



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1HXU / pdb_00001hxu
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Deposited on : 2001-01-17
Resolution : 3.00 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

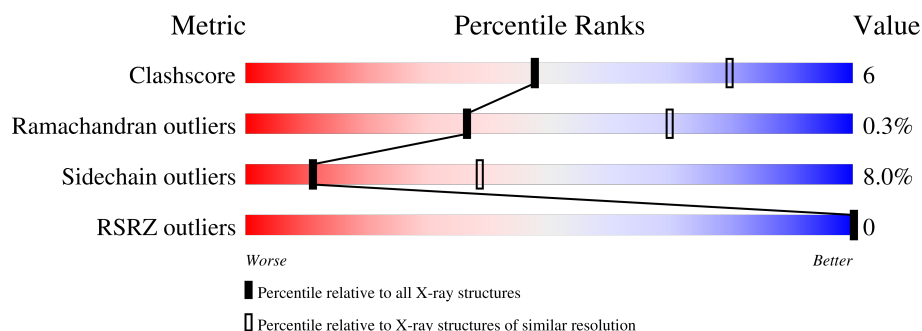
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	340	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2640 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 OUTER MEMBRANE PROTEIN F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	126	0	0
			2634	1659	440	532	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	LYS	VAL	engineered mutation	UNP P02931
A	131	LYS	GLY	engineered mutation	UNP P02931

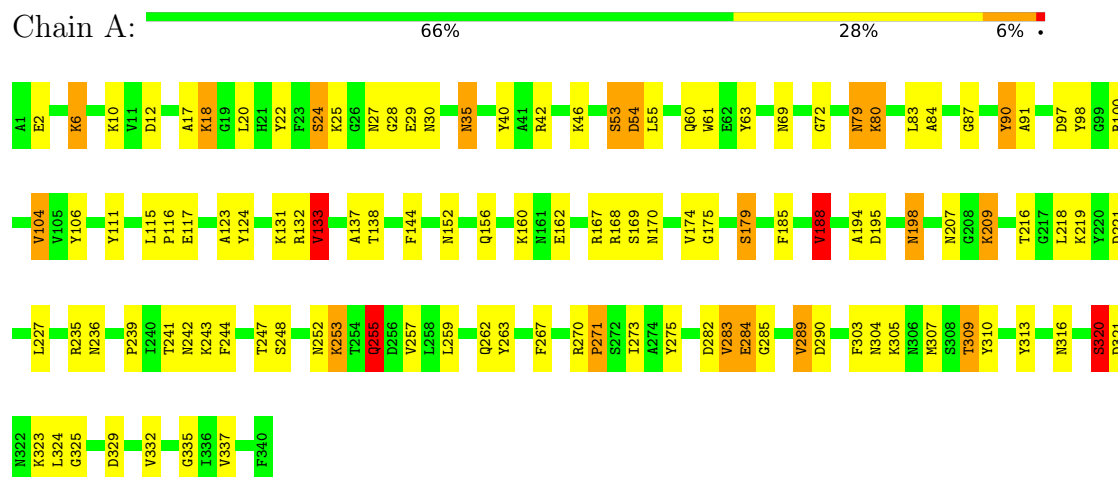
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		

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: OUTER MEMBRANE PROTEIN F



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.67Å 119.67Å 53.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00 8.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.00) 93.2 (8.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.264 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 90.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2640	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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	0.99	9/2690 (0.3%)	2.21	82/3635 (2.3%)

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	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	THR	C-N	-19.95	1.08	1.33
1	A	30	ASN	C-N	-19.82	1.06	1.33
1	A	285	GLY	C-N	-15.54	1.11	1.33
1	A	6	LYS	CA-CB	-11.71	1.33	1.53
1	A	242	ASN	C-N	-10.66	1.19	1.34
1	A	320	SER	C-N	-9.90	1.19	1.33
1	A	24	SER	C-N	-9.62	1.19	1.33
1	A	305	LYS	CB-CG	6.00	1.70	1.52
1	A	321	ASP	C-N	-6.00	1.25	1.33

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	VAL	O-C-N	-44.69	72.77	122.83
1	A	235	ARG	CD-NE-CZ	17.69	149.17	124.40
1	A	30	ASN	CA-C-N	15.28	147.47	122.87
1	A	30	ASN	C-N-CA	15.28	147.47	122.87
1	A	285	GLY	CA-C-N	15.24	137.91	122.97
1	A	285	GLY	C-N-CA	15.24	137.91	122.97
1	A	10	LYS	CA-CB-CG	12.60	139.30	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ASN	O-C-N	-11.75	107.90	122.35
1	A	54	ASP	CA-CB-CG	11.42	124.02	112.60
1	A	6	LYS	CB-CA-C	10.92	128.76	109.65
1	A	285	GLY	O-C-N	-10.91	113.98	122.71
1	A	46	LYS	CA-CB-CG	10.52	135.15	114.10
1	A	227	LEU	CA-C-O	-9.44	110.50	120.70
1	A	242	ASN	O-C-N	-8.84	111.46	122.68
1	A	221	ASP	CA-CB-CG	8.59	121.19	112.60
1	A	247	THR	CA-C-N	8.55	141.01	121.87
1	A	247	THR	C-N-CA	8.55	141.01	121.87
1	A	304	ASN	CA-CB-CG	8.32	120.92	112.60
1	A	247	THR	O-C-N	-8.17	113.36	122.84
1	A	104	VAL	N-CA-C	7.74	118.52	110.62
1	A	290	ASP	CA-CB-CG	7.58	120.18	112.60
1	A	18	LYS	CA-CB-CG	7.57	129.25	114.10
1	A	168	ARG	CD-NE-CZ	7.55	134.97	124.40
1	A	316	ASN	OD1-CG-ND2	7.50	130.10	122.60
1	A	198	ASN	CA-CB-CG	-7.33	105.27	112.60
1	A	262	GLN	OE1-CD-NE2	7.30	129.90	122.60
1	A	167	ARG	NE-CZ-NH2	7.21	125.69	119.20
1	A	152	ASN	CA-CB-CG	7.17	119.77	112.60
1	A	320	SER	O-C-N	-7.16	112.91	122.43
1	A	35	ASN	CA-CB-CG	7.14	119.74	112.60
1	A	255	GLN	N-CA-CB	7.09	121.71	110.65
1	A	69	ASN	CA-CB-CG	6.99	119.59	112.60
1	A	100	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	A	337	VAL	N-CA-C	6.90	117.83	107.75
1	A	69	ASN	O-C-N	-6.90	114.20	123.10
1	A	133	VAL	CB-CA-C	-6.85	100.68	110.82
1	A	104	VAL	CA-C-O	-6.85	113.83	120.95
1	A	132	ARG	NH1-CZ-NH2	6.83	128.19	119.30
1	A	79	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	323	LYS	CG-CD-CE	6.68	126.67	111.30
1	A	30	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	98	TYR	CA-C-O	-6.42	113.62	121.06
1	A	29	GLU	N-CA-C	6.37	119.04	111.33
1	A	132	ARG	NE-CZ-NH2	-6.37	113.47	119.20
1	A	144	PHE	CA-CB-CG	-6.32	107.48	113.80
1	A	244	PHE	CA-CB-CG	-6.21	107.59	113.80
1	A	28	GLY	CA-C-N	6.15	128.80	120.38
1	A	28	GLY	C-N-CA	6.15	128.80	120.38
1	A	329	ASP	CA-CB-CG	6.08	118.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	VAL	CB-CA-C	-5.98	100.01	110.71
1	A	316	ASN	N-CA-CB	-5.92	101.03	109.85
1	A	100	ARG	CA-C-O	-5.83	113.73	120.49
1	A	170	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	55	LEU	N-CA-C	5.79	117.84	108.34
1	A	209	LYS	CG-CD-CE	5.68	124.36	111.30
1	A	248	SER	N-CA-C	5.65	117.11	108.52
1	A	53	SER	CA-CB-OG	-5.64	99.82	111.10
1	A	179	SER	CA-C-O	5.64	127.31	120.99
1	A	271	PRO	CA-C-O	-5.64	114.79	121.67
1	A	20	LEU	CA-C-O	5.61	127.27	120.99
1	A	257	VAL	CB-CA-C	-5.58	101.47	110.28
1	A	267	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	195	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	42	ARG	CA-CB-CG	5.49	125.08	114.10
1	A	72	GLY	CA-C-N	5.45	131.96	121.54
1	A	72	GLY	C-N-CA	5.45	131.96	121.54
1	A	185	PHE	N-CA-CB	5.45	119.52	110.63
1	A	316	ASN	CB-CA-C	5.45	118.60	109.89
1	A	243	LYS	N-CA-C	5.42	117.94	111.71
1	A	22	TYR	CA-CB-CG	5.35	123.54	113.90
1	A	169	SER	N-CA-C	5.33	117.98	110.14
1	A	12	ASP	CA-C-O	-5.32	114.61	120.30
1	A	137	ALA	CA-C-O	-5.30	114.49	120.32
1	A	2	GLU	CA-C-O	-5.27	115.29	120.98
1	A	90	TYR	N-CA-C	5.25	117.20	108.02
1	A	106	TYR	CA-C-O	5.20	125.81	119.05
1	A	325	GLY	N-CA-C	-5.18	107.91	115.63
1	A	25	LYS	CA-C-O	5.18	128.46	121.89
1	A	236	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	100	ARG	CB-CG-CD	5.11	123.05	111.30
1	A	270	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	239	PRO	O-C-N	-5.06	117.43	123.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	VAL	Mainchain
1	A	17	ALA	Mainchain
1	A	194	ALA	Mainchain
1	A	283	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	320	SER	Mainchain

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	2634	0	2455	27	0
2	A	6	0	0	0	0
All	All	2640	0	2455	27	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 6.

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:A:179:SER:HB3	1:A:188:VAL:HG13	1.58	0.85
1:A:54:ASP:HB3	1:A:91:ALA:HB2	1.67	0.76
1:A:179:SER:CB	1:A:188:VAL:HG13	2.28	0.63
1:A:18:LYS:HD3	1:A:40:TYR:CZ	2.33	0.63
1:A:289:VAL:HG21	1:A:324:LEU:HG	1.81	0.62
1:A:259:LEU:HD12	1:A:275:TYR:HD2	1.70	0.56
1:A:24:SER:HB2	1:A:35:ASN:HB2	1.90	0.53
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.45	0.52
1:A:117:GLU:HB2	1:A:310:TYR:CE1	2.46	0.51
1:A:263:TYR:O	1:A:271:PRO:HD2	2.10	0.51
1:A:309:THR:HG22	1:A:335:GLY:O	2.11	0.50
1:A:115:LEU:HB3	1:A:116:PRO:HD2	1.94	0.50
1:A:313:TYR:CD1	1:A:332:VAL:HG22	2.49	0.47
1:A:255:GLN:HE21	1:A:255:GLN:HB3	1.59	0.46
1:A:253:LYS:HE3	1:A:282:ASP:OD2	2.16	0.46
1:A:123:ALA:O	1:A:131:LYS:HD2	2.16	0.45
1:A:61:TRP:HA	1:A:83:LEU:O	2.15	0.45
1:A:160:LYS:HD2	1:A:162:GLU:HG3	1.99	0.45
1:A:79:ASN:O	1:A:80:LYS:HB3	2.19	0.42
1:A:90:TYR:O	1:A:91:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HD13	1:A:273:ILE:HA	1.91	0.42
1:A:174:VAL:HG12	1:A:175:GLY:N	2.34	0.42
1:A:138:THR:OG1	1:A:156:GLN:HG3	2.20	0.41
1:A:87:GLY:HA3	1:A:97:ASP:HB3	2.01	0.41
1:A:111:TYR:CZ	1:A:219:LYS:HD3	2.55	0.40
1:A:60:GLN:O	1:A:84:ALA:HA	2.21	0.40
1:A:303:PHE:HB2	1:A:307:MET:HB3	2.03	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	338/340 (99%)	314 (93%)	23 (7%)	1 (0%)	36 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	GLU

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	264/264 (100%)	243 (92%)	21 (8%)	11 38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	27	ASN
1	A	53	SER
1	A	80	LYS
1	A	104	VAL
1	A	124	TYR
1	A	133	VAL
1	A	188	VAL
1	A	198	ASN
1	A	207	ASN
1	A	209	LYS
1	A	216	THR
1	A	218	LEU
1	A	241	THR
1	A	252	ASN
1	A	253	LYS
1	A	255	GLN
1	A	284	GLU
1	A	289	VAL
1	A	309	THR
1	A	320	SER

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

Mol	Chain	Res	Type
1	A	223	ASN
1	A	317	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	24:SER	C	25:LYS	N	1.19
1	A	242:ASN	C	243:LYS	N	1.19
1	A	320:SER	C	321:ASP	N	1.19
1	A	285:GLY	C	286:ILE	N	1.11
1	A	247:THR	C	248:SER	N	1.08
1	A	30:ASN	C	31:SER	N	1.06

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	326/340 (95%)	-0.69	0 100 100	14, 26, 49, 59	5 (1%)

There are no RSRZ outliers to report.

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.