



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 07:49 AM GMT

PDB ID : 1WCM
Title : COMPLETE 12-SUBUNIT RNA POLYMERASE II AT 3.8 ANG
Authors : Armache, K.-J.; Mitterweger, S.; Meinhart, A.; Cramer, P.
Deposited on : 2004-11-17
Resolution : 3.80 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>

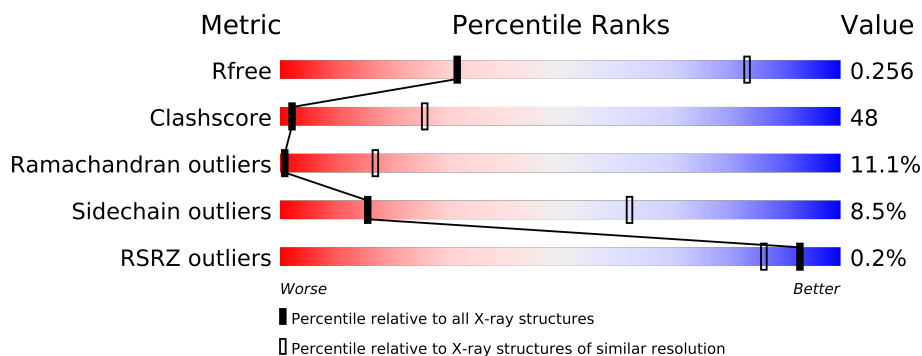
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.80 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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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	1733	
2	B	1224	
3	C	318	
4	D	177	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30945 atoms, of which 0 are hydrogen 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 II LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SECOND LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

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

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 POLYMERASE II 32 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	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	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19 KD 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	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2 KDA POLYPEPTIDE.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II AND III 8.3 KDA POLYPEPTIDE.

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	115	Total	C	N	O	S	0	0	1
			920	590	157	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
			363	224	72	63	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

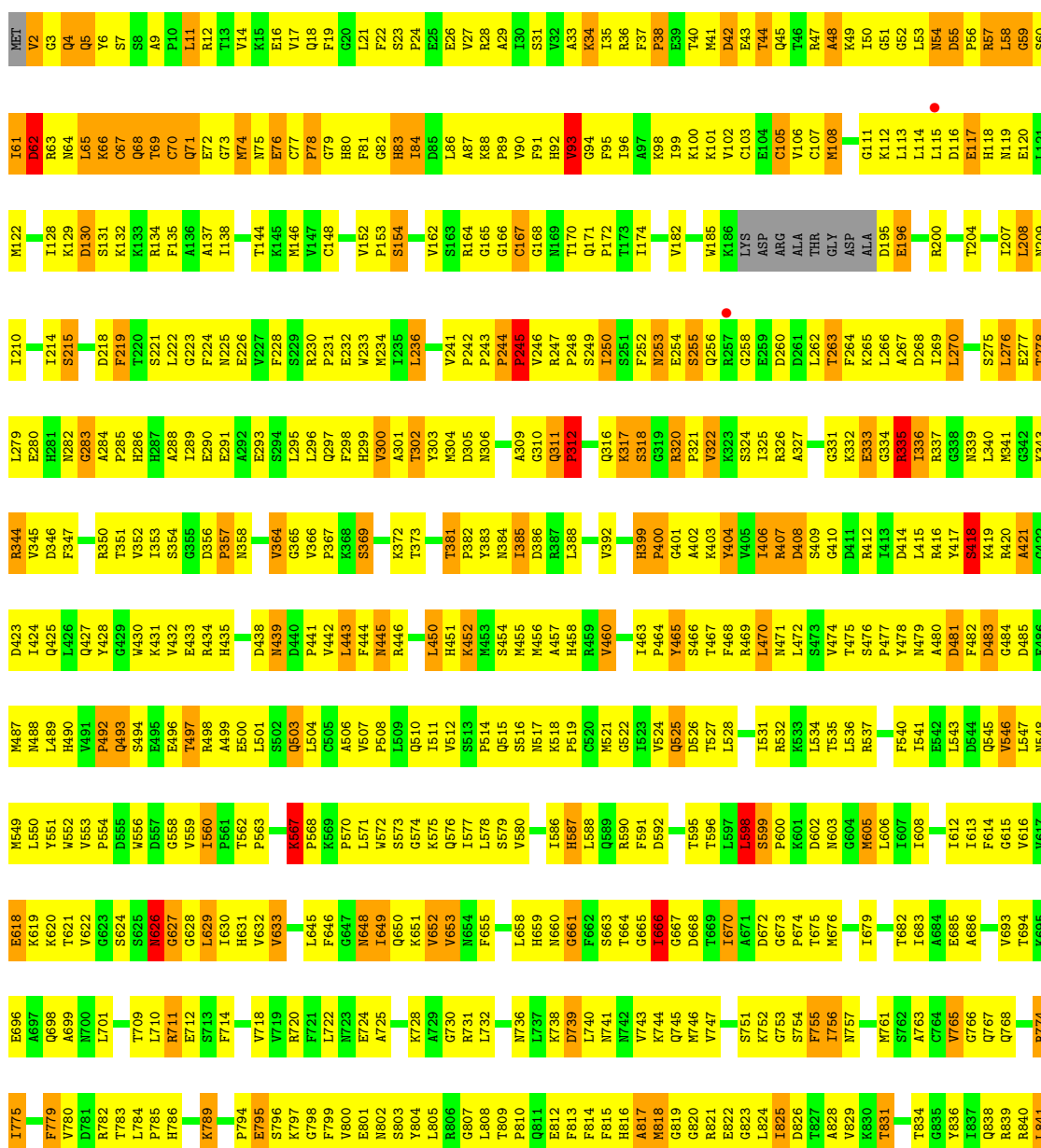
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Mg	0	0
			1	1		

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

Chain A:



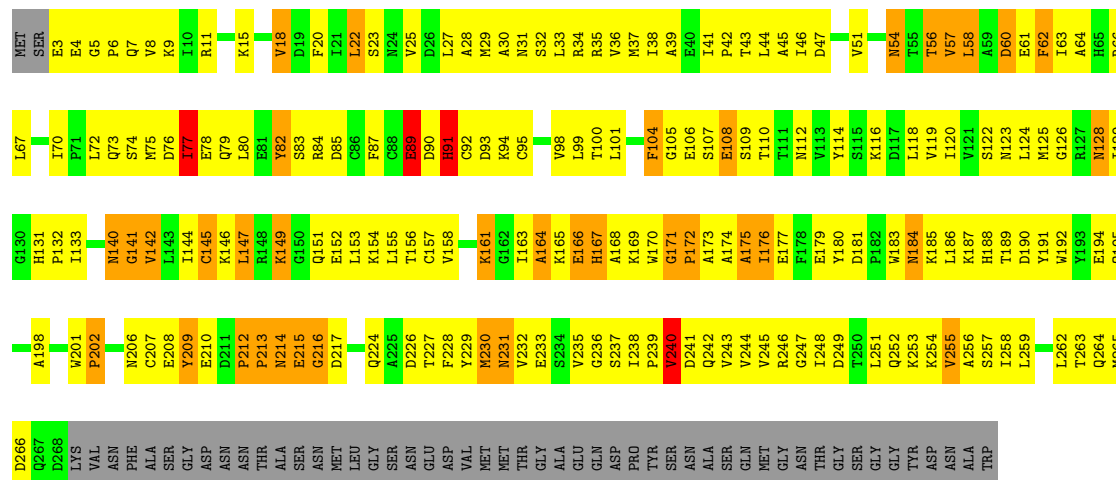


I1139	F1069	D998	S933	M868	T806	C741	Y679	S614	T549	V479	G410	GLY	L273	E194	F129
A1140	M1072	M999	K934	S889	T807	E742	T880	M615	D550	S480	P411	ILE	L276	C195	V130
A1143	F1073	F1000	D935	T870	A808	I743	W881	R617	M552	L483	L412	LYS	K277	F196	K133
A1144	N1074	F1002	A937	S872	M809	T745	S683	R620	P553	R484	L414	K345	K278	D198	K134
S1145	T1077	A1003	S938	T873	E810	S746	L684	R620	I554	R485	Q415	K347	Q277	M199	ARG
F1146			T339		Y811	W747	L685	E621	I555	Y486			D279	G200	THR
L1147			P940	P877		L748		K622	T556	T487	K418	Y351	T280	G201	
	K1080	V1007	L941	Q878	R815	L749	E687	E623	F567	Y488	T419		T281	Y202	
R1150	P1008	P1008	R942	R879	R816	G750	G688	L624	F567	Y488	T419		T282	Y202	GLU
L1151	M1082	L1009	S943	T880	L817	G751	G688	L624	S489	S489	F421		T283	F204	ALA
M1152	A1083	L1010	T944	N881	P818	A752	V690	I626	S559	S489	F421		T284	I204	ILE
L1153	G1084	I1011	E945	T882	A819	A753	E691	F627	E560	T491			T285	I205	ASP
A1154	I1085	I1012		L883	G820		Y682	T628	G562	S483	L424		T286	M206	VAL
S1155	F1086	M1013		R884	Q821	I756	I693	D629	M563	H494	D427		F287	G207	PRO
D1156	F1087		V949		N822	P757	D694	A630	L566	H494	I428		R287	K210	GLY
A1157	G1088	A1016	D950	T888	R823	F758	E695	L631	L566	H494	I428		R288	L211	ARG
F1158	P1089	I1017	Q951	T889	I824	F759	E696	G631	L566	H494	F429		R289	V211	GLU
R1159	T1090	P1018	V952	Y890	V825	D760	E697	G631	L566	H494	F429		R290	L212	LEU
V1160	S1019	L953	L953	D891	A826	H761	E698	G631	L566	H494	F429		R291	L213	LYS
H1161	R1020	V954		K992	I827		E699	G631	L566	H494	F429		R292	L214	LYS
C1163	M1021	T955	T955	L893	Y830	S764	I701	P636	H572	P501	GLU		R293	A214	TYR
G1164	T1022	T956	T956	D894	Y831	S765	L702	F638	S574	F502	ALA		R294	R217	GLU
L1165	H1025	Q958	Q958	G897	G832	R766	I703	T639	S574	F502	ALA		R295	R217	LEU
C1166	L1026	L1027	D959	L893	Y833	R767	A704	V640	D576	ASP	HIS		R296	Q224	ALA
G1167	I1027			L893	N834	T768	R705	V640	D576	ASP	HIS		R297	R225	GLU
L1168	E1028	E1028	F963	A900	Q835	T769	Q706	E642	A577	GLY	PHE		R298	F226	GLU
M1169	C1029	V964		A900	Q835	T769	Q706	E642	A577	GLY	PHE		R299	F226	SER
T1170	L1030	K965	K965	G902	D837	S771	E708	E644	R579	LEU	MET		R300	K227	GLU
V1171	L1031	V903	V903	G902	D837	S771	E708	E644	R579	LEU	MET		R301	K227	GLU
I1172	S1032	S1032	V966	R904	S838	A772	D709	E644	R579	LEU	MET		R302	K227	GLU
A1173	A1033	A1033		R904	S838	A772	D709	E644	R579	LEU	MET		R303	K227	GLU
K1174	V1034	S906	T971	V905	R840	G774	L711	H648	F581	P511	A450		R304	A229	ASP
L1175	A1035	A1035	T971	S906	R841	G775	P712	H649	F581	P511	A450		R305	A230	SER
N1176	A1036	A1036	K972	E908	Q843	A777	A715	R649	F581	P511	A450		R306	R231	GLU
G1177	R1108	G1109	T973	D909	S844	W778	ASN	V653	G588	H516	L453		R307	S252	SER
H1178	G1109	P1110	T974	V910	S845	W779	GLU	V653	G588	H516	L453		R308	S252	GLU
Q1179	M1040	E1041	Q975	I911	S845	W779	GLU	V653	G588	H516	L453		R309	S252	SER
F1180	E1041	E1041	Q975	I911	S845	W779	GLU	V653	G588	H516	L453		R310	S252	GLU
E1181	A1044	A1044	Q977	G913	S845	W779	GLU	V653	G588	H516	L453		R311	S252	GLU
C1182	S1045	S1045	Q977	G913	S845	W779	GLU	V653	G588	H516	L453		R312	S252	GLU
K1183	P1046	P1046	Q977	G913	S845	W779	GLU	V653	G588	H516	L453		R313	S252	GLU
G1184	F1047	F1047	Q981	T915	S851	Y785	D722	L661	A594	V522	L461		R314	S252	GLU
C1185			A981	T915	S851	Y785	D722	L661	A594	V522	L461		R315	S252	GLU
D1186	I1050	I1050	S982	I918	S853	W787	P725	H662	L596	P524	T463		R316	S252	GLU
N1187	T1051	T1051	R983	S919	L854	W788	A726	H662	L596	P524	T463		R317	S252	GLU
K1188	R1124	R1124	H984	S919	L854	W788	A726	H662	L596	P524	T463		R318	S252	GLU
I1189	D1125	D1125	Q985	ASP	F856	W792	R728	T664	R601	T527	W466		R319	S252	GLU
D1190	G1126	G1126	Q986	ASP	F856	W792	R728	T664	R601	T527	W466		R320	S252	GLU
I1191	G1127	G1127	Q986	ASP	F856	W792	R728	T664	R601	T527	W466		R321	S252	GLU
Y1192			T989	GLU	S858	W794	R730	T664	R601	T527	W466		R322	S252	GLU
Q1193	G1131	G1131	T990	GLU	S858	W794	R730	T664	R601	T527	W466		R323	S252	GLU
I1194	E1132	E1132	G991	LEU	M860	L796	S732	T664	R601	T527	W466		R324	S252	GLU
H1195	L1059	L1059	G991	LEU	M860	L796	S732	T664	R601	T527	W466		R325	S252	GLU
L1196	R1060	R1060	T992	GLN	D861	Y797	H733	T664	R601	T527	W466		R326	S252	GLU
E1197	E1134	E1134	T993	GLN	D861	Y797	H733	T664	R601	T527	W466		R327	S252	GLU
P1197	R1135	R1135	T994	ARG	E863	Y798	H734	T664	R601	T527	W466		R328	S252	GLU
Y1198	Q1065	Q1065	T994	THR	E864	Q800	A735	T664	R601	T527	W466		R329	S252	GLU
A1199	S1066	S1066	T995	ALA	K865	R801	T736	T664	R601	T527	W466		R330	S252	GLU
C1197	R1067	R1067	T996	ALA	K865	R801	T736	T664	R601	T527	W466		R331	S252	GLU
L1199	Y1199	Y1199	T997	THR	Y866	R802	T738	T664	R601	T527	W466		R332	S252	GLU
A1200	M1138	M1138	E997	HIS	G967	L803		T664	R601	T527	W466		R333	S252	GLU



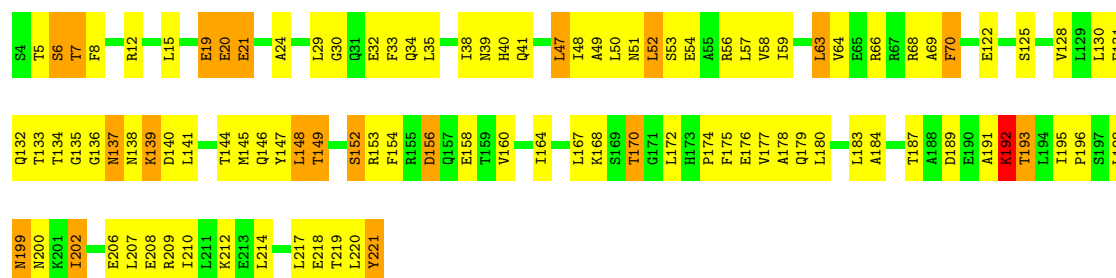
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45 KDA POLYPEPTIDE

Chain C:



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

Chain D:



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

Chain E:



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

Chain F:



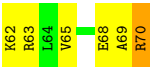
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K:



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

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.72Å 395.13Å 284.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 47.39 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.80) 99.2 (47.39-3.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.285 0.225 , 0.256	Depositor DCC
R_{free} test set	2439 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	116.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 36.2	EDS
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 121835 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30945	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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, 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	0.48	0/11339	0.73	4/15334 (0.0%)
2	B	0.47	0/8890	0.70	1/11990 (0.0%)
3	C	0.52	0/2133	0.76	0/2891
4	D	0.45	0/1365	0.71	1/1837 (0.1%)
5	E	0.43	0/1788	0.64	0/2406
6	F	0.53	0/691	0.78	0/933
7	G	0.53	0/1368	0.74	0/1844
8	H	0.40	0/1086	0.66	0/1470
9	I	0.48	0/989	0.77	0/1331
10	J	0.54	0/541	0.89	1/727 (0.1%)
11	K	0.50	0/938	0.68	0/1267
12	L	0.55	0/365	0.79	0/485
All	All	0.48	0/31493	0.72	7/42515 (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
3	C	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	10	CYS	CA-CB-SG	8.66	129.59	114.00
1	A	1403	GLU	N-CA-C	5.38	125.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	C-N-CD	5.34	139.62	128.40
2	B	1185	CYS	N-CA-C	-5.30	96.69	111.00
1	A	452	LYS	N-CA-C	-5.21	96.94	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
3	C	82	TYR	Sidechain

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	11140	0	11217	1180	0
2	B	8720	0	8745	919	0
3	C	2095	0	2051	244	0
4	D	1356	0	1319	114	0
5	E	1752	0	1776	154	0
6	F	679	0	701	84	0
7	G	1340	0	1357	150	0
8	H	1068	0	1040	104	0
9	I	971	0	927	94	0
10	J	532	0	542	93	0
11	K	920	0	929	83	0
12	L	363	0	386	45	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	30945	0	30990	2984	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 48.

The worst 5 of 2984 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:CYS:O	1:A:78:PRO:O	1.65	1.14
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.30	1.11
7:G:138:THR:HG22	7:G:139:ILE:H	1.12	1.09
1:A:53:LEU:HD23	1:A:54:ASN:N	1.69	1.06
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.69	1.06

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	1406/1733 (81%)	949 (68%)	293 (21%)	164 (12%)	1	15
2	B	1077/1224 (88%)	735 (68%)	221 (20%)	121 (11%)	1	16
3	C	264/318 (83%)	159 (60%)	66 (25%)	39 (15%)	0	9
4	D	173/177 (98%)	122 (70%)	34 (20%)	17 (10%)	1	21
5	E	212/215 (99%)	148 (70%)	49 (23%)	15 (7%)	2	33
6	F	82/155 (53%)	64 (78%)	14 (17%)	4 (5%)	3	45
7	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	2	33
8	H	129/146 (88%)	84 (65%)	29 (22%)	16 (12%)	1	14
9	I	117/122 (96%)	80 (68%)	29 (25%)	8 (7%)	2	35
10	J	63/70 (90%)	37 (59%)	10 (16%)	16 (25%)	0	2
11	K	113/120 (94%)	89 (79%)	18 (16%)	6 (5%)	3	42
12	L	44/70 (63%)	19 (43%)	14 (32%)	11 (25%)	0	2
All	All	3849/4521 (85%)	2617 (68%)	803 (21%)	429 (11%)	1	17

5 of 429 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	48	ALA
1	A	54	ASN
1	A	55	ASP
1	A	57	ARG

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	1239/1520 (82%)	1135 (92%)	104 (8%)	16	63
2	B	952/1061 (90%)	866 (91%)	86 (9%)	14	59
3	C	234/274 (85%)	212 (91%)	22 (9%)	13	56
4	D	140/159 (88%)	124 (89%)	16 (11%)	8	45
5	E	196/197 (100%)	187 (95%)	9 (5%)	37	83
6	F	74/137 (54%)	65 (88%)	9 (12%)	7	42
7	G	152/152 (100%)	142 (93%)	10 (7%)	24	73
8	H	117/128 (91%)	111 (95%)	6 (5%)	33	81
9	I	113/116 (97%)	99 (88%)	14 (12%)	7	41
10	J	60/65 (92%)	54 (90%)	6 (10%)	11	53
11	K	99/102 (97%)	92 (93%)	7 (7%)	21	70
12	L	40/57 (70%)	37 (92%)	3 (8%)	19	67
All	All	3416/3968 (86%)	3124 (92%)	292 (8%)	15	62

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	485	ARG
2	B	956	THR
9	I	85	PHE
2	B	516	ASN
2	B	701	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	236	HIS
2	B	734	HIS
9	I	12	ASN
2	B	363	HIS
2	B	484	ASN

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 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.

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	1416/1733 (81%)	-0.10	3 (0%) 93 86	19, 87, 162, 200	0
2	B	1097/1224 (89%)	-0.09	4 (0%) 90 79	23, 97, 166, 194	0
3	C	266/318 (83%)	-0.15	0 100 100	37, 81, 139, 160	0
4	D	177/177 (100%)	-0.07	0 100 100	52, 108, 147, 165	0
5	E	214/215 (99%)	-0.07	0 100 100	57, 142, 187, 193	0
6	F	84/155 (54%)	-0.27	0 100 100	25, 59, 105, 124	0
7	G	171/171 (100%)	-0.10	0 100 100	57, 84, 114, 138	0
8	H	133/146 (91%)	0.15	0 100 100	101, 139, 175, 184	0
9	I	119/122 (97%)	0.13	1 (0%) 83 64	74, 130, 159, 200	0
10	J	65/70 (92%)	-0.25	0 100 100	42, 79, 120, 127	0
11	K	115/120 (95%)	-0.11	0 100 100	42, 83, 114, 123	0
12	L	46/70 (65%)	-0.01	0 100 100	76, 137, 168, 177	0
All	All	3903/4521 (86%)	-0.09	8 (0%) 93 86	19, 94, 166, 200	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	7.1
2	B	133	LYS	2.7
9	I	119	THR	2.7
2	B	882	THR	2.6
1	A	257	ARG	2.4

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(\AA^2)	Q<0.9
14	MG	A	2458	1/1	0.17	0.56	56,56,56,56	0
13	ZN	L	1071	1/1	0.12	-0.44	115,115,115,115	0
13	ZN	B	2225	1/1	0.15	-0.65	44,44,44,44	0
13	ZN	I	1121	1/1	0.12	-0.83	90,90,90,90	0
13	ZN	C	1269	1/1	0.08	-0.88	39,39,39,39	0
13	ZN	A	2457	1/1	0.09	-1.40	44,44,44,44	0
13	ZN	A	2456	1/1	0.09	-1.81	86,86,86,86	0
13	ZN	J	1066	1/1	0.15	-2.44	65,65,65,65	0
13	ZN	I	1122	1/1	0.07	-2.65	156,156,156,156	0

6.5 Other polymers

There are no such residues in this entry.