



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:32 PM UTC

PDB ID : 8ASC / pdb_00008asc
Title : Ku70/80 binds to the Ku-binding motif of PAXX
Authors : Seif El Dahan, M.; Ropars, V.; Charbonnier, J.B.
Deposited on : 2022-08-19
Resolution : 2.95 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
Mogul : 2022.3.0, CSD as543be (2022)
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

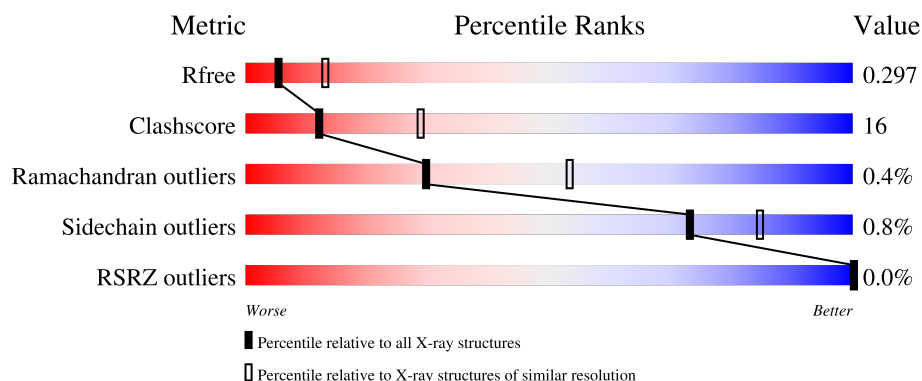
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

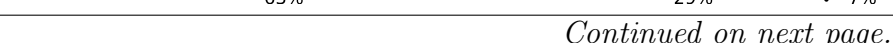
The reported resolution of this entry is 2.95 Å.

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.



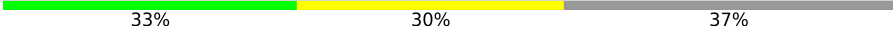
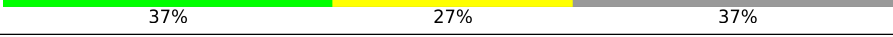
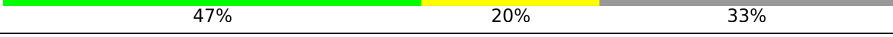
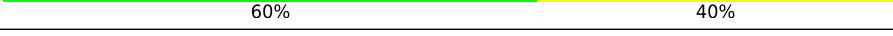
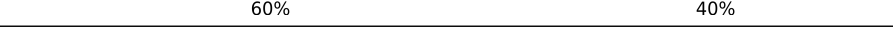
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	544	 63% 28% • 8%
1	E	544	 58% 32% • 9%
1	K	544	 60% 30% • 8%
1	O	544	 59% 32% 8%
2	B	572	 63% 29% • 7%

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Mol	Chain	Length	Quality of chain
2	F	572	
2	L	572	
2	P	572	
3	C	30	
3	G	30	
3	M	30	
3	Q	30	
4	D	15	
4	H	15	
4	N	15	
4	R	15	
5	J	28	
5	T	28	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 36383 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4027	2576	681	752	18			
1	E	497	Total	C	N	O	S	0	0	0
			4015	2569	683	745	18			
1	K	502	Total	C	N	O	S	0	0	0
			4052	2590	686	758	18			
1	O	498	Total	C	N	O	S	0	0	0
			4023	2575	684	746	18			

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	531	Total	C	N	O	S	0	0	0
			4248	2720	715	790	23			
2	F	537	Total	C	N	O	S	0	0	0
			4282	2736	720	803	23			
2	L	530	Total	C	N	O	S	0	0	0
			4238	2712	715	788	23			
2	P	531	Total	C	N	O	S	0	0	0
			4242	2714	713	792	23			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP P13010
B	-15	HIS	-	expression tag	UNP P13010
B	-14	HIS	-	expression tag	UNP P13010
B	-13	HIS	-	expression tag	UNP P13010
B	-12	HIS	-	expression tag	UNP P13010
B	-11	HIS	-	expression tag	UNP P13010
B	-10	HIS	-	expression tag	UNP P13010
B	-9	HIS	-	expression tag	UNP P13010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P13010
B	-7	HIS	-	expression tag	UNP P13010
B	-6	HIS	-	expression tag	UNP P13010
B	-5	GLU	-	expression tag	UNP P13010
B	-4	ASN	-	expression tag	UNP P13010
B	-3	LEU	-	expression tag	UNP P13010
B	-2	TYR	-	expression tag	UNP P13010
B	-1	PHE	-	expression tag	UNP P13010
B	0	GLN	-	expression tag	UNP P13010
B	1	GLY	-	expression tag	UNP P13010
F	-16	MET	-	initiating methionine	UNP P13010
F	-15	HIS	-	expression tag	UNP P13010
F	-14	HIS	-	expression tag	UNP P13010
F	-13	HIS	-	expression tag	UNP P13010
F	-12	HIS	-	expression tag	UNP P13010
F	-11	HIS	-	expression tag	UNP P13010
F	-10	HIS	-	expression tag	UNP P13010
F	-9	HIS	-	expression tag	UNP P13010
F	-8	HIS	-	expression tag	UNP P13010
F	-7	HIS	-	expression tag	UNP P13010
F	-6	HIS	-	expression tag	UNP P13010
F	-5	GLU	-	expression tag	UNP P13010
F	-4	ASN	-	expression tag	UNP P13010
F	-3	LEU	-	expression tag	UNP P13010
F	-2	TYR	-	expression tag	UNP P13010
F	-1	PHE	-	expression tag	UNP P13010
F	0	GLN	-	expression tag	UNP P13010
F	1	GLY	-	expression tag	UNP P13010
L	-16	MET	-	initiating methionine	UNP P13010
L	-15	HIS	-	expression tag	UNP P13010
L	-14	HIS	-	expression tag	UNP P13010
L	-13	HIS	-	expression tag	UNP P13010
L	-12	HIS	-	expression tag	UNP P13010
L	-11	HIS	-	expression tag	UNP P13010
L	-10	HIS	-	expression tag	UNP P13010
L	-9	HIS	-	expression tag	UNP P13010
L	-8	HIS	-	expression tag	UNP P13010
L	-7	HIS	-	expression tag	UNP P13010
L	-6	HIS	-	expression tag	UNP P13010
L	-5	GLU	-	expression tag	UNP P13010
L	-4	ASN	-	expression tag	UNP P13010
L	-3	LEU	-	expression tag	UNP P13010

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	TYR	-	expression tag	UNP P13010
L	-1	PHE	-	expression tag	UNP P13010
L	0	GLN	-	expression tag	UNP P13010
L	1	GLY	-	expression tag	UNP P13010
P	-16	MET	-	initiating methionine	UNP P13010
P	-15	HIS	-	expression tag	UNP P13010
P	-14	HIS	-	expression tag	UNP P13010
P	-13	HIS	-	expression tag	UNP P13010
P	-12	HIS	-	expression tag	UNP P13010
P	-11	HIS	-	expression tag	UNP P13010
P	-10	HIS	-	expression tag	UNP P13010
P	-9	HIS	-	expression tag	UNP P13010
P	-8	HIS	-	expression tag	UNP P13010
P	-7	HIS	-	expression tag	UNP P13010
P	-6	HIS	-	expression tag	UNP P13010
P	-5	GLU	-	expression tag	UNP P13010
P	-4	ASN	-	expression tag	UNP P13010
P	-3	LEU	-	expression tag	UNP P13010
P	-2	TYR	-	expression tag	UNP P13010
P	-1	PHE	-	expression tag	UNP P13010
P	0	GLN	-	expression tag	UNP P13010
P	1	GLY	-	expression tag	UNP P13010

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	19	Total	C	N	O	P	0	0	0
			393	185	76	113	19			
3	G	20	Total	C	N	O	P	0	0	0
			412	194	79	119	20			
3	M	19	Total	C	N	O	P	0	0	0
			393	185	76	113	19			
3	Q	20	Total	C	N	O	P	0	0	0
			412	194	79	119	20			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	14	Total	C	N	O	P	0	0	0
			285	134	52	85	14			

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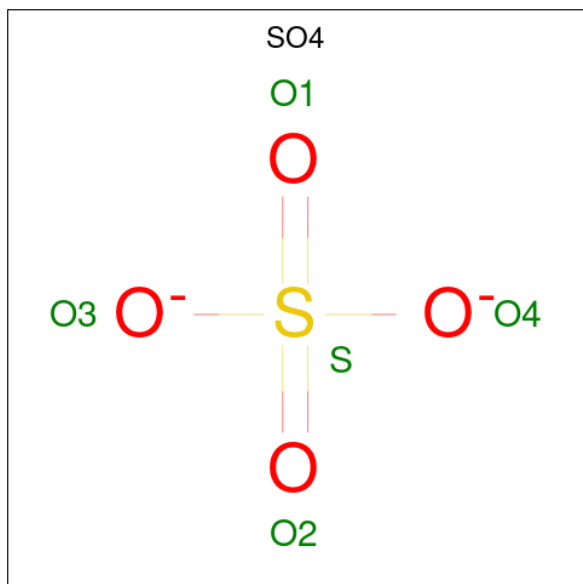
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	15	Total	C	N	O	P	0	0	0
			304	143	55	91	15			
4	N	14	Total	C	N	O	P	0	0	0
			285	134	52	85	14			
4	R	15	Total	C	N	O	P	0	0	0
			304	143	55	91	15			

- Molecule 5 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	28	Total	C	N	O	S	0	0	0
			214	132	41	40	1			
5	T	28	Total	C	N	O	S	0	0	0
			214	132	41	40	1			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	P	1	Total	O	S	0	0
			5	4	1		

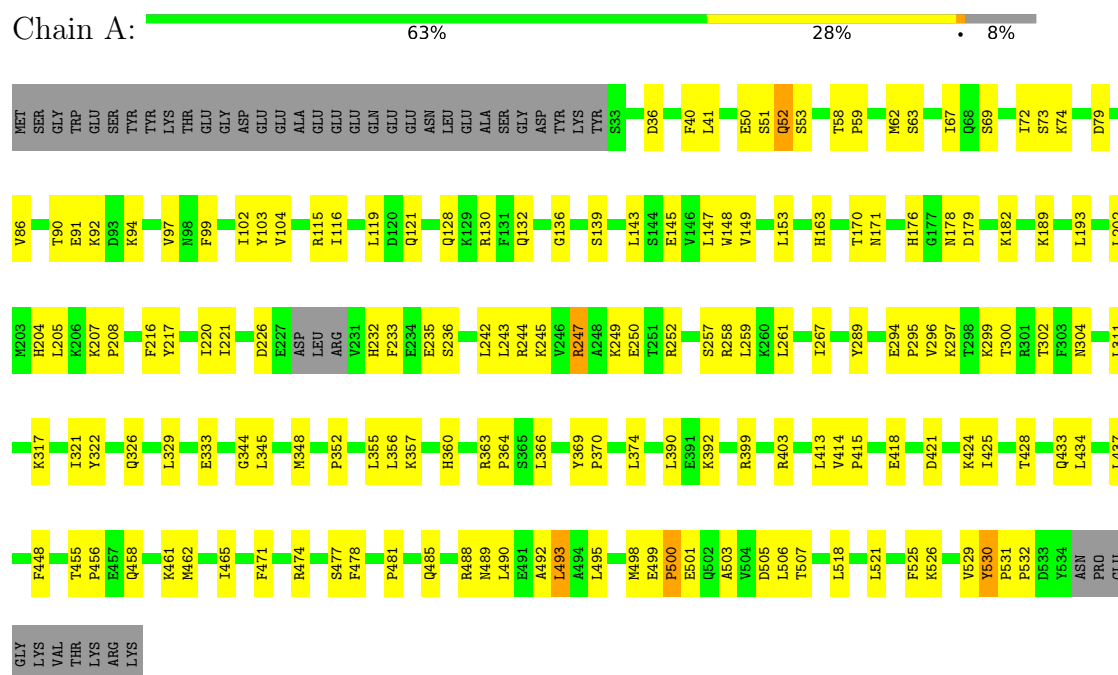
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	O 1	0	0
7	E	6	Total 6	O 6	0	0
7	F	3	Total 3	O 3	0	0
7	K	4	Total 4	O 4	0	0
7	L	2	Total 2	O 2	0	0
7	N	1	Total 1	O 1	0	0
7	O	3	Total 3	O 3	0	0

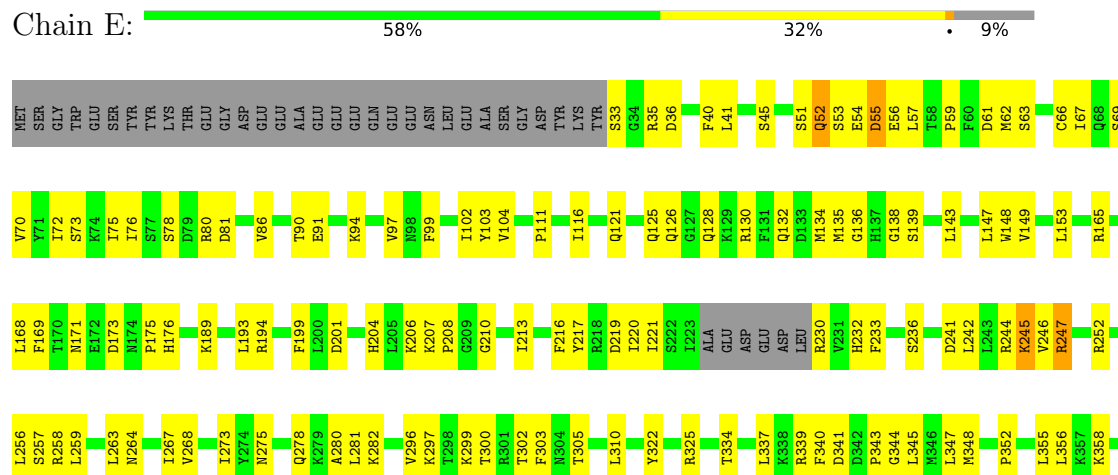
3 Residue-property plots

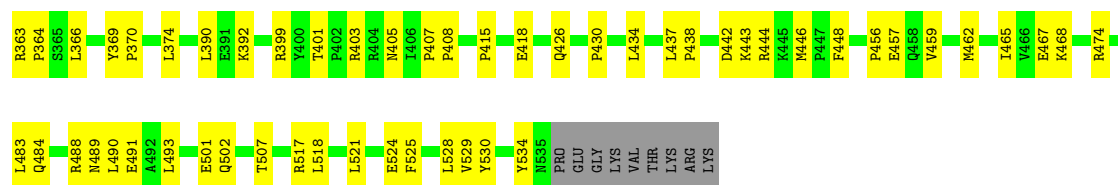
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: X-ray repair cross-complementing protein 6



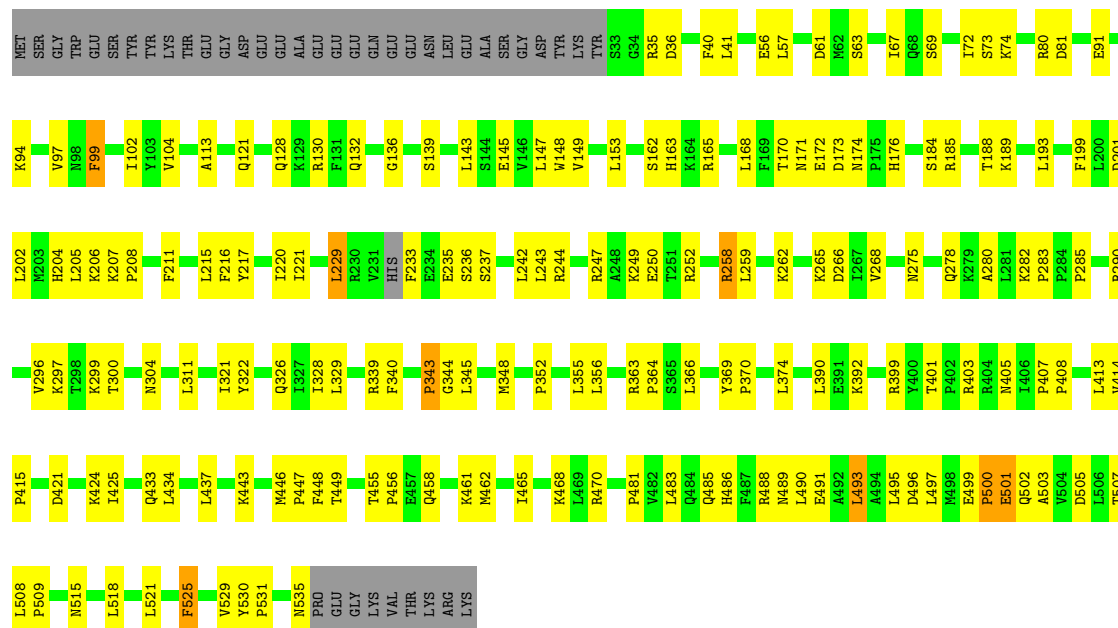
- Molecule 1: X-ray repair cross-complementing protein 6





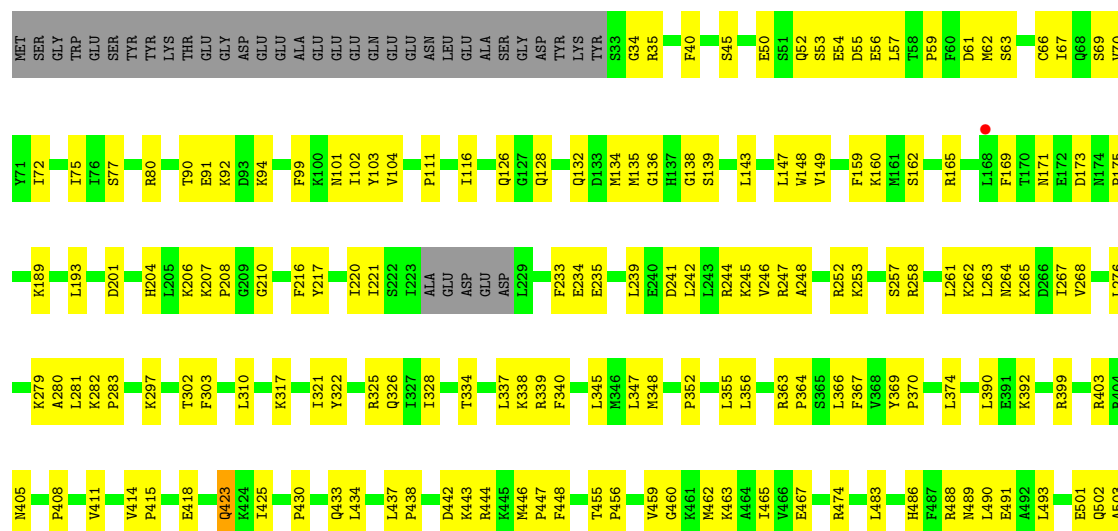
• Molecule 1: X-ray repair cross-complementing protein 6

Chain K: 60% 30% 8%



• Molecule 1: X-ray repair cross-complementing protein 6

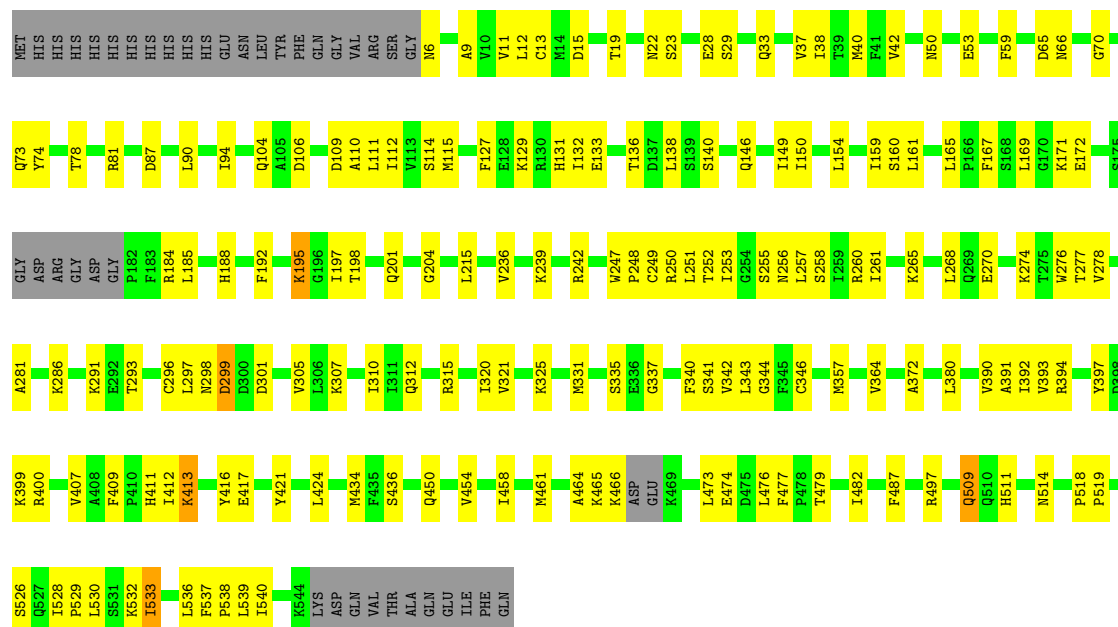
Chain O: 59% 32% 8%





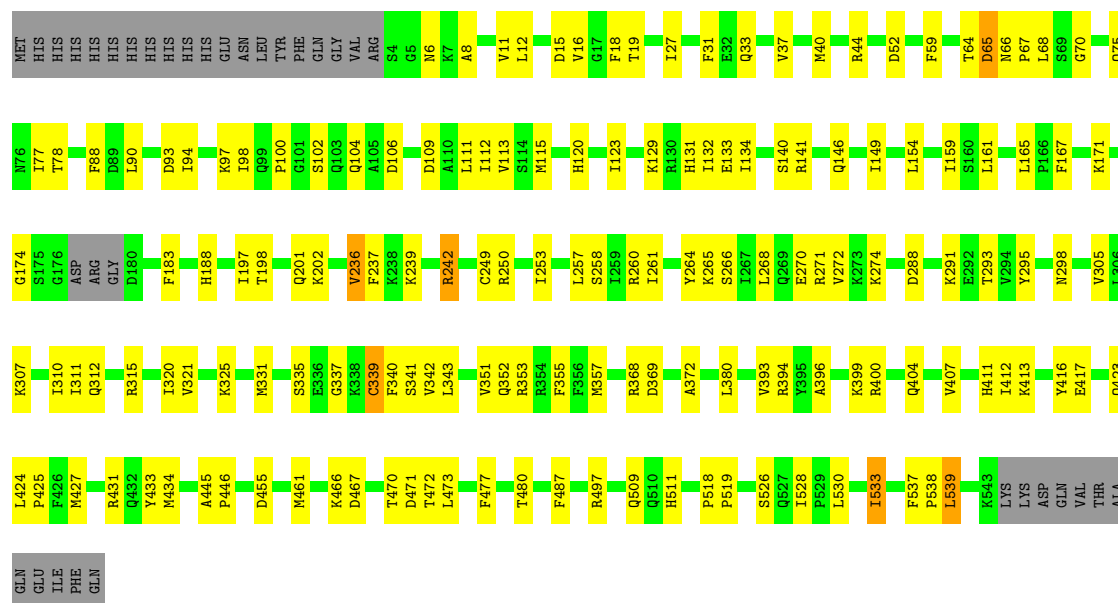
• Molecule 2: X-ray repair cross-complementing protein 5

Chain B: 63% 29% 7%



• Molecule 2: X-ray repair cross-complementing protein 5

Chain F: 66% 27% 6%

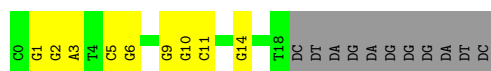


• Molecule 2: X-ray repair cross-complementing protein 5

[illegible]

R497	A383	I267	I159	G63	Met
Q509	D386	L268	S160	T64	HIS
Q510	D387	Q269	L161	D65	HIS
H511	D388	R271	L165	P67	HIS
P518	D389	V272	L166	L68	HIS
P519	P390	K273	F167	S69	HIS
S526	A391	K274	G170	G70	HIS
Q527	I392	A281	G170	G71	HIS
I528	V393	L284	LYS	D72	HIS
P529	V395	L284	GLU	Q73	HIS
L530	V396	K291	ASP	N76	GLU
S531	A396	K291	GLY	I77	LEU
K532	K399	V295	SER	T78	TYR
I533	R400	C296	GLY	R81	PRO
P537	V407	N298	ASP	D87	GLN
P538	A408	D299	ARG	F88	VAL
L539	F409	D300	GLY	D89	ARG
I540	I412	R301	F183	L90	S4
K543	E417	E302	R184	L91	G5
LYS	LYS	K307	L185	I94	N6
ASP	Y421	I310	H188	P100	K7
GLN	L424	I311	L194	G101	V11
VAL	L424	Q312	L194	S102	L12
THR	R431	R315	E199	Q103	D15
ALA	Q432	Q320	K202	Q104	V16
GLN	Y433	V321	K202	A105	G17
ILE	D455	V321	S226	D106	F18
PRO	M461	K325	V236	D109	T19
GLN	K465	M331	F237	A110	S23
	K466	S335	K238	L111	I27
	D467	F336	R239	I112	E28
	D471	G337	R242	M115	S29
	T472	K338	R247	D116	P30
	E473	C339	P248	I123	F31
	E474	F340	C249	G124	I38
	F477	V342	R250	K125	T39
	F478	L343	L251	K126	M40
	T479		T252	H131	F41
	K481	Q352	N256	I132	V42
	I482	T480	G254	E133	Q43
	P485	F355	T255	I134	R44
	R486	F356	S258	S140	Q45
	F487	K357	I259	Q146	F57
	L495	A372	R260	I149	V57
	H496	T380	I261	I150	L58
	L496	L380	K265	L154	F59

Chain C: 33% 30% 37%



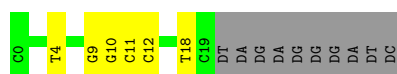
- Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*A P*TP*AP*T)-3')



- Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*A P*TP*AP*T)-3')



- Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*A P*TP*AP*T)-3')



- Molecule 4: DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3')

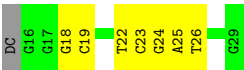


- Molecule 4: DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3')



- Molecule 4: DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3')

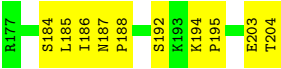




- Molecule 4: DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3')



- Molecule 5: Protein PAXX



- Molecule 5: Protein PAXX



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.02Å 428.57Å 96.06Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	45.32 – 2.95 45.32 – 2.95	Depositor EDS
% Data completeness (in resolution range)	23.9 (45.32-2.95) 21.9 (45.32-2.95)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.252 , 0.298 0.249 , 0.297	Depositor DCC
R_{free} test set	2001 reflections (5.85%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	1.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	36383	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: SO4

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	0.32	0/4105	0.83	8/5529 (0.1%)
1	E	0.28	0/4093	0.81	3/5512 (0.1%)
1	K	0.32	0/4129	0.83	10/5561 (0.2%)
1	O	0.32	0/4101	0.84	7/5523 (0.1%)
2	B	0.29	0/4334	0.79	2/5842 (0.0%)
2	F	0.28	0/4369	0.81	4/5892 (0.1%)
2	L	0.29	0/4324	0.79	6/5831 (0.1%)
2	P	0.27	0/4329	0.80	4/5840 (0.1%)
3	C	0.17	0/441	0.35	0/679
3	G	0.20	0/462	0.36	0/711
3	M	0.21	0/441	0.41	0/679
3	Q	0.20	0/462	0.37	0/711
4	D	0.23	0/318	0.40	0/488
4	H	0.24	0/339	0.45	0/520
4	N	0.24	0/318	0.40	0/488
4	R	0.25	0/339	0.43	0/520
5	J	0.17	0/218	0.40	0/290
5	T	0.13	0/218	0.47	0/290
All	All	0.29	0/37340	0.78	44/50906 (0.1%)

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
2	F	0	1

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	GLU	N-CA-C	-9.24	96.59	110.07
1	K	500	PRO	CA-C-N	7.26	132.80	121.99
1	K	500	PRO	C-N-CA	7.26	132.80	121.99
1	K	258	ARG	CG-CD-NE	6.99	127.37	112.00
2	L	69	SER	CA-C-N	6.45	130.17	121.01

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	65	ASP	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	4027	0	4101	153	0
1	E	4015	0	4099	167	0
1	K	4052	0	4128	171	0
1	O	4023	0	4110	170	0
2	B	4248	0	4299	134	0
2	F	4282	0	4312	135	0
2	L	4238	0	4281	131	0
2	P	4242	0	4278	144	0
3	C	393	0	213	13	0
3	G	412	0	224	11	0
3	M	393	0	213	18	0
3	Q	412	0	224	10	0
4	D	285	0	157	10	0
4	H	304	0	168	10	0
4	N	285	0	157	8	0
4	R	304	0	168	9	0
5	J	214	0	212	12	0
5	T	214	0	212	8	0
6	A	5	0	0	0	0
6	F	5	0	0	0	0
6	K	5	0	0	0	0
6	P	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
7	E	6	0	0	0	0
7	F	3	0	0	0	0
7	K	4	0	0	1	0
7	L	2	0	0	0	0
7	N	1	0	0	0	0
7	O	3	0	0	0	0
All	All	36383	0	35556	1120	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 16.

The worst 5 of 1120 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:F:250:ARG:HD3	2:F:258:SER:HB3	1.37	1.06
2:L:400:ARG:NH2	3:M:10:DG:O3'	1.93	1.02
1:O:339:ARG:HA	1:O:405:ASN:HA	1.44	0.99
1:A:207:LYS:HD2	1:A:208:PRO:HD2	1.48	0.96
1:A:493:LEU:HD13	2:B:321:VAL:HG11	1.46	0.96

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	495/544 (91%)	478 (97%)	15 (3%)	2 (0%)	30 53
1	E	493/544 (91%)	474 (96%)	16 (3%)	3 (1%)	21 45
1	K	498/544 (92%)	484 (97%)	13 (3%)	1 (0%)	43 66
1	O	494/544 (91%)	472 (96%)	21 (4%)	1 (0%)	43 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	525/572 (92%)	513 (98%)	11 (2%)	1 (0%)	43	66
2	F	533/572 (93%)	517 (97%)	14 (3%)	2 (0%)	30	53
2	L	524/572 (92%)	507 (97%)	15 (3%)	2 (0%)	30	53
2	P	527/572 (92%)	506 (96%)	18 (3%)	3 (1%)	21	45
5	J	26/28 (93%)	24 (92%)	2 (8%)	0	100	100
5	T	26/28 (93%)	23 (88%)	3 (12%)	0	100	100
All	All	4141/4520 (92%)	3998 (96%)	128 (3%)	15 (0%)	30	53

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	TYR
1	E	55	ASP
2	L	302	GLU
2	P	69	SER
2	P	125	LYS

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	453/492 (92%)	451 (100%)	2 (0%)	84	92
1	E	452/492 (92%)	448 (99%)	4 (1%)	70	83
1	K	456/492 (93%)	451 (99%)	5 (1%)	65	80
1	O	453/492 (92%)	450 (99%)	3 (1%)	76	87
2	B	478/513 (93%)	472 (99%)	6 (1%)	61	78
2	F	481/513 (94%)	477 (99%)	4 (1%)	73	85
2	L	476/513 (93%)	472 (99%)	4 (1%)	73	85
2	P	477/513 (93%)	473 (99%)	4 (1%)	73	85
5	J	23/23 (100%)	23 (100%)	0	100	100
5	T	23/23 (100%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3772/4066 (93%)	3740 (99%)	32 (1%)	73 85

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	236	VAL
2	P	331	MET
2	F	236	VAL
1	E	247	ARG
2	P	533	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	360	HIS
2	L	514	ASN
1	K	433	GLN
2	L	119	GLN
1	O	101	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are 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	$\# Z > 2$
6	SO4	A	601	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	P	601	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	K	601	-	4,4,4	0.24	0	6,6,6	0.10	0
6	SO4	F	601	-	4,4,4	0.23	0	6,6,6	0.09	0

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	499/544 (91%)	-1.73	0 100 100	51, 105, 175, 256	0
1	E	497/544 (91%)	-1.79	0 100 100	46, 80, 134, 187	0
1	K	502/544 (92%)	-1.79	0 100 100	43, 112, 181, 235	0
1	O	498/544 (91%)	-1.77	1 (0%) 91 90	44, 81, 136, 204	0
2	B	531/572 (92%)	-1.71	0 100 100	44, 92, 161, 227	0
2	F	537/572 (93%)	-1.74	0 100 100	47, 84, 145, 208	0
2	L	530/572 (92%)	-1.74	0 100 100	33, 93, 159, 257	0
2	P	531/572 (92%)	-1.75	0 100 100	45, 83, 137, 194	0
3	C	19/30 (63%)	-2.14	0 100 100	105, 146, 174, 176	0
3	G	20/30 (66%)	-2.22	0 100 100	106, 143, 164, 174	0
3	M	19/30 (63%)	-2.17	0 100 100	102, 148, 184, 186	0
3	Q	20/30 (66%)	-2.34	0 100 100	108, 145, 172, 187	0
4	D	14/15 (93%)	-2.28	0 100 100	130, 154, 191, 201	0
4	H	15/15 (100%)	-2.22	0 100 100	106, 123, 176, 193	0
4	N	14/15 (93%)	-2.32	0 100 100	134, 143, 180, 223	0
4	R	15/15 (100%)	-2.28	0 100 100	114, 131, 185, 213	0
5	J	28/28 (100%)	-1.75	0 100 100	83, 104, 141, 161	0
5	T	28/28 (100%)	-1.75	0 100 100	77, 107, 149, 165	0
All	All	4317/4700 (91%)	-1.77	1 (0%) 100 100	33, 92, 163, 257	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	168	LEU	2.2

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	SO4	A	601	5/5	0.97	0.02	98,103,110,110	0
6	SO4	K	601	5/5	0.98	0.02	81,82,87,90	0
6	SO4	F	601	5/5	0.99	0.06	70,72,77,77	0
6	SO4	P	601	5/5	0.99	0.02	79,80,84,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.