



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2022 – 02:06 PM EDT

PDB ID : 7S00
Title : X-ray structure of the phage AR9 non-virion RNA polymerase core
Authors : Leiman, P.G.; Sokolova, M.L.; Fraser, A.
Deposited on : 2021-08-28
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

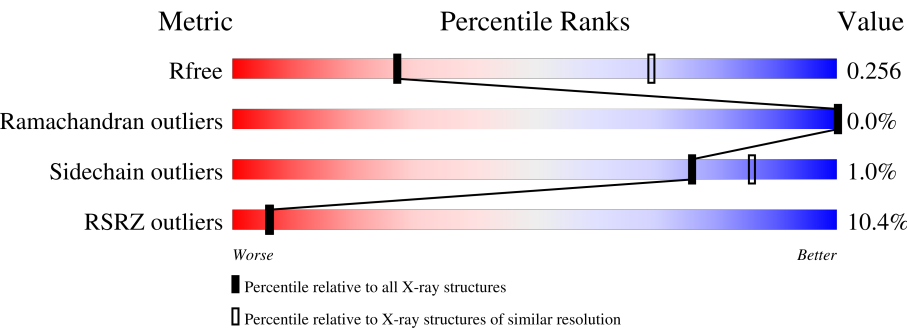
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	c	496	<div><div>9%</div><div>96%</div><div>..</div></div>
1	e	496	<div><div>11%</div><div>97%</div><div>..</div></div>
2	C	665	<div><div>5%</div><div>95%</div><div>..</div></div>
2	E	665	<div><div>8%</div><div>96%</div><div>..</div></div>
3	D	631	<div><div>4%</div><div>76%</div><div>24%</div></div>
3	F	631	<div><div>14%</div><div>94%</div><div>6%</div></div>
4	d	448	<div><div>17%</div><div>89%</div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
4	f	448	<div> <div style="width: 14%;"></div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> </div> <div>14%91%8%</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33894 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 beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	484	Total	C	N	O	S	0	0	0
			4003	2580	658	754	11			
1	e	484	Total	C	N	O	S	0	0	0
			4003	2580	658	754	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	640	Total	C	N	O	S	0	1	0
			5208	3296	857	1031	24			
2	E	640	Total	C	N	O	S	0	1	0
			5208	3296	857	1031	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	481	Total	C	N	O	S	0	0	0
			3893	2481	640	757	15			
3	F	596	Total	C	N	O	S	0	0	0
			4853	3092	791	952	18			

- Molecule 4 is a protein called DNA-directed RNA polymerase beta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	410	Total	C	N	O	S	0	0	0
			3362	2182	541	631	8			
4	f	410	Total	C	N	O	S	0	0	0
			3362	2182	541	631	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-21	MET	-	expression tag	UNP A0A172JIH0
d	-20	GLY	-	expression tag	UNP A0A172JIH0
d	-19	SER	-	expression tag	UNP A0A172JIH0
d	-18	SER	-	expression tag	UNP A0A172JIH0
d	-17	HIS	-	expression tag	UNP A0A172JIH0
d	-16	HIS	-	expression tag	UNP A0A172JIH0
d	-15	HIS	-	expression tag	UNP A0A172JIH0
d	-14	HIS	-	expression tag	UNP A0A172JIH0
d	-13	HIS	-	expression tag	UNP A0A172JIH0
d	-12	HIS	-	expression tag	UNP A0A172JIH0
d	-11	SER	-	expression tag	UNP A0A172JIH0
d	-10	SER	-	expression tag	UNP A0A172JIH0
d	-9	GLY	-	expression tag	UNP A0A172JIH0
d	-8	GLU	-	expression tag	UNP A0A172JIH0
d	-7	ASN	-	expression tag	UNP A0A172JIH0
d	-6	LEU	-	expression tag	UNP A0A172JIH0
d	-5	TYR	-	expression tag	UNP A0A172JIH0
d	-4	PHE	-	expression tag	UNP A0A172JIH0
d	-3	GLN	-	expression tag	UNP A0A172JIH0
d	-2	GLY	-	expression tag	UNP A0A172JIH0
d	-1	HIS	-	expression tag	UNP A0A172JIH0
d	0	HIS	-	expression tag	UNP A0A172JIH0
f	-21	MET	-	expression tag	UNP A0A172JIH0
f	-20	GLY	-	expression tag	UNP A0A172JIH0
f	-19	SER	-	expression tag	UNP A0A172JIH0
f	-18	SER	-	expression tag	UNP A0A172JIH0
f	-17	HIS	-	expression tag	UNP A0A172JIH0
f	-16	HIS	-	expression tag	UNP A0A172JIH0
f	-15	HIS	-	expression tag	UNP A0A172JIH0
f	-14	HIS	-	expression tag	UNP A0A172JIH0
f	-13	HIS	-	expression tag	UNP A0A172JIH0
f	-12	HIS	-	expression tag	UNP A0A172JIH0
f	-11	SER	-	expression tag	UNP A0A172JIH0
f	-10	SER	-	expression tag	UNP A0A172JIH0
f	-9	GLY	-	expression tag	UNP A0A172JIH0
f	-8	GLU	-	expression tag	UNP A0A172JIH0
f	-7	ASN	-	expression tag	UNP A0A172JIH0
f	-6	LEU	-	expression tag	UNP A0A172JIH0
f	-5	TYR	-	expression tag	UNP A0A172JIH0
f	-4	PHE	-	expression tag	UNP A0A172JIH0
f	-3	GLN	-	expression tag	UNP A0A172JIH0
f	-2	GLY	-	expression tag	UNP A0A172JIH0
f	-1	HIS	-	expression tag	UNP A0A172JIH0

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Chain	Residue	Modelled	Actual	Comment	Reference
f	0	HIS	-	expression tag	UNP A0A172JIH0

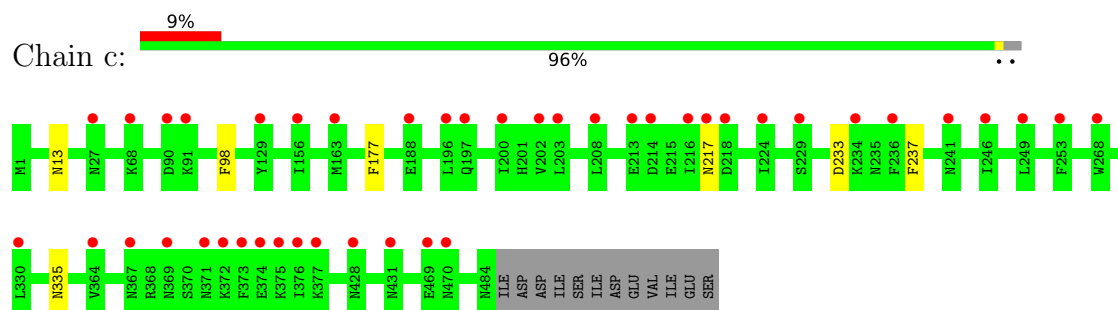
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Zn 1	0	0
5	F	1	Total 1	Zn 1	0	0

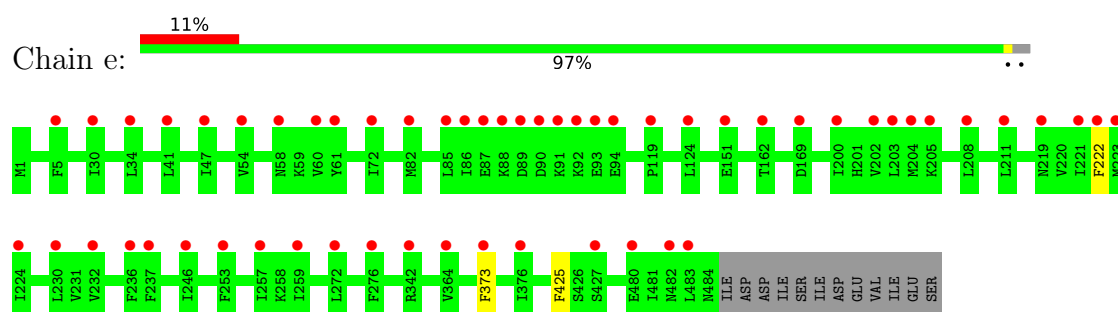
3 Residue-property plots [i](#)

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.

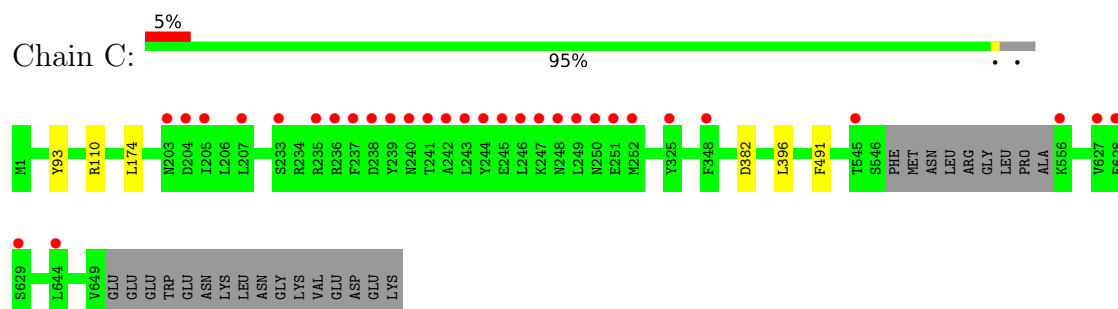
- Molecule 1: DNA-directed RNA polymerase beta subunit



- Molecule 1: DNA-directed RNA polymerase beta subunit

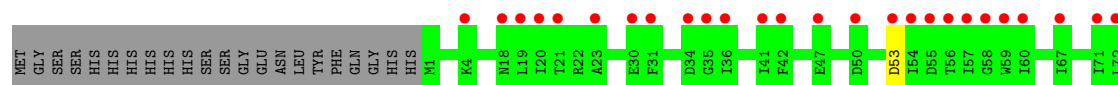


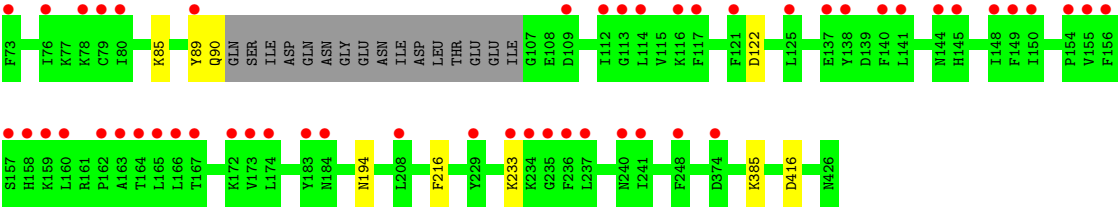
- Molecule 2: DNA-directed RNA polymerase



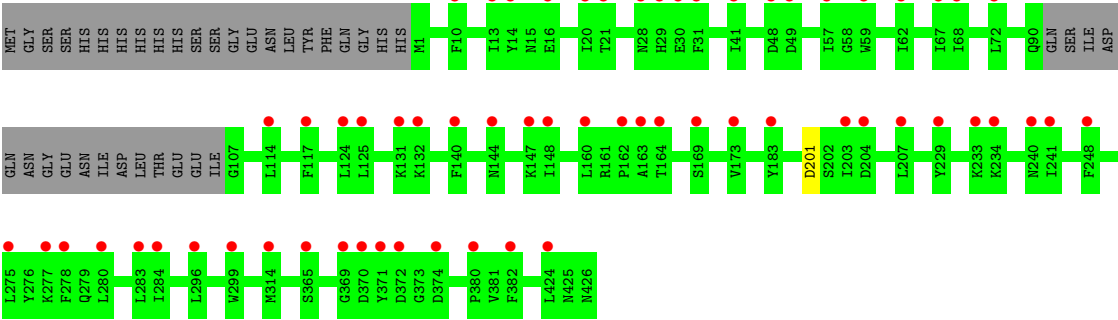
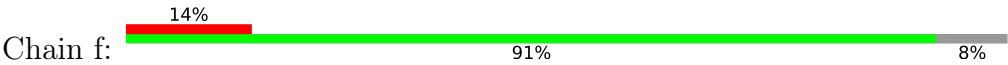
- Molecule 2: DNA-directed RNA polymerase







● Molecule 4: DNA-directed RNA polymerase beta' subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.86Å 166.27Å 307.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.30 49.42 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.42-3.30) 98.6 (49.42-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.258 0.220 , 0.256	Depositor DCC
R_{free} test set	4308 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	107.3	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 96.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33894	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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

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	c	0.26	0/4082	0.48	0/5502
1	e	0.26	0/4082	0.47	0/5502
2	C	0.27	0/5308	0.48	0/7156
2	E	0.26	0/5308	0.47	0/7156
3	D	0.25	0/3952	0.44	0/5328
3	F	0.25	0/4932	0.44	0/6650
4	d	0.25	0/3431	0.44	0/4630
4	f	0.25	0/3431	0.44	0/4630
All	All	0.26	0/34526	0.46	0/46554

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	482/496 (97%)	473 (98%)	9 (2%)	0	100	100
1	e	482/496 (97%)	474 (98%)	8 (2%)	0	100	100
2	C	637/665 (96%)	625 (98%)	12 (2%)	0	100	100
2	E	637/665 (96%)	627 (98%)	10 (2%)	0	100	100
3	D	477/631 (76%)	471 (99%)	6 (1%)	0	100	100
3	F	594/631 (94%)	584 (98%)	10 (2%)	0	100	100
4	d	406/448 (91%)	398 (98%)	8 (2%)	0	100	100
4	f	406/448 (91%)	399 (98%)	6 (2%)	1 (0%)	47	77
All	All	4121/4480 (92%)	4051 (98%)	69 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	f	201	ASP

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	c	457/469 (97%)	450 (98%)	7 (2%)	65	81
1	e	457/469 (97%)	454 (99%)	3 (1%)	84	90
2	C	587/608 (96%)	581 (99%)	6 (1%)	76	86
2	E	587/608 (96%)	583 (99%)	4 (1%)	84	90
3	D	445/590 (75%)	441 (99%)	4 (1%)	78	87
3	F	555/590 (94%)	549 (99%)	6 (1%)	73	85
4	d	375/409 (92%)	365 (97%)	10 (3%)	44	71
4	f	375/409 (92%)	375 (100%)	0	100	100
All	All	3838/4152 (92%)	3798 (99%)	40 (1%)	76	86

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	13	ASN
1	c	98	PHE
1	c	177	PHE
1	c	217	ASN
1	c	233	ASP
1	c	237	PHE
1	c	335	ASN
2	C	93	TYR
2	C	110	ARG
2	C	174	LEU
2	C	382	ASP
2	C	396	LEU
2	C	491	PHE
3	D	68	TYR
3	D	267	GLN
3	D	292	ASP
3	D	541	PHE
4	d	53	ASP
4	d	85	LYS
4	d	89	TYR
4	d	90	GLN
4	d	122	ASP
4	d	194	ASN
4	d	216	PHE
4	d	233	LYS
4	d	385	LYS
4	d	416	ASP
1	e	222	PHE
1	e	373	PHE
1	e	425	PHE
2	E	491	PHE
2	E	501	TRP
2	E	516	GLU
2	E	528	TYR
3	F	68	TYR
3	F	293	ASP
3	F	457	ARG
3	F	541	PHE
3	F	569	ASP
3	F	587	ARG

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

Mol	Chain	Res	Type
4	d	15	ASN
4	d	180	ASN
4	d	377	ASN
4	f	247	ASN
4	f	377	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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	c	484/496 (97%)	0.57	43 (8%) 9 10	57, 129, 227, 365	0
1	e	484/496 (97%)	0.56	56 (11%) 4 4	109, 173, 251, 319	0
2	C	640/665 (96%)	0.37	31 (4%) 30 28	49, 92, 202, 317	0
2	E	640/665 (96%)	0.51	51 (7%) 12 11	98, 151, 214, 279	0
3	D	481/631 (76%)	0.33	24 (4%) 28 27	54, 112, 194, 261	0
3	F	596/631 (94%)	0.80	87 (14%) 2 2	121, 175, 272, 329	0
4	d	410/448 (91%)	0.94	78 (19%) 1 1	71, 179, 259, 367	0
4	f	410/448 (91%)	0.83	63 (15%) 2 2	123, 196, 278, 427	0
All	All	4145/4480 (92%)	0.60	433 (10%) 6 6	49, 152, 250, 427	0

All (433) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	450	PHE	9.6
4	f	49	ASP	9.1
2	E	557	SER	8.7
3	F	429	VAL	8.5
3	F	491	ILE	7.9
4	d	112	ILE	7.8
3	F	453	LYS	7.4
2	C	241	THR	7.2
4	f	30	GLU	7.1
3	F	452	LEU	7.0
4	d	20	ILE	6.9
1	e	89	ASP	6.8
4	d	183	TYR	6.8
2	C	237	PHE	6.6
3	D	596	ASP	6.5
4	d	229	TYR	6.5

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Mol	Chain	Res	Type	RSRZ
4	d	234	LYS	6.2
1	c	214	ASP	6.0
4	d	117	PHE	6.0
3	F	415	VAL	6.0
4	d	160	LEU	5.9
2	C	244	TYR	5.8
1	e	88	LYS	5.7
1	c	216	ILE	5.7
2	C	242	ALA	5.7
2	C	238	ASP	5.5
3	F	567	LEU	5.5
3	F	447	PHE	5.4
1	e	90	ASP	5.3
4	d	36	ILE	5.3
4	d	163	ALA	5.2
1	e	87	GLU	5.0
3	F	571	ASP	5.0
4	d	156	PHE	5.0
1	e	94	GLU	4.9
2	C	245	GLU	4.9
4	f	370	ASP	4.9
2	C	248	ASN	4.9
4	d	89	TYR	4.9
3	F	409	PHE	4.9
3	F	394	HIS	4.9
3	F	426	ASN	4.8
4	f	163	ALA	4.8
4	d	240	ASN	4.8
1	e	364	VAL	4.8
4	d	241	ILE	4.8
4	f	147	LYS	4.8
1	c	236	PHE	4.7
3	D	324	ASN	4.7
2	E	598	TYR	4.6
4	d	233	LYS	4.6
3	F	451	THR	4.5
3	D	583	TYR	4.5
4	f	10	PHE	4.5
1	e	272	LEU	4.5
2	C	644	LEU	4.5
3	F	468	PHE	4.4
3	F	431	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
3	F	511	GLU	4.4
2	C	556	LYS	4.4
4	d	114	LEU	4.4
1	e	482	ASN	4.4
4	f	117	PHE	4.4
1	e	93	GLU	4.4
3	F	465	MET	4.4
4	d	159	LYS	4.4
2	E	485	PRO	4.3
1	e	85	LEU	4.3
4	f	169	SER	4.2
1	c	371	ASN	4.2
1	e	91	LYS	4.2
2	C	251	GLU	4.2
4	f	299	TRP	4.2
4	d	121	PHE	4.2
4	d	184	ASN	4.2
4	f	31	PHE	4.1
4	d	31	PHE	4.1
4	f	48	ASP	4.1
4	d	60	ILE	4.1
2	C	243	LEU	4.1
4	f	283	LEU	4.1
2	C	240	ASN	4.1
4	f	277	LYS	4.0
2	C	239	TYR	4.0
3	F	458	PHE	4.0
1	e	208	LEU	4.0
3	F	413	PHE	4.0
1	c	200	ILE	4.0
1	e	253	PHE	4.0
1	c	196	LEU	4.0
2	E	475	PHE	4.0
2	C	235	ARG	4.0
3	F	596	ASP	4.0
2	E	556	LYS	4.0
3	D	394	HIS	3.9
4	d	18	ASN	3.9
4	f	372	ASP	3.9
1	c	376	ILE	3.9
4	d	125	LEU	3.9
4	f	148	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	c	197	GLN	3.9
2	C	249	LEU	3.9
1	c	469	GLU	3.9
3	F	66	ILE	3.8
4	d	41	ILE	3.8
1	e	47	ILE	3.8
3	F	428	THR	3.8
3	D	593	LEU	3.8
2	C	233	SER	3.8
3	D	230	PHE	3.7
3	F	474	LYS	3.7
4	d	174	LEU	3.6
4	d	21	THR	3.6
2	C	252	MET	3.6
4	f	160	LEU	3.6
1	c	224	ILE	3.6
3	F	430	ILE	3.6
2	E	279	LEU	3.6
2	E	452	VAL	3.6
1	e	237	PHE	3.6
3	F	463	SER	3.6
4	d	149	PHE	3.5
2	C	205	ILE	3.5
4	d	67	ILE	3.5
4	f	204	ASP	3.5
4	f	59	TRP	3.5
3	F	446	VAL	3.5
3	F	502	PHE	3.5
2	E	484	ILE	3.5
4	f	240	ASN	3.4
2	C	628	GLU	3.4
1	e	92	LYS	3.4
2	E	566	LEU	3.4
3	F	512	LEU	3.4
3	F	400	SER	3.4
1	c	253	PHE	3.4
3	F	461	ILE	3.4
4	d	42	PHE	3.4
1	e	246	ILE	3.4
3	F	490	GLU	3.4
3	F	478	ASP	3.4
4	d	57	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
4	d	113	GLY	3.3
3	D	395	LEU	3.3
4	d	155	VAL	3.3
4	d	55	ASP	3.3
2	C	246	LEU	3.3
3	F	424	VAL	3.3
1	c	428	ASN	3.3
4	d	19	LEU	3.3
4	d	109	ASP	3.3
3	F	405	TRP	3.2
2	C	348	PHE	3.2
1	c	369	ASN	3.2
1	c	367	ASN	3.2
3	F	306	VAL	3.2
3	F	436	PHE	3.2
4	f	132	LYS	3.2
3	F	208	GLY	3.2
2	E	567	TYR	3.2
1	e	203	LEU	3.2
4	f	241	ILE	3.2
1	c	246	ILE	3.1
4	f	41	ILE	3.1
1	c	218	ASP	3.1
2	E	479	ILE	3.1
2	E	205	ILE	3.1
4	d	235	GLY	3.1
4	f	62	ILE	3.1
2	E	372	ASN	3.1
1	e	224	ILE	3.1
4	d	158	HIS	3.1
3	F	467	LEU	3.1
4	f	114	LEU	3.1
4	f	131	LYS	3.1
2	E	206	LEU	3.1
4	f	68	ILE	3.1
1	c	377	LYS	3.1
4	f	125	LEU	3.1
1	c	431	ASN	3.1
2	C	236	ARG	3.1
1	e	276	PHE	3.1
4	d	162	PRO	3.0
4	f	284	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	454	SER	3.0
3	F	462	SER	3.0
4	f	29	HIS	3.0
4	f	13	ILE	3.0
2	E	262	ASP	3.0
1	e	200	ILE	3.0
4	d	72	LEU	3.0
1	e	72	ILE	3.0
4	f	162	PRO	3.0
2	E	270	ILE	3.0
1	e	41	LEU	3.0
1	c	68	LYS	2.9
4	d	59	TRP	2.9
2	C	627	VAL	2.9
2	E	306	LEU	2.9
2	E	317	VAL	2.9
1	e	151	GLU	2.9
1	e	376	ILE	2.9
2	E	644	LEU	2.9
4	f	124	LEU	2.9
4	d	167	THR	2.9
2	E	476	LEU	2.9
4	d	237	LEU	2.9
4	f	278	PHE	2.9
3	F	456	ASN	2.8
2	C	203	ASN	2.8
3	D	567	LEU	2.8
3	D	361	TYR	2.8
4	f	203	ILE	2.8
4	f	248	PHE	2.8
2	E	390	GLU	2.8
3	D	59	VAL	2.8
4	d	79	CYS	2.8
3	F	460	SER	2.8
3	F	53	GLU	2.8
2	E	595	LEU	2.8
4	f	140	PHE	2.8
1	c	163	MET	2.8
2	C	545	THR	2.8
1	c	156	ILE	2.8
1	c	208	LEU	2.8
4	f	28	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
4	d	138	TYR	2.8
4	f	380	PRO	2.8
4	d	76	ILE	2.8
4	d	148	ILE	2.8
3	F	11	LEU	2.8
1	c	90	ASP	2.8
2	E	176	ASP	2.8
3	D	57	LEU	2.7
4	d	35	GLY	2.7
1	e	30	ILE	2.7
4	f	57	ILE	2.7
1	e	119	PRO	2.7
4	f	72	LEU	2.7
4	d	144	ASN	2.7
1	e	483	LEU	2.7
3	F	592	ASN	2.7
3	F	469	LEU	2.7
4	f	280	LEU	2.7
1	c	373	PHE	2.7
2	E	371	GLY	2.7
2	E	495	ILE	2.7
1	e	222	PHE	2.7
4	d	47	GLU	2.7
1	e	221	ILE	2.7
1	c	372	LYS	2.7
4	f	173	VAL	2.7
3	F	402	LYS	2.6
1	c	213	GLU	2.6
1	c	203	LEU	2.6
4	d	166	LEU	2.6
4	f	365	SER	2.6
4	d	164	THR	2.6
2	E	231	ILE	2.6
2	E	424	ILE	2.6
4	d	157	SER	2.6
3	F	420	ILE	2.6
4	d	145	HIS	2.6
4	d	173	VAL	2.6
1	c	27	ASN	2.6
4	d	140	PHE	2.6
4	d	58	GLY	2.6
4	d	137	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
4	f	14	TYR	2.6
4	d	34	ASP	2.6
4	f	371	TYR	2.6
1	c	470	ASN	2.6
1	e	202	VAL	2.6
1	c	91	LYS	2.6
3	F	10	ILE	2.6
3	F	503	ALA	2.6
4	d	116	LYS	2.6
4	f	374	ASP	2.6
3	F	477	LEU	2.6
1	c	375	LYS	2.5
1	e	86	ILE	2.5
2	E	175	GLU	2.5
2	E	480	ILE	2.5
2	E	325	TYR	2.5
3	F	412	ASN	2.5
4	d	141	LEU	2.5
4	d	53	ASP	2.5
3	F	212	ASN	2.5
3	F	398	THR	2.5
4	d	78	LYS	2.5
3	F	457	ARG	2.5
1	e	169	ASP	2.5
4	f	275	LEU	2.5
4	f	20	ILE	2.5
2	E	427	PHE	2.5
3	F	286	THR	2.5
2	E	350	MET	2.5
2	E	107	LEU	2.5
1	e	205	LYS	2.5
3	D	55	ILE	2.5
3	D	320	TYR	2.5
4	f	207	LEU	2.5
4	f	382	PHE	2.5
3	F	473	LEU	2.5
3	F	466	ARG	2.5
1	e	204	MET	2.4
3	F	389	LEU	2.4
3	F	392	ALA	2.4
1	c	374	GLU	2.4
1	e	480	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	488	GLN	2.4
1	e	211	LEU	2.4
4	d	50	ASP	2.4
2	E	95	LEU	2.4
4	f	16	GLU	2.4
1	e	54	VAL	2.4
2	E	545	THR	2.4
4	d	73	PHE	2.4
4	d	71	ILE	2.4
4	f	67	ILE	2.4
1	c	202	VAL	2.4
1	e	60	VAL	2.4
4	d	208	LEU	2.4
2	E	460	MET	2.4
2	E	348	PHE	2.4
1	e	219	ASN	2.4
2	E	582	LEU	2.4
2	E	624	LEU	2.4
2	E	487	CYS	2.4
3	D	74	LEU	2.4
2	C	204	ASP	2.3
4	d	30	GLU	2.3
1	c	364	VAL	2.3
4	d	54	ILE	2.3
4	d	172	LYS	2.3
4	d	236	PHE	2.3
3	F	493	LEU	2.3
4	f	183	TYR	2.3
3	D	343	LYS	2.3
2	E	609	ILE	2.3
3	D	229	LEU	2.3
4	f	314	MET	2.3
1	c	129	TYR	2.3
1	e	342	ARG	2.3
2	C	250	ASN	2.3
3	D	7	LEU	2.3
3	D	576	LYS	2.3
3	F	464	PRO	2.3
1	e	58	ASN	2.3
1	c	229	SER	2.3
2	E	448	PHE	2.3
2	C	207	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	f	144	ASN	2.2
2	C	629	SER	2.2
1	c	234	LYS	2.2
4	d	80	ILE	2.2
4	f	21	THR	2.2
2	C	325	TYR	2.2
3	D	551	ASN	2.2
4	f	234	LYS	2.2
3	F	36	VAL	2.2
2	E	244	TYR	2.2
4	f	296	LEU	2.2
1	c	241	ASN	2.2
3	F	60	ASP	2.2
1	e	34	LEU	2.2
4	f	424	LEU	2.2
4	d	23	ALA	2.2
1	e	236	PHE	2.2
3	F	133	PHE	2.2
1	c	330	LEU	2.2
2	E	329	LYS	2.2
4	d	4	LYS	2.2
1	e	162	THR	2.2
3	F	422	PRO	2.2
3	D	88	MET	2.2
3	F	441	GLU	2.2
3	D	321	LEU	2.2
3	F	594	LYS	2.2
1	e	5	PHE	2.2
2	E	456	GLU	2.2
3	F	440	GLU	2.2
1	c	249	LEU	2.1
1	e	124	LEU	2.1
3	F	361	TYR	2.1
3	F	506	ILE	2.1
4	f	233	LYS	2.1
1	e	373	PHE	2.1
4	f	164	THR	2.1
3	F	88	MET	2.1
4	d	165	LEU	2.1
2	E	259	PHE	2.1
2	E	442	VAL	2.1
3	D	27	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	37	LYS	2.1
3	F	427	GLY	2.1
3	F	287	LYS	2.1
3	F	489	PHE	2.1
3	F	209	ALA	2.1
3	F	448	ASP	2.1
1	e	257	ILE	2.1
2	C	247	LYS	2.1
3	F	197	THR	2.1
3	F	179	ILE	2.1
3	F	508	ASP	2.1
3	F	416	ASN	2.1
1	c	188	GLU	2.1
1	e	232	VAL	2.1
1	e	230	LEU	2.1
1	e	427	SER	2.1
3	F	72	ILE	2.1
2	E	177	ALA	2.1
4	d	56	THR	2.1
1	e	82	MET	2.1
4	d	374	ASP	2.1
4	d	154	PRO	2.0
4	f	369	GLY	2.0
1	c	268	TRP	2.0
1	e	223	MET	2.0
3	F	513	SER	2.0
4	d	248	PHE	2.0
1	e	61	TYR	2.0
4	f	229	TYR	2.0
1	c	217	ASN	2.0
3	D	302	LEU	2.0
3	F	150	LEU	2.0
3	D	359	LYS	2.0
2	E	251	GLU	2.0
1	e	259	ILE	2.0
2	E	486	ILE	2.0
3	F	496	LEU	2.0
4	d	150	ILE	2.0
3	F	305	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

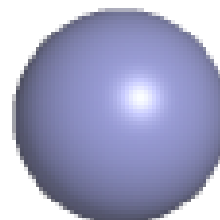
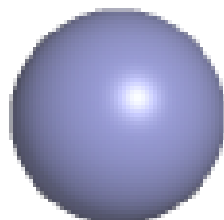
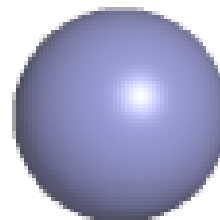
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

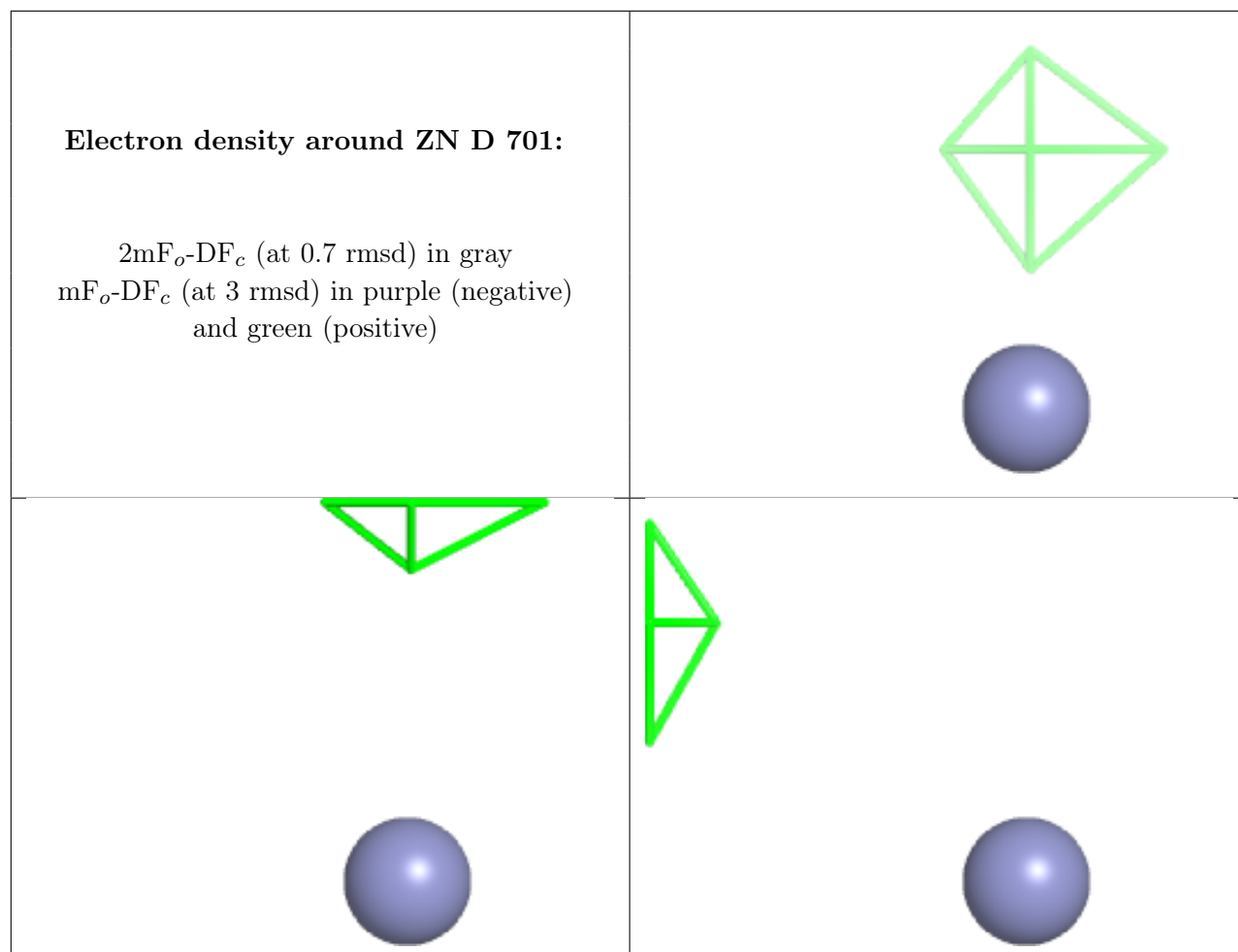
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	F	701	1/1	0.71	0.15	188,188,188,188	0
5	ZN	D	701	1/1	0.91	0.17	135,135,135,135	0

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 ZN F 701:

$2mF_o-DF_c$ (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.