



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 12:10 PM EDT

PDB ID : 9D92 / pdb_00009d92
Title : Structure of Z4 c3i
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Deposited on : 2024-08-20
Resolution : 3.06 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:

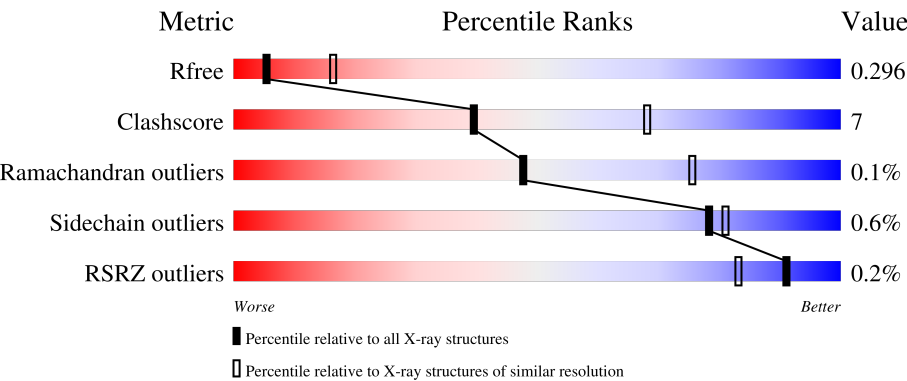
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.06 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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	A	244	75%16%10%
1	AA00	244	88%.10%
1	BAA0	244	% 89%.10%
1	C	244	74%16%10%
1	D	244	83%7%10%

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Mol	Chain	Length	Quality of chain
1	E	244	 A horizontal bar chart showing the quality of chain E. The bar is divided into three segments: a green segment representing 73%, a yellow segment representing 17%, and a grey segment representing 10%.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10006 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 Z4 c3i.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	0	0	0
			1666	1027	282	357			
1	C	220	Total	C	N	O	0	0	0
			1666	1027	282	357			
1	D	220	Total	C	N	O	0	0	0
			1666	1027	282	357			
1	E	220	Total	C	N	O	0	0	0
			1666	1027	282	357			
1	AA00	220	Total	C	N	O	0	0	0
			1666	1027	282	357			
1	BAA0	220	Total	C	N	O	0	0	0
			1666	1027	282	357			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	C	2	Total	O	0	0
			2	2		
2	D	2	Total	O	0	0
			2	2		
2	E	3	Total	O	0	0
			3	3		
2	AA00	2	Total	O	0	0
			2	2		

Chain AA00:

88%

10%



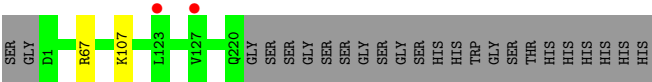
● Molecule 1: Z4 c3i

Chain BAA0:

%

89%

10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.66Å 72.15Å 119.52Å 90.00° 109.78° 90.00°	Depositor
Resolution (Å)	34.75 – 3.06 34.75 – 3.06	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.75-3.06) 98.0 (34.75-3.06)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.06Å)	Xtriage
Refinement program	PHENIX 2.1_6048	Depositor
R, R_{free}	0.240 , 0.299 0.242 , 0.296	Depositor DCC
R_{free} test set	1992 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10006	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9251e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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](#)

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	0.08	0/1668	0.21	0/2249
1	AA00	0.08	0/1668	0.21	0/2249
1	BAA0	0.08	0/1668	0.20	0/2249
1	C	0.07	0/1668	0.20	0/2249
1	D	0.06	0/1668	0.18	0/2249
1	E	0.07	0/1668	0.18	0/2249
All	All	0.07	0/10008	0.20	0/13494

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	1666	0	1726	26	0
1	AA00	1666	0	0	0	0
1	BAA0	1666	0	0	0	0
1	C	1666	0	1726	24	0
1	D	1666	0	1726	11	0
1	E	1666	0	1726	28	0
2	A	1	0	0	0	0
2	AA00	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3	0	0	2	0
All	All	10006	0	6904	81	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.

All (81) 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:19:SER:OG	1:E:202:GLU:OE2	2.03	0.77
1:C:180:GLN:NE2	1:C:218:GLU:OE2	2.19	0.76
1:A:128:GLU:HG2	1:A:155:LEU:HD21	1.70	0.73
1:E:86:LEU:HD12	1:E:119:GLU:HG3	1.71	0.70
1:C:54:LYS:NZ	1:C:154:GLU:OE2	2.25	0.69
1:D:181:ASP:OD2	1:D:183:THR:OG1	2.13	0.66
1:A:86:LEU:HD11	1:A:115:ALA:HB1	1.78	0.64
1:E:180:GLN:NE2	1:E:218:GLU:OE1	2.32	0.62
1:C:102:ILE:HG23	1:C:116:LEU:HD21	1.83	0.61
1:C:154:GLU:OE2	1:C:157:ARG:NH2	2.33	0.60
1:A:165:LEU:HD12	1:A:195:ILE:HG23	1.85	0.59
1:E:177:LYS:NZ	1:E:214:GLU:OE1	2.33	0.59
1:C:1:ASP:OD2	1:C:3:THR:OG1	2.20	0.59
1:C:128:GLU:HG3	1:C:155:LEU:HD21	1.85	0.59
1:C:25:LEU:HD22	1:C:55:ILE:HG23	1.87	0.57
1:A:141:ASP:OD1	1:A:142:SER:N	2.39	0.55
1:E:47:LYS:NZ	2:E:301:HOH:O	2.38	0.55
1:A:12:ILE:HG23	1:E:209:ILE:HG23	1.88	0.55
1:E:25:LEU:HD22	1:E:55:ILE:HG23	1.90	0.54
1:C:205:LEU:HD22	1:E:15:ILE:HG23	1.90	0.53
1:A:135:ILE:O	1:A:139:SER:OG	2.24	0.53
1:E:54:LYS:O	1:E:58:THR:OG1	2.25	0.53
1:E:181:ASP:HB3	1:E:184:VAL:HG12	1.91	0.53
1:D:14:THR:O	1:D:18:THR:OG1	2.25	0.53
1:D:41:ASP:OD2	1:D:44:VAL:N	2.38	0.52
1:E:214:GLU:HA	1:E:217:LYS:HE2	1.89	0.52
1:E:128:GLU:HG2	1:E:155:LEU:HD21	1.91	0.52
1:A:49:LEU:HD23	1:A:147:LEU:HD11	1.91	0.52
1:D:29:ILE:HG21	1:D:69:ALA:HA	1.91	0.51
1:E:26:ARG:HD2	1:E:68:GLN:HB2	1.92	0.51
1:E:54:LYS:HG2	1:E:154:GLU:OE2	2.10	0.51
1:D:41:ASP:OD2	1:D:44:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ALA:HA	1:C:137:ILE:HD12	1.94	0.50
1:A:108:ARG:HH11	1:A:108:ARG:HB3	1.76	0.50
1:C:135:ILE:HG23	1:C:175:LEU:HD11	1.94	0.50
1:A:209:ILE:HG23	1:C:12:ILE:HG23	1.94	0.49
1:D:114:LEU:HB2	1:D:147:LEU:HD11	1.94	0.49
1:C:196:ALA:HB1	1:C:205:LEU:HD23	1.94	0.49
1:A:25:LEU:HD22	1:A:55:ILE:HG23	1.95	0.49
1:D:132:LYS:O	1:D:136:LYS:HG2	2.13	0.49
1:E:54:LYS:NZ	2:E:301:HOH:O	2.46	0.48
1:A:88:LYS:HA	1:A:91:GLU:HG3	1.96	0.48
1:C:13:SER:OG	1:C:17:ARG:NH1	2.47	0.48
1:E:146:SER:O	1:E:187:LYS:NZ	2.47	0.48
1:E:185:LEU:HD22	1:E:215:ILE:HG23	1.95	0.47
1:E:22:GLU:OE2	1:E:26:ARG:NH1	2.47	0.47
1:A:17:ARG:NH2	1:A:154:GLU:OE1	2.47	0.47
1:A:38:GLU:N	1:A:38:GLU:OE1	2.47	0.47
1:D:25:LEU:HD22	1:D:55:ILE:HG23	1.96	0.47
1:A:49:LEU:HB3	1:A:147:LEU:HD21	1.97	0.47
1:C:82:THR:HG22	1:C:108:ARG:HD3	1.95	0.47
1:C:100:GLU:O	1:C:103:GLU:HG2	2.16	0.46
1:E:93:GLU:N	1:E:93:GLU:OE1	2.48	0.46
1:A:70:ARG:HH21	1:A:83:ARG:HH12	1.62	0.46
1:E:1:ASP:OD2	1:E:3:THR:OG1	2.30	0.46
1:A:21:SER:OG	1:E:202:GLU:OE2	2.31	0.46
1:A:93:GLU:OE1	1:A:93:GLU:N	2.49	0.46
1:C:57:PHE:HA	1:C:60:ILE:HG23	1.98	0.46
1:E:94:ASP:OD2	1:E:97:GLU:N	2.43	0.44
1:D:49:LEU:HB3	1:D:147:LEU:HD12	1.99	0.44
1:A:85:LEU:HB3	1:A:105:LEU:HD21	2.00	0.44
1:A:119:GLU:OE2	1:A:123:LEU:HD22	2.17	0.44
1:C:49:LEU:HD11	1:C:111:GLU:HG2	2.00	0.44
1:D:185:LEU:HD13	1:D:219:ALA:HB2	2.00	0.43
1:E:13:SER:OG	1:E:17:ARG:NH1	2.51	0.43
1:C:165:LEU:HD22	1:C:195:ILE:HG23	2.01	0.42
1:C:128:GLU:OE1	1:C:128:GLU:N	2.35	0.42
1:E:193:SER:OG	1:E:197:ARG:NH1	2.52	0.42
1:C:153:SER:O	1:C:157:ARG:HG3	2.19	0.42
1:E:139:SER:HB2	1:E:140:LYS:HZ3	1.82	0.42
1:A:5:LEU:HD11	1:E:220:GLN:HG2	2.02	0.41
1:A:189:ILE:HG22	1:C:11:VAL:HG21	2.02	0.41
1:C:220:GLN:HE21	1:E:5:LEU:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLU:OE2	1:C:98:LYS:HE3	2.20	0.41
1:C:185:LEU:HG	1:C:215:ILE:HG23	2.01	0.41
1:A:66:ALA:HB1	1:A:118:ALA:O	2.21	0.41
1:A:147:LEU:HD23	1:A:147:LEU:HA	1.93	0.41
1:A:22:GLU:HG3	1:A:62:ASN:HD21	1.86	0.41
1:E:105:LEU:HD23	1:E:105:LEU:HA	1.96	0.41
1:D:29:ILE:HD13	1:D:69:ALA:HB2	2.04	0.40
1:A:82:THR:HG23	1:A:105:LEU:HD22	2.03	0.40

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	218/244 (89%)	212 (97%)	6 (3%)	0	100	100
1	AA00	218/244 (89%)	213 (98%)	4 (2%)	1 (0%)	24	52
1	BAA0	218/244 (89%)	210 (96%)	8 (4%)	0	100	100
1	C	218/244 (89%)	212 (97%)	6 (3%)	0	100	100
1	D	218/244 (89%)	213 (98%)	5 (2%)	0	100	100
1	E	218/244 (89%)	216 (99%)	2 (1%)	0	100	100
All	All	1308/1464 (89%)	1276 (98%)	31 (2%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA00	139	SER

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	180/198 (91%)	180 (100%)	0	100	100
1	AA00	180/198 (91%)	176 (98%)	4 (2%)	45	67
1	BAA0	180/198 (91%)	178 (99%)	2 (1%)	65	76
1	C	180/198 (91%)	180 (100%)	0	100	100
1	D	180/198 (91%)	180 (100%)	0	100	100
1	E	180/198 (91%)	180 (100%)	0	100	100
All	All	1080/1188 (91%)	1074 (99%)	6 (1%)	78	81

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

Mol	Chain	Res	Type
1	AA00	93	GLU
1	AA00	157	ARG
1	AA00	158	GLN
1	AA00	171	ASP
1	BAA0	67	ARG
1	BAA0	107	LYS

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

Mol	Chain	Res	Type
1	A	220	GLN
1	C	180	GLN
1	D	180	GLN
1	E	62	ASN
1	E	220	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	220/244 (90%)	-0.43	0	100	100	57, 86, 123, 147	0
1	AA00	220/244 (90%)	-0.43	0	100	100	65, 94, 124, 142	0
1	BAA0	220/244 (90%)	-0.46	2 (0%)	81	61	59, 88, 122, 143	0
1	C	220/244 (90%)	-0.28	1 (0%)	87	72	62, 88, 129, 139	2 (0%)
1	D	220/244 (90%)	-0.49	0	100	100	59, 88, 119, 132	0
1	E	220/244 (90%)	-0.54	0	100	100	56, 86, 121, 140	0
All	All	1320/1464 (90%)	-0.44	3 (0%)	91	83	56, 88, 124, 147	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BAA0	123	LEU	3.4
1	BAA0	127	VAL	2.3
1	C	34	GLU	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.