



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:03 AM GMT

PDB ID : 4KMU
Title : X-ray crystal structure of the Escherichia coli RNA polymerase in complex with Rifampin
Authors : Murakami, K.S.
Deposited on : 2013-05-08
Resolution : 3.85 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

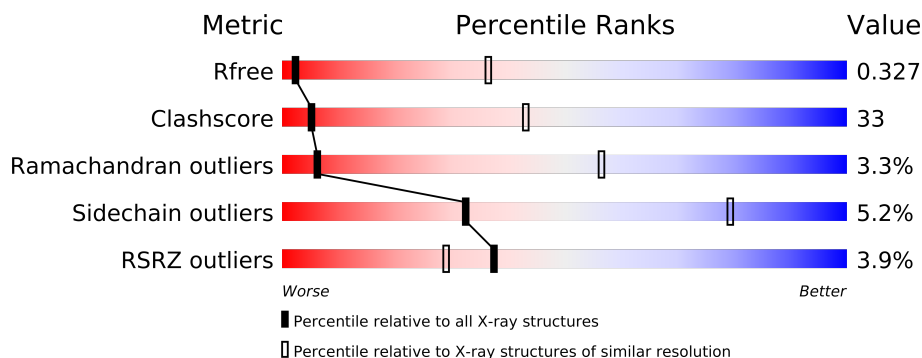
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 3.85 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}	66092	1013 (4.30-3.42)
Clashscore	79885	1145 (4.22-3.50)
Ramachandran outliers	78287	1091 (4.22-3.50)
Sidechain outliers	78261	1081 (4.22-3.50)
RSRZ outliers	66119	1014 (4.30-3.42)

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.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	F	329	
1	G	329	
2	C	1342	
2	H	1342	
3	D	1407	
3	I	1407	
4	E	91	
4	J	91	
5	X	613	
5	Y	613	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
8	MG	I	1503	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56315 atoms, of which 116 are hydrogens 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 polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

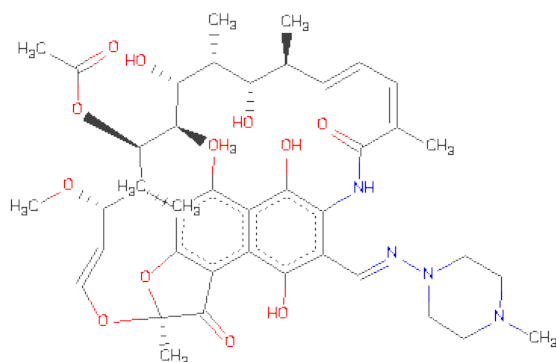
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



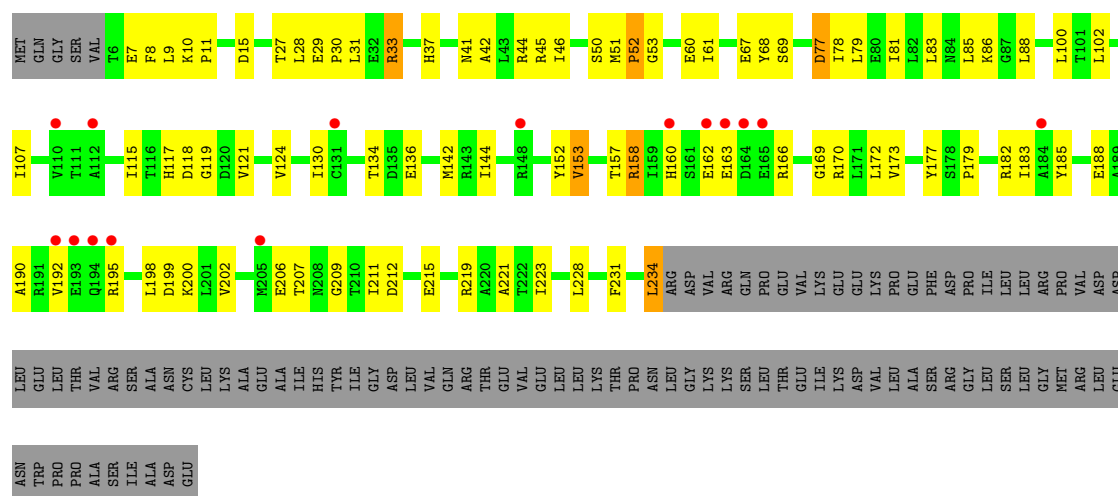
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			117	43	58	4	12		
6	H	1	Total	C	H	N	O	0	0
			117	43	58	4	12		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

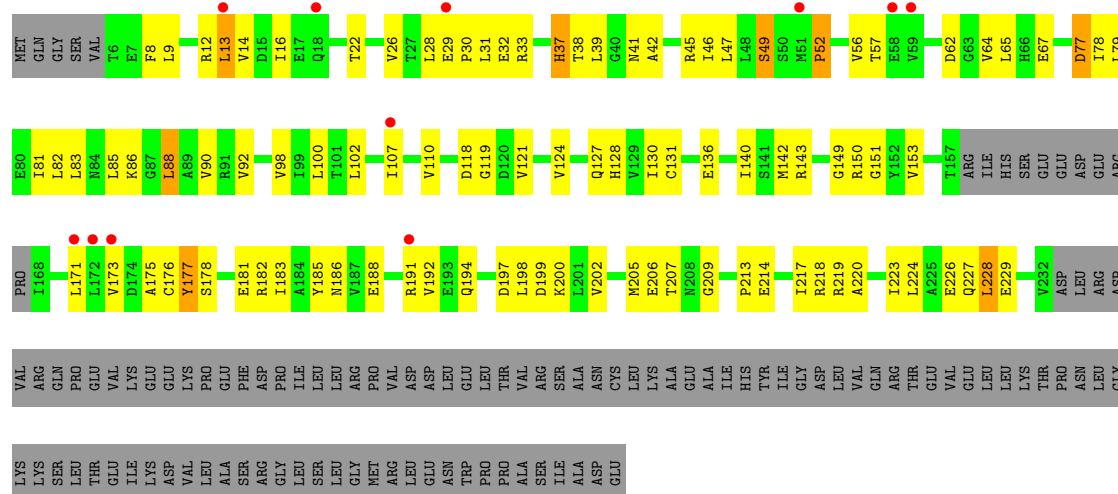
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



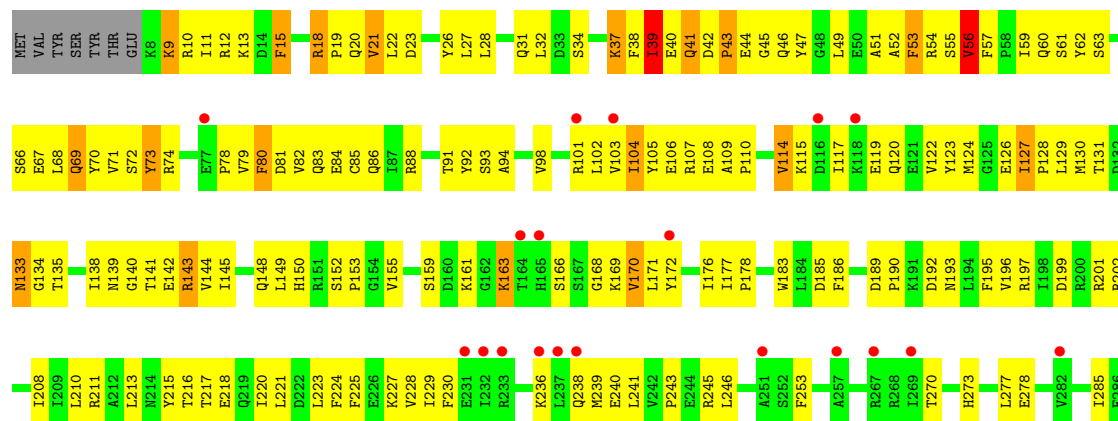
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



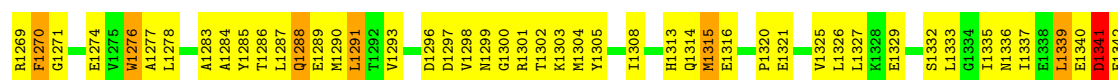
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:



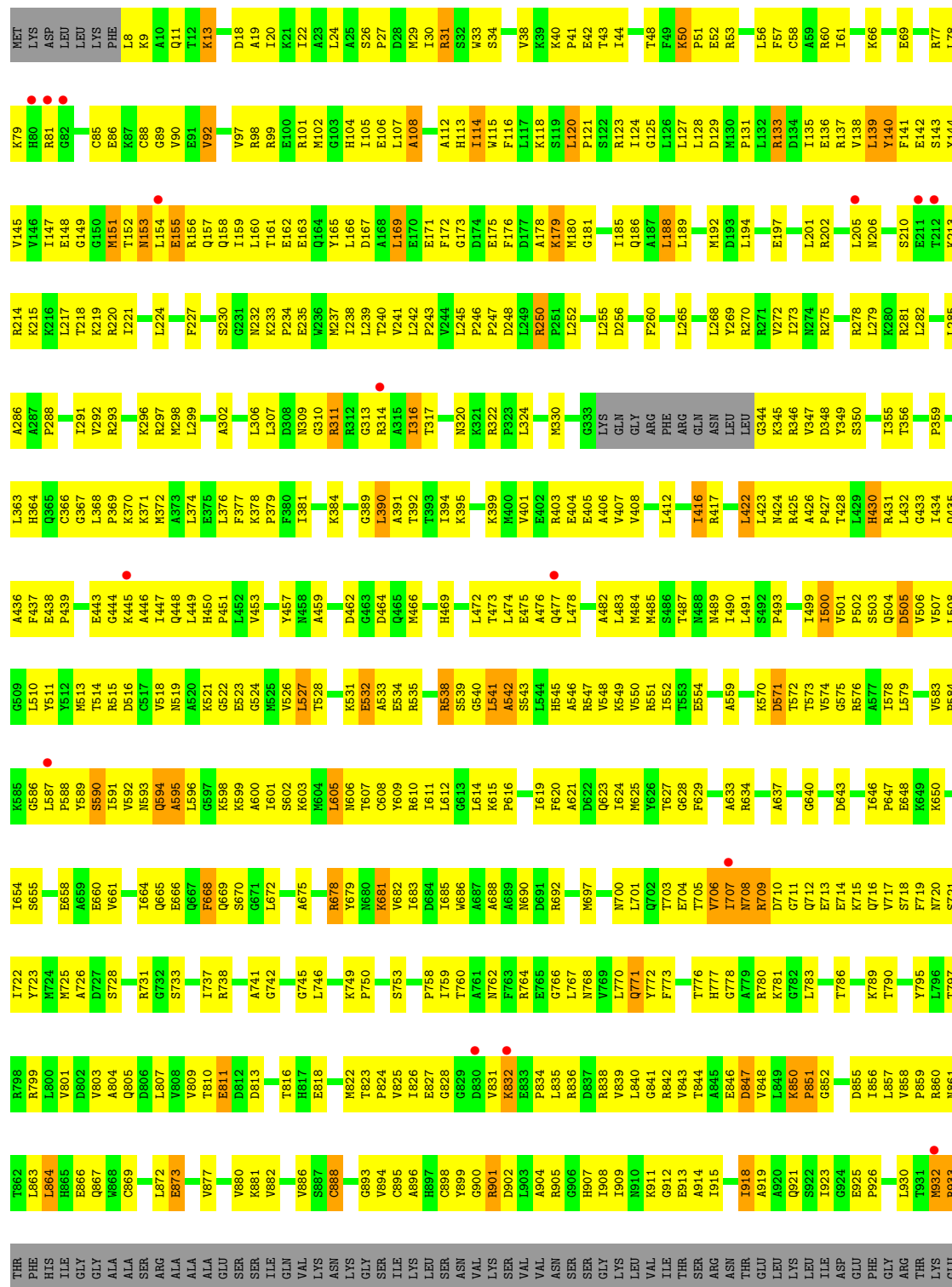


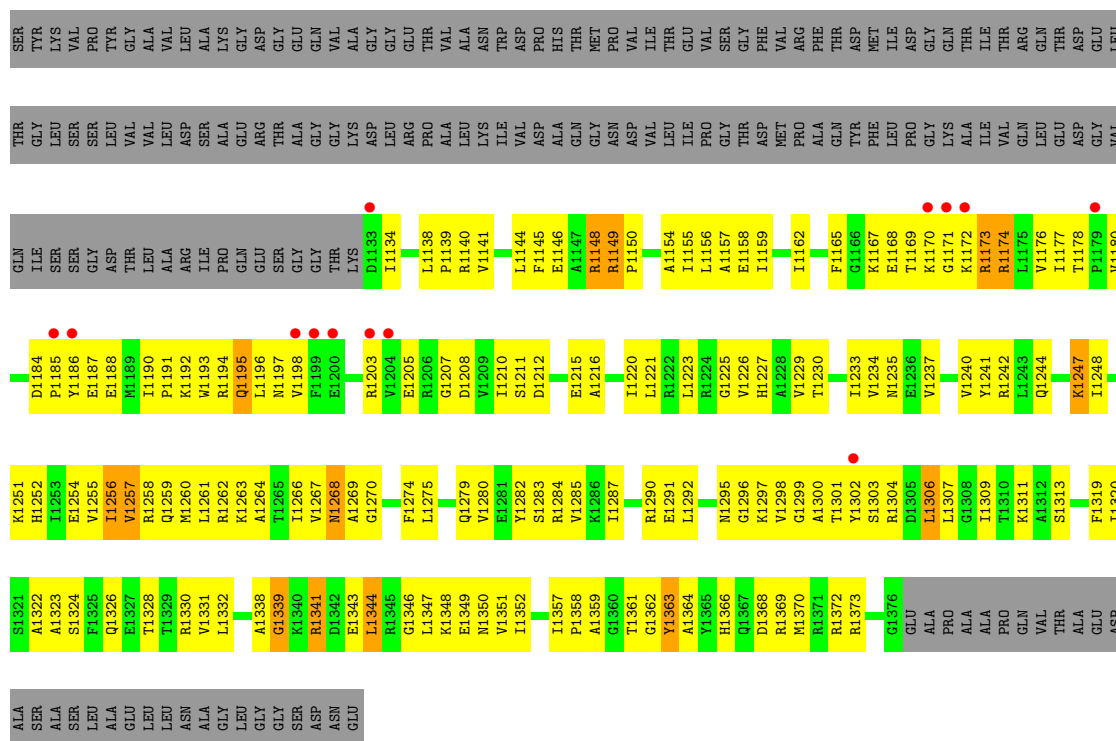
G1189	H1116	L1042	L1967	E892	Y726	V654	N573	A495	T426	E334	R211	I138	L68
L1199	M1119	A1043	E966	T893	V727	V655	S574	K496	T427	F337	R216	I139	Q89
L1200	M1120	P1044	A969	Q894	D728	Q658	L575	P497	D427	T338	T216	G140	Y70
L1201	K1122	G1045	G970	L896	A729	Q659	S576	A500	M429	T339	T217	T141	S72
G1202	L1047	V1046	L971	T896	I732	V660	Y577	E504	D342	D342	E218	E142	Y73
D1203	K1127	P1043	L976	E898	V733	V681	A579	E505	K431	H843	Q219	R143	R74
L1204	M1128	A1054	A976	E813	I734	S622	Q580	F506	L432	G344	I220	V144	
L1205	M1129	A1055	A977	L901	K735	V683	T881	F507	L433	G345		I145	P78
L1206	V1056	V1056	Y978	L902	V736	G664	N582	S508	D434	Y346	L223	V146	P79
S1207	L1132	K1057	L979	T897	I733	A665	G585		I347			S147	F80
G1208	K1133	R1058	Y980	L905	D739	S666	F586	L511	K436		F230	Q148	D81
Q1209	R1059	T1060	Y981	E908	E740	L687	F587	S512	M437	L351	F231	L149	V82
I1210	R1211		G982	E909	M741	I688	L587	Q513	G436		I232	H150	
L1212	A1140	D1064	Y984	A910	Y742	P689	E588	F514	K439	T356	K236	R151	Q86
L1213	R1141	K1065	E985	S911	P743	F670	T589	M515	L360		L237	S152	I87
L1214	L1142	M1066	E986	D912	A746	L671	Y590	D516	S361	L360	Q238	P153	R88
G1215	E1143		F987	Y913	G747	E672	Y591	Q517	A362				
R1216	F1144	H1070	K988	V913	I748	H673	R592	N518	D446		L241	F156	T91
L1217	I1145	K1073	L989	S916	D749	R678	V599	N519	H447	E365		F157	Y92
Q1218	Q1146	G1074	D990	T830	N752	A679	T600	P520	L448	I366	R245	D158	S93
E1219	R1147		K991	L918	L753	L680	D601	L521		Y367	L246	S159	A94
	A1148	V1075	L992	L918		N681	E602	E523	R452	R368		D160	P95
R1223		I1076	P993	P921	Y756		I603	I524	I453	M369	A251	K181	L96
P1224	G1152	S1077	R994	N922		N684	S807	I524	R454	G374		G182	R97
V1225	A1153	K1078	G923	Q923	S759	N685	S807	H526	E458	E374	F253	K183	Y98
T1226	L1154	I1079	R996	Y924	N760	Q686	E610	H526	E458	D254	E264	T184	K99
V1227	R1156	P1080	Y997	S925	T763	R687	E611	R528	M459	P376	I255	S166	L100
G1228	Q1157	K1081	L998	Q926	T763	Q688	E611	R528		T377		S167	R101
Y1229	K1158	I1082	F998	T927	T763	A689	Y614	R529	M462	R378		G168	I102
M1230	V1159	E1083	L1000	V933	T764	V690	V615		Q463	R377		K189	V103
L1231	D1160	P1084	G1001	Y933	I765	P691	V616	P535	P464	E379	V263	V170	I104
M1232	S1161	M1085	L1002	R936	N766	K697	A617	L538	R465	L384	E264	E106	
L1233	P1086	K1087	T1003	S936	Q767	P698	Q618	T539	V466		I269	Y172	R107
K1234	Y1087		D1004	K941	M768	L699	A619		Q467	M173		A174	E108
L1235	E1164	E1005	E1005	D942	P769			A543	L468	A174	H273	R175	A109
S1165	S1165	E1006	E1006	K943	C770	V700	L623		V469	L388		I176	P110
D1237	D1166	P1093	K1007	K943	V771	G701		V547	R470		V287	I177	
L1238	E1167	L1008	Q1008	R944	S772	T702	H628	R548	E472	E392	I292	P178	
V1239	E1168	M1009	N1009	A945	G774	E705	F629	D549	V475	D393		S182	I117
D1240		Q1010	Q1010	E946	E775	E706	D632	V550	K476	R394	V287	E183	K118
L1241	R1171	L1098	L1013	L946	L783	A707	L633	H551	V475	Y395	A298	L184	E119
K1242	L1172	M1099	L1014	E947	A784		V634	P552	E477	V400	K299	F186	Q120
M1243	A1173	P1100	L1014	E948	D785			H554	R478				E121
	E1174	G1102	A1015	S663	G786	V710	D632	H554	L479	M403	D303	D189	Y123
M1175	M1175	P1103	E1016	Q869	S787	D711	R637	Y555	S480	K404	E304	P190	M124
R1177	L1176	K1017	Q1017	V872	G787	S712	S638	G556	F405	F405		L309	G125
S1105	S1105	S1105	D1019	E876	S788	G713	K639	R557	N406	N406	L309	I310	E126
G1178	G1178	E1020	E1020	V877	E793	V714	S643	V558	R407	S408	C311	P128	I127
G1179	M1180	M1107	K1028	V877	L794	T715	L644	C559	L486				E126
M1180	P1181	N1108	D959	L883	A795	V717	F645	E562	N487				P128
Q1256	I1182	L1109	L960	V884	L796	V718	S646	T563	R488				L129
Q1257	R1183	K1032	S961	S663	L796	K718	R647	P564	P489	R411	L317	M130	M130
P1258	T1184	R1033	E962	K886		K719	R647	P564	Q490	E412		L204	D132
L1259	P1185	R1034	E963	V887	N799	R720			D491	E413		P205	T131
	V1186	L1112	E964	T888	M800	R720	V850	N568	D492	I414		A206	N133
Q1264	F1187	L1113	L965	P889	R801	V724			M492			T207	G134
		E1114	Q965	P889	V802	Q725	M653	I572	M494			I208	T135
Q1268		T1115	I966										



• Molecule 3: DNA-directed RNA polymerase subunit beta'

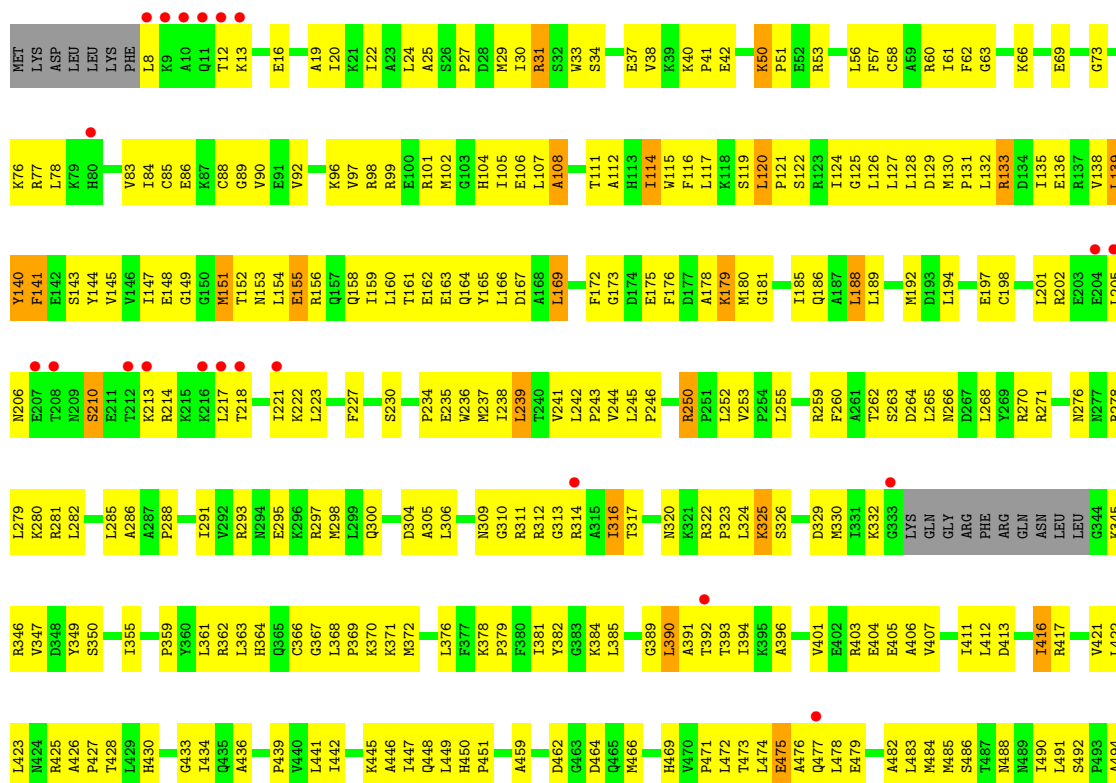
Chain D:





• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain I:



- Chain J:

Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis shows amino acid frequencies for positions 1 through 22. The 10th position (V20) is highlighted with a red dot, indicating a high information content. The sequence logo shows that the 10th position is highly conserved for Valine (V).

- Chain X:

L607	S442	Q345	N271	GLU	S133	LEU
R608	F522	Q346	N271	ASP	V134	ALA
S609	I523	A444		GLU	A135	GLU
PHE	D445	E350	R274	ASP	E136	ASN
LEU	Q446		V275	GLU	P137	THR
ASP	A447	I363	M276	GLU	P138	ALA
	R448	T354	M277	ASP	E139	ASP
E529	T449	I355	D278	GLY	A140	GLU
L530	R450	E356	R279	ASP	T141	ASP
	I451	Q357	V280	ASP	T142	ALA
T536	I452	V358		ASP	I143	ALA
	Q453	E359	M288	SER	L144	GLU
	V454	D360	R289	ALA	L145	ALA
L540	R455		L290	ASP	A146	ALA
R541	M456	R363	C291	ASP	Q147	ALA
A542	A542	R364	V292	ASP	Y148	GLN
A543	I457	R365	E293	ASN		VAL
T544	E458	E366	Q294	SER	V151	LEU
H545	T459	I367	C295	I212	A152	SER
B546	I460	G368	R296	D213	E153	SER
V547	R461	E369	M297		E154	VAL
	L462	R374	P298	L216	GLU	GLU
L551	K463		R299	A217	ALA	SER
A556	R464		K300	R218	ARG	GLU
	R465		N301		LEU	ILE
R560	I466	K377	F302	L224	SER	GLY
M561	M470	E378	I303	R225	ASP	ARG
R562	L471	V380	T304	A226	LEU	THR
F563			L305	Q227	ILE	T95
G564	R476	L384	F306	Y228	THR	D96
I565	E477		T307	V229	GLY	P97
D566	P478	V387	G308		PHE	T98
M567	A484	S389	N309	A237	VAL	R99
N568	R485	I390	T311	K238	ASP	M100
T569	R486		S312	G239	PRO	Y101
D570	M487	T395	D313	R240	ASN	
T571			S314	S241	ALA	D39
T572			T314	H242	GLU	
V576	P490	Q400	W315	A243	GLU	M105
	E491	F401	F316	T244	ASP	V108
	R495	L402	N317	A245	LEU	I44
F580		P403	A318	Q246	ALA	L111
D581	I500	L404	A319	E247	PRO	L112
V582		T405		E248	THR	R113
T583	E503	Q406	N322	I249	ALA	E114
B584	P504	E407	N323	L249	THR	G115
		G408	K324	K251	HIS	I116
T587	M507	I410	P325	L252	GLY	T117
					VAL	D118
A592	I511	Y421	V333	V255	SER	I119
L595	G512	R422	E335	F256	GLU	A120
R596	D513	R423	E336	K257	LEU	V55
K597	D514	G424	V337	Q258	SER	M56
L598	E515	Y425		F259	GLN	E57
R599	D516					E58
H600	S517	I435	A340	V262	GLU	A59
	H518		L341	P263	ASP	P60
P601	H518		Q342	K264	LEU	
S602	L519	I439	K343	Q265	ASP	D64
			L244	F266	ASP	LEU
					ASP	MET

- Chain Y:

[illegible]

G126	G127	G128	G129	G130	G131	G132	G133	G134	G135	G136	G137	G138	G139	G140	G141	G142	G143	G144	G145	G146	G147	G148	G149	G150	G151	G152	G153	G154	G155	G156	G157	G158	G159	G160	G161	G162	G163	G164	G165	G166	G167	G168	G169	G170	G171	G172	G173	G174	G175	G176	G177	G178	G179	G180	G181	G182	G183	G184	G185	G186	G187	G188	G189	G190	G191	G192	G193	G194	G195	G196	G197	G198	G199	G200	G201	G202	G203	G204	G205	G206	G207	G208	G209	G210	G211	G212	G213	G214	G215	G216	G217	G218	G219	G220	G221	G222	G223	G224	G225	G226	G227	G228	G229	G230	G231	G232	G233	G234	G235	G236	G237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	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	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.52Å 203.87Å 307.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.85 30.75 – 3.81	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.97-3.85) 85.5 (30.75-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.264 , 0.321 0.270 , 0.327	Depositor DCC
R_{free} test set	4853 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	112.9	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , -7.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 103271 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	56315	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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, RFP, 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	0.19	0/2548	0.38	0/3454
1	B	0.20	0/1725	0.42	0/2337
1	F	0.20	0/1797	0.41	0/2436
1	G	0.20	0/1690	0.41	0/2290
2	C	0.21	0/10690	0.42	0/14423
2	H	0.22	0/10690	0.42	0/14423
3	D	0.20	0/9198	0.42	0/12413
3	I	0.20	0/9198	0.42	0/12413
4	E	0.19	0/710	0.38	0/956
4	J	0.19	0/607	0.39	0/817
5	X	0.20	0/4253	0.39	0/5719
5	Y	0.20	0/3783	0.39	0/5083
All	All	0.21	0/56889	0.41	0/76764

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	2514	0	2566	170	0
1	B	1706	0	1738	108	0
1	F	1775	0	1800	77	0
1	G	1671	0	1706	92	0
2	C	10523	0	10546	800	0
2	H	10523	0	10546	701	0
3	D	9060	0	9257	808	0
3	I	9060	0	9257	751	0
4	E	708	0	719	51	0
4	J	605	0	612	44	0
5	X	4198	0	4250	243	0
5	Y	3732	0	3809	211	0
6	C	59	58	0	6	0
6	H	59	58	0	12	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56199	116	56806	3749	0

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 33.

The worst 5 of 3749 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.20	1.17
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.26	1.14
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.29	1.14
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.30	1.12
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.28	1.12

There are no symmetry-related clashes.

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	321/329 (98%)	254 (79%)	52 (16%)	15 (5%)	4	45
1	B	217/329 (66%)	188 (87%)	23 (11%)	6 (3%)	8	60
1	F	227/329 (69%)	194 (86%)	28 (12%)	5 (2%)	10	65
1	G	213/329 (65%)	188 (88%)	20 (9%)	5 (2%)	10	64
2	C	1333/1342 (99%)	1066 (80%)	225 (17%)	42 (3%)	6	57
2	H	1333/1342 (99%)	1065 (80%)	222 (17%)	46 (4%)	6	55
3	D	1154/1407 (82%)	919 (80%)	193 (17%)	42 (4%)	5	54
3	I	1154/1407 (82%)	925 (80%)	192 (17%)	37 (3%)	6	57
4	E	88/91 (97%)	76 (86%)	7 (8%)	5 (6%)	3	40
4	J	74/91 (81%)	64 (86%)	5 (7%)	5 (7%)	2	34
5	X	511/613 (83%)	444 (87%)	54 (11%)	13 (2%)	9	62
5	Y	454/613 (74%)	410 (90%)	33 (7%)	11 (2%)	9	64
All	All	7079/8222 (86%)	5793 (82%)	1054 (15%)	232 (3%)	6	56

5 of 232 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	B	20	SER
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/286 (98%)	270 (96%)	11 (4%)	43	85
1	B	189/286 (66%)	184 (97%)	5 (3%)	59	90
1	F	197/286 (69%)	191 (97%)	6 (3%)	53	89
1	G	185/286 (65%)	180 (97%)	5 (3%)	57	90
2	C	1150/1157 (99%)	1084 (94%)	66 (6%)	29	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	1150/1157 (99%)	1084 (94%)	66 (6%)	29	76
3	D	971/1168 (83%)	911 (94%)	60 (6%)	26	74
3	I	971/1168 (83%)	913 (94%)	58 (6%)	27	75
4	E	74/75 (99%)	72 (97%)	2 (3%)	57	90
4	J	65/75 (87%)	63 (97%)	2 (3%)	52	89
5	X	460/540 (85%)	442 (96%)	18 (4%)	43	85
5	Y	407/540 (75%)	388 (95%)	19 (5%)	36	82
All	All	6100/7024 (87%)	5782 (95%)	318 (5%)	32	79

5 of 318 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	6	VAL
2	H	46	GLN
3	I	1306	LEU
5	X	136	GLU
5	X	607	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	31	GLN
5	X	437	GLN
5	Y	242	HIS
5	X	28	ASN
5	X	242	HIS

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 8 ligands modelled in this entry, 6 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	$\# Z > 2$
6	RFP	C	1401	-	63,63,63	2.39	11 (17%)	94,94,94	2.28	30 (31%)
6	RFP	H	1401	-	63,63,63	2.45	11 (17%)	94,94,94	2.03	28 (29%)

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
6	RFP	C	1401	-	-	0/60/85/85	0/1/5/5
6	RFP	H	1401	-	-	1/60/85/85	0/1/5/5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	RFP	O3-C6	12.62	1.57	1.37
6	H	1401	RFP	O3-C6	12.49	1.57	1.37
6	H	1401	RFP	C15-N1	6.99	1.50	1.35
6	C	1401	RFP	C12-C11	-6.34	1.36	1.54
6	C	1401	RFP	C15-N1	6.32	1.48	1.35

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	RFP	C2-C3-C43	-6.88	115.01	123.70
6	C	1401	RFP	O4-C11-C5	-6.16	122.02	132.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1401	RFP	C41-C42-N4	5.98	117.42	110.82
6	H	1401	RFP	O4-C11-C5	-5.93	122.40	132.35
6	C	1401	RFP	O7-C35-C36	5.32	121.14	111.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1401	RFP	C29-C28-C27-C26

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 ⓘ

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	323/329 (98%)	0.26	6 (1%) 64 47	0, 73, 165, 263	0
1	B	221/329 (67%)	0.50	16 (7%) 15 14	3, 97, 189, 266	0
1	F	229/329 (69%)	0.58	15 (6%) 18 16	16, 121, 201, 266	0
1	G	217/329 (65%)	0.53	11 (5%) 27 22	39, 111, 186, 215	0
2	C	1335/1342 (99%)	0.17	41 (3%) 47 35	0, 48, 166, 284	0
2	H	1335/1342 (99%)	0.33	60 (4%) 32 25	1, 86, 201, 341	0
3	D	1160/1407 (82%)	0.18	28 (2%) 56 41	0, 40, 157, 284	0
3	I	1160/1407 (82%)	0.31	48 (4%) 35 27	1, 52, 180, 322	0
4	E	90/91 (98%)	-0.04	1 (1%) 77 60	0, 40, 109, 159	0
4	J	76/91 (83%)	0.35	2 (2%) 53 39	5, 76, 155, 167	0
5	X	517/613 (84%)	0.36	25 (4%) 29 23	3, 99, 228, 365	0
5	Y	458/613 (74%)	0.33	28 (6%) 21 18	2, 102, 219, 328	0
All	All	7121/8222 (86%)	0.29	281 (3%) 37 29	0, 70, 190, 365	0

The worst 5 of 281 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1002	LEU	12.6
3	I	10	ALA	8.6
5	X	319	ALA	8.2
5	X	36	VAL	8.2
2	H	1001	GLY	8.1

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	MG	I	1503	1/1	0.73	3.30	20,20,20,20	0
6	RFP	H	1401	59/59	0.36	1.51	20,20,20,20	0
6	RFP	C	1401	59/59	0.30	0.95	20,20,20,20	0
8	MG	D	1503	1/1	0.17	-0.10	24,24,24,24	0
7	ZN	I	1502	1/1	0.18	-0.30	49,49,49,49	0
7	ZN	D	1502	1/1	0.16	-0.68	8,8,8,8	0
7	ZN	D	1501	1/1	0.09	-1.23	54,54,54,54	0
7	ZN	I	1501	1/1	0.05	-1.45	60,60,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.