



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:32 AM GMT

PDB ID : 3AOI  
Title : RNA polymerase-Gfh1 complex (Crystal type 2)  
Authors : Tagami, S.; Sekine, S.; Kumarevel, T.; Yamamoto, M.; Yokoyama, S.; RIKEN  
Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2010-09-30  
Resolution : 4.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

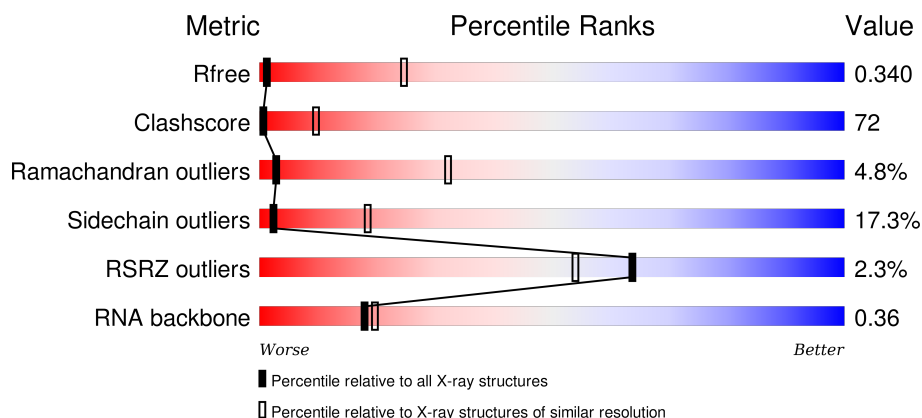
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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))
$R_{free}$	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)
RNA backbone	2183	1087 (5.60-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div></div> <div>19%44%8%29%</div> </div>
1	B	315	<div> <div></div> <div>21%42%8%29%</div> </div>
1	F	315	<div> <div>%</div> <div>20%43%9%29%</div> </div>
1	G	315	<div> <div></div> <div>22%39%10%29%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	315	
1	L	315	
2	C	1119	
2	H	1119	
2	M	1119	
3	D	1524	
3	I	1524	
3	N	1524	
4	E	99	
4	J	99	
4	O	99	
5	P	27	
5	R	27	
5	T	27	
6	Q	32	
6	S	32	
6	U	32	
7	X	156	
7	Y	156	
7	Z	156	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 73646 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 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	F	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	G	224	Total	C	N	O	S	0	0	0
			1764	1126	307	329	2			
1	K	225	Total	C	N	O	S	0	0	0
			1769	1129	308	330	2			
1	L	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1083	Total	C	N	O	S	0	0	0
			8550	5413	1525	1588	24			
2	H	1080	Total	C	N	O	S	0	0	0
			8524	5395	1521	1584	24			
2	M	1084	Total	C	N	O	S	0	0	0
			8555	5413	1528	1590	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1316	Total	C	N	O	S	0	0	0
			10384	6574	1840	1941	29			
3	I	1262	Total	C	N	O	S	0	0	0
			9965	6314	1765	1858	28			
3	N	1327	Total	C	N	O	S	0	0	0
			10475	6634	1852	1961	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			
4	J	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			
4	O	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

- Molecule 5 is a DNA chain called DNA (5'-D(\*GP\*GP\*TP\*CP\*TP\*GP\*TP\*AP\*TP\*CP\*AP\*CP\*GP\*AP\*GP\*CP\*CP\*A\*CP\*CP\*GP\*CP\*CP\*GP\*CP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	7	Total	C	N	O	P	0	0	0
			136	65	25	40	6			
5	R	6	Total	C	N	O	P	0	0	0
			119	57	24	33	5			
5	T	5	Total	C	N	O	P	0	0	0
			98	47	19	28	4			

- Molecule 6 is a RNA chain called RNA (5'-R(\*CP\*CP\*CP\*GP\*GP\*AP\*AP\*GP\*AP\*UP\*CP\*AP\*UP\*CP\*UP\*UP\*CP\*CP\*GP\*GP\*GP\*GP\*GP\*AP\*U\*GP\*CP\*GP\*GP\*CP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	Q	7	Total	C	N	O	P	0	0	0
			152	68	31	47	6			
6	S	8	Total	C	N	O	P	0	0	0
			172	77	33	55	7			
6	U	7	Total	C	N	O	P	0	0	0
			152	68	31	47	6			

- Molecule 7 is a protein called Anti-cleavage anti-GreA transcription factor Gfh1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	X	154	Total	C	N	O	S	0	0	0
			1189	730	212	243	4			
7	Y	152	Total	C	N	O	S	0	0	0
			1169	719	207	239	4			
7	Z	152	Total	C	N	O	S	0	0	0
			1169	719	207	239	4			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	1	Total 1	Zn 1	0	0
8	D	1	Total 1	Zn 1	0	0
8	N	1	Total 1	Zn 1	0	0

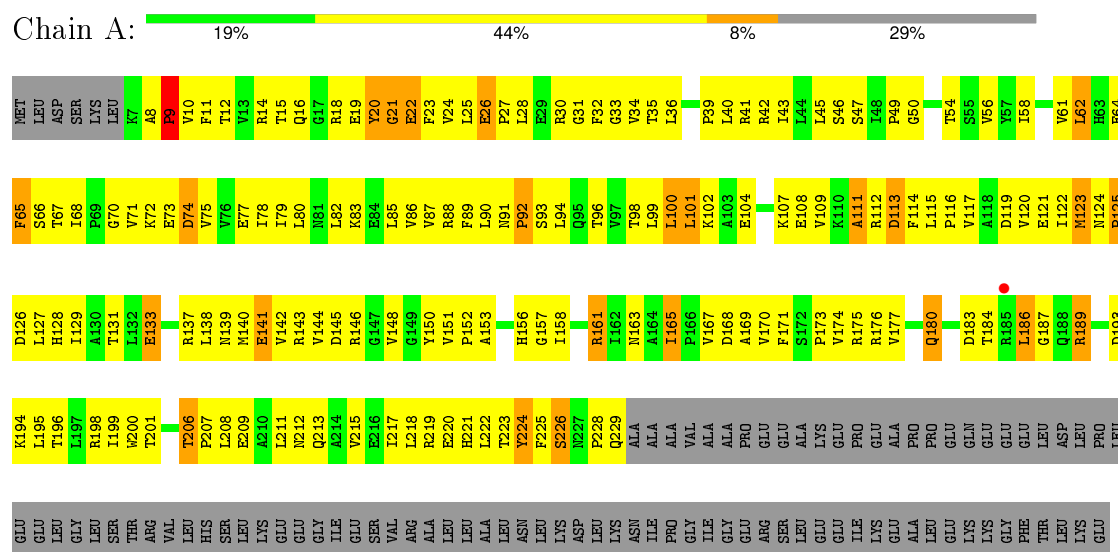
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total 1	Mg 1	0	0
9	S	1	Total 1	Mg 1	0	0
9	N	1	Total 1	Mg 1	0	0

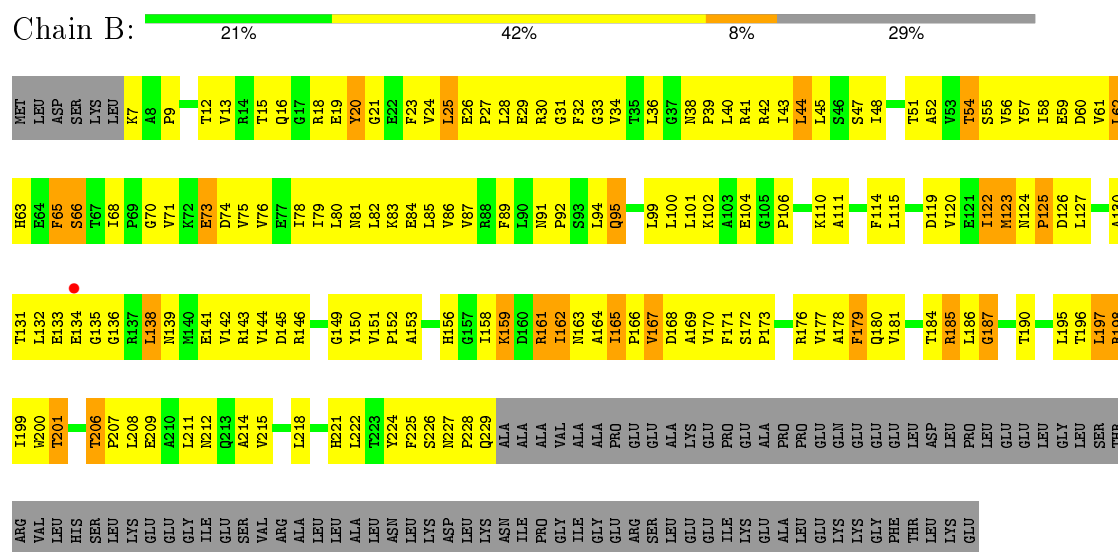
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

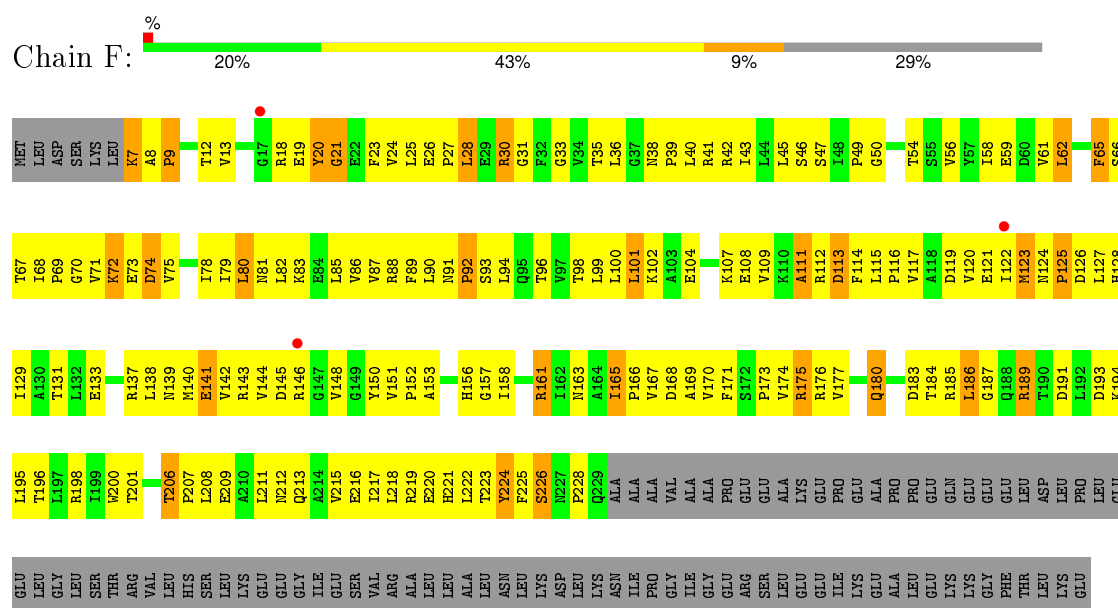
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



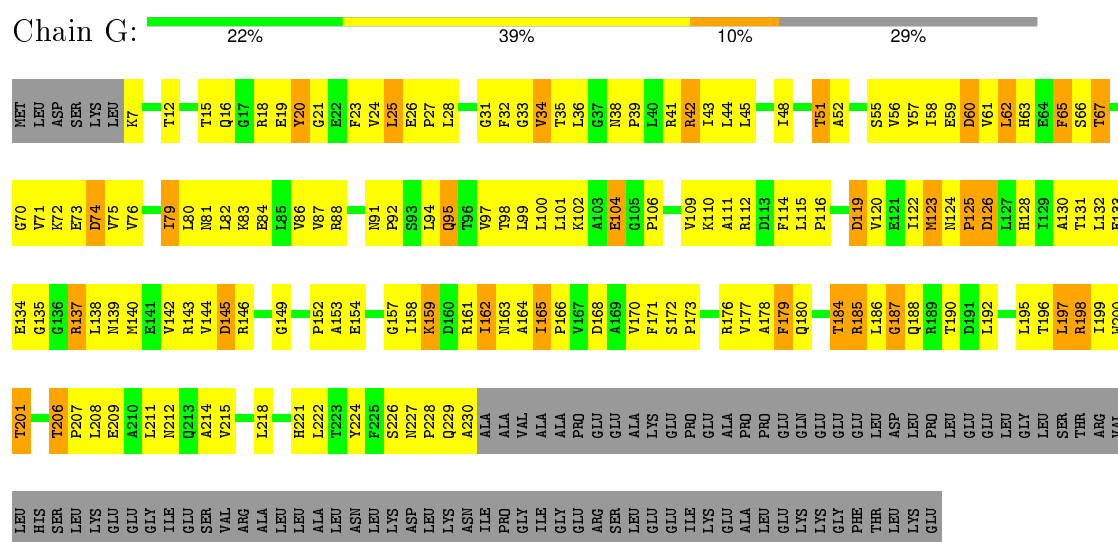
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



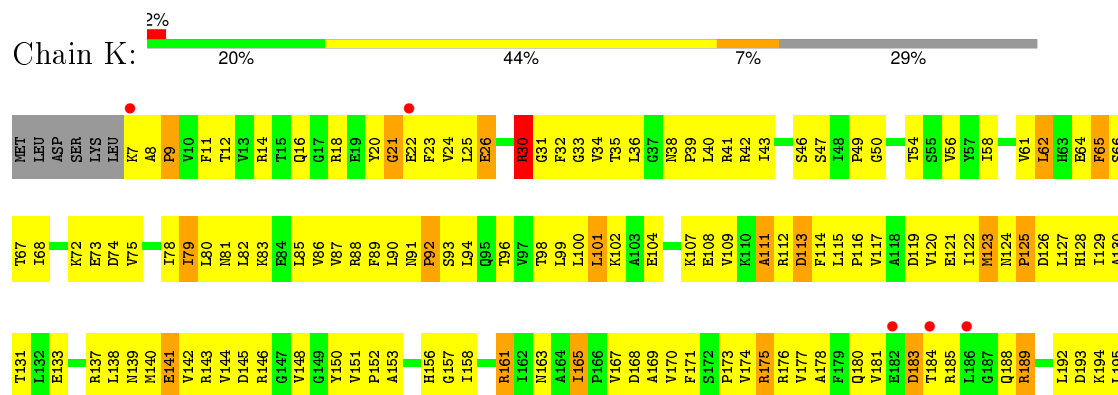
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



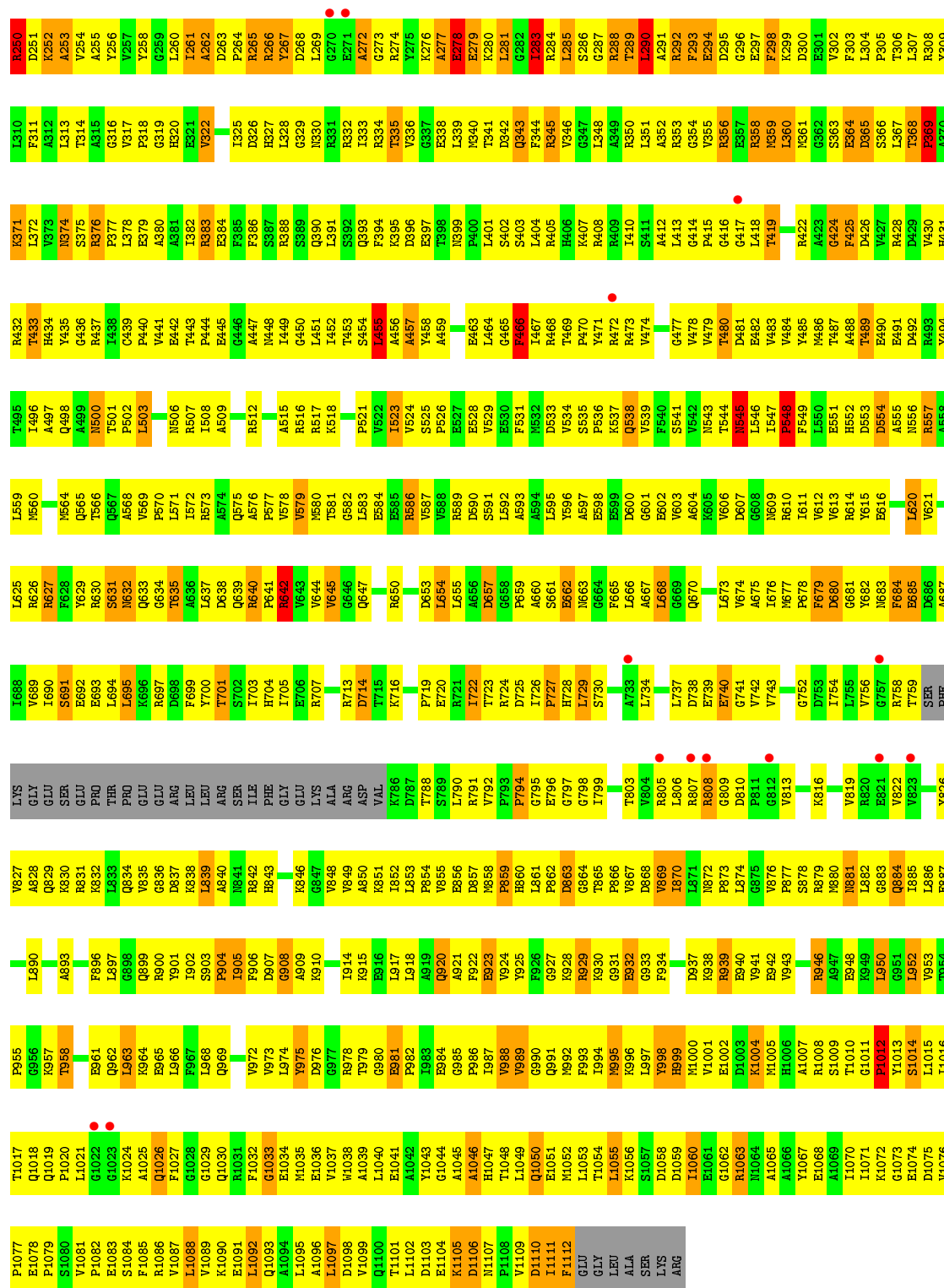
• Molecule 1: DNA-directed RNA polymerase subunit alpha











G1028	L966	I902	L839	THR	E692	S631	Q565	A497	H434	R369	R308	P247	K185	D124	G63
G1029	F967	S903	A840	PRO	E693	N632	T566	Q498	Y435	A370	T309	P248	V186	G125	L64
G1030	L968	P904	N841	GLU	L694	Q633	Q567	A499	G436	K371	T310	K249	K187	G126	V65
R1031	Q969	I905	N842	GLU	L695	Q634	A568	N500	R437	L372	F311	R260	K188	F127	L66
F1032	F1032	F906	N843	ARG	K696	T635	V569	T501	I438	V373	A312	D251	R189	I128	D67
G1033	V972	D907	L843	LEU	K697	A636	P570	P502	C439	N374	L313	K252	K190	I129	F68
E1034	R973	G908	K846	LEU	D698	L637	L571	L503	R440	S375	T314	A253	F191	N130	L69
M1035	L974	A909	G847	ARG	F699	D638	I572		V441	K376	K315	V284	P192	G131	E70
E1036	Y975	K910	N848	SER	K700	Q639	R573	N506	A442	P377	G316	A255	L193	A132	Y71
M1037	R976	E911	N849	ILE	T701	R640	A574	R507	T443	K378	T317	V256	P194	D133	R72
M1038	G977		A850	PRO	S702	P641	Q575	L508	P444	E379	P318	V257	L195	R134	L73
A1039	R978	I914	K851	GLY	H703	N642	A576	A509		A380	G319	Y258	L196	V135	G74
L1040	T979	H704	N852	GLU	H704	N643	P577		A447	A381	G320	G259	L197	I136	E75
E1041	G980	K915	L853	LYS	I705	V644	V578	R512	N448	I382	E321	L260	R198	V137	P76
A1042	P981	E916	N854		E706	V645	V579	V513	A449	E383	V322	T261	V199	G138	F77
Y1043	R982	L917	N855		E707	G646	M580	V514	G450	E384	V323	A262	V199	Q139	F78
G1044	E983	R918	D856		Y708	Q647	T581	A515	L451		R324	P264	G201	I140	P79
A1045	E984	Q920	D857			N648	G582	R516	I452	R388	L325	G263	Y202	H141	Q80
A1046	G985	A921	N858		D714	N649	L583	R517	T453		R326	R265	D203	R142	D81
H1047	P986	F922	N859			N650	E584	K518	S454	L391	R327	R266	Q204	S143	E82
T1048	R987	E923	H860		P719	D653	R586	P521	A456	S392	L328	Y267	Q205	P144	C83
L1049	V988	R924	L861		E720	L654	V587	V522	A457	F394	G329	D268	T206	G145	R84
Q1050	P989	Y925	P862		R721	L655	V588	I523	A458	K395	R331	L269	G208	V146	E85
M1051	G990	F926	D863		I722	L656	V589	V524	A459	I396	R332	G270	A208	Y147	K86
E1052	Q991	G927	G864		R723	D657	D590	S525	R460		T333	E271	R209	D87	D87
M1053	N992	K928	T865		R724	G658	S591		V461	E397	T334	A272	E210	P150	L88
F1054	F993	R929	P866		I725	P659	S592	E528	L462	N398	R334	G273	L211	D151	T89
T1055	L994	K930	N867		I726	N659	L592		T469	N399	T335	R274	G212	P152	Y90
K1056	G995	G931	D868		R727	A660	A593		E463	P400	V336	Y275	A213	A153	Q91
S1057	K996	E932	N869		H728	S661		F531	L464	L401	G337	K276	Y214	R154	A92
D1058	L997	G933	L870		I729	N662	A597		G465	S402	E338	A277	G215	P155	P93
I1059	Y998	F934	L871		S730	N663		D533	F466	S403	L339	E278	E216	G156	L94
E1060	E999	D937	N872			G664	D600	V534	L467	L404	R340	E279	L217	R157	A96
E1061	M1000	L837	P873		L734	F665	E601	S535	R468	H405	T342	K280	V218	Y158	R97
G1062	V1001	K938	L874		R735	L666	G802	P536	T469	E406	D342	L281	Q219	L159	L98
R1063	E1002	R939	G875		D736	A667	V603	K537	P470	R407	D343	G282	G220	A160	Q99
M1064	D1003	E940	V876		L737	L668	A604	Q538	Y471	R408	F344	I283	L221	S161	L98
A1065	K1004	V941	P877		D738	G669	V605	V539	R472	E409	R345	R284	M222	I182	L00
A1066	M1005	E942	S878		E739	Q670	V606	F540	G475	I410	V346	L285	M223	I163	L101
Y1067	H1006	V943	N879		E740	N671	D607	S541	V474	S411	G347		E224	P164	H102
E1068	A1007		N880		V742	V672	G808	N543	G476	L413	L348	T289	S225	L165	K103
A1069	R1008	R946	N881		V743	L673	N809	N544	G477	G414	R350	L290	V226	P166	D104
I1070	S1009	E947	L882			V674	R610	T544	V478	P415	L351	A291	A228	K167	L107
L1071	T1010	E948	G883		V749	A675	I611	N545	V479	L418	A352	R292	M229	G168	L108
K1072	G1011	K949	Q884			L676	V612	L546		T419	R353	F293	R230	P170	K109
E1073	P1012	L950	N885		V754	N677	E616	P548	D481	T419	R356	D295	E232	W171	D111
E1074	Y1013	G951	L886		L755	P678	V613	F549	E482		R357	G296	L235	D173	V113
D1075	S1014	L952	E887		V756	F679	N617		V483	R422	R358	E297	I236	L174	F114
V1076	T954	V953	T888		V757	D680	G681		V484	A423	R359	F298	I236	E175	L115
P1077	P1017	P955	N889		V758	N682	V682		V485	G424	R359	F298	I236	V176	L115
E1078	Q1018	G956	L890		T759	N683	V682		V486	P425	L360	R299	I237	V176	L115
	Q1019	K957			SER	F684	E622		P487	D426	R361	D300	L238	E177	G116
V1081	P1020	T958	A893		PHE	E685			A488	V427	G362	E301	F239	P178	H117
E1082	L1021		F896		LYS	N686	L625		T489	D428	S363	V302	T240	M179	I118
S1083	G1022		L897		GLY	A687	R626		E490	M299	E364	F303	L241	G180	P119
E1084	G1023		N898		GLU	L688	R627		E491	V430	D365	L304	L242	V181	L120
F1085	K1024	Q962	G886		SER	L689	F628		D492	R431	S366	L304	R243	V182	M121
R1086	A1025	K964	Q899		GLU	N690	V629		D492	R432	L367	T306	P244	S183	T122
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	F1027	E965	Y901		PRO	S691	R630								







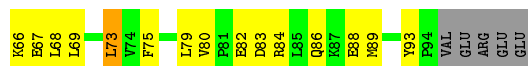
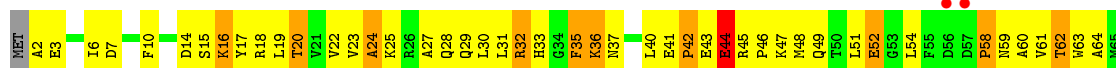




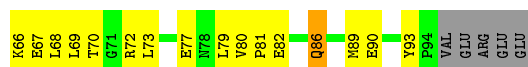
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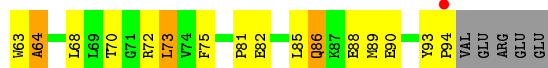
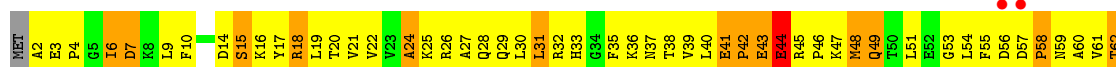
- Molecule 4: DNA-directed RNA polymerase subunit omega



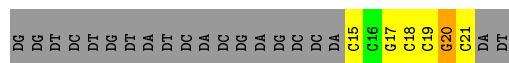
- Molecule 4: DNA-directed RNA polymerase subunit omega



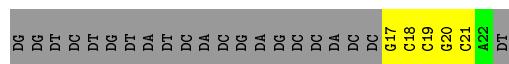
- Molecule 4: DNA-directed RNA polymerase subunit omega



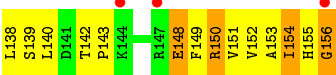
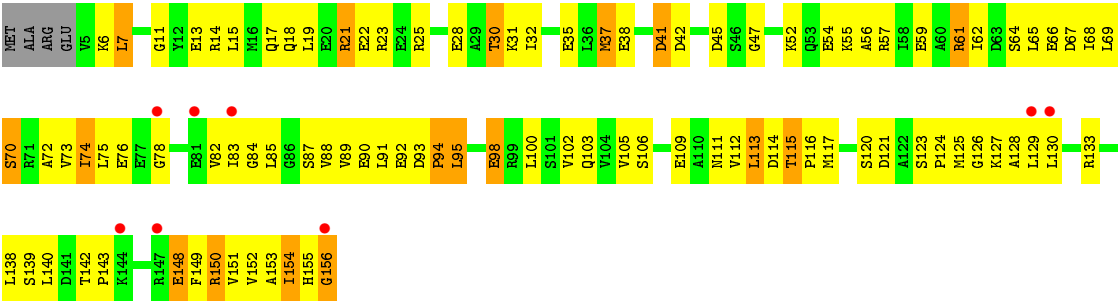
- Molecule 5: DNA (5'-D(\*GP\*GP\*TP\*CP\*TP\*GP\*TP\*AP\*TP\*CP\*AP\*CP\*GP\*AP\*GP\*CP\*CP\*A\*CP\*CP\*GP\*CP\*CP\*GP\*CP\*AP\*T)-3')



- Molecule 5: DNA (5'-D(\*GP\*GP\*TP\*CP\*TP\*GP\*TP\*AP\*TP\*CP\*AP\*CP\*GP\*AP\*GP\*CP\*CP\*A\*CP\*CP\*GP\*CP\*CP\*GP\*CP\*AP\*T)-3')



- Chain Y: 



● Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.23Å 264.51Å 193.93Å 90.00° 116.68° 90.00°	Depositor
Resolution (Å)	47.57 – 4.30 47.57 – 4.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.57-4.30) 97.7 (47.57-4.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 4.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.317 , 0.338 0.320 , 0.340	Depositor DCC
$R_{free}$ test set	3392 reflections (3.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	128.7	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 107.1	EDS
Estimated twinning fraction	0.054 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 112834 reflections	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	73646	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.48	0/1791	0.76	0/2436
1	B	0.47	0/1791	0.71	1/2436 (0.0%)
1	F	0.48	0/1791	0.75	0/2436
1	G	0.47	0/1796	0.70	1/2443 (0.0%)
1	K	0.50	0/1801	0.76	0/2450
1	L	0.48	0/1791	0.70	1/2436 (0.0%)
2	C	0.49	0/8713	0.78	5/11785 (0.0%)
2	H	0.51	0/8686	0.78	3/11750 (0.0%)
2	M	0.51	0/8717	0.81	6/11792 (0.1%)
3	D	0.50	0/10559	0.77	5/14272 (0.0%)
3	I	0.50	0/10131	0.79	6/13685 (0.0%)
3	N	0.49	0/10653	0.79	8/14403 (0.1%)
4	E	0.47	0/768	0.72	1/1035 (0.1%)
4	J	0.47	0/768	0.73	1/1035 (0.1%)
4	O	0.49	0/768	0.77	1/1035 (0.1%)
5	P	0.89	0/151	1.70	3/230 (1.3%)
5	R	0.81	0/133	1.04	0/203
5	T	0.84	0/109	0.89	0/166
6	Q	1.05	0/170	1.04	0/265
6	S	1.02	0/192	0.92	0/299
6	U	0.94	0/170	0.97	2/265 (0.8%)
7	X	0.56	1/1198 (0.1%)	0.70	1/1608 (0.1%)
7	Y	0.64	1/1178 (0.1%)	0.66	0/1582
7	Z	0.65	1/1178 (0.1%)	0.68	1/1582 (0.1%)
All	All	0.51	3/75003 (0.0%)	0.78	46/101629 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	5
2	H	0	1
2	M	0	3
3	D	0	2
3	I	0	4
3	N	0	5
6	Q	0	1
6	S	0	1
All	All	0	22

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	156	GLY	C-OXT	16.27	1.54	1.23
7	Y	156	GLY	C-OXT	16.19	1.54	1.23
7	X	156	GLY	C-OXT	11.06	1.44	1.23

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	20	DG	N9-C1'-C2'	9.98	131.56	112.60
5	P	20	DG	O4'-C1'-C2'	8.43	112.64	105.90
3	I	1209	LEU	N-CA-C	-8.04	89.28	111.00
3	N	1209	LEU	N-CA-C	-7.97	89.49	111.00
3	N	142	LEU	CA-CB-CG	7.29	132.07	115.30

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	267	TYR	Sidechain
2	C	589	ARG	Sidechain
2	C	642	ARG	Sidechain
2	C	71	TYR	Sidechain
2	C	735	ARG	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	1759	0	1805	209	3
1	B	1759	0	1805	263	2
1	F	1759	0	1805	195	3
1	G	1764	0	1810	253	3
1	K	1769	0	1815	202	0
1	L	1759	0	1805	220	0
2	C	8550	0	8654	1412	1
2	H	8524	0	8626	1521	0
2	M	8555	0	8658	1519	1
3	D	10384	0	10615	1752	3
3	I	9965	0	10206	1707	1
3	N	10475	0	10699	1791	3
4	E	754	0	769	94	0
4	J	754	0	769	116	0
4	O	754	0	769	111	0
5	P	136	0	79	3	0
5	R	119	0	68	12	0
5	T	98	0	57	8	0
6	Q	152	0	78	10	0
6	S	172	0	88	12	0
6	U	152	0	79	12	0
7	X	1189	0	1205	141	0
7	Y	1169	0	1186	151	0
7	Z	1169	0	1186	146	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
8	N	1	0	0	0	0
9	D	1	0	0	0	0
9	N	1	0	0	0	0
9	S	1	0	0	0	0
All	All	73646	0	74636	10729	10

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 72.

The worst 5 of 10729 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:50:PHE:CD2	3:N:522:PRO:HD3	1.20	1.62
2:H:182:VAL:HG11	2:H:193:LEU:CD2	1.09	1.56
2:H:1090:LYS:HE3	3:I:90:MET:SD	1.45	1.55
2:H:182:VAL:CG1	2:H:193:LEU:HD21	1.13	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:783:ARG:NH1	7:Y:41:ASP:CB	1.67	1.53

The worst 5 of 10 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:CD1	1:F:59:GLU:OE1[2_455]	1.51	0.69
3:D:1182:GLU:OE2	1:G:112:ARG:NE[1_655]	1.61	0.59
1:B:162:ILE:CG1	3:N:976:GLN:NE2[1_655]	1.90	0.30
1:A:100:LEU:CD1	1:F:59:GLU:CD[2_455]	1.97	0.23
2:C:223:ASP:O	3:N:562:ALA:O[2_444]	2.02	0.18

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/315 (70%)	191 (86%)	22 (10%)	8 (4%)	4	40
1	B	221/315 (70%)	191 (86%)	27 (12%)	3 (1%)	14	59
1	F	221/315 (70%)	191 (86%)	20 (9%)	10 (4%)	3	34
1	G	222/315 (70%)	193 (87%)	26 (12%)	3 (1%)	14	59
1	K	223/315 (71%)	193 (86%)	21 (9%)	9 (4%)	4	37
1	L	221/315 (70%)	188 (85%)	28 (13%)	5 (2%)	8	50
2	C	1077/1119 (96%)	864 (80%)	150 (14%)	63 (6%)	2	28
2	H	1074/1119 (96%)	867 (81%)	145 (14%)	62 (6%)	2	28
2	M	1078/1119 (96%)	871 (81%)	149 (14%)	58 (5%)	2	30
3	D	1306/1524 (86%)	1062 (81%)	186 (14%)	58 (4%)	3	34
3	I	1252/1524 (82%)	1012 (81%)	177 (14%)	63 (5%)	3	31
3	N	1317/1524 (86%)	1052 (80%)	196 (15%)	69 (5%)	2	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	91/99 (92%)	67 (74%)	17 (19%)	7 (8%)	1	20
4	J	91/99 (92%)	70 (77%)	14 (15%)	7 (8%)	1	20
4	O	91/99 (92%)	68 (75%)	16 (18%)	7 (8%)	1	20
7	X	152/156 (97%)	132 (87%)	16 (10%)	4 (3%)	7	47
7	Y	150/156 (96%)	135 (90%)	12 (8%)	3 (2%)	9	53
7	Z	150/156 (96%)	131 (87%)	16 (11%)	3 (2%)	9	53
All	All	9158/10584 (86%)	7478 (82%)	1238 (14%)	442 (5%)	3	32

5 of 442 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	GLY
2	C	23	VAL
2	C	40	GLU
2	C	44	ILE
2	C	152	PRO

### 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	196/273 (72%)	164 (84%)	32 (16%)	3	21
1	B	196/273 (72%)	166 (85%)	30 (15%)	3	24
1	F	196/273 (72%)	167 (85%)	29 (15%)	4	26
1	G	196/273 (72%)	164 (84%)	32 (16%)	3	21
1	K	196/273 (72%)	164 (84%)	32 (16%)	3	21
1	L	196/273 (72%)	164 (84%)	32 (16%)	3	21
2	C	912/941 (97%)	737 (81%)	175 (19%)	2	14
2	H	909/941 (97%)	736 (81%)	173 (19%)	2	14
2	M	912/941 (97%)	746 (82%)	166 (18%)	2	16
3	D	1113/1279 (87%)	928 (83%)	185 (17%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	1068/1279 (84%)	878 (82%)	190 (18%)	2	17
3	N	1124/1279 (88%)	937 (83%)	187 (17%)	3	21
4	E	82/88 (93%)	72 (88%)	10 (12%)	6	33
4	J	82/88 (93%)	72 (88%)	10 (12%)	6	33
4	O	82/88 (93%)	67 (82%)	15 (18%)	2	16
7	X	130/131 (99%)	115 (88%)	15 (12%)	7	35
7	Y	128/131 (98%)	104 (81%)	24 (19%)	2	15
7	Z	128/131 (98%)	110 (86%)	18 (14%)	4	28
All	All	7846/8955 (88%)	6491 (83%)	1355 (17%)	2	18

5 of 1355 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	691	SER
3	I	778	LEU
3	N	1297	GLU
2	H	870	ILE
3	I	138	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 252 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	834	GLN
3	I	973	GLN
3	N	1465	ASN
2	H	969	GLN
3	I	463	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Q	6/32 (18%)	1 (16%)	0
6	S	7/32 (21%)	2 (28%)	0
6	U	6/32 (18%)	2 (33%)	0
All	All	19/96 (19%)	5 (26%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Q	11	C
6	S	13	G
6	S	16	G
6	U	11	C
6	U	12	G

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	223/315 (70%)	-0.14	1 (0%) 93 90	82, 143, 203, 231	0
1	B	223/315 (70%)	-0.22	1 (0%) 93 90	86, 150, 211, 231	0
1	F	223/315 (70%)	0.02	3 (1%) 79 71	88, 145, 202, 231	0
1	G	224/315 (71%)	-0.19	0 100 100	74, 150, 204, 231	0
1	K	225/315 (71%)	0.08	5 (2%) 65 56	77, 152, 205, 231	0
1	L	223/315 (70%)	-0.20	1 (0%) 93 90	71, 146, 208, 231	0
2	C	1083/1119 (96%)	-0.13	14 (1%) 79 71	46, 150, 225, 231	0
2	H	1080/1119 (96%)	-0.15	15 (1%) 78 69	32, 148, 226, 231	0
2	M	1084/1119 (96%)	-0.03	23 (2%) 67 57	51, 150, 227, 231	0
3	D	1316/1524 (86%)	-0.04	30 (2%) 64 54	91, 161, 249, 285	0
3	I	1262/1524 (82%)	0.09	54 (4%) 39 30	91, 160, 246, 285	0
3	N	1327/1524 (87%)	0.03	25 (1%) 70 61	91, 162, 250, 284	0
4	E	93/99 (93%)	0.11	2 (2%) 65 56	91, 182, 231, 231	0
4	J	93/99 (93%)	0.05	3 (3%) 51 40	98, 176, 231, 231	0
4	O	93/99 (93%)	-0.02	3 (3%) 51 40	90, 172, 231, 231	0
5	P	7/27 (25%)	0.52	0 100 100	199, 200, 200, 200	0
5	R	6/27 (22%)	1.01	0 100 100	200, 200, 200, 200	0
5	T	5/27 (18%)	0.79	0 100 100	199, 200, 200, 200	0
6	Q	7/32 (21%)	1.19	1 (14%) 4 4	195, 200, 200, 200	0
6	S	8/32 (25%)	2.35	6 (75%) 0 1	200, 200, 200, 200	0
6	U	7/32 (21%)	1.54	2 (28%) 1 2	194, 200, 200, 200	0
7	X	154/156 (98%)	0.15	7 (4%) 37 29	97, 175, 229, 231	0
7	Y	152/156 (97%)	0.16	8 (5%) 30 23	88, 174, 228, 231	0
7	Z	152/156 (97%)	0.24	7 (4%) 36 28	95, 172, 228, 231	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	9270/10761 (86%)	-0.02	211 (2%) 64 54	32, 156, 231, 285	0

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	56	ASP	6.3
3	I	191	LEU	5.7
3	I	1301	LYS	5.7
3	I	1292	VAL	5.6
2	C	270	GLY	5.2

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	ZN	N	2001	1/1	0.90	0.07	-1.54	115,115,115,115	0
8	ZN	I	2003	1/1	0.99	0.09	-1.65	115,115,115,115	0
8	ZN	D	2002	1/1	0.96	0.03	-1.81	115,115,115,115	0
9	MG	S	2005	1/1	0.97	0.85	-	115,115,115,115	0
9	MG	N	2006	1/1	0.96	0.44	-	115,115,115,115	0
9	MG	D	2004	1/1	0.99	0.12	-	115,115,115,115	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.