



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 10:40 AM GMT

PDB ID : 2E2J
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with GMPCPP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 3.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

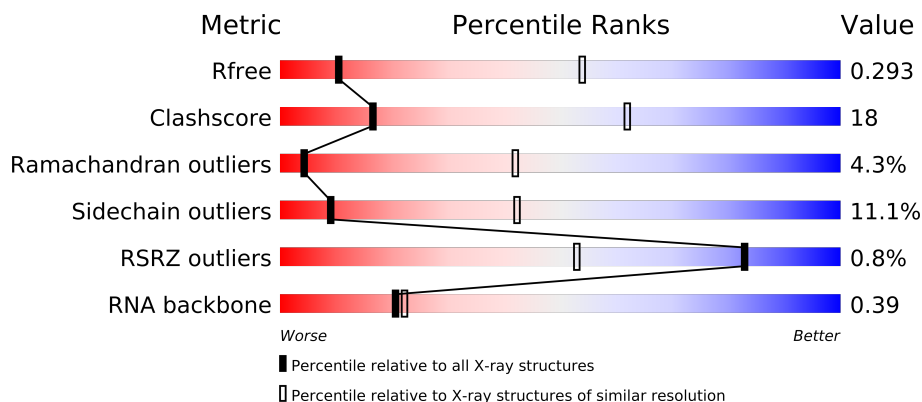
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	R	9	
2	T	27	
3	N	13	
4	A	1733	
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	

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Mol	Chain	Length	Quality of chain
13	L	70	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
15	MG	A	2002	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29206 atoms, of which 0 are hydrogen and 0 are deuterium.

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 5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

- Molecule 2 is a DNA chain called 27-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	27	Total	C	N	O	P	0	0	0
			546	261	102	157	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	13	Total	C	N	O	P	0	0	0
			266	127	44	82	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1105	Total	C	N	O	S	0	0	0
			8782	5560	1537	1630	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			696	445	118	130	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypep-

tide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

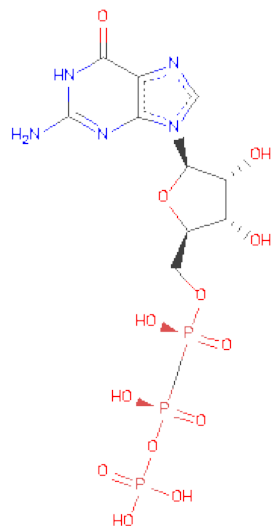
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is PHOSPHOMETHYLPHOSPHONICACID GUANYLATE ESTER (three-letter code: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).



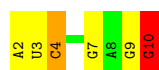
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	T	1	32	11	5	13	3	0	0

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: 5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3'

Chain R: 



- Molecule 2: 27-MER DNA template strand

Chain T: 



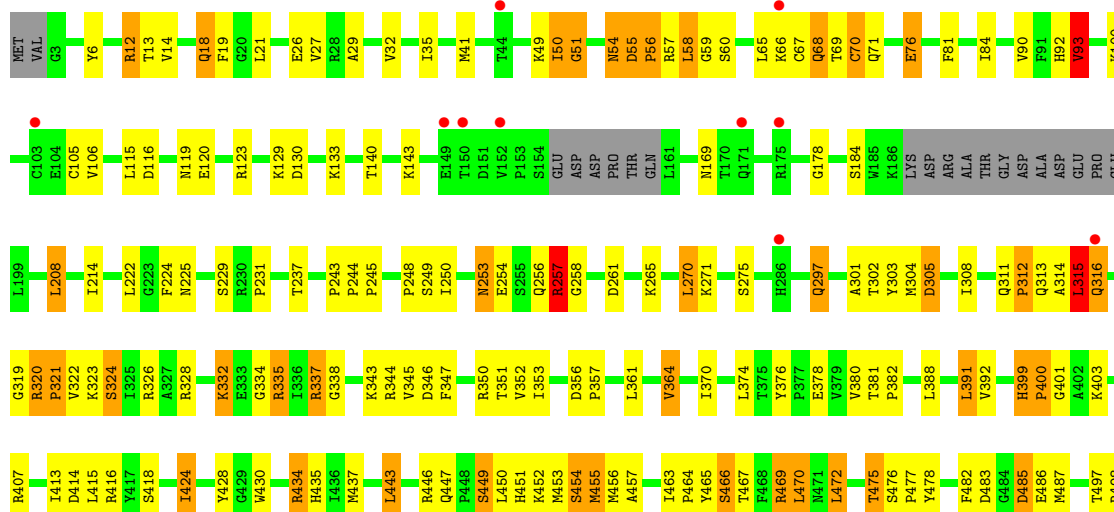
- Molecule 3: 5'-D(P*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*A)-3'

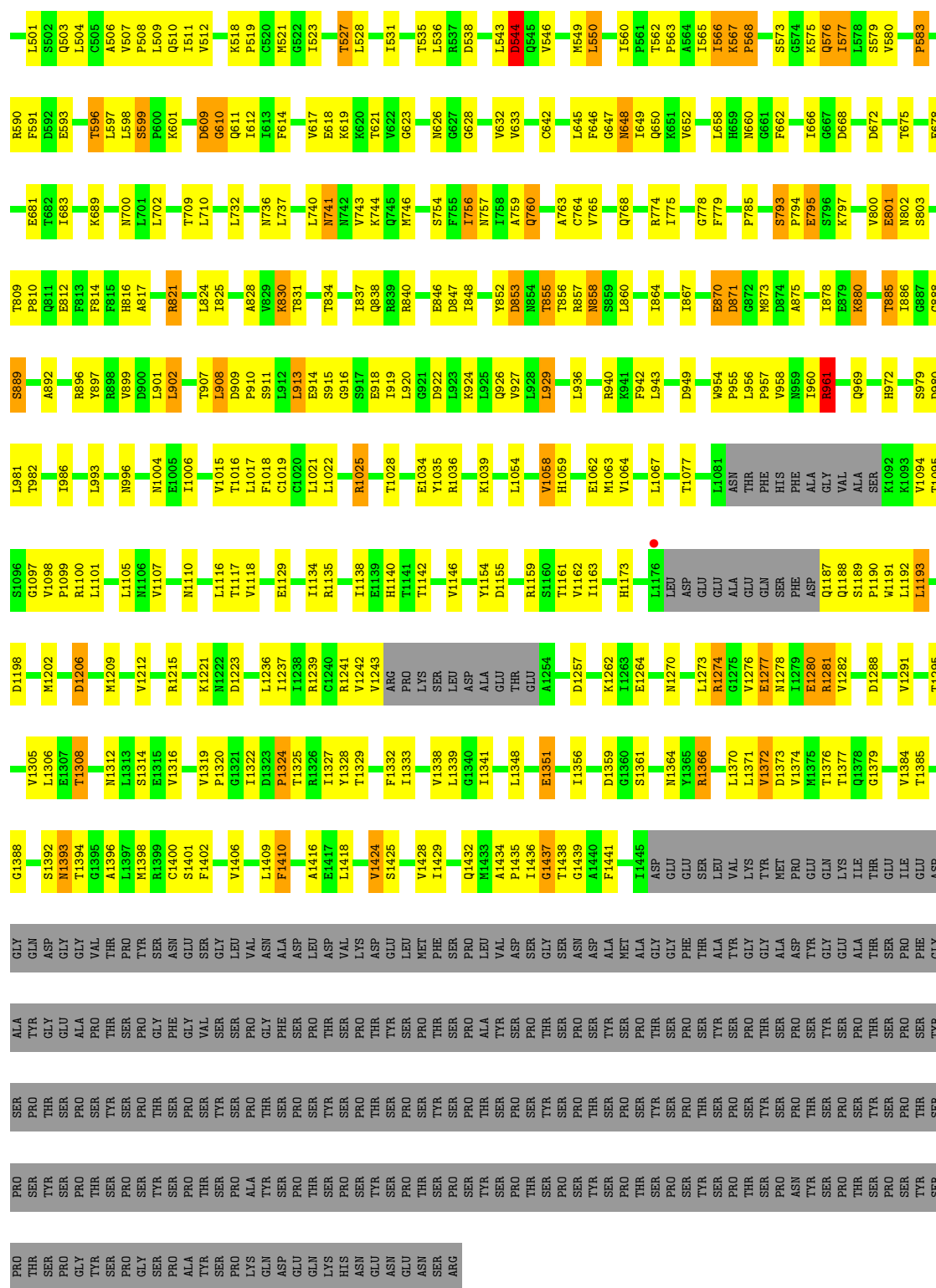
Chain N: 



- Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A: 

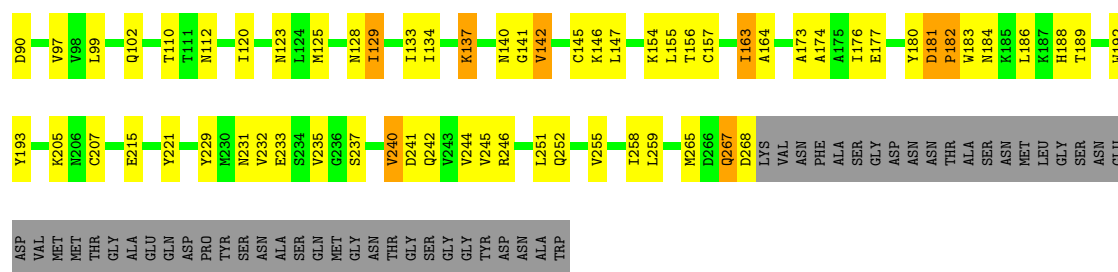




● Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide

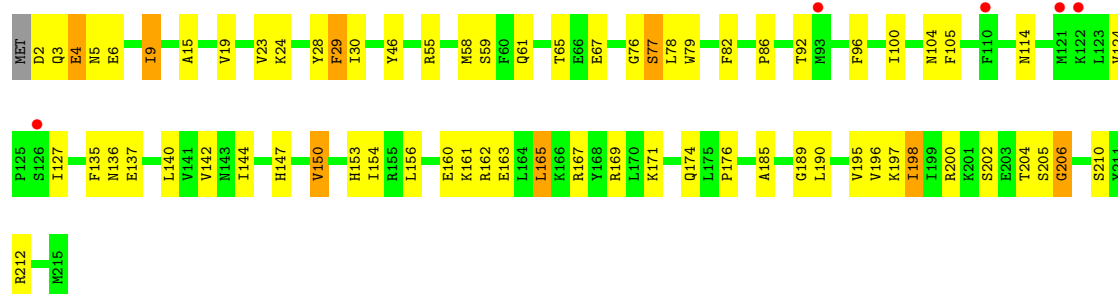
Chain B:





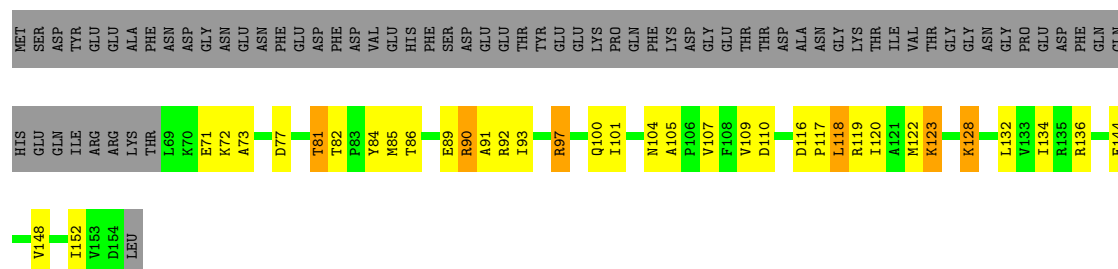
- Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:



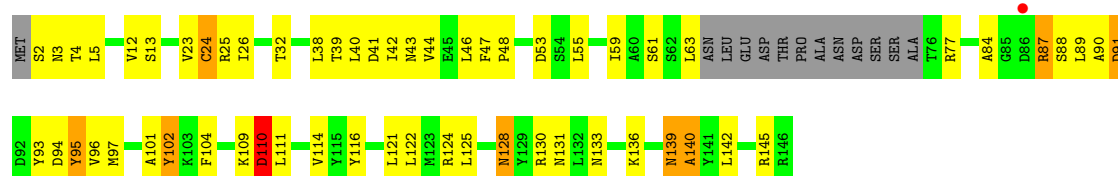
- Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



- Molecule 10: DNA-directed RNA polymerase II subunit 9

Chain I:





- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.14Å 222.02Å 194.65Å 90.00° 101.36° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.14 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-3.50) 94.6 (50.14-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.306 0.245 , 0.293	Depositor DCC
R_{free} test set	2511 reflections (3.08%)	DCC
Wilson B-factor (Å ²)	101.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 84062 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29206	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, G2P

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	R	1.15	1/223 (0.4%)	1.88	8/345 (2.3%)
2	T	0.99	0/612	1.78	19/941 (2.0%)
3	N	1.15	2/296 (0.7%)	1.84	9/453 (2.0%)
4	A	0.61	0/11163	0.70	2/15091 (0.0%)
5	B	0.63	0/8952	0.72	1/12071 (0.0%)
6	C	0.61	0/2139	0.70	0/2899
7	E	0.56	0/1788	0.64	0/2406
8	F	0.57	0/708	0.66	0/956
9	H	0.53	0/1086	0.68	0/1470
10	I	0.62	0/989	0.68	0/1331
11	J	0.66	0/541	0.74	0/727
12	K	0.67	0/937	0.69	0/1265
13	L	0.60	0/365	0.78	0/485
All	All	0.64	3/29799 (0.0%)	0.78	39/40440 (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
4	A	0	3
5	B	0	4
6	C	0	1
9	H	1	1
11	J	0	1
All	All	1	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	2	DC	OP3-P	-10.47	1.48	1.61
1	R	2	A	OP3-P	-9.50	1.49	1.61
3	N	13	DT	C5-C7	5.64	1.53	1.50

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	12	DG	O4'-C1'-N9	13.05	117.14	108.00
2	T	25	DG	O4'-C1'-N9	11.72	116.20	108.00
3	N	4	DG	O4'-C1'-N9	10.88	115.62	108.00
2	T	21	DT	O4'-C4'-C3'	-10.45	99.73	106.00
2	T	25	DG	C1'-O4'-C4'	-9.85	100.25	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	H	110	ASP	CA

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1392	SER	Peptide
4	A	257	ARG	Peptide
4	A	258	GLY	Peptide
5	B	293	PRO	Peptide
5	B	478	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	199	0	98	3	0
2	T	546	0	304	5	0
3	N	266	0	149	0	0
4	A	10969	0	11067	410	0
5	B	8782	0	8816	419	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2101	0	2056	86	0
7	E	1752	0	1776	47	0
8	F	696	0	720	31	0
9	H	1068	0	1040	46	0
10	I	971	0	927	26	0
11	J	532	0	542	43	0
12	K	919	0	929	39	0
13	L	363	0	386	10	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	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	T	32	0	14	1	0
All	All	29206	0	28824	1043	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

The worst 5 of 1043 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:H:109:LYS:HB3	9:H:110:ASP:CA	1.54	1.34
9:H:109:LYS:CB	9:H:110:ASP:HA	1.49	1.31
4:A:399:HIS:CB	4:A:400:PRO:HD3	1.65	1.27
5:B:635:ARG:CG	5:B:636:PRO:HD2	1.65	1.24
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.73	1.18

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	
4	A	1383/1733 (80%)	1136 (82%)	182 (13%)	65 (5%)	4	39
5	B	1087/1224 (89%)	918 (84%)	124 (11%)	45 (4%)	4	44
6	C	265/318 (83%)	222 (84%)	34 (13%)	9 (3%)	6	50
7	E	212/215 (99%)	180 (85%)	25 (12%)	7 (3%)	6	51
8	F	84/155 (54%)	73 (87%)	10 (12%)	1 (1%)	19	75
9	H	129/146 (88%)	101 (78%)	23 (18%)	5 (4%)	5	45
10	I	117/122 (96%)	95 (81%)	18 (15%)	4 (3%)	6	50
11	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	6	51
12	K	112/120 (93%)	97 (87%)	11 (10%)	4 (4%)	5	49
13	L	44/70 (63%)	25 (57%)	11 (25%)	8 (18%)	0	3
All	All	3496/4173 (84%)	2903 (83%)	443 (13%)	150 (4%)	4	42

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	55	ASP
4	A	93	VAL
4	A	248	PRO
4	A	321	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	
4	A	1218/1520 (80%)	1083 (89%)	135 (11%)	9	42
5	B	959/1061 (90%)	852 (89%)	107 (11%)	9	41
6	C	235/274 (86%)	215 (92%)	20 (8%)	15	58
7	E	196/197 (100%)	182 (93%)	14 (7%)	21	67
8	F	76/137 (56%)	67 (88%)	9 (12%)	8	38
9	H	117/128 (91%)	103 (88%)	14 (12%)	7	37
10	I	113/116 (97%)	96 (85%)	17 (15%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	60/65 (92%)	53 (88%)	7 (12%)	8	38
12	K	99/102 (97%)	86 (87%)	13 (13%)	6	32
13	L	40/57 (70%)	32 (80%)	8 (20%)	2	11
All	All	3113/3657 (85%)	2769 (89%)	344 (11%)	9	42

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	249	ARG
5	B	737	THR
11	J	9	SER
5	B	366	GLN
5	B	510	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	686	ASN
5	B	878	GLN
9	H	134	ASN
5	B	734	HIS
5	B	794	ASN

5.3.3 RNA ⓘ

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

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	4	C
1	R	10	G

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 10 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	$\# Z > 2$
16	G2P	T	3000	-	34,34,34	1.83	3 (8%)	51,54,54	3.08	7 (13%)

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
16	G2P	T	3000	-	-	0/20/38/38	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	3000	G2P	PB-C3A	7.15	1.86	1.79
16	T	3000	G2P	PA-C3A	5.21	1.84	1.79
16	T	3000	G2P	C2-N3	3.50	1.37	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	3000	G2P	C6-C5-N7	-18.81	131.61	134.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	3000	G2P	PG-O3B-PB	-4.18	117.54	131.81
16	T	3000	G2P	C5-C4-N3	-4.15	119.93	125.94
16	T	3000	G2P	N3-C4-N9	3.85	132.56	126.91
16	T	3000	G2P	C4'-O4'-C1'	3.84	113.92	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	R	9/9 (100%)	-0.06	0 100 100	98, 111, 151, 169	0
2	T	27/27 (100%)	0.49	4 (14%) 3 3	100, 203, 234, 238	0
3	N	13/13 (100%)	0.73	1 (7%) 13 7	197, 219, 252, 258	0
4	A	1395/1733 (80%)	0.03	11 (0%) 83 53	61, 99, 161, 173	0
5	B	1105/1224 (90%)	0.02	8 (0%) 84 56	64, 94, 139, 155	0
6	C	267/318 (83%)	-0.18	0 100 100	74, 89, 122, 144	0
7	E	214/215 (99%)	0.00	5 (2%) 57 27	79, 116, 155, 159	0
8	F	86/155 (55%)	-0.17	0 100 100	75, 105, 145, 156	0
9	H	133/146 (91%)	0.12	1 (0%) 83 53	100, 118, 146, 148	0
10	I	119/122 (97%)	-0.12	0 100 100	84, 103, 123, 142	0
11	J	65/70 (92%)	-0.15	0 100 100	69, 87, 107, 112	0
12	K	114/120 (95%)	-0.09	0 100 100	73, 95, 112, 115	0
13	L	46/70 (65%)	0.10	0 100 100	102, 147, 159, 163	0
All	All	3593/4222 (85%)	0.00	30 (0%) 83 53	61, 99, 157, 258	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	5.0
4	A	44	THR	4.1
2	T	3	DC	4.0
5	B	883	LEU	3.8
2	T	2	DA	3.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	MG	A	2002	1/1	0.37	7.69	76,76,76,76	0
16	G2P	T	3000	32/32	0.26	1.86	125,129,158,158	0
14	ZN	I	203	1/1	0.12	0.04	101,101,101,101	0
14	ZN	C	319	1/1	0.12	-0.32	90,90,90,90	0
15	MG	A	2001	1/1	0.18	-0.37	67,67,67,67	0
14	ZN	A	1735	1/1	0.15	-0.53	153,153,153,153	0
14	ZN	I	204	1/1	0.10	-0.77	90,90,90,90	0
14	ZN	J	101	1/1	0.16	-1.38	77,77,77,77	0
14	ZN	A	1734	1/1	0.09	-1.51	165,165,165,165	0
14	ZN	B	1307	1/1	0.08	-1.76	138,138,138,138	0
14	ZN	L	105	1/1	0.05	-2.41	146,146,146,146	0

6.5 Other polymers ⓘ

There are no such residues in this entry.