



Full wwPDB X-ray Structure Validation 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 full wwPDB validation 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>

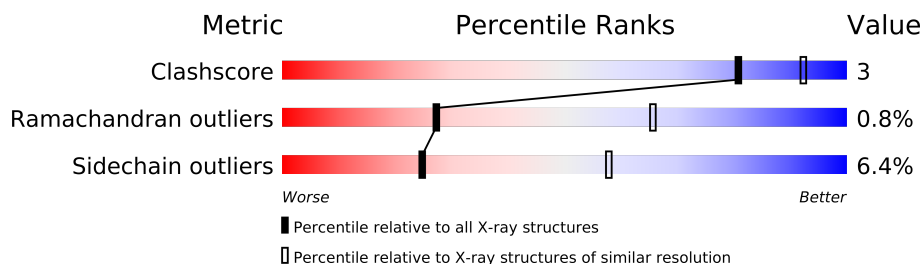
The following versions of software and data (see [references](#)) were used in the production of this report:

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)






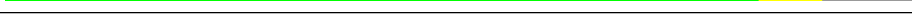

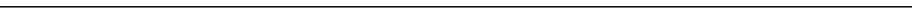
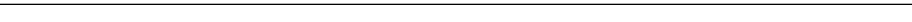



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The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

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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			

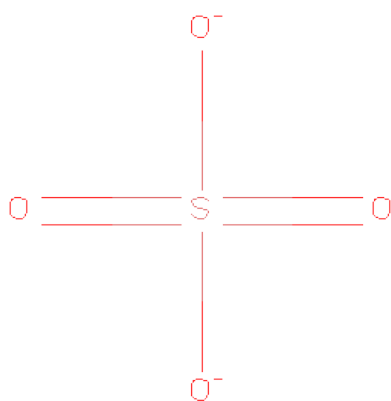
- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

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

GLU	ALA	TLE	GLN	ALA
PHE	GLY	PRO	LEU	TLE
ILE	ASN	TYR	TYR	ALA
PRO	GLU	LEU	SER	ASP
LYS	ASP	SER	GLY	GLU
SER	LYS	LEU	LEU	ASN
THR	ILE	LEU	LEU	ARG
ALA	LEU	LEU	LEU	ILE
ALA	CYS	GLY	VAL	ASP
SER	TYR	TYR	TYR	SER
TYR	ILE	LEU	GLY	ASP
ILE	ALA	ASN	ASN	LYS
ALA	ILE	ARG	ARG	LEU
THR	ILE	ARG	VAL	THR
MET	MET	VAL	ASN	ASP
LYS	HIS	ASN	ASN	SER
VAL	LEU	ASN	ASN	ALA
PRO	ASP	LYS	LYS	ASP
PHE	ASN	THR	THR	ASP
LYS	PHE	LYS	LEU	VAL
LEU	ILE	LEU	LEU	ASP
PRO	VAL	LEU	LEU	SER
GLU	GLU	GLU	GLU	VAL
MET	ILE	ARG	ARG	ALA
THR	THR	LEU	LEU	THR
ARG	PRO	ASN	ASN	ALA
ARG	LEU	SER	SER	SER
GLY	ALA	PRO	PRO	LYS
ARG	HIS	PRO	LEU	LYS
GLY	GLU	GLU	LEU	ASP
PRO	LEU	ILE	GLU	LEU
ARG	ASN	ASN	LEU	PRO
ARG	LEU	VAL	VAL	THR
	LYS	ASP	ASP	ARG
	PRO	GLY	GLY	ALA
	SER	ILE	ILE	GLN
	LYE	THR	THR	GLN
	VAL	VAL	VAL	ASN
	ARG	ILE	LYS	ASN
	VAL	VAL	PRO	ARG
	LEU	LEU	GLY	THR
	ALA	ALA	GLN	PRO
	ILE	PHE	LEU	ALA
	VAL	VAL	THR	ALA
	LYS	ARG	GLN	ASN
	GLY	SER	PRO	ILE
	ALA	ALA	SER	ASP
	THR	THR	GLN	ALA
	VAL	VAL	MET	THR
	ALA	ALA	SER	ASP
	GLN	GLN	LYS	VAL
	ALA	THR	LEU	GLU

● Molecule 3: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34

Chain 3:

● Molecule 3: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34

Chain N:

- Molecule 3: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34

Chain N: 

[illegible]

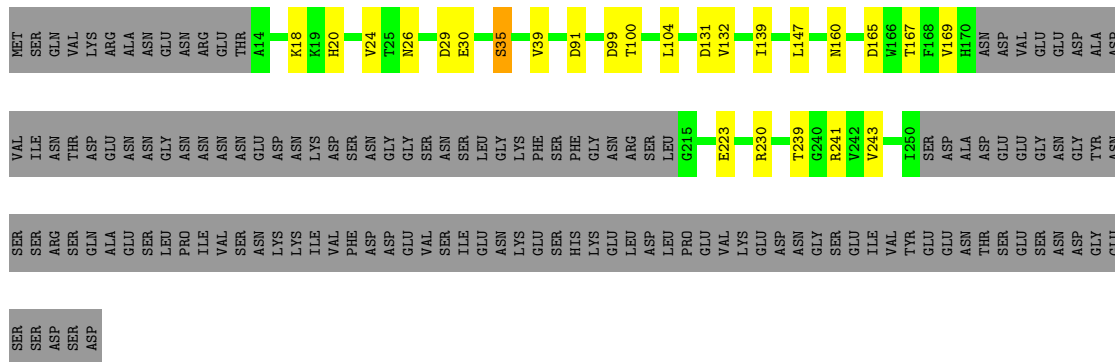
● Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain 4: 

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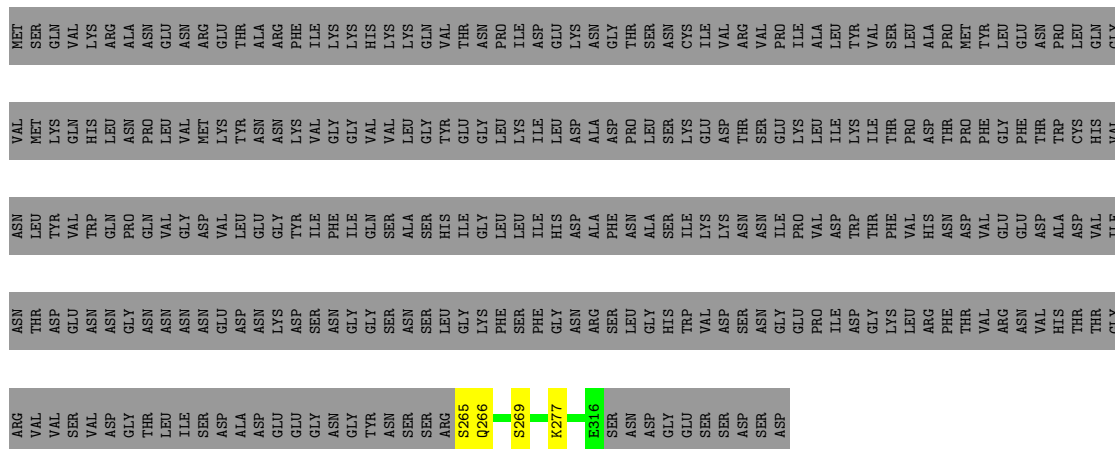
- Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain G:



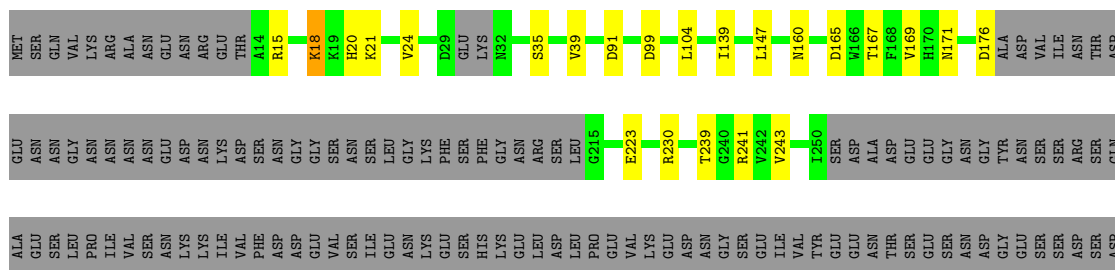
- Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain 0:



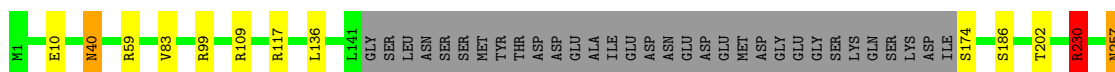
● Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

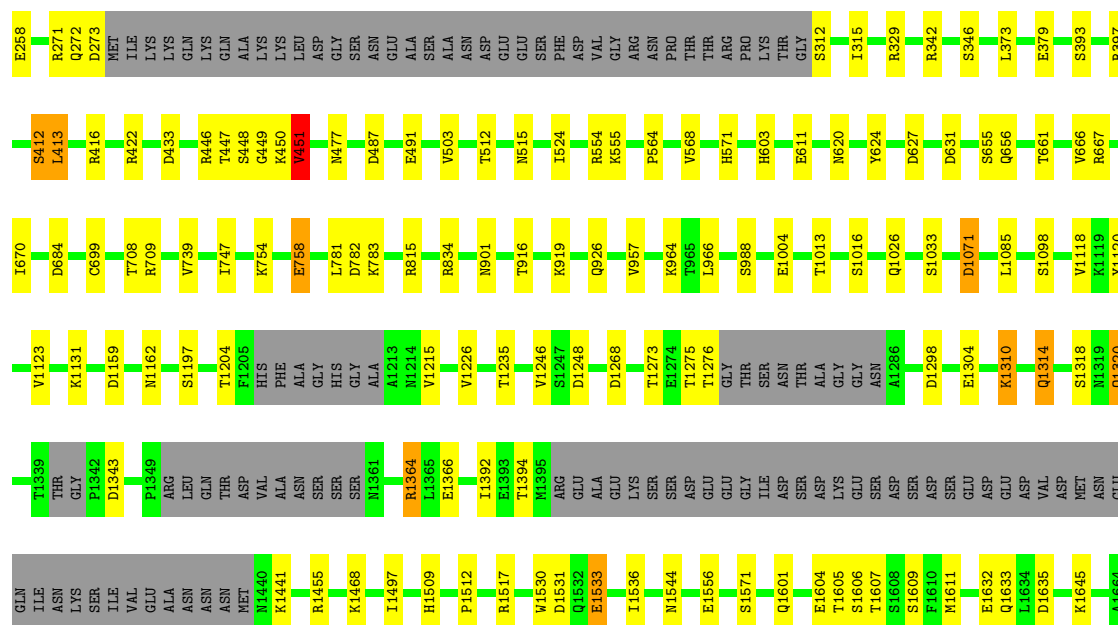
Chain V:



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

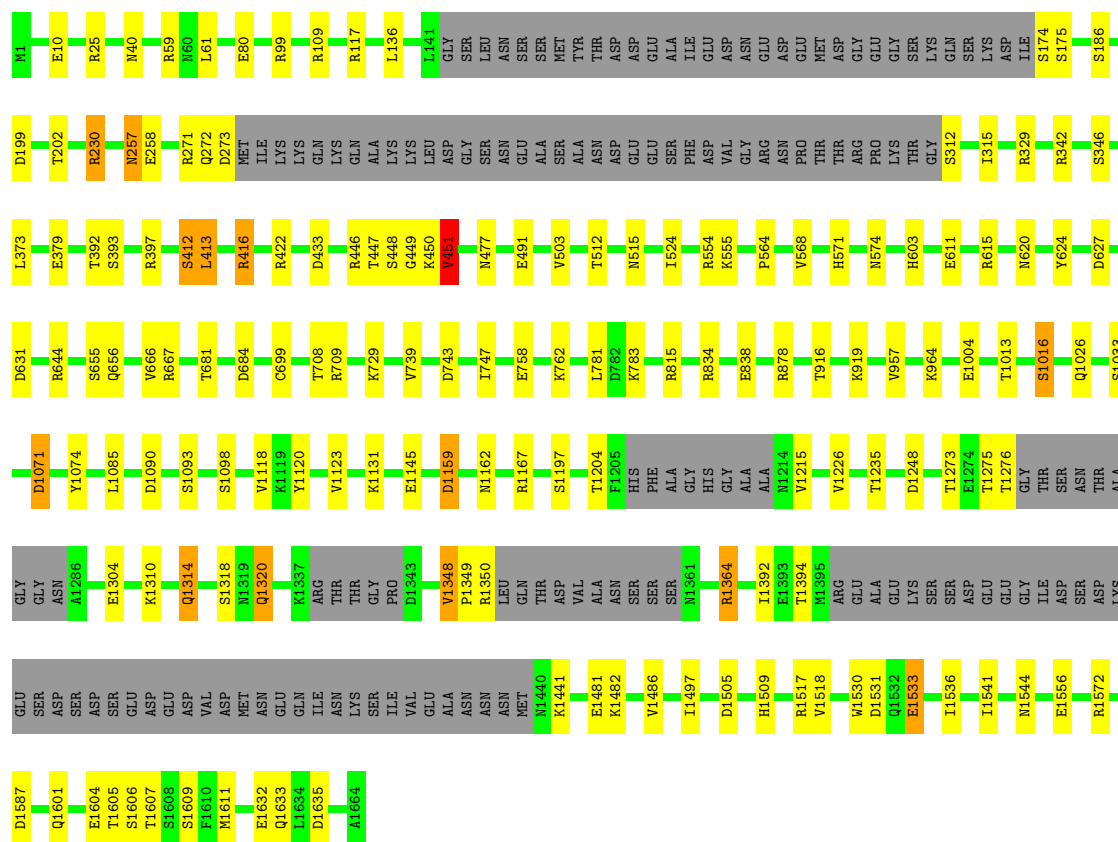
Chain A:





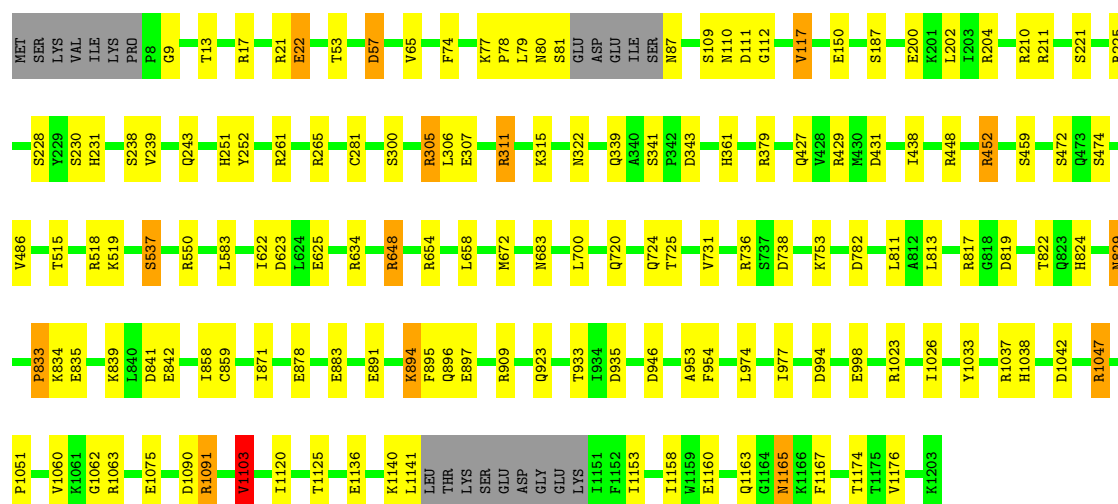
• Molecule 5: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190

Chain P:



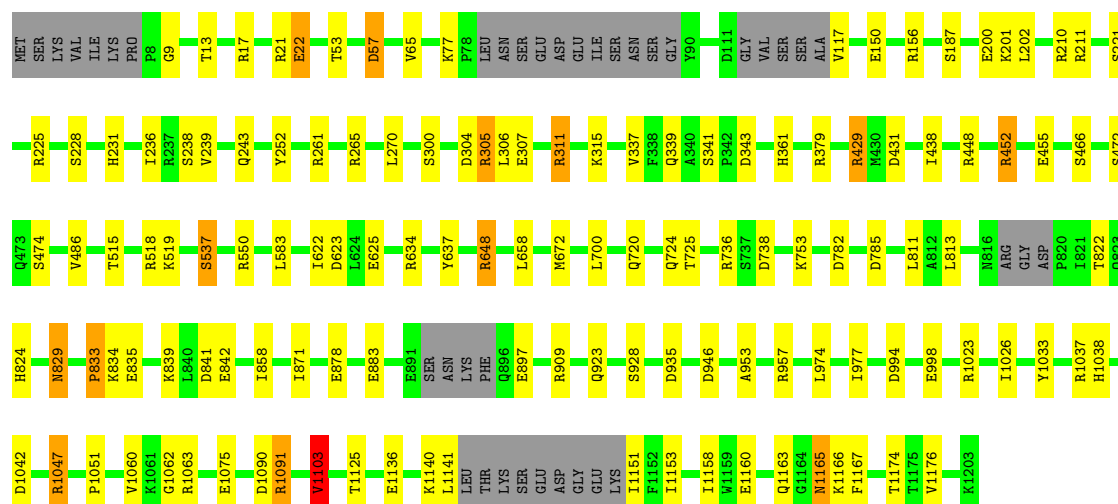
• Molecule 6: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

Chain B:



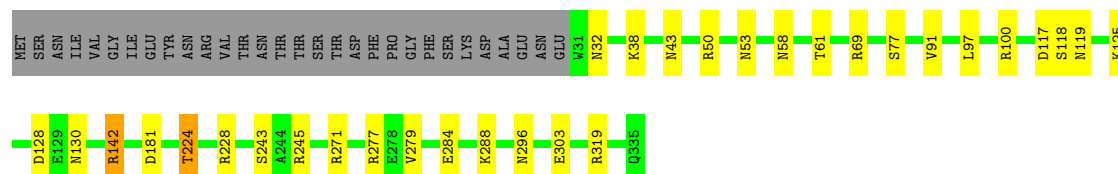
• Molecule 6: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

Chain Q:



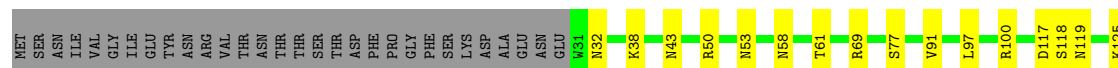
• Molecule 7: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain C:



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

Chain R:



- Molecule 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:



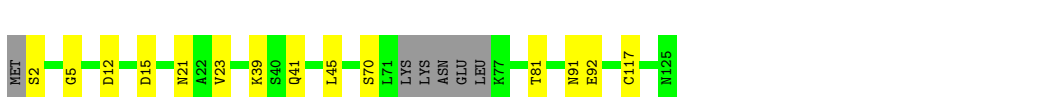
- Molecule 12: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

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:



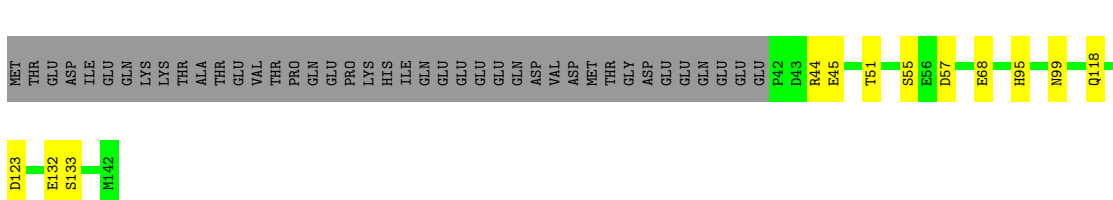
- Molecule 13: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

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	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
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E132	S133	M142
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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

All (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
7	R	58	ASN	CG-ND2	-6.37	1.17	1.32
6	B	859	CYS	CB-SG	-6.18	1.71	1.82

All (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
6	B	452	ARG	NE-CZ-NH2	-13.35	113.62	120.30
5	A	397	ARG	NE-CZ-NH1	13.31	126.96	120.30
6	Q	550	ARG	NE-CZ-NH1	13.09	126.84	120.30
6	B	448	ARG	NE-CZ-NH2	-12.99	113.80	120.30
5	A	329	ARG	NE-CZ-NH2	-12.94	113.83	120.30
6	Q	648	ARG	NE-CZ-NH2	-12.92	113.84	120.30
5	A	59	ARG	NE-CZ-NH1	12.84	126.72	120.30
6	Q	452	ARG	NE-CZ-NH1	12.83	126.72	120.30
5	A	329	ARG	NE-CZ-NH1	12.79	126.70	120.30
5	A	59	ARG	NE-CZ-NH2	-12.76	113.92	120.30
6	B	429	ARG	NE-CZ-NH2	-12.75	113.93	120.30
5	P	397	ARG	NE-CZ-NH2	-12.74	113.93	120.30
6	Q	634	ARG	NE-CZ-NH2	-12.74	113.93	120.30
9	T	167	ARG	NE-CZ-NH2	-12.59	114.00	120.30
5	P	342	ARG	NE-CZ-NH2	-12.58	114.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	167	ARG	NE-CZ-NH2	-12.54	114.03	120.30
9	E	167	ARG	NE-CZ-NH1	12.53	126.57	120.30
5	A	416	ARG	NE-CZ-NH2	-12.46	114.07	120.30
6	B	261	ARG	NE-CZ-NH1	12.46	126.53	120.30
6	B	448	ARG	NE-CZ-NH1	12.40	126.50	120.30
5	P	422	ARG	NE-CZ-NH2	-12.32	114.14	120.30
14	K	44	ARG	NE-CZ-NH2	-12.31	114.14	120.30
6	B	634	ARG	NE-CZ-NH2	-12.23	114.19	120.30
6	Q	634	ARG	NE-CZ-NH1	12.23	126.42	120.30
5	P	59	ARG	NE-CZ-NH2	-12.19	114.20	120.30
6	B	452	ARG	NE-CZ-NH1	12.19	126.39	120.30
6	B	261	ARG	NE-CZ-NH2	-12.14	114.23	120.30
6	B	429	ARG	NE-CZ-NH1	12.12	126.36	120.30
5	P	416	ARG	NE-CZ-NH2	-12.06	114.27	120.30
5	P	342	ARG	NE-CZ-NH1	12.04	126.32	120.30
5	P	422	ARG	NE-CZ-NH1	11.98	126.29	120.30
14	K	44	ARG	NE-CZ-NH1	11.98	126.29	120.30
6	Q	261	ARG	NE-CZ-NH1	11.93	126.27	120.30
5	P	416	ARG	NE-CZ-NH1	11.86	126.23	120.30
7	R	142	ARG	NE-CZ-NH2	-11.84	114.38	120.30
9	T	167	ARG	NE-CZ-NH1	11.84	126.22	120.30
5	A	1364	ARG	NE-CZ-NH2	-11.82	114.39	120.30
5	A	397	ARG	NE-CZ-NH2	-11.81	114.39	120.30
5	P	59	ARG	NE-CZ-NH1	11.79	126.19	120.30
5	P	329	ARG	NE-CZ-NH1	11.78	126.19	120.30
4	G	241	ARG	NE-CZ-NH1	11.78	126.19	120.30
6	Q	261	ARG	NE-CZ-NH2	-11.75	114.42	120.30
5	P	329	ARG	NE-CZ-NH2	-11.70	114.45	120.30
6	Q	648	ARG	NE-CZ-NH1	11.67	126.14	120.30
5	A	422	ARG	NE-CZ-NH2	-11.65	114.47	120.30
4	G	241	ARG	NE-CZ-NH2	-11.64	114.48	120.30
7	C	142	ARG	NE-CZ-NH2	-11.50	114.55	120.30
6	Q	429	ARG	NE-CZ-NH2	-11.50	114.55	120.30
6	Q	448	ARG	NE-CZ-NH1	11.42	126.01	120.30
7	C	142	ARG	NE-CZ-NH1	11.41	126.01	120.30
5	P	230	ARG	NE-CZ-NH2	-11.41	114.59	120.30
5	P	230	ARG	NE-CZ-NH1	11.32	125.96	120.30
7	R	142	ARG	NE-CZ-NH1	11.31	125.95	120.30
5	A	422	ARG	NE-CZ-NH1	11.30	125.95	120.30
6	Q	448	ARG	NE-CZ-NH2	-11.29	114.66	120.30
5	A	342	ARG	NE-CZ-NH2	-11.24	114.68	120.30
14	Z	44	ARG	NE-CZ-NH2	-11.20	114.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1364	ARG	NE-CZ-NH2	-11.20	114.70	120.30
5	A	1364	ARG	NE-CZ-NH1	11.11	125.85	120.30
5	A	416	ARG	NE-CZ-NH1	11.09	125.84	120.30
6	B	634	ARG	NE-CZ-NH1	11.08	125.84	120.30
6	Q	1023	ARG	NE-CZ-NH1	10.87	125.74	120.30
14	Z	44	ARG	NE-CZ-NH1	10.82	125.71	120.30
5	A	230	ARG	NE-CZ-NH2	-10.81	114.89	120.30
5	A	230	ARG	NE-CZ-NH1	10.74	125.67	120.30
5	P	1364	ARG	NE-CZ-NH1	10.70	125.65	120.30
6	B	550	ARG	NE-CZ-NH2	-10.63	114.98	120.30
4	V	241	ARG	NE-CZ-NH2	-10.62	114.99	120.30
6	B	648	ARG	NE-CZ-NH2	-10.60	115.00	120.30
6	Q	429	ARG	NE-CZ-NH1	10.60	125.60	120.30
4	V	241	ARG	NE-CZ-NH1	10.03	125.31	120.30
6	B	550	ARG	NE-CZ-NH1	9.81	125.21	120.30
6	B	1023	ARG	NE-CZ-NH1	9.56	125.08	120.30
5	A	342	ARG	NE-CZ-NH1	9.15	124.87	120.30
6	B	648	ARG	NE-CZ-NH1	8.97	124.78	120.30
5	A	397	ARG	CD-NE-CZ	6.93	133.31	123.60
6	B	261	ARG	CD-NE-CZ	6.89	133.24	123.60
9	T	167	ARG	CD-NE-CZ	6.72	133.01	123.60
5	A	59	ARG	CD-NE-CZ	6.63	132.88	123.60
5	P	397	ARG	CD-NE-CZ	6.58	132.81	123.60
5	P	59	ARG	CD-NE-CZ	6.55	132.77	123.60
6	B	452	ARG	CD-NE-CZ	6.54	132.75	123.60
5	A	329	ARG	CD-NE-CZ	6.42	132.58	123.60
5	P	329	ARG	CD-NE-CZ	6.37	132.52	123.60
6	B	448	ARG	CD-NE-CZ	6.33	132.47	123.60
6	Q	550	ARG	CD-NE-CZ	6.29	132.41	123.60
14	K	44	ARG	CD-NE-CZ	6.26	132.37	123.60
6	Q	452	ARG	CD-NE-CZ	6.25	132.35	123.60
6	Q	634	ARG	CD-NE-CZ	6.25	132.35	123.60
5	A	416	ARG	CD-NE-CZ	6.18	132.25	123.60
5	P	422	ARG	CD-NE-CZ	6.17	132.24	123.60
6	B	634	ARG	CD-NE-CZ	6.17	132.23	123.60
7	R	142	ARG	CD-NE-CZ	6.13	132.18	123.60
6	B	429	ARG	CD-NE-CZ	6.13	132.18	123.60
5	A	422	ARG	CD-NE-CZ	6.12	132.16	123.60
4	G	241	ARG	CD-NE-CZ	6.03	132.05	123.60
5	P	416	ARG	CD-NE-CZ	6.00	131.99	123.60
7	C	142	ARG	CD-NE-CZ	5.99	131.98	123.60
6	Q	1023	ARG	CD-NE-CZ	5.95	131.93	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	167	ARG	CD-NE-CZ	5.90	131.86	123.60
14	Z	44	ARG	CD-NE-CZ	5.82	131.75	123.60
6	Q	261	ARG	CD-NE-CZ	5.81	131.74	123.60
6	Q	448	ARG	CD-NE-CZ	5.81	131.73	123.60
5	A	1364	ARG	CD-NE-CZ	5.74	131.63	123.60
6	Q	1103	VAL	CB-CA-C	-5.73	100.51	111.40
5	A	342	ARG	CD-NE-CZ	5.67	131.54	123.60
5	P	1364	ARG	CD-NE-CZ	5.67	131.53	123.60
6	B	1103	VAL	CB-CA-C	-5.60	100.76	111.40
6	Q	429	ARG	CD-NE-CZ	5.55	131.38	123.60
5	P	342	ARG	CD-NE-CZ	5.55	131.37	123.60
5	P	230	ARG	CD-NE-CZ	5.51	131.32	123.60
6	B	550	ARG	CD-NE-CZ	5.48	131.27	123.60
4	V	241	ARG	CD-NE-CZ	5.44	131.22	123.60
6	Q	648	ARG	CD-NE-CZ	5.43	131.20	123.60
6	B	648	ARG	CD-NE-CZ	5.42	131.18	123.60
6	B	1023	ARG	CD-NE-CZ	5.29	131.01	123.60
5	A	230	ARG	CD-NE-CZ	5.21	130.89	123.60
5	P	1071	ASP	N-CA-C	-5.09	97.27	111.00
5	A	1071	ASP	N-CA-C	-5.03	97.41	111.00

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
17	3	1	0	0	0	0
17	A	96	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
6:B:894:LYS:O	6:B:896:GLN:N	2.11	0.83
7:R:100:ARG:NH2	13:Y:3:VAL:O	2.12	0.81
7:R:303:GLU:OE1	13:Y:43:ARG:NH2	2.14	0.81
6:Q:518:ARG:NH2	6:Q:537:SER:O	2.15	0.79
6:Q:878:GLU:OE2	6:Q:909:ARG:NH1	2.16	0.77
6:B:878:GLU:OE2	6:B:909:ARG:NH1	2.17	0.77
6:Q:77:LYS:NZ	6:Q:438:ILE:O	2.18	0.77
6:B:974:LEU:O	13:J:47:ARG:NH1	2.18	0.76
5:P:834:ARG:NH2	6:Q:994:ASP:OD1	2.19	0.76
6:Q:974:LEU:O	13:Y:47:ARG:NH1	2.20	0.75
6:B:211:ARG:NH2	6:B:243:GLN:OE1	2.19	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:B:518:ARG:NH2	6:B:537:SER:O	2.21	0.74
5:P:1248:ASP:OD1	5:P:1517:ARG:NH1	2.22	0.72
5:P:524:ILE:O	5:P:554:ARG:NH1	2.22	0.72
5:A:1120:TYR:O	9:E:207:ARG:NH2	2.22	0.71
6:Q:211:ARG:NH2	6:Q:243:GLN:OE1	2.24	0.71
5:A:524:ILE:O	5:A:554:ARG:NH1	2.23	0.71
6:Q:623:ASP:O	6:Q:648:ARG:NH2	2.24	0.71
6:B:1165:ASN:OD1	6:B:1165:ASN:N	2.24	0.70
5:A:99:ARG:O	5:A:109:ARG:NH2	2.24	0.70
5:A:1246:VAL:O	5:A:1517:ARG:NH2	2.25	0.69
5:A:477:ASN:OD1	6:B:1047:ARG:NH1	2.26	0.69
6:Q:431:ASP:OD1	6:Q:452:ARG:NH2	2.26	0.69
7:R:125:LYS:O	7:R:130:ASN:ND2	2.26	0.68
6:Q:1165:ASN:N	6:Q:1165:ASN:OD1	2.24	0.68
5:A:964:LYS:NZ	6:B:672:MET:O	2.27	0.67
5:P:477:ASN:OD1	6:Q:1047:ARG:NH1	2.27	0.67
7:C:125:LYS:O	7:C:130:ASN:ND2	2.27	0.67
6:Q:923:GLN:NE2	6:Q:953:ALA:O	2.28	0.67
6:Q:341:SER:OG	6:Q:343:ASP:OD1	2.12	0.66
12:I:43:SER:N	17:I:2001:HOH:O	2.28	0.66
9:T:55:ARG:NH2	9:T:113:GLN:OE1	2.29	0.65
5:P:699:CYS:O	5:P:815:ARG:NH1	2.29	0.65
6:B:341:SER:OG	6:B:343:ASP:OD1	2.13	0.65
5:P:99:ARG:O	5:P:109:ARG:NH2	2.29	0.65
5:P:109:ARG:NH1	5:P:230:ARG:O	2.28	0.65
6:B:700:LEU:N	16:B:2204:SO4:O2	2.30	0.65
5:A:109:ARG:NH1	5:A:230:ARG:O	2.29	0.65
6:B:923:GLN:NE2	6:B:953:ALA:O	2.30	0.64
5:A:834:ARG:NH2	6:B:994:ASP:OD1	2.31	0.64
5:A:1366:GLU:OE2	6:B:204:ARG:NH2	2.31	0.63
5:P:1556:GLU:OE2	9:T:212:ARG:NH1	2.32	0.63
5:P:964:LYS:NZ	6:Q:672:MET:O	2.31	0.63
11:W:25:ARG:NH1	11:W:27:GLU:OE2	2.32	0.63
5:P:1120:TYR:O	9:T:207:ARG:NH2	2.32	0.63
6:Q:946:ASP:OD2	13:Y:48:ARG:NH2	2.33	0.61
5:A:926:GLN:NE2	17:A:2061:HOH:O	2.33	0.61
6:B:251:HIS:ND1	17:B:2014:HOH:O	2.31	0.61
5:A:449:GLY:O	5:A:451:VAL:N	2.34	0.61
5:P:449:GLY:O	5:P:451:VAL:N	2.34	0.61
5:P:1004:GLU:OE2	6:Q:519:LYS:NZ	2.34	0.61
2:2:11:GLU:N	2:2:86:LYS:O	2.34	0.60
6:Q:935:ASP:OD1	7:R:69:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:63:ASP:OD2	3:N:66:LYS:NZ	2.35	0.60
11:H:25:ARG:NH1	11:H:27:GLU:OE2	2.34	0.60
5:A:699:CYS:O	5:A:815:ARG:NH1	2.35	0.60
6:B:110:ASN:O	6:B:112:GLY:N	2.35	0.59
6:B:829:ASN:OD1	6:B:829:ASN:N	2.36	0.58
5:A:758:GLU:N	17:A:2042:HOH:O	2.36	0.58
2:M:11:GLU:N	2:M:86:LYS:O	2.36	0.58
9:E:55:ARG:NH2	9:E:113:GLN:OE1	2.36	0.58
6:B:935:ASP:OD1	7:C:69:ARG:NH2	2.37	0.58
6:Q:210:ARG:NH2	6:Q:625:GLU:OE2	2.37	0.58
5:A:1556:GLU:OE2	9:E:212:ARG:NH1	2.37	0.57
5:A:1004:GLU:OE2	6:B:519:LYS:NZ	2.37	0.57
3:3:69:SER:OG	3:3:70:LEU:N	2.35	0.57
4:4:265:SER:OG	4:4:266:GLN:N	2.38	0.57
9:T:159:ASP:OD1	9:T:162:ARG:NH1	2.37	0.57
3:3:63:ASP:OD2	3:3:66:LYS:NZ	2.37	0.57
6:Q:21:ARG:NH1	6:Q:22:GLU:OE1	2.38	0.57
5:A:1235:THR:O	5:A:1544:ASN:ND2	2.38	0.57
8:S:48:GLU:OE2	8:S:90:LYS:NZ	2.38	0.57
9:E:159:ASP:OD1	9:E:162:ARG:NH1	2.39	0.56
6:Q:700:LEU:N	16:Q:2204:SO4:O2	2.38	0.56
6:B:109:SER:OG	6:B:891:GLU:OE2	2.24	0.56
5:P:491:GLU:OE2	5:P:815:ARG:NH2	2.39	0.55
4:G:20:HIS:O	4:G:20:HIS:ND1	2.38	0.55
6:B:946:ASP:OD2	13:J:48:ARG:NH2	2.39	0.55
5:A:916:THR:O	5:A:919:LYS:NZ	2.40	0.55
4:V:20:HIS:ND1	4:V:20:HIS:O	2.39	0.55
6:Q:829:ASN:OD1	6:Q:829:ASN:N	2.36	0.55
5:A:491:GLU:OE2	5:A:815:ARG:NH2	2.40	0.55
3:N:69:SER:OG	3:N:70:LEU:N	2.37	0.55
6:B:21:ARG:NH1	6:B:22:GLU:OE1	2.40	0.55
12:X:91:ASN:OD1	12:X:92:GLU:N	2.40	0.54
6:B:841:ASP:OD1	6:B:842:GLU:N	2.40	0.54
4:O:265:SER:OG	4:O:266:GLN:N	2.40	0.54
6:B:654:ARG:NH1	17:B:2043:HOH:O	2.38	0.54
1:1:34:CYS:CB	1:1:51:CYS:SG	2.95	0.54
6:Q:1151:ILE:HG12	4:V:21:LYS:NZ	2.21	0.53
7:R:284:GLU:O	7:R:288:LYS:NZ	2.41	0.53
6:Q:472:SER:OG	6:Q:474:SER:O	2.27	0.53
14:Z:55:SER:OG	14:Z:57:ASP:OD1	2.26	0.52
6:B:307:GLU:OE2	6:B:311:ARG:NH1	2.43	0.52
7:R:117:ASP:OD1	7:R:119:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:Q:337:VAL:N	17:Q:2002:HOH:O	2.42	0.52
8:D:48:GLU:OE2	8:D:90:LYS:NZ	2.43	0.51
6:B:1047:ARG:NH2	6:B:1051:PRO:O	2.43	0.51
5:P:916:THR:O	5:P:919:LYS:NZ	2.44	0.51
5:A:40:ASN:N	5:A:40:ASN:OD1	2.44	0.51
6:B:74:PHE:N	17:B:2007:HOH:O	2.43	0.51
6:Q:841:ASP:OD1	6:Q:842:GLU:N	2.44	0.50
5:P:1314:GLN:OE1	5:P:1318:SER:OG	2.29	0.50
7:C:117:ASP:OD1	7:C:119:ASN:ND2	2.44	0.50
1:L:34:CYS:CB	1:L:51:CYS:SG	2.99	0.50
6:B:252:TYR:OH	6:B:305:ARG:NH1	2.44	0.50
12:I:91:ASN:OD1	12:I:92:GLU:N	2.45	0.50
14:K:55:SER:OG	14:K:57:ASP:OD1	2.28	0.49
5:P:1541:ILE:O	9:T:147:HIS:NE2	2.45	0.49
6:Q:252:TYR:OH	6:Q:305:ARG:NH1	2.45	0.49
6:Q:307:GLU:OE2	6:Q:311:ARG:NH1	2.46	0.49
7:C:284:GLU:O	7:C:288:LYS:NZ	2.46	0.49
1:L:45:ALA:O	1:L:47:ARG:N	2.46	0.48
5:A:1530:TRP:O	9:E:14:ARG:NH2	2.46	0.48
6:B:210:ARG:NH2	6:B:625:GLU:OE2	2.46	0.48
5:P:1090:ASP:OD2	5:P:1093:SER:OG	2.32	0.48
6:B:472:SER:OG	6:B:474:SER:O	2.31	0.48
5:P:412:SER:OG	5:P:413:LEU:N	2.46	0.48
6:Q:1047:ARG:NH2	6:Q:1051:PRO:O	2.46	0.48
6:B:933:THR:N	17:B:2050:HOH:O	2.46	0.48
5:P:568:VAL:O	5:P:571:HIS:ND1	2.47	0.48
5:A:568:VAL:O	5:A:571:HIS:ND1	2.47	0.48
4:G:35:SER:OG	4:G:132:VAL:N	2.46	0.48
5:P:1320:GLN:OE1	5:P:1497:ILE:N	2.47	0.48
5:A:412:SER:OG	5:A:413:LEU:N	2.47	0.47
5:A:901:ASN:OD1	17:A:2057:HOH:O	2.20	0.47
5:P:644:ARG:NH2	10:U:116:ASP:OD1	2.47	0.47
6:Q:1090:ASP:OD2	6:Q:1091:ARG:NH1	2.47	0.47
5:A:1314:GLN:OE1	5:A:1318:SER:OG	2.32	0.47
6:B:265:ARG:NH2	6:B:339:GLN:OE1	2.48	0.47
5:A:487:ASP:OD2	14:K:95:HIS:NE2	2.48	0.47
7:R:319:ARG:NH2	14:Z:132:GLU:OE2	2.48	0.47
6:B:238:SER:OG	6:B:361:HIS:ND1	2.48	0.47
5:P:1530:TRP:O	9:T:14:ARG:NH2	2.49	0.46
6:B:1103:VAL:HG22	6:B:1176:VAL:HG22	1.97	0.46
4:G:26:ASN:ND2	4:G:131:ASP:OD2	2.48	0.46
5:P:1348:VAL:HA	5:P:1349:PRO:HD3	1.68	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:I:23:VAL:O	12:I:39:LYS:NZ	2.49	0.46
6:Q:1103:VAL:HG22	6:Q:1176:VAL:HG22	1.98	0.46
1:1:45:ALA:O	1:1:47:ARG:N	2.48	0.46
4:4:294:GLU:OE1	6:B:1120:ILE:HD13	2.16	0.46
5:P:762:LYS:N	17:P:2019:HOH:O	2.48	0.46
5:A:1248:ASP:OD1	5:A:1517:ARG:NH1	2.49	0.45
7:R:296:ASN:OD1	7:R:296:ASN:N	2.48	0.45
5:P:603:HIS:NE2	5:P:624:TYR:OH	2.50	0.45
6:Q:57:ASP:OD1	6:Q:57:ASP:N	2.49	0.45
5:A:1320:GLN:OE1	5:A:1497:ILE:N	2.50	0.45
5:P:273:ASP:OD1	5:P:273:ASP:N	2.50	0.45
4:V:91:ASP:OD1	4:V:104:LEU:N	2.49	0.45
5:P:257:ASN:OD1	5:P:258:GLU:N	2.50	0.45
7:C:53:ASN:OD1	7:C:271:ARG:NH2	2.49	0.45
6:B:1153:ILE:HA	6:B:1153:ILE:HD13	1.79	0.45
6:Q:201:LYS:NZ	6:Q:466:SER:O	2.50	0.44
12:I:74:ASN:N	12:I:74:ASN:OD1	2.50	0.44
6:Q:156:ARG:NE	6:Q:455:GLU:OE2	2.50	0.44
6:B:1158:ILE:HA	6:B:1167:PHE:O	2.17	0.44
9:T:161:LYS:NZ	9:T:193:GLY:O	2.50	0.44
6:Q:265:ARG:NH2	6:Q:339:GLN:OE1	2.51	0.44
6:Q:1158:ILE:HA	6:Q:1167:PHE:O	2.17	0.44
7:C:296:ASN:OD1	7:C:296:ASN:N	2.49	0.44
6:Q:637:TYR:N	17:Q:2003:HOH:O	2.50	0.44
7:C:319:ARG:NH2	14:K:132:GLU:OE2	2.50	0.44
2:2:59:ARG:NH2	12:X:12:ASP:OD2	2.51	0.44
5:A:257:ASN:OD1	5:A:258:GLU:N	2.51	0.44
6:B:431:ASP:OD1	6:B:452:ARG:NH1	2.51	0.44
3:3:63:ASP:OD1	3:3:65:SER:OG	2.36	0.44
6:Q:785:ASP:OD2	6:Q:957:ARG:NH2	2.51	0.44
5:P:1016:SER:OG	5:P:1197:SER:OG	2.36	0.43
12:X:23:VAL:O	12:X:39:LYS:NZ	2.51	0.43
8:D:23:HIS:CD2	10:F:58:PHE:CE1	3.06	0.43
4:V:165:ASP:OD1	4:V:165:ASP:N	2.52	0.43
11:H:124:ARG:NH1	17:H:2009:HOH:O	2.51	0.43
6:B:623:ASP:O	6:B:648:ARG:NH1	2.51	0.43
5:P:1145:GLU:OE2	5:P:1167:ARG:NE	2.51	0.43
6:B:322:ASN:ND2	2:M:108:LEU:O	2.52	0.43
6:Q:238:SER:OG	6:Q:361:HIS:ND1	2.51	0.43
6:Q:736:ARG:NH1	6:Q:738:ASP:OD1	2.51	0.43
6:B:57:ASP:OD1	6:B:57:ASP:N	2.52	0.43
4:G:29:ASP:OD1	4:G:30:GLU:N	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:1298:ASP:OD1	5:A:1468:LYS:NZ	2.51	0.43
5:A:603:HIS:NE2	5:A:624:TYR:OH	2.51	0.43
6:B:1160:GLU:OE1	5:P:40:ASN:ND2	2.52	0.43
4:V:160:ASN:N	4:V:160:ASN:OD1	2.52	0.43
5:P:40:ASN:OD1	5:P:40:ASN:N	2.50	0.42
5:P:512:THR:N	5:P:515:ASN:OD1	2.52	0.42
5:P:615:ARG:NH2	6:Q:928:SER:O	2.52	0.42
5:A:1268:ASP:OD1	12:I:61:ARG:NH2	2.52	0.42
9:T:114:ASN:N	9:T:114:ASN:OD1	2.52	0.42
7:R:53:ASN:OD1	7:R:271:ARG:NH2	2.52	0.42
4:G:160:ASN:N	4:G:160:ASN:OD1	2.52	0.42
4:G:165:ASP:OD1	4:G:165:ASP:N	2.52	0.42
11:W:105:GLU:OE2	11:W:115:TYR:OH	2.37	0.42
6:B:1090:ASP:OD2	6:B:1091:ARG:NH1	2.53	0.42
6:Q:200:GLU:OE2	6:Q:736:ARG:NH2	2.52	0.42
5:P:681:THR:O	5:P:729:LYS:NZ	2.52	0.42
5:P:574:ASN:OD1	5:P:574:ASN:N	2.53	0.42
6:Q:1160:GLU:HG2	6:Q:1166:LYS:HG2	2.02	0.42
4:G:91:ASP:OD1	4:G:104:LEU:N	2.53	0.42
5:P:743:ASP:N	5:P:743:ASP:OD1	2.52	0.42
4:V:15:ARG:O	4:V:18:LYS:NZ	2.53	0.41
5:A:1016:SER:OG	5:A:1197:SER:OG	2.38	0.41
5:P:631:ASP:OD1	5:P:631:ASP:N	2.51	0.41
9:E:161:LYS:NZ	9:E:193:GLY:O	2.53	0.41
5:P:1074:TYR:OH	5:P:1159:ASP:O	2.38	0.41
11:H:105:GLU:OE2	11:H:115:TYR:OH	2.38	0.41
6:B:200:GLU:OE2	6:B:736:ARG:NH2	2.54	0.41
11:W:98:TYR:OH	11:W:139:ASN:ND2	2.53	0.41
14:Z:57:ASP:OD1	14:Z:57:ASP:N	2.53	0.41
6:B:427:GLN:OE1	6:B:452:ARG:NH1	2.54	0.41
3:N:63:ASP:OD1	3:N:65:SER:OG	2.39	0.41
5:P:1348:VAL:HG11	6:Q:270:LEU:CD1	2.51	0.41
5:A:512:THR:N	5:A:515:ASN:OD1	2.54	0.41
6:B:230:SER:OG	6:B:252:TYR:O	2.39	0.41
5:P:1235:THR:O	5:P:1544:ASN:ND2	2.54	0.41
5:A:754:LYS:N	5:A:782:ASP:OD2	2.54	0.41
7:R:128:ASP:OD1	7:R:128:ASP:N	2.54	0.41
6:Q:1153:ILE:HA	6:Q:1153:ILE:HD13	1.72	0.41
6:B:736:ARG:NH1	6:B:738:ASP:OD1	2.54	0.40
5:P:1482:LYS:NZ	6:Q:304:ASP:OD1	2.54	0.40
6:Q:515:THR:O	6:Q:518:ARG:N	2.54	0.40
5:P:392:THR:OG1	5:P:433:ASP:OD2	2.40	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:P:25:ARG:NE	5:P:80:GLU:OE2	2.54	0.40
7:C:128:ASP:OD1	7:C:128:ASP:N	2.54	0.40
5:A:631:ASP:N	5:A:631:ASP:OD1	2.55	0.40
6:B:683:ASN:OD1	3:N:154:ARG:NH2	2.54	0.40
6:B:515:THR:O	6:B:518:ARG:N	2.54	0.40
5:P:1533:GLU:OE2	9:T:14:ARG:NH2	2.54	0.40
5:A:433:ASP:OD2	4:O:277:LYS:NZ	2.53	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
12	I	41	GLN
5	P	1533	GLU
7	R	224	THR
8	S	99	LEU
12	X	41	GLN
5	A	412	SER
5	A	448	SER
5	A	1394	THR
5	A	1533	GLU

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Mol	Chain	Res	Type
6	B	817	ARG
6	B	1140	LYS
8	D	98	GLY
9	E	50	MET
12	I	5	GLY
5	P	412	SER
5	P	448	SER
5	P	1348	VAL
5	P	1394	THR
5	P	1606	SER
9	T	50	MET
12	X	5	GLY
1	1	46	VAL
2	2	85	LYS
5	A	450	LYS
6	B	78	PRO
4	G	99	ASP
12	I	21	ASN
1	L	46	VAL
2	M	85	LYS
5	P	450	LYS
8	S	98	GLY
4	V	99	ASP
12	X	21	ASN
1	1	43	THR
3	3	115	SER
6	B	834	LYS
4	G	100	THR
1	L	43	THR
2	M	36	THR
3	N	115	SER
5	P	564	PRO
5	P	1572	ARG
6	Q	834	LYS
6	Q	1140	LYS
2	2	36	THR
5	A	451	VAL
5	A	564	PRO
6	B	80	ASN
6	B	117	VAL
6	B	1062	GLY
6	B	1063	ARG

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Mol	Chain	Res	Type
7	C	32	ASN
5	P	451	VAL
6	Q	1062	GLY
6	Q	1063	ARG
7	R	32	ASN
3	3	70	LEU
5	A	1512	PRO
6	Q	9	GLY
6	B	9	GLY
3	N	70	LEU
3	N	39	PRO
6	Q	833	PRO
9	T	206	GLY
6	B	833	PRO
6	B	954	PHE

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

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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

All (492) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	38	LEU
1	1	55	ILE
1	1	66	GLN
2	2	17	ASP
2	2	18	GLN
2	2	31	ARG
2	2	65	TYR
2	2	77	VAL
2	2	84	GLU
2	2	98	SER
2	2	109	ARG
3	3	51	GLN
3	3	81	THR
3	3	124	THR

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Mol	Chain	Res	Type
3	3	135	LYS
3	3	153	VAL
3	3	167	LYS
3	3	178	GLU
4	4	269	SER
5	A	10	GLU
5	A	40	ASN
5	A	83	VAL
5	A	117	ARG
5	A	136	LEU
5	A	174	SER
5	A	186	SER
5	A	202	THR
5	A	230	ARG
5	A	257	ASN
5	A	271	ARG
5	A	272	GLN
5	A	273	ASP
5	A	312	SER
5	A	315	ILE
5	A	346	SER
5	A	373	LEU
5	A	379	GLU
5	A	393	SER
5	A	413	LEU
5	A	446	ARG
5	A	447	THR
5	A	451	VAL
5	A	503	VAL
5	A	555	LYS
5	A	611	GLU
5	A	627	ASP
5	A	655	SER
5	A	656	GLN
5	A	661	THR
5	A	666	VAL
5	A	670	ILE
5	A	684	ASP
5	A	708	THR
5	A	709	ARG
5	A	739	VAL
5	A	747	ILE

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Mol	Chain	Res	Type
5	A	758	GLU
5	A	783	LYS
5	A	957	VAL
5	A	966	LEU
5	A	988	SER
5	A	1013	THR
5	A	1026	GLN
5	A	1033	SER
5	A	1071	ASP
5	A	1085	LEU
5	A	1098	SER
5	A	1118	VAL
5	A	1123	VAL
5	A	1131	LYS
5	A	1159	ASP
5	A	1162	ASN
5	A	1204	THR
5	A	1215	VAL
5	A	1226	VAL
5	A	1273	THR
5	A	1275	THR
5	A	1276	THR
5	A	1304	GLU
5	A	1310	LYS
5	A	1314	GLN
5	A	1320	GLN
5	A	1364	ARG
5	A	1392	ILE
5	A	1441	LYS
5	A	1455	ARG
5	A	1509	HIS
5	A	1531	ASP
5	A	1533	GLU
5	A	1536	ILE
5	A	1571	SER
5	A	1601	GLN
5	A	1604	GLU
5	A	1605	THR
5	A	1607	THR
5	A	1609	SER
5	A	1611	MET
5	A	1632	GLU

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Mol	Chain	Res	Type
5	A	1633	GLN
5	A	1635	ASP
5	A	1645	LYS
6	B	13	THR
6	B	17	ARG
6	B	22	GLU
6	B	53	THR
6	B	57	ASP
6	B	65	VAL
6	B	79	LEU
6	B	81	SER
6	B	87	ASN
6	B	117	VAL
6	B	150	GLU
6	B	187	SER
6	B	202	LEU
6	B	221	SER
6	B	225	ARG
6	B	228	SER
6	B	231	HIS
6	B	239	VAL
6	B	300	SER
6	B	305	ARG
6	B	306	LEU
6	B	311	ARG
6	B	315	LYS
6	B	379	ARG
6	B	459	SER
6	B	486	VAL
6	B	537	SER
6	B	583	LEU
6	B	622	ILE
6	B	658	LEU
6	B	720	GLN
6	B	724	GLN
6	B	725	THR
6	B	731	VAL
6	B	753	LYS
6	B	782	ASP
6	B	811	LEU
6	B	813	LEU
6	B	819	ASP

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Mol	Chain	Res	Type
6	B	822	THR
6	B	824	HIS
6	B	829	ASN
6	B	833	PRO
6	B	835	GLU
6	B	839	LYS
6	B	858	ILE
6	B	871	ILE
6	B	883	GLU
6	B	894	LYS
6	B	897	GLU
6	B	977	ILE
6	B	998	GLU
6	B	1026	ILE
6	B	1033	TYR
6	B	1037	ARG
6	B	1038	HIS
6	B	1042	ASP
6	B	1047	ARG
6	B	1060	VAL
6	B	1075	GLU
6	B	1091	ARG
6	B	1103	VAL
6	B	1125	THR
6	B	1136	GLU
6	B	1141	LEU
6	B	1163	GLN
6	B	1165	ASN
6	B	1174	THR
7	C	38	LYS
7	C	43	ASN
7	C	50	ARG
7	C	61	THR
7	C	77	SER
7	C	91	VAL
7	C	97	LEU
7	C	118	SER
7	C	142	ARG
7	C	181	ASP
7	C	224	THR
7	C	228	ARG
7	C	243	SER

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Mol	Chain	Res	Type
7	C	245	ARG
7	C	277	ARG
7	C	279	VAL
8	D	15	THR
8	D	29	GLN
8	D	38	GLN
8	D	46	GLU
8	D	80	THR
8	D	99	LEU
9	E	31	THR
9	E	33	GLU
9	E	41	ASP
9	E	74	ASP
9	E	77	SER
9	E	90	VAL
9	E	92	THR
9	E	93	MET
9	E	107	THR
9	E	131	THR
9	E	136	ASN
9	E	142	VAL
9	E	162	ARG
9	E	177	ARG
10	F	59	GLN
10	F	87	LYS
10	F	99	LEU
10	F	109	VAL
4	G	18	LYS
4	G	24	VAL
4	G	35	SER
4	G	39	VAL
4	G	139	ILE
4	G	147	LEU
4	G	167	THR
4	G	169	VAL
4	G	223	GLU
4	G	230	ARG
4	G	239	THR
4	G	243	VAL
11	H	3	ASN
11	H	39	THR
11	H	108	SER

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Mol	Chain	Res	Type
11	H	112	ILE
12	I	2	SER
12	I	15	ASP
12	I	45	LEU
12	I	70	SER
12	I	74	ASN
12	I	81	THR
12	I	117	CYS
13	J	3	VAL
13	J	9	SER
13	J	10	CYS
13	J	14	VAL
13	J	27	GLU
13	J	45	CYS
13	J	48	ARG
14	K	45	GLU
14	K	51	THR
14	K	68	GLU
14	K	99	ASN
14	K	118	GLN
14	K	123	ASP
14	K	133	SER
1	L	38	LEU
1	L	55	ILE
1	L	66	GLN
2	M	17	ASP
2	M	18	GLN
2	M	31	ARG
2	M	44	LYS
2	M	48	LYS
2	M	65	TYR
2	M	77	VAL
2	M	84	GLU
2	M	98	SER
2	M	109	ARG
3	N	51	GLN
3	N	124	THR
3	N	135	LYS
3	N	153	VAL
3	N	167	LYS
3	N	178	GLU
4	O	269	SER

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Mol	Chain	Res	Type
5	P	10	GLU
5	P	61	LEU
5	P	117	ARG
5	P	136	LEU
5	P	174	SER
5	P	175	SER
5	P	186	SER
5	P	199	ASP
5	P	202	THR
5	P	257	ASN
5	P	271	ARG
5	P	272	GLN
5	P	312	SER
5	P	315	ILE
5	P	346	SER
5	P	373	LEU
5	P	379	GLU
5	P	393	SER
5	P	413	LEU
5	P	416	ARG
5	P	446	ARG
5	P	447	THR
5	P	451	VAL
5	P	503	VAL
5	P	555	LYS
5	P	611	GLU
5	P	627	ASP
5	P	655	SER
5	P	656	GLN
5	P	666	VAL
5	P	684	ASP
5	P	708	THR
5	P	709	ARG
5	P	739	VAL
5	P	747	ILE
5	P	758	GLU
5	P	783	LYS
5	P	878	ARG
5	P	957	VAL
5	P	1013	THR
5	P	1016	SER
5	P	1026	GLN

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Mol	Chain	Res	Type
5	P	1033	SER
5	P	1071	ASP
5	P	1085	LEU
5	P	1098	SER
5	P	1118	VAL
5	P	1123	VAL
5	P	1131	LYS
5	P	1159	ASP
5	P	1162	ASN
5	P	1204	THR
5	P	1215	VAL
5	P	1226	VAL
5	P	1273	THR
5	P	1275	THR
5	P	1276	THR
5	P	1304	GLU
5	P	1310	LYS
5	P	1314	GLN
5	P	1320	GLN
5	P	1350	ARG
5	P	1364	ARG
5	P	1392	ILE
5	P	1441	LYS
5	P	1481	GLU
5	P	1486	VAL
5	P	1505	ASP
5	P	1509	HIS
5	P	1518	VAL
5	P	1531	ASP
5	P	1536	ILE
5	P	1587	ASP
5	P	1601	GLN
5	P	1604	GLU
5	P	1605	THR
5	P	1607	THR
5	P	1609	SER
5	P	1611	MET
5	P	1632	GLU
5	P	1633	GLN
5	P	1635	ASP
6	Q	13	THR
6	Q	17	ARG

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Mol	Chain	Res	Type
6	Q	22	GLU
6	Q	53	THR
6	Q	57	ASP
6	Q	65	VAL
6	Q	117	VAL
6	Q	150	GLU
6	Q	187	SER
6	Q	202	LEU
6	Q	221	SER
6	Q	225	ARG
6	Q	228	SER
6	Q	231	HIS
6	Q	236	ILE
6	Q	239	VAL
6	Q	300	SER
6	Q	305	ARG
6	Q	306	LEU
6	Q	311	ARG
6	Q	315	LYS
6	Q	379	ARG
6	Q	429	ARG
6	Q	486	VAL
6	Q	537	SER
6	Q	583	LEU
6	Q	622	ILE
6	Q	658	LEU
6	Q	720	GLN
6	Q	724	GLN
6	Q	725	THR
6	Q	753	LYS
6	Q	782	ASP
6	Q	811	LEU
6	Q	813	LEU
6	Q	822	THR
6	Q	824	HIS
6	Q	829	ASN
6	Q	833	PRO
6	Q	835	GLU
6	Q	839	LYS
6	Q	858	ILE
6	Q	871	ILE
6	Q	883	GLU

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Mol	Chain	Res	Type
6	Q	897	GLU
6	Q	977	ILE
6	Q	998	GLU
6	Q	1026	ILE
6	Q	1033	TYR
6	Q	1037	ARG
6	Q	1038	HIS
6	Q	1042	ASP
6	Q	1047	ARG
6	Q	1060	VAL
6	Q	1075	GLU
6	Q	1091	ARG
6	Q	1103	VAL
6	Q	1125	THR
6	Q	1136	GLU
6	Q	1141	LEU
6	Q	1163	GLN
6	Q	1165	ASN
6	Q	1174	THR
7	R	38	LYS
7	R	43	ASN
7	R	50	ARG
7	R	61	THR
7	R	77	SER
7	R	91	VAL
7	R	97	LEU
7	R	118	SER
7	R	128	ASP
7	R	142	ARG
7	R	181	ASP
7	R	224	THR
7	R	228	ARG
7	R	243	SER
7	R	245	ARG
7	R	277	ARG
7	R	279	VAL
8	S	15	THR
8	S	29	GLN
8	S	38	GLN
8	S	46	GLU
8	S	80	THR
8	S	99	LEU

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Mol	Chain	Res	Type
9	T	4	GLU
9	T	31	THR
9	T	33	GLU
9	T	41	ASP
9	T	74	ASP
9	T	77	SER
9	T	90	VAL
9	T	92	THR
9	T	93	MET
9	T	107	THR
9	T	131	THR
9	T	136	ASN
9	T	142	VAL
9	T	162	ARG
9	T	167	ARG
9	T	177	ARG
10	U	59	GLN
10	U	87	LYS
10	U	99	LEU
10	U	109	VAL
4	V	18	LYS
4	V	24	VAL
4	V	35	SER
4	V	39	VAL
4	V	139	ILE
4	V	147	LEU
4	V	167	THR
4	V	169	VAL
4	V	171	ASN
4	V	176	ASP
4	V	223	GLU
4	V	230	ARG
4	V	239	THR
4	V	243	VAL
11	W	3	ASN
11	W	39	THR
11	W	108	SER
11	W	112	ILE
12	X	2	SER
12	X	15	ASP
12	X	45	LEU
12	X	70	SER

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Mol	Chain	Res	Type
12	X	81	THR
12	X	117	CYS
13	Y	3	VAL
13	Y	9	SER
13	Y	10	CYS
13	Y	14	VAL
13	Y	27	GLU
13	Y	45	CYS
13	Y	48	ARG
14	Z	45	GLU
14	Z	51	THR
14	Z	68	GLU
14	Z	99	ASN
14	Z	118	GLN
14	Z	123	ASP
14	Z	133	SER

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.