



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 01:13 AM GMT

PDB ID : 4C2M
Title : Structure of RNA polymerase I at 2.8 Å resolution
Authors : Engel, C.; Sainsbury, S.; Cheung, A.C.; Kostrewa, D.; Cramer, P.
Deposited on : 2013-08-19
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

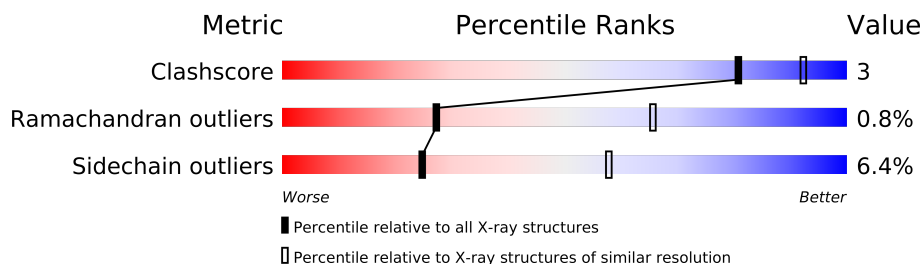
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)







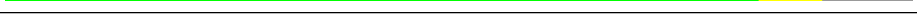

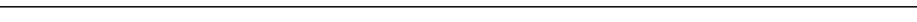
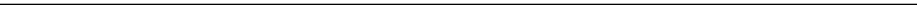



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	70	
1	L	70	
2	2	415	
2	M	415	
3	3	233	
3	N	233	
4	4	326	
4	G	326	
4	O	326	
4	V	326	
5	A	1664	
5	P	1664	
6	B	1203	
6	Q	1203	
7	C	335	
7	R	335	
8	D	137	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	S	137	
9	E	215	
9	T	215	
10	F	155	
10	U	155	
11	H	146	
11	W	146	
12	I	125	
12	X	125	
13	J	70	
13	Y	70	
14	K	142	
14	Z	142	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 69107 atoms, of which 0 are hydrogen and 0 are deuterium.

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 POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			
1	L	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	103	Total	C	N	O		0	0	0
			814	517	134	163				
2	M	108	Total	C	N	O		0	0	0
			856	543	142	171				

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	145	Total	C	N	O	S	0	0	0
			1152	735	189	224	4			
3	N	145	Total	C	N	O	S	0	0	0
			1151	735	188	224	4			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	54	Total	C	N	O		0	0	0
			430	262	69	99				
4	G	193	Total	C	N	O	S	0	0	0
			1526	985	262	274	5			
4	O	52	Total	C	N	O		0	0	0
			413	253	64	96				
4	V	197	Total	C	N	O	S	0	0	0
			1557	1001	266	285	5			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	1521	Total	C	N	O	S	0	0	0
			12019	7579	2088	2290	62			
5	P	1518	Total	C	N	O	S	0	0	0
			12000	7567	2085	2286	62			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	1182	Total	C	N	O	S	0	0	0
			9386	5934	1648	1753	51			
6	Q	1164	Total	C	N	O	S	0	0	0
			9261	5862	1623	1725	51			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	305	Total	C	N	O	S	0	0	0
			2423	1539	416	460	8			
7	R	305	Total	C	N	O	S	0	0	0
			2423	1539	416	460	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	D	58	Total	C	N	O	0	0	0
			459	289	78	92			
8	S	59	Total	C	N	O	0	0	0
			467	293	79	95			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	E	212	Total	C	N	O	S	0	0	0
			1735	1102	306	316	11			
9	T	212	Total	C	N	O	S	0	0	0
			1735	1102	306	316	11			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			
10	U	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	131	Total	C	N	O	S	0	0	0
			1052	664	176	208	4			
11	W	131	Total	C	N	O	S	0	0	0
			1052	664	176	208	4			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	124	Total	C	N	O	S	0	0	0
			943	584	160	190	9			
12	X	119	Total	C	N	O	S	0	0	0
			900	557	152	182	9			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			
13	Y	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			

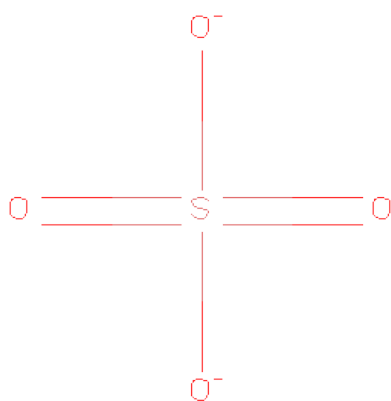
- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	101	Total	C	N	O	S	0	0	0
			793	496	130	162	5			
14	Z	100	Total	C	N	O	S	0	0	0
			786	491	129	161	5			

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	P	2	Total 2	Zn 2	0	0
15	J	1	Total 1	Zn 1	0	0
15	1	1	Total 1	Zn 1	0	0
15	B	1	Total 1	Zn 1	0	0
15	I	2	Total 2	Zn 2	0	0
15	A	2	Total 2	Zn 2	0	0
15	X	2	Total 2	Zn 2	0	0
15	Q	1	Total 1	Zn 1	0	0
15	L	1	Total 1	Zn 1	0	0
15	Y	1	Total 1	Zn 1	0	0

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total 5	O 4	S 1	0	0
16	Q	1	Total 5	O 4	S 1	0	0

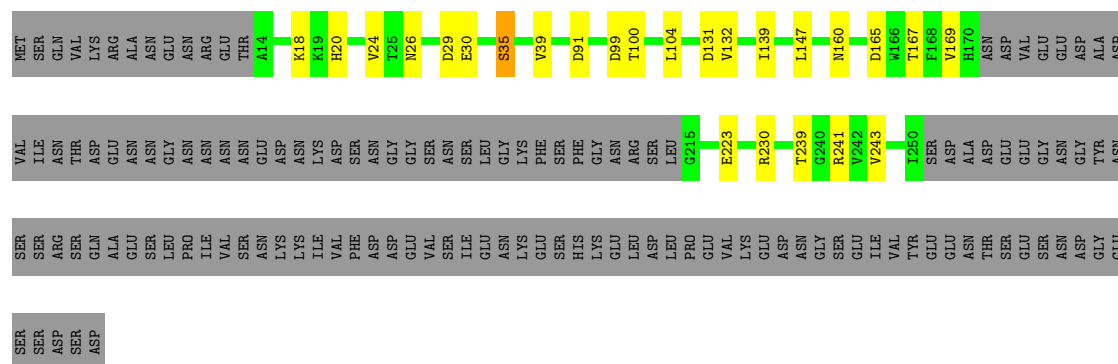
- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	3	1	Total O 1 1	0	0
17	A	96	Total O 96 96	0	0
17	B	62	Total O 62 62	0	0
17	C	1	Total O 1 1	0	0
17	D	3	Total O 3 3	0	0
17	E	4	Total O 4 4	0	0
17	F	4	Total O 4 4	0	0
17	G	1	Total O 1 1	0	0
17	H	10	Total O 10 10	0	0
17	I	3	Total O 3 3	0	0
17	N	3	Total O 3 3	0	0
17	O	1	Total O 1 1	0	0
17	P	43	Total O 43 43	0	0
17	Q	15	Total O 15 15	0	0
17	R	1	Total O 1 1	0	0
17	S	1	Total O 1 1	0	0
17	T	4	Total O 4 4	0	0
17	U	4	Total O 4 4	0	0
17	V	2	Total O 2 2	0	0
17	W	1	Total O 1 1	0	0
17	X	2	Total O 2 2	0	0



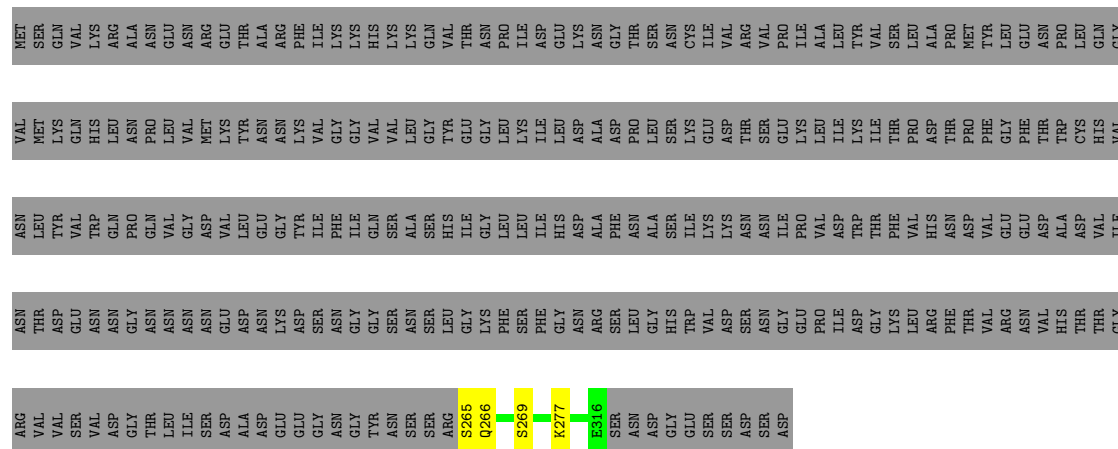
- Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain G:



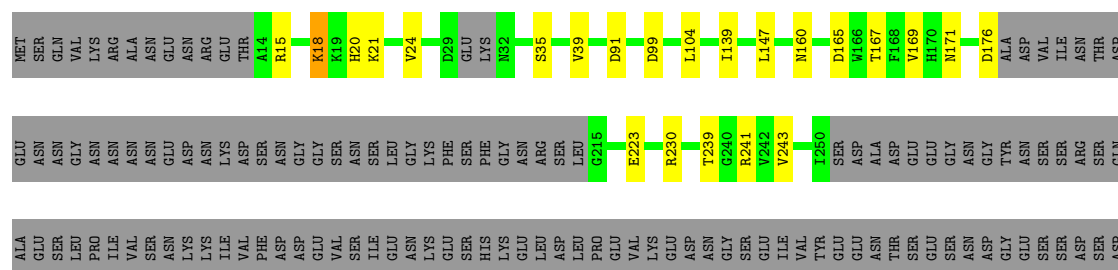
- Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain O:



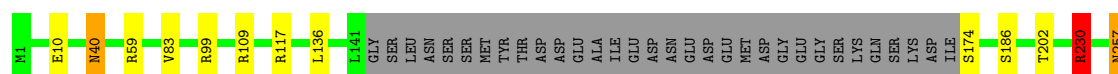
- Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

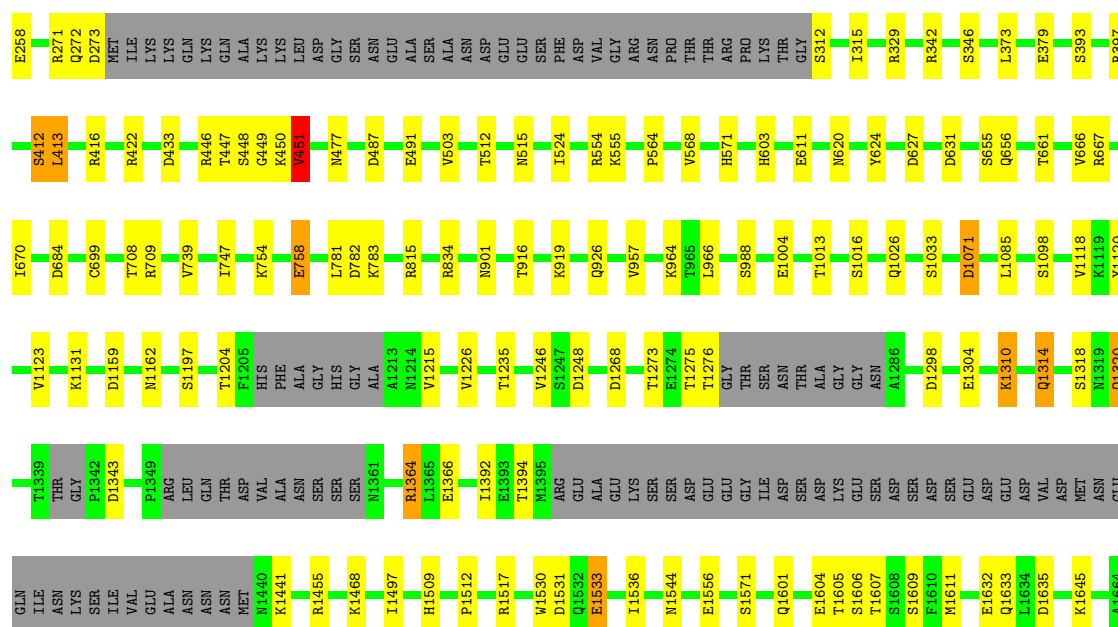
Chain V:



- Molecule 5: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190

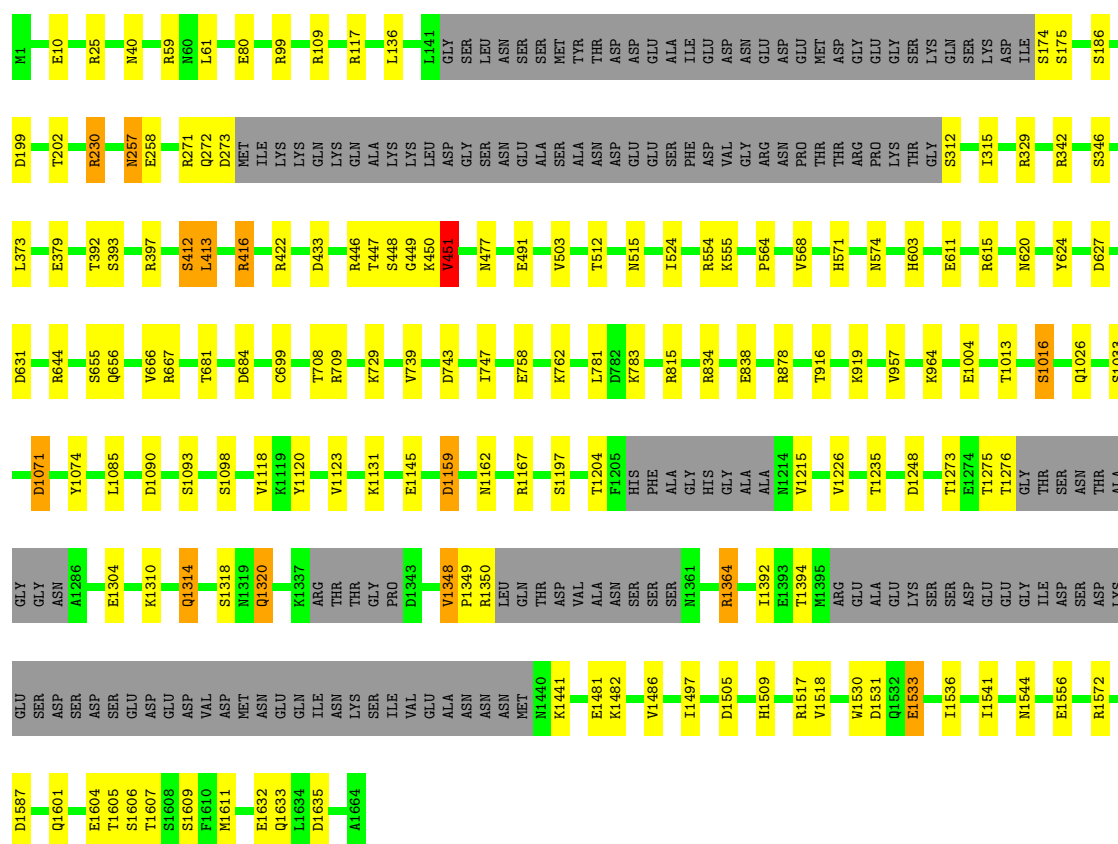
Chain A:





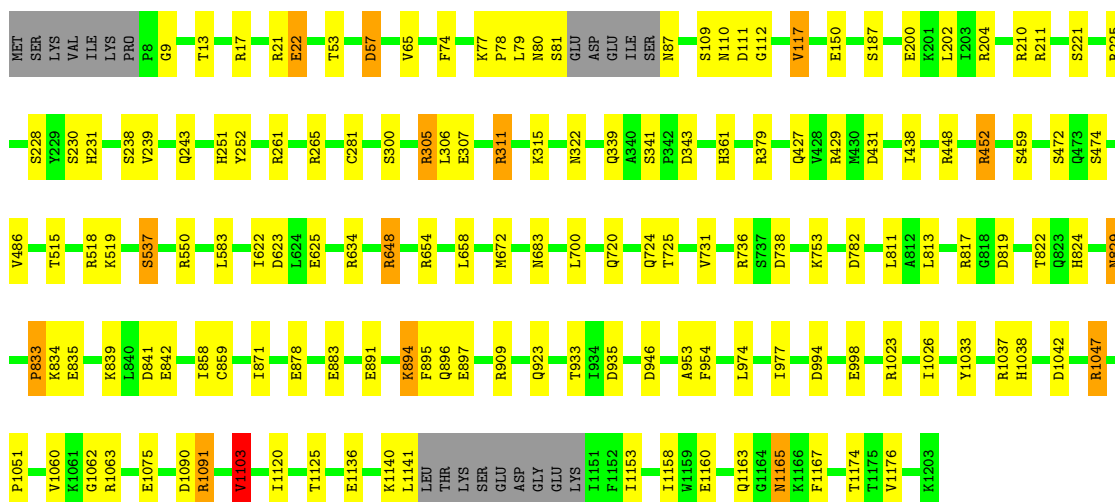
• Molecule 5: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190

Chain P:



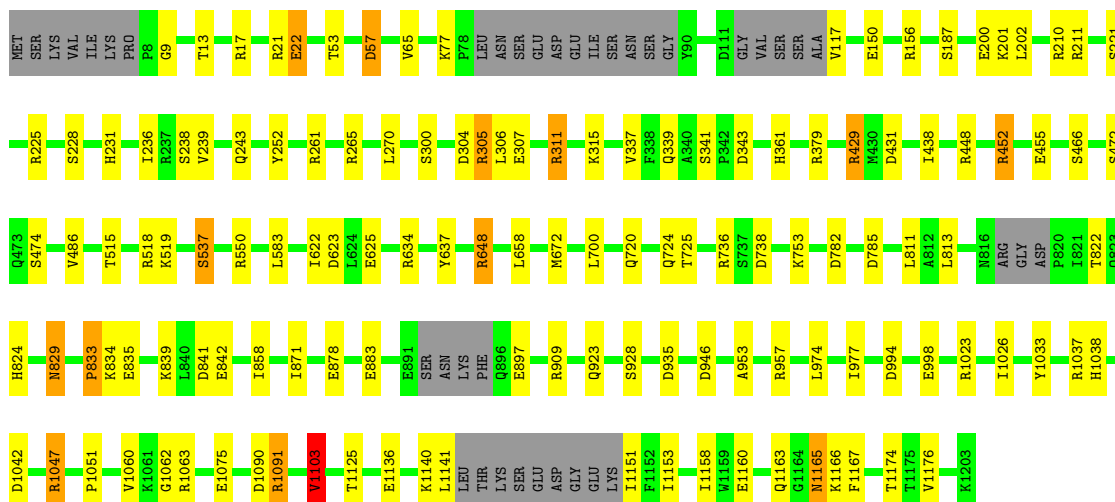
• Molecule 6: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

Chain B:



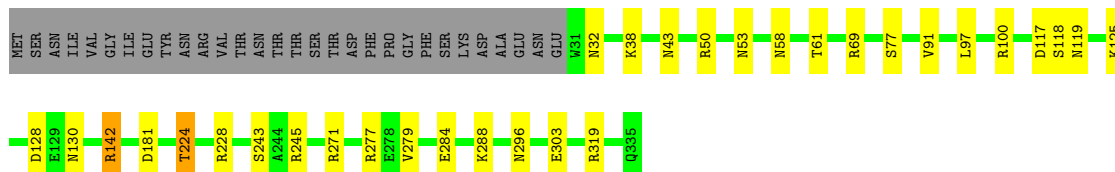
● Molecule 6: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

Chain Q:



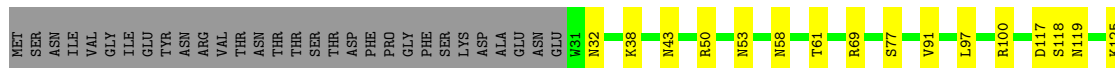
● Molecule 7: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain C:



- Molecule 7: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

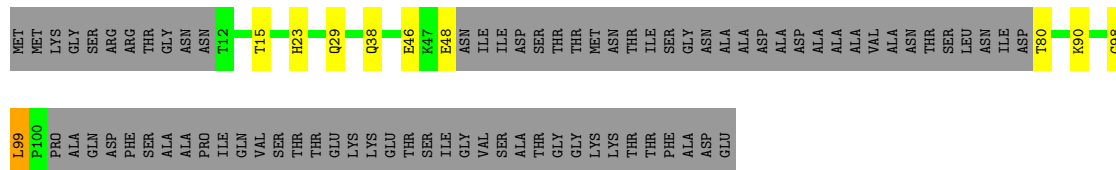
Chain R:





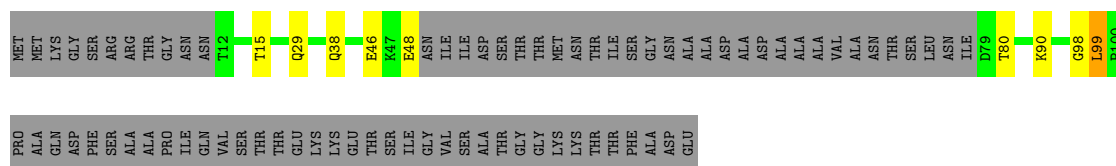
• Molecule 8: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

Chain D:



• Molecule 8: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

Chain S:



• Molecule 9: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



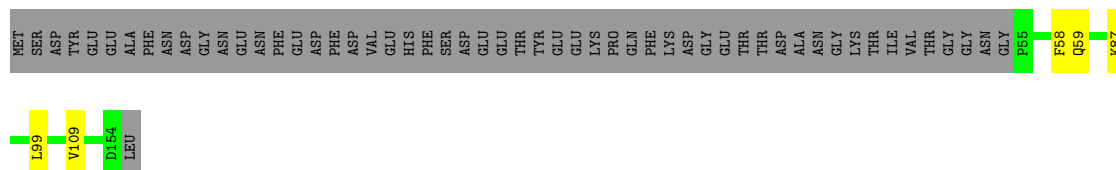
• Molecule 9: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain T:



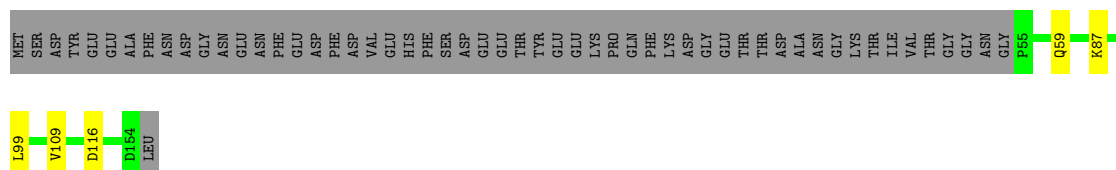
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain U:



- Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



- Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain W:



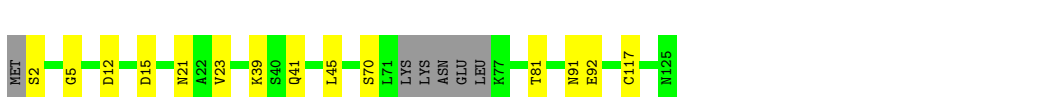
- Molecule 12: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain I:



- Molecule 12: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain X:



- Molecule 13: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



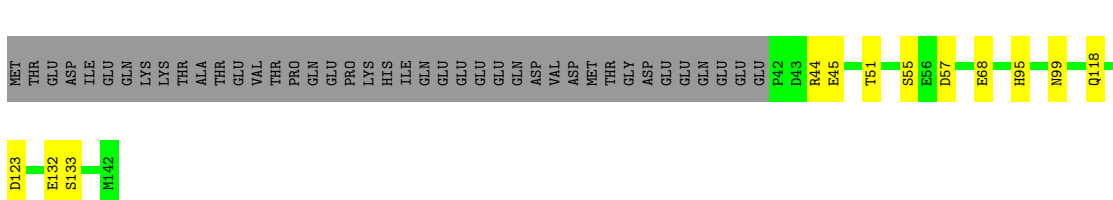
- Molecule 13: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain Y:



- Molecule 14: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain K:



- Molecule 14: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain Z:

MET	THR	GLU	ASP	ILE	GLU	GLN	LYS	LYS	THR	ALA	THR	GLU	VAL	THR	PRO	GLN	GLU	PRO	LYS	HIS	ILE	GLN	GLU	GLU	GLU	GLN	ASP	VAL	ASP	MET	THR	GLY	ASP	GLU	GLU	GLN	GLU	GLU	GLU	PRO	D43	R44	E45	T51	S55	S56	D57	E68	N99	Q118	D123
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------

E132	S133	M142
------	------	------

4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.74Å 139.02Å 209.55Å 108.06° 95.40° 93.85°	Depositor
Resolution (Å)	39.29 – 2.80	Depositor
% Data completeness (in resolution range)	99.9 (39.29-2.80)	Depositor
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.169 , 0.210	Depositor
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.250	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 320921 reflections	Xtriage
Total number of atoms	69107	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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	1	0.38	0/354	0.58	0/468
1	L	0.42	0/354	0.60	0/468
2	2	0.34	0/829	0.53	0/1114
2	M	0.40	0/872	0.55	0/1170
3	3	0.35	0/1174	0.52	0/1584
3	N	0.40	0/1172	0.55	0/1580
4	4	0.38	0/434	0.58	0/584
4	G	0.37	0/1564	0.66	3/2127 (0.1%)
4	O	0.42	0/417	0.60	0/562
4	V	0.38	0/1594	0.65	3/2168 (0.1%)
5	A	0.49	0/12236	0.75	25/16523 (0.2%)
5	P	0.45	0/12216	0.73	25/16495 (0.2%)
6	B	0.50	2/9594 (0.0%)	0.78	25/12967 (0.2%)
6	Q	0.43	0/9465	0.76	25/12789 (0.2%)
7	C	0.46	2/2475 (0.1%)	0.67	3/3354 (0.1%)
7	R	0.43	2/2475 (0.1%)	0.66	3/3354 (0.1%)
8	D	0.40	0/465	0.58	0/630
8	S	0.41	0/473	0.59	0/641
9	E	0.40	0/1771	0.66	3/2383 (0.1%)
9	T	0.41	0/1771	0.67	3/2383 (0.1%)
10	F	0.46	0/838	0.59	0/1129
10	U	0.43	0/838	0.59	0/1129
11	H	0.42	0/1070	0.61	0/1449
11	W	0.40	0/1070	0.60	0/1449
12	I	0.43	0/956	0.59	0/1288
12	X	0.42	0/912	0.58	0/1229
13	J	0.57	1/578 (0.2%)	0.59	0/775
13	Y	0.42	0/578	0.58	0/775
14	K	0.46	0/804	0.79	3/1083 (0.3%)
14	Z	0.42	0/796	0.75	3/1072 (0.3%)
All	All	0.45	7/70145 (0.0%)	0.71	124/94722 (0.1%)

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
5	A	0	2
5	P	0	1
All	All	0	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	10	CYS	CB-SG	7.66	1.95	1.82
6	B	281	CYS	CB-SG	-6.93	1.70	1.82
7	C	58	ASN	CG-ND2	-6.88	1.15	1.32
7	R	58	ASN	CG-OD1	-6.67	1.09	1.24
7	C	58	ASN	CG-OD1	-6.47	1.09	1.24

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	1023	ARG	NE-CZ-NH2	-14.08	113.26	120.30
6	Q	550	ARG	NE-CZ-NH2	-13.79	113.41	120.30
6	B	1023	ARG	NE-CZ-NH2	-13.75	113.43	120.30
5	P	397	ARG	NE-CZ-NH1	13.48	127.04	120.30
6	Q	452	ARG	NE-CZ-NH2	-13.35	113.62	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1343	ASP	Peptide
5	A	781	LEU	Peptide
5	P	781	LEU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	352	0	0	2	0
1	L	352	0	0	2	0
2	2	814	0	0	2	0
2	M	856	0	0	2	0
3	3	1152	0	0	3	0
3	N	1151	0	4	4	0
4	4	430	0	0	2	0
4	G	1526	0	0	7	0
4	O	413	0	0	2	0
4	V	1557	0	0	6	0
5	A	12019	0	74	37	1
5	P	12000	0	60	45	1
6	B	9386	0	784	49	0
6	Q	9261	0	784	45	0
7	C	2423	0	0	10	0
7	R	2423	0	0	10	0
8	D	459	0	0	2	0
8	S	467	0	0	1	0
9	E	1735	0	0	6	0
9	T	1735	0	0	9	0
10	F	823	0	0	1	0
10	U	823	0	0	1	0
11	H	1052	0	0	3	0
11	W	1052	0	0	3	0
12	I	943	0	0	5	0
12	X	900	0	0	3	0
13	J	569	0	0	4	0
13	Y	569	0	0	4	0
14	K	793	0	0	3	0
14	Z	786	0	0	3	0
15	1	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
15	P	2	0	0	0	0
15	Q	1	0	0	0	0
15	X	2	0	0	0	0
15	Y	1	0	0	0	0
16	B	5	0	0	1	0
16	Q	5	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	3	1	0	0	0	0
17	A	96	0	0	3	0
17	B	62	0	0	4	0
17	C	1	0	0	0	0
17	D	3	0	0	0	0
17	E	4	0	0	0	0
17	F	4	0	0	0	0
17	G	1	0	0	0	0
17	H	10	0	0	1	0
17	I	3	0	0	1	0
17	N	3	0	0	0	0
17	O	1	0	0	0	0
17	P	43	0	0	1	0
17	Q	15	0	0	2	0
17	R	1	0	0	0	0
17	S	1	0	0	0	0
17	T	4	0	0	0	0
17	U	4	0	0	0	0
17	V	2	0	0	0	0
17	W	1	0	0	0	0
17	X	2	0	0	0	0
All	All	69107	0	1706	233	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 233 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:620:ASN:OD1	5:A:667:ARG:NH2	2.01	0.93
6:B:77:LYS:NZ	6:B:438:ILE:O	2.07	0.86
5:P:620:ASN:OD1	5:P:667:ARG:NH2	2.10	0.85
7:C:100:ARG:NH2	13:J:3:VAL:O	2.10	0.84
7:C:303:GLU:OE1	13:J:43:ARG:NH2	2.11	0.83

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:1310:LYS:NZ	5:P:838:GLU:OE2[1_556]	2.07	0.13

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	1	42/70 (60%)	37 (88%)	3 (7%)	2 (5%)	4	10
1	L	42/70 (60%)	36 (86%)	4 (10%)	2 (5%)	4	10
2	2	99/415 (24%)	93 (94%)	4 (4%)	2 (2%)	11	35
2	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	12	37
3	3	139/233 (60%)	122 (88%)	15 (11%)	2 (1%)	16	49
3	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	10	32
4	4	52/326 (16%)	49 (94%)	3 (6%)	0	100	100
4	G	189/326 (58%)	174 (92%)	13 (7%)	2 (1%)	21	57
4	O	50/326 (15%)	46 (92%)	4 (8%)	0	100	100
4	V	191/326 (59%)	175 (92%)	15 (8%)	1 (0%)	38	76
5	A	1505/1664 (90%)	1434 (95%)	62 (4%)	9 (1%)	33	72
5	P	1502/1664 (90%)	1433 (95%)	59 (4%)	10 (1%)	30	69
6	B	1176/1203 (98%)	1116 (95%)	47 (4%)	13 (1%)	21	57
6	Q	1152/1203 (96%)	1104 (96%)	42 (4%)	6 (0%)	38	76
7	C	303/335 (90%)	288 (95%)	13 (4%)	2 (1%)	30	69
7	R	303/335 (90%)	289 (95%)	12 (4%)	2 (1%)	30	69
8	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	5	16
8	S	55/137 (40%)	51 (93%)	2 (4%)	2 (4%)	5	17
9	E	210/215 (98%)	198 (94%)	11 (5%)	1 (0%)	38	76
9	T	210/215 (98%)	199 (95%)	9 (4%)	2 (1%)	22	60
10	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
10	U	98/155 (63%)	98 (100%)	0	0	100	100
11	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
11	W	127/146 (87%)	119 (94%)	8 (6%)	0	100	100
12	I	122/125 (98%)	107 (88%)	12 (10%)	3 (2%)	9	28
12	X	115/125 (92%)	102 (89%)	10 (9%)	3 (3%)	8	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
13	Y	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
14	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
14	Z	98/142 (69%)	92 (94%)	6 (6%)	0	100	100
All	All	8537/11124 (77%)	8066 (94%)	400 (5%)	71 (1%)	27	65

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	1606	SER
6	B	111	ASP
6	B	895	PHE
7	C	224	THR
8	D	99	LEU

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	1	39/57 (68%)	36 (92%)	3 (8%)	18	45
1	L	39/57 (68%)	36 (92%)	3 (8%)	18	45
2	2	93/371 (25%)	85 (91%)	8 (9%)	15	40
2	M	98/371 (26%)	88 (90%)	10 (10%)	11	29
3	3	135/220 (61%)	128 (95%)	7 (5%)	32	68
3	N	135/220 (61%)	129 (96%)	6 (4%)	39	75
4	4	52/291 (18%)	51 (98%)	1 (2%)	69	94
4	G	171/291 (59%)	159 (93%)	12 (7%)	21	52
4	O	50/291 (17%)	49 (98%)	1 (2%)	68	94
4	V	175/291 (60%)	161 (92%)	14 (8%)	17	44
5	A	1345/1465 (92%)	1263 (94%)	82 (6%)	26	61
5	P	1343/1465 (92%)	1261 (94%)	82 (6%)	26	61
6	B	1033/1053 (98%)	965 (93%)	68 (7%)	24	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Q	1019/1053 (97%)	956 (94%)	63 (6%)	26	60
7	C	269/296 (91%)	253 (94%)	16 (6%)	28	62
7	R	269/296 (91%)	252 (94%)	17 (6%)	25	59
8	D	55/116 (47%)	49 (89%)	6 (11%)	9	26
8	S	56/116 (48%)	50 (89%)	6 (11%)	10	26
9	E	194/197 (98%)	180 (93%)	14 (7%)	21	50
9	T	194/197 (98%)	178 (92%)	16 (8%)	17	43
10	F	90/137 (66%)	86 (96%)	4 (4%)	39	75
10	U	90/137 (66%)	86 (96%)	4 (4%)	39	75
11	H	115/128 (90%)	111 (96%)	4 (4%)	48	83
11	W	115/128 (90%)	111 (96%)	4 (4%)	48	83
12	I	109/110 (99%)	102 (94%)	7 (6%)	25	58
12	X	104/110 (94%)	98 (94%)	6 (6%)	28	63
13	J	64/65 (98%)	57 (89%)	7 (11%)	9	26
13	Y	64/65 (98%)	57 (89%)	7 (11%)	9	26
14	K	91/130 (70%)	84 (92%)	7 (8%)	18	45
14	Z	90/130 (69%)	83 (92%)	7 (8%)	18	45
All	All	7696/9854 (78%)	7204 (94%)	492 (6%)	25	58

5 of 492 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	39	THR
5	P	257	ASN
4	V	18	LYS
12	I	74	ASN
2	M	17	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
6	B	1163	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 14 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	$\# Z > 2$
16	SO4	B	2204	-	4,4,4	0.30	0	6,6,6	0.41	0
16	SO4	Q	2204	-	4,4,4	0.30	0	6,6,6	0.42	0

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
16	SO4	B	2204	-	-	0/0/0/0	0/0/0/0
16	SO4	Q	2204	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.