



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 11:07 PM EDT

PDB ID : 6BLO
Title : Pol II elongation complex with an abasic lesion at i+1 position
Authors : Wang, W.; Wang, D.
Deposited on : 2017-11-10
Resolution : 3.40 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

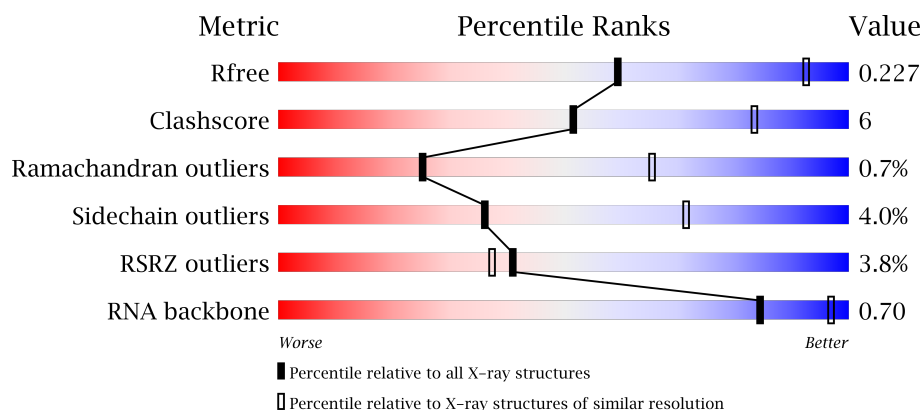
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)
RNA backbone	2435	1009 (3.96-2.84)

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	1733	<div> <div>4%</div> <div>62%</div> <div>16%</div> <div>•</div> <div>21%</div> </div>
2	B	1224	<div> <div>•</div> <div>71%</div> <div>17%</div> <div>•</div> <div>10%</div> </div>
3	C	318	<div> <div>65%</div> <div>17%</div> <div>•</div> <div>16%</div> </div>
4	E	215	<div> <div>12%</div> <div>87%</div> <div>11%</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	T	29	
12	R	8	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28206 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	1372	Total	C	N	O	S	0	0	0
			10784	6802	1887	2034	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8726	5526	1530	1615	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	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	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	130	Total	C	N	O	S	0	0	0
			1043	660	173	206	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	115	Total	C	N	O	S	0	0	0
			935	575	170	180	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	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 11 is a DNA chain called DNA (5'-D(P*AP*(3DR)P*CP*TP*CP*TP*CP*GP*A P*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	11	Total	C	N	O	P	0	0	0
			214	102	35	66	11			

- Molecule 12 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	8	Total	C	N	O	P	0	0	0
			175	78	35	54	8			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

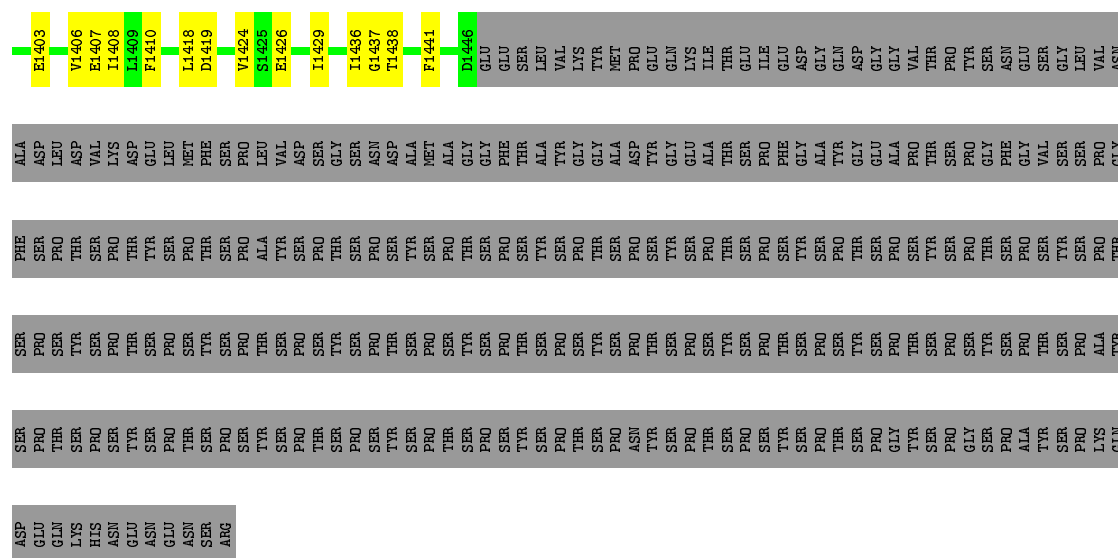
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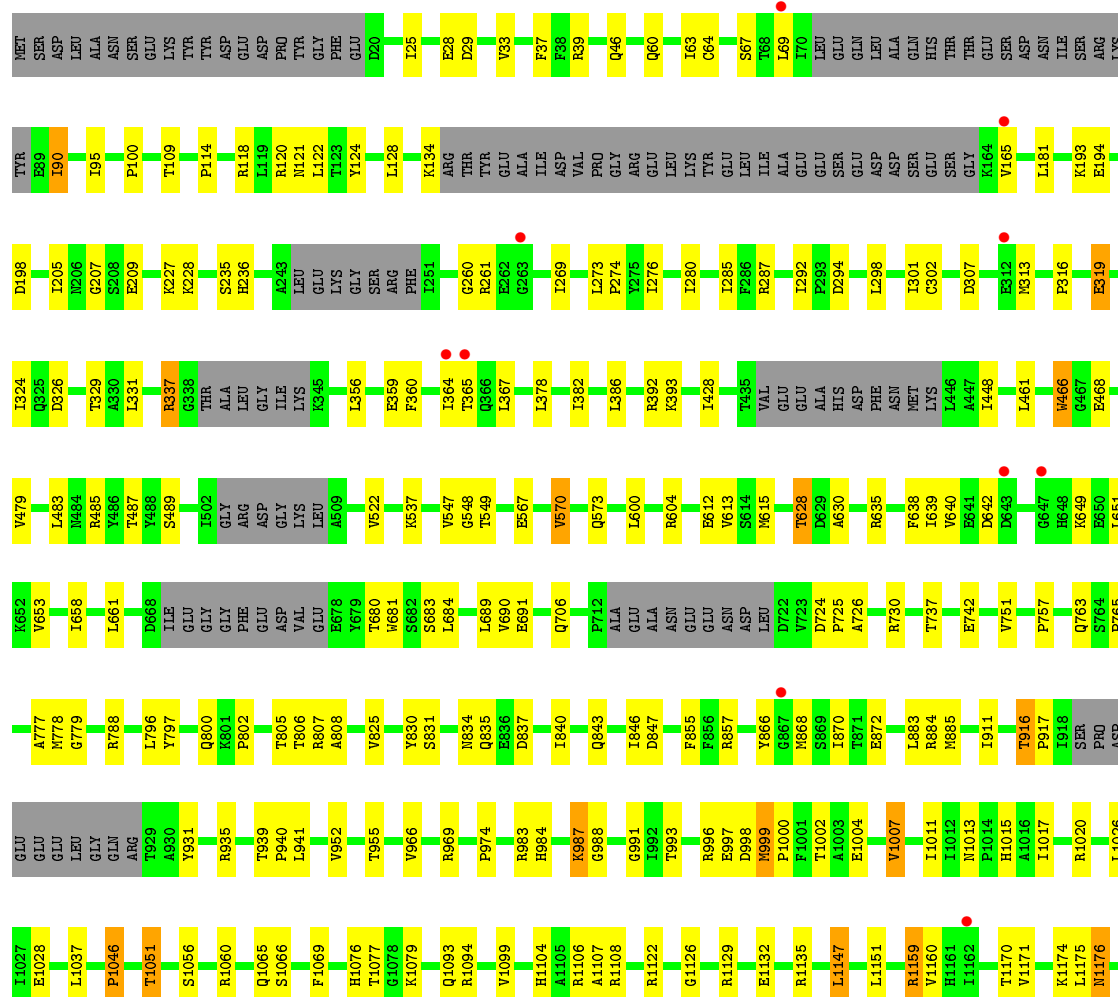
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



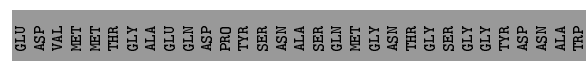
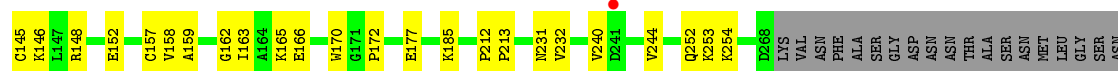
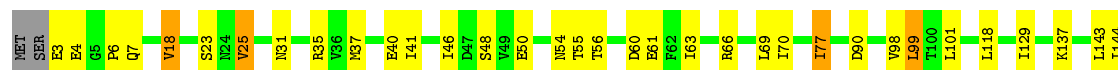
● Molecule 2: DNA-directed RNA polymerase II subunit RPB2





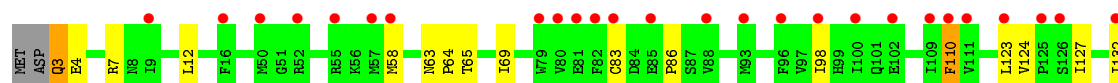
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 65% 17% 16%



- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 12% 87% 11%



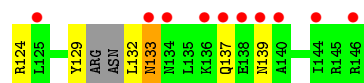
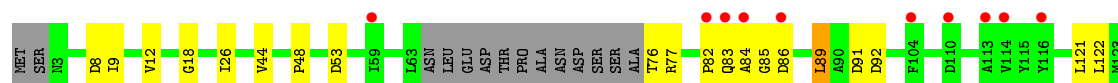
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 43% 10% 46%



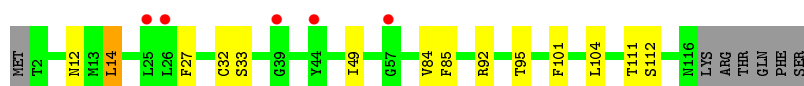
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 14% 71% 16% 11%



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

Chain I: 4% 83% 11% 6%



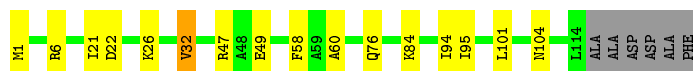
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 74% 16% 7%



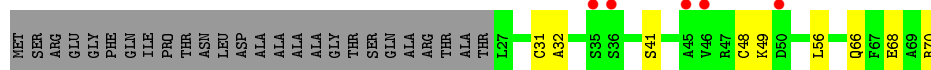
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 82% 13% 5%



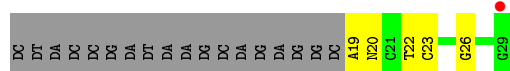
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 7% 50% 13% 37%



- Molecule 11: DNA (5'-D(P*AP*(3DR)P*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')

Chain T: 3% 21% 17% 62%



- Molecule 12: RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*G)-3')

Chain R: 88% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.55Å 222.28Å 193.77Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	63.48 – 3.40 95.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	86.6 (63.48-3.40) 86.7 (95.99-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.203 , 0.227 0.202 , 0.227	Depositor DCC
R_{free} test set	4034 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	28206	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 3DR

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	0.22	0/10975	0.38	0/14838
2	B	0.22	0/8896	0.39	0/11996
3	C	0.22	0/2133	0.38	0/2891
4	E	0.21	0/1780	0.36	0/2395
5	F	0.21	0/691	0.38	0/933
6	H	0.22	0/1060	0.39	0/1434
7	I	0.22	0/953	0.36	0/1284
8	J	0.22	0/541	0.38	0/727
9	K	0.22	0/937	0.36	0/1265
10	L	0.21	0/353	0.36	0/468
11	T	0.55	0/225	0.91	0/342
12	R	0.15	0/196	0.64	0/304
All	All	0.22	0/28740	0.39	0/38877

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	10784	0	10871	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8726	0	8759	128	0
3	C	2095	0	2051	36	0
4	E	1744	0	1772	13	0
5	F	679	0	701	10	0
6	H	1043	0	1015	15	0
7	I	935	0	886	8	0
8	J	532	0	542	10	0
9	K	919	0	929	11	0
10	L	351	0	375	5	0
11	T	214	0	122	6	0
12	R	175	0	87	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28206	0	28110	362	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 6.

The worst 5 of 362 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)
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.61	0.83
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.62	0.82
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.65	0.79
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.70	0.73
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.72	0.70

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	1358/1733 (78%)	1249 (92%)	99 (7%)	10 (1%)	25	65
2	B	1077/1224 (88%)	989 (92%)	80 (7%)	8 (1%)	25	65
3	C	264/318 (83%)	248 (94%)	14 (5%)	2 (1%)	22	62
4	E	211/215 (98%)	198 (94%)	12 (6%)	1 (0%)	32	71
5	F	82/155 (53%)	76 (93%)	6 (7%)	0	100	100
6	H	124/146 (85%)	109 (88%)	13 (10%)	2 (2%)	11	48
7	I	113/122 (93%)	102 (90%)	11 (10%)	0	100	100
8	J	63/70 (90%)	59 (94%)	4 (6%)	0	100	100
9	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	20	61
10	L	42/70 (60%)	34 (81%)	7 (17%)	1 (2%)	7	40
All	All	3446/4173 (83%)	3171 (92%)	250 (7%)	25 (1%)	25	65

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	110	CYS
1	A	322	VAL
1	A	1437	GLY
2	B	468	GLU

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	1196/1520 (79%)	1137 (95%)	59 (5%)	29	66
2	B	952/1061 (90%)	915 (96%)	37 (4%)	37	72
3	C	234/274 (85%)	227 (97%)	7 (3%)	46	78
4	E	195/197 (99%)	189 (97%)	6 (3%)	45	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	74/137 (54%)	70 (95%)	4 (5%)	26	63
6	H	114/128 (89%)	110 (96%)	4 (4%)	41	74
7	I	109/116 (94%)	107 (98%)	2 (2%)	64	85
8	J	60/65 (92%)	57 (95%)	3 (5%)	28	65
9	K	99/102 (97%)	97 (98%)	2 (2%)	60	84
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3072/3657 (84%)	2948 (96%)	124 (4%)	36	71

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1374	VAL
2	B	549	THR
6	H	89	LEU
1	A	1400	CYS
2	B	134	LYS

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

Mol	Chain	Res	Type
2	B	762	ASN
2	B	984	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	7/8 (87%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	8	G

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	$\# Z > 2$
11	3DR	T	20	11	8,11,12	1.68	2 (25%)	8,14,17	0.89	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
11	3DR	T	20	11	-	0/3/15/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	20	3DR	O5'-C5'	-2.49	1.41	1.44
11	T	20	3DR	O4'-C4'	-2.37	1.40	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	20	3DR	3	0

5.5 Carbohydrates ⓘ

There are no carbohydrates 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

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 [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	1372/1733 (79%)	0.32	61 (4%) 35 32	19, 76, 172, 296	0
2	B	1097/1224 (89%)	0.13	12 (1%) 80 76	19, 59, 133, 245	0
3	C	266/318 (83%)	0.11	1 (0%) 92 90	24, 60, 106, 189	0
4	E	213/215 (99%)	0.69	26 (12%) 5 5	44, 112, 190, 264	0
5	F	84/155 (54%)	0.03	1 (1%) 79 75	38, 75, 123, 159	0
6	H	130/146 (89%)	1.02	20 (15%) 2 2	58, 100, 155, 217	0
7	I	115/122 (94%)	0.33	5 (4%) 36 33	33, 78, 117, 175	0
8	J	65/70 (92%)	-0.07	0 100 100	26, 46, 100, 141	0
9	K	114/120 (95%)	0.01	0 100 100	31, 64, 108, 131	0
10	L	44/70 (62%)	0.66	5 (11%) 6 6	34, 114, 210, 228	0
11	T	10/29 (34%)	0.52	1 (10%) 8 8	70, 86, 170, 209	0
12	R	8/8 (100%)	0.20	0 100 100	62, 71, 139, 193	0
All	All	3518/4210 (83%)	0.27	132 (3%) 41 37	19, 70, 160, 296	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	139	ASN	5.8
2	B	643	ASP	5.7
4	E	93	MET	5.6
1	A	105	CYS	4.9
4	E	100	ILE	4.7

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. 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
11	3DR	T	20	11/12	0.88	0.25	-	143,150,185,188	0

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
13	ZN	I	202	1/1	0.99	0.18	0.49	55,55,55,55	0
13	ZN	C	401	1/1	0.98	0.20	0.08	53,53,53,53	0
13	ZN	B	1301	1/1	0.98	0.11	-1.25	99,99,99,99	0
13	ZN	I	201	1/1	0.99	0.12	-1.27	71,71,71,71	0
13	ZN	J	101	1/1	1.00	0.16	-1.30	42,42,42,42	0
13	ZN	A	1802	1/1	0.95	0.13	-1.75	97,97,97,97	0
13	ZN	L	101	1/1	0.97	0.07	-2.19	130,130,130,130	0
13	ZN	A	1801	1/1	0.64	0.07	-3.39	188,188,188,188	0
14	MG	A	1803	1/1	0.97	0.19	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.