



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:03 PM GMT

PDB ID : 4K4X
Title : Coxsackievirus B3 polymerase elongation complex (r2_form), rna
Authors : Gong, P.; Peersen, O.B.
Deposited on : 2013-04-12
Resolution : 2.37 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

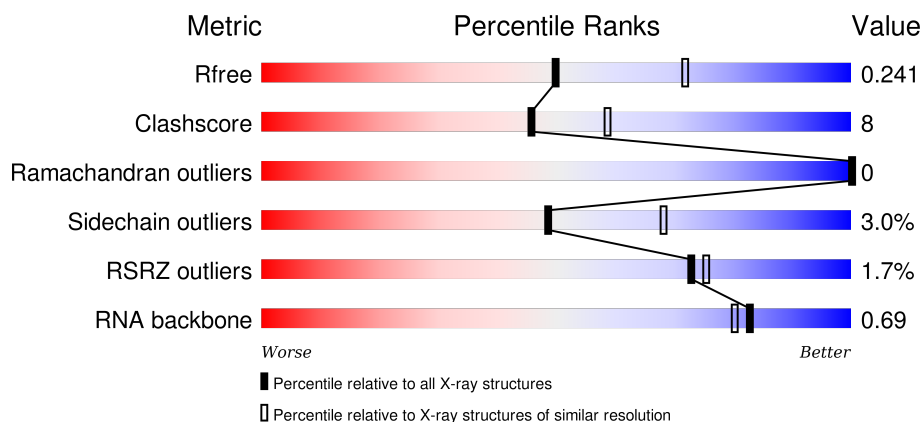
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)
RNA backbone	2183	1092 (2.90-1.86)

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. 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	472	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 82%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 16% .. </div> </div>
1	E	472	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 82%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 15% .. </div> </div>
1	I	472	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 17%, green 80%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 17% .. </div> </div>
1	M	472	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 82%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 15% .. </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	24	
2	F	24	
2	J	24	
2	N	24	
3	C	14	
3	G	14	
3	K	14	
3	O	14	
4	D	9	
4	H	9	
4	L	9	
4	P	9	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18197 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3693	2372	614	685	22			
1	E	463	Total	C	N	O	S	0	0	0
			3693	2372	614	685	22			
1	I	463	Total	C	N	O	S	0	0	0
			3693	2372	614	685	22			
1	M	463	Total	C	N	O	S	0	0	0
			3693	2372	614	685	22			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ILE	LEU	VARIANT	UNP Q66338
A	463	GLY	-	EXPRESSION TAG	UNP Q66338
A	464	SER	-	EXPRESSION TAG	UNP Q66338
A	465	SER	-	EXPRESSION TAG	UNP Q66338
A	466	SER	-	EXPRESSION TAG	UNP Q66338
A	467	HIS	-	EXPRESSION TAG	UNP Q66338
A	468	HIS	-	EXPRESSION TAG	UNP Q66338
A	469	HIS	-	EXPRESSION TAG	UNP Q66338
A	470	HIS	-	EXPRESSION TAG	UNP Q66338
A	471	HIS	-	EXPRESSION TAG	UNP Q66338
A	472	HIS	-	EXPRESSION TAG	UNP Q66338
E	252	ILE	LEU	VARIANT	UNP Q66338
E	463	GLY	-	EXPRESSION TAG	UNP Q66338
E	464	SER	-	EXPRESSION TAG	UNP Q66338
E	465	SER	-	EXPRESSION TAG	UNP Q66338
E	466	SER	-	EXPRESSION TAG	UNP Q66338
E	467	HIS	-	EXPRESSION TAG	UNP Q66338
E	468	HIS	-	EXPRESSION TAG	UNP Q66338
E	469	HIS	-	EXPRESSION TAG	UNP Q66338
E	470	HIS	-	EXPRESSION TAG	UNP Q66338
E	471	HIS	-	EXPRESSION TAG	UNP Q66338

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	472	HIS	-	EXPRESSION TAG	UNP Q66338
I	252	ILE	LEU	VARIANT	UNP Q66338
I	463	GLY	-	EXPRESSION TAG	UNP Q66338
I	464	SER	-	EXPRESSION TAG	UNP Q66338
I	465	SER	-	EXPRESSION TAG	UNP Q66338
I	466	SER	-	EXPRESSION TAG	UNP Q66338
I	467	HIS	-	EXPRESSION TAG	UNP Q66338
I	468	HIS	-	EXPRESSION TAG	UNP Q66338
I	469	HIS	-	EXPRESSION TAG	UNP Q66338
I	470	HIS	-	EXPRESSION TAG	UNP Q66338
I	471	HIS	-	EXPRESSION TAG	UNP Q66338
I	472	HIS	-	EXPRESSION TAG	UNP Q66338
M	252	ILE	LEU	VARIANT	UNP Q66338
M	463	GLY	-	EXPRESSION TAG	UNP Q66338
M	464	SER	-	EXPRESSION TAG	UNP Q66338
M	465	SER	-	EXPRESSION TAG	UNP Q66338
M	466	SER	-	EXPRESSION TAG	UNP Q66338
M	467	HIS	-	EXPRESSION TAG	UNP Q66338
M	468	HIS	-	EXPRESSION TAG	UNP Q66338
M	469	HIS	-	EXPRESSION TAG	UNP Q66338
M	470	HIS	-	EXPRESSION TAG	UNP Q66338
M	471	HIS	-	EXPRESSION TAG	UNP Q66338
M	472	HIS	-	EXPRESSION TAG	UNP Q66338

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total 338	C 151	N 58	O 113	P 16	0	0	0
2	F	16	Total 338	C 151	N 58	O 113	P 16	0	0	0
2	J	16	Total 338	C 151	N 58	O 113	P 16	0	0	0
2	N	16	Total 338	C 151	N 58	O 113	P 16	0	0	0

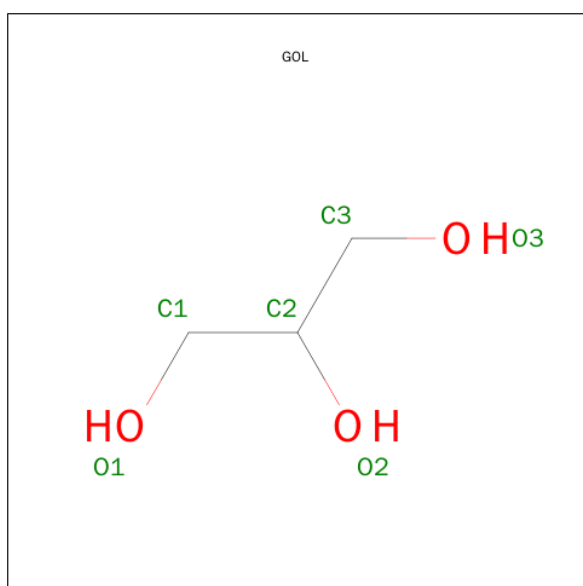
- Molecule 3 is a RNA chain called RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	P	0	0	0
			283	126	55	89	13			
3	G	13	Total	C	N	O	P	0	0	0
			283	126	55	89	13			
3	K	13	Total	C	N	O	P	0	0	0
			283	126	55	89	13			
3	O	13	Total	C	N	O	P	0	0	0
			283	126	55	89	13			

- Molecule 4 is a RNA chain called RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			
4	H	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			
4	L	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			
4	P	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	M	1	Total	Mg	0	0
			1	1		
6	E	1	Total	Mg	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	161	Total	O	0	0
			161	161		
7	B	17	Total	O	0	0
			17	17		
7	C	22	Total	O	0	0
			22	22		
7	E	120	Total	O	0	0
			120	120		
7	F	18	Total	O	0	0
			18	18		
7	G	11	Total	O	0	0
			11	11		
7	I	153	Total	O	0	0
			153	153		
7	J	19	Total	O	0	0
			19	19		
7	K	21	Total	O	0	0
			21	21		
7	M	156	Total	O	0	0
			156	156		
7	N	16	Total	O	0	0
			16	16		

Continued on next page...

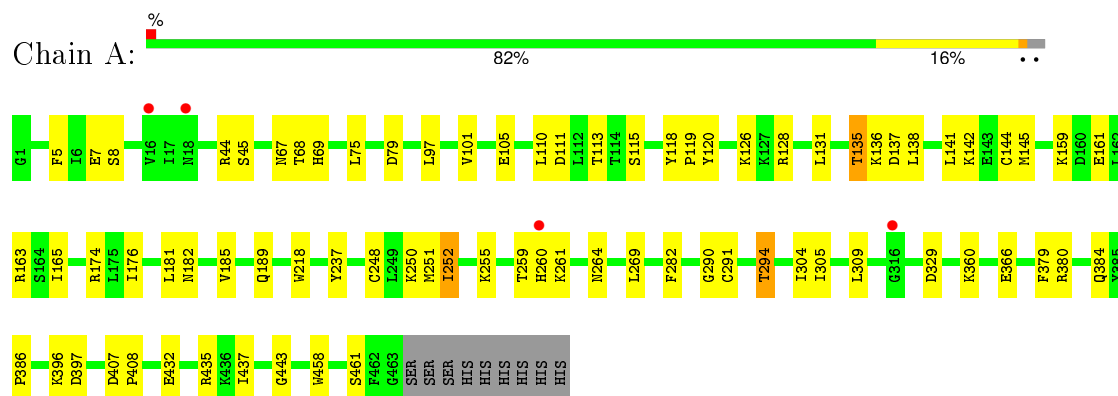
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	O	15	Total	O	0	0
			15	15		

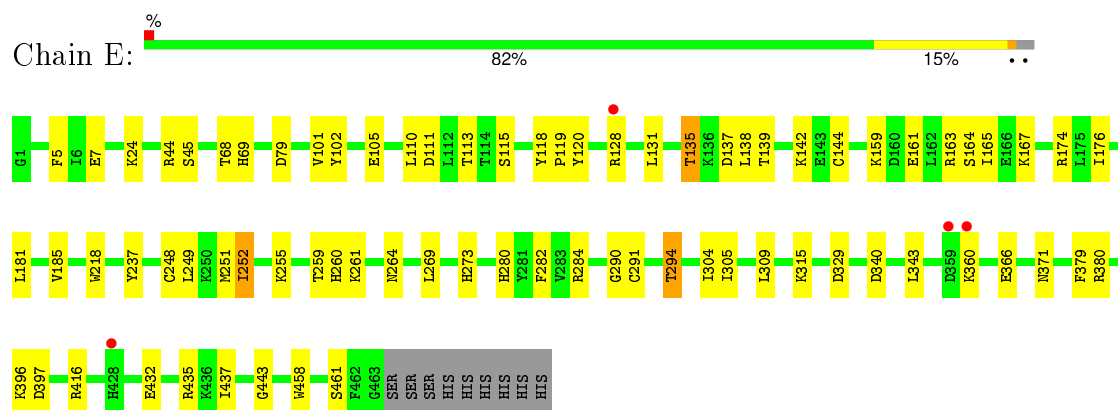
3 Residue-property plots

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.

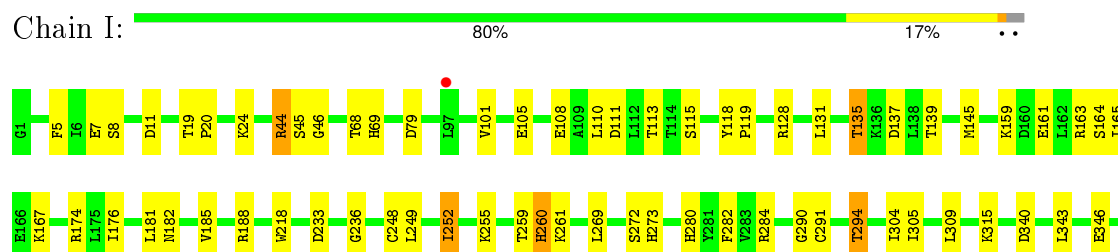
• Molecule 1: RNA-dependent RNA polymerase

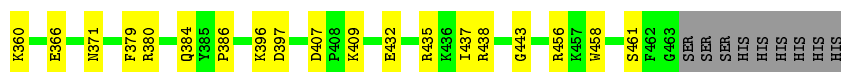


• Molecule 1: RNA-dependent RNA polymerase

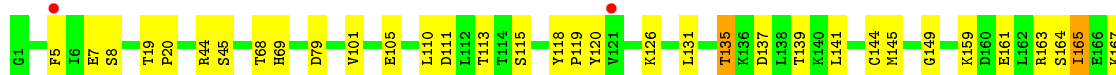
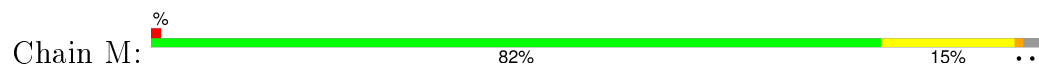


• Molecule 1: RNA-dependent RNA polymerase





- Molecule 1: RNA-dependent RNA polymerase



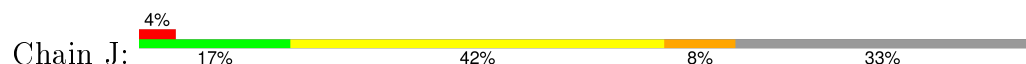
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3')



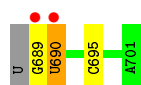
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3')



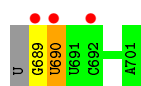
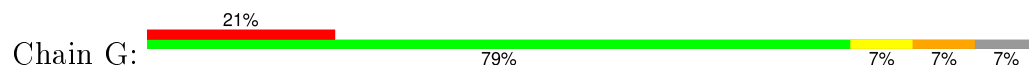
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3')



- Molecule 3: RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')



- Molecule 3: RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')



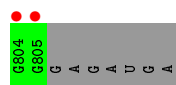
- Molecule 3: RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')



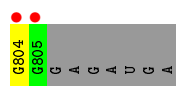
- Molecule 3: RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')



- Molecule 4: RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



- Molecule 4: RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



- Molecule 4: RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



- Molecule 4: RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.00Å 61.01Å 195.14Å 90.02° 89.98° 78.36°	Depositor
Resolution (Å)	44.01 – 2.37 44.01 – 2.37	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.01-2.37) 97.6 (44.01-2.37)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.37Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.241 0.202 , 0.241	Depositor DCC
R_{free} test set	5507 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.4	EDS
Estimated twinning fraction	0.467 for -h,-k,l 0.459 for -k,-h,-l 0.466 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 109344 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18197	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.44	0/3786	0.57	0/5125
1	E	0.44	0/3786	0.58	0/5125
1	I	0.45	0/3786	0.59	0/5125
1	M	0.45	0/3786	0.58	0/5125
2	B	0.56	0/376	0.92	0/583
2	F	0.55	0/376	0.92	0/583
2	J	0.54	0/376	0.91	0/583
2	N	0.53	0/376	0.94	0/583
3	C	0.55	0/317	0.88	0/493
3	G	0.59	0/317	0.93	0/493
3	K	0.54	0/317	0.87	0/493
3	O	0.53	0/317	0.87	0/493
4	D	0.29	0/51	0.61	0/78
4	H	0.32	0/51	0.86	0/78
4	L	0.34	0/51	0.74	0/78
4	P	0.48	0/51	1.03	0/78
All	All	0.46	0/18120	0.65	0/25116

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	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	272	SER	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	3693	0	3661	46	0
1	E	3693	0	3661	57	0
1	I	3693	0	3661	59	0
1	M	3693	0	3661	52	1
2	B	338	0	173	12	0
2	F	338	0	173	12	0
2	J	338	0	173	10	0
2	N	338	0	173	11	0
3	C	283	0	142	4	0
3	G	283	0	142	3	0
3	K	283	0	142	3	0
3	O	283	0	142	4	0
4	D	46	0	23	0	0
4	H	46	0	23	1	0
4	L	46	0	23	0	0
4	P	46	0	23	0	0
5	A	12	0	16	0	1
5	E	6	0	8	0	0
5	I	6	0	8	2	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
6	I	1	0	0	0	0
6	M	1	0	0	0	0
7	A	161	0	0	6	0
7	B	17	0	0	0	0
7	C	22	0	0	1	0
7	E	120	0	0	8	0
7	F	18	0	0	0	0
7	G	11	0	0	0	0
7	I	153	0	0	11	0
7	J	19	0	0	0	0
7	K	21	0	0	1	0
7	M	156	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	16	0	0	0	0
7	O	15	0	0	0	0
All	All	18197	0	16028	253	1

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 8.

The worst 5 of 253 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)
3:C:689:G:H22	3:G:689:G:H22	1.25	0.83
3:C:689:G:H1	3:G:689:G:H1	1.27	0.82
3:K:689:G:H22	3:O:689:G:H22	1.27	0.81
3:K:689:G:H1	3:O:689:G:H1	1.29	0.81
1:E:290:GLY:H	1:E:294:THR:HG21	1.48	0.77

All (1) 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)
1:M:284:ARG:NH1	5:A:501:GOL:O2[1_556]	2.17	0.03

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	461/472 (98%)	446 (97%)	15 (3%)	0	100	100
1	E	461/472 (98%)	444 (96%)	17 (4%)	0	100	100
1	I	461/472 (98%)	446 (97%)	15 (3%)	0	100	100
1	M	461/472 (98%)	445 (96%)	16 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1844/1888 (98%)	1781 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	404/413 (98%)	391 (97%)	13 (3%)	46	66
1	E	404/413 (98%)	393 (97%)	11 (3%)	52	71
1	I	404/413 (98%)	391 (97%)	13 (3%)	46	66
1	M	404/413 (98%)	392 (97%)	12 (3%)	48	68
All	All	1616/1652 (98%)	1567 (97%)	49 (3%)	48	68

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	360	LYS
1	I	105	GLU
1	M	260	HIS
1	I	8	SER
1	I	135	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	273	HIS
1	M	273	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	15/24 (62%)	5 (33%)	0
2	F	15/24 (62%)	5 (33%)	0
2	J	15/24 (62%)	5 (33%)	0
2	N	15/24 (62%)	5 (33%)	0
3	C	12/14 (85%)	1 (8%)	0
3	G	12/14 (85%)	1 (8%)	0
3	K	12/14 (85%)	1 (8%)	0
3	O	12/14 (85%)	1 (8%)	0
4	D	1/9 (11%)	0	0
4	H	1/9 (11%)	0	0
4	L	1/9 (11%)	0	0
4	P	1/9 (11%)	0	0
All	All	112/188 (59%)	24 (21%)	0

5 of 24 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	598	A
2	B	602	C
2	B	610	G
2	B	611	A
2	B	612	A

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
5	GOL	A	501	-	5,5,5	0.40	0	5,5,5	0.27	0
5	GOL	A	502	-	5,5,5	0.32	0	5,5,5	0.47	0
5	GOL	E	501	-	5,5,5	0.30	0	5,5,5	0.60	0
5	GOL	I	501	-	5,5,5	0.28	0	5,5,5	0.60	0

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
5	GOL	A	501	-	-	0/4/4/4	0/0/0/0
5	GOL	A	502	-	-	0/4/4/4	0/0/0/0
5	GOL	E	501	-	-	0/4/4/4	0/0/0/0
5	GOL	I	501	-	-	0/4/4/4	0/0/0/0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GOL	0	1
5	I	501	GOL	2	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 ⓘ

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	463/472 (98%)	0.07	4 (0%) 85 87	26, 40, 59, 95	0
1	E	463/472 (98%)	0.04	4 (0%) 85 87	28, 41, 60, 94	0
1	I	463/472 (98%)	0.04	1 (0%) 95 96	27, 41, 59, 95	0
1	M	463/472 (98%)	0.08	5 (1%) 82 84	26, 41, 59, 94	0
2	B	16/24 (66%)	0.14	0 100 100	36, 53, 117, 118	0
2	F	16/24 (66%)	0.33	1 (6%) 23 27	37, 54, 117, 119	0
2	J	16/24 (66%)	0.44	1 (6%) 23 27	35, 53, 118, 118	0
2	N	16/24 (66%)	0.28	0 100 100	35, 54, 117, 118	0
3	C	13/14 (92%)	0.86	2 (15%) 3 3	32, 58, 125, 129	0
3	G	13/14 (92%)	0.88	3 (23%) 1 1	31, 60, 125, 129	0
3	K	13/14 (92%)	0.62	2 (15%) 3 3	31, 58, 126, 128	0
3	O	13/14 (92%)	0.87	2 (15%) 3 3	31, 58, 125, 130	0
4	D	2/9 (22%)	3.12	2 (100%) 0 0	125, 125, 125, 132	0
4	H	2/9 (22%)	4.47	2 (100%) 0 0	126, 126, 126, 133	0
4	L	2/9 (22%)	4.05	2 (100%) 0 0	127, 127, 127, 133	0
4	P	2/9 (22%)	3.88	2 (100%) 0 0	124, 124, 124, 132	0
All	All	1976/2076 (95%)	0.10	33 (1%) 73 75	26, 41, 64, 133	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	689	G	7.3
3	C	689	G	6.4
4	H	804	G	6.2
3	G	689	G	5.7
4	P	804	G	5.1

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MG	E	502	1/1	0.95	0.11	-0.84	48,48,48,48	0
5	GOL	I	501	6/6	0.96	0.11	-0.89	37,41,42,45	0
5	GOL	A	502	6/6	0.96	0.10	-1.00	37,41,43,45	0
5	GOL	E	501	6/6	0.97	0.09	-1.49	37,42,42,43	0
6	MG	I	502	1/1	0.96	0.09	-1.51	42,42,42,42	0
5	GOL	A	501	6/6	0.98	0.10	-1.56	38,41,46,47	0
6	MG	A	503	1/1	0.94	0.03	-2.86	47,47,47,47	0
6	MG	M	501	1/1	0.94	0.15	-	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.