Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 12:52 AM EST

PDB ID	:	4II1
Title	:	Crystal structure of the zinc finger of ZGPAT
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Deposited on	:	2012-12-19
Resolution	:	2.65 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:

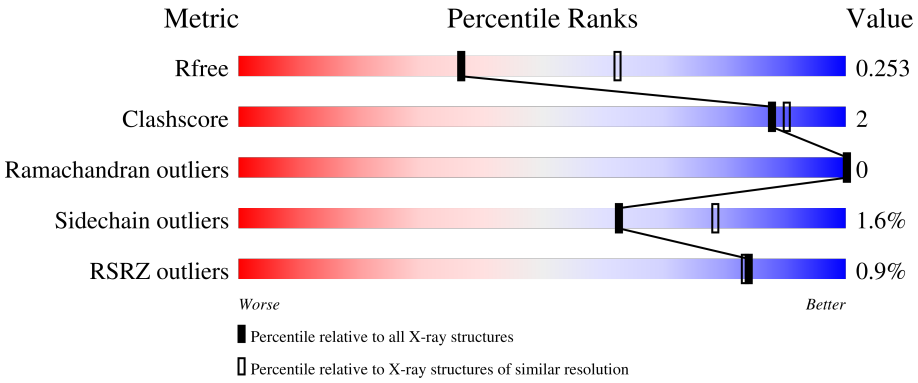
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	167	77% 5% 19%
1	B	167	% 78% 5% 17%
1	C	167	% 74% • 22%
1	D	167	2% 77% 6% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	A	902	-	-	-	X
3	UNX	D	903	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3977 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 Zinc finger CCCH-type with G patch domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1010	644	171	190	5			
1	B	139	Total	C	N	O	S	0	0	0
			1034	659	170	200	5			
1	C	130	Total	C	N	O	S	0	0	0
			913	587	154	167	5			
1	D	138	Total	C	N	O	S	0	1	0
			997	642	166	184	5			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	MET	-	expression tag	UNP Q8N5A5
A	103	HIS	-	expression tag	UNP Q8N5A5
A	104	HIS	-	expression tag	UNP Q8N5A5
A	105	HIS	-	expression tag	UNP Q8N5A5
A	106	HIS	-	expression tag	UNP Q8N5A5
A	107	HIS	-	expression tag	UNP Q8N5A5
A	108	HIS	-	expression tag	UNP Q8N5A5
A	109	SER	-	expression tag	UNP Q8N5A5
A	110	SER	-	expression tag	UNP Q8N5A5
A	111	GLY	-	expression tag	UNP Q8N5A5
A	112	ARG	-	expression tag	UNP Q8N5A5
A	114	ASN	-	expression tag	UNP Q8N5A5
A	115	LEU	-	expression tag	UNP Q8N5A5
A	116	TYR	-	expression tag	UNP Q8N5A5
A	117	PHE	-	expression tag	UNP Q8N5A5
A	118	GLN	-	expression tag	UNP Q8N5A5
A	119	GLY	-	expression tag	UNP Q8N5A5
B	102	MET	-	expression tag	UNP Q8N5A5
B	103	HIS	-	expression tag	UNP Q8N5A5
B	104	HIS	-	expression tag	UNP Q8N5A5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	105	HIS	-	expression tag	UNP Q8N5A5
B	106	HIS	-	expression tag	UNP Q8N5A5
B	107	HIS	-	expression tag	UNP Q8N5A5
B	108	HIS	-	expression tag	UNP Q8N5A5
B	109	SER	-	expression tag	UNP Q8N5A5
B	110	SER	-	expression tag	UNP Q8N5A5
B	111	GLY	-	expression tag	UNP Q8N5A5
B	112	ARG	-	expression tag	UNP Q8N5A5
B	114	ASN	-	expression tag	UNP Q8N5A5
B	115	LEU	-	expression tag	UNP Q8N5A5
B	116	TYR	-	expression tag	UNP Q8N5A5
B	117	PHE	-	expression tag	UNP Q8N5A5
B	118	GLN	-	expression tag	UNP Q8N5A5
B	119	GLY	-	expression tag	UNP Q8N5A5
C	102	MET	-	expression tag	UNP Q8N5A5
C	103	HIS	-	expression tag	UNP Q8N5A5
C	104	HIS	-	expression tag	UNP Q8N5A5
C	105	HIS	-	expression tag	UNP Q8N5A5
C	106	HIS	-	expression tag	UNP Q8N5A5
C	107	HIS	-	expression tag	UNP Q8N5A5
C	108	HIS	-	expression tag	UNP Q8N5A5
C	109	SER	-	expression tag	UNP Q8N5A5
C	110	SER	-	expression tag	UNP Q8N5A5
C	111	GLY	-	expression tag	UNP Q8N5A5
C	112	ARG	-	expression tag	UNP Q8N5A5
C	114	ASN	-	expression tag	UNP Q8N5A5
C	115	LEU	-	expression tag	UNP Q8N5A5
C	116	TYR	-	expression tag	UNP Q8N5A5
C	117	PHE	-	expression tag	UNP Q8N5A5
C	118	GLN	-	expression tag	UNP Q8N5A5
C	119	GLY	-	expression tag	UNP Q8N5A5
D	102	MET	-	expression tag	UNP Q8N5A5
D	103	HIS	-	expression tag	UNP Q8N5A5
D	104	HIS	-	expression tag	UNP Q8N5A5
D	105	HIS	-	expression tag	UNP Q8N5A5
D	106	HIS	-	expression tag	UNP Q8N5A5
D	107	HIS	-	expression tag	UNP Q8N5A5
D	108	HIS	-	expression tag	UNP Q8N5A5
D	109	SER	-	expression tag	UNP Q8N5A5
D	110	SER	-	expression tag	UNP Q8N5A5
D	111	GLY	-	expression tag	UNP Q8N5A5
D	112	ARG	-	expression tag	UNP Q8N5A5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	114	ASN	-	expression tag	UNP Q8N5A5
D	115	LEU	-	expression tag	UNP Q8N5A5
D	116	TYR	-	expression tag	UNP Q8N5A5
D	117	PHE	-	expression tag	UNP Q8N5A5
D	118	GLN	-	expression tag	UNP Q8N5A5
D	119	GLY	-	expression tag	UNP Q8N5A5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

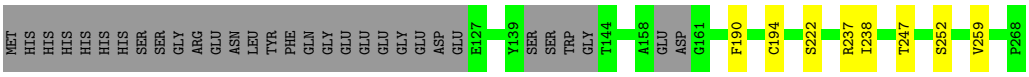
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total X 5 5	0	0
3	B	4	Total X 4 4	0	0
3	C	3	Total X 3 3	0	0
3	D	7	Total X 7 7	0	0

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.

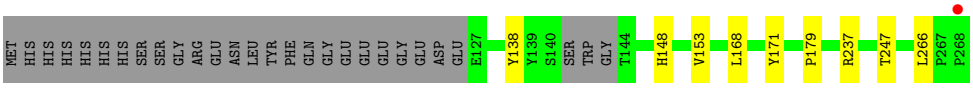
• Molecule 1: Zinc finger CCCH-type with G patch domain-containing protein

Chain A:



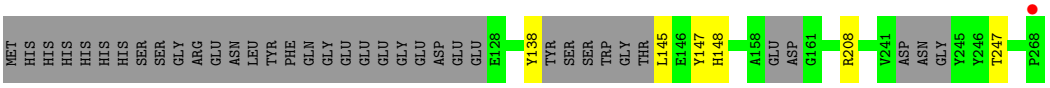
• Molecule 1: Zinc finger CCCH-type with G patch domain-containing protein

Chain B:



• Molecule 1: Zinc finger CCCH-type with G patch domain-containing protein

Chain C:



• Molecule 1: Zinc finger CCCH-type with G patch domain-containing protein

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.17Å 87.07Å 76.57Å 90.00° 95.65° 90.00°	Depositor
Resolution (Å)	37.80 – 2.65 34.11 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.80-2.65) 98.8 (34.11-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.65Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.208 , 0.242 0.227 , 0.253	Depositor DCC
R_{free} test set	985 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3977	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, UNX

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	0.46	0/1034	0.63	0/1407
1	B	0.48	0/1060	0.61	0/1444
1	C	0.44	0/935	0.61	0/1278
1	D	0.48	0/1027	0.62	0/1404
All	All	0.46	0/4056	0.62	0/5533

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

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	1010	0	932	3	0
1	B	1034	0	943	4	0
1	C	913	0	793	5	0
1	D	997	0	885	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	7	0	0	0	0
All	All	3977	0	3553	15	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 2.

All (15) 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:C:208:ARG:NH1	1:D:229:GLN:O	2.23	0.70
1:B:153:VAL:HG11	1:B:168:LEU:HD12	1.77	0.66
1:B:168:LEU:HD13	1:B:179:PRO:HB3	1.83	0.59
1:C:145:LEU:HD23	1:D:228:HIS:HE1	1.71	0.56
1:A:190:PHE:HB2	1:A:194:CYS:HB2	1.88	0.54
1:B:171:TYR:CG	1:B:266:LEU:HD11	2.43	0.53
1:C:138:TYR:HB3	1:C:148:HIS:HD2	1.75	0.52
1:C:147:TYR:CE2	1:D:230:ASP:HA	2.45	0.52
1:A:222:SER:HB2	1:A:238:ILE:HD12	1.93	0.51
1:D:247:THR:HG22	1:D:259:VAL:HG22	1.94	0.49
1:D:168:LEU:HD13	1:D:179:PRO:HB3	1.96	0.47
1:A:247:THR:HG22	1:A:259:VAL:HG22	1.95	0.47
1:C:208:ARG:HD2	1:D:230:ASP:C	2.34	0.47
1:B:138:TYR:CD1	1:B:148:HIS:HB2	2.52	0.44
1:D:138:TYR:CE2	1:D:148:HIS:HB2	2.56	0.41

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	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
1	B	135/167 (81%)	132 (98%)	3 (2%)	0	100	100
1	C	122/167 (73%)	120 (98%)	2 (2%)	0	100	100
1	D	135/167 (81%)	132 (98%)	3 (2%)	0	100	100
All	All	522/668 (78%)	512 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	101/142 (71%)	99 (98%)	2 (2%)	55	73
1	B	104/142 (73%)	102 (98%)	2 (2%)	57	74
1	C	81/142 (57%)	80 (99%)	1 (1%)	71	84
1	D	92/142 (65%)	91 (99%)	1 (1%)	73	85
All	All	378/568 (66%)	372 (98%)	6 (2%)	62	78

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	ARG
1	A	252	SER
1	B	237	ARG
1	B	247	THR
1	C	247	THR
1	D	237	ARG

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

Mol	Chain	Res	Type
1	C	148	HIS
1	D	211	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 4 are monoatomic and 19 are unknown - 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

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, 95^{th} 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	136/167 (81%)	-0.21	0	100	100	41, 62, 93, 104	0
1	B	139/167 (83%)	-0.08	1 (0%)	87	87	39, 64, 89, 98	0
1	C	130/167 (77%)	0.07	1 (0%)	86	85	46, 73, 99, 107	0
1	D	138/167 (82%)	0.06	3 (2%)	62	57	39, 66, 98, 126	0
All	All	543/668 (81%)	-0.04	5 (0%)	84	83	39, 65, 95, 126	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	PRO	3.6
1	D	245	TYR	3.5
1	D	253	LEU	2.5
1	D	190	PHE	2.3
1	C	268	PRO	2.1

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

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^{th} 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
3	UNX	D	903	1/1	0.65	0.49	30,30,30,30	0
3	UNX	D	908	1/1	0.76	0.29	30,30,30,30	0
3	UNX	A	902	1/1	0.77	0.46	30,30,30,30	0
3	UNX	B	903	1/1	0.80	0.18	30,30,30,30	0
3	UNX	B	905	1/1	0.81	0.09	30,30,30,30	0
3	UNX	D	907	1/1	0.84	0.30	30,30,30,30	0
3	UNX	D	904	1/1	0.84	0.27	30,30,30,30	0
3	UNX	C	902	1/1	0.85	0.34	30,30,30,30	0
3	UNX	D	902	1/1	0.88	0.21	30,30,30,30	0
3	UNX	D	905	1/1	0.88	0.42	30,30,30,30	0
3	UNX	D	906	1/1	0.90	0.43	30,30,30,30	0
3	UNX	C	903	1/1	0.91	0.50	30,30,30,30	0
3	UNX	B	904	1/1	0.91	0.20	30,30,30,30	0
3	UNX	A	905	1/1	0.92	0.24	30,30,30,30	0
3	UNX	A	904	1/1	0.93	0.37	30,30,30,30	0
3	UNX	B	902	1/1	0.93	0.36	30,30,30,30	0
3	UNX	A	906	1/1	0.94	0.15	30,30,30,30	0
3	UNX	A	903	1/1	0.95	0.08	30,30,30,30	0
3	UNX	C	904	1/1	0.96	0.10	30,30,30,30	0
2	ZN	C	901	1/1	0.98	0.10	74,74,74,74	0
2	ZN	B	901	1/1	0.98	0.07	78,78,78,78	0
2	ZN	D	901	1/1	0.99	0.12	76,76,76,76	0
2	ZN	A	901	1/1	0.99	0.08	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.