Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:39 PM GMT

PDB ID	:	1UNV
Title	:	STRUCTURE BASED ENGINEERING OF INTERNAL MOLECULAR SURFACES OF FOUR HELIX BUNDLES
Authors	:	Yadav, M.K.; Redman, J.E.; Alvarez-Gutierrez, J.M.; Zhang, Y.; Stout, C.D.; Ghadiri, M.R.
Deposited on	:	2003-09-15
Resolution	:	2.14 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

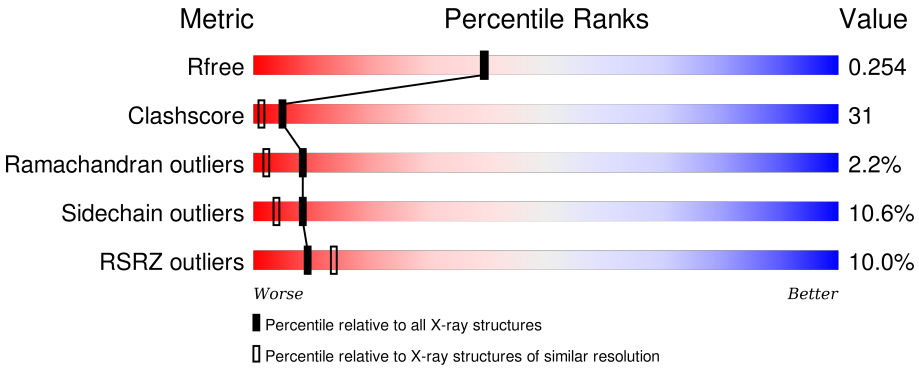
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.14 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}	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	34	6% 21% 24% 21% 9% 26%
1	B	34	9% 9% 35% 21% 9% 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 424 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 GENERAL CONTROL PROTEIN GCN4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	25	Total	C	N	O	0	0	0
			208	134	35	39			
1	B	25	Total	C	N	O	0	0	0
			212	136	35	41			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	THR	VAL	ENGINEERED MUTATION	UNP P03069
A	12	ILE	LEU	CONFLICT	UNP P03069
A	16	LEU	ASN	CONFLICT	UNP P03069
A	19	ILE	LEU	CONFLICT	UNP P03069
A	23	LEU	VAL	CONFLICT	UNP P03069
A	26	ILE	LEU	CONFLICT	UNP P03069
A	30	LEU	VAL	CONFLICT	UNP P03069
B	9	THR	VAL	ENGINEERED MUTATION	UNP P03069
B	12	ILE	LEU	CONFLICT	UNP P03069
B	16	LEU	ASN	CONFLICT	UNP P03069
B	19	ILE	LEU	CONFLICT	UNP P03069
B	23	LEU	VAL	CONFLICT	UNP P03069
B	26	ILE	LEU	CONFLICT	UNP P03069
B	30	LEU	VAL	CONFLICT	UNP P03069

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

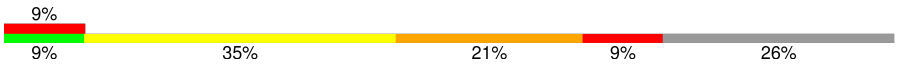
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: GENERAL CONTROL PROTEIN GCN4

Chain A:

- Molecule 1: GENERAL CONTROL PROTEIN GCN4

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	78.09Å 78.09Å 78.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.05 – 2.14 27.61 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.6 (55.05-2.14) 97.3 (27.61-2.07)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.241 , 0.302 0.250 , 0.254	Depositor DCC
R_{free} test set	222 reflections (4.92%)	DCC
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 9082 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	424	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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 21.33 % 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 7.1753e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	3.24	29/209 (13.9%)	2.63	15/277 (5.4%)
1	B	3.68	31/213 (14.6%)	2.30	14/283 (4.9%)
All	All	3.47	60/422 (14.2%)	2.47	29/560 (5.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	SER	CB-OG	-14.65	1.23	1.42
1	B	11	GLU	CD-OE1	11.72	1.38	1.25
1	A	20	GLU	CD-OE2	10.69	1.37	1.25
1	B	11	GLU	CD-OE2	10.01	1.36	1.25
1	B	8	LYS	CD-CE	9.80	1.75	1.51
1	B	8	LYS	CE-NZ	9.64	1.73	1.49
1	A	15	LYS	CD-CE	9.55	1.75	1.51
1	B	28	LYS	CD-CE	9.44	1.74	1.51
1	B	20	GLU	CD-OE2	-9.22	1.15	1.25
1	B	7	ASP	CB-CG	8.88	1.70	1.51
1	B	20	GLU	CB-CG	8.77	1.68	1.52
1	B	7	ASP	CA-CB	8.68	1.73	1.53
1	A	28	LYS	CD-CE	8.55	1.72	1.51
1	A	17	TYR	CE1-CZ	-8.54	1.27	1.38
1	B	14	SER	C-O	8.52	1.39	1.23
1	B	14	SER	CA-CB	8.47	1.65	1.52
1	B	22	GLU	CD-OE1	-8.47	1.16	1.25
1	A	9	THR	CB-CG2	-8.12	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ASN	N-CA	7.96	1.62	1.46
1	A	15	LYS	CE-NZ	7.75	1.68	1.49
1	A	25	ARG	NE-CZ	7.71	1.43	1.33
1	B	6	GLU	CA-CB	7.62	1.70	1.53
1	A	10	GLU	CD-OE2	-7.09	1.17	1.25
1	B	6	GLU	CG-CD	6.94	1.62	1.51
1	A	19	ILE	N-CA	6.84	1.60	1.46
1	B	21	ASN	CA-C	6.83	1.70	1.52
1	B	10	GLU	CD-OE1	6.79	1.33	1.25
1	B	13	LEU	CG-CD1	6.55	1.76	1.51
1	B	22	GLU	CG-CD	6.53	1.61	1.51
1	B	29	LEU	CG-CD1	6.39	1.75	1.51
1	A	23	LEU	C-O	-6.33	1.11	1.23
1	A	10	GLU	CA-CB	6.32	1.67	1.53
1	A	17	TYR	CD1-CE1	6.28	1.48	1.39
1	A	9	THR	CA-CB	6.16	1.69	1.53
1	A	28	LYS	CE-NZ	6.08	1.64	1.49
1	B	24	ALA	CA-CB	6.02	1.65	1.52
1	B	18	HIS	C-O	5.95	1.34	1.23
1	B	28	LYS	CG-CD	5.88	1.72	1.52
1	A	20	GLU	C-O	5.86	1.34	1.23
1	A	17	TYR	CE2-CZ	5.72	1.46	1.38
1	B	8	LYS	CB-CG	5.71	1.68	1.52
1	A	32	GLU	CG-CD	5.64	1.60	1.51
1	A	25	ARG	CG-CD	5.63	1.66	1.51
1	B	27	LYS	CD-CE	5.63	1.65	1.51
1	A	8	LYS	CD-CE	5.60	1.65	1.51
1	A	22	GLU	CD-OE2	5.59	1.31	1.25
1	A	21	ASN	CB-CG	5.53	1.63	1.51
1	B	13	LEU	N-CA	5.53	1.57	1.46
1	B	10	GLU	CD-OE2	5.45	1.31	1.25
1	A	8	LYS	CG-CD	5.42	1.70	1.52
1	A	8	LYS	N-CA	5.28	1.56	1.46
1	A	8	LYS	CB-CG	5.27	1.66	1.52
1	B	6	GLU	N-CA	5.27	1.56	1.46
1	A	22	GLU	CB-CG	5.24	1.62	1.52
1	A	23	LEU	CG-CD1	-5.15	1.32	1.51
1	A	28	LYS	CG-CD	5.11	1.69	1.52
1	B	22	GLU	CB-CG	-5.06	1.42	1.52
1	A	15	LYS	N-CA	5.05	1.56	1.46
1	B	9	THR	CA-CB	-5.01	1.40	1.53
1	B	7	ASP	C-O	5.01	1.32	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	LEU	CB-CG-CD2	-14.78	85.87	111.00
1	A	25	ARG	NE-CZ-NH2	11.84	126.22	120.30
1	B	11	GLU	OE1-CD-OE2	11.03	136.54	123.30
1	B	7	ASP	CB-CG-OD1	8.89	126.30	118.30
1	A	11	GLU	OE1-CD-OE2	8.83	133.90	123.30
1	A	8	LYS	N-CA-C	8.21	133.18	111.00
1	B	6	GLU	OE1-CD-OE2	-7.98	113.72	123.30
1	A	25	ARG	CB-CG-CD	7.53	131.18	111.60
1	A	27	LYS	CD-CE-NZ	-7.45	94.58	111.70
1	A	25	ARG	NH1-CZ-NH2	-6.73	112.00	119.40
1	B	28	LYS	CD-CE-NZ	6.71	127.14	111.70
1	B	14	SER	CA-CB-OG	-6.61	93.36	111.20
1	B	29	LEU	CB-CG-CD1	6.39	121.87	111.00
1	B	12	ILE	CG1-CB-CG2	-6.14	97.89	111.40
1	A	10	GLU	N-CA-CB	5.91	121.23	110.60
1	B	29	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	15	LYS	CD-CE-NZ	-5.76	98.44	111.70
1	A	10	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	B	25	ARG	CB-CG-CD	5.72	126.47	111.60
1	A	22	GLU	CG-CD-OE1	-5.62	107.06	118.30
1	B	17	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	A	29	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	23	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	A	15	LYS	CA-CB-CG	5.31	125.09	113.40
1	B	6	GLU	CA-CB-CG	5.24	124.93	113.40
1	B	30	LEU	N-CA-C	5.18	125.00	111.00
1	A	10	GLU	CG-CD-OE1	5.14	128.59	118.30
1	B	11	GLU	CG-CD-OE2	-5.06	108.17	118.30
1	A	25	ARG	CB-CA-C	-5.03	100.34	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	8	LYS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	GLU	Mainchain
1	A	8	LYS	Mainchain

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	208	0	224	12	1
1	B	212	0	225	17	1
2	A	3	0	0	2	0
2	B	1	0	0	0	0
All	All	424	0	449	27	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 31.

All (27) 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:29:LEU:CD1	1:B:29:LEU:CG	1.75	1.61
1:A:15:LYS:CD	1:A:15:LYS:CE	1.75	1.60
1:B:28:LYS:CE	1:B:28:LYS:CD	1.74	1.59
1:B:13:LEU:CD1	1:B:13:LEU:CG	1.76	1.58
1:B:8:LYS:CD	1:B:8:LYS:CE	1.75	1.57
1:A:15:LYS:NZ	1:A:15:LYS:CE	1.68	1.52
1:B:8:LYS:NZ	1:B:8:LYS:CE	1.73	1.51
1:A:15:LYS:CG	1:A:15:LYS:CE	2.65	0.74
1:B:13:LEU:CB	1:B:13:LEU:CD1	2.68	0.70
1:A:15:LYS:CD	1:A:15:LYS:NZ	2.60	0.65
1:B:6:GLU:OE2	1:B:10:GLU:OE1	2.18	0.62
1:B:29:LEU:CD1	1:B:29:LEU:HG	2.14	0.58
1:A:25:ARG:O	1:A:29:LEU:HD13	2.06	0.56
1:B:13:LEU:CD2	1:B:13:LEU:CD1	2.78	0.54
1:A:18:HIS:HE1	2:A:2003:HOH:O	1.93	0.52
1:B:6:GLU:O	1:B:7:ASP:CB	2.62	0.48
1:A:18:HIS:CE1	2:A:2003:HOH:O	2.66	0.47
1:B:29:LEU:CD2	1:B:29:LEU:CD1	2.87	0.46
1:A:23:LEU:O	1:A:27:LYS:HG3	2.18	0.43
1:B:18:HIS:O	1:B:22:GLU:HG3	2.19	0.43
1:A:17:TYR:CE1	1:B:15:LYS:HE2	2.54	0.43
1:A:8:LYS:HE3	1:A:9:THR:H	1.84	0.42
1:B:28:LYS:CE	1:B:28:LYS:CG	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLU:O	1:B:7:ASP:HB3	2.21	0.41
1:B:6:GLU:CD	1:B:10:GLU:OE1	2.59	0.41
1:A:8:LYS:HB2	1:A:8:LYS:HE3	1.81	0.41
1:A:32:GLU:O	1:B:29:LEU:HD12	2.21	0.41

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:25:ARG:NH1	1:B:27:LYS:NZ[18_545]	1.94	0.26

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	23/34 (68%)	20 (87%)	3 (13%)	0	100	100
1	B	23/34 (68%)	22 (96%)	0	1 (4%)	3	0
All	All	46/68 (68%)	42 (91%)	3 (6%)	1 (2%)	8	2

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	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 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	23/31 (74%)	20 (87%)	3 (13%)	5 2
1	B	24/31 (77%)	22 (92%)	2 (8%)	14 8
All	All	47/62 (76%)	42 (89%)	5 (11%)	8 4

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	9	THR
1	A	29	LEU
1	B	6	GLU
1	B	29	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	25/34 (73%)	0.38	2 (8%) 15 20	36, 45, 72, 97	0
1	B	25/34 (73%)	0.66	3 (12%) 6 9	34, 47, 76, 100	0
All	All	50/68 (73%)	0.52	5 (10%) 9 14	34, 47, 82, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	5.5
1	B	6	GLU	5.3
1	A	31	GLY	5.0
1	B	29	LEU	3.6
1	A	32	GLU	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.