



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 14, 2025 – 05:01 PM JST

PDB ID : 8KAL / pdb_00008kal
Title : Crystal structure of SpyCas9 in complex with sgRNA and 17nt target DNA
Authors : Chen, Y.; Chen, J.; Liu, L.
Deposited on : 2023-08-03
Resolution : 3.16 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

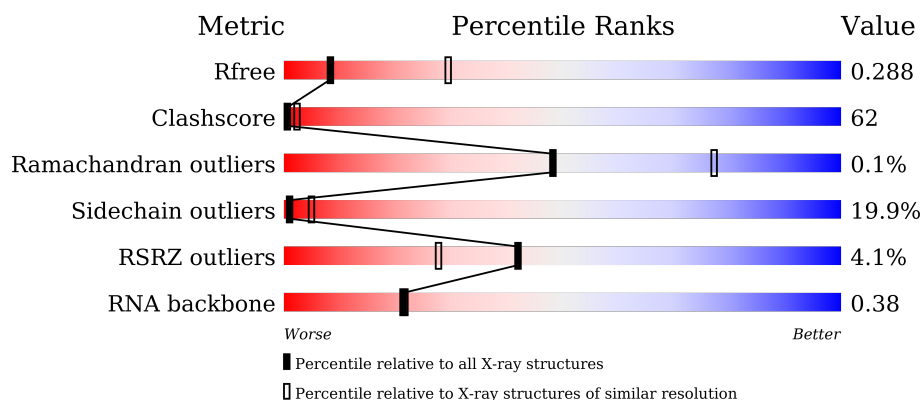
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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}	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)
RNA backbone	3690	1016 (3.42-2.90)

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	98	<div> <div>11%</div> <div>48%</div> <div>32%</div> <div>5%</div> </div>
1	E	98	<div> <div>16%</div> <div>49%</div> <div>28%</div> </div>
2	B	1368	<div> <div>4%</div> <div>30%</div> <div>52%</div> <div>14%</div> </div>
2	G	1368	<div> <div>4%</div> <div>32%</div> <div>52%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	25	
3	H	25	
4	D	11	
4	J	11	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27214 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 RNA chain called RNA (98-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	P	0	0	0
			2009	899	362	654	94			
1	E	95	Total	C	N	O	P	0	0	0
			2029	908	365	661	95			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1326	Total	C	N	O	S	0	0	0
			10821	6892	1877	2030	22			
2	G	1326	Total	C	N	O	S	0	0	0
			10822	6892	1879	2029	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
G	10	ALA	ASP	engineered mutation	UNP Q99ZW2
G	840	ALA	HIS	engineered mutation	UNP Q99ZW2

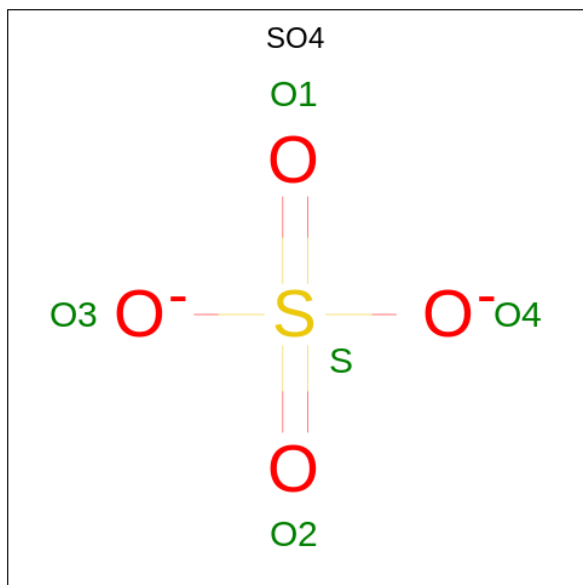
- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			505	243	93	145	24			
3	H	25	Total	C	N	O	P	0	0	0
			505	243	93	145	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			
4	J	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		

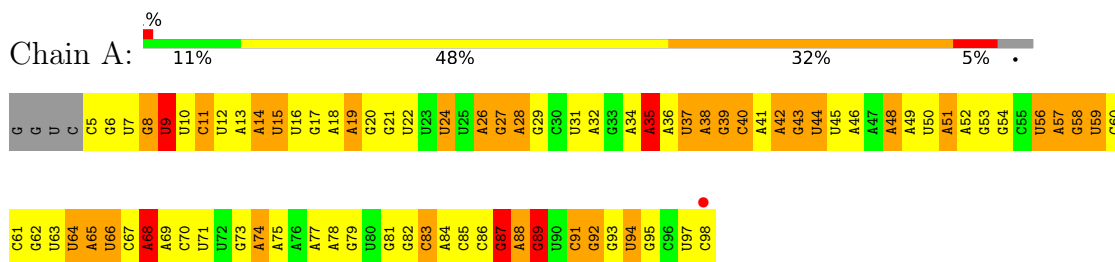
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	B	26	Total	O	0	0
			26	26		
6	C	1	Total	O	0	0
			1	1		
6	E	3	Total	O	0	0
			3	3		
6	G	29	Total	O	0	0
			29	29		
6	H	1	Total	O	0	0
			1	1		

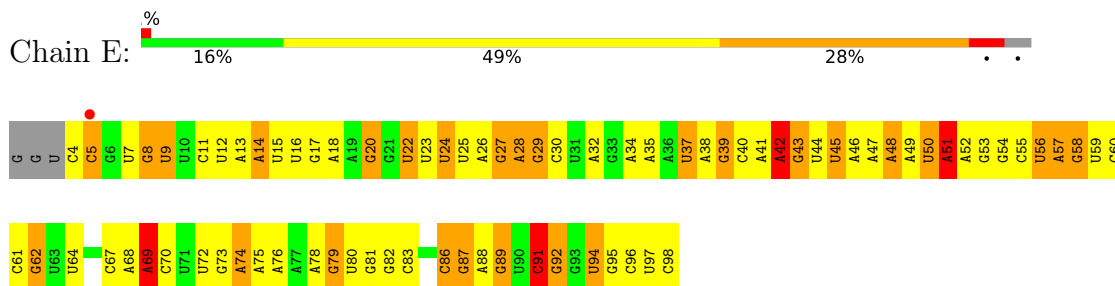
3 Residue-property plots [i](#)

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.

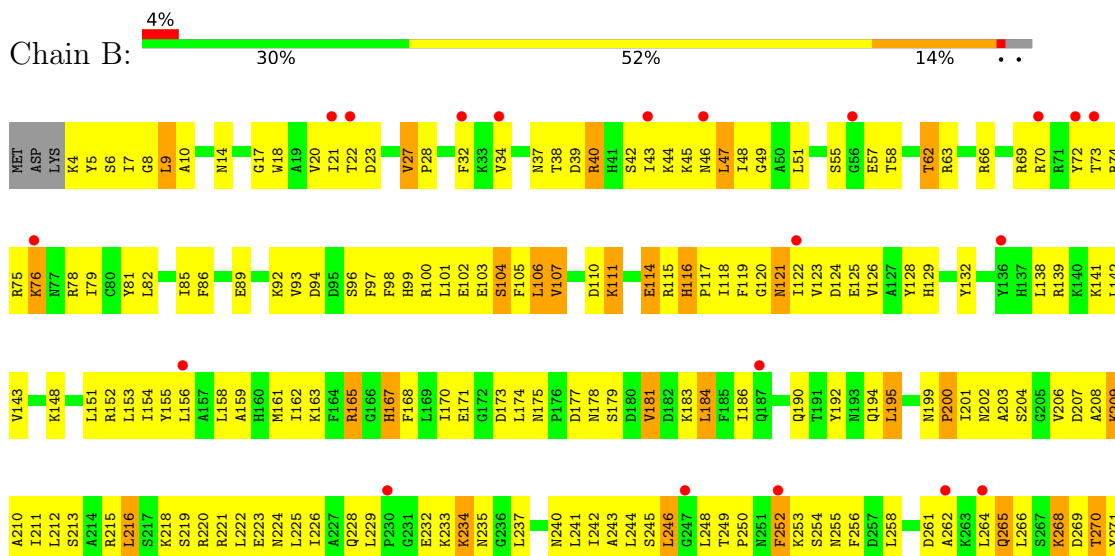
- Molecule 1: RNA (98-MER)



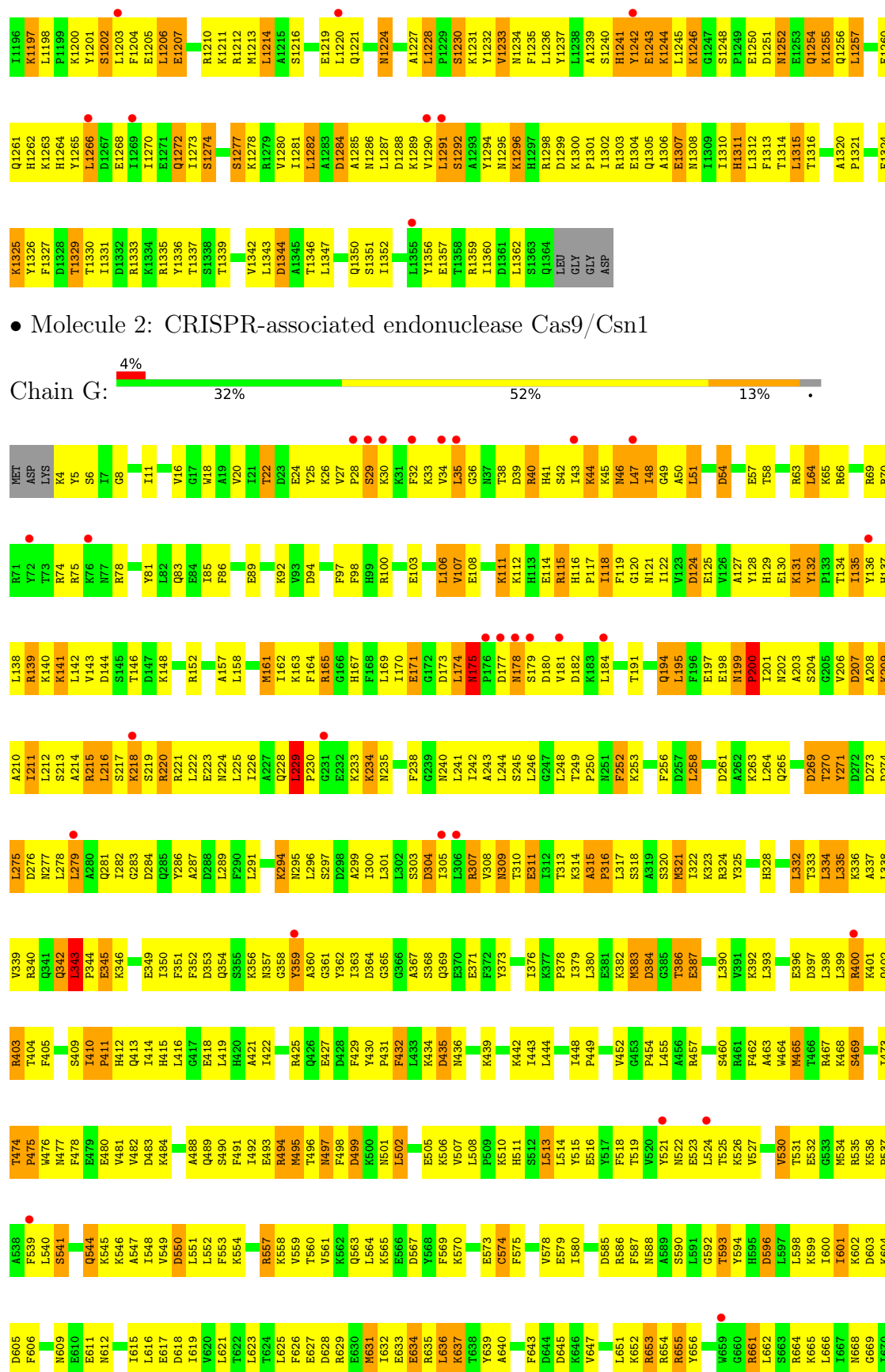
- Molecule 1: RNA (98-MER)

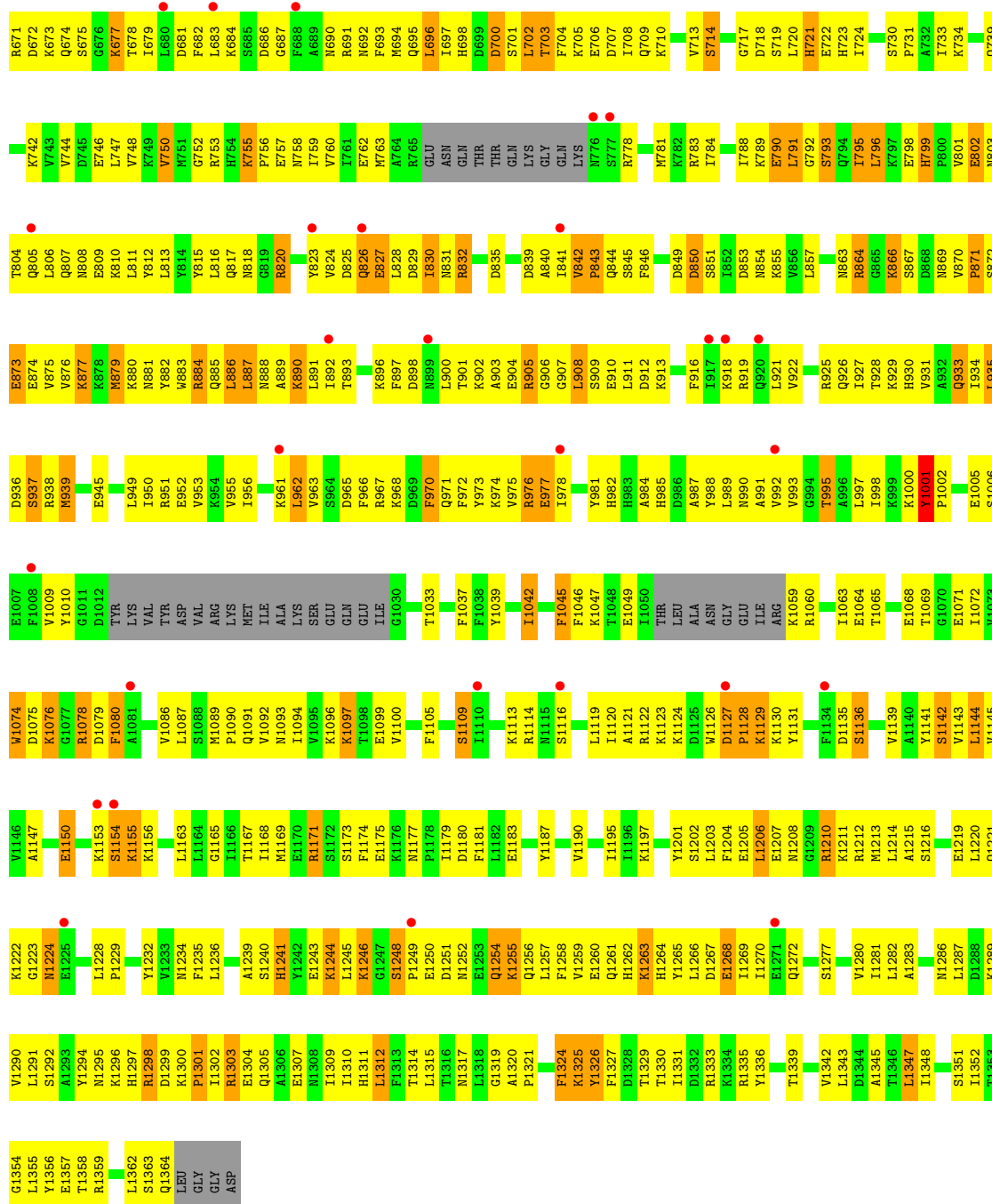


- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



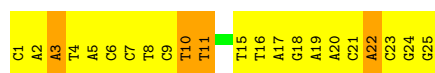
Y1131	F1134	D1135	S1136	P1137	T1138	V1139	A1140	S1142	V1143	I1144	V1145	V1146	A1147	K1148	V1149	E1150	K1151	G1152	K1153	S1154	K1155	K1156	L1157	K1158	S1159	V1160	K1161	L1164	G1165	T1166	T1167	M1168	M1169	E1170	R1171	F1174	E1175	K1176	M1177	P1178	I1179	D1180	F1181	L1182	E1183	A1184	K1185	Y1187	K1191	K1192	D1193	L1194	I1195				
THR	LEU	ALA	ASN	GLY	GLU	ILE	ARG	R1060	P1061	L1062	E1064	W1074	D1075	F1080	A1081	T1082	V1083	VAL	ASP	VAL	ARG	LYS	MET	Q1091	V1092	A1093	L1094	V1095	V1100	Q1101	T1102	F1105	S1106	K1107	E1108	S1109	T1110	F1111	Y1112	K1113	R1114	A1121	R1122	K1123	D1127	P1128	L1129	K1130									
H983	A984	A987	Y988	L989	N990	A991	V992	T995	Y1001	P1002	E1005	S1006	E1007	F1008	V1009	D1012	T1013	L1014	VAL	ASP	VAL	ARG	LYS	ILE	ALA	LYS	SER	GLU	GLN	GLU	K961	L962	V963	S964	D965	R966	R967	K968	D969	F970	Q971	F972	Y973	K974	V975	R976	E977	F1045	F1046	K1047	N980	L981	H982				
D850	S851	L852	D853	N854	K855	V856	L857	T858	R859	D861	R864	G865	K866	S867	V870	P871	S872	K873	E874	L875	V876	K877	W883	E884	Q885	L886	L887	N888	M889	Y890	T893	Q894	K895	K896	F897	L900	T901	K902	A903	E904	R905	G906	G907	L908	S909	E910	L911	D912	K913	A914	G915	F916	I917				
E722	H723	A724	L725	K726	L727	S730	P731	A732	L733	K734	V735	G736	L737	L738	Q739	T740	V743	V744	D745	E746	D681	L682	L683	K684	S685	G686	L687	N688	D689	M690	D691	F692	E693	M694	Q695	L696	L697	H698	K699	L700	S701	L702	T703	F704	K705	E706	D707	L708	Q709	K710	A711	Q712	D718	S719	L720	H721	I724
E785	E786	G787	L788	K789	E790	L791	G792	S793	L794	L796	H799	P800	V801	E802	N803	L806	K810	L811	Y812	L813	Y814	Y815	L816	Q817	N818	Q819	R820	D821	Y822	Y823	V824	E827	L828	D829	L830	N831	R832	L833	S834	D835	Y836	D837	V838	D839	A840	V842	P843	Q844	S845	F846	K848	D849					
D850	S851	L852	D853	N854	K855	V856	L857	T858	R859	D861	R864	G865	K866	S867	V870	P871	S872	K873	E874	L875	V876	K877	W883	E884	Q885	L886	L887	N888	M889	Y890	T893	Q894	K895	K896	F897	L900	T901	K902	A903	E904	R905	G906	G907	L908	S909	E910	L911	D912	K913	A914	G915	F916	I917				
K918	R919	Q920	E923	T924	R925	Q926	L927	T928	K929	H930	V931	A932	Q933	I934	L935	D936	S937	R938	P939	N940	D944	E945	N946	D947	K948	L949	P950	R951	E952	V953	A954	L958	K961	L962	V963	S964	D965	R966	R967	K968	D969	F970	Q971	F972	Y973	K974	V975	R976	E977	F1045	F1046	K1047	N980	L981	H982		
H983	A984	A987	Y988	L989	N990	A991	V992	T995	Y1001	P1002	E1005	S1006	E1007	F1008	V1009	D1012	T1013	L1014	VAL	ASP	VAL	ARG	LYS	MET	Q1091	V1092	A1093	L1094	V1095	V1100	Q1101	T1102	F1105	S1106	K1107	E1108	S1109	T1110	F1111	Y1112	K1113	R1114	A1121	R1122	K1123	D1127	P1128	L1129	K1130								
THR	LEU	ALA	ASN	GLY	GLU	ILE	ARG	R1060	P1061	L1062	E1064	W1074	D1075	F1080	A1081	T1082	V1083	VAL	ASP	VAL	ARG	LYS	MET	Q1091	V1092	A1093	L1094	V1095	V1100	Q1101	T1102	F1105	S1106	K1107	E1108	S1109	T1110	F1111	Y1112	K1113	R1114	A1121	R1122	K1123	D1127	P1128	L1129	K1130									
D272	D273	D274	L275	D276	D277	L278	L279	A280	Q281	L282	Q283	D284	Q285	Y286	A287	D288	L289	F290	L291	A292	K293	N295	L296	S297	D298	A299	I300	L301	L302	S303	D304	I305	L306	R307	V308	N309	T310	E311	I312	T313	K314	A315	P316	L317	S320	K323	R324	H328	L332	T333	L334	L335	K336	A337			





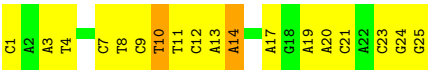
• Molecule 3: DNA (25-MER)

Chain C: 12% 72% 16%

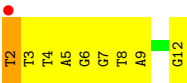


• Molecule 3: DNA (25-MER)

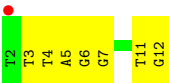
Chain H: 28% 64% 8%



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



● Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*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	362.05Å 70.96Å 200.10Å 90.00° 101.52° 90.00°	Depositor
Resolution (Å)	50.17 – 3.16 50.17 – 3.16	Depositor EDS
% Data completeness (in resolution range)	65.6 (50.17-3.16) 65.6 (50.17-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.251 , 0.288 0.248 , 0.288	Depositor DCC
R_{free} test set	4281 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	27214	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6562e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.87	1/2249 (0.0%)	1.58	39/3503 (1.1%)
1	E	0.84	0/2271	1.55	31/3537 (0.9%)
2	B	0.62	11/11013 (0.1%)	0.73	29/14802 (0.2%)
2	G	0.60	9/11013 (0.1%)	0.71	22/14799 (0.1%)
3	C	1.25	2/566 (0.4%)	1.24	6/870 (0.7%)
3	H	1.38	2/566 (0.4%)	1.21	1/870 (0.1%)
4	D	1.40	2/251 (0.8%)	1.27	0/387
4	J	1.29	2/251 (0.8%)	1.20	0/387
All	All	0.71	29/28180 (0.1%)	0.97	128/39155 (0.3%)

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	10	DT	C3'-O3'	-7.60	1.34	1.44
4	J	3	DT	C1'-N1	6.21	1.57	1.49
4	D	3	DT	N1-C2	5.78	1.42	1.38
4	J	4	DT	C3'-O3'	-5.67	1.36	1.44
3	H	14	DA	N9-C4	-5.66	1.34	1.37

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	A	O5'-P-OP2	-9.27	97.36	105.70
2	B	684	LYS	N-CA-C	-9.20	86.15	111.00
1	E	51	A	C8-N9-C4	-9.21	102.12	105.80
2	G	506	LYS	N-CA-C	-9.19	86.20	111.00
2	G	507	VAL	N-CA-CB	-9.01	91.67	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2009	0	1009	110	0
1	E	2029	0	1020	127	0
2	B	10821	0	10948	1507	0
2	G	10822	0	10967	1594	0
3	C	505	0	283	31	0
3	H	505	0	283	23	0
4	D	225	0	129	18	0
4	J	225	0	129	6	0
5	B	5	0	0	0	0
5	G	5	0	0	1	0
6	A	3	0	0	0	0
6	B	26	0	0	7	0
6	C	1	0	0	0	0
6	E	3	0	0	1	0
6	G	29	0	0	10	0
6	H	1	0	0	0	0
All	All	27214	0	24768	3234	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 62.

The worst 5 of 3234 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:G:530:VAL:CG1	2:G:537:PRO:HB3	1.21	1.65
2:B:181:VAL:HG11	2:B:300:ILE:CD1	1.14	1.59
2:G:279:LEU:CD1	2:G:287:ALA:HB2	1.28	1.59
2:G:279:LEU:HD11	2:G:287:ALA:CB	1.21	1.59
2:G:870:VAL:CG2	2:G:908:LEU:CD2	1.77	1.59

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	
2	B	1318/1368 (96%)	1279 (97%)	38 (3%)	1 (0%)	48	77
2	G	1318/1368 (96%)	1273 (97%)	43 (3%)	2 (0%)	44	72
All	All	2636/2736 (96%)	2552 (97%)	81 (3%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	PRO
2	G	200	PRO
2	G	230	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	
2	B	1185/1225 (97%)	943 (80%)	242 (20%)	1	4
2	G	1186/1225 (97%)	957 (81%)	229 (19%)	1	5
All	All	2371/2450 (97%)	1900 (80%)	471 (20%)	1	5

5 of 471 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1291	LEU
2	G	1205	GLU
2	G	220	ARG

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Mol	Chain	Res	Type
2	G	1155	LYS
2	G	886	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	235	ASN
2	G	497	ASN
2	G	281	GLN
2	G	342	GLN
2	G	690	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	93/98 (94%)	31 (33%)	4 (4%)
1	E	94/98 (95%)	24 (25%)	3 (3%)
All	All	187/196 (95%)	55 (29%)	7 (3%)

5 of 55 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	11	C
1	A	20	G
1	A	24	U
1	A	27	G

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	68	A
1	E	8	G
1	E	42	A
1	E	27	G
1	A	42	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

2 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	$\# Z > 2$
5	SO4	B	1401	-	4,4,4	0.98	0	6,6,6	1.66	1 (16%)
5	SO4	G	1401	-	4,4,4	0.98	0	6,6,6	1.66	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	1401	SO4	O4-S-O3	3.83	125.39	109.06
5	G	1401	SO4	O4-S-O3	3.83	125.39	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1401	SO4	1	0

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	94/98 (95%)	-0.12	1 (1%) 77 62	27, 56, 107, 151	0
1	E	95/98 (96%)	-0.26	1 (1%) 77 62	31, 56, 109, 125	0
2	B	1326/1368 (96%)	0.12	60 (4%) 39 25	24, 57, 90, 137	0
2	G	1326/1368 (96%)	0.12	56 (4%) 41 27	25, 57, 89, 123	0
3	C	25/25 (100%)	-0.01	0 100 100	32, 47, 96, 107	0
3	H	25/25 (100%)	-0.16	0 100 100	34, 47, 99, 112	0
4	D	11/11 (100%)	0.19	1 (9%) 16 11	48, 65, 121, 133	0
4	J	11/11 (100%)	0.40	1 (9%) 16 11	35, 60, 114, 132	0
All	All	2913/3004 (96%)	0.10	120 (4%) 42 28	24, 57, 93, 151	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1134	PHE	5.5
2	G	76	LYS	4.2
2	B	539	PHE	4.1
2	B	46	ASN	4.1
2	G	305	ILE	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 monosaccharides 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(\AA^2)	Q<0.9
5	SO4	G	1401	5/5	0.80	0.10	78,81,95,107	0
5	SO4	B	1401	5/5	0.84	0.24	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.