



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

PDB ID : 3K1F
Title : Crystal structure of RNA Polymerase II in complex with TFIIB
Authors : Kostrewa, D.; Zeller, M.E.; Armache, K.-J.; Seizl, M.; Leike, K.; Thomm, M.; Cramer, P.
Deposited on : 2009-09-27
Resolution : 4.30 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
<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

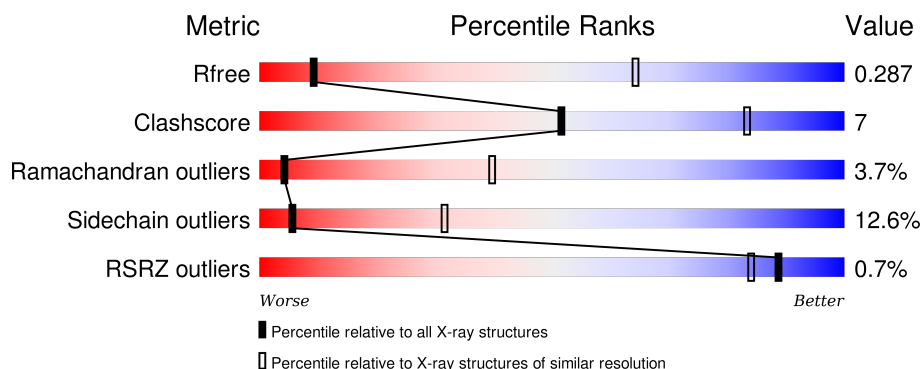
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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))
R_{free}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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>59%</div> <div>19%</div> <div>•</div> <div>18%</div> </div>
2	B	1224	<div> <div>64%</div> <div>24%</div> <div>•</div> <div>8%</div> </div>
3	C	318	<div> <div>63%</div> <div>19%</div> <div>•</div> <div>16%</div> </div>
4	D	221	<div> <div>2%</div> <div>58%</div> <div>21%</div> <div>•</div> <div>19%</div> </div>
5	E	215	<div> <div>•</div> <div>74%</div> <div>23%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	197	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 32332 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	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1120	Total	C	N	O	S	0	0	0
			8910	5639	1560	1656	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 polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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 polymerases I, II, and III subunit RPABC5.

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 subunit RPB11.

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 polymerases I, II, and III subunit RPABC4.

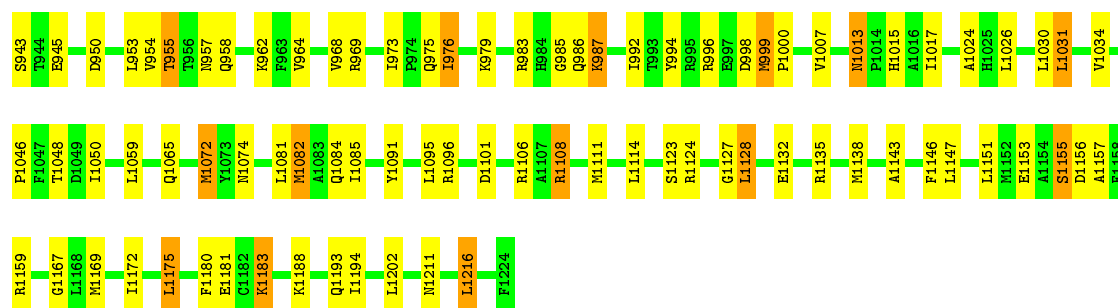
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a protein called Transcription initiation factor IIB.

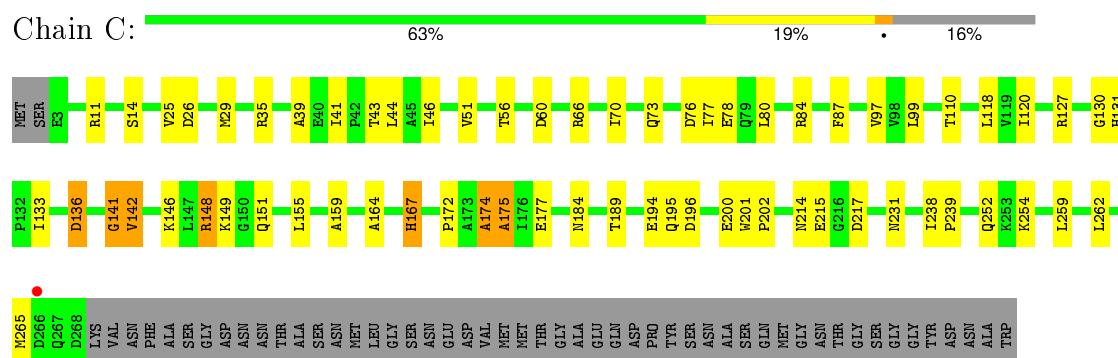
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	185	Total	C	N	O	S	0	0	0
			1083	662	207	210	4			

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

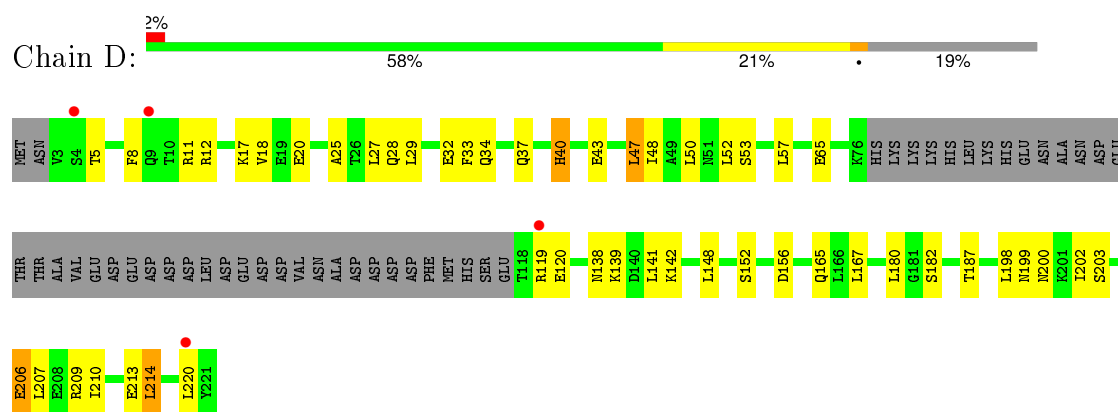
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total 1	Zn 1	0	0
14	B	1	Total 1	Zn 1	0	0
14	I	2	Total 2	Zn 2	0	0
14	C	1	Total 1	Zn 1	0	0
14	A	2	Total 2	Zn 2	0	0
14	L	1	Total 1	Zn 1	0	0
14	M	1	Total 1	Zn 1	0	0



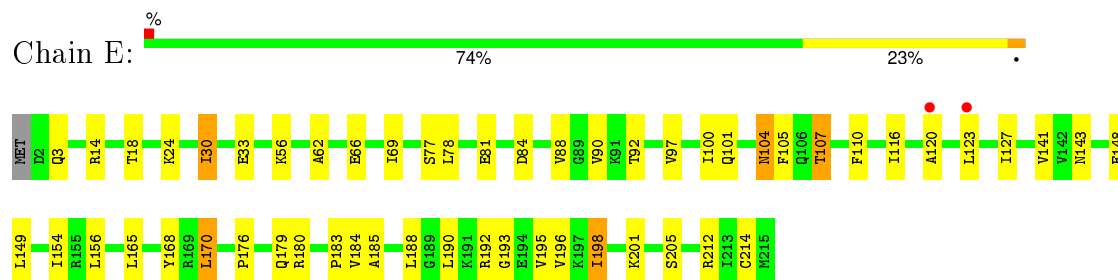
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

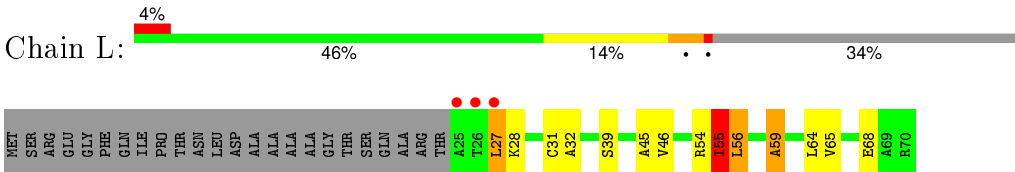


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

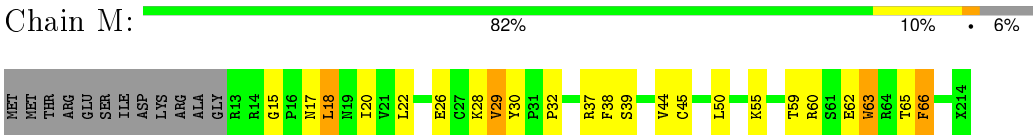


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2





• Molecule 13: Transcription initiation factor IIB



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.97Å 408.27Å 275.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.69 – 4.30 39.69 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.69-4.30) 99.4 (39.69-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 4.28Å)	Xtriage
Refinement program	BUSTER 2.7.0	Depositor
R, R_{free}	0.220 , 0.255 0.250 , 0.287	Depositor DCC
R_{free} test set	2055 reflections (2.45%)	DCC
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.780	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 111.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 83919 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	32332	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: 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	A	0.44	0/11342	0.72	0/15337
2	B	0.44	0/9084	0.69	0/12251
3	C	0.43	0/2133	0.71	0/2891
4	D	0.42	0/1444	0.68	0/1935
5	E	0.43	0/1788	0.66	0/2406
6	F	0.46	0/717	0.75	0/967
7	G	0.41	0/1368	0.74	0/1844
8	H	0.45	0/1094	0.74	0/1481
9	I	0.41	0/989	0.73	0/1331
10	J	0.45	0/541	0.74	0/727
11	K	0.44	0/937	0.64	0/1265
12	L	0.49	0/365	0.78	0/485
13	M	0.43	0/449	0.72	0/609
All	All	0.44	0/32251	0.71	0/43529

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	11143	0	11217	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8910	0	8926	135	0
3	C	2095	0	2051	31	0
4	D	1434	0	1460	18	0
5	E	1752	0	1776	27	0
6	F	705	0	731	15	0
7	G	1340	0	1357	28	0
8	H	1076	0	1046	21	0
9	I	971	0	927	12	0
10	J	532	0	542	13	0
11	K	919	0	929	15	0
12	L	363	0	386	5	0
13	M	1083	0	578	12	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
14	M	1	0	0	0	0
All	All	32332	0	31926	434	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 7.

The worst 5 of 434 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:567:LYS:HB2	1:A:568:PRO:HD3	1.48	0.94
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.60	0.83
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.62	0.82
1:A:225:ASN:HD22	1:A:228:PHE:H	1.28	0.81
3:C:142:VAL:H	10:J:16:ASP:HB3	1.46	0.79

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	1406/1733 (81%)	1215 (86%)	137 (10%)	54 (4%)	4	39
2	B	1102/1224 (90%)	938 (85%)	126 (11%)	38 (3%)	5	42
3	C	264/318 (83%)	219 (83%)	37 (14%)	8 (3%)	5	44
4	D	174/221 (79%)	147 (84%)	20 (12%)	7 (4%)	4	37
5	E	212/215 (99%)	192 (91%)	16 (8%)	4 (2%)	10	54
6	F	85/155 (55%)	74 (87%)	11 (13%)	0	100	100
7	G	169/171 (99%)	145 (86%)	21 (12%)	3 (2%)	11	55
8	H	130/146 (89%)	97 (75%)	18 (14%)	15 (12%)	0	9
9	I	117/122 (96%)	96 (82%)	19 (16%)	2 (2%)	11	56
10	J	63/70 (90%)	51 (81%)	7 (11%)	5 (8%)	1	19
11	K	112/120 (93%)	101 (90%)	10 (9%)	1 (1%)	21	67
12	L	44/70 (63%)	34 (77%)	5 (11%)	5 (11%)	0	10
13	M	54/197 (27%)	43 (80%)	8 (15%)	3 (6%)	2	29
All	All	3932/4762 (83%)	3352 (85%)	435 (11%)	145 (4%)	4	40

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	65	LEU
1	A	66	LYS
1	A	167	CYS
1	A	311	GLN

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	1239/1520 (82%)	1071 (86%)	168 (14%)	5	29
2	B	972/1061 (92%)	847 (87%)	125 (13%)	5	31
3	C	234/274 (85%)	210 (90%)	24 (10%)	9	40
4	D	160/200 (80%)	138 (86%)	22 (14%)	4	29
5	E	196/197 (100%)	181 (92%)	15 (8%)	16	55
6	F	77/137 (56%)	68 (88%)	9 (12%)	7	35
7	G	152/152 (100%)	135 (89%)	17 (11%)	7	37
8	H	118/128 (92%)	102 (86%)	16 (14%)	5	29
9	I	113/116 (97%)	103 (91%)	10 (9%)	12	48
10	J	60/65 (92%)	53 (88%)	7 (12%)	7	35
11	K	99/102 (97%)	87 (88%)	12 (12%)	6	33
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	25
13	M	52/62 (84%)	40 (77%)	12 (23%)	1	8
All	All	3512/4071 (86%)	3069 (87%)	443 (13%)	5	31

5 of 443 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	365	THR
2	B	801	LYS
10	J	26	GLN
2	B	393	LYS
2	B	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	516	ASN
2	B	1015	HIS
8	H	33	GLN
2	B	518	HIS
2	B	878	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 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 ⓘ

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	1416/1733 (81%)	-0.24	6 (0%) 93 90	53, 106, 168, 238	0
2	B	1120/1224 (91%)	-0.18	6 (0%) 91 88	53, 122, 192, 238	0
3	C	266/318 (83%)	-0.27	1 (0%) 93 90	63, 117, 167, 202	0
4	D	178/221 (80%)	0.02	4 (2%) 65 56	65, 132, 190, 228	0
5	E	214/215 (99%)	-0.04	2 (0%) 85 80	74, 138, 210, 245	0
6	F	87/155 (56%)	-0.38	0 100 100	56, 88, 114, 128	0
7	G	171/171 (100%)	-0.28	0 100 100	64, 108, 146, 188	0
8	H	134/146 (91%)	-0.04	1 (0%) 89 84	101, 144, 209, 224	0
9	I	119/122 (97%)	0.29	6 (5%) 32 25	103, 170, 220, 232	0
10	J	65/70 (92%)	-0.29	0 100 100	78, 114, 152, 177	0
11	K	114/120 (95%)	-0.19	0 100 100	74, 120, 143, 198	0
12	L	46/70 (65%)	0.23	3 (6%) 22 16	81, 152, 165, 202	0
13	M	56/197 (28%)	-0.22	0 100 100	89, 117, 157, 174	0
All	All	3986/4762 (83%)	-0.18	29 (0%) 89 84	53, 118, 192, 245	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1455	PRO	3.8
12	L	26	THR	3.4
4	D	9	GLN	3.0
1	A	1173	HIS	2.9
1	A	69	THR	2.9

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 [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(\AA^2)	Q<0.9
14	ZN	I	3004	1/1	0.98	0.16	-1.64	196,196,196,196	0
14	ZN	A	3008	1/1	0.97	0.07	-1.70	65,65,65,65	0
14	ZN	C	3002	1/1	0.98	0.06	-1.76	62,62,62,62	0
14	ZN	I	3003	1/1	0.97	0.07	-1.80	151,151,151,151	0
14	ZN	M	3009	1/1	0.98	0.06	-2.01	71,71,71,71	0
14	ZN	J	3001	1/1	0.94	0.16	-2.06	124,124,124,124	0
14	ZN	L	3005	1/1	0.96	0.07	-2.17	190,190,190,190	0
14	ZN	A	3006	1/1	0.95	0.05	-3.22	130,130,130,130	0
14	ZN	B	3007	1/1	0.97	0.06	-	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.