



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 11:14 PM BST

PDB ID : 6OVR
Title : X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter variant -1G
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2019-05-08
Resolution : 2.84 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 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) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

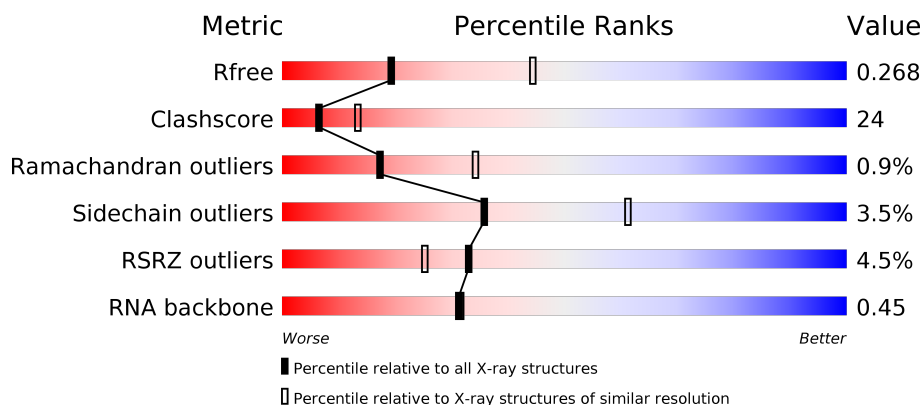
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)
RNA backbone	3102	1077 (3.10-2.58)

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 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	315	<div> <div>46%</div> <div>24%</div> <div>28%</div> </div>
1	B	315	<div> <div>35%</div> <div>36%</div> <div>29%</div> </div>
2	C	1119	<div> <div>4%</div> <div>61%</div> <div>35%</div> </div>
3	D	1524	<div> <div>3%</div> <div>59%</div> <div>36%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>59%32%5%</div></div>
5	F	423	<div><div></div><div>12%45%34%18%</div></div>
6	G	22	<div><div></div><div>14%50%32%5%14%</div></div>
7	H	27	<div><div></div><div>11%44%22%30%</div></div>
8	I	8	<div><div></div><div>25%38%25%38%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28535 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1107	Total	C	N	O	S	0	0	0
			8726	5523	1551	1628	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total	C	N	O	S	0	0	0
			11722	7431	2065	2191	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2790	1760	508	518	4			

- Molecule 6 is a DNA chain called DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	19	Total	C	N	O	P	0	0	0
			387	183	75	110	19			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	19	Total	C	N	O	P	0	0	0
			394	188	76	112	18			

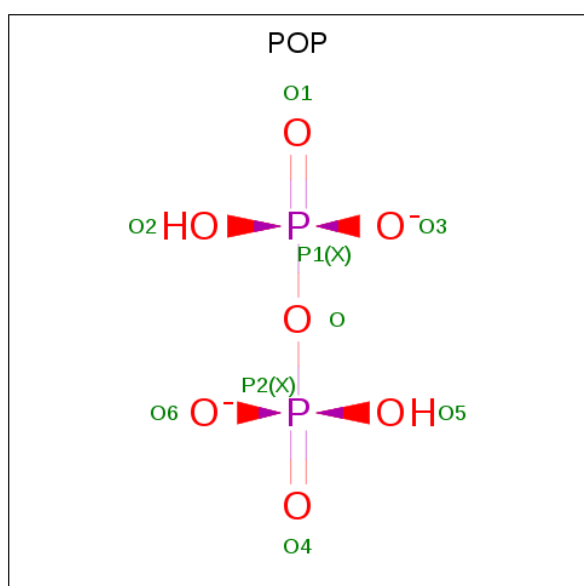
- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	8	Total	C	N	O	P	0	0	0
			193	80	40	63	10			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	P	0	0
			9	7	2		

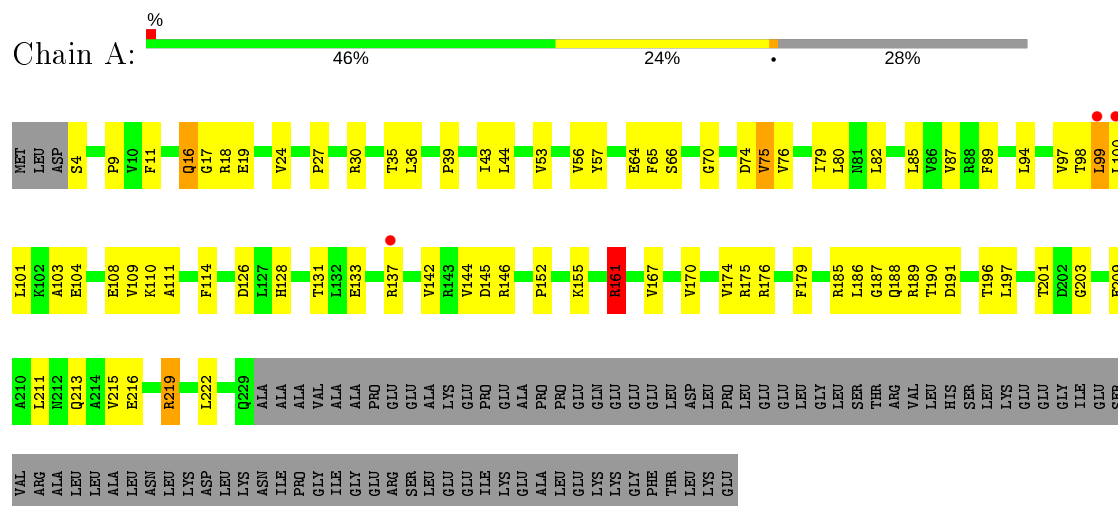
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

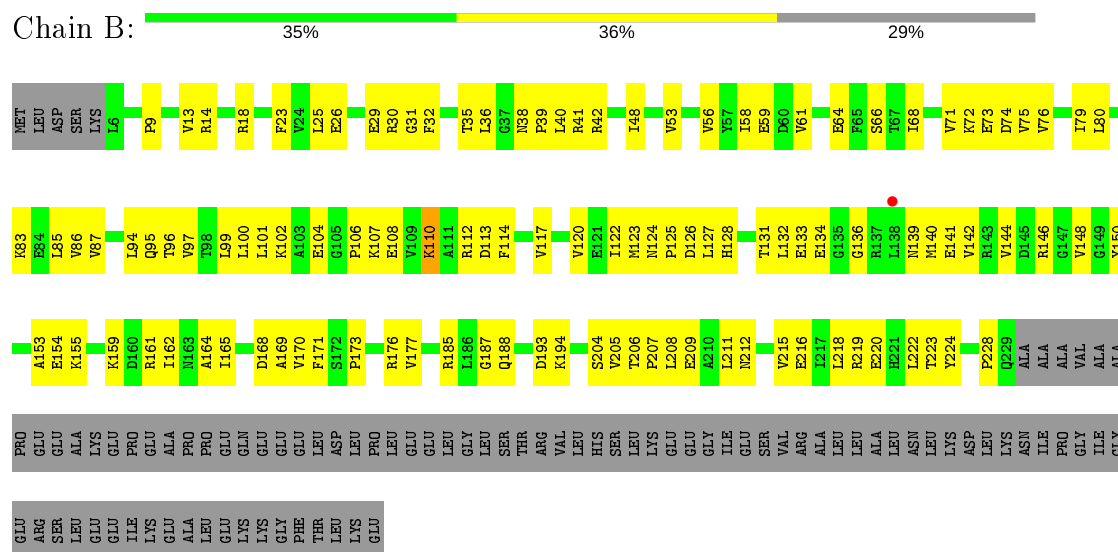
3 Residue-property plots

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

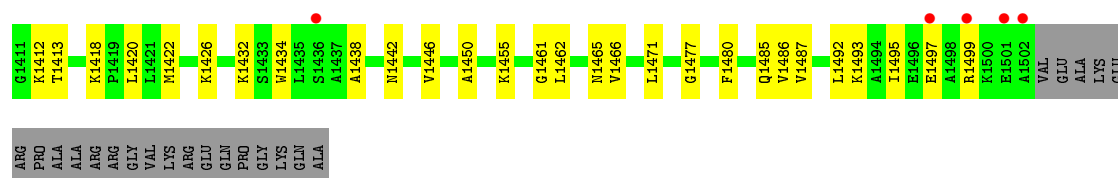


• Molecule 2: DNA-directed RNA polymerase subunit beta

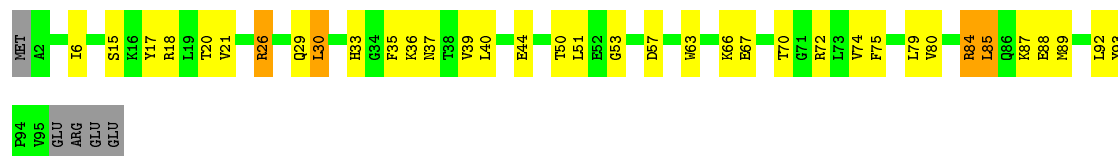




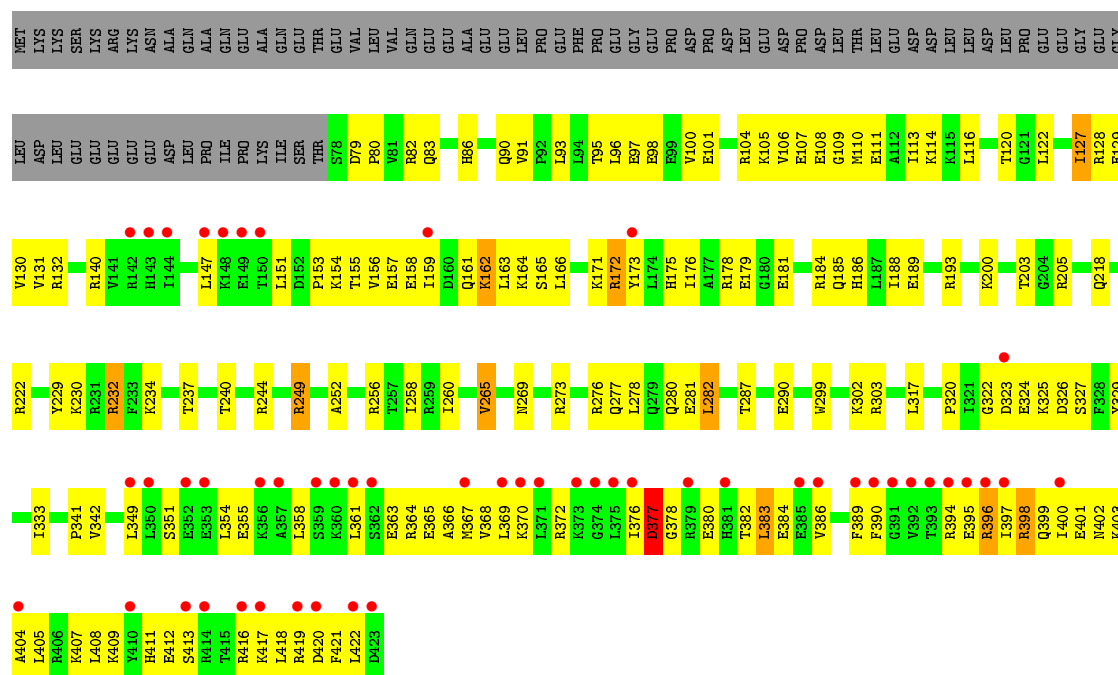
K1301	T1234	R1108	L881	D682	Q575	R486	A398	L333	E247	P172	T97
E1302	Q1235	E1109	L881	I603	D579	A467	A401	L335	P243	P173	P98
Y1303	L1236	A1110	K684	K684	D579	R488	Y401	T334	Y249	G174	A99
K1304	T1237	D1111	I885	D685	A580	R489	D405	L335	R252	L178	H101
P1306	ARG	G1112	E886	E686	L581	A490	D406	E338	R253	L179	H102
K1307	THR	C1113	A887	V687	L582	K491	V407	K339	E254	K180	H103
E1308	PHE	T1114	E888	K688	R587	K494	E408	E339	D181	F104	F105
A1309	HIS	D1126	A889	D689	R587	K495	V409	K343	V258	G182	V105
R1310	THR	E1127	V890	L691	S602	L496	S410	D344	V259	E183	K106
L1311	GLY	V1128	V895	L695	L603	R500	T411	E184	E184	E184	S110
V1312	VAL	T1129	K896	L695	R613	R500	G412	V347	E266	V186	K111
L1313	ALA	R1130	E896	V689	R613	L503	D413	Q348	G267	K187	I112
K1314	ALA	R1137	L899	V689	R622	L503	V420	Q348	A268	G188	I112
D1315	GLY	L1137	L899	V700	R622	L503	V420	Q348	A268	G188	I112
G1316	ALA	E1141	L899	V700	R622	L503	V420	Q348	A268	G188	I112
D1317	ALA	E1142	L899	V700	R622	L503	V420	Q348	A268	G188	I112
Y1318	ASP	G1143	L899	V700	R622	L503	V420	Q348	A268	G188	I112
L1318	ILE	L1144	L899	V700	R622	L503	V420	Q348	A268	G188	I112
T1326	THR	Y1145	L899	V700	R622	L503	V420	Q348	A268	G188	I112
R1327	Q1254	V1148	L899	V700	R622	L503	V420	Q348	A268	G188	I112
D1331	R1258	R1151	L899	V700	R622	L503	V420	Q348	A268	G188	I112
P1332	R1258	V1155	L899	V700	R622	L503	V420	Q348	A268	G188	I112
H1333	R1258	V1155	L899	V700	R622	L503	V420	Q348	A268	G188	I112
L1336	R1258	V1155	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1343	R1266	V1155	L899	V700	R622	L503	V420	Q348	A268	G188	I112
V1344	R1267	V1155	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1351	P1268	V1155	L899	V700	R622	L503	V420	Q348	A268	G188	I112
L1363	K1271	R1164	L899	V700	R622	L503	V420	Q348	A268	G188	I112
H1364	I1271	Y1165	L899	V700	R622	L503	V420	Q348	A268	G188	I112
D1365	A1272	L1166	L899	V700	R622	L503	V420	Q348	A268	G188	I112
K1366	S1275	S1167	L899	V700	R622	L503	V420	Q348	A268	G188	I112
V1371	E1276	M1168	L899	V700	R622	L503	V420	Q348	A268	G188	I112
R1372	I1277	V1171	L899	V700	R622	L503	V420	Q348	A268	G188	I112
Q1373	D1278	A1177	L899	V700	R622	L503	V420	Q348	A268	G188	I112
Q1374	G1279	V1188	L899	V700	R622	L503	V420	Q348	A268	G188	I112
M1375	V1280	R1189	L899	V700	R622	L503	V420	Q348	A268	G188	I112
V1379	L1282	R1197	L899	V700	R622	L503	V420	Q348	A268	G188	I112
D1386	T1286	Y1198	L899	V700	R622	L503	V420	Q348	A268	G188	I112
S1387	E1287	G1199	L899	V700	R622	L503	V420	Q348	A268	G188	I112
L1390	K1288	V1200	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1391	L1289	K1203	L899	V700	R622	L503	V420	Q348	A268	G188	I112
W1398	S1291	G1204	L899	V700	R622	L503	V420	Q348	A268	G188	I112
D1399	V1292	C1204	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1405	F1293	P1214	L899	V700	R622	L503	V420	Q348	A268	G188	I112
A1409	W1294	I1217	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1410	S1295	T1217	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1410	E1296	A1225	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1410	E1297	E1297	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1410	G1298	G1298	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1410	F1299	F1299	L899	V700	R622	L503	V420	Q348	A268	G188	I112
E1410	S1300	S1300	L899	V700	R622	L503	V420	Q348	A268	G188	I112



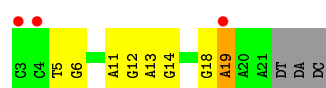
- Molecule 4: DNA-directed RNA polymerase subunit omega



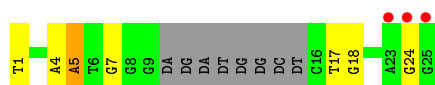
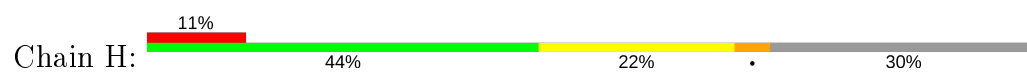
- Molecule 5: RNA polymerase sigma factor SigA



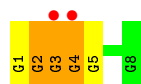
- Molecule 6: DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*GP*AP*AP*A)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP*AP*GP*G)-3')



● Molecule 8: RNA (5'-D*(GTP))-R(P*GP*GP*GP*GP*GP*GP*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	185.90Å 101.42Å 295.19Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	41.69 – 2.84 41.69 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.5 (41.69-2.84) 96.5 (41.69-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.222 , 0.268 0.222 , 0.268	Depositor DCC
R_{free} test set	1994 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28535	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: GTP, ZN, MG, POP

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	0.50	1/1814 (0.1%)	0.70	1/2466 (0.0%)
1	B	0.53	0/1799	0.72	0/2447
2	C	0.52	3/8892 (0.0%)	0.72	5/12028 (0.0%)
3	D	0.57	3/11928 (0.0%)	0.75	12/16127 (0.1%)
4	E	0.52	0/775	0.80	3/1045 (0.3%)
5	F	0.58	5/2835 (0.2%)	0.74	6/3816 (0.2%)
6	G	1.14	1/434 (0.2%)	1.06	1/666 (0.2%)
7	H	0.87	0/442	1.00	2/680 (0.3%)
8	I	0.79	0/181	1.36	1/283 (0.4%)
All	All	0.57	13/29100 (0.0%)	0.75	31/39558 (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
1	A	0	1
3	D	0	2
5	F	0	1
All	All	0	4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	249	ARG	CB-CG	10.78	1.81	1.52
2	C	37	GLU	CB-CG	-10.32	1.32	1.52
2	C	37	GLU	CD-OE1	-8.63	1.16	1.25
5	F	249	ARG	CZ-NH2	-8.59	1.21	1.33
5	F	249	ARG	NE-CZ	8.53	1.44	1.33

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	249	ARG	NE-CZ-NH2	13.02	126.81	120.30
6	G	19	DA	O4'-C4'-C3'	-8.25	101.05	106.00
5	F	249	ARG	NH1-CZ-NH2	-7.98	110.62	119.40
3	D	513	ILE	CG1-CB-CG2	-7.95	93.91	111.40
3	D	35	ARG	NE-CZ-NH2	-7.32	116.64	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Peptide
3	D	1129	THR	Peptide
3	D	65	ARG	Peptide
5	F	389	PHE	Peptide

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	1782	0	1834	86	0
1	B	1767	0	1816	118	0
2	C	8726	0	8814	428	0
3	D	11722	0	11950	601	13
4	E	761	0	778	43	0
5	F	2790	0	2853	183	11
6	G	387	0	212	9	0
7	H	394	0	217	9	0
8	I	193	0	88	3	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	9	0	0	0	0
11	D	2	0	0	0	0
All	All	28535	0	28562	1358	13

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 24.

The worst 5 of 1358 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)
5:F:249:ARG:CG	5:F:249:ARG:CB	1.81	1.58
3:D:371:ILE:CD1	3:D:372:ASP:H	1.36	1.38
2:C:605:LYS:HB3	2:C:610:ARG:NH2	1.35	1.36
3:D:411:THR:O	5:F:178:ARG:NH2	1.58	1.36
3:D:411:THR:C	5:F:178:ARG:NH2	1.90	1.23

The worst 5 of 13 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)
3:D:301:GLY:N	5:F:249:ARG:NH1[4_1349]	1.44	0.76
3:D:300:LYS:O	5:F:249:ARG:NE[4_1349]	1.58	0.62
3:D:302:GLN:N	5:F:249:ARG:NH2[4_1349]	1.66	0.54
3:D:302:GLN:N	5:F:249:ARG:CZ[4_1349]	1.77	0.43
3:D:300:LYS:C	5:F:249:ARG:NE[4_1349]	1.80	0.40

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	224/315 (71%)	211 (94%)	13 (6%)	0	100	100
1	B	222/315 (70%)	202 (91%)	18 (8%)	2 (1%)	17	34
2	C	1101/1119 (98%)	1036 (94%)	53 (5%)	12 (1%)	14	30
3	D	1480/1524 (97%)	1398 (94%)	71 (5%)	11 (1%)	22	42
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/423 (81%)	316 (92%)	23 (7%)	5 (2%)	10	22
All	All	3463/3795 (91%)	3252 (94%)	181 (5%)	30 (1%)	17	34

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	GLU
2	C	363	SER
2	C	418	LEU
2	C	419	THR
3	D	486	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	199/273 (73%)	192 (96%)	7 (4%)	36	61
1	B	197/273 (72%)	194 (98%)	3 (2%)	65	82
2	C	931/941 (99%)	892 (96%)	39 (4%)	30	54
3	D	1250/1279 (98%)	1213 (97%)	37 (3%)	41	65
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	60
5	F	296/371 (80%)	281 (95%)	15 (5%)	24	45
All	All	2956/3225 (92%)	2852 (96%)	104 (4%)	36	61

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	929	ARG
3	D	316	GLN
5	F	355	GLU
2	C	1026	GLN
3	D	190	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1047	HIS
3	D	529	GLN

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Mol	Chain	Res	Type
5	F	248	ASN
3	D	33	ASN
3	D	151	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	7/8 (87%)	3 (42%)	2 (28%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	3	G
8	I	4	G
8	I	5	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	1	GTP
8	I	4	G

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
10	POP	C	1201	-	6,8,8	0.51	0	13,13,13	1.31	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	POP	C	1201	-	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
10	C	1201	POP	P2-O-P1	-2.86	123.03	132.83

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	226/315 (71%)	-0.11	3 (1%) 77 74	71, 95, 118, 132	0
1	B	224/315 (71%)	-0.02	1 (0%) 92 91	68, 96, 127, 146	0
2	C	1107/1119 (98%)	0.16	48 (4%) 35 27	54, 94, 165, 203	0
3	D	1484/1524 (97%)	0.13	47 (3%) 47 41	49, 87, 149, 204	0
4	E	94/99 (94%)	0.01	0 100 100	64, 102, 152, 157	0
5	F	346/423 (81%)	0.65	52 (15%) 2 1	62, 107, 206, 228	0
6	G	19/22 (86%)	0.63	3 (15%) 2 1	66, 123, 229, 241	0
7	H	19/27 (70%)	0.11	3 (15%) 2 1	92, 125, 233, 239	0
8	I	7/8 (87%)	1.04	2 (28%) 0 0	68, 83, 172, 195	0
All	All	3526/3852 (91%)	0.17	159 (4%) 33 25	49, 94, 165, 241	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	392	VAL	9.6
5	F	397	ILE	8.2
5	F	376	ILE	8.1
5	F	396	ARG	8.0
5	F	374	GLY	7.7

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
10	POP	C	1201	9/9	0.91	0.15	78,95,107,114	0
9	MG	D	2001	1/1	0.92	0.25	48,48,48,48	0
9	MG	B	1001	1/1	0.93	0.37	78,78,78,78	0
11	ZN	D	2002	1/1	0.97	0.12	113,113,113,113	0
11	ZN	D	2003	1/1	0.99	0.28	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.