



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 04:00 PM UTC

PDB ID : 3GTL / pdb_00003gtl
Title : Backtracked RNA polymerase II complex with 13mer with G<>U mismatch
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.38 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

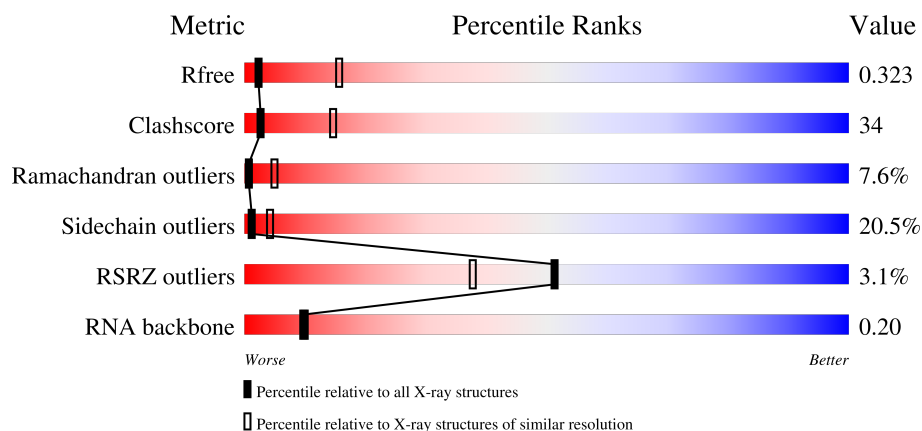
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)
RNA backbone	3983	1122 (3.76-3.00)

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	1733	
2	B	1224	
3	C	318	
4	E	215	

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	13	
12	T	28	
13	N	14	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 29256 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 subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	12	Total	C	N	O	P	0	0	0
			257	116	49	81	11			

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 13 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total 2	Zn 2	0	0
14	B	1	Total 1	Zn 1	0	0
14	C	1	Total 1	Zn 1	0	0
14	I	2	Total 2	Zn 2	0	0
14	J	1	Total 1	Zn 1	0	0
14	L	1	Total 1	Zn 1	0	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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.

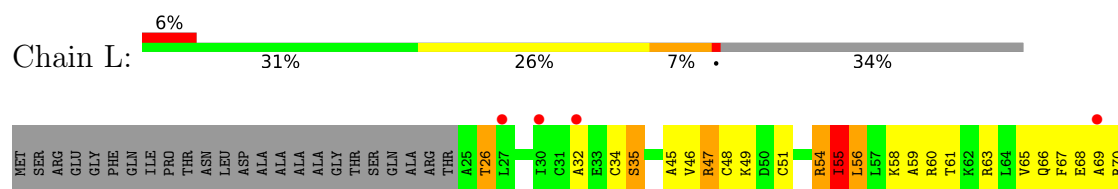
- Chain A: 2% 33% 34% 12% 20%

Sequence logo for Chain A showing amino acid conservation. The y-axis represents information content in bits (0.00 to 2.00). The x-axis shows amino acids: MET, VAL, G3, Q4, N169, Q5, Y6, S7, L11, R12, R13, T13, V14, K15, E16, V17, Q18, R19, K20, F19, G20, L21, V27, I30, S31, R36, F37, P38, E39, T40, M41, D42, E43, T44, Q45, T46, R47, A48, K129, D130, I50, G51, L52, G53, N54, D55, P56, R57, L58, C67, Q68, T69, P153, K154, G155, ASP, PRO, THR, C70, E76, C77, P78, G79, H80.

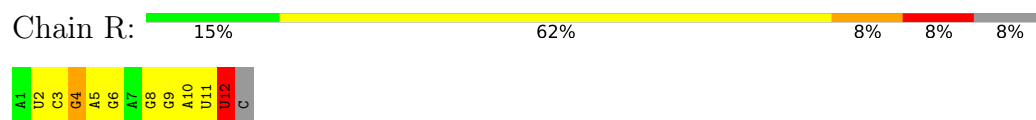


LEU	GLY	GLN	ARG	THR	ALA	ASN	SER	GLU	LYS	TYR	GLU	TYR	ASP	ASP	GLU	ASP	PRO	TYR	LYS	PHE	GLY	D20	E21	I25	T26	A27	E28	D29	S30	W31	A32	V33	I34	S35	A36	F37	F38	Q39	E40	A41	R42	L43	V44	S45	Q46	Q47	L48	V49	D50	D51	T52	I53	Q54	P55	R56	S57	T58	V59	W60	X61	Y62	Z63			
LEU	GLN	GLU	LEU	LEU	ALA	GLN	HIS	THR	THR	GLU	GLU	GLU	THR	SER	GLU	ASP	ASP	GLU	LYS	TYR	GLY	I90	K94	T98	K99	P100	M101	E102	S103	W104	A105	D106	V107	T108	I109	L110	K111	L112	K113	E114	A115	R116	L117	F118	D119	M120	N121	L122	Q123	V124	W125	F126	T127	I128	Q129	P130	R131	S132	T133	V134	W135	X136	Y137	Z138	
LEU	LYS	TYR	TYR	ILE	ALA	GLU	GLU	GLU	SER	GLU	GLU	GLU	GLU	ASP	ASP	ASP	SER	GLU	GLU	GLY	K164	V165	F166	G167	R168	L169	L170	R171	S172	S173	S174	S175	D176	L177	R178	I179	Y180	L181	E182	A183	C184	P185	F186	R187	D188	M189	N190	L191	T192	Q193	V194	W195	F196	T197	I198	Q199	P200	R201	S202	T203	V204	W205	X206	Y207	Z208
T222	V223	V224	Q225	F226	K227	K228	S232	P233	I234	H235	H236	V237	A238	I240	L244	E245	K246	G247	S248	R249	F250	I251	T252	T253	V256	K257	L258	R261	E262	G263	S264	T268	I269	L273	P274	V275	I276	K277	Q278	D279	V283	I284	T285	F286	R287	K358	L359	F360	L361	I291	I292	P293													
D294	G295	E296	I297	I301	C302	Y303	D304	V305	N306	D307	H308	Q309	M310	E312	M313	L314	K315	P316	D320	G321	F322	V323	I324	Q325	D326	R327	E328	T329	D332	G335	ARG	ARG	GLY	THR	ALA	LEU	GLY	ILE	LYS	K345	E346	K347	R348	I349	T355	L356	Q357	K358	L424	T425	F360	L361	I291	I292	P293										
I364	T365	Q366	F370	E371	S372	R373	F377	L378	G379	Y380	H381	N382	N383	R384	L385	L386	L387	C388	A389	L390	D391	R392	K393	Q394	Q395	D396	D397	R398	F401	K404	R405	L406	D407	L408	A409	G410	P411	LEU	GLY	ILE	LYS	K345	E346	K347	R348	I349	T355	L356	Q357	K358	L424	T425	F360	L361	I291	I292	P293								
R430	Q433	Q434	T435	V436	E437	GLU	ALA	HIS	ASP	PHE	ASN	MET	LYS	L446	A447	I448	K451	T452	I453	T454	L457	K458	Y459	A460	L461	A462	T463	G464	M465	W466	G467	E468	Q469	K470	A471	M472	M473	S474	S475	R476	A477	G478	V479	S480	Q481	V482	L483	N484	R485	Y486	T487	Y488	S489	S490	T491	L492									
S493	H494	L495	R496	L497	T498	N499	T500	P501	I502	ARG	ASP	GLY	LYS	A509	B512	Q513	L514	H515	N516	T517	H518	W519	G520	L521	P524	A525	E526	T527	P528	E529	O530	Q531	A532	C533	G534	L535	V536	K537	S540	L541	M542	S543	C544	T545	S546	V547	G548	T549	D550	P551	M552	P553	T554	I555											
E560	P565	L566	E567	D568	V569	V570	A577	V582	H587	G588	V589	H590	R591	N592	L600	E601	E604	R605	K606	E612	V613	S614	M615	L616	L619	L624	K625	L626	F627	T628	G631	R632	V633	Y634	R635	P636	L637	F638	L639	V640	E641	D642	S645	H646	K649	E650																			
L651	K652	V653	R654	K655	G656	H657	L658	T664	D668	ILE	GLU	GLY	PHE	GLU	VAL	GLU	E678	Y679	T680	V681	S682	S683	L684	L685	N686	L689	V690	E691	Y692	I693	D694	E698	I701	L702	L703	A704	Y705	Q706	P707	E708	D709	L710	E711	P712	Y713	E714	A715	ASN	GLU	GLU	ASN	ASP													
LEU	D722	R728	I729	R730	V731	S732	H733	H734	A735	T736	F738	I739	H740	E741	C742	I743	H744	P745	S746	M747	T748	L749	G750	V751	A752	A753	S754	I755	I756	P757	F758	N762	Q763	S764	P765	R766	N767	T768	Y769	Q770	M773	G774	K775	D776	A777	M778	G779	V780	L781	F782	T783	N784	V787												
R788	M789	D790	T791	M792	A793	L796	Y797	Y798	M800	K801	P802	L803	G804	T805	T806	R807	A808	M809	E810	Y811	L812	K813	F814	R815	E816	L817	P818	I819	H820	Q821	R822	K823	L824	R825	A826	R827	R828	P829	R830	S831	D832	V833	R834	Q835	E836	D837	S838	M839	L840	R841	M842	Q843	R844	ASN	ASP	L846	D847	R848	P849						
G849	L850	F851	F855	F856	R857	S858	Y859	M860	D861	K864	K865	Y866	T871	E872	T873	R879	T880	N881	L882	L883	K884	R885	T886	N887	D891	D894	D895	D896	G897	L898	T899	A900	G902	V903	R904	V905	S906	D909	V910	I911	D912	G913	T916	P917	N918	S919	R924	S925	ASP	GLU	GLU	D947	G985	Q986	K987	G988									
LEU	GLY	GLN	ARG	THR	ALA	ASN	SER	GLU	LYS	TYR	GLU	TYR	ASP	ASP	GLU	ASP	PRO	TYR	LYS	PHE	GLY	D20	E21	I25	T26	A27	E28	D29	S30	W31	A32	V33	I34	S35	A36	F37	F38	Q39	E40	A41	R42	L43	V44	S45	Q46	Q47	L48	V49	D50	D51	T52	I53	Q54	P55	R56	S57	T58	V59	W60	X61	Y62	Z63			

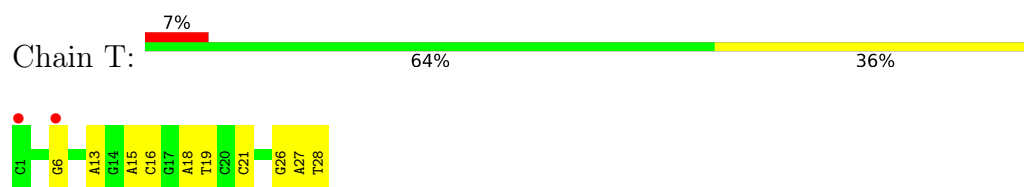
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



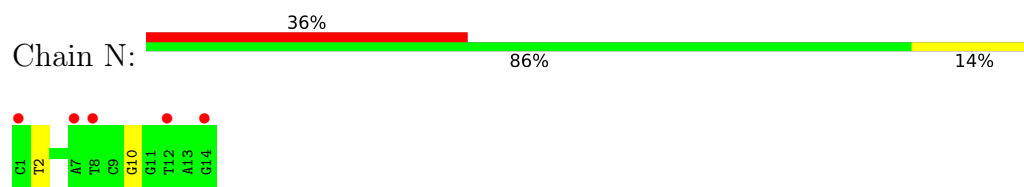
- Molecule 11: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*UP*C)-3')



- Molecule 12: DNA (28-MER)



- Molecule 13: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.53Å 222.28Å 194.81Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	50.00 – 3.38 50.00 – 3.38	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-3.38) 91.2 (50.00-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.270 , 0.322 0.277 , 0.323	Depositor DCC
R_{free} test set	4515 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	95.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 107.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29256	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.74	3/11163 (0.0%)	1.08	48/15091 (0.3%)
2	B	0.78	2/8963 (0.0%)	1.12	43/12086 (0.4%)
3	C	0.81	1/2133 (0.0%)	1.14	11/2891 (0.4%)
4	E	0.59	0/1788	0.94	3/2406 (0.1%)
5	F	0.62	0/691	0.91	0/933
6	H	0.62	0/1086	0.97	5/1470 (0.3%)
7	I	0.57	0/989	0.94	3/1331 (0.2%)
8	J	1.00	1/541 (0.2%)	1.33	5/727 (0.7%)
9	K	0.71	0/937	1.17	6/1265 (0.5%)
10	L	0.80	0/365	1.08	1/485 (0.2%)
11	R	0.77	1/288 (0.3%)	1.27	2/448 (0.4%)
12	T	0.39	0/634	1.05	1/975 (0.1%)
13	N	0.30	0/317	0.83	1/488 (0.2%)
All	All	0.74	8/29895 (0.0%)	1.08	129/40596 (0.3%)

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
8	J	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	9	SER	N-CA	8.58	1.56	1.46
2	B	751	VAL	CA-CB	7.80	1.65	1.54
11	R	12	U	C1'-N1	6.40	1.57	1.47
1	A	366	VAL	N-CA	6.36	1.51	1.46
1	A	527	THR	CA-CB	6.20	1.64	1.53

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	VAL	N-CA-C	10.10	120.96	110.36
9	K	65	HIS	CA-C-N	9.54	131.77	119.84
9	K	65	HIS	C-N-CA	9.54	131.77	119.84
2	B	1122	ARG	N-CA-C	-9.50	102.19	113.88
8	J	9	SER	N-CA-C	9.50	121.33	110.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	4	PRO	Peptide

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	10969	0	11071	810	0
2	B	8792	0	8823	798	0
3	C	2095	0	2051	166	0
4	E	1752	0	1776	58	0
5	F	679	0	701	43	0
6	H	1068	0	1040	63	0
7	I	971	0	930	47	0
8	J	532	0	543	72	0
9	K	919	0	929	68	0
10	L	363	0	387	18	0
11	R	257	0	131	15	0
12	T	566	0	316	18	0
13	N	284	0	161	1	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29256	0	28859	1958	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 34.

The worst 5 of 1958 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:B:636:PRO:CB	2:B:637:LEU:HA	1.49	1.35
2:B:848:ARG:HD2	8:J:7:CYS:O	1.32	1.26
2:B:827:ILE:HG23	2:B:1012:ILE:CD1	1.68	1.24
2:B:1002:THR:CG2	2:B:1006:ILE:HG12	1.66	1.24
1:A:482:PHE:CD1	2:B:836:GLU:HB3	1.73	1.23

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	1383/1733 (80%)	1021 (74%)	249 (18%)	113 (8%)	0	4
2	B	1088/1224 (89%)	820 (75%)	186 (17%)	82 (8%)	1	5
3	C	264/318 (83%)	192 (73%)	48 (18%)	24 (9%)	0	3
4	E	212/215 (99%)	177 (84%)	28 (13%)	7 (3%)	3	17
5	F	82/155 (53%)	58 (71%)	20 (24%)	4 (5%)	1	11
6	H	129/146 (88%)	101 (78%)	19 (15%)	9 (7%)	1	6
7	I	117/122 (96%)	84 (72%)	22 (19%)	11 (9%)	0	3
8	J	63/70 (90%)	50 (79%)	10 (16%)	3 (5%)	2	11
9	K	112/120 (93%)	88 (79%)	18 (16%)	6 (5%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	44/70 (63%)	25 (57%)	12 (27%)	7 (16%)	0	0
All	All	3494/4173 (84%)	2616 (75%)	612 (18%)	266 (8%)	1	5

5 of 266 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	55	ASP
1	A	130	ASP
1	A	226	GLU
1	A	248	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1520 (80%)	953 (78%)	265 (22%)	1	3
2	B	960/1061 (90%)	756 (79%)	204 (21%)	1	3
3	C	234/274 (85%)	176 (75%)	58 (25%)	1	2
4	E	196/197 (100%)	175 (89%)	21 (11%)	6	23
5	F	74/137 (54%)	63 (85%)	11 (15%)	3	12
6	H	117/128 (91%)	98 (84%)	19 (16%)	2	10
7	I	113/116 (97%)	89 (79%)	24 (21%)	1	3
8	J	60/65 (92%)	45 (75%)	15 (25%)	0	1
9	K	99/102 (97%)	84 (85%)	15 (15%)	3	11
10	L	40/57 (70%)	33 (82%)	7 (18%)	2	8
All	All	3111/3657 (85%)	2472 (80%)	639 (20%)	1	4

5 of 639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1185	CYS

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Mol	Chain	Res	Type
6	H	123	MET
3	C	43	THR
2	B	1175	LEU
3	C	243	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	744	HIS
2	B	1177	HIS
9	K	52	ASN
2	B	767	ASN
2	B	957	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/13 (84%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	11	U
11	R	12	U

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry

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

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 [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	1395/1733 (80%)	0.12	31 (2%) 62 46	13, 87, 161, 194	0
2	B	1106/1224 (90%)	0.24	47 (4%) 40 29	16, 81, 127, 148	0
3	C	266/318 (83%)	-0.16	2 (0%) 82 70	45, 75, 113, 128	0
4	E	214/215 (99%)	-0.11	2 (0%) 81 68	72, 122, 161, 166	0
5	F	84/155 (54%)	-0.16	2 (2%) 59 44	67, 91, 112, 121	0
6	H	133/146 (91%)	0.40	11 (8%) 17 15	97, 117, 137, 140	0
7	I	119/122 (97%)	0.27	4 (3%) 48 35	79, 104, 123, 134	0
8	J	65/70 (92%)	-0.13	0 100 100	24, 67, 95, 101	0
9	K	114/120 (95%)	-0.24	1 (0%) 81 68	60, 82, 96, 97	0
10	L	46/70 (65%)	0.65	4 (8%) 16 14	86, 138, 153, 154	0
11	R	12/13 (92%)	-0.24	0 100 100	53, 77, 140, 150	0
12	T	28/28 (100%)	0.86	2 (7%) 22 18	52, 198, 323, 324	0
13	N	14/14 (100%)	1.76	5 (35%) 1 1	287, 311, 319, 321	0
All	All	3596/4228 (85%)	0.13	111 (3%) 51 38	13, 86, 153, 324	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	I	13	MET	4.9
5	F	155	LEU	4.7
13	N	7	DA	4.4
2	B	883	LEU	4.3
2	B	335	GLY	4.1

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($\text{\AA}^2$)	Q<0.9
15	MG	A	1736	1/1	0.94	0.14	61,61,61,61	0
14	ZN	I	203	1/1	0.95	0.05	98,98,98,98	0
14	ZN	A	1735	1/1	0.95	0.05	148,148,148,148	0
14	ZN	A	1734	1/1	0.97	0.09	150,150,150,150	0
14	ZN	B	1307	1/1	0.97	0.05	112,112,112,112	0
14	ZN	I	204	1/1	0.99	0.03	101,101,101,101	0
14	ZN	J	101	1/1	0.99	0.09	66,66,66,66	0
14	ZN	L	105	1/1	0.99	0.03	135,135,135,135	0
14	ZN	C	319	1/1	0.99	0.07	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.