



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:44 AM UTC

PDB ID : 4CQ4 / pdb_00004cq4
Title : C-terminal fragment of Af1503-sol: transmembrane receptor Af1503 from *Archaeoglobus fulgidus* engineered for solubility
Authors : Hartmann, M.D.; Dunin-Horkawicz, S.; Hulko, M.; Martin, J.; Coles, M.; Lupas, A.N.
Deposited on : 2014-02-11
Resolution : 1.70 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

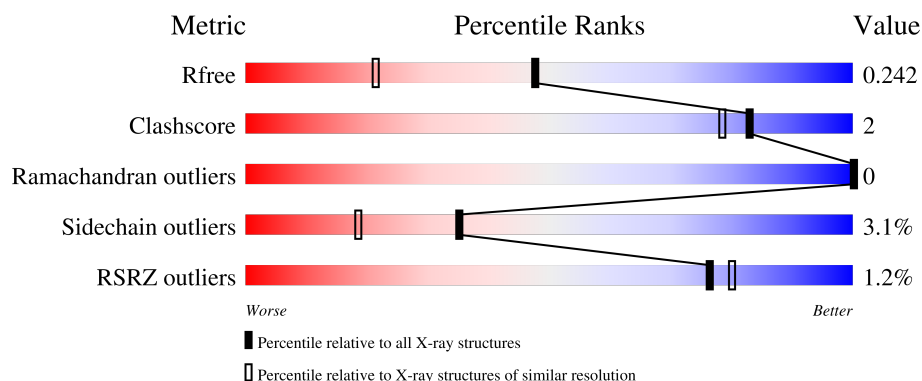
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	309	2% 31% 66%
1	B	309	29% 67%
1	C	309	30% 67%
1	D	309	29% 67%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3465 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 ENGINEERED VERSION OF TRANSMEMBRANE RECEPTOR AF1503.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			782	480	138	163	1			
1	B	102	Total	C	N	O	S	0	0	0
			747	462	129	155	1			
1	C	102	Total	C	N	O	S	0	2	0
			768	471	136	160	1			
1	D	102	Total	C	N	O	S	0	4	0
			786	483	138	164	1			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	LYS	TYR	engineered mutation	UNP O28769
A	256	ASN	TYR	engineered mutation	UNP O28769
A	257	LEU	ALA	engineered mutation	UNP O28769
A	259	THR	GLY	engineered mutation	UNP O28769
A	260	LEU	ILE	engineered mutation	UNP O28769
A	263	ASP	ALA	engineered mutation	UNP O28769
A	264	ARG	ILE	engineered mutation	UNP O28769
A	266	GLU	ILE	engineered mutation	UNP O28769
A	267	GLN	VAL	engineered mutation	UNP O28769
A	268	ILE	PHE	engineered mutation	UNP O28769
A	270	ASN	ILE	engineered mutation	UNP O28769
A	271	ASP	VAL	engineered mutation	UNP O28769
A	274	SER	VAL	engineered mutation	UNP O28769
A	275	THR	PHE	engineered mutation	UNP O28769
B	255	LYS	TYR	engineered mutation	UNP O28769
B	256	ASN	TYR	engineered mutation	UNP O28769
B	257	LEU	ALA	engineered mutation	UNP O28769
B	259	THR	GLY	engineered mutation	UNP O28769
B	260	LEU	ILE	engineered mutation	UNP O28769
B	263	ASP	ALA	engineered mutation	UNP O28769

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	ARG	ILE	engineered mutation	UNP O28769
B	266	GLU	ILE	engineered mutation	UNP O28769
B	267	GLN	VAL	engineered mutation	UNP O28769
B	268	ILE	PHE	engineered mutation	UNP O28769
B	270	ASN	ILE	engineered mutation	UNP O28769
B	271	ASP	VAL	engineered mutation	UNP O28769
B	274	SER	VAL	engineered mutation	UNP O28769
B	275	THR	PHE	engineered mutation	UNP O28769
C	255	LYS	TYR	engineered mutation	UNP O28769
C	256	ASN	TYR	engineered mutation	UNP O28769
C	257	LEU	ALA	engineered mutation	UNP O28769
C	259	THR	GLY	engineered mutation	UNP O28769
C	260	LEU	ILE	engineered mutation	UNP O28769
C	263	ASP	ALA	engineered mutation	UNP O28769
C	264	ARG	ILE	engineered mutation	UNP O28769
C	266	GLU	ILE	engineered mutation	UNP O28769
C	267	GLN	VAL	engineered mutation	UNP O28769
C	268	ILE	PHE	engineered mutation	UNP O28769
C	270	ASN	ILE	engineered mutation	UNP O28769
C	271	ASP	VAL	engineered mutation	UNP O28769
C	274	SER	VAL	engineered mutation	UNP O28769
C	275	THR	PHE	engineered mutation	UNP O28769
D	255	LYS	TYR	engineered mutation	UNP O28769
D	256	ASN	TYR	engineered mutation	UNP O28769
D	257	LEU	ALA	engineered mutation	UNP O28769
D	259	THR	GLY	engineered mutation	UNP O28769
D	260	LEU	ILE	engineered mutation	UNP O28769
D	263	ASP	ALA	engineered mutation	UNP O28769
D	264	ARG	ILE	engineered mutation	UNP O28769
D	266	GLU	ILE	engineered mutation	UNP O28769
D	267	GLN	VAL	engineered mutation	UNP O28769
D	268	ILE	PHE	engineered mutation	UNP O28769
D	270	ASN	ILE	engineered mutation	UNP O28769
D	271	ASP	VAL	engineered mutation	UNP O28769
D	274	SER	VAL	engineered mutation	UNP O28769
D	275	THR	PHE	engineered mutation	UNP O28769

- Molecule 2 is water.

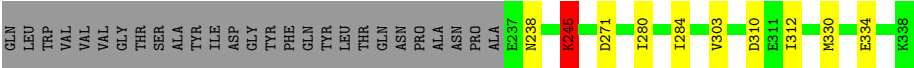
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	87	Total O 87 87	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	96	Total 96	O 96	0	0
2	C	103	Total 103	O 103	0	0
2	D	96	Total 96	O 96	0	0

GLU THR MET PRO GLU TYR ASN LEU LEU LEU LEU LYS ILE THR GLU ASN PRO GLU ALA PRO LYS ASN PRO VAL CYS GLY TYR THR HIS TRP ASP PRO GLU THR PRO GLU LYS GLU ILE PRO LYS TYR CYS HIS TYR THR THR ILE LYS VAL THR ASP PRO ILE LYS ASP GLY



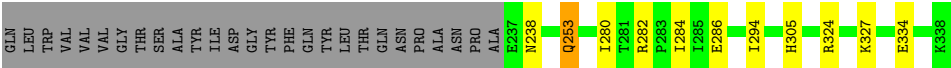
● Molecule 1: ENGINEERED VERSION OF TRANSMEMBRANE RECEPTOR AF1503



MET THR SER SER ALA GLU ALA LYS GLY VAL THR THR VAL SER GLN TYR LEU THR LYS VAL MET LYS ALA GLN ASP LEU LEU ALA THR ILE GLU ALA LYS THR MET LYS LEU ASN LYS THR MET THR THR PHE SER LEU

ILE GLN ASP PRO VAL PHE ARG SER SER LEU ALA GLN ARG TRP GLY ALA LYS TYR THR TRP VAL GLY ALA GLY ASN LYS VAL ALA GLY ARG ASP VAL VAL ILE LEU THR HIS PRO ALA PHE THR GLY GLN TYR LYS TYR LEU GLY VAL ASP VAL VAL MET LEU ARG TRP ASN

GLU THR MET PRO GLU TYR ASN LEU LEU LEU LEU LYS ILE THR GLU ASN PRO GLU ALA PRO LYS ASN PRO VAL CYS GLY TYR THR HIS TRP ASP PRO GLU THR PRO GLU LYS GLU ILE PRO LYS TYR LEU CYS HIS TYR TRP LYS PRO THR THR ILE VAL VAL THR ASP PRO ILE SER LYS TRP ASP GLY



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.07Å 48.04Å 95.19Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	37.67 – 1.70 37.67 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.67-1.70) 99.4 (37.67-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.243 0.198 , 0.242	Depositor DCC
R_{free} test set	2187 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3465	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.71% 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	1.11	0/785	1.16	5/1063 (0.5%)
1	B	1.17	1/749 (0.1%)	1.14	1/1013 (0.1%)
1	C	1.21	0/776	1.20	3/1048 (0.3%)
1	D	1.27	2/800 (0.2%)	1.27	1/1080 (0.1%)
All	All	1.19	3/3110 (0.1%)	1.19	10/4204 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	282	ARG	C-O	-6.07	1.18	1.24
1	D	294	ILE	N-CA	5.47	1.53	1.46
1	B	298	ASN	N-CA	5.01	1.52	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	SER	N-CA-C	5.91	117.39	111.07
1	C	245	LYS	N-CA-C	5.89	118.48	111.71
1	D	253	GLN	CB-CG-CD	-5.68	102.94	112.60
1	A	234	ASN	CA-C-N	-5.49	114.11	120.04
1	A	234	ASN	C-N-CA	-5.49	114.11	120.04
1	C	303	VAL	CA-C-N	5.44	125.41	120.03
1	C	303	VAL	C-N-CA	5.44	125.41	120.03
1	A	255	LYS	N-CA-C	5.43	117.19	111.28
1	A	303	VAL	CA-C-N	-5.19	115.38	120.52
1	A	303	VAL	C-N-CA	-5.19	115.38	120.52

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	782	0	793	4	0
1	B	747	0	757	5	0
1	C	768	0	789	7	0
1	D	786	0	816	3	0
2	A	87	0	0	1	0
2	B	96	0	0	0	0
2	C	103	0	0	1	0
2	D	96	0	0	1	0
All	All	3465	0	3155	15	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 2.

All (15) 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:335:GLU:OE2	2:A:2085:HOH:O	2.14	0.65
1:B:239:ILE:HD11	1:C:312:ILE:HG12	1.87	0.56
1:C:280:ILE:HG22	1:C:284:ILE:HD12	1.89	0.54
1:A:280:ILE:HD13	1:B:280:ILE:HG21	1.90	0.54
1:D:286:GLU:OE1	1:D:305:HIS:NE2	2.36	0.48
1:D:280:ILE:HG22	1:D:284[A]:ILE:HD12	1.96	0.48
1:A:241:SER:O	1:A:245:LYS:HD3	2.15	0.47
1:C:330:MET:O	1:C:334:GLU:HG3	2.16	0.46
1:B:282:ARG:CB	1:B:283:PRO:HD3	2.46	0.46
1:D:324:ARG:NH2	2:D:2063:HOH:O	2.50	0.45
1:B:237:GLU:O	1:C:310:ASP:HB3	2.18	0.43
1:C:271:ASP:OD2	2:C:2032:HOH:O	2.22	0.42
1:B:311:GLU:OE2	1:C:238:ASN:HB2	2.20	0.41
1:A:284:ILE:HD11	1:A:312:ILE:HD12	2.03	0.41

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	104/309 (34%)	103 (99%)	1 (1%)	0	100	100
1	B	100/309 (32%)	99 (99%)	1 (1%)	0	100	100
1	C	102/309 (33%)	101 (99%)	1 (1%)	0	100	100
1	D	104/309 (34%)	103 (99%)	1 (1%)	0	100	100
All	All	410/1236 (33%)	406 (99%)	4 (1%)	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	83/261 (32%)	82 (99%)	1 (1%)	63	51
1	B	78/261 (30%)	74 (95%)	4 (5%)	21	7
1	C	84/261 (32%)	83 (99%)	1 (1%)	63	51
1	D	88/261 (34%)	84 (96%)	4 (4%)	24	9
All	All	333/1044 (32%)	323 (97%)	10 (3%)	35	19

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	B	274	SER

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Mol	Chain	Res	Type
1	B	312	ILE
1	B	326	LEU
1	B	338	LYS
1	C	245	LYS
1	D	238	ASN
1	D	253	GLN
1	D	327	LYS
1	D	334	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	B	252	GLN
1	C	252	GLN
1	C	256	ASN
1	D	270	ASN
1	D	307	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 ⓘ

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 [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	106/309 (34%)	0.49	5 (4%) 36 40	16, 28, 42, 56	0
1	B	102/309 (33%)	0.25	0 100 100	16, 26, 39, 46	0
1	C	102/309 (33%)	-0.00	0 100 100	12, 22, 37, 59	2 (1%)
1	D	102/309 (33%)	-0.04	0 100 100	9, 21, 34, 46	4 (3%)
All	All	412/1236 (33%)	0.18	5 (1%) 76 80	9, 25, 40, 59	6 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	ALA	4.9
1	A	337	LEU	2.6
1	A	295	ALA	2.3
1	A	304	PRO	2.1
1	A	296	GLU	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.