35 26	47, 82, 139, 189	0
9	L	92/92 (100%)	-0.01	2 (2%) 62 47	42, 81, 125, 200	0
9	X	92/92 (100%)	0.34	2 (2%) 62 47	52, 102, 140, 159	0
10	N	64/66 (96%)	0.19	1 (1%) 70 56	60, 90, 124, 174	0
10	Y	64/66 (96%)	0.35	5 (7%) 19 16	61, 98, 145, 185	0
11	P	43/48 (89%)	0.45	0 100 100	48, 101, 137, 154	0
11	Z	43/48 (89%)	0.60	3 (6%) 22 18	64, 100, 144, 180	0
All	All	6058/6678 (90%)	0.25	217 (3%) 46 33	23, 88, 153, 202	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	K	51	ILE	5.8
6	U	2	SER	5.0
3	B	625	TYR	4.9
1	A	707	LEU	4.5
6	F	14	TYR	4.5

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	MG	A	1003	1/1	0.85	0.17	57,57,57,57	0
13	MG	Q	1003	1/1	0.96	0.13	60,60,60,60	0
12	ZN	B	2001	1/1	0.98	0.05	91,91,91,91	0
12	ZN	R	2001	1/1	0.98	0.03	101,101,101,101	0
14	F3S	D	1001	7/7	0.98	0.05	79,80,80,80	0
14	F3S	S	1001	7/7	0.98	0.05	111,111,112,113	0
12	ZN	Z	1001	1/1	0.99	0.08	106,106,106,106	0
12	ZN	P	1001	1/1	0.99	0.06	103,103,103,103	0
12	ZN	Q	1002	1/1	0.99	0.03	89,89,89,89	0
12	ZN	A	1002	1/1	0.99	0.03	87,87,87,87	0
12	ZN	Y	1001	1/1	0.99	0.02	93,93,93,93	0
12	ZN	N	1001	1/1	1.00	0.02	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.