



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:28 pm GMT

PDB ID : 5O4W
Title : Protein structure determination by electron diffraction using a single three-dimensional nanocrystal
Authors : Clabbers, M.T.B.; van Genderen, E.; Wan, W.; Wieggers, E.L.; Gruene, T.; Abrahams, J.P.
Deposited on : 2017-05-31
Resolution : 2.11 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

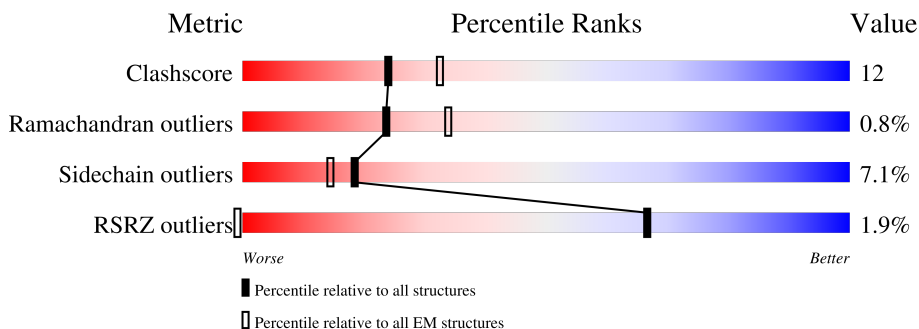
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.11 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RSRZ outliers	127900	0

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	129	 4% 65% 32% .
1	B	129	 74% 22% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

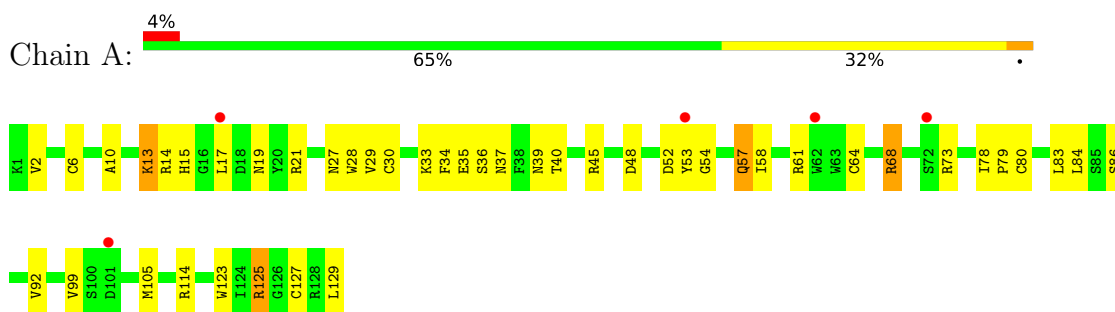
- Molecule 1 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	129	Total	C	N	O	S	0	0
			1000	613	193	184	10		
1	B	129	Total	C	N	O	S	0	0
			1000	613	193	184	10		

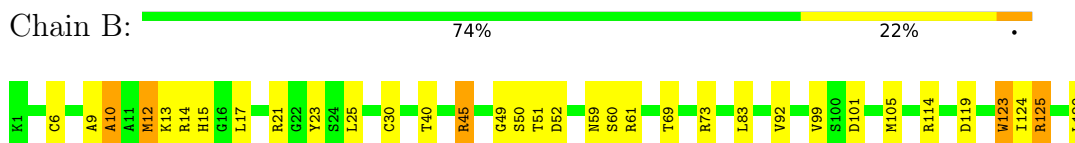
3 Residue-property plots [i](#)

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. 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. 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: Lysozyme C



- Molecule 1: Lysozyme C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.56Å 68.05Å 32.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.46 – 2.11 41.46 – 2.11	Depositor EDS
% Data completeness (in resolution range)	48.4 (41.46-2.11) 48.4 (41.46-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.335 , 0.350 0.347 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	2000	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.89% 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

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	1.00	3/1020 (0.3%)	1.25	8/1379 (0.6%)
1	B	0.84	1/1020 (0.1%)	1.29	11/1379 (0.8%)
All	All	0.92	4/2040 (0.2%)	1.27	19/2758 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	ARG	CZ-NH1	10.82	1.47	1.33
1	A	114	ARG	CZ-NH1	10.63	1.46	1.33
1	A	68	ARG	CZ-NH1	-10.59	1.19	1.33
1	B	123	TRP	CB-CG	-5.20	1.40	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	ARG	NE-CZ-NH1	21.71	131.15	120.30
1	A	125	ARG	NE-CZ-NH1	17.50	129.05	120.30
1	A	114	ARG	NE-CZ-NH2	-14.48	113.06	120.30
1	A	68	ARG	NE-CZ-NH1	-12.98	113.81	120.30
1	A	125	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	A	21	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	B	125	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	B	14	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	B	119	ASP	CB-CG-OD1	-8.81	110.37	118.30
1	B	114	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	114	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	B	101	ASP	CB-CG-OD1	8.11	125.59	118.30
1	A	45	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	45	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	114	ARG	NH1-CZ-NH2	-6.05	112.74	119.40
1	B	119	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	21	ARG	NH1-CZ-NH2	5.76	125.73	119.40
1	B	61	ARG	NE-CZ-NH2	5.37	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ARG	NE-CZ-NH1	5.36	122.98	120.30

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	1000	0	965	24	1
1	B	1000	0	959	22	1
All	All	2000	0	1924	46	1

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 12.

All (46) 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:B:45:ARG:NH1	1:B:51:THR:OG1	2.19	0.76
1:A:64:CYS:HG	1:A:80:CYS:HG	1.29	0.75
1:A:36:SER:HB3	1:A:57:GLN:NE2	2.09	0.68
1:A:28:TRP:CH2	1:A:99:VAL:HG11	2.30	0.66
1:A:17:LEU:HD11	1:A:92:VAL:HG13	1.78	0.64
1:A:2:VAL:HG22	1:A:39:ASN:OD1	1.97	0.64
1:B:6:CYS:O	1:B:9:ALA:O	2.16	0.64
1:B:17:LEU:HD11	1:B:92:VAL:HG13	1.80	0.62
1:A:54:GLY:O	1:A:57:GLN:NE2	2.31	0.61
1:A:6:CYS:SG	1:A:127:CYS:HB3	2.42	0.59
1:A:29:VAL:HG12	1:A:123:TRP:CZ3	2.40	0.56
1:B:23:TYR:CD1	1:B:105:MET:HG3	2.40	0.56
1:A:15:HIS:HB3	1:A:92:VAL:HG11	1.88	0.54
1:A:33:LYS:HB2	1:A:123:TRP:HH2	1.74	0.53
1:B:12:MET:HE1	1:B:17:LEU:HB3	1.92	0.52
1:A:27:ASN:HA	1:A:30:CYS:SG	2.50	0.52
1:A:28:TRP:HH2	1:A:99:VAL:HG11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:MET:HE2	1:B:25:LEU:HD12	1.92	0.51
1:A:58:ILE:HD12	1:A:83:LEU:HD22	1.93	0.51
1:A:36:SER:HB3	1:A:57:GLN:HE21	1.77	0.50
1:B:30:CYS:HB2	1:B:123:TRP:CD1	2.46	0.50
1:A:53:TYR:CD2	1:A:80:CYS:SG	3.05	0.50
1:B:9:ALA:O	1:B:10:ALA:HB3	2.12	0.49
1:A:78:ILE:HG22	1:A:79:PRO:O	2.13	0.48
1:A:10:ALA:HA	1:A:13:LYS:HB2	1.96	0.48
1:B:15:HIS:HB3	1:B:92:VAL:HG11	1.95	0.48
1:B:21:ARG:O	1:B:21:ARG:NH1	2.47	0.47
1:B:23:TYR:CE1	1:B:105:MET:HG3	2.50	0.46
1:B:12:MET:CE	1:B:25:LEU:HD12	2.47	0.45
1:B:9:ALA:O	1:B:10:ALA:CB	2.63	0.45
1:B:60:SER:OG	1:B:69:THR:HG21	2.16	0.45
1:A:33:LYS:HE2	1:A:34:PHE:CZ	2.52	0.45
1:A:52:ASP:OD1	1:A:57:GLN:OE1	2.34	0.45
1:B:25:LEU:HD23	1:B:124:ILE:HG21	1.99	0.44
1:A:68:ARG:O	1:A:68:ARG:CG	2.66	0.43
1:A:33:LYS:HB2	1:A:123:TRP:CH2	2.53	0.43
1:B:13:LYS:HE3	1:B:129:LEU:HB3	2.00	0.43
1:A:40:THR:HG21	1:A:86:SER:HA	2.00	0.43
1:A:30:CYS:HA	1:A:123:TRP:CE2	2.54	0.42
1:B:52:ASP:OD1	1:B:59:ASN:ND2	2.46	0.42
1:B:12:MET:SD	1:B:17:LEU:HD13	2.60	0.41
1:B:49:GLY:O	1:B:69:THR:HG22	2.19	0.41
1:B:50:SER:HA	1:B:69:THR:CG2	2.51	0.41
1:B:21:ARG:HG2	1:B:99:VAL:HG22	2.03	0.41
1:B:50:SER:HA	1:B:69:THR:HG22	2.02	0.40
1:A:35:GLU:HB3	1:A:57:GLN:HG2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:O	1:B:125:ARG:CZ[1_554]	2.19	0.01

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 PDB entries followed by that with respect to all EM entries.

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	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	14
1	B	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	14
All	All	254/258 (98%)	234 (92%)	18 (7%)	2 (1%)	24	14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	ALA
1	A	48	ASP

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 PDB entries followed by that with respect to all EM entries.

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	105/105 (100%)	94 (90%)	11 (10%)	7	3
1	B	105/105 (100%)	101 (96%)	4 (4%)	33	33
All	All	210/210 (100%)	195 (93%)	15 (7%)	18	11

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	ARG
1	A	19	ASN
1	A	37	ASN

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Mol	Chain	Res	Type
1	A	57	GLN
1	A	61	ARG
1	A	73	ARG
1	A	84	LEU
1	A	105	MET
1	A	125	ARG
1	A	129	LEU
1	B	12	MET
1	B	40	THR
1	B	73	ARG
1	B	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	27	ASN
1	A	37	ASN
1	A	46	ASN
1	A	57	GLN
1	A	74	ASN
1	A	103	ASN
1	B	15	HIS
1	B	27	ASN
1	B	39	ASN
1	B	46	ASN
1	B	65	ASN
1	B	74	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](#)

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.