



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 01:52 AM UTC

PDB ID : 1I6H / pdb_00001i6h
Title : RNA POLYMERASE II ELONGATION COMPLEX
Authors : Gnatt, A.L.; Cramer, P.; Kornberg, R.D.
Deposited on : 2001-03-02
Resolution : 3.30 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

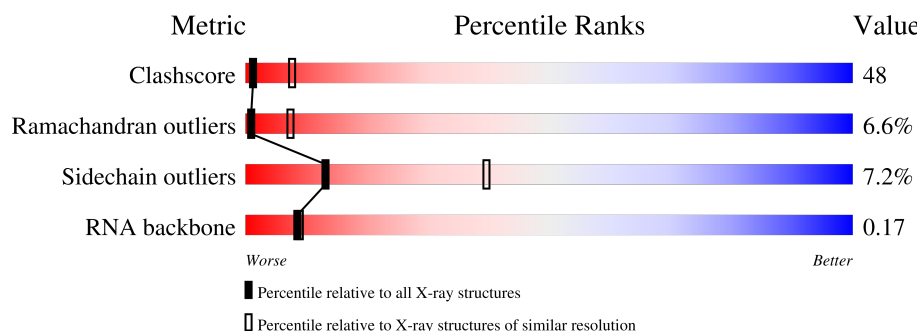
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	13	15% 69% 15%
2	R	9	11% 56% 11% 22%
3	A	1733	27% 43% 9% • 20%
4	B	1224	28% 51% 10% • 10%
5	C	318	33% 40% 10% • 16%
6	E	215	39% 56% 5%

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Mol	Chain	Length	Quality of chain
7	F	155	15%34%5%46%
8	H	146	27%52%12%•9%
9	I	122	30%53%12%••
10	J	70	26%51%14%•7%
11	K	120	34%55%5%•5%
12	L	70	13%30%20%•34%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28430 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 DNA chain called 5'-D(P*AP*AP*AP*TP*GP*CP*CP*TP*GP*GP*TP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	13	Total	C	N	O	P	0	0	0
			267	127	47	80	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	9	Total	C	N	O	P	0	0	0
			196	87	39	61	9			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1381	Total	C	N	O	S	0	0	0
			10857	6851	1899	2046	61			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1097	Total	C	N	O	S	0	0	0
			8721	5526	1523	1618	54			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

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

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	R	1	Total	Mg	0	0
			1	1		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

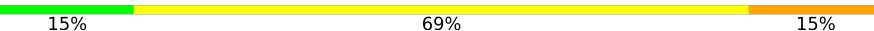
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	1	Total	Zn	0	0
			1	1		
14	C	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	J	1	Total	Zn	0	0
			1	1		
14	L	1	Total	Zn	0	0
			1	1		

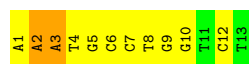
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

- Molecule 1: 5'-D(P*AP*AP*AP*TP*GP*CP*CP*TP*GP*GP*TP*CP*T)-3'

Chain D: 

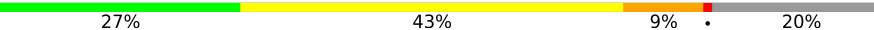


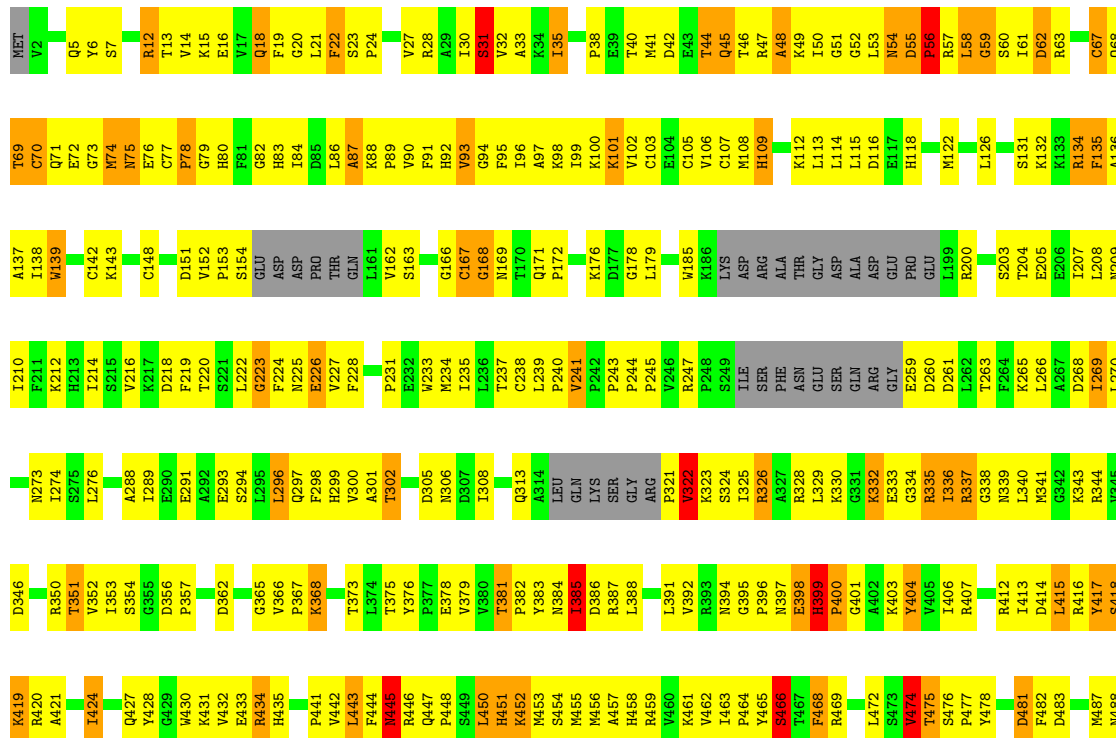
- Molecule 2: 5'-R(P*GP*AP*CP*CP*AP*GP*GP*CP*A)-3'

Chain R: 



- Molecule 3: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

Chain A: 

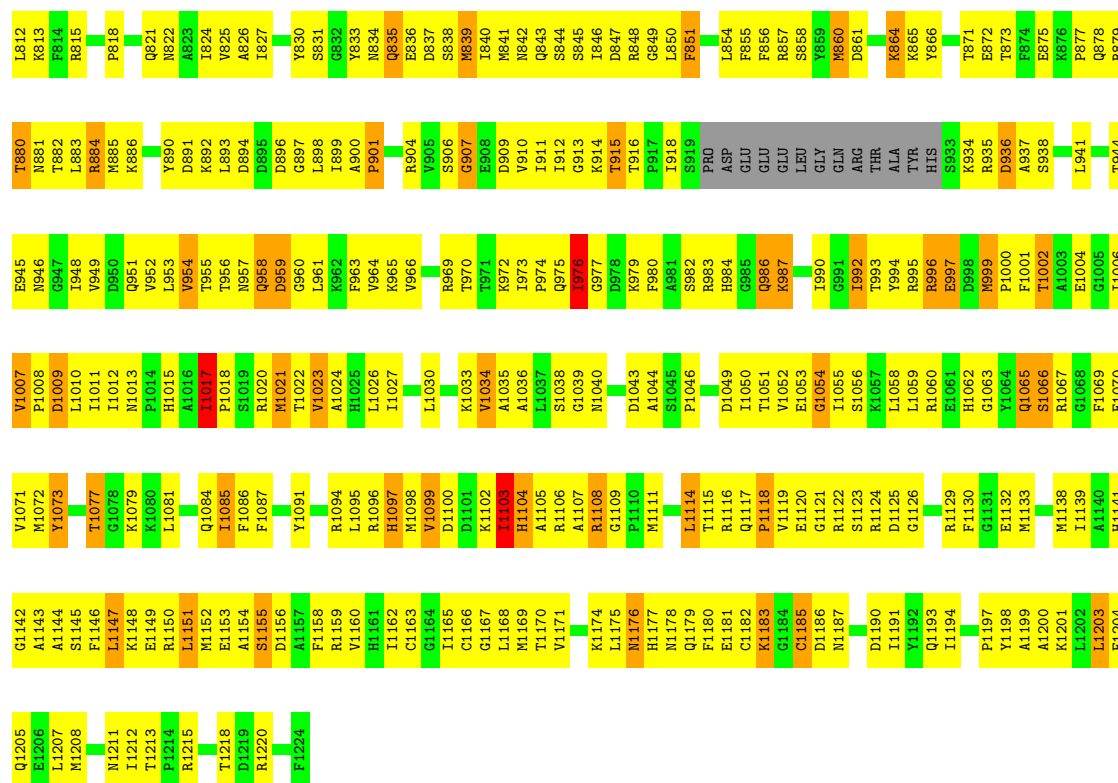




SER	TYR	SER	PRO	THR	SER	PRO	ASN	SER	TYR	PRO	THR	SER	PRO	SER	TYR	PRO	THR	SER	PRO	GLY	TYR	SER	GLY	SER	ALA	TYR	PRO	PRO	GLN	ASP	GLU	GLN	LYS	HIS	ASN	GLU	ASN	GLU	ASN	SER	ARG
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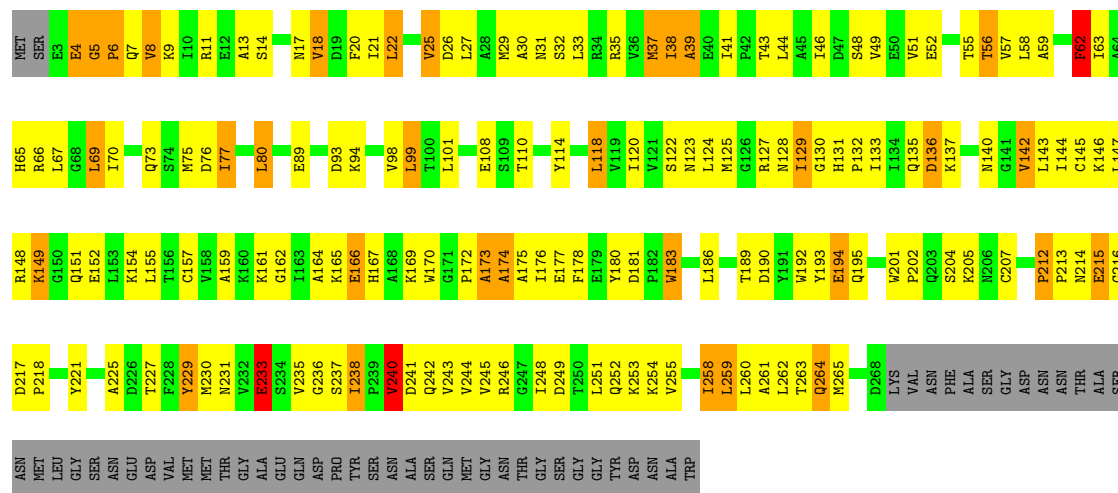
Chain B: 28% 51% 10% • 10%





• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE

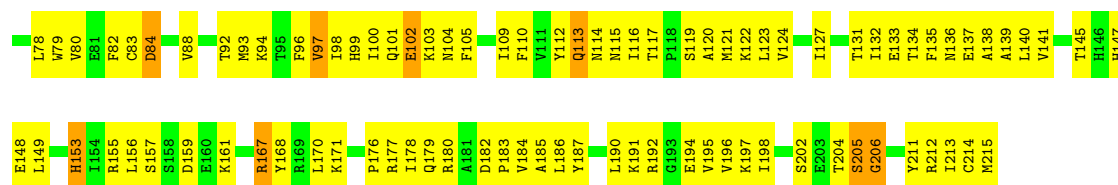
Chain C: 33% 40% 10% 16%



• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

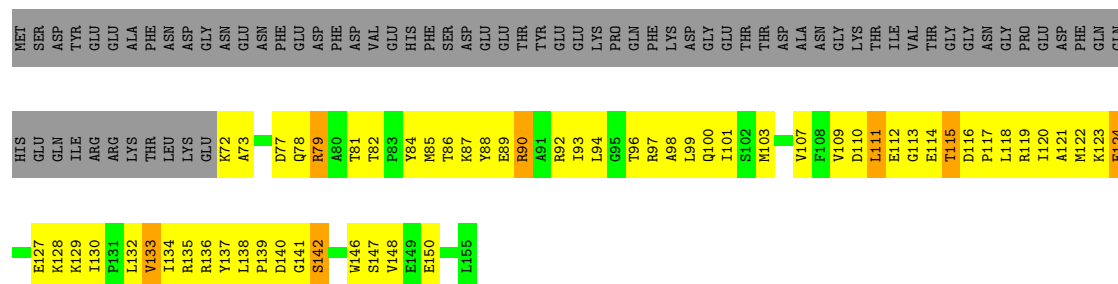
Chain E: 39% 56% 5%





• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F: 15% 34% 5% 46%



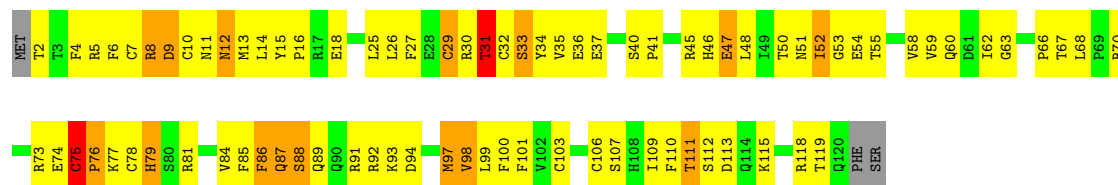
• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

Chain H: 27% 52% 12% 9%



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I: 30% 53% 12% . .

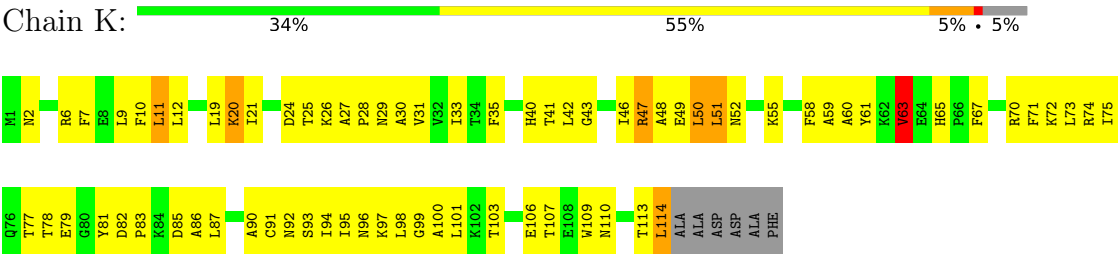


• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

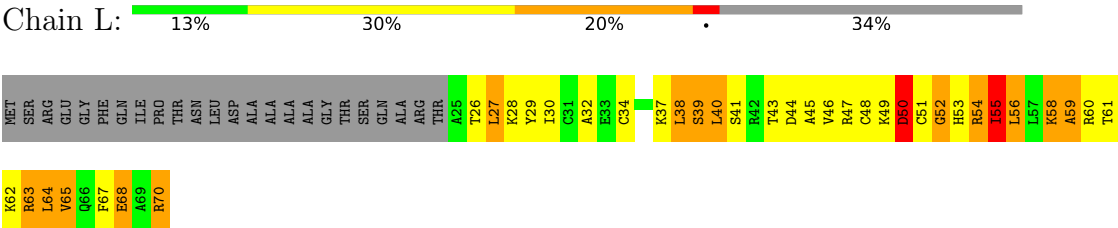
Chain J: 26% 51% 14% . 7%



● Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE



● Molecule 12: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.30Å 220.70Å 191.30Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28430	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	D	0.61	0/298	1.01	1/456 (0.2%)
2	R	1.28	2/219 (0.9%)	1.73	8/338 (2.4%)
3	A	0.53	0/11048	1.07	74/14936 (0.5%)
4	B	0.56	0/8891	1.07	58/11990 (0.5%)
5	C	0.59	0/2133	1.19	27/2891 (0.9%)
6	E	0.42	0/1788	1.03	12/2406 (0.5%)
7	F	0.48	0/691	0.99	4/933 (0.4%)
8	H	0.46	0/1086	1.11	11/1470 (0.7%)
9	I	0.53	0/989	1.10	7/1331 (0.5%)
10	J	0.67	0/541	1.09	4/727 (0.6%)
11	K	0.53	0/937	0.95	3/1265 (0.2%)
12	L	0.54	0/366	1.10	5/485 (1.0%)
All	All	0.55	2/28987 (0.0%)	1.08	214/39228 (0.5%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	9	A	P-OP2	6.72	1.62	1.49
2	R	9	A	P-OP1	5.43	1.59	1.49

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	296	GLU	N-CA-C	-12.31	97.62	112.89
5	C	173	ALA	N-CA-C	11.19	123.48	111.28
2	R	9	A	N9-C1'-C2'	-11.15	95.27	112.00
3	A	452	LYS	N-CA-C	-10.91	97.29	112.45
3	A	474	VAL	N-CA-C	-10.76	102.57	112.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2	DA	Sidechain

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	D	267	0	148	31	0
2	R	196	0	100	25	0
3	A	10857	0	10959	1110	0
4	B	8721	0	8746	938	0
5	C	2095	0	2052	175	0
6	E	1752	0	1776	143	0
7	F	679	0	701	68	0
8	H	1068	0	1040	134	0
9	I	971	0	933	108	0
10	J	532	0	544	78	0
11	K	919	0	929	93	0
12	L	364	0	388	57	0
13	R	1	0	0	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	1	0
14	J	1	0	0	1	0
14	L	1	0	0	0	0
All	All	28430	0	28316	2692	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 48.

The worst 5 of 2692 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:A:567:LYS:HB2	3:A:568:PRO:HD2	1.18	1.17
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.15
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.13
4:B:345:LYS:HA	4:B:348:ARG:HE	1.11	1.13
3:A:353:ILE:HD13	3:A:487:MET:HE3	1.23	1.12

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	
3	A	1365/1733 (79%)	1021 (75%)	253 (18%)	91 (7%)	1	7
4	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	1	8
5	C	264/318 (83%)	208 (79%)	39 (15%)	17 (6%)	1	8
6	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	2	14
7	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	2	17
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	2
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	5
10	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	8
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	14	43
12	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	0
All	All	3465/4173 (83%)	2654 (77%)	583 (17%)	228 (7%)	1	7

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	31	SER
3	A	48	ALA
3	A	55	ASP
3	A	56	PRO
3	A	74	MET

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	
3	A	1206/1520 (79%)	1123 (93%)	83 (7%)	14	41
4	B	952/1061 (90%)	874 (92%)	78 (8%)	10	35
5	C	234/274 (85%)	218 (93%)	16 (7%)	14	42
6	E	196/197 (100%)	192 (98%)	4 (2%)	48	68
7	F	74/137 (54%)	68 (92%)	6 (8%)	11	36
8	H	117/128 (91%)	113 (97%)	4 (3%)	32	59
9	I	113/116 (97%)	105 (93%)	8 (7%)	13	40
10	J	60/65 (92%)	54 (90%)	6 (10%)	7	27
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	22
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	13
All	All	3091/3657 (84%)	2869 (93%)	222 (7%)	13	40

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	556	THR
12	L	70	ARG
4	B	999	MET
12	L	65	VAL
10	J	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	744	HIS
4	B	1179	GLN
4	B	822	ASN
4	B	1065	GLN
5	C	112	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	3	C
2	R	9	A

There are no RNA pucker outliers to report.

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 ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.