



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 31, 2021 – 01:10 PM EDT

PDB ID : 7KEE
Title : RNA polymerase II elongation complex with unnatural base dTPT3, rNaMTP bound to E-site
Authors : Oh, J.; Wang, D.
Deposited on : 2020-10-10
Resolution : 3.45 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 : 2.23.1
buster-report : 1.1.7 (2018)
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) : 2.23.1

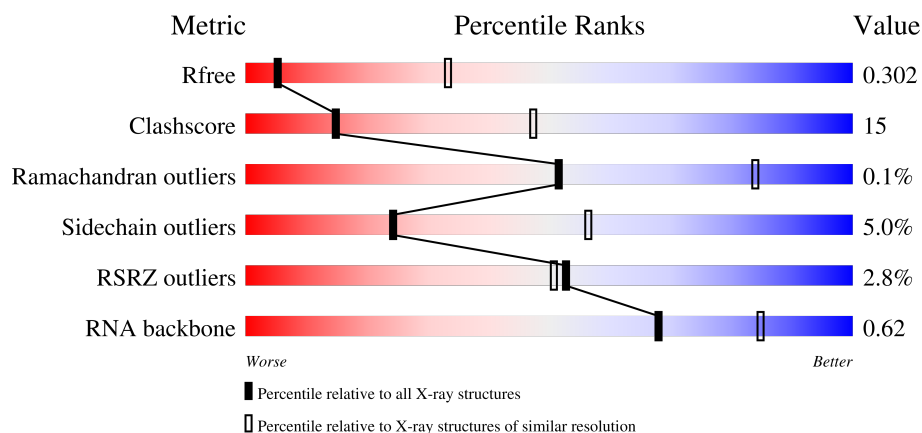
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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	1733	<div> <div>2%</div> <div>50%</div> <div>28%</div> <div>20%</div> </div>
2	B	1224	<div> <div>3%</div> <div>57%</div> <div>32%</div> <div>10%</div> </div>
3	C	318	<div> <div>%</div> <div>57%</div> <div>26%</div> <div>16%</div> </div>
4	E	215	<div> <div>7%</div> <div>66%</div> <div>31%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	10	
12	T	29	
13	N	16	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29039 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1390	Total	C	N	O	S	0	0	0
			10898	6875	1903	2059	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

- Molecule 12 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	24	Total	C	N	O	P	0	0	0
			490	235	87	142	24			

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	11	Total	C	N	O	P	0	0	0
			222	107	34	70	11			

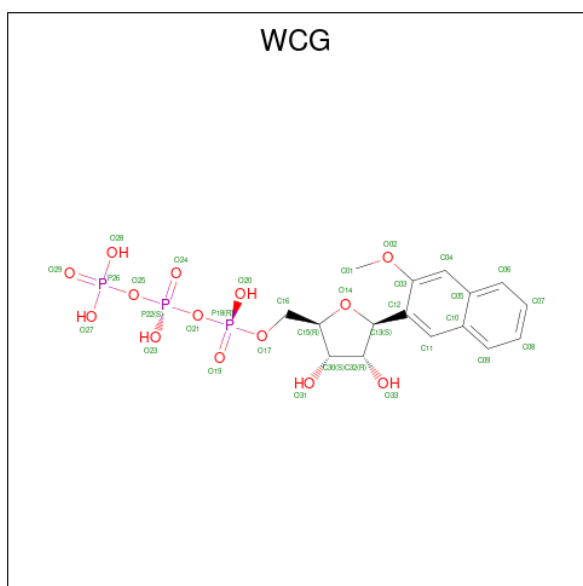
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

- Molecule 16 is (1S)-1,4-anhydro-5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-1-(3-methoxynaphthalen-2-yl)-D-ribitol (three-letter code: WCG) (formula: C₁₆H₂₁O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

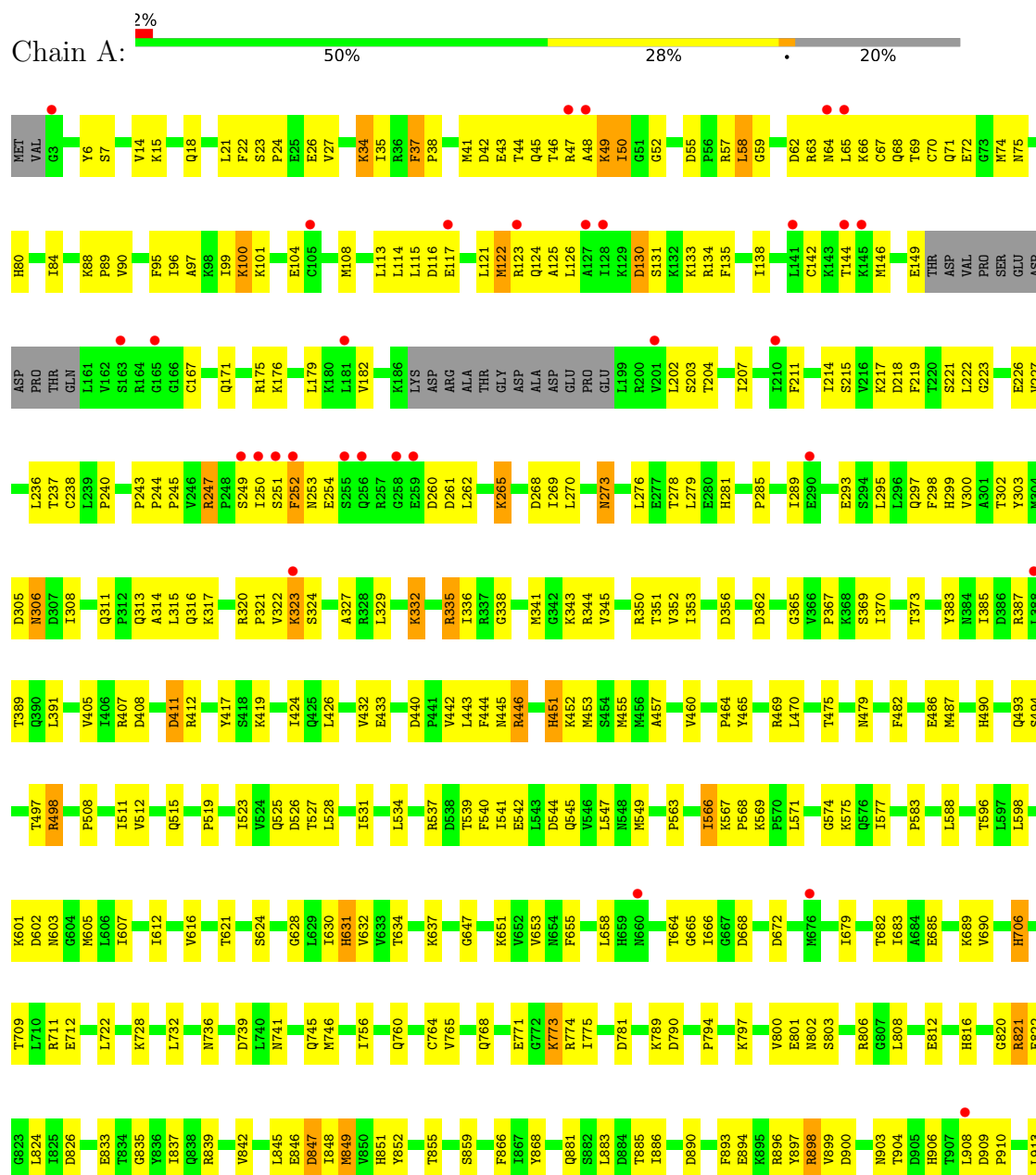


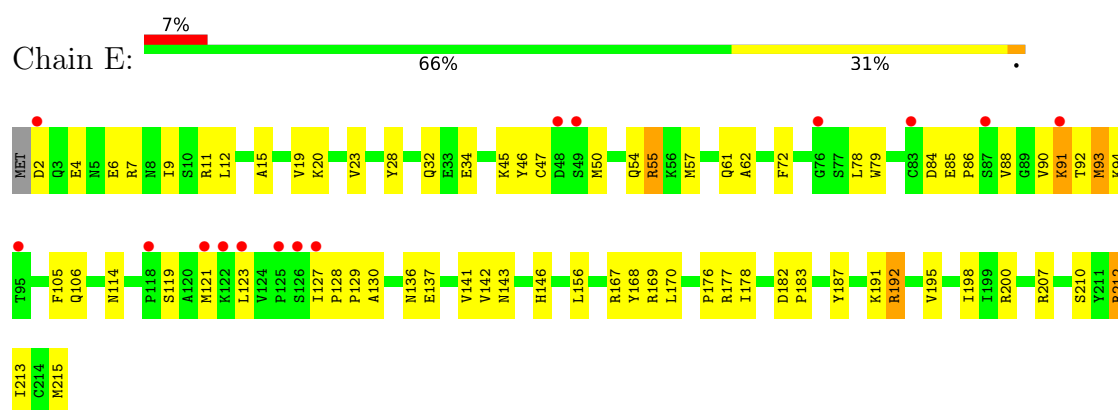
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total 33	C 16	O 14	P 3	0	0

3 Residue-property plots

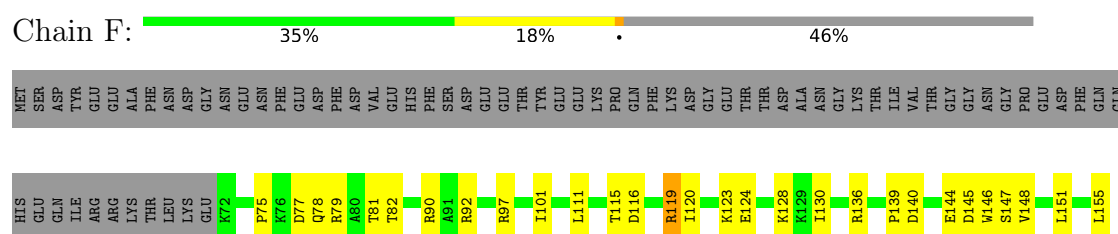
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 II subunit RPB1

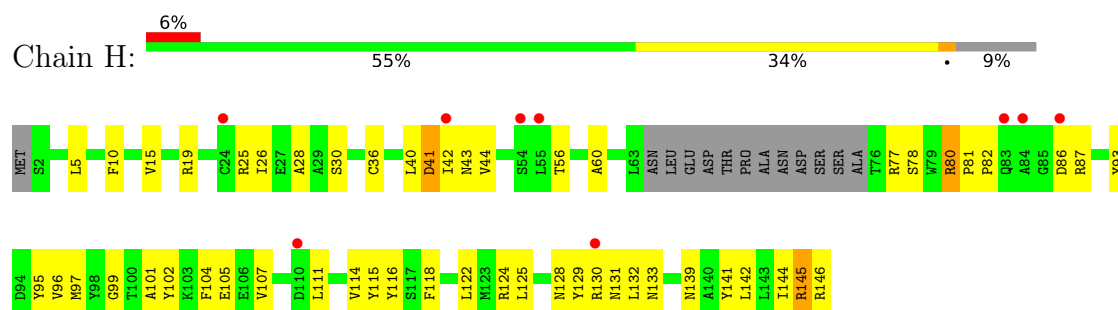




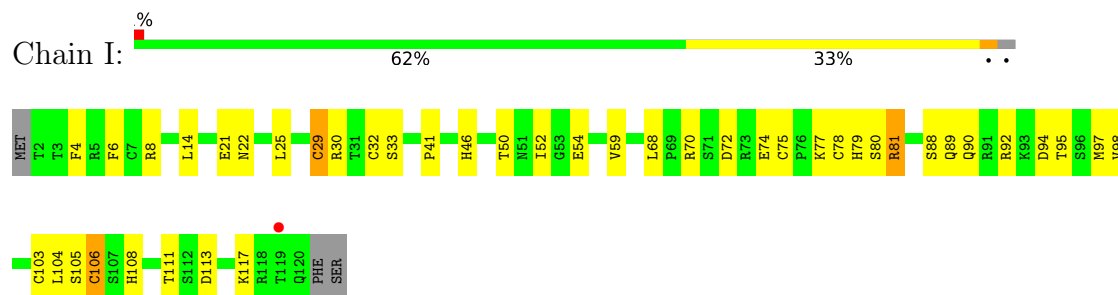
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



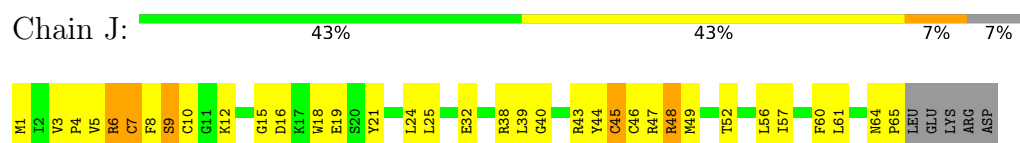
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



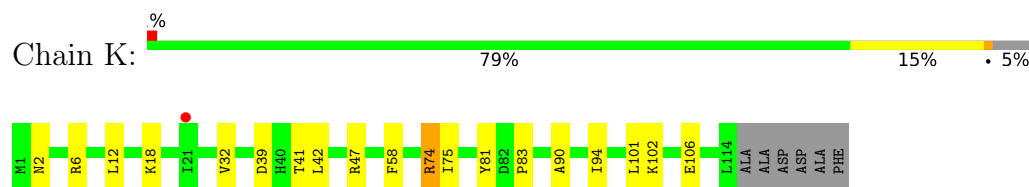
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



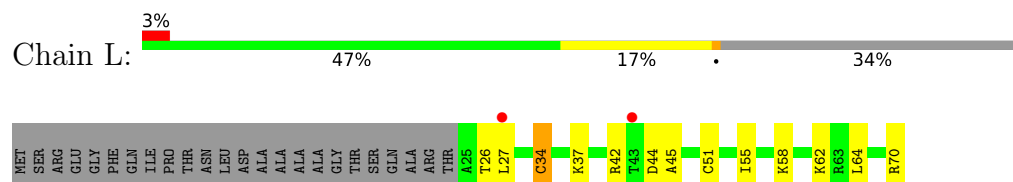
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



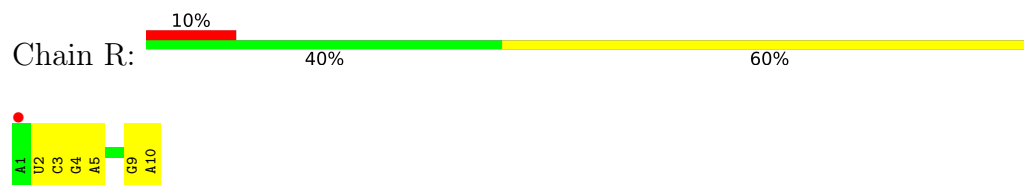
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



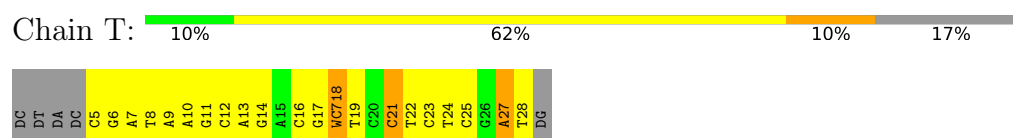
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



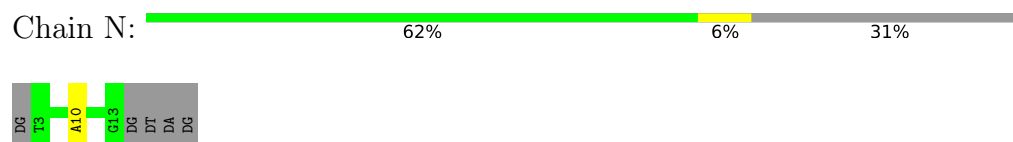
- Molecule 11: RNA



- Molecule 12: Template strand DNA



- Molecule 13: Non-template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.54Å 222.74Å 194.66Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	49.15 – 3.45 49.15 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-3.45) 99.8 (49.15-3.45)	Depositor EDS
R_{merge}	0.66	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.259 , 0.302 0.259 , 0.302	Depositor DCC
R_{free} test set	1930 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29039	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: ZN, WC7, MG, WCG

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	0.31	2/11091 (0.0%)	0.59	9/15000 (0.1%)
2	B	0.32	3/8963 (0.0%)	0.58	4/12086 (0.0%)
3	C	0.28	0/2133	0.52	0/2891
4	E	0.27	0/1788	0.48	0/2406
5	F	0.28	0/691	0.48	0/933
6	H	0.29	0/1086	0.54	0/1470
7	I	0.28	0/989	0.47	0/1331
8	J	0.37	0/541	0.51	0/727
9	K	0.27	0/937	0.46	0/1265
10	L	0.23	0/365	0.52	0/485
11	R	0.53	0/243	1.10	0/378
12	T	0.76	0/524	1.16	4/803 (0.5%)
13	N	0.69	0/246	1.21	1/377 (0.3%)
All	All	0.33	5/29597 (0.0%)	0.60	18/40152 (0.0%)

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	8
3	C	0	1
4	E	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	822	ASN	CG-OD1	-8.49	1.05	1.24
2	B	822	ASN	CG-ND2	7.50	1.51	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	ASN	CG-OD1	-7.07	1.08	1.24
2	B	822	ASN	CB-CG	-6.52	1.36	1.51
1	A	306	ASN	CG-ND2	5.60	1.46	1.32

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	822	ASN	CB-CG-OD1	29.15	179.91	121.60
1	A	306	ASN	CB-CG-OD1	24.03	169.65	121.60
1	A	306	ASN	CB-CG-ND2	-15.29	80.01	116.70
2	B	822	ASN	CB-CG-ND2	-14.26	82.47	116.70
1	A	306	ASN	CB-CA-C	-12.23	85.93	110.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1106	ASN	Peptide
1	A	1187	GLN	Peptide
1	A	130	ASP	Peptide
1	A	49	LYS	Peptide
1	A	566	ILE	Peptide

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	A	10898	0	10959	400	0
2	B	8792	0	8824	316	0
3	C	2095	0	2051	59	0
4	E	1752	0	1776	44	0
5	F	679	0	701	20	0
6	H	1068	0	1040	37	0
7	I	971	0	932	25	0
8	J	532	0	542	34	0
9	K	919	0	929	15	0
10	L	363	0	388	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	216	0	109	5	0
12	T	490	0	259	23	0
13	N	222	0	127	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	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	B	33	0	0	2	0
All	All	29039	0	28637	873	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 15.

The worst 5 of 873 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)
1:A:821:ARG:NH2	2:B:524:PRO:O	1.80	1.13
1:A:821:ARG:HH21	2:B:514:LEU:HD13	1.23	1.04
1:A:525:GLN:O	2:B:1015:HIS:NE2	1.90	1.02
1:A:821:ARG:NH2	2:B:514:LEU:HD13	1.76	1.01
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.49	0.94

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
1	A	1378/1733 (80%)	1272 (92%)	103 (8%)	3 (0%)	47 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1088/1224 (89%)	1011 (93%)	76 (7%)	1 (0%)	51	84
3	C	264/318 (83%)	259 (98%)	4 (2%)	1 (0%)	34	70
4	E	212/215 (99%)	201 (95%)	11 (5%)	0	100	100
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
6	H	129/146 (88%)	113 (88%)	16 (12%)	0	100	100
7	I	117/122 (96%)	110 (94%)	7 (6%)	0	100	100
8	J	63/70 (90%)	56 (89%)	7 (11%)	0	100	100
9	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
10	L	44/70 (63%)	40 (91%)	4 (9%)	0	100	100
All	All	3489/4173 (84%)	3248 (93%)	236 (7%)	5 (0%)	51	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	90	ASP
1	A	50	ILE
1	A	1188	GLN
2	B	1040	ASN
1	A	1107	VAL

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	1206/1520 (79%)	1149 (95%)	57 (5%)	26	59
2	B	960/1061 (90%)	919 (96%)	41 (4%)	29	61
3	C	234/274 (85%)	220 (94%)	14 (6%)	19	51
4	E	196/197 (100%)	181 (92%)	15 (8%)	13	42
5	F	74/137 (54%)	72 (97%)	2 (3%)	44	73
6	H	117/128 (91%)	112 (96%)	5 (4%)	29	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	113/116 (97%)	102 (90%)	11 (10%)	8	32
8	J	60/65 (92%)	53 (88%)	7 (12%)	5	24
9	K	99/102 (97%)	97 (98%)	2 (2%)	55	79
10	L	40/57 (70%)	38 (95%)	2 (5%)	24	56
All	All	3099/3657 (85%)	2943 (95%)	156 (5%)	24	56

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	61	GLN
7	I	88	SER
4	E	93	MET
6	H	80	ARG
8	J	45	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	171	GLN
2	B	60	GLN
2	B	395	GLN
2	B	538	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	8/10 (80%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	5	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
12	WC7	T	18	12	17,23,24	1.86	3 (17%)	17,33,36	1.72	4 (23%)

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
12	WC7	T	18	12	-	1/4/21/22	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	WC7	C5-C4	4.96	1.48	1.40
12	T	18	WC7	C5-S1	-4.33	1.59	1.67
12	T	18	WC7	C1-C2	2.47	1.39	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	18	WC7	C3-C4-S3	-4.96	108.78	111.74
12	T	18	WC7	C6-C3-C4	2.48	113.97	108.07
12	T	18	WC7	C2-C1-N1	2.24	125.69	120.68
12	T	18	WC7	C6-C3-C2	-2.21	129.00	136.72

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	T	18	WC7	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	18	WC7	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	WCG	B	2101	-	31,35,35	3.43	14 (45%)	46,54,54	2.31	10 (21%)

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	WCG	B	2101	-	-	13/24/40/40	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	2101	WCG	O14-C13	-8.83	1.31	1.44
16	B	2101	WCG	C30-C15	-8.76	1.30	1.53
16	B	2101	WCG	O14-C15	8.08	1.63	1.45
16	B	2101	WCG	O02-C03	4.48	1.44	1.37
16	B	2101	WCG	C04-C03	4.41	1.44	1.36

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	2101	WCG	O02-C03-C12	6.70	122.24	115.83
16	B	2101	WCG	C15-O14-C13	-6.36	101.58	109.42
16	B	2101	WCG	O02-C03-C04	-5.95	117.55	125.24
16	B	2101	WCG	P22-O25-P26	-5.50	113.94	132.83
16	B	2101	WCG	P22-O21-P18	-4.28	118.12	132.83

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

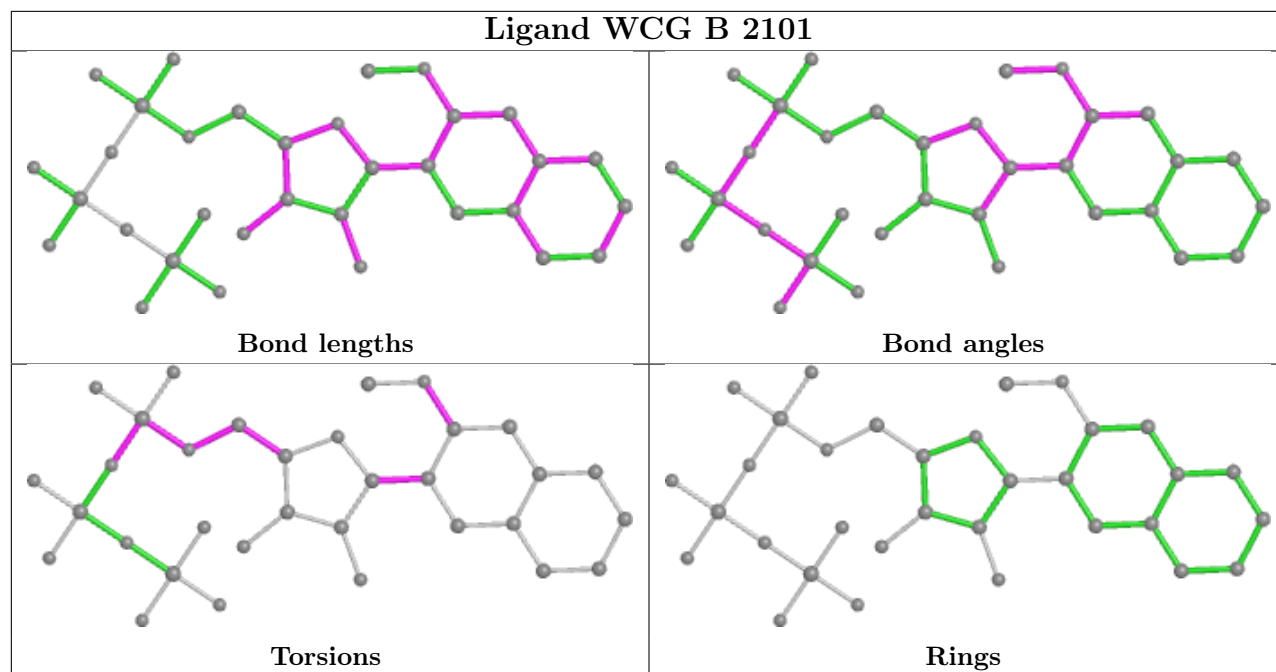
Mol	Chain	Res	Type	Atoms
16	B	2101	WCG	C03-C12-C13-C32
16	B	2101	WCG	C03-C12-C13-O14
16	B	2101	WCG	C11-C12-C13-C32
16	B	2101	WCG	C11-C12-C13-O14
16	B	2101	WCG	C16-O17-P18-O19

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	2101	WCG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1390/1733 (80%)	0.10	35 (2%) 57 54	42, 80, 142, 183	0
2	B	1106/1224 (90%)	0.18	34 (3%) 49 47	44, 77, 126, 177	0
3	C	266/318 (83%)	-0.04	3 (1%) 80 77	49, 77, 107, 155	0
4	E	214/215 (99%)	0.20	15 (7%) 16 18	58, 97, 152, 170	0
5	F	84/155 (54%)	-0.10	0 100 100	50, 81, 104, 116	0
6	H	133/146 (91%)	0.41	9 (6%) 17 19	75, 106, 151, 172	0
7	I	119/122 (97%)	-0.06	1 (0%) 86 82	62, 87, 114, 149	0
8	J	65/70 (92%)	-0.10	0 100 100	56, 73, 103, 118	0
9	K	114/120 (95%)	-0.06	1 (0%) 84 81	46, 73, 100, 112	0
10	L	46/70 (65%)	0.39	2 (4%) 35 34	58, 114, 151, 177	0
11	R	10/10 (100%)	0.33	1 (10%) 7 9	79, 91, 147, 164	0
12	T	23/29 (79%)	-0.09	0 100 100	92, 124, 203, 213	0
13	N	11/16 (68%)	0.13	0 100 100	152, 174, 203, 204	0
All	All	3581/4228 (84%)	0.11	101 (2%) 53 51	42, 81, 140, 213	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	83	CYS	6.5
2	B	248	SER	6.4
2	B	870	ILE	6.2
2	B	472	ALA	5.7
10	L	27	LEU	5.4

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
12	WC7	T	18	21/22	0.85	0.26	97,104,113,117	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

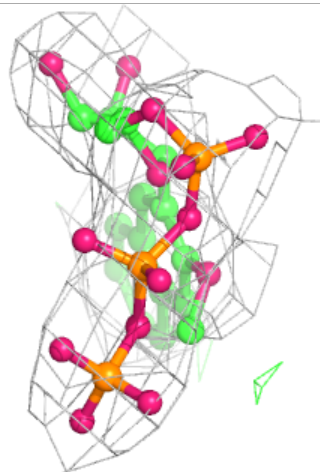
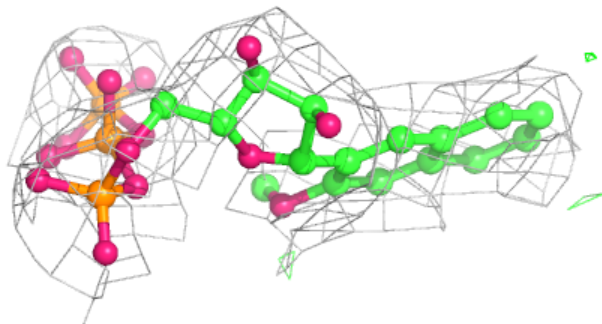
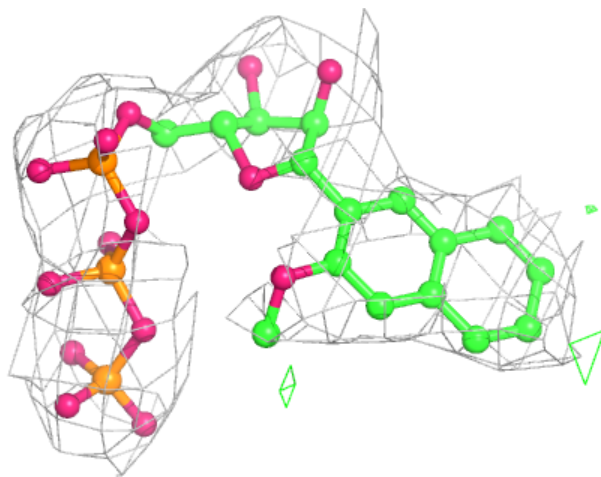
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ZN	A	1801	1/1	0.77	0.17	193,193,193,193	0
14	ZN	B	2102	1/1	0.88	0.10	121,121,121,121	0
16	WCG	B	2101	33/33	0.88	0.19	79,116,204,209	0
14	ZN	I	202	1/1	0.90	0.12	76,76,76,76	0
14	ZN	C	401	1/1	0.90	0.13	76,76,76,76	0
14	ZN	J	101	1/1	0.92	0.18	70,70,70,70	0
15	MG	A	1803	1/1	0.93	0.19	53,53,53,53	0
14	ZN	A	1802	1/1	0.95	0.11	116,116,116,116	0
14	ZN	L	101	1/1	0.95	0.06	120,120,120,120	0
14	ZN	I	201	1/1	0.98	0.15	71,71,71,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around WCG B 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.