



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 12, 2022 – 02:02 PM EST

PDB ID : 7S1T  
Title : Structure of the human POT1-TPP1 complex  
Authors : Aramburu, T.; Skordalakes, E.  
Deposited on : 2021-09-02  
Resolution : 2.90 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](mailto: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.

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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	:	2.25
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)	:	2.25

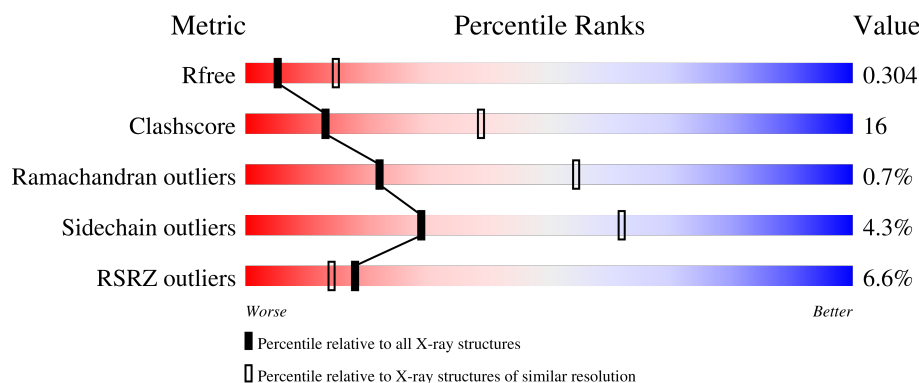
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	313	<div> <div>4%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	D	313	<div> <div>7%</div> <div>63%</div> <div>32%</div> <div>..</div> </div>
1	G	313	<div> <div>6%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>
1	J	313	<div> <div>10%</div> <div>60%</div> <div>36%</div> <div>..</div> </div>
2	B	93	<div> <div>2%</div> <div>52%</div> <div>27%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	93	
2	H	93	
2	K	93	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11776 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 Protection of telomeres protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2393	1528	398	451	16			
1	D	302	Total	C	N	O	S	0	0	0
			2393	1528	398	451	16			
1	G	302	Total	C	N	O	S	0	0	0
			2393	1528	398	451	16			
1	J	302	Total	C	N	O	S	0	0	0
			2393	1528	398	451	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	SER	-	expression tag	UNP Q9NUX5
A	323	ASN	-	expression tag	UNP Q9NUX5
A	324	ILE	-	expression tag	UNP Q9NUX5
D	322	SER	-	expression tag	UNP Q9NUX5
D	323	ASN	-	expression tag	UNP Q9NUX5
D	324	ILE	-	expression tag	UNP Q9NUX5
G	322	SER	-	expression tag	UNP Q9NUX5
G	323	ASN	-	expression tag	UNP Q9NUX5
G	324	ILE	-	expression tag	UNP Q9NUX5
J	322	SER	-	expression tag	UNP Q9NUX5
J	323	ASN	-	expression tag	UNP Q9NUX5
J	324	ILE	-	expression tag	UNP Q9NUX5

- Molecule 2 is a protein called Adrenocortical dysplasia protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	S	0	0	0
			550	338	91	114	7			
2	E	74	Total	C	N	O	S	0	0	0
			550	338	91	114	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	74	Total	C	N	O	S	0	0	0
			550	338	91	114	7			
2	K	74	Total	C	N	O	S	0	0	0
			550	338	91	114	7			

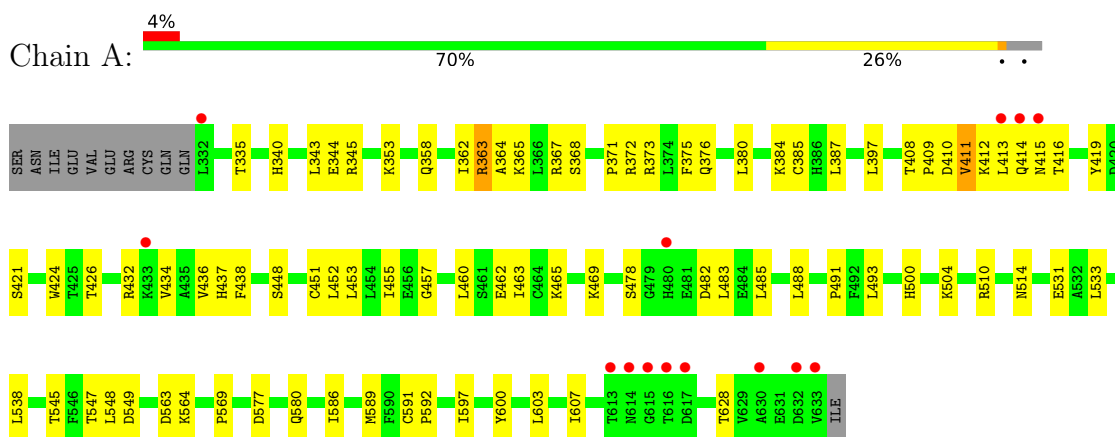
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		

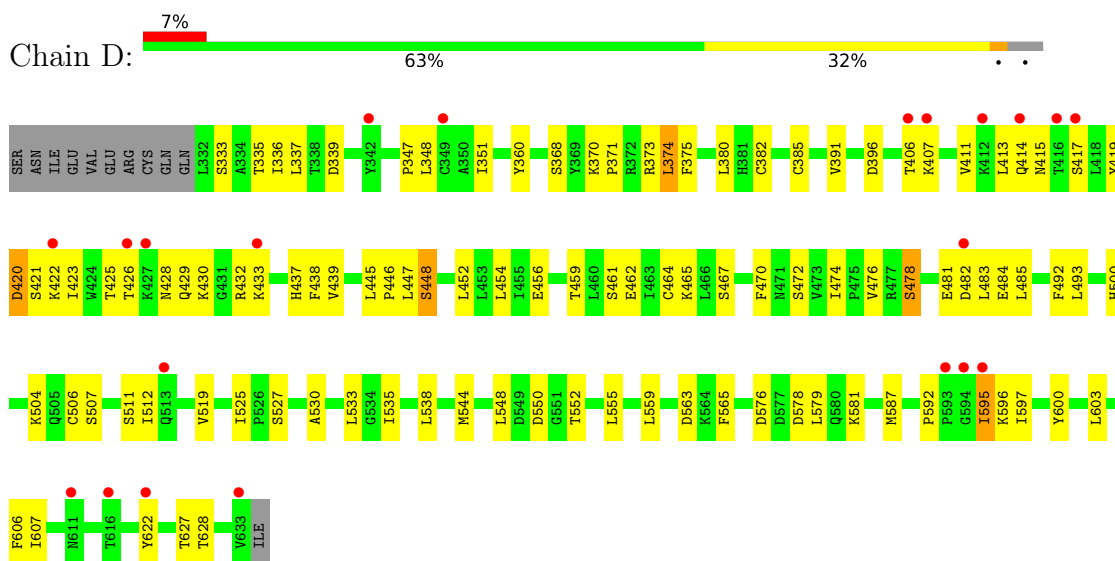
### 3 Residue-property plots [i](#)

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: Protection of telomeres protein 1

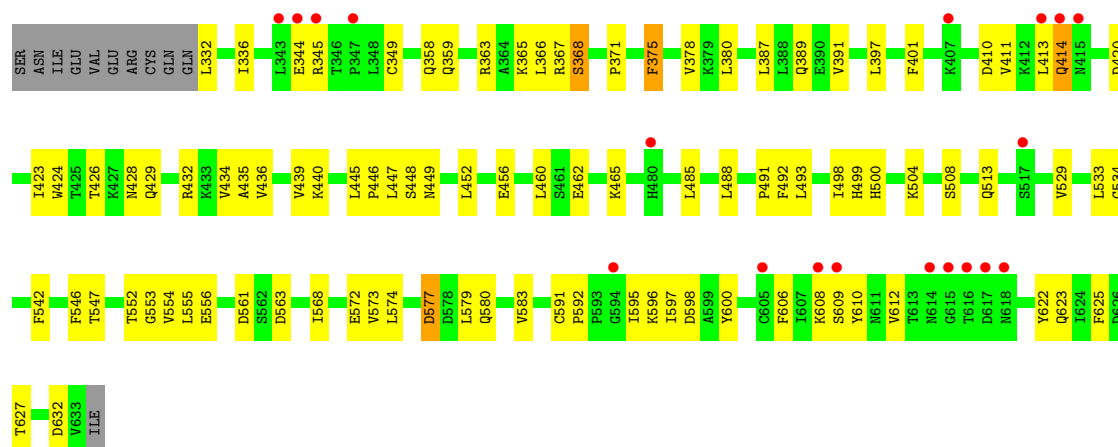


#### • Molecule 1: Protection of telomeres protein 1

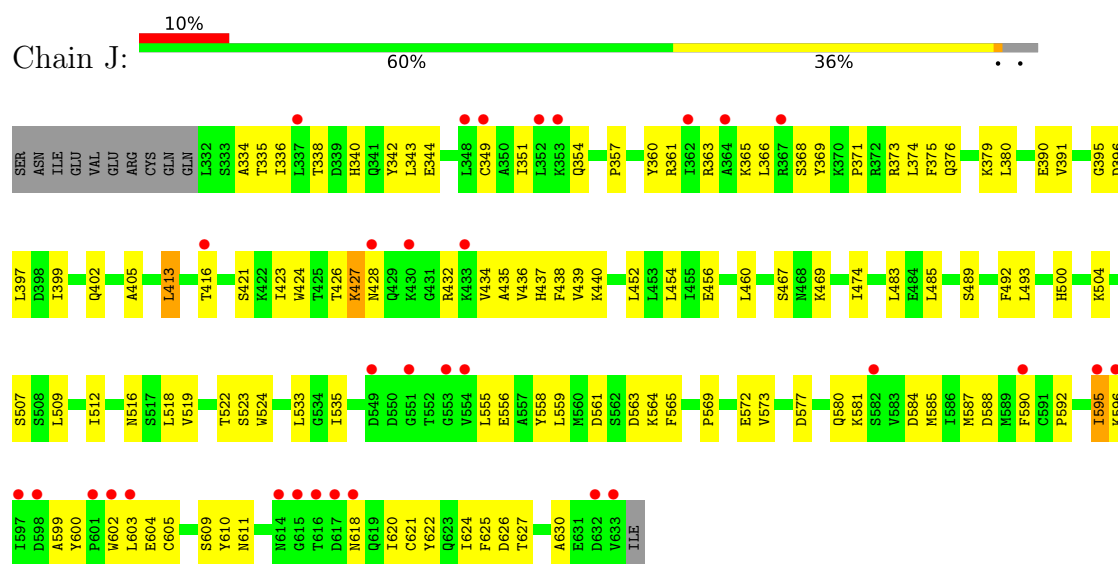


#### • Molecule 1: Protection of telomeres protein 1

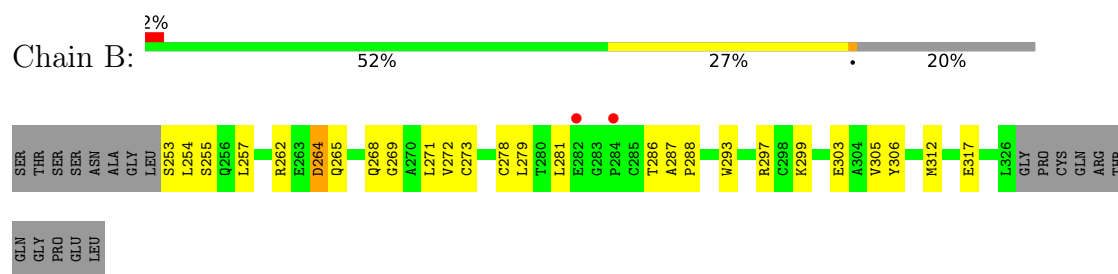




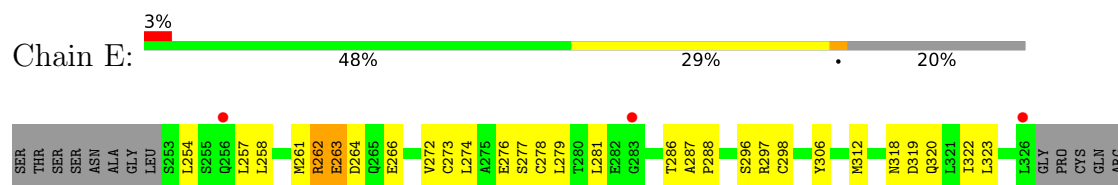
• Molecule 1: Protection of telomeres protein 1



• Molecule 2: Adrenocortical dysplasia protein homolog



• Molecule 2: Adrenocortical dysplasia protein homolog



THR  
GLN  
GLY  
PRO  
GLU  
LEU

● Molecule 2: Adrenocortical dysplasia protein homolog



SER THR SER SER SER ASN ALA GLY LEU S253 L254 L257 L258 D259 E260 M261 R262 E263 D264 Q265 E266 H267 Q268 G269 A270 L271 V272 C273 E276 S277 C278 L279 T280 L281 E282 G283 P284 C285 T291 H292 W293 R297 Y306 P309 S310 S311 M312 E317 N318 L321 L326 GLY

PRO  
CYS  
GLN  
ARG  
THR  
GLN  
GLY  
PRO  
GLU  
LEU

● Molecule 2: Adrenocortical dysplasia protein homolog



SER THR SER SER SER ASN ALA GLY LEU S253 Q256 L257 L258 D259 E260 M261 R262 E263 D264 L271 L274 L281 P284 C285 R297 C298 T301 V305 Y306 T307 V308 L313 I322 L326 GLY PRO CYS GLN ARG THR GLN GLY PRO GLU LEU



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.88Å 70.98Å 103.79Å 76.76° 84.61° 70.55°	Depositor
Resolution (Å)	36.44 – 2.90 36.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.7 (36.44-2.90) 89.8 (36.44-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.250 , 0.307 0.248 , 0.304	Depositor DCC
$R_{free}$ test set	1848 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.28	0/2443	0.51	0/3314
1	D	0.28	0/2443	0.51	0/3314
1	G	0.31	0/2443	0.50	0/3314
1	J	0.30	0/2443	0.51	0/3314
2	B	0.49	0/558	0.59	0/760
2	E	0.31	0/558	0.58	0/760
2	H	0.45	0/558	0.59	0/760
2	K	0.25	0/558	0.44	0/760
All	All	0.31	0/12004	0.52	0/16296

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	2393	0	2404	87	0
1	D	2393	0	2404	90	0
1	G	2393	0	2404	80	0
1	J	2393	0	2404	87	0
2	B	550	0	537	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	550	0	537	30	0
2	H	550	0	537	28	0
2	K	550	0	537	17	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
All	All	11776	0	11764	383	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 16.

The worst 5 of 383 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:408:THR:CG2	1:A:409:PRO:HD2	1.61	1.31
1:G:359:GLN:OE1	1:G:608:LYS:HE2	1.48	1.09
1:J:375:PHE:HD1	2:K:297:ARG:HG2	1.17	1.05
1:J:375:PHE:CD1	2:K:297:ARG:HG2	1.91	1.05
1:A:408:THR:HG23	1:A:409:PRO:HD2	1.08	1.04

There are no symmetry-related clashes.

## 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	A	300/313 (96%)	276 (92%)	22 (7%)	2 (1%)	22 54
1	D	300/313 (96%)	274 (91%)	21 (7%)	5 (2%)	9 31
1	G	300/313 (96%)	271 (90%)	28 (9%)	1 (0%)	41 71
1	J	300/313 (96%)	262 (87%)	37 (12%)	1 (0%)	41 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	72/93 (77%)	68 (94%)	4 (6%)	0	100	100
2	E	72/93 (77%)	67 (93%)	5 (7%)	0	100	100
2	H	72/93 (77%)	60 (83%)	11 (15%)	1 (1%)	11	36
2	K	72/93 (77%)	67 (93%)	5 (7%)	0	100	100
All	All	1488/1624 (92%)	1345 (90%)	133 (9%)	10 (1%)	22	54

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	448	SER
1	A	414	GLN
2	H	263	GLU
1	A	411	VAL
1	D	339	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	A	275/286 (96%)	270 (98%)	5 (2%)	59	85
1	D	275/286 (96%)	265 (96%)	10 (4%)	35	69
1	G	275/286 (96%)	266 (97%)	9 (3%)	38	72
1	J	275/286 (96%)	264 (96%)	11 (4%)	31	65
2	B	64/79 (81%)	60 (94%)	4 (6%)	18	46
2	E	64/79 (81%)	58 (91%)	6 (9%)	8	26
2	H	64/79 (81%)	56 (88%)	8 (12%)	4	14
2	K	64/79 (81%)	59 (92%)	5 (8%)	12	34
All	All	1356/1460 (93%)	1298 (96%)	58 (4%)	29	62

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	467	SER
2	K	260	GLU
2	B	264	ASP
2	K	259	ASP
2	H	268	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	539	GLN
1	J	611	ASN
2	B	320	GLN
2	B	268	GLN
1	D	358	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	302/313 (96%)	0.18	14 (4%) 32 29	40, 64, 112, 164	0
1	D	302/313 (96%)	0.36	21 (6%) 16 12	41, 68, 115, 161	0
1	G	302/313 (96%)	0.24	19 (6%) 20 16	39, 72, 105, 161	0
1	J	302/313 (96%)	0.63	32 (10%) 6 4	39, 77, 134, 158	0
2	B	74/93 (79%)	0.32	2 (2%) 54 50	48, 78, 101, 115	0
2	E	74/93 (79%)	0.26	3 (4%) 37 32	43, 79, 118, 125	0
2	H	74/93 (79%)	0.36	6 (8%) 12 9	51, 82, 107, 113	0
2	K	74/93 (79%)	0.26	2 (2%) 54 50	54, 82, 103, 171	0
All	All	1504/1624 (92%)	0.34	99 (6%) 18 14	39, 71, 121, 171	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	LEU	7.4
1	A	632	ASP	5.6
2	K	256	GLN	5.6
1	J	615	GLY	5.5
1	A	415	ASN	5.1

### 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

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, 95<sup>th</sup> 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.

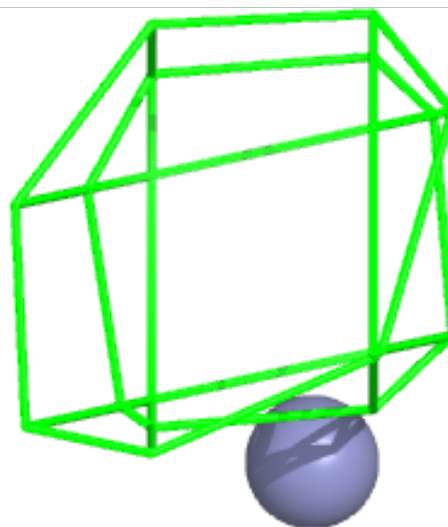
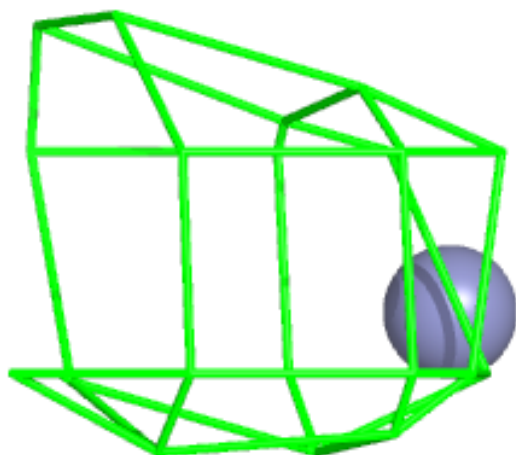
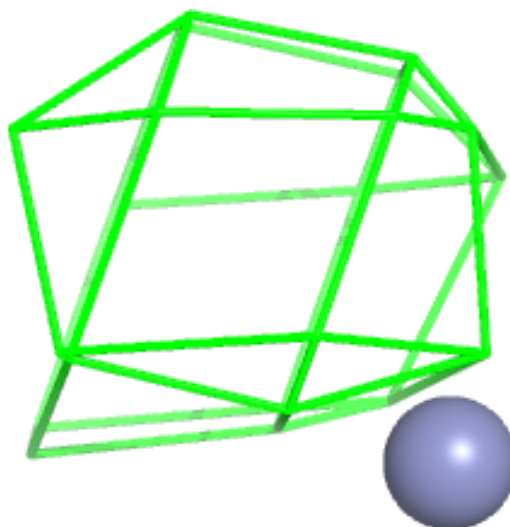
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	G	701	1/1	0.93	0.19	72,72,72,72	0
3	ZN	A	701	1/1	0.94	0.13	61,61,61,61	0
3	ZN	D	701	1/1	0.95	0.12	69,69,69,69	0
3	ZN	J	701	1/1	0.96	0.15	69,69,69,69	0

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.



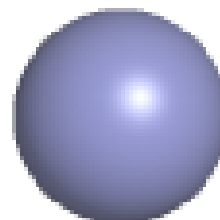
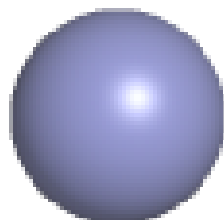
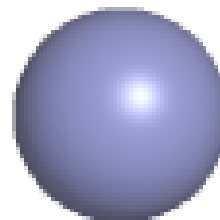
**Electron density around ZN G 701:**

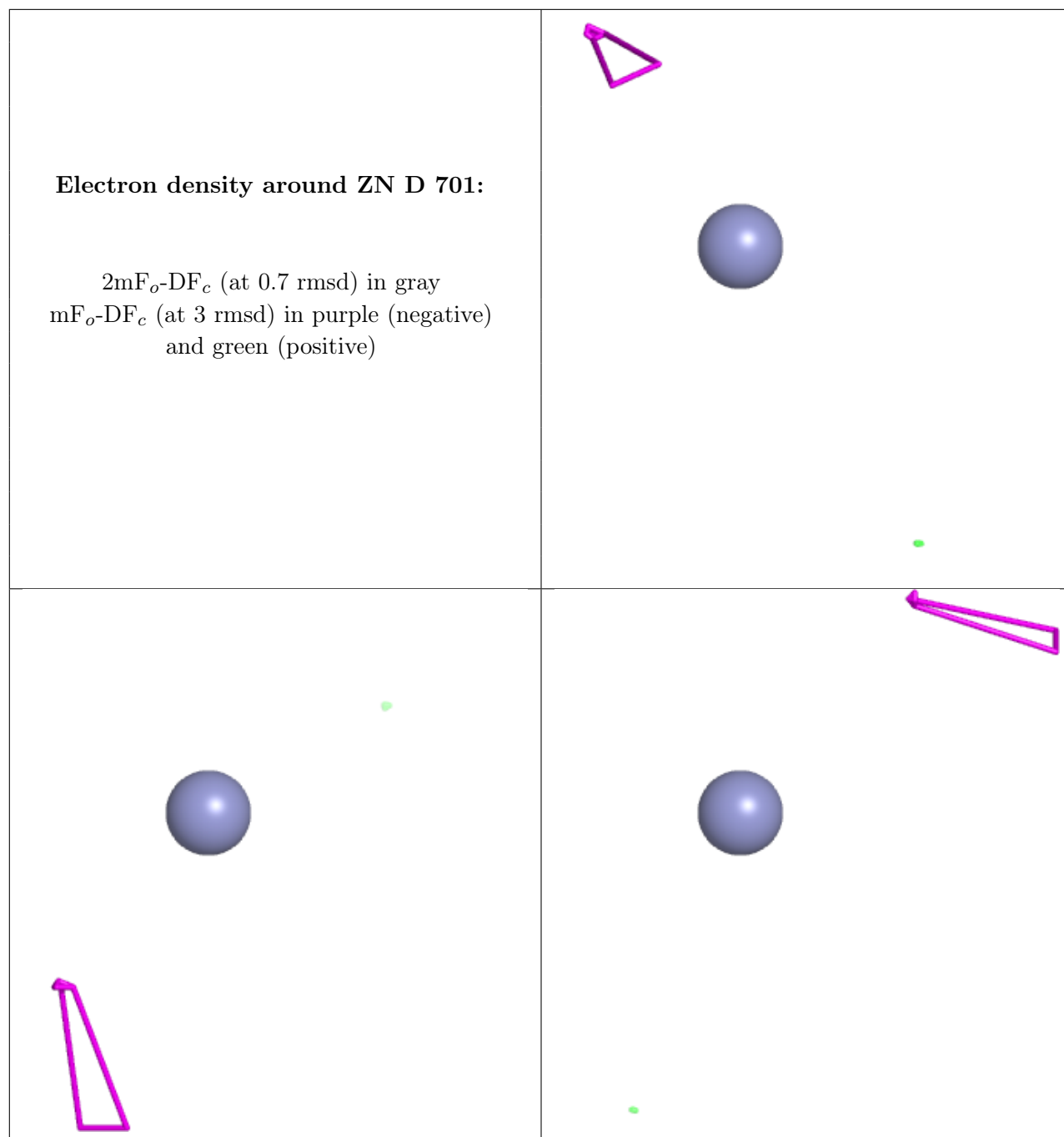
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

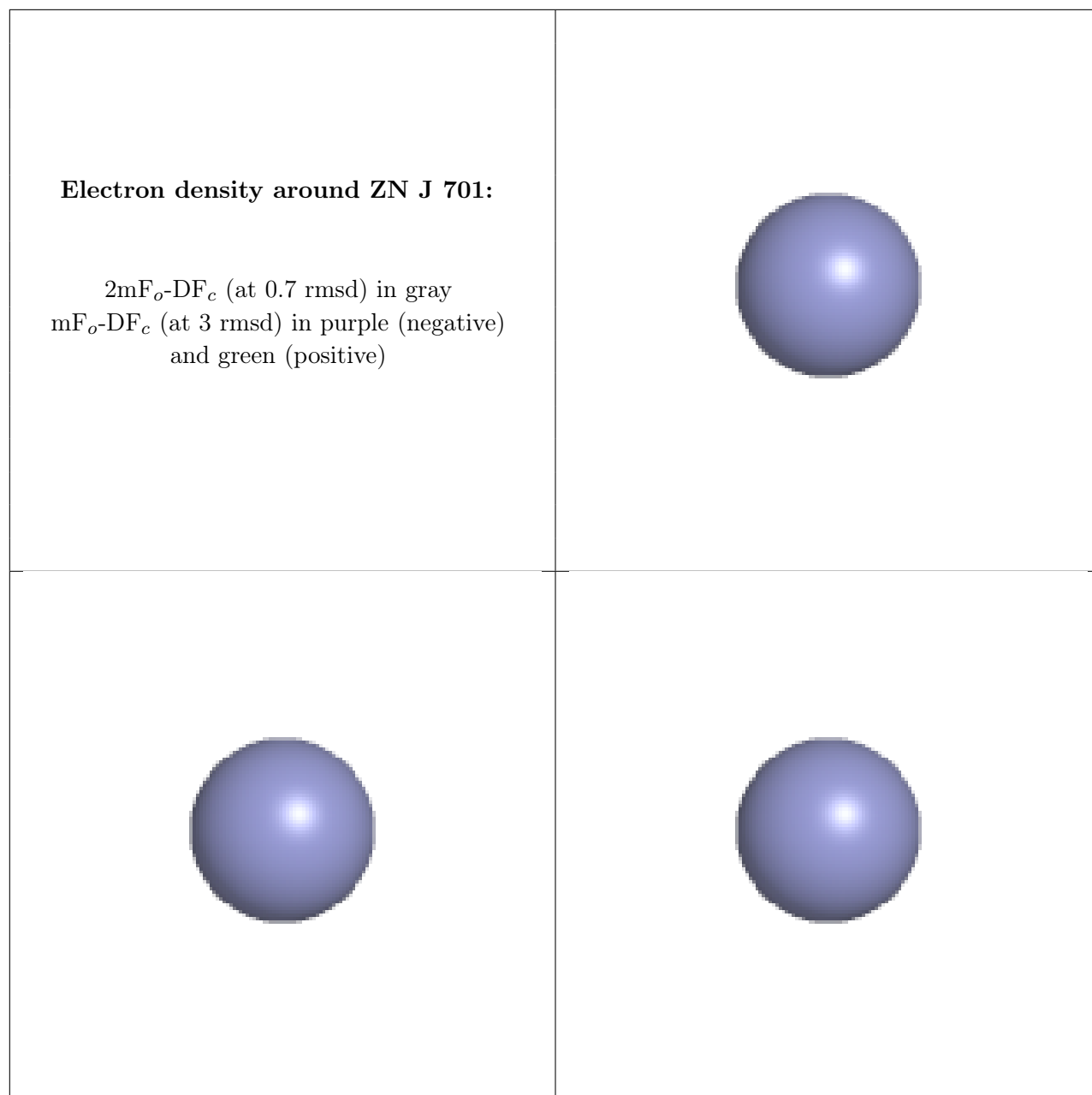


**Electron density around ZN A 701:**

$2mF_o-DF_c$  (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.