



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 04:05 PM UTC

PDB ID : 2A6E / pdb_00002a6e
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

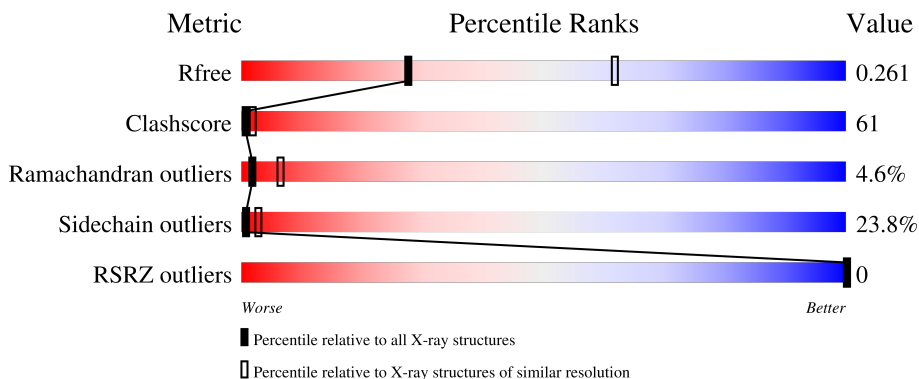
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	

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Mol	Chain	Length	Quality of chain
2	M	1119	 24% 56% 19% .
3	D	1524	 21% 49% 19% . 9%
3	N	1524	 22% 50% 18% . 9%
4	E	99	 22% 53% 17% . .
4	O	99	 27% 42% 24% . .
5	F	423	 18% 46% 16% . 18%
5	P	423	 22% 49% 10% . 18%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 58679 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	B	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	K	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	L	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1119	Total 8829	C 5581	N 1577	O 1647	S 24	0	0	0
2	M	1119	Total 8829	C 5581	N 1577	O 1647	S 24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1392	Total 10797	C 6819	N 1925	O 2020	S 33	0	0	0
3	N	1392	Total 10797	C 6819	N 1925	O 2020	S 33	0	0	0

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	95	Total 769	C 488	N 133	O 144	S 4	0	0	0
4	O	95	Total 769	C 488	N 133	O 144	S 4	0	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		
6	N	2	Total	Zn	0	0
			2	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	191	Total	O	0	0
			191	191		
8	B	181	Total	O	0	0
			181	181		
8	C	767	Total	O	0	0
			767	767		
8	D	1100	Total	O	0	0
			1100	1100		
8	E	93	Total	O	0	0
			93	93		
8	F	333	Total	O	0	0
			333	333		
8	K	151	Total	O	0	0
			151	151		
8	L	179	Total	O	0	0
			179	179		
8	M	739	Total	O	0	0
			739	739		

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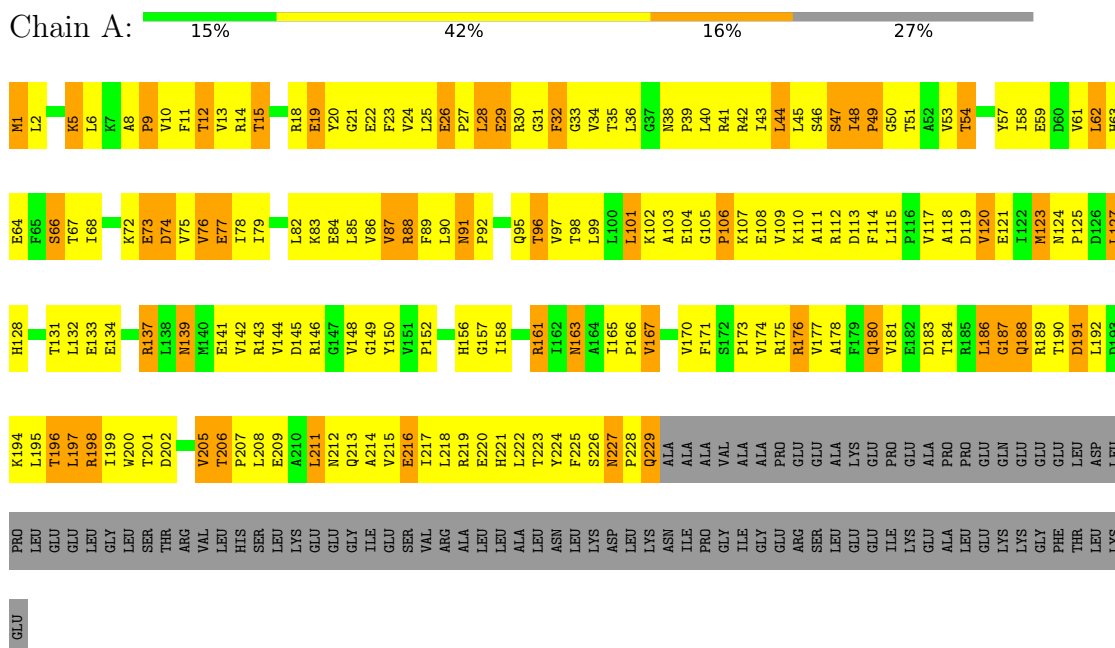
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	1038	Total 1038	O 1038	0	0
8	O	78	Total 78	O 78	0	0
8	P	267	Total 267	O 267	0	0

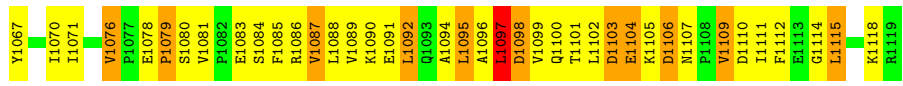
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

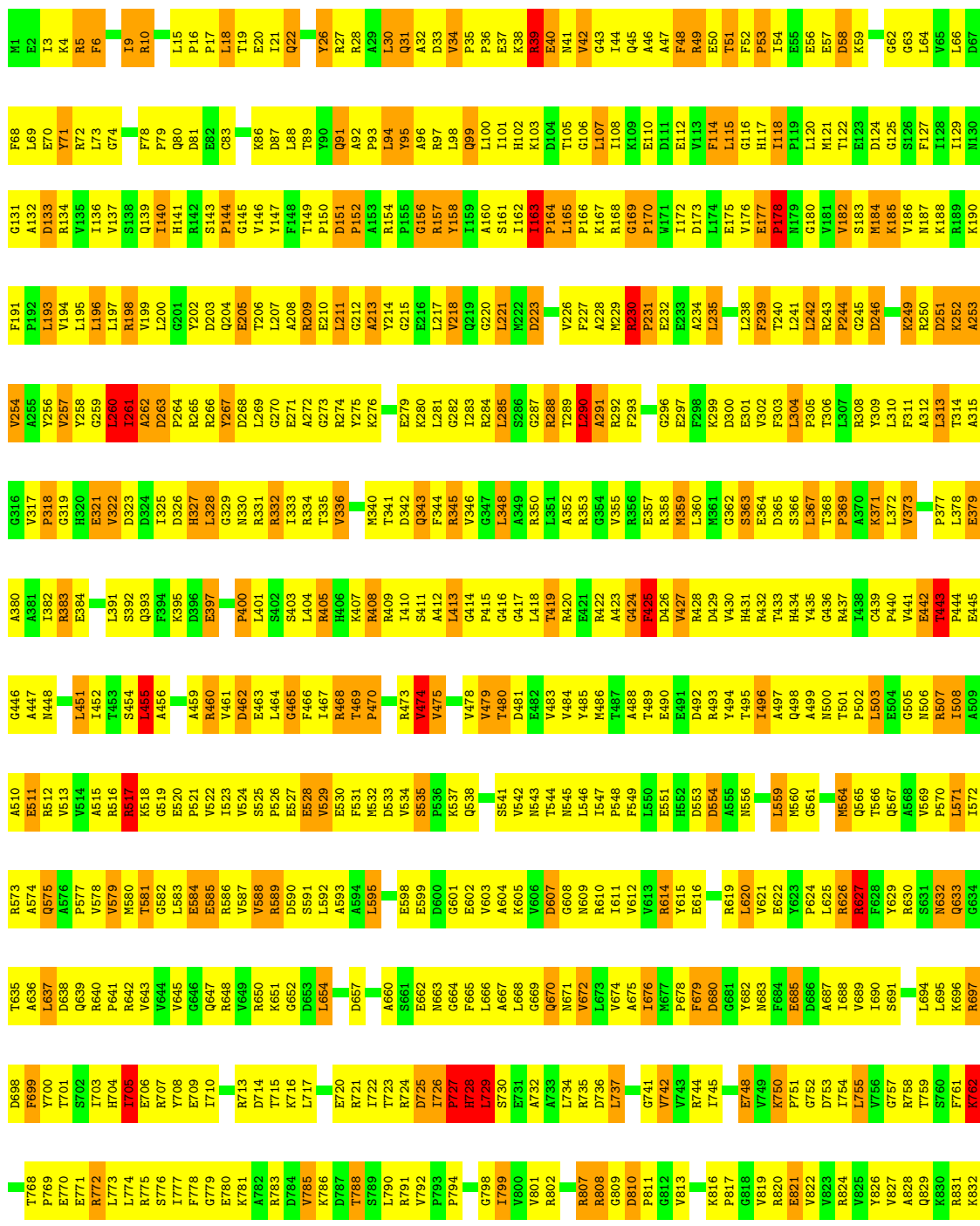
- Molecule 1: DNA-directed RNA polymerase alpha chain



V943	V944	R879	R816	W749	V689	Q566	P502	V441	L378	A315	D251	N187	D124	G62	E2	W1
L944	L945	M680	P817	K750	L690	T566	L503	E442	E379	G316	K251	K188	G125	G63	E1	E1
R946	R947	N881	G818	P751	S691	Q567	E504	T443	A380	P317	K252	K189	S126	G64	E2	E2
L882	L883	N882	W819	G752	E692	A568	E505	P444	A381	A253	K253	K190	F127	V65	E3	E3
Q848	Q849	G883	R820	D753	G693	V569	M506	E445	R382	G319	V254	F191	I128	L66	E4	E4
K949	K950	Q884	E821	L754	L694	P570	R507	E446	R383	A255	A255	P192	I129	D67	E5	E5
L980	L981	T885	W822	L755	L695	L571	I508	A447	E384	E321	Y256	L193	G133	F68	E6	E6
G951	G952	L886	V623	K696	K636	A509	A509	R448	F385	F257	Y258	V194	D133	F69	E7	E7
L952	L953	G957	R824	R697	L637	R572	A510	I449	F386	F387	Y259	L195	R134	E70	E8	E8
W953	W954	L890	W826	D698	D638	A574	E511	R450	G387	G326	G259	L196	R135	Y71	E9	E9
T954	T955	G891	W827	F699	F639	Q575	R512	L451	R388	H327	L260	L197	W116	Y72	E10	E10
F955	F956	L892	A828	Y700	Y700	A576	V513	L452	L391	L328	L261	R198	W137	Y73	E11	E11
G956	G957	G763	G763	W701	P641	P577	V514	T453	L392	G329	A262	V199	S138	Y74	E12	E12
K957	K958	E764	E764	S702	R642	W578	A515	S454	S392	M330	D283	L200	Q139	Y75	E13	E13
T958	T959	E764	E764	L703	V643	W579	R516	L455	Q393	R331	P264	G201	I140	Y76	E14	E14
P959	P960	L705	L705	H704	V644	M580	R517	L456	F394	R332	R265	Y201	H141	Y77	E15	E15
G960	G961	R769	R769	I705	V645	T581	R518	A457	K395	I333	R266	D203	H142	Y78	E16	E16
Q962	Q963	R707	R707	E706	G646	G582	G519	Y458	K396	K334	Y267	D204	F148	Y79	E17	E17
R900	R901	R707	R707	R706	G647	L583	F520	A459	K397	T335	Y268	E205	F149	Y80	E18	E18
Y901	Y902	E771	E771	Y708	R648	E584	F521	R480	R398	W336	L289	T206	G145	Y81	E19	E19
Q903	Q904	R778	R778	E709	E585	E591	V522	W461	R399	G337	G270	T207	V146	Y82	E20	E20
R904	R905	L773	L773	R710	R650	R586	F523	D462	P400	E338	E271	A208	Y147	Y83	E21	E21
P905	P906	L774	L774	E711	K651	V587	W524	E463	L401	L339	A272	R209	F148	Y84	E22	E22
F906	F907	R775	R775	A712	G652	W588	S525	L464	S402	M340	G273	E210	T149	Y85	E23	E23
Q908	Q909	S776	S776	R713	D653	R589	P526	G465	S403	T341	R274	L211	P150	Y86	E24	E24
R909	R910	I777	I777	D714	L654	D590	E527	F466	L404	D342	Y275	G212	D151	Y87	E25	E25
G908	G909	F778	F778	W715	L655	S591	V529	L467	R405	Q343	K276	A213	D152	Y88	E26	E26
A909	A910	R779	R779	K716	A656	L592	W529	R468	H406	F344	Y214	G215	P155	Y89	E27	E27
E911	E912	E780	E780	L717	D657	L595	E530	T469	K407	R345	E279	G215	G156	Y90	E28	E28
F912	F913	K781	K781	G718	G658	L596	F531	P470	R408	K280	K280	E216	G156	Y91	E29	E29
L974	L975	W782	W782	P719	P659	W596	M532	Y471	R409	G347	L281	L217	L94	Y92	E30	E30
Y975	Y976	R783	R783	E720	A660	A597	D533	R472	I410	L348	G282	V218	Y95	Y93	E31	E31
D977	D978	R721	R721	S661	S661	E598	V534	R473	A412	A349	F283	Q219	Y96	Y94	E32	E32
G977	G978	I722	I722	E662	E662	G601	P536	W474	A413	R350	L285	G220	Y97	Y95	E33	E33
R978	R979	R723	R723	G664	G664	E602	F536	V475	L413	L351	L285	L221	Y98	Y96	E34	E34
W979	W980	D725	D725	F665	F665	V603	K537	V475	G414	A352	S286	M222	Y99	Y97	E35	E35
G980	G981	L726	L726	L666	L666	A604	Q538	W478	P415	V355	R288	D223	I163	Y100	E36	E36
E981	E982	P727	P727	A667	A667	R605	V542	T480	G416	R356	T289	E224	P164	Y101	E37	E37
R982	R983	H728	H728	L668	L668	V606	M543	D481	L417	E357	L290	S225	L165	Y102	E38	E38
E984	E985	L729	L729	G669	G669	D607	M543	E482	L418	R358	A291	F227	L166	Y103	E39	E39
G985	G986	S730	S730	O670	O670	G608	L546	V483	T419	M359	R428	A228	K167	Y104	E40	E40
F986	F987	E731	E731	M671	M671	M609	L547	V484	R420	L360	R292	M229	R168	Y105	E41	E41
Y925	Y926	A732	A732	R610	R610	R610	P548	Y485	E421	K361	G287	R230	G169	Y106	E42	E42
F926	F927	R733	R733	L673	L673	L611	F549	M486	R422	G362	K289	P231	W171	Y107	E43	E43
G927	G928	L734	L734	V674	V674	V612	F549	T487	G416	S363	D300	E232	W172	Y108	E44	E44
E929	E930	R735	R735	A675	A675	V613	L550	T487	L417	E364	D301	E232	I172	Y109	E45	E45
K930	K931	D736	D736	L676	L676	G614	E551	A488	G417	D365	E301	E233	D173	Y110	E46	E46
E932	E933	L737	L737	M677	M677	Y615	H552	T489	L418	V427	V302	A234	L174	Y111	E47	E47
Y924	Y925	D738	D738	P678	P678	E616	D554	E491	R420	S366	F303	L235	E175	Y112	E48	E48
G933	G934	E739	E739	R679	R679	A585	A585	W492	D429	L367	L304	I236	W176	Y113	E49	E49
F934	F935	W804	W804	D680	D680	L620	M556	W492	V430	T366	P305	R237	E177	Y114	E50	E50
G935	G936	E741	E741	G681	G681	V621	R493	Y494	H431	P369	T306	L238	P178	Y115	E51	E51
D937	D938	W805	W805	V742	V742	E622	R493	T494	R432	L307	T306	L238	L115	Y116	E52	E52
Y938	Y939	L810	L810	W743	W743	G623	A588	T495	R432	M179	L307	F239	L115	Y117	E53	E53
R939	R940	P811	P811	V743	V743	G624	M560	I496	H434	K371	L307	F239	G180	Y118	E54	E54
E940	E941	G812	G812	R744	R744	L625	M560	A497	Y435	L372	L304	L241	G180	Y119	E55	E55
E1002	E1003	W813	W813	L745	L745	R626	G581	Q498	G436	W373	P305	R237	G180	Y120	E56	E56
K1004	K1005	E746	E746	G746	G746	R627	S582	A499	R437	N374	T306	L238	G180	Y121	E57	E57
		E748	E748	E748	E748	R627	M563	A499	R437	S375	T306	L238	G180	Y122	E58	E58
		L815	L815	L815	L815	F628	M564	T501	P440	R376	G244	G244	G180	Y123	E59	E59



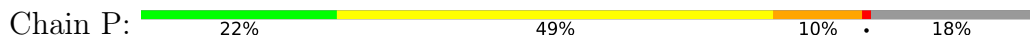
● Molecule 2: DNA-directed RNA polymerase beta chain



I949	G950	I951	I952	D953	A954	V955	I956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000	E1001	K1002	V1003	T1004	T1005	T1006	T1007	T1008	K1009	M1010	M1018	P1019																																																																																																																													
G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948																																																																																											
V820	V821	A822	L823	A824	N825	A826	L827	K828	V829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948																																																												
D689	A690	E691	E692	E693	V694	L695	H696	K697	K698	L699	L700	L701	L702	N703	C642	C643	L644	P645	K646	R647	M648	L649	L650	E651	K654	P655	F656	L657	L658	K659	K660	M661	E662	E663	K664	G665	L666	A667	P668	N669	V670	K671	A672	C673	R674	E675	E676	F677	F678	F679	F680	F681	F682	F683	F684	F685	F686	F687	F688	F689	F690	F691	F692	F693	F694	F695	F696	F697	F698	F699	F700	F701	F702	F703	F704	F705	F706	F707	F708	F709	F710	F711	F712	F713	F714	F715	F716	F717	F718	F719	F720	F721	F722	F723	F724	F725	F726	F727	F728	F729	F730	F731	F732	F733	F734	F735	F736	F737	F738	F739	F740	F741	F742	F743	F744	F745	F746	F747	F748	F749	F750	F751	F752	F753	F754	F755	F756	F757	F758	F759	F760	F761	F762	F763	F764	F765	F766	F767	F768	F769	F770	F771	F772	F773	F774	F775	F776	F777	F778	F779	F780	F781	F782	F783	F784	F785	F786	F787	F788	F789	F790	F791	F792	F793	F794	F795	F796	F797	F798	F799	F800	G803	L804	E805	F806	A807	T808	P809	E810	E811	A812	L813	A814	E815	E816	E817	L818	G819
E820	V821	A822	L823	A824	N825	A826	L827	K828	V829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948																																																												
R884	E885	V886	A887	E888	A889	V890	E891	D892	E893	K894	A895	K896	K897	M898	E899	L894	L895	Q900	Q901	L902	Q906	E907	K908	N909	S910	L911	D912	E913	L914	V915	Y916	Q917	A918	F919	L920	R921	L922	G923	M924	E925	K926	L927	V928	A929	L930	L931	D932	E1001	L1002	V1003	T1004	Q1005	A1006	V1007	F1008	K1009	M1010	M1018	P1019																																																																																																																																	
E122	L123	E124	Q125	V126	L127	Y128	F129	E130	G131	Y132	L133	V134	L135	D136	P137	G138	K139	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																		
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170	L171	P172	G173	L174	L175	V176	D177	L178	V179	K180	L181																																																																																																																																					
E183	E184	V185	V186	K187	G188	L191	A192	P193	G194	V195	V196	S197	R198	L199	D200	L204	Y205	R206	V145	P146	V147	E148	K149	R150	L151	R152	L153	L154	D155	E156	E157	Y158	R159	A160	L161	R162	Y163	W164	G165	Q166	E167	T168	Y169	P170																																																																																																																																																

MET	LEU	P124	H186	T251	Q312	K373	Q312	H186	T251	Q312	K373
LYS	ASP	D126	L187	A252	E313	G374	E313	L187	A252	E313	G374
LYS	LEU	L126	I188	D253	S316	I375	S316	I188	D253	S316	I375
SER	GLU	I127	E189	Q254	L317	I376	L317	E189	Q254	L317	I376
ARG	GLU	R128	A190	R255	E318	D377	E318	A190	R255	E318	D377
ARG	GLU	E129	N191	A256	G319	G378	G319	N191	A256	G319	G378
LYS	GLU	V130	L192	T257	T319	ARG	T319	L192	T257	T319	ARG
ASN	GLU	Y131	R193	L258	P320	GLU	P320	R193	L258	P320	GLU
ASP	ASP	Y132	R194	L259	I321	HIS	I321	R194	L259	I321	HIS
ALA	LEU	A133	V196	I260	G322	THR	G322	V196	I260	G322	THR
ALA	PRO	K134	P196	P261	D323	THR	D323	P196	P261	D323	THR
GLN	ILE	I135	S197	V262	G324	GLN	G324	S197	V262	G324	GLN
GLU	PRO	L136	A198	H263	K325	GLU	K325	A198	H263	K325	GLU
ALA	K74	G137	A199	H264	D326	ALA	D326	K74	G137	A199	ALA
GLN	I75	A138	K200	V265	S327	GLN	S327	I75	A138	K200	GLN
GLU	S76	A139	K201	E266	F328	GLU	F328	S76	A139	K201	GLU
THR	T77	R140	Y202	T267	F390	THR	F390	T77	R140	Y202	THR
GLU	S78	V141	T203	L268	G330	GLU	G330	S78	V141	T203	GLU
VAL	D79	R142	G204	N269	D331	VAL	D331	D79	R142	G204	VAL
LEU	P80	H143	R205	K270	F332	LEU	F332	P80	H143	R205	LEU
VAL	V81	I144	R206	L271	L333	VAL	L333	V81	I144	R206	VAL
GLN	R82	P145	S208	Q272	I334	GLN	I334	R82	P145	S208	GLN
GLU	Q83	G146	F209	R273	P334	GLU	P334	Q83	G146	F209	GLU
GLU	Y84	L147	S208	R274	D335	GLU	D335	Y84	L147	S208	GLU
ALA	L85	L147	F209	T274	E336	ALA	E336	L85	L147	F209	ALA
GLU	H86	K148	L210	A275	H337	GLU	H337	H86	K148	L210	GLU
GLU	H86	E149	D211	R276	L338	GLU	L338	H86	E149	D211	GLU
GLU	E87	T150	L212	Q277	P339	GLU	P339	E87	T150	L212	GLU
LEU	I88	L151	I213	L278	S340	LEU	S340	I88	L151	I213	LEU
PRO	V91	D152	E215	Q279	P941	PRO	P941	V91	D152	E215	PRO
GLU	P92	P153	G216	Q280	K403	GLU	K403	P92	P153	G216	GLU
PHE	P93	K154	E281	E281	A404	PHE	A404	P93	K154	E281	PHE
PRO	L93	T155	N217	L282	L405	PRO	L405	L93	T155	N217	PRO
GLU	L94	T155	Q218	L282	L406	GLU	L406	L94	T155	Q218	GLU
GLY	T95	E157	Q219	G283	K407	GLY	K407	T95	E157	Q219	GLY
GLU	T96	E157	G219	R284	L408	GLU	L408	T96	E157	G219	GLU
PRO	E97	E159	R222	R284	L408	PRO	L408	E97	E159	R222	PRO
ASP	E98	I159	R222	P286	K409	ASP	K409	E98	I159	R222	ASP
PRO	E99	D160	Y224	T287	Y410	PRO	Y410	E99	D160	Y224	PRO
ASP	V100	L163	E225	Y288	H411	ASP	H411	V100	L163	E225	ASP
LEU	E101	K164	E226	E289	E412	LEU	E412	E101	K164	E226	LEU
GLU	L102	S165	F227	E290	S413	GLU	S413	L102	S165	F227	GLU
ASP	L105	L166	E228	I291	R414	ASP	R414	L105	L166	E228	ASP
PRO	V106	P167	R231	A292	T415	PRO	T415	V106	P167	R231	PRO
LEU	E107	K168	R232	E293	R416	LEU	R416	E107	K168	R232	LEU
ALA	E108	H170	R233	M295	K417	ALA	K417	E108	H170	R233	ALA
GLU	G109	K171	F233	G296	L418	GLU	L418	G109	K171	F233	GLU
ASP	A112	K171	K234	P297	R419	ASP	R419	A112	K171	K234	ASP
LEU	A112	Y173	F235	Q298	F421	LEU	F421	A112	Y173	F235	LEU
ASP	I113	L174	S236	M299	L422	ASP	L422	I113	L174	S236	ASP
LEU	K114	H175	T240	D300	L361	LEU	L361	K114	H175	T240	LEU
LEU	K115	I176	W241	A301	K360	LEU	K360	K115	I176	W241	LEU
ASP	L116	A177	W242	R303	E365	ASP	E365	L116	A177	W242	ASP
LEU	S117	R178	I243	V304	A366	LEU	A366	S117	R178	I243	LEU
PRO	E118	R178	R244	E305	M367	PRO	M367	E118	R178	R244	PRO
GLU	I119	E187	Q245	E306	V368	GLU	V368	I119	E187	Q245	GLU
GLU	T120	E181	A246	L369	L369	GLU	L369	T120	E181	A246	GLU
GLY	G121	R184	T247	K309	K370	GLY	K370	G121	R184	T247	GLY
GLY	L122	L184	M248	A311	L371	GLY	L371	L122	L184	M248	GLY
GLY	D123	L184	R372	R372	R372	GLY	R372	D123	L184	R372	GLY

• Molecule 5: RNA polymerase sigma factor rpoD



MET	LEU	D126	Q185	R256	T319	ARG
LYS	ASP	L126	H186	R256	P320	GLU
LYS	LEU	I127	L187	T257	I321	HIS
SER	GLU	R128	I188	I258	G322	THR
ARG	GLU	E129	E189	R259	D323	LEU
ARG	GLU	V130	A190	I260	E324	GLU
ASN	GLU	Y131	N191	P261	K325	GLU
ASP	GLU	R132	L192	V262	D326	ASP
ALA	ASP	A133	R193	H263	F390	ALA
GLN	LEU	K134	L194	M264	G329	GLN
ALA	PRO	I135	V196	E266	G330	ALA
GLN	ILE	I136	S197	G137	D331	GLN
GLU	PRO	L137	A198	T267	F332	GLU
ALA	K74	S138	L268	I268	F332	ALA
GLN	I75	A139	N269	M269	I333	GLN
GLU	S76	A139	K201	K270	G333	GLU
THR	T77	R140	L271	L271	D335	THR
GLU	S78	V141	T203	L272	E336	GLU
VAL	D79	R142	G204	R273	Q399	VAL
LEU	P80	H143	R205	T274	I400	LEU
VAL	V81	I144	R206	T274	E401	VAL
GLN	R82	P145	S208	A275	M402	GLN
GLU	Q83	G146	L207	R276	K403	GLU
GLU	Y84	L147	S208	Q277	S340	GLU
GLU	L85	L147	F209	L278	A404	GLU
ALA	H86	K148	L210	L278	L405	ALA
GLU	H86	E149	L210	Q279	R406	GLU
GLU	E87	T150	D211	Q280	K407	GLU
GLU	E87	L151	L212	Q280	L407	GLU
LEU	I88	L151	I213	G283	L408	LEU
LEU	D152	D152	I213	G283	K409	LEU
PRO	P153	P153	Q214	R284	Y410	PRO
GLU	K154	K154	E215	E285	H411	GLU
PHE	P92	T155	G216	P286	E412	PHE
PRO	L93	T155	N217	T287	L416	PRO
GLU	L94	T155	Q218	Y288	K417	GLU
GLY	T95	E157	G219	E289	L418	GLY
GLY	T96	E157	R222	E289	L418	GLY
PRO	E97	E159	I221	E290	R419	PRO
PRO	E97	D160	I291	I291	D420	PRO
ASP	E98	I160	A292	A292	F421	ASP
PRO	E99	D160	A223	A292	L422	PRO
ASP	V100	L163	V224	M295	D423	ASP
LEU	E101	K164	E225	G296	L423	LEU
GLU	L102	S165	K226	P297	L423	GLU
ASP	L105	L166	R232	G298	L361	ASP
PRO	V106	P167	R233	M299	L361	PRO
LEU	E107	K168	R234	K302	E363	LEU
ALA	E108	H170	R234	R303	E363	ALA
GLU	G109	K171	Y238	V304	E365	GLU
ASP	A112	K171	W242	T307	A366	ASP
LEU	A112	Y173	I243	M367	M367	LEU
LEU	A112	L174	R244	V368	V368	LEU
LEU	I113	H175	R244	L369	L369	LEU
LEU	K114	I176	Q245	K370	K370	LEU
LEU	K115	A177	A246	I310	I310	LEU
ASP	L116	A177	I247	A311	A311	ASP
LEU	S117	R178	I247	Q312	Q312	LEU
LEU	E118	E179	N248	R313	R313	LEU
PRO	E119	G180	R249	P314	P314	PRO
GLU	T120	E181	A250	G374	G374	GLU
GLU	G121	E181	I251	L375	L375	GLU
GLY	A182	A182	A252	I376	I376	GLY
GLY	L122	L122	L317	D377	D377	GLY
GLY	D123	L184	E318	G378	G378	GLY

4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 25.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.80) 92.0 (25.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.268 0.226 , 0.261	Depositor DCC
R_{free} test set	21166 reflections (5.78%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.068 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	58679	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	0.88	3/1838 (0.2%)	1.22	9/2498 (0.4%)
1	B	0.78	0/1838	1.09	7/2498 (0.3%)
1	K	0.79	0/1838	1.15	7/2498 (0.3%)
1	L	0.75	1/1838 (0.1%)	1.08	9/2498 (0.4%)
2	C	0.91	5/8997 (0.1%)	1.28	73/12164 (0.6%)
2	M	0.89	6/8997 (0.1%)	1.27	72/12164 (0.6%)
3	D	0.95	11/10975 (0.1%)	1.33	99/14836 (0.7%)
3	N	0.92	13/10975 (0.1%)	1.32	95/14836 (0.6%)
4	E	0.92	0/783	1.36	6/1054 (0.6%)
4	O	0.95	2/783 (0.3%)	1.39	10/1054 (0.9%)
5	F	0.81	2/2812 (0.1%)	1.19	13/3781 (0.3%)
5	P	0.80	0/2812	1.17	11/3781 (0.3%)
All	All	0.89	43/54486 (0.1%)	1.27	411/73662 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	9.24	1.44	1.33
3	D	82	LYS	CA-C	8.55	1.64	1.52
2	C	163	ILE	CA-CB	8.41	1.62	1.53
2	M	163	ILE	CA-CB	8.23	1.62	1.53
1	A	48	ILE	CA-C	8.08	1.60	1.52

The worst 5 of 411 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	207	PHE	CA-C-N	16.60	140.59	119.84
3	D	207	PHE	C-N-CA	16.60	140.59	119.84
3	N	207	PHE	CA-C-N	16.53	140.50	119.84
3	N	207	PHE	C-N-CA	16.53	140.50	119.84
2	C	177	GLU	CA-C-N	14.79	138.33	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	1806	0	1861	219	0
1	B	1806	0	1861	208	0
1	K	1806	0	1861	212	0
1	L	1806	0	1861	208	0
2	C	8829	0	8933	1217	0
2	M	8829	0	8933	1131	0
3	D	10797	0	10873	1489	0
3	N	10797	0	10873	1385	0
4	E	769	0	775	99	0
4	O	769	0	775	113	0
5	F	2771	0	2844	345	0
5	P	2771	0	2844	346	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
8	A	191	0	0	37	0
8	B	181	0	0	35	0
8	C	767	0	0	175	0
8	D	1100	0	0	235	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	93	0	0	14	0
8	F	333	0	0	58	0
8	K	151	0	0	30	0
8	L	179	0	0	49	0
8	M	739	0	0	195	0
8	N	1038	0	0	224	0
8	O	78	0	0	24	0
8	P	267	0	0	62	0
All	All	58679	0	54294	6567	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

The worst 5 of 6567 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)
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.28	1.11
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.12	1.08
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.36	1.04
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.14	1.04
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.20	1.04

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	6 23
1	B	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	6 23
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	6 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	6	23
2	C	1117/1119 (100%)	917 (82%)	150 (13%)	50 (4%)	2	7
2	M	1117/1119 (100%)	907 (81%)	159 (14%)	51 (5%)	2	6
3	D	1388/1524 (91%)	1123 (81%)	191 (14%)	74 (5%)	1	5
3	N	1388/1524 (91%)	1110 (80%)	195 (14%)	83 (6%)	1	3
4	E	93/99 (94%)	74 (80%)	16 (17%)	3 (3%)	3	11
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	3	11
5	F	341/423 (81%)	283 (83%)	42 (12%)	16 (5%)	2	6
5	P	341/423 (81%)	285 (84%)	40 (12%)	16 (5%)	2	6
All	All	6786/7590 (89%)	5582 (82%)	892 (13%)	312 (5%)	2	6

5 of 312 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO

5.3.2 Protein sidechains [i](#)

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	202/273 (74%)	147 (73%)	55 (27%)	0	1
1	B	202/273 (74%)	161 (80%)	41 (20%)	1	4
1	K	202/273 (74%)	155 (77%)	47 (23%)	1	3
1	L	202/273 (74%)	155 (77%)	47 (23%)	1	3
2	C	941/941 (100%)	724 (77%)	217 (23%)	1	3
2	M	941/941 (100%)	723 (77%)	218 (23%)	1	3
3	D	1123/1279 (88%)	832 (74%)	291 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	1123/1279 (88%)	842 (75%)	281 (25%)	0	2
4	E	83/87 (95%)	61 (74%)	22 (26%)	0	2
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	2
5	F	295/370 (80%)	224 (76%)	71 (24%)	1	2
5	P	295/370 (80%)	250 (85%)	45 (15%)	3	10
All	All	5692/6446 (88%)	4335 (76%)	1357 (24%)	1	3

5 of 1357 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	637	LEU
3	N	794	GLN
2	M	808	ARG
2	M	635	THR
3	N	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 197 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	390	GLN
2	M	1050	GLN
2	M	538	GLN
2	M	834	GLN
3	N	507	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-1.72	0 100 100	38, 65, 92, 117	0
1	B	229/315 (72%)	-1.66	0 100 100	53, 95, 115, 121	0
1	K	229/315 (72%)	-1.75	0 100 100	41, 66, 93, 122	0
1	L	229/315 (72%)	-1.70	0 100 100	52, 94, 114, 127	0
2	C	1119/1119 (100%)	-1.70	0 100 100	23, 81, 110, 119	0
2	M	1119/1119 (100%)	-1.72	0 100 100	27, 79, 109, 122	0
3	D	1392/1524 (91%)	-1.71	0 100 100	17, 68, 113, 130	0
3	N	1392/1524 (91%)	-1.72	0 100 100	27, 69, 110, 138	0
4	E	95/99 (95%)	-1.64	0 100 100	47, 85, 115, 133	0
4	O	95/99 (95%)	-1.76	0 100 100	40, 76, 97, 111	0
5	F	345/423 (81%)	-1.69	0 100 100	46, 84, 112, 131	0
5	P	345/423 (81%)	-1.69	0 100 100	54, 87, 112, 125	0
All	All	6818/7590 (89%)	-1.71	0 100 100	17, 77, 111, 138	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	N	9002	1/1	0.99	0.02	64,64,64,64	0
6	ZN	D	7112	1/1	1.00	0.01	75,75,75,75	0
6	ZN	N	7059	1/1	1.00	0.01	100,100,100,100	0
6	ZN	N	7113	1/1	1.00	0.01	87,87,87,87	0
7	MG	D	9001	1/1	1.00	0.01	67,67,67,67	0
6	ZN	D	7058	1/1	1.00	0.03	109,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.