



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:19 PM UTC

PDB ID : 1W4V / pdb_00001w4v
Title : structure of the oxidised form of human thioredoxin 2
Authors : Smeets, A.; Evrard, C.; Declercq, J.P.
Deposited on : 2004-07-30
Resolution : 1.80 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

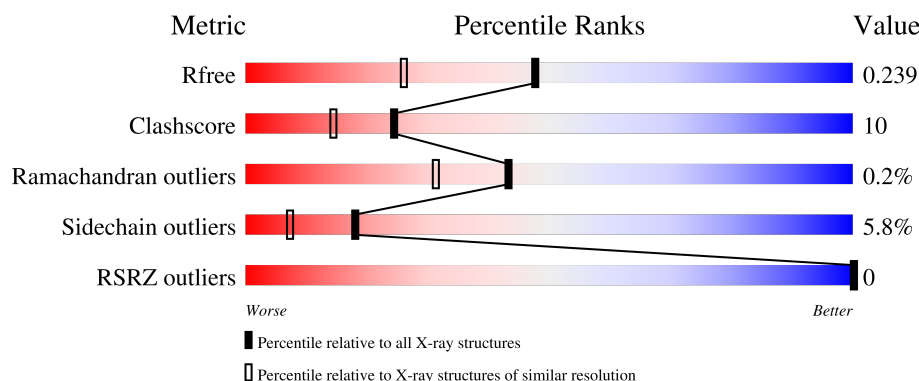
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	119	
1	B	119	
1	C	119	
1	D	119	
1	E	119	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	119	74% 12% • • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5837 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 THIOREDOXIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	0	0
			853	541	143	164	5			
1	B	110	Total	C	N	O	S	0	0	0
			853	541	143	164	5			
1	C	107	Total	C	N	O	S	0	0	0
			833	530	138	160	5			
1	D	109	Total	C	N	O	S	0	0	0
			843	535	140	163	5			
1	E	110	Total	C	N	O	S	0	0	0
			853	541	143	164	5			
1	F	108	Total	C	N	O	S	0	0	0
			839	533	139	162	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	127	Total	O	0	0
			127	127		
2	B	145	Total	O	0	0
			145	145		
2	C	101	Total	O	0	0
			101	101		
2	D	105	Total	O	0	0
			105	105		
2	E	135	Total	O	0	0
			135	135		
2	F	150	Total	O	0	0
			150	150		

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: THIOREDOXIN, MITOCHONDRIAL

Chain A: 



• Molecule 1: THIOREDOXIN, MITOCHONDRIAL

Chain B: 



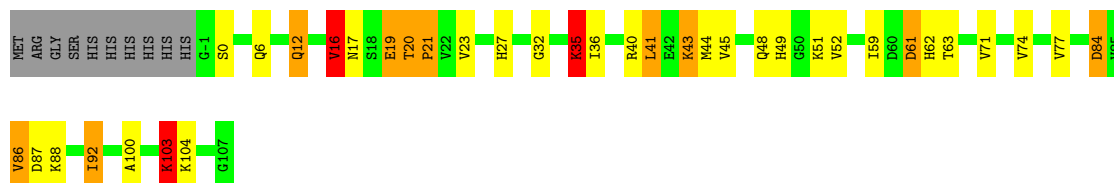
• Molecule 1: THIOREDOXIN, MITOCHONDRIAL

Chain C: 



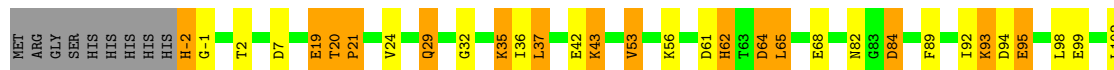
• Molecule 1: THIOREDOXIN, MITOCHONDRIAL

Chain D: 



• Molecule 1: THIOREDOXIN, MITOCHONDRIAL

Chain E: 





MET	ARG	GLY	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	GLY	SO	T1	T2	D10	F11	Q12	R13	R14	E19	T20	L11	E12	K17	Q18	G19	G50	K51	V52	D64	L65	M80	K88	D94	K103	G107
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.06Å 49.14Å 78.71Å 87.75° 82.77° 79.20°	Depositor
Resolution (Å)	19.32 – 1.80 19.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.32-1.80) 99.4 (19.32-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.169 , 0.228 0.214 , 0.239	Depositor DCC
R_{free} test set	3368 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5837	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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	0.62	0/869	1.67	8/1175 (0.7%)
1	B	0.66	0/869	1.58	5/1175 (0.4%)
1	C	0.61	1/848 (0.1%)	1.82	19/1147 (1.7%)
1	D	0.56	0/858	1.95	22/1160 (1.9%)
1	E	0.62	0/869	1.88	21/1175 (1.8%)
1	F	0.92	4/854 (0.5%)	1.87	17/1155 (1.5%)
All	All	0.67	5/5167 (0.1%)	1.80	92/6987 (1.3%)

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	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	50	GLY	N-CA	14.57	1.64	1.45
1	F	51	LYS	N-CA	14.08	1.64	1.46
1	F	80	MET	SD-CE	-5.56	1.65	1.79
1	F	50	GLY	C-O	5.32	1.31	1.24
1	C	50	GLY	N-CA	5.18	1.53	1.45

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	14	ARG	NE-CZ-NH2	-13.17	107.35	119.20
1	F	51	LYS	N-CA-C	-12.68	97.83	113.18
1	F	49	HIS	CA-C-N	9.56	136.41	120.91
1	F	49	HIS	C-N-CA	9.56	136.41	120.91
1	C	106	ILE	N-CA-C	9.52	119.53	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	84	ASP	CB-CA-C	-8.46	93.89	109.37
1	E	53	VAL	CG1-CB-CG2	7.99	128.38	110.80
1	F	20	THR	OG1-CB-CG2	-7.92	93.45	109.30
1	C	106	ILE	O-C-N	-7.89	113.81	121.94
1	E	19	GLU	CB-CG-CD	7.82	125.90	112.60
1	B	61	ASP	CA-CB-CG	7.78	120.38	112.60
1	C	14	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	E	68	GLU	N-CA-C	7.77	119.75	111.28
1	F	52	VAL	CA-C-O	7.66	129.11	121.45
1	D	6	GLN	OE1-CD-NE2	7.50	130.10	122.60
1	A	99	GLU	N-CA-C	-7.49	103.05	111.14
1	E	37	LEU	N-CA-C	7.21	119.14	111.28
1	D	71	VAL	CA-C-O	-6.98	112.48	120.65
1	E	20	THR	OG1-CB-CG2	-6.96	95.39	109.30
1	D	100	ALA	N-CA-C	6.94	118.85	111.28
1	A	29	GLN	CB-CG-CD	6.73	124.04	112.60
1	F	14	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	E	99	GLU	CA-CB-CG	-6.66	100.79	114.10
1	F	50	GLY	CA-C-N	-6.56	108.78	121.58
1	F	50	GLY	C-N-CA	-6.56	108.78	121.58
1	A	16	VAL	N-CA-C	-6.54	104.12	110.72
1	F	64	ASP	N-CA-C	6.53	118.06	111.07
1	C	17	ASN	N-CA-CB	6.47	120.33	110.44
1	D	84	ASP	CA-CB-CG	6.46	119.06	112.60
1	F	47	LYS	N-CA-C	6.44	120.60	112.87
1	C	53	VAL	CB-CA-C	6.39	120.10	110.90
1	C	14	ARG	N-CA-C	6.37	121.05	113.28
1	D	103	LYS	N-CA-C	-6.34	104.45	111.36
1	D	19	GLU	CB-CG-CD	6.30	123.32	112.60
1	D	35	LYS	CD-CE-NZ	6.28	131.99	111.90
1	A	23	VAL	CB-CA-C	6.23	120.12	110.83
1	D	0	SER	N-CA-CB	6.20	122.65	111.37
1	F	51	LYS	CA-C-O	6.17	127.00	119.11
1	C	17	ASN	CA-CB-CG	6.15	118.75	112.60
1	E	-1	GLY	O-C-N	-6.15	114.70	122.70
1	C	49	HIS	CA-C-N	6.15	133.64	121.53
1	C	49	HIS	C-N-CA	6.15	133.64	121.53
1	A	6	GLN	OE1-CD-NE2	6.14	128.74	122.60
1	D	17	ASN	N-CA-C	6.11	119.77	112.93
1	C	19	GLU	N-CA-C	-6.07	105.36	112.89
1	F	12	GLN	N-CA-C	-5.96	104.70	111.07
1	E	53	VAL	N-CA-CB	-5.93	100.97	111.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	LEU	CD1-CG-CD2	-5.91	97.81	110.80
1	F	20	THR	CB-CA-C	5.90	117.72	108.63
1	A	29	GLN	CA-CB-CG	5.86	125.81	114.10
1	C	53	VAL	N-CA-CB	-5.83	102.67	112.47
1	E	64	ASP	CB-CG-OD1	5.82	131.79	118.40
1	D	12	GLN	CA-CB-CG	5.79	125.68	114.10
1	E	99	GLU	N-CA-CB	5.77	118.61	110.12
1	C	1	THR	CA-CB-OG1	5.76	118.24	109.60
1	C	97	GLN	N-CA-C	-5.69	105.15	111.36
1	A	-1	GLY	N-CA-C	5.68	120.98	113.37
1	C	20	THR	N-CA-C	-5.68	102.28	110.40
1	E	32	GLY	CA-C-O	-5.67	113.41	121.52
1	E	21	PRO	CB-CA-C	5.67	118.65	111.39
1	C	1	THR	CA-CB-CG2	-5.60	100.99	110.50
1	B	83	GLY	N-CA-C	5.56	123.00	115.32
1	E	35	LYS	CG-CD-CE	5.54	124.05	111.30
1	E	93	LYS	CA-C-N	5.54	132.12	121.54
1	E	93	LYS	C-N-CA	5.54	132.12	121.54
1	B	95	GLU	N-CA-C	5.52	117.30	111.28
1	F	19	GLU	N-CA-CB	-5.51	102.01	110.44
1	E	95	GLU	N-CA-CB	5.48	118.11	109.94
1	D	92	ILE	CA-C-N	5.47	131.53	121.85
1	D	92	ILE	C-N-CA	5.47	131.53	121.85
1	E	84	ASP	N-CA-C	5.46	118.62	109.95
1	E	62	HIS	CA-CB-CG	-5.40	108.40	113.80
1	D	88	LYS	CA-CB-CG	5.38	124.86	114.10
1	D	61	ASP	N-CA-C	-5.37	106.77	113.38
1	E	93	LYS	CB-CG-CD	5.36	123.62	111.30
1	D	16	VAL	CG1-CB-CG2	-5.30	99.13	110.80
1	D	86	VAL	O-C-N	5.22	128.72	122.03
1	E	-2	HIS	CA-C-O	-5.21	111.94	120.80
1	D	36	ILE	N-CA-C	-5.17	106.64	111.45
1	C	8	GLY	O-C-N	-5.16	119.21	121.07
1	D	12	GLN	CB-CA-C	5.16	119.35	110.79
1	D	21	PRO	CB-CA-C	-5.13	104.82	111.39
1	B	82	ASN	N-CA-CB	5.13	118.95	111.62
1	C	16	VAL	N-CA-C	-5.13	105.50	110.42
1	D	61	ASP	OD1-CG-OD2	-5.09	110.69	122.90
1	F	94	ASP	N-CA-CB	5.09	117.71	110.44
1	D	43	LYS	CG-CD-CE	-5.08	99.61	111.30
1	F	41	LEU	CD1-CG-CD2	5.05	121.92	110.80
1	C	86	VAL	N-CA-C	5.05	118.94	113.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLU	N-CA-CB	5.04	117.53	110.12
1	D	21	PRO	N-CA-CB	5.03	107.55	103.32
1	B	23	VAL	CG1-CB-CG2	-5.02	99.75	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	106	ILE	Peptide

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	853	0	849	20	0
1	B	853	0	849	9	0
1	C	833	0	834	9	0
1	D	843	0	842	31	0
1	E	853	0	849	25	0
1	F	839	0	839	9	0
2	A	127	0	0	9	0
2	B	145	0	0	7	0
2	C	101	0	0	4	0
2	D	105	0	0	8	0
2	E	135	0	0	13	0
2	F	150	0	0	6	0
All	All	5837	0	5062	100	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 10.

All (100) 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:E:29:GLN:H	1:E:29:GLN:HE21	1.11	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:LYS:HG2	1:D:44:MET:CE	2.00	0.91
1:D:43:LYS:HG2	1:D:44:MET:HE3	1.60	0.82
1:C:2:THR:HG23	1:C:56:LYS:HE2	1.64	0.80
1:D:12:GLN:HA	1:D:16:VAL:CG2	2.13	0.78
1:C:1:THR:HG22	2:C:2001:HOH:O	1.82	0.78
1:D:20:THR:HG22	1:D:21:PRO:O	1.83	0.77
1:B:-2:HIS:HB3	2:B:2004:HOH:O	1.85	0.76
1:D:59:ILE:HD13	1:D:74:VAL:HG11	1.67	0.76
1:E:29:GLN:H	1:E:29:GLN:NE2	1.86	0.73
1:D:23:VAL:HG11	1:D:41:LEU:HD11	1.68	0.72
1:A:90:VAL:O	2:A:2106:HOH:O	2.07	0.72
1:E:37:LEU:HD12	1:E:98:LEU:HD11	1.71	0.71
1:D:12:GLN:O	1:D:16:VAL:HG23	1.92	0.69
1:D:44:MET:HA	1:D:44:MET:HE2	1.74	0.69
1:C:10:ASP:OD1	1:C:14:ARG:HD2	1.92	0.69
1:D:92:ILE:HG13	2:D:2039:HOH:O	1.93	0.68
1:F:10:ASP:OD1	1:F:14:ARG:HD2	1.93	0.68
1:A:27:HIS:HD2	2:A:2047:HOH:O	1.76	0.68
1:B:51:LYS:HE3	2:B:2084:HOH:O	1.93	0.67
1:D:49:HIS:HD2	2:D:2057:HOH:O	1.83	0.62
1:A:33:PRO:HB3	1:A:92:ILE:HG13	1.81	0.61
1:D:23:VAL:CG1	1:D:41:LEU:HD11	2.31	0.61
1:B:61:ASP:HB3	2:B:2093:HOH:O	2.03	0.58
1:F:50:GLY:CA	2:F:2091:HOH:O	2.51	0.58
1:E:43:LYS:NZ	2:E:2060:HOH:O	2.36	0.57
1:D:43:LYS:CG	1:D:44:MET:HE3	2.34	0.57
1:E:104:LYS:HE3	2:E:2046:HOH:O	2.05	0.56
1:E:20:THR:HG23	1:E:21:PRO:O	2.06	0.56
1:D:12:GLN:NE2	1:D:16:VAL:HG21	2.20	0.56
1:F:50:GLY:C	1:F:52:VAL:N	2.57	0.55
1:D:44:MET:HE2	1:D:44:MET:CA	2.36	0.55
1:A:51:LYS:HE2	2:A:2070:HOH:O	2.05	0.55
1:D:23:VAL:HG13	1:D:77:VAL:CG1	2.38	0.54
1:E:2:THR:OG1	1:E:56:LYS:NZ	2.40	0.54
1:F:50:GLY:HA2	2:F:2091:HOH:O	2.08	0.53
1:E:36:ILE:HD13	2:E:2018:HOH:O	2.07	0.53
1:D:61:ASP:HB2	1:D:62:HIS:CD2	2.43	0.53
1:D:27:HIS:HE1	2:D:2009:HOH:O	1.91	0.53
1:E:7:ASP:HA	1:E:62:HIS:HE1	1.73	0.53
1:E:37:LEU:CD1	1:E:98:LEU:HD11	2.38	0.53
1:E:92:ILE:HG13	1:E:93:LYS:H	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:THR:CG2	1:D:21:PRO:O	2.57	0.51
1:A:29:GLN:HG3	2:A:2075:HOH:O	2.10	0.51
1:D:32:GLY:HA2	1:D:35:LYS:HD3	1.92	0.51
1:F:47:LYS:HD2	2:F:2142:HOH:O	2.10	0.51
1:D:59:ILE:HD13	1:D:74:VAL:CG1	2.39	0.51
1:E:56:LYS:HE3	2:E:2010:HOH:O	2.10	0.50
1:A:99:GLU:HG2	1:A:103:LYS:HE3	1.94	0.50
1:A:23:VAL:HG13	1:A:77:VAL:CG1	2.41	0.50
1:E:84:ASP:HA	2:E:2106:HOH:O	2.11	0.50
1:B:88:LYS:NZ	2:B:2120:HOH:O	2.43	0.50
1:A:24:VAL:O	1:A:77:VAL:HA	2.13	0.49
1:D:49:HIS:CD2	2:D:2057:HOH:O	2.63	0.49
1:D:104:LYS:NZ	2:D:2101:HOH:O	2.31	0.49
1:D:103:LYS:HB3	1:D:103:LYS:HE3	1.52	0.48
1:A:35:LYS:NZ	1:D:84:ASP:OD2	2.35	0.48
1:E:82:ASN:ND2	2:E:2103:HOH:O	2.41	0.48
1:E:7:ASP:HA	1:E:62:HIS:CE1	2.49	0.48
1:C:1:THR:HA	1:C:53:VAL:HG23	1.94	0.48
1:E:64:ASP:HB3	2:E:2085:HOH:O	2.14	0.48
1:D:40:ARG:O	1:D:44:MET:HG2	2.14	0.47
1:F:50:GLY:N	2:F:2091:HOH:O	2.47	0.47
1:E:-2:HIS:CE1	2:E:2005:HOH:O	2.67	0.46
1:E:42:GLU:OE2	1:E:56:LYS:NZ	2.40	0.46
1:D:59:ILE:HG21	1:D:74:VAL:HG11	1.98	0.45
1:A:92:ILE:CD1	2:D:2102:HOH:O	2.65	0.45
1:B:27:HIS:HE1	2:B:2013:HOH:O	1.99	0.45
1:E:65:LEU:HD12	2:E:2090:HOH:O	2.18	0.44
1:A:36:ILE:HD11	1:D:86:VAL:HG21	1.98	0.44
1:F:103:LYS:HD3	2:F:2146:HOH:O	2.17	0.44
1:A:88:LYS:NZ	2:A:2105:HOH:O	2.49	0.44
1:E:29:GLN:HG3	2:E:2035:HOH:O	2.17	0.43
1:F:2:THR:HG21	1:F:42:GLU:HG2	2.00	0.43
1:C:49:HIS:CE1	2:C:2054:HOH:O	2.71	0.43
1:A:6:GLN:HG3	2:A:2014:HOH:O	2.18	0.43
1:D:12:GLN:HA	1:D:16:VAL:HG21	1.96	0.43
1:C:88:LYS:CE	2:C:2077:HOH:O	2.65	0.43
1:D:87:ASP:OD1	2:D:2083:HOH:O	2.22	0.43
1:A:92:ILE:HD13	1:A:92:ILE:HG21	1.85	0.42
1:C:52:VAL:HG23	1:C:106:ILE:HD11	2.01	0.42
1:A:-2:HIS:N	2:A:2003:HOH:O	2.52	0.42
1:F:88:LYS:NZ	2:F:2127:HOH:O	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PRO:HB3	1:A:92:ILE:CG1	2.47	0.42
1:A:6:GLN:C	1:A:62:HIS:HE1	2.28	0.42
1:B:61:ASP:CB	2:B:2093:HOH:O	2.63	0.42
1:D:45:VAL:HG13	1:D:52:VAL:HG13	2.01	0.41
1:E:61:ASP:HB2	1:E:62:HIS:HD2	1.84	0.41
1:A:27:HIS:HE1	2:A:2009:HOH:O	2.02	0.41
1:A:92:ILE:HD13	2:D:2102:HOH:O	2.19	0.41
1:B:27:HIS:HD2	2:B:2054:HOH:O	2.02	0.41
1:E:-2:HIS:HB3	2:E:2002:HOH:O	2.20	0.41
1:E:64:ASP:CG	2:E:2087:HOH:O	2.64	0.41
1:E:19:GLU:C	2:E:2039:HOH:O	2.63	0.41
1:E:89:PHE:CD1	1:E:93:LYS:HD3	2.56	0.41
1:A:-2:HIS:HD2	2:A:2003:HOH:O	2.04	0.41
1:D:48:GLN:O	1:D:51:LYS:HE2	2.21	0.41
1:B:81:LYS:HG3	1:C:36:ILE:HD11	2.02	0.41
1:C:88:LYS:NZ	2:C:2078:HOH:O	2.44	0.41
1:B:74:VAL:HA	1:B:75:PRO:C	2.46	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	108/119 (91%)	105 (97%)	3 (3%)	0	100	100
1	B	108/119 (91%)	105 (97%)	3 (3%)	0	100	100
1	C	105/119 (88%)	103 (98%)	2 (2%)	0	100	100
1	D	107/119 (90%)	103 (96%)	4 (4%)	0	100	100
1	E	108/119 (91%)	102 (94%)	5 (5%)	1 (1%)	14	5
1	F	106/119 (89%)	102 (96%)	4 (4%)	0	100	100
All	All	642/714 (90%)	620 (97%)	21 (3%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	94	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	95/103 (92%)	91 (96%)	4 (4%)	26	14
1	B	95/103 (92%)	93 (98%)	2 (2%)	47	36
1	C	93/103 (90%)	87 (94%)	6 (6%)	15	5
1	D	94/103 (91%)	87 (93%)	7 (7%)	13	4
1	E	95/103 (92%)	87 (92%)	8 (8%)	10	3
1	F	94/103 (91%)	88 (94%)	6 (6%)	16	6
All	All	566/618 (92%)	533 (94%)	33 (6%)	18	7

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	36	ILE
1	A	41	LEU
1	A	65	LEU
1	B	65	LEU
1	B	81	LYS
1	C	1	THR
1	C	2	THR
1	C	41	LEU
1	C	53	VAL
1	C	65	LEU
1	C	88	LYS
1	D	16	VAL
1	D	19	GLU
1	D	20	THR
1	D	35	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	41	LEU
1	D	63	THR
1	D	103	LYS
1	E	24	VAL
1	E	29	GLN
1	E	35	LYS
1	E	43	LYS
1	E	53	VAL
1	E	65	LEU
1	E	95	GLU
1	E	102	LEU
1	F	0	SER
1	F	14	ARG
1	F	41	LEU
1	F	47	LYS
1	F	65	LEU
1	F	103	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	27	HIS
1	A	62	HIS
1	A	82	ASN
1	B	4	ASN
1	B	6	GLN
1	B	27	HIS
1	C	4	ASN
1	C	48	GLN
1	D	12	GLN
1	D	27	HIS
1	D	62	HIS
1	D	82	ASN
1	E	17	ASN
1	E	29	GLN
1	E	48	GLN
1	E	62	HIS
1	F	4	ASN
1	F	17	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 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	110/119 (92%)	-1.53	0 100 100	7, 11, 18, 29	0
1	B	110/119 (92%)	-1.56	0 100 100	8, 11, 18, 32	0
1	C	107/119 (89%)	-1.48	0 100 100	7, 12, 19, 24	0
1	D	109/119 (91%)	-1.33	0 100 100	2, 6, 13, 16	0
1	E	110/119 (92%)	-1.47	0 100 100	4, 12, 21, 33	0
1	F	108/119 (90%)	-1.47	0 100 100	8, 12, 18, 29	0
All	All	654/714 (91%)	-1.47	0 100 100	2, 11, 19, 33	0

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.