



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4UOS / pdb_00004uos
Title : Thermodynamic hyperstability in parametrically designed helical bundles
Authors : Oberdorfer, G.; Huang, P.; Pei, X.Y.; Xu, C.; Gonen, T.; Nannenga, B.; DiMaio, D.; Rogers, J.; Luisi, B.F.; Baker, D.
Deposited on : 2014-06-09
Resolution : 1.63 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

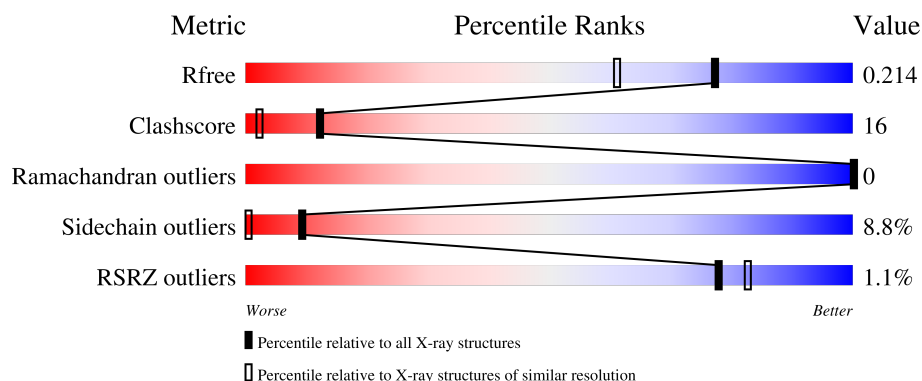
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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 $\leq 5\%$. 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	191	51% 38% 8% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1857 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 DESIGNED HELICAL BUNDLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	188	1555	1003	249	282	21	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	PDB 4UOS
A	0	GLY	-	cloning artifact	PDB 4UOS

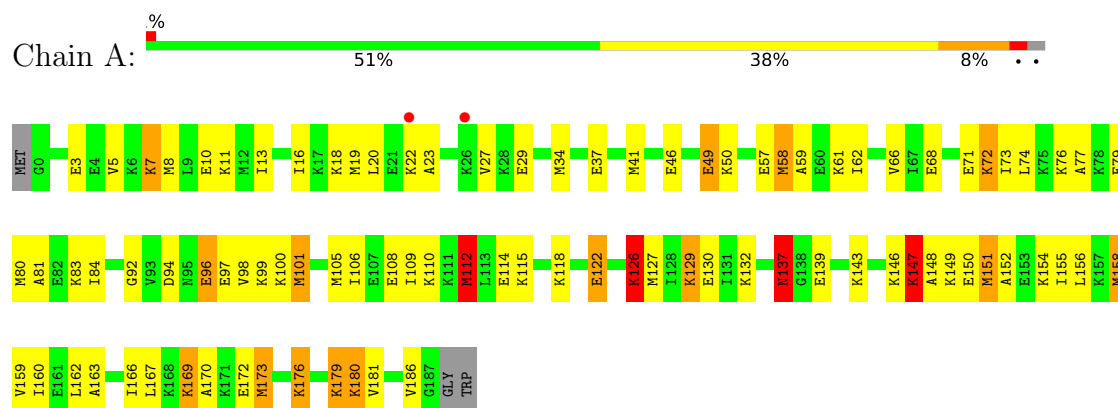
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	302	Total	O	0	0
			302	302		

3 Residue-property plots

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: DESIGNED HELICAL BUNDLE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	29.46Å 72.15Å 51.26Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	23.60 – 1.63 23.60 – 1.63	Depositor EDS
% Data completeness (in resolution range)	97.4 (23.60-1.63) 97.4 (23.60-1.63)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.53Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.193 , 0.206 0.204 , 0.214	Depositor DCC
R_{free} test set	1524 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1857	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.54% 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

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	2.00	66/1563 (4.2%)	1.22	17/2038 (0.8%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58[A]	MET	CA-C	8.20	1.63	1.52
1	A	58[B]	MET	CA-C	8.20	1.63	1.52
1	A	8[A]	MET	CA-C	7.64	1.62	1.52
1	A	8[B]	MET	CA-C	7.64	1.62	1.52
1	A	173[A]	MET	CA-C	7.44	1.62	1.52
1	A	173[B]	MET	CA-C	7.44	1.62	1.52
1	A	92	GLY	C-O	-7.20	1.16	1.24
1	A	169	LYS	C-O	-6.71	1.16	1.24
1	A	149	LYS	C-O	-6.55	1.16	1.24
1	A	108	GLU	C-O	-6.54	1.16	1.24
1	A	170	ALA	C-O	-6.49	1.16	1.24
1	A	62	ILE	C-O	-6.44	1.16	1.24
1	A	74	LEU	C-O	-6.42	1.16	1.24
1	A	98	VAL	C-O	-6.38	1.16	1.24
1	A	159	VAL	C-O	-6.38	1.16	1.24
1	A	84	ILE	C-O	-6.36	1.17	1.24
1	A	27	VAL	C-O	-6.22	1.16	1.24
1	A	152	ALA	C-O	-6.18	1.16	1.24
1	A	13	ILE	C-O	-6.14	1.16	1.24
1	A	19	MET	C-O	-6.14	1.16	1.24
1	A	16	ILE	C-O	-6.00	1.17	1.24
1	A	126[A]	LYS	C-O	-5.93	1.17	1.24
1	A	126[B]	LYS	C-O	-5.93	1.17	1.24
1	A	154	LYS	C-O	-5.90	1.17	1.24
1	A	10	GLU	C-O	-5.89	1.17	1.24
1	A	109	ILE	C-O	-5.89	1.17	1.24
1	A	76	LYS	C-O	-5.86	1.17	1.24
1	A	155	ILE	C-O	-5.81	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	GLU	C-O	-5.81	1.17	1.24
1	A	106	ILE	C-O	-5.79	1.17	1.24
1	A	163	ALA	C-O	-5.79	1.17	1.24
1	A	156	LEU	C-O	-5.74	1.17	1.24
1	A	160	ILE	C-O	-5.73	1.17	1.24
1	A	59	ALA	C-O	-5.72	1.17	1.24
1	A	137	ASN	C-O	-5.70	1.16	1.24
1	A	5	VAL	C-O	-5.68	1.17	1.24
1	A	181	VAL	C-O	-5.63	1.17	1.24
1	A	127	MET	C-O	-5.63	1.17	1.24
1	A	83	LYS	C-O	-5.52	1.17	1.24
1	A	158	MET	C-O	-5.51	1.17	1.24
1	A	112	MET	C-O	-5.49	1.17	1.24
1	A	66	VAL	C-O	-5.49	1.17	1.24
1	A	166	ILE	C-O	-5.47	1.18	1.24
1	A	3	GLU	C-O	-5.46	1.17	1.24
1	A	20	LEU	C-O	-5.43	1.17	1.24
1	A	101	MET	C-O	-5.38	1.17	1.24
1	A	81	ALA	C-O	-5.37	1.17	1.24
1	A	22	LYS	C-O	-5.35	1.17	1.24
1	A	110	LYS	C-O	-5.34	1.17	1.24
1	A	186	VAL	C-O	-5.29	1.18	1.24
1	A	151	MET	C-O	-5.27	1.17	1.24
1	A	73	ILE	C-O	-5.27	1.18	1.24
1	A	79	GLU	C-O	-5.24	1.18	1.24
1	A	105	MET	C-O	-5.24	1.18	1.24
1	A	118	LYS	C-O	-5.23	1.18	1.24
1	A	77	ALA	C-O	-5.22	1.18	1.24
1	A	147	LYS	C-O	-5.21	1.18	1.24
1	A	167	LEU	C-O	-5.21	1.18	1.24
1	A	172	GLU	C-O	-5.15	1.18	1.24
1	A	71	GLU	C-O	-5.14	1.18	1.24
1	A	72	LYS	C-O	-5.13	1.18	1.24
1	A	148	ALA	C-O	-5.11	1.18	1.24
1	A	23	ALA	C-O	-5.09	1.18	1.24
1	A	99	LYS	C-O	-5.08	1.18	1.24
1	A	68	GLU	C-O	-5.00	1.18	1.24
1	A	132	LYS	C-O	-5.00	1.18	1.24

All (17) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173[A]	MET	CA-C-O	12.94	134.26	120.55
1	A	173[B]	MET	CA-C-O	12.94	134.26	120.55
1	A	173[A]	MET	N-CA-C	8.76	120.82	111.28
1	A	173[B]	MET	N-CA-C	8.76	120.82	111.28
1	A	8[A]	MET	CA-C-O	7.95	128.98	120.55
1	A	8[B]	MET	CA-C-O	7.95	128.98	120.55
1	A	96	GLU	N-CA-C	7.01	119.00	111.36
1	A	58[A]	MET	CA-C-O	6.35	127.28	120.55
1	A	58[B]	MET	CA-C-O	6.35	127.28	120.55
1	A	172	GLU	O-C-N	5.85	128.32	122.12
1	A	7	LYS	CA-C-N	-5.52	112.82	120.38
1	A	7	LYS	C-N-CA	-5.52	112.82	120.38
1	A	57	GLU	O-C-N	5.50	127.73	122.07
1	A	57	GLU	CA-C-N	-5.12	113.62	120.54
1	A	57	GLU	C-N-CA	-5.12	113.62	120.54
1	A	151	MET	CG-SD-CE	-5.11	89.66	100.90
1	A	94	ASP	N-CA-C	5.06	116.83	110.91

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	1555	0	1796	52	0
2	A	302	0	0	22	0
All	All	1857	0	1796	52	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.

All (52) 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:130:GLU:HB2	2:A:2238:HOH:O	1.44	1.15
1:A:169:LYS:NZ	1:A:173[A]:MET:HE2	1.71	1.06
1:A:112:MET:HE3	2:A:2223:HOH:O	1.62	0.98
1:A:122[B]:GLU:O	1:A:126[B]:LYS:HD2	1.67	0.95
1:A:126[B]:LYS:HD3	2:A:2232:HOH:O	1.67	0.91
1:A:147:LYS:HZ2	1:A:147:LYS:HB2	1.40	0.86
1:A:34:MET:HA	1:A:58[A]:MET:HE2	1.58	0.84
1:A:147:LYS:HB2	1:A:147:LYS:NZ	1.90	0.84
1:A:7:LYS:O	1:A:11:LYS:HG2	1.80	0.81
1:A:11:LYS:HD3	2:A:2038:HOH:O	1.82	0.80
1:A:169:LYS:HZ2	1:A:173[A]:MET:HE2	1.48	0.77
1:A:180:LYS:HD3	2:A:2296:HOH:O	1.85	0.76
1:A:143:LYS:HE2	2:A:2126:HOH:O	1.94	0.68
1:A:158:MET:HG3	2:A:2273:HOH:O	1.95	0.67
1:A:126[B]:LYS:NZ	2:A:2236:HOH:O	2.25	0.66
1:A:112:MET:HA	1:A:112:MET:HE2	1.79	0.65
1:A:58[A]:MET:HE3	2:A:2091:HOH:O	1.98	0.63
1:A:41:MET:HE1	2:A:2136:HOH:O	2.01	0.60
1:A:169:LYS:HZ1	1:A:173[A]:MET:HE2	1.62	0.59
1:A:34:MET:HA	1:A:58[A]:MET:CE	2.33	0.58
1:A:46:GLU:OE1	1:A:50:LYS:HE3	2.03	0.58
1:A:137:ASN:ND2	1:A:139:GLU:HG3	2.19	0.58
1:A:41:MET:CE	2:A:2136:HOH:O	2.52	0.56
1:A:101:MET:HE3	1:A:176:LYS:HZ2	1.71	0.56
1:A:126[A]:LYS:HD2	2:A:2232:HOH:O	2.06	0.55
1:A:101:MET:HE3	1:A:176:LYS:NZ	2.21	0.55
1:A:122[A]:GLU:O	1:A:126[A]:LYS:HG2	2.07	0.54
1:A:115:LYS:HE2	1:A:162:LEU:HD21	1.90	0.53
1:A:158:MET:CG	2:A:2273:HOH:O	2.55	0.53
1:A:112:MET:HG3	2:A:2215:HOH:O	2.09	0.52
1:A:96:GLU:HG3	1:A:100:LYS:HE3	1.91	0.51
1:A:101:MET:SD	1:A:180:LYS:HG3	2.52	0.50
1:A:34:MET:HA	1:A:58[B]:MET:HE3	1.93	0.50
1:A:169:LYS:NZ	1:A:173[A]:MET:CE	2.61	0.49
1:A:137:ASN:HD21	1:A:139:GLU:HG3	1.78	0.49
1:A:137:ASN:C	1:A:137:ASN:HD22	2.22	0.48
1:A:49:GLU:H	1:A:49:GLU:CD	2.22	0.47
1:A:143:LYS:HG2	2:A:2126:HOH:O	2.16	0.45
1:A:11:LYS:CE	2:A:2016:HOH:O	2.64	0.45
1:A:11:LYS:CD	2:A:2038:HOH:O	2.53	0.45
1:A:18:LYS:NZ	2:A:2061:HOH:O	2.50	0.44
1:A:179:LYS:HE3	1:A:179:LYS:HB2	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:HG2	2:A:2227:HOH:O	2.18	0.44
1:A:37:GLU:HG3	1:A:41:MET:HE2	1.99	0.43
1:A:129:LYS:HB3	1:A:129:LYS:HE2	1.67	0.43
1:A:112:MET:HA	1:A:112:MET:CE	2.49	0.43
1:A:146:LYS:O	1:A:150:GLU:HG3	2.20	0.42
1:A:58[A]:MET:CE	2:A:2091:HOH:O	2.63	0.42
1:A:112:MET:HE1	2:A:2228:HOH:O	2.18	0.41
1:A:34:MET:CA	1:A:58[A]:MET:HE2	2.40	0.41
1:A:122[A]:GLU:O	1:A:126[A]:LYS:HE2	2.20	0.41
1:A:180:LYS:CD	2:A:2296:HOH:O	2.56	0.40

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	191/191 (100%)	190 (100%)	1 (0%)	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	175/172 (102%)	158 (90%)	17 (10%)	8 0

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	49	GLU
1	A	61	LYS
1	A	72	LYS
1	A	80	MET
1	A	112	MET
1	A	122[A]	GLU
1	A	122[B]	GLU
1	A	126[A]	LYS
1	A	126[B]	LYS
1	A	129	LYS
1	A	137	ASN
1	A	147	LYS
1	A	151	MET
1	A	176	LYS
1	A	179	LYS
1	A	180	LYS

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

Mol	Chain	Res	Type
1	A	137	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	188/191 (98%)	0.23	2 (1%) 78 83	16, 29, 39, 42	5 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	LYS	2.7
1	A	22	LYS	2.1

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 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.