



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:28 PM UTC

PDB ID : 5UAQ / pdb_00005uaq
Title : Escherichia coli RNA polymerase RpoB H526Y mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.60 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

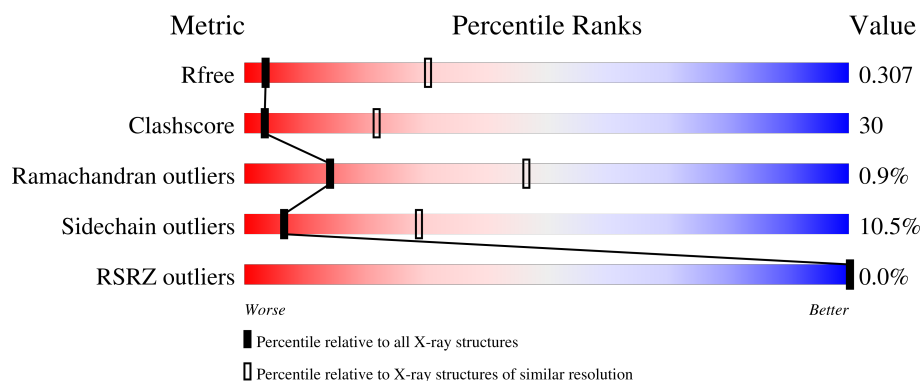
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	329	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	48% 45% 6%
3	D	1407	35% 40% 8% 17%
3	J	1407	36% 39% 7% 18%
4	E	91	63% 32% • •
4	K	91	% 49% 36% • 13%
5	F	613	38% 34% • 24%
5	L	613	35% 37% 5% 23%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55699 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2403	1505	421	469	8			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1044	295	327	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10572	6634	1839	2056	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10568	6632	1838	2055	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	526	TYR	HIS	engineered mutation	UNP P0A8V2
I	526	TYR	HIS	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9029	5676	1620	1687	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	467	Total	C	N	O	S	0	0	0
			3806	2385	677	721	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

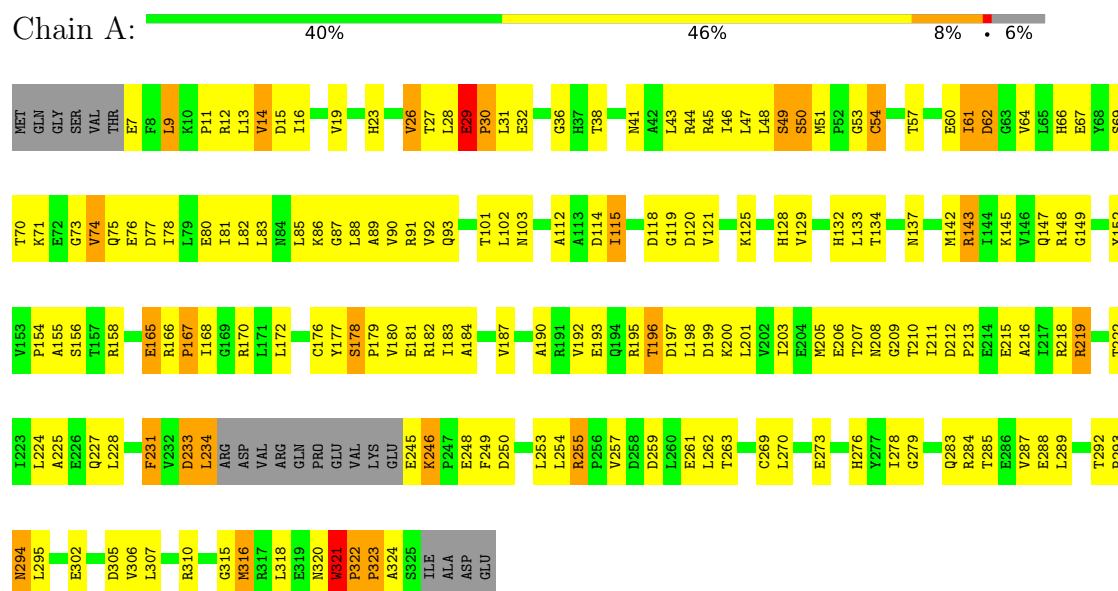
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

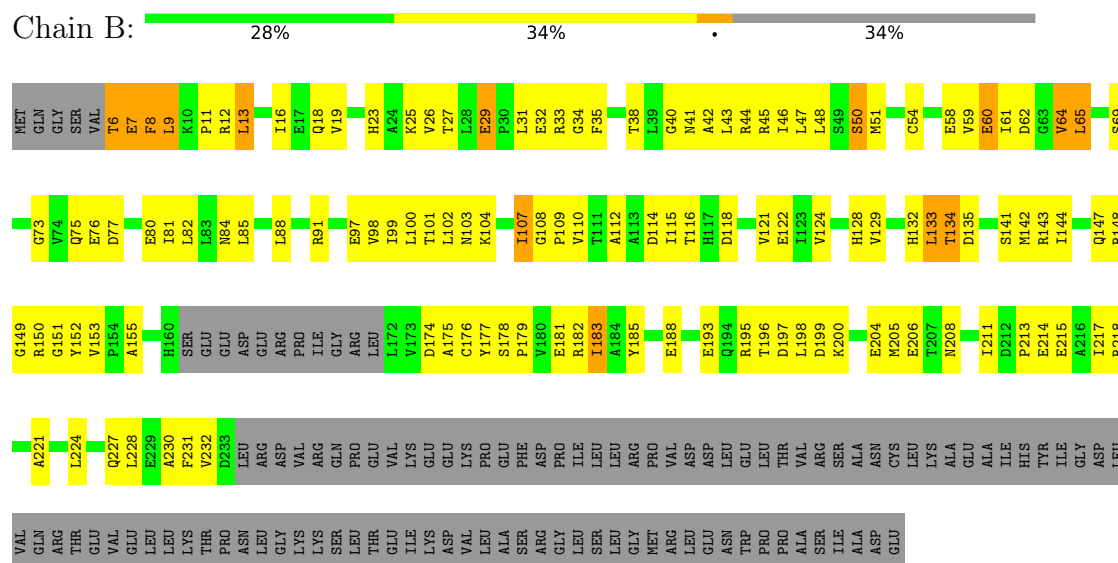
3 Residue-property plots

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 subunit alpha

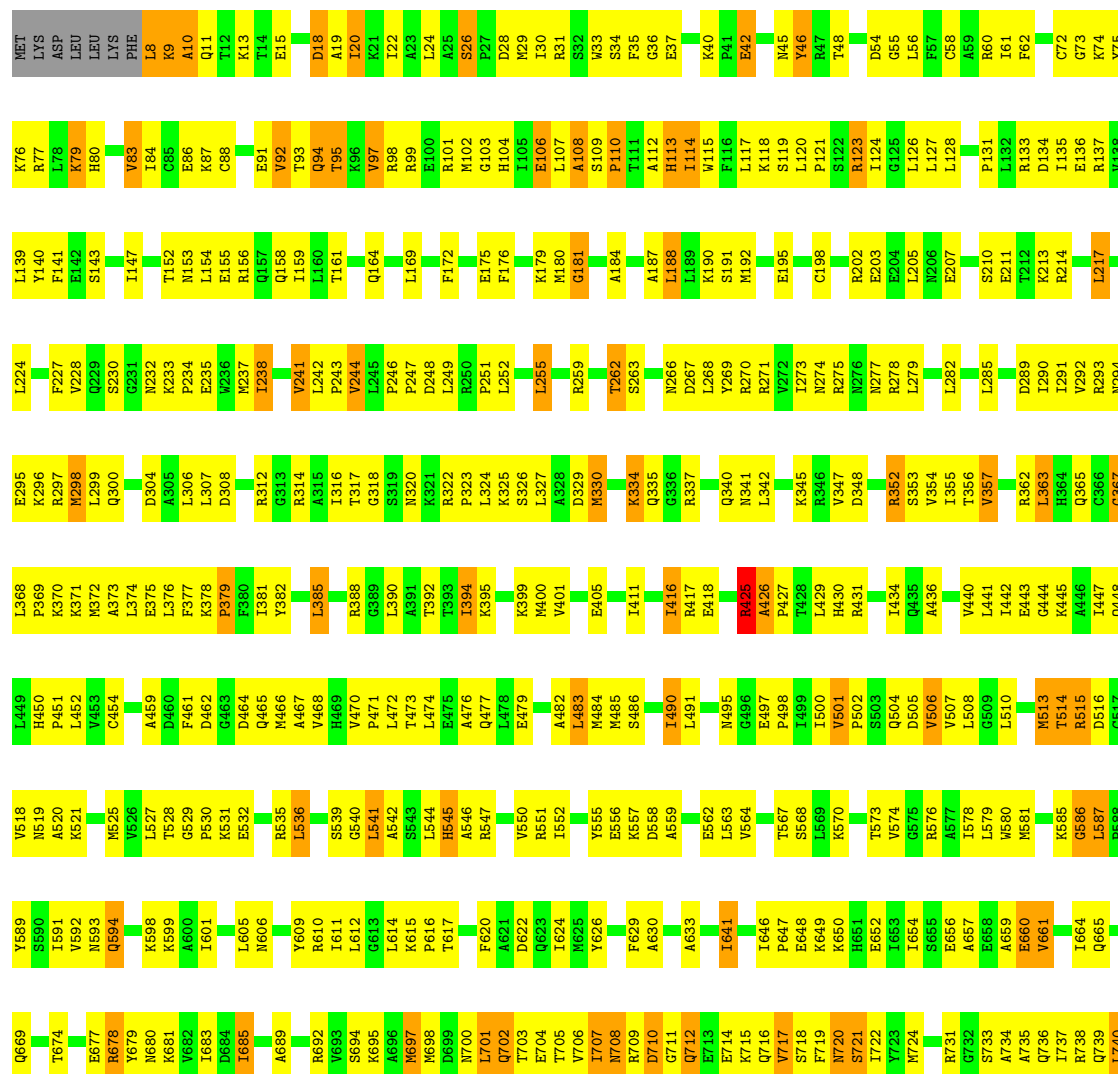


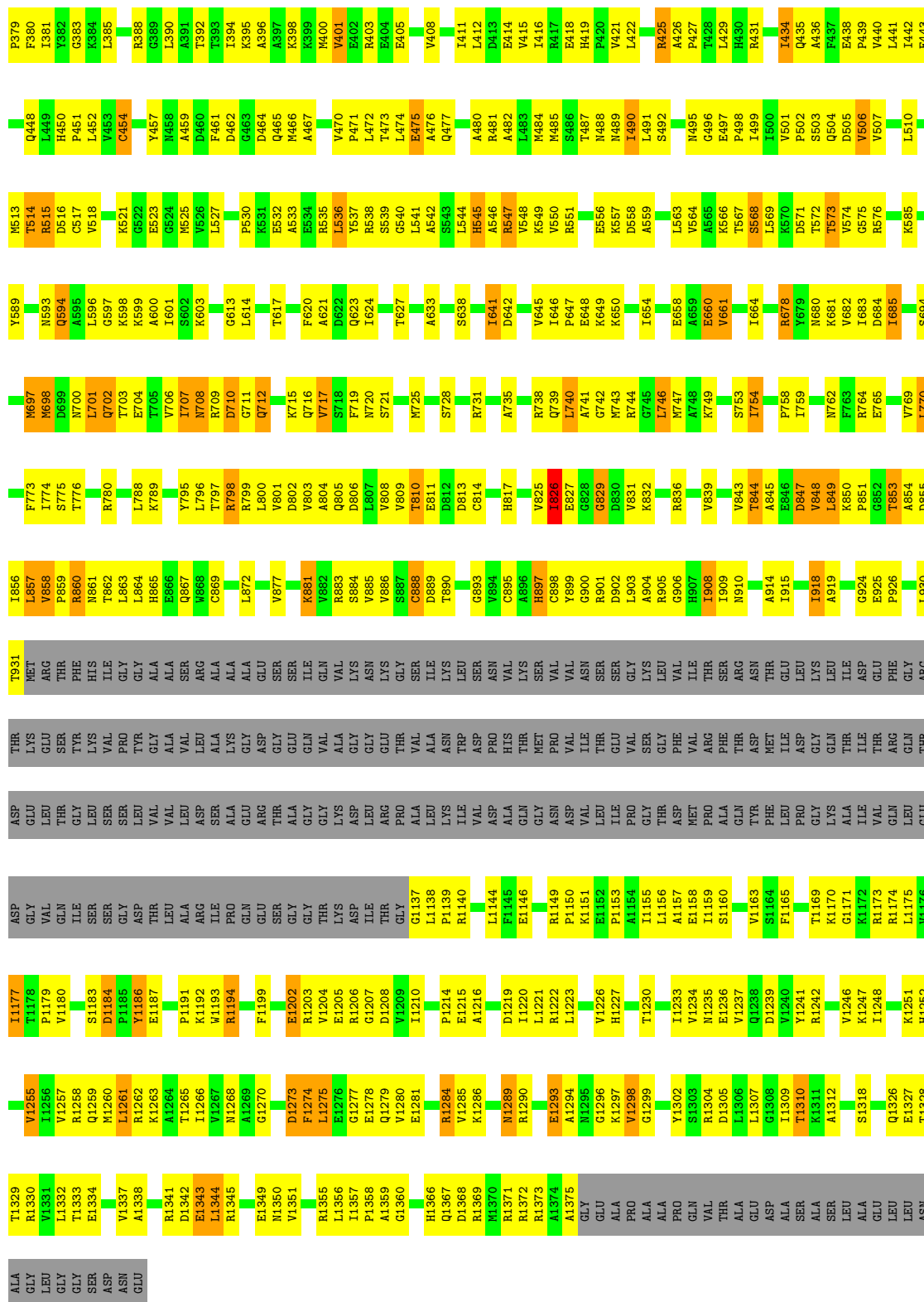
• Molecule 1: DNA-directed RNA polymerase subunit alpha



Y1149	I1079	K1007	F906	E825	K755	A679	V615	G544	E379	R473	G544	V927	L213	N139
D1150	P1081	Q1008		D826	Y756	L680	I616		A380	A474		A298	Y215	G140
L1216	M1080	M1009	S911	R827	T757	M681	A617	V547	R389	V475	V547	K299	Y215	E142
A1152	I1082	Q1010	D912	F828	R758	G682	Q618	R548	E382	E477	D549	D300	L221	
	E1083	L1011	V913	T829	S759	A683	A619	E549	S383	R478	V550	Y301		
F1221	D1084	E1012		T830	W760	N684	N620	V550	L384	L479	H551	I302		I145
R1156	M1085	Q1013	S916	I831	Q761	N685	S621	H551			F224		F224	V146
Q1157	P1086	L1014	S917	H832	W762	Q686	R622	P552	N387		F225		F225	V146
V1159	Y1087			R833	T763	R687	L623	T553	L388	G482		T306		Q148
D1160	G1091			Q834	G764		D624	G556	F390	D483				L149
L1161		L1021	V931	E835	Y765		E625	G556	R389	L484		L309	V228	H150
	V1094	K1022		L836	W768		E626	R557	F390	D485		C311	F230	R151
F1164	D1095	H1023	R936	A637			G627	V558	R394	T486		A312	E231	S152
Y1231	I1096	E1024		W839	L773		F629	C559	Y395	L487		A313		
		F1025	E940	S840	G774	K697	V630	I561	D396	M488			N235	F156
	M1099	E1026	K941	R841	E775	P698	E631	F562	L397	N314			K236	F157
L1235	P1100	K1027	D942	D842	P776	L699	D632	F562	S398	Q490			L237	D158
W1237	L1101		K943				L633	T563	A399	D491		L317	Q238	S159
L1238	G1102	E1030	R944	I850	R779	G701	V634	P564	V400	M492		S318	M239	D160
V1239	P1103	R1033	L946		D781	T702	G703	E565	G401	I493		L319	E240	
D1240	L1043	L1042		W857	G780	G703	C636	G566	N494	N494		D320	L241	
D1241	S1105	K1034		G858	D781	T703	R635	P567	K404			L321	V242	
K1242	R1106	K1035	M951	E859	W782	E704	R637	N568	L409	K496		L322		
M1243	M1107		Q952		L783	W705	S638	I569	P497	I498		A323	R245	G168
	M1108	Q1038	L953	L862	A784	R706	G640	G570	L409			K324	L246	K169
R1246	G1039	G1039		S863		A707	S642	N573	E412	S499		L325	R247	V170
S1247	I1109	D1040	K958	K864	S788				E413			Q327	T250	L171
T1248	Q1111	L1041	D959	L865	D790	W710	F645	Y578	I419	K503		S328		Y172
G1249	L1112	L1042	L960	D866	L791	S712	S646		D423	F506		G329	E256	A174
S1250	L1113	L1043	S961	E867	G792	G713	R647	N582				H330		
I1251	E1114	P1044	E962		E793	W714	D648	E583	V428	Q510		R332	V261	R176
S1252	T1115	G1045	E963		L794		Q649	F584	S512	L511			V263	I177
L1253	H1116	V1046		W871	A795	W717	V650	G585	Q513	S512		T335	E264	Y179
V1254	L1117	L1047	L967	R872	L796	A718	D651	F586				L336		
T1255	G1118	K1048	R974	I873	G797	K719	D51	L587	D434	D516			R268	W183
Q1256	M1119	I1049	I975	W877	Q798	R720	F652	L587		Q517		G344	I269	I184
Q1257	A1120		R976	T878	M800	G721	M653	F588	I445	N518		P345	L270	D185
	G1123	Y1052		G879	R801	W724	D654	T589	R451	N519		Y346	A271	
K1262	I1124	Y1053	L979	D880	W802	Q725	S656	F591	D446	P520		R271		D189
Q1264		R1058	V980	D881	R802	W726	T657	R592	H447	L521		I347	R272	
F1265	M1129	L1059		I882		Y727	Q658	K593	L448	L521			H273	P190
G1266	A1130	I1060	V984	L883	R805	D728	Q659	F594		S522		V953	I274	K191
Q1267	M1131	Q1061	E985	L883	P806	W727	V660	T595	R451	E523		R275	R275	D192
Q1268		P1062	A986	K886	W808	A729	V661	D596	I453	N524		T356	Q276	N193
	Q1134		E987	V887	N808			G597	R454	T525		N357		L194
L1199	Q1135	K1065	K988					V598	R454	Y526		D358	D280	F195
K1200	Q1136	K1066	L989		R811	I732	S662	F599	S455	K527		R359	D381	V196
L1201	E1137	M1066	L989	R890	F812	W736	A665	V599	V456	L360		L360	V282	D199
G1202		Q1067	D990	C891	E813	R737	S666	T600	R451	R529		G361	K283	I999
V1275	D1203		K991	E892	D814	E738	L687	D601	I453	N524		A362	L284	R200
L1204	L1204	L1204	L992	T893	S815	D739	G739	E602	R454	T526		L363	I285	R201
P1205	K1140	H1071	G1071	Q894	L816	E740	F670	F603	R454	Y526		V864	F286	R202
A1277	R1141	G1071	P983	Q894	L816	E740	L671	E602	S455	K527		V864	F286	R202
L1278	R1142	N1072	R994	L995	L817	W741	L671	H604	S455	R528		E365	V287	K203
E1279	E1143	K1073	D995	T896	R818		H604	T605	V456	L360		E365		
	F1144	G1074	R996	R897	S819	E745	F672	F605	V466	L538		G467	P288	I208
Q1209	I1145	V1075	W997	E898	E820		H673	V605	G467	T539		M369	V288	L209
I1210	Q1146	I1076		E399	R821	G747	A676	A608	V469	R470		M370		I209
R1211	L1147	S1077	L1002			I748			E541	R470			I292	L210
L1212	A1148	K1078		T095	R824		N677	I609	R542	R470		T377		R211
Y1213									F472					







V582	V497	S428	E350	D267	V130	ASP
T583	L498	T429	T351	Y268	Q131	ALA
R584	K499	Y430		L269	C132	ASP
E585	I500	A431		V270	S133	ASP
R586	A501		T354	N271	V134	LEU
I587	K502	W433		S272		MET
R588		W434	Q357	M273	Y137	LEU
Q589	I505	I435	V358	R274	F138	ALA
I590	S506	R436	K359	V275	E139	GLU
	M507	Q437	D360	M276		ASN
	E508		I361	M277	Y143	THR
K597		S442	N362	D278		ALA
L598	G512		R363	R279	Y148	ASP
R599	D513		R364	V280		GLU
H600	D514	Q446	N365	R281	V151	ASP
P601	E515	A447	S366	E219		ALA
S602	E516	R448	I367	K220	E154	ALA
R603	D516	T449	I368	F221		GLU
S604	S517	I450	G368	A222	R157	ALA
E605	H518	R451	E369	E223	L158	ALA
L519	L519	I452	A370	L224	S159	ALA
G520	G520		K371	R225	D160	GLN
L530	L530	M456	A372	A226	L161	VAL
P531	P531	I457	R373			LEU
L532	L532	R458	R374	C294	G164	SER
D533	D533	T459		K295	F165	SER
		I460	N383	K296	V166	VAL
T536		M461	L384	M297	D167	GLU
L540	L540	K462	R385	P298		PRO
T544	T544	L463	L386	K299	ALA	ASN
V547	V547	R464	V387	K300	GLU	GLU
T552	T552	R465	I388	N301	ALA	ILE
E555	E555	I466	S389	F302	GLU	GLY
A556	A556		I390	I303	ARG	
K557	K557	M470	K393	T304	T94	T94
V558	V558	L471	Y394	L305	T95	T95
L559	L559	Q472	T395	F306	D96	D96
R560	R560	E473	N396		P97	P97
M561	M561	M474	R397	E310	V98	V98
		G475	G398	T311	R99	R99
		R476	L399	S312	M100	M100
		E477	Q400	D313	Y101	Y101
		P478	F401	T314	M102	M102
		T479	L402	W315	R103	R103
		R480		F316	E104	E104
		E481		N317	M105	M105
		E482	I405	A318		
		L483	Q406	A319	T112	T112
		A484	E407	I320	G115	G115
		E485	G408			
		R486	M409	L330	ASP	ASP
		M487		S334	LEU	LEU
		L488	L412		D118	D118
		M489	F419	L341	I119	I119
		P490	E420	Q342	R122	R122
		E491	Y421	K343	I123	I123
		D492	R422	L344	E124	E124
		K493	K426	Q345	GLU	GLU
		I494	R495	Q346	ASP	ASP
		F495	D581	F427	I127	I127
					N128	N128
					Q129	Q129

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.36Å 206.28Å 308.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.60 29.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.90-3.60) 93.5 (29.90-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.246 , 0.305 0.248 , 0.307	Depositor DCC
R_{free} test set	2000 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	142.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 109.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55699	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: MG, ZN

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	0.87	0/2435	1.28	20/3300 (0.6%)
1	B	0.77	0/1692	1.17	3/2293 (0.1%)
1	G	0.59	0/1751	1.22	7/2373 (0.3%)
1	H	0.57	0/1686	1.08	7/2285 (0.3%)
2	C	1.23	5/10741 (0.0%)	1.37	70/14492 (0.5%)
2	I	0.82	0/10737	1.13	26/14487 (0.2%)
3	D	1.27	3/9246 (0.0%)	1.39	41/12478 (0.3%)
3	J	1.07	2/9168 (0.0%)	1.25	29/12374 (0.2%)
4	E	0.68	0/693	0.95	0/935
4	K	0.35	0/629	0.75	0/847
5	F	0.92	0/3857	1.21	9/5184 (0.2%)
5	L	0.81	1/3872 (0.0%)	1.09	2/5205 (0.0%)
All	All	1.02	11/56507 (0.0%)	1.25	214/76253 (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
1	A	0	2
1	G	0	1
2	C	0	11
2	I	0	2
3	D	0	12
3	J	0	9
5	F	0	1
5	L	0	1
All	All	0	39

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	811	ASN	CB-CG	-8.81	1.30	1.52
3	J	307	LEU	CG-CD2	-6.91	1.29	1.52
2	C	1076	ILE	CB-CG2	-6.62	1.30	1.52
3	D	426	ALA	C-N	-5.64	1.20	1.33
2	C	1079	ILE	C-N	5.62	1.45	1.33

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	109	ALA	CA-C-N	15.51	136.53	119.93
2	I	109	ALA	C-N-CA	15.51	136.53	119.93
2	C	109	ALA	CA-C-N	14.05	134.97	119.93
2	C	109	ALA	C-N-CA	14.05	134.97	119.93
2	C	762	ASN	CA-C-N	-9.17	104.69	122.02

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	TRP	Peptide
1	A	49	SER	Mainchain
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
2	C	473	ARG	Mainchain

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	2403	0	2453	202	0
1	B	1672	0	1694	120	0
1	G	1730	0	1756	149	0
1	H	1667	0	1689	127	1
2	C	10572	0	10584	698	3
2	I	10568	0	10578	636	0
3	D	9107	0	9308	652	0
3	J	9029	0	9225	612	0
4	E	691	0	695	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	27	0
5	F	3806	0	3873	226	2
5	L	3821	0	3884	211	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	55699	0	56373	3395	3

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 30.

The worst 5 of 3395 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)
1:A:27:THR:O	1:A:28:LEU:HD12	1.10	1.23
2:I:27:LEU:O	2:I:528:ARG:NH1	1.78	1.17
1:A:27:THR:O	1:A:28:LEU:CD1	1.93	1.17
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.36	1.08
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.16	1.08

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:ASP:OD1	5:F:554:ARG:NH2[4_455]	1.99	0.21
2:C:44:GLU:OE1	5:F:596:ARG:NH1[4_455]	2.05	0.15
2:C:940:GLU:OE1	1:H:139:SER:OG[4_455]	2.05	0.15

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	305/329 (93%)	271 (89%)	25 (8%)	9 (3%)	3	25
1	B	213/329 (65%)	191 (90%)	20 (9%)	2 (1%)	14	46
1	G	222/329 (68%)	182 (82%)	28 (13%)	12 (5%)	1	14
1	H	213/329 (65%)	193 (91%)	20 (9%)	0	100	100
2	C	1338/1342 (100%)	1225 (92%)	103 (8%)	10 (1%)	18	51
2	I	1338/1342 (100%)	1226 (92%)	100 (8%)	12 (1%)	14	46
3	D	1162/1407 (83%)	1074 (92%)	79 (7%)	9 (1%)	16	49
3	J	1151/1407 (82%)	1064 (92%)	82 (7%)	5 (0%)	30	61
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	461/613 (75%)	422 (92%)	37 (8%)	2 (0%)	30	61
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	43	72
All	All	7030/8222 (86%)	6424 (91%)	544 (8%)	62 (1%)	14	46

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	30	PRO
1	A	324	ALA
1	B	232	VAL
2	C	345	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	268/286 (94%)	247 (92%)	21 (8%)	11	38
1	B	184/286 (64%)	163 (89%)	21 (11%)	5	26
1	G	191/286 (67%)	176 (92%)	15 (8%)	11	37
1	H	183/286 (64%)	162 (88%)	21 (12%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1155/1157 (100%)	1036 (90%)	119 (10%)	7	30
2	I	1154/1157 (100%)	1037 (90%)	117 (10%)	7	30
3	D	975/1168 (84%)	863 (88%)	112 (12%)	5	25
3	J	967/1168 (83%)	859 (89%)	108 (11%)	6	27
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	27
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	39
5	F	416/540 (77%)	374 (90%)	42 (10%)	7	30
5	L	418/540 (77%)	374 (90%)	44 (10%)	6	29
All	All	6050/7024 (86%)	5417 (90%)	633 (10%)	6	29

5 of 633 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	1198	LEU
3	J	1275	LEU
3	J	18	ASP
2	I	1180	MET
3	J	573	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	518	HIS
5	L	600	HIS
2	I	761	GLN
5	L	579	GLN
5	L	294	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	309/329 (93%)	-0.57	0 100 100	99, 147, 225, 245	0
1	B	217/329 (65%)	-0.45	0 100 100	112, 194, 254, 272	0
1	G	224/329 (68%)	-0.49	0 100 100	163, 206, 241, 270	0
1	H	217/329 (65%)	-0.47	0 100 100	146, 213, 252, 285	0
2	C	1340/1342 (99%)	-0.60	0 100 100	74, 121, 234, 285	0
2	I	1340/1342 (99%)	-0.57	0 100 100	86, 159, 261, 388	0
3	D	1166/1407 (82%)	-0.62	0 100 100	72, 112, 215, 264	0
3	J	1155/1407 (82%)	-0.61	0 100 100	86, 138, 229, 274	0
4	E	89/91 (97%)	-0.52	0 100 100	147, 183, 216, 241	0
4	K	79/91 (86%)	-0.45	1 (1%) 75 48	202, 277, 319, 350	0
5	F	467/613 (76%)	-0.56	0 100 100	93, 165, 290, 340	0
5	L	469/613 (76%)	-0.63	0 100 100	116, 178, 288, 353	0
All	All	7072/8222 (86%)	-0.58	1 (0%) 100 100	72, 147, 251, 388	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	16	ARG	2.0

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
6	MG	D	1501	1/1	0.85	0.12	87,87,87,87	0
6	MG	J	1501	1/1	0.91	0.13	94,94,94,94	0
7	ZN	D	1502	1/1	0.95	0.06	134,134,134,134	0
7	ZN	J	1503	1/1	0.96	0.04	97,97,97,97	0
7	ZN	J	1502	1/1	0.99	0.04	131,131,131,131	0
7	ZN	D	1503	1/1	1.00	0.07	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.