



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:56 AM GMT

PDB ID : 2JA5
Title : CPD lesion containing RNA Polymerase II elongation complex A
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on : 2006-11-23
Resolution : 3.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

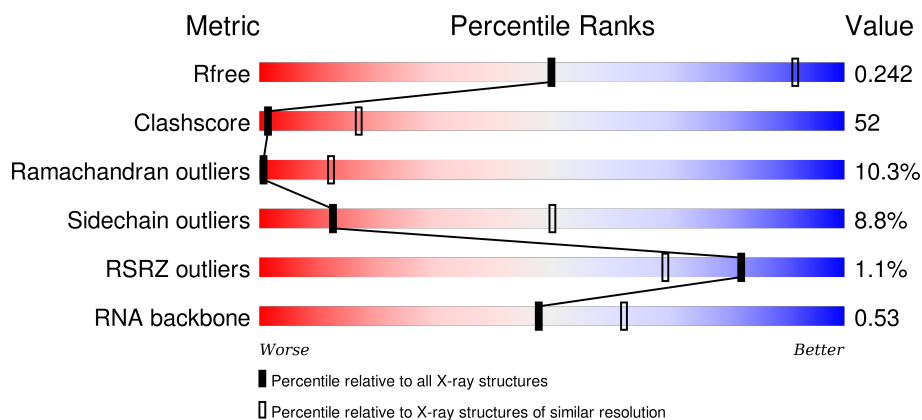
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.






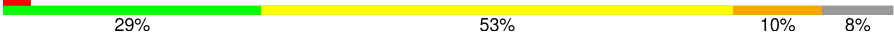
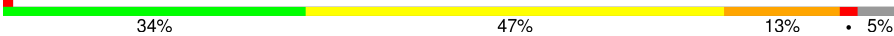
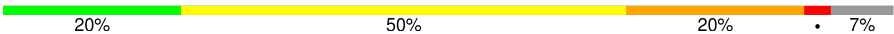
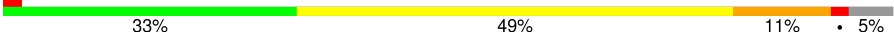
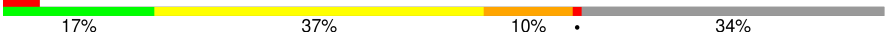
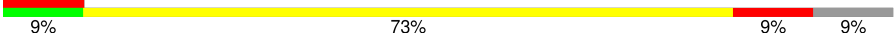

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1733	<div> <div></div> <div> <div></div> <div>26%</div> <div>45%</div> <div>10%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div></div> <div> <div></div> <div>27%</div> <div>52%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>25%</div> <div>49%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>
4	D	221	<div> <div></div> <div> <div></div> <div>25%</div> <div>41%</div> <div>12%</div> <div>•</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	P	11	
14	T	25	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31660 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 II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8866	5614	1553	1644	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	10	Total	C	N	O	P	0	0	0
			212	96	41	66	9			

- Molecule 14 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TTP*TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	11	Total	Br	C	N	O	P	0	0	0
			219	1	106	34	68	10			

- Molecule 15 is a DNA chain called 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
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- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

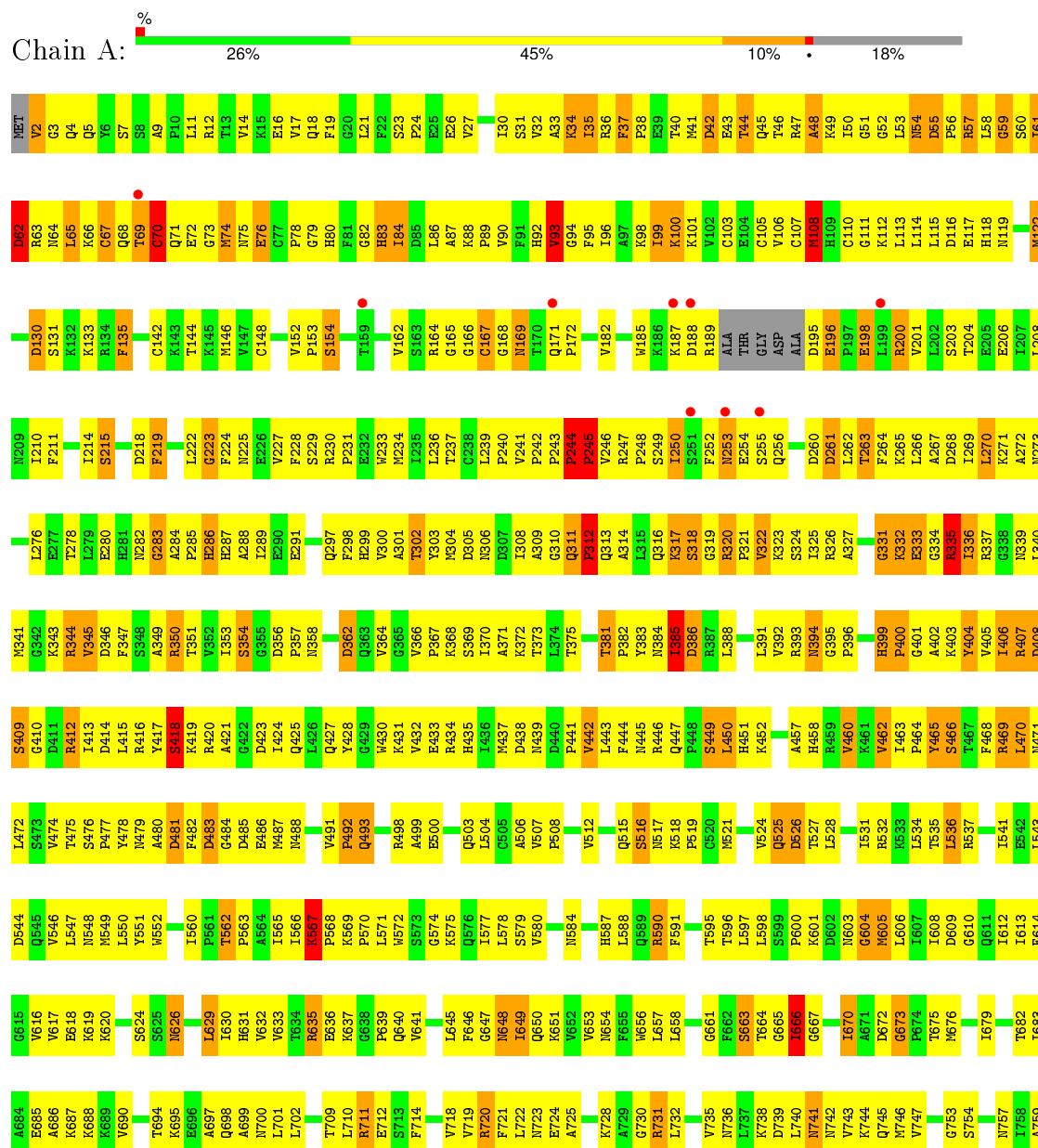
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	8	Total	Zn	0	0
			8	8		

3 Residue-property plots

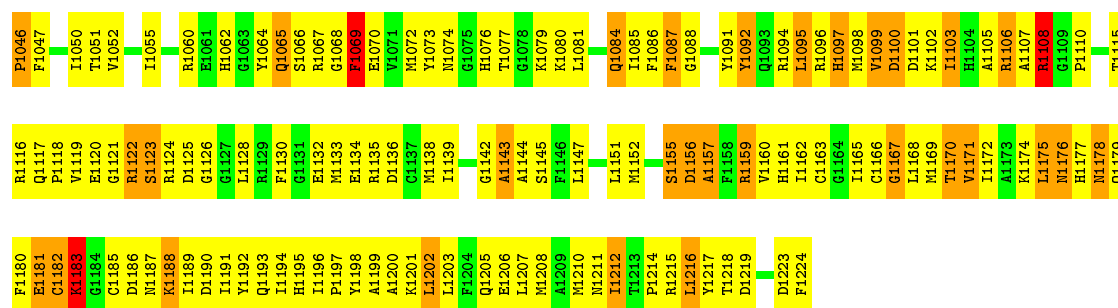
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 II LARGEST SUBUNIT

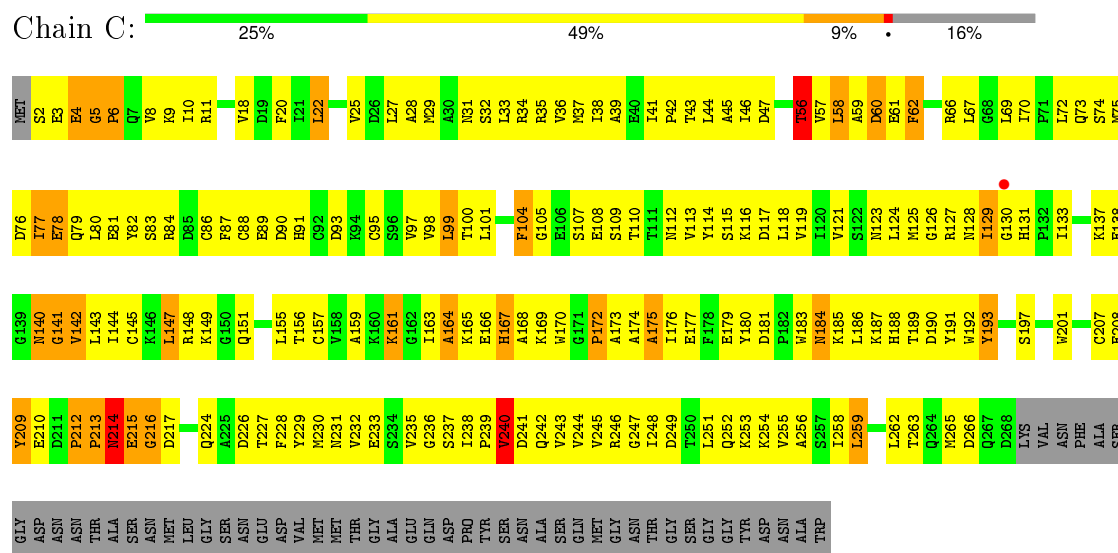




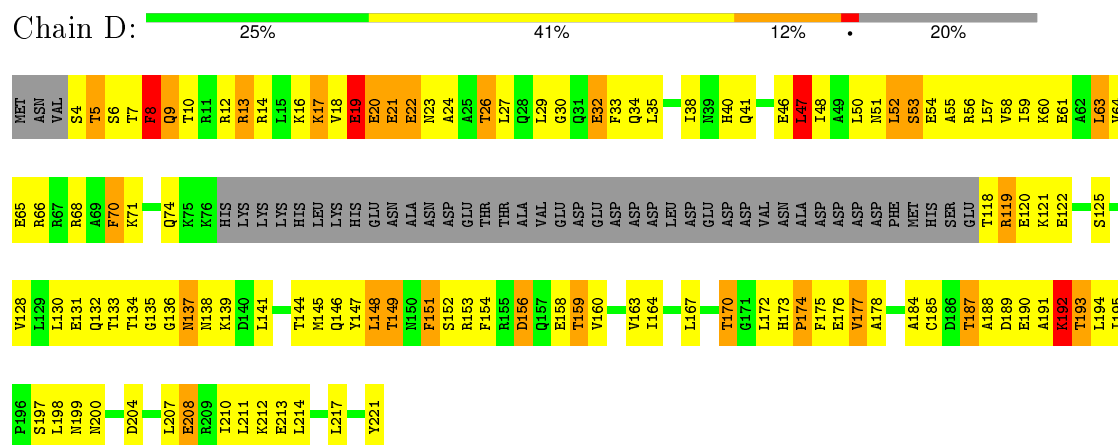
Q986	Y98	Y731	ILE	T602	B529	A460	K393	E328	L258	D188	L128	B65	MET
Q987	P799	S732	GLU	L603	G530	L461	D394	T329	Y259	L189	F129	D66	SER
G988	Q800	H733	GLY	R604	Q531	A462	Q395	A330	G260	V130	V130	S67	ASP
T989	P802	H734	PHE	R605	A532	T463	D396	L331	D261	K191	D131	LEU	ALA
G990	T805	T737	GLU	K606	K537	G464	D397	D332	E262	K132	K132	I70	ASN
G991	T806	T738	ASP	D608	N538	N465	D399	F333	G263	K193	K193	LEU	SER
G992	T807	T739	VAL	I609	L539	N466	R400	I334	S264	E194	L192	GLU	GLU
G993	R807	H740	GLU	P611	S540	G467	F401	G336	S265	K196	L192	GLU	LYS
G994	A808	C741	GLU	B612	N542	Q469	Q402	R337	A266	F197	T197	ALA	TYR
G995	N809	E742	GLU	P613	N542	Q470	K403	G338	T268	D198	T198	GLN	TYR
G996	B810	E743	T680	V613	V647	K471	K404	T339	I269	M199	I199	HIS	ASP
G997	B811	H744	H681	S614	N546	A472	R405	A340	LEU	ALA	ILE	THR	GLU
G998	L812	P745	S682	R615	G546	N473		A343	L273	T204	T204	THR	ASP
G999	S813	S746	S683	I616	T549	S474	L408	T343	P274	I205	I205	GLU	PRO
G1000	F814	M747	L684	D617	D550	S475	A409	K344	Y275	M206	M206	SER	TYR
F1001	R815	I748	D618	P651	P651		Q410	K345	I276	G207	G207	ASP	GLY
T1002	R816	L749	N686	N552	N552	V479	P411	E346	K277	ARG	ARG	ASN	F18
A1003	E816	G750	N687	R620	P653	S480	L412	K347	Q278	K210	K210	ILE	E19
E1004	P818	V751	G688	B621	I554	Q481	L413	R348	D279	V211	V211	SER	D20
G1005	A819	A752	L689	B622	I555	Q482	A414	R348	P281	L212	L212	ARG	A23
T1006	G820	A753	V690	B623	I555	N483		Y351	P281	L213	L213	LYS	P24
V1007	Q821	A753	E691	L624	F557	N484	T419	K355	I282	A214	A214	TYR	T25
P1008	N822	I756	Y692	K625	L558	R495	L420	L356	LEU	D215	D215	GLU	T26
P1009	A823	P757	I693	I626	S559	Y486	F421	Q357	ILE	E216	E216	I90	T27
L1010	I824	F758	E696	P627	E560	T487		K358	ALA	R217	R217	GLU	E28
I1011	V825	P759	E697	D629	N561		L424	F358	R287	G220	G220	GLU	D29
E1012	A826	D760	E698	D629	N561	S490	T425	K359	I95	N221	N221	SER	S30
N1013	I827	H761	E698	D630	N563	T491	K426	F360	Y96	N221	N221	GLU	Y97
P1014	A828	N762	E699	B633	Y569	R496	D427	L361	T291	V223	V223	ASP	T98
H1015	G829	Q763	S700	V634	N570	R497	F429	P362	I292	Q224	Q224	ASP	T34
A1016	B830	S764	I701	R635	N571	T498	R430	H363	P293	V225	V225	SER	S35
I1017	S831	P765	L702	P636	P571	N499	Y431	I364	D294	F226	F226	GLU	A36
S1019	G832	R766	A704	L637	P575		N432	Q366	E296	K227	K227	SER	F37
R1020	Y833	N767	M705	F638	P575	I502	Q433	L367	I297	K228	K228	GLY	F38
H1021	Q835	Y769	Q706	I639	A577	GLY	R434	E368	L298	A229	A229	E104	R39
T1022	B836	Q770	P707	B641	N578	ARG		G369	E299	A230	A230	S105	E40
V1023	D837	S771	E708	D642	N579	ASP	E437	F370	H300	F166	F166	D106	K41
A1024	S838	A772	D709	D643	N580	GLY	GLU	E371		G107	G107	G107	K42
H1025	N839	F771	L710	B644	N581	LYS	ALA	S372	Y303	G168	G168	V108	L43
L1026	R841	Q776	E711	B644	N582	LEU	HIS	R373	D304	R169	R169	T109	V44
I1027	N842	A777	P712	K649	N583	ALA	ASP		V305	S235	S235	H110	S45
K965	N843	N778	A713	B650	G584	K510	PHE	F376	W308	H236	H236	A111	Q46
V966	Q843	L782	E714	L651	N585	P511	ASN	F377	Q309	V237	V237	L112	Q47
G1029	S844	L782	A715	R652	N586	R512	MET	L378		A238	A238	Y113	L48
L1030	S845		ASN	R653	N587	Q513	LYS	G379	Q309	E239	E239	P114	
L1031	I846	Y785	GLU	R654	G588	L514	L446	Y380	M310	R175	R175	Q115	F51
V1034	D847	N786	GLU	K655	N589	H515	A447	N381	E312	K176	K176	E116	N52
A1035	R848	R787	ASN	G656	N590	N516	T448	I382	R241	S176	S176	K177	Q53
A1036	G849	R788	ASP	G657	N591	T517	N449	N383	L314	N178	N178	A117	F54
L1037	L850	N789	LEU	I658	N592	H518	A450	I384	K315	C179	C179	R118	V55
S1038	F851	D790	ASP	A659	N593	W519	K451	L385	P316	Y180	Y180	R120	D56
G1039	R852	T791	D722	R660	A594	G520	T452	L386	C317	K246	K246	N121	V57
N1040	S853	N792	D724	L661	N597	L521	L453	L387		G247	G247	T122	T58
E1041	L854	A793			N597	L521	T454	C388	F322	S248	S248	T123	
G1042	F855	N794	K727	B665	N598	A525		A389	W323	R249	R249	Y124	D61
D1043	P856	I795	R728	Y666	T599	E526	L457	L390	I324			S125	I62
A1044	N857	L796	I729	Y667	L600	T527	K458	D391		I254	I254	S126	I63
S1045	S858	Y797	R730	D668	N601	P528	Y459	R392	R327			G127	O54



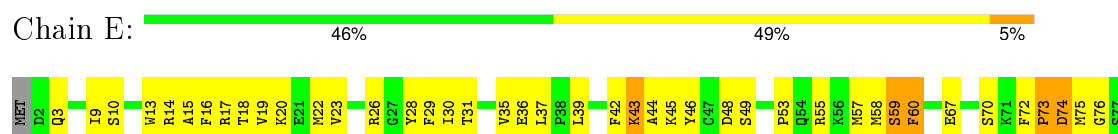
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE

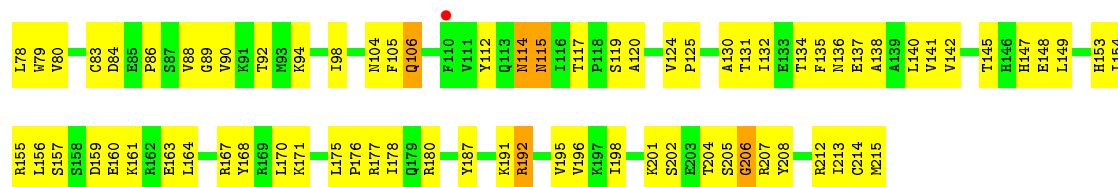


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE



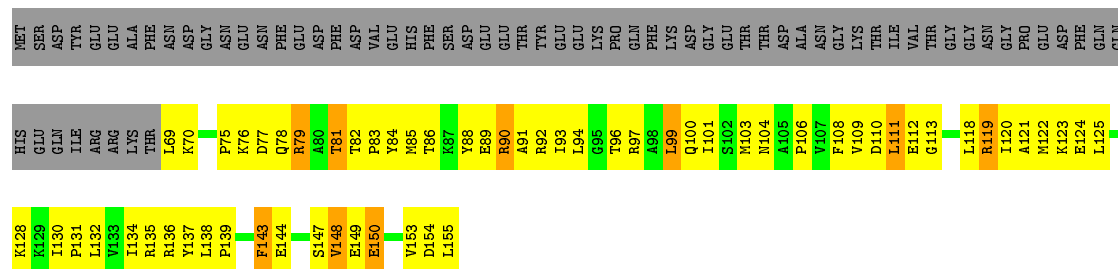
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE





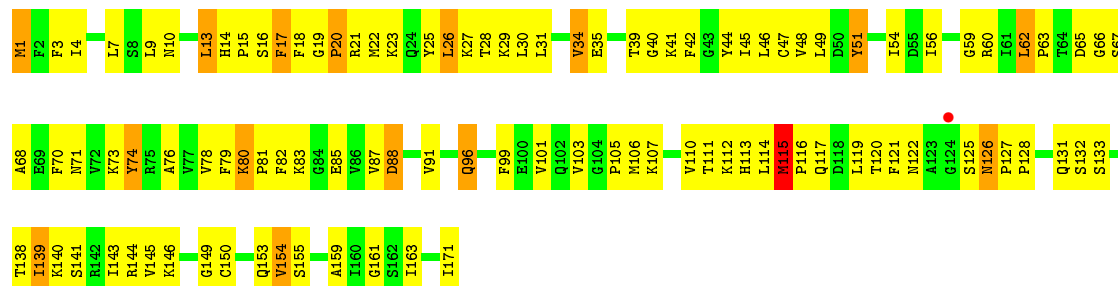
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

Chain F: 17% 34% 6% 44%



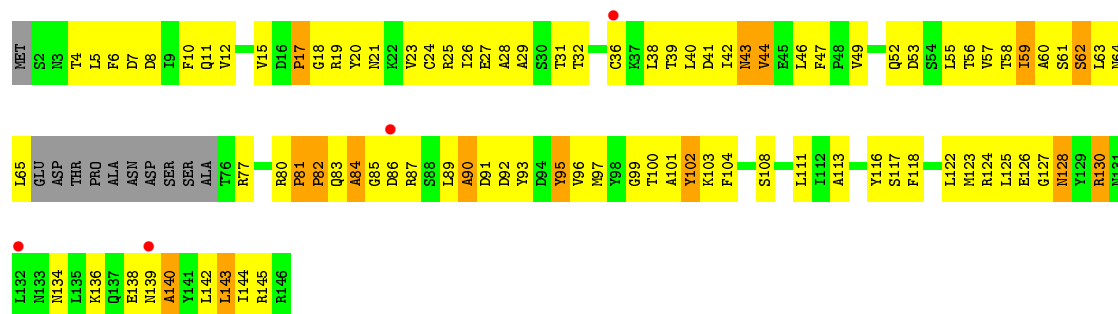
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

Chain G: 39% 52% 9%



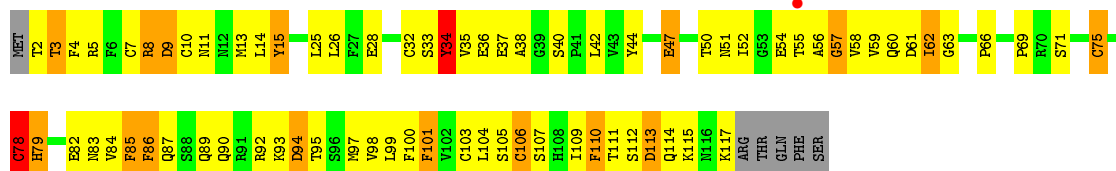
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

Chain H: 3% 29% 53% 10% 8%

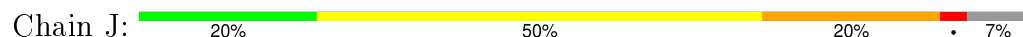


- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

Chain I: 34% 47% 13% 5%



• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10



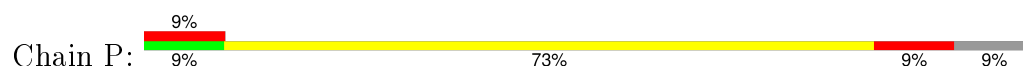
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE



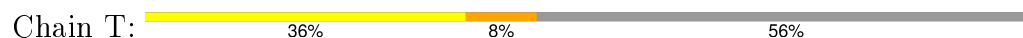
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE



• Molecule 13: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'



• Molecule 14: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TTP*TP*TP*CP*CP *BRUP*GP*GP*TP*CP*AP*TP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.21Å 392.21Å 284.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 48.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.80) 99.0 (48.98-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270 , 0.280 0.227 , 0.242	Depositor DCC
R_{free} test set	2412 reflections (2.08%)	DCC
Wilson B-factor (Å ²)	99.7	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 70.2	EDS
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 235886 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31660	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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, 0.375 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: MG, ZN, BRU

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	0/11385	0.73	1/15393 (0.0%)
2	B	0.46	0/9037	0.71	2/12181 (0.0%)
3	C	0.48	0/2138	0.72	0/2896
4	D	0.43	0/1437	0.68	1/1925 (0.1%)
5	E	0.43	0/1788	0.63	0/2406
6	F	0.55	0/716	0.77	0/964
7	G	0.48	0/1368	0.73	0/1844
8	H	0.40	0/1102	0.67	0/1492
9	I	0.41	0/962	0.68	0/1295
10	J	0.50	0/541	0.79	1/727 (0.1%)
11	K	0.90	6/937 (0.6%)	1.02	11/1265 (0.9%)
12	L	0.44	0/366	0.70	0/485
13	P	1.13	1/237 (0.4%)	1.22	2/368 (0.5%)
14	T	1.05	0/220	1.33	0/335
All	All	0.50	7/32234 (0.0%)	0.74	18/43576 (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
1	A	0	1
2	B	0	1
14	T	0	2
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	112	GLN	CA-C	9.87	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	N-CA	9.16	1.64	1.46
11	K	112	GLN	CB-CG	9.05	1.76	1.52
11	K	112	GLN	N-CA	8.12	1.62	1.46
11	K	112	GLN	CG-CD	6.57	1.66	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	113	THR	N-CA-C	9.53	136.74	111.00
13	P	1	U	N1-C1'-C2'	9.37	126.18	114.00
11	K	112	GLN	N-CA-C	8.61	134.26	111.00
11	K	114	LEU	CB-CG-CD1	8.38	125.24	111.00
11	K	114	LEU	N-CA-C	7.93	132.41	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
2	B	486	TYR	Sidechain
14	T	19	DT	Sidechain
14	T	20	DC	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	11186	0	11266	1286	0
2	B	8866	0	8898	1020	0
3	C	2101	0	2055	267	0
4	D	1427	0	1451	141	0
5	E	1752	0	1776	127	0
6	F	705	0	730	84	0
7	G	1340	0	1357	161	0
8	H	1084	0	1057	123	0
9	I	944	0	899	101	0
10	J	532	0	542	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	919	0	929	109	0
12	L	364	0	386	43	0
13	P	212	0	109	20	0
14	T	219	0	125	31	0
16	A	1	0	0	0	0
17	A	8	0	0	0	0
All	All	31660	0	31580	3314	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 52.

The worst 5 of 3314 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)
11:K:112:GLN:CB	11:K:112:GLN:CG	1.77	1.62
11:K:112:GLN:CA	11:K:112:GLN:C	1.78	1.51
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.18	1.17
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.26	1.17
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.12	1.15

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	1410/1733 (81%)	975 (69%)	289 (20%)	146 (10%)	1	12
2	B	1096/1224 (90%)	781 (71%)	200 (18%)	115 (10%)	1	11
3	C	264/318 (83%)	171 (65%)	65 (25%)	28 (11%)	0	11
4	D	173/221 (78%)	124 (72%)	31 (18%)	18 (10%)	1	12
5	E	212/215 (99%)	154 (73%)	44 (21%)	14 (7%)	1	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	84/155 (54%)	69 (82%)	11 (13%)	4 (5%)	3	32
7	G	169/171 (99%)	131 (78%)	28 (17%)	10 (6%)	2	27
8	H	131/146 (90%)	82 (63%)	32 (24%)	17 (13%)	0	7
9	I	114/122 (93%)	80 (70%)	23 (20%)	11 (10%)	1	14
10	J	63/70 (90%)	37 (59%)	12 (19%)	14 (22%)	0	1
11	K	112/120 (93%)	85 (76%)	16 (14%)	11 (10%)	1	14
12	L	44/70 (63%)	18 (41%)	17 (39%)	9 (20%)	0	2
All	All	3872/4565 (85%)	2707 (70%)	768 (20%)	397 (10%)	1	12

5 of 397 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1244/1520 (82%)	1129 (91%)	115 (9%)	11	48
2	B	967/1061 (91%)	884 (91%)	83 (9%)	13	51
3	C	235/274 (86%)	214 (91%)	21 (9%)	12	50
4	D	159/200 (80%)	135 (85%)	24 (15%)	3	25
5	E	196/197 (100%)	192 (98%)	4 (2%)	63	87
6	F	77/137 (56%)	69 (90%)	8 (10%)	9	42
7	G	152/152 (100%)	141 (93%)	11 (7%)	18	58
8	H	119/128 (93%)	113 (95%)	6 (5%)	30	70
9	I	110/116 (95%)	98 (89%)	12 (11%)	8	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	60/65 (92%)	53 (88%)	7 (12%)	7	36
11	K	99/102 (97%)	89 (90%)	10 (10%)	9	43
12	L	40/57 (70%)	36 (90%)	4 (10%)	9	43
All	All	3458/4009 (86%)	3153 (91%)	305 (9%)	12	50

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	429	PHE
2	B	909	ASP
9	I	94	ASP
2	B	496	ARG
2	B	682	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	515	HIS
2	B	842	ASN
9	I	12	ASN
2	B	516	ASN
2	B	734	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	9/11 (81%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	10	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
14	BRU	T	22	13,14	13,21,22	2.05	3 (23%)	16,30,33	4.03	3 (18%)

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
14	BRU	T	22	13,14	-	0/3/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	22	BRU	C6-N1	2.95	1.39	1.35
14	T	22	BRU	C4-N3	3.20	1.39	1.33
14	T	22	BRU	C4-C5	5.46	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	22	BRU	C5-C4-N3	-7.96	115.51	124.00
14	T	22	BRU	C5-C6-N1	2.02	123.75	119.79
14	T	22	BRU	C4-N3-C2	13.58	126.98	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	22	BRU	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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, 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	1421/1733 (81%)	-0.31	12 (0%) 87 77	12, 73, 146, 189	0
2	B	1115/1224 (91%)	-0.22	17 (1%) 76 62	12, 83, 154, 191	0
3	C	267/318 (83%)	-0.37	1 (0%) 93 87	30, 69, 125, 150	0
4	D	177/221 (80%)	-0.15	0 100 100	53, 104, 145, 162	0
5	E	214/215 (99%)	-0.16	1 (0%) 91 85	45, 126, 174, 178	0
6	F	87/155 (56%)	-0.51	0 100 100	17, 49, 91, 119	0
7	G	171/171 (100%)	-0.23	1 (0%) 90 82	53, 77, 115, 126	0
8	H	135/146 (92%)	0.23	4 (2%) 54 37	87, 128, 162, 171	0
9	I	116/122 (95%)	-0.03	1 (0%) 85 74	69, 122, 151, 173	0
10	J	65/70 (92%)	-0.59	0 100 100	35, 66, 109, 118	0
11	K	114/120 (95%)	-0.30	2 (1%) 71 56	33, 73, 102, 140	0
12	L	46/70 (65%)	0.35	3 (6%) 22 13	69, 141, 161, 169	0
13	P	10/11 (90%)	0.00	1 (10%) 9 6	71, 85, 160, 163	0
14	T	10/25 (40%)	-0.34	0 100 100	72, 96, 137, 158	0
All	All	3948/4601 (85%)	-0.25	43 (1%) 82 69	12, 82, 154, 191	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	113	THR	6.4
11	K	114	LEU	6.4
2	B	882	THR	5.4
2	B	471	LYS	3.8
8	H	139	ASN	3.6

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	BRU	T	22	20/21	0.87	0.18	-	59,61,68,69	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
17	ZN	A	2460	1/1	0.99	0.14	-0.46	69,69,69,69	0
17	ZN	A	2463	1/1	0.99	0.13	-1.12	42,42,42,42	0
17	ZN	A	2462	1/1	0.99	0.07	-1.24	23,23,23,23	0
17	ZN	A	2461	1/1	0.98	0.08	-1.37	163,163,163,163	0
17	ZN	A	2465	1/1	0.99	0.07	-1.86	31,31,31,31	0
17	ZN	A	2459	1/1	0.99	0.04	-2.05	115,115,115,115	0
17	ZN	A	2458	1/1	1.00	0.14	-2.29	51,51,51,51	0
17	ZN	A	2464	1/1	0.98	0.07	-2.87	82,82,82,82	0
16	MG	A	2457	1/1	1.00	0.15	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.