



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:52 PM EDT

PDB ID : 7Q3K / pdb_00007q3k
Title : Computationally designed thioredoxin subjected to stability optimizing mutations.
Authors : Norrild, R.K.; Johansson, K.E.; O'Shea, C.; Lindorff-Larsen, K.; Winther, J.R.; Morth, J.P.
Deposited on : 2021-10-27
Resolution : 2.25 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

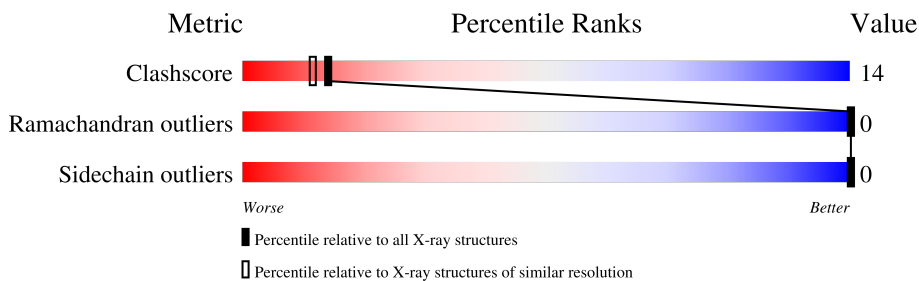
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	112	59% 34% 7%
1	B	112	67% 26% 7%
1	C	112	59% 34% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	201	-	-	X	-

2 Entry composition [i](#)

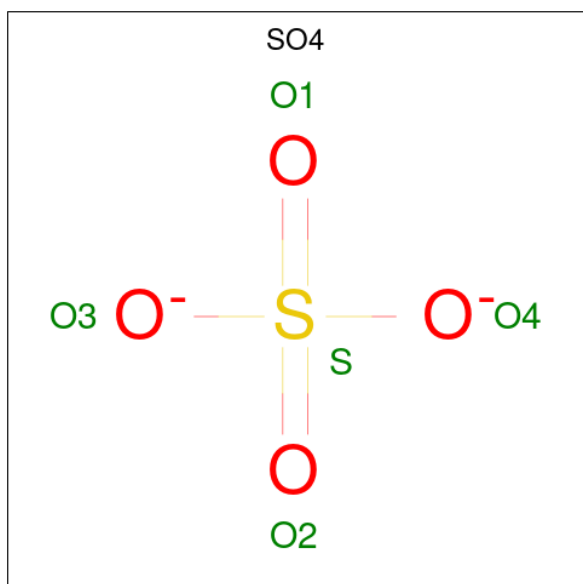
There are 2 unique types of molecules in this entry. The entry contains 2551 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 eMM9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			847	556	135	155	1			
1	B	104	Total	C	N	O	S	0	0	0
			847	556	135	155	1			
1	C	104	Total	C	N	O	S	0	0	0
			847	556	135	155	1			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

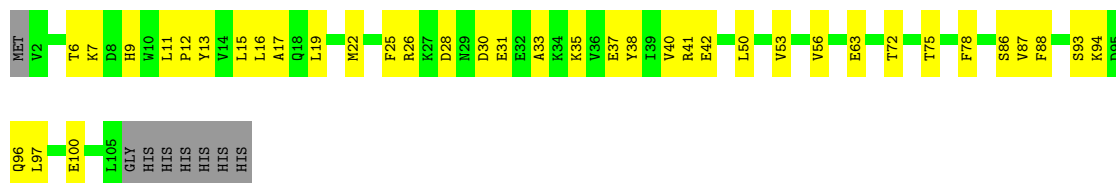
3 Residue-property plots [i](#)

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.

Note EDS failed to run properly.

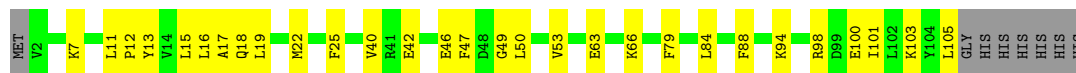
• Molecule 1: eMM9

Chain A: 



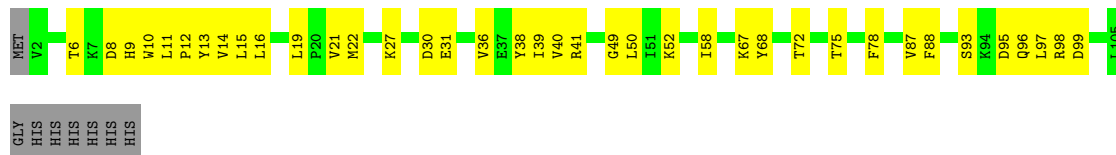
• Molecule 1: eMM9

Chain B: 



• Molecule 1: eMM9

Chain C: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	70.85Å 70.85Å 75.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.57 – 2.25	Depositor
% Data completeness (in resolution range)	99.9 (47.57-2.25)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.286 , 0.301	Depositor
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.855	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l 0.477 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
Total number of atoms	2551	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.51	0/863	0.61	0/1168
1	B	0.53	0/863	0.64	0/1168
1	C	0.39	0/863	0.63	0/1168
All	All	0.48	0/2589	0.63	0/3504

There are no bond length outliers.

There are no bond angle outliers.

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	847	0	879	26	0
1	B	847	0	879	24	0
1	C	847	0	879	25	0
2	A	5	0	0	0	0
2	B	5	0	0	2	0
All	All	2551	0	2637	74	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 14.

All (74) 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:88:PHE:HZ	1:A:100:GLU:HG3	1.35	0.91
1:A:88:PHE:CZ	1:A:100:GLU:HG3	2.12	0.85
1:B:66:LYS:NZ	1:C:8:ASP:OD2	2.16	0.79
1:B:7:LYS:HD3	1:B:63:GLU:HG3	1.65	0.78
1:C:12:PRO:HA	1:C:16:LEU:HD12	1.67	0.76
1:C:72:THR:O	1:C:75:THR:OG1	2.06	0.73
1:B:22:MET:HE3	1:B:40:VAL:HG13	1.70	0.72
1:A:42:GLU:OE1	1:A:94:LYS:NZ	2.17	0.71
1:A:22:MET:HE3	1:A:40:VAL:HG13	1.71	0.70
1:A:7:LYS:HD3	1:A:63:GLU:HG3	1.72	0.70
1:A:6:THR:HB	1:A:9:HIS:ND1	2.13	0.64
1:A:72:THR:O	1:A:75:THR:OG1	2.15	0.63
1:A:12:PRO:HA	1:A:16:LEU:HD12	1.81	0.61
1:C:9:HIS:HB3	1:C:13:TYR:CD2	2.37	0.59
1:A:11:LEU:HD12	1:A:15:LEU:HB2	1.84	0.59
1:B:88:PHE:CZ	1:B:100:GLU:HG3	2.37	0.59
1:C:95:ASP:O	1:C:99:ASP:HB2	2.04	0.57
1:A:38:TYR:HA	1:A:41:ARG:HD3	1.87	0.55
1:B:100:GLU:O	1:B:103:LYS:N	2.39	0.55
1:B:42:GLU:OE1	1:B:94:LYS:NZ	2.31	0.55
1:B:19:LEU:N	2:B:201:SO4:O3	2.27	0.55
1:C:93:SER:HB3	1:C:96:GLN:CD	2.32	0.54
1:B:13:TYR:O	1:B:17:ALA:HB2	2.08	0.53
1:A:11:LEU:HA	1:A:15:LEU:HB2	1.91	0.53
1:C:27:LYS:HG2	1:C:58:ILE:HD11	1.90	0.51
1:A:87:VAL:C	1:A:88:PHE:HD1	2.19	0.51
1:B:12:PRO:HA	1:B:16:LEU:HD12	1.92	0.51
1:B:49:GLY:O	1:B:50:LEU:HD12	2.12	0.49
1:C:22:MET:HE3	1:C:40:VAL:HG13	1.95	0.49
1:A:87:VAL:O	1:A:88:PHE:HD1	1.96	0.49
1:C:38:TYR:CD1	1:C:41:ARG:HD3	2.48	0.48
1:B:18:GLN:N	2:B:201:SO4:O3	2.46	0.48
1:C:11:LEU:HD12	1:C:15:LEU:HB2	1.96	0.48
1:A:78:PHE:HB2	1:A:86:SER:OG	2.14	0.48
1:C:30:ASP:OD1	1:C:31:GLU:N	2.46	0.47
1:B:11:LEU:HD12	1:B:15:LEU:HB2	1.96	0.47
1:C:10:TRP:CZ2	1:C:14:VAL:HG11	2.49	0.47
1:C:21:VAL:HG22	1:C:52:LYS:HB3	1.96	0.47
1:A:13:TYR:O	1:A:17:ALA:HB2	2.14	0.47
1:C:49:GLY:C	1:C:50:LEU:HD12	2.39	0.47
1:A:7:LYS:CD	1:A:63:GLU:HG3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:TRP:CZ3	1:C:14:VAL:HG21	2.50	0.46
1:A:30:ASP:HB3	1:A:33:ALA:HB3	1.96	0.46
1:C:36:VAL:HA	1:C:39:ILE:HD12	1.96	0.46
1:C:87:VAL:O	1:C:88:PHE:HD1	1.99	0.46
1:B:63:GLU:CD	1:B:63:GLU:H	2.24	0.46
1:A:37:GLU:O	1:A:41:ARG:HG3	2.16	0.45
1:C:36:VAL:O	1:C:40:VAL:HG23	2.17	0.45
1:A:25:PHE:CD1	1:A:56:VAL:HB	2.52	0.45
1:A:93:SER:O	1:A:96:GLN:N	2.49	0.45
1:A:88:PHE:CD2	1:A:97:LEU:HD23	2.52	0.44
1:B:50:LEU:HD23	1:B:105:LEU:HD21	2.00	0.44
1:B:47:PHE:CE2	1:B:101:ILE:HG21	2.53	0.43
1:B:49:GLY:C	1:B:50:LEU:HD12	2.43	0.43
1:C:6:THR:HB	1:C:9:HIS:ND1	2.33	0.43
1:C:12:PRO:HA	1:C:16:LEU:CD1	2.43	0.43
1:B:46:GLU:OE1	1:B:98:ARG:HD3	2.17	0.43
1:B:22:MET:O	1:B:53:VAL:HA	2.17	0.43
1:A:19:LEU:HD22	1:A:50:LEU:O	2.18	0.43
1:B:79:PHE:CD1	1:B:84:LEU:HA	2.54	0.42
1:B:88:PHE:CE2	1:B:100:GLU:HG3	2.55	0.42
1:C:19:LEU:HD22	1:C:50:LEU:O	2.19	0.42
1:B:25:PHE:N	1:B:25:PHE:CD1	2.87	0.42
1:B:50:LEU:HB3	1:B:105:LEU:HD21	2.02	0.42
1:C:95:ASP:OD1	1:C:98:ARG:NH2	2.48	0.42
1:A:26:ARG:NH1	1:A:28:ASP:OD1	2.50	0.41
1:C:78:PHE:HZ	1:C:97:LEU:HD22	1.85	0.41
1:B:25:PHE:N	1:B:25:PHE:HD1	2.18	0.41
1:A:31:GLU:O	1:A:35:LYS:HG2	2.21	0.41
1:C:67:LYS:HD3	1:C:68:TYR:CE2	2.55	0.41
1:C:9:HIS:HA	1:C:12:PRO:HG2	2.03	0.41
1:A:9:HIS:CD2	1:A:13:TYR:CZ	3.09	0.40
1:A:22:MET:O	1:A:53:VAL:HA	2.22	0.40
1:B:100:GLU:O	1:B:101:ILE:C	2.64	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	102/112 (91%)	94 (92%)	8 (8%)	0	100	100
1	B	102/112 (91%)	96 (94%)	6 (6%)	0	100	100
1	C	102/112 (91%)	96 (94%)	6 (6%)	0	100	100
All	All	306/336 (91%)	286 (94%)	20 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	94/101 (93%)	94 (100%)	0	100	100
1	B	94/101 (93%)	94 (100%)	0	100	100
1	C	94/101 (93%)	94 (100%)	0	100	100
All	All	282/303 (93%)	282 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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](#)

2 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.