



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:42 AM UTC

PDB ID : 6OKM / pdb_00006okm
Title : Human OX40R (TNFRSF4) bound to Fab 3C8
Authors : Boenig, G.; Ultsch, M.H.; Harris, S.F.
Deposited on : 2019-04-14
Resolution : 2.10 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

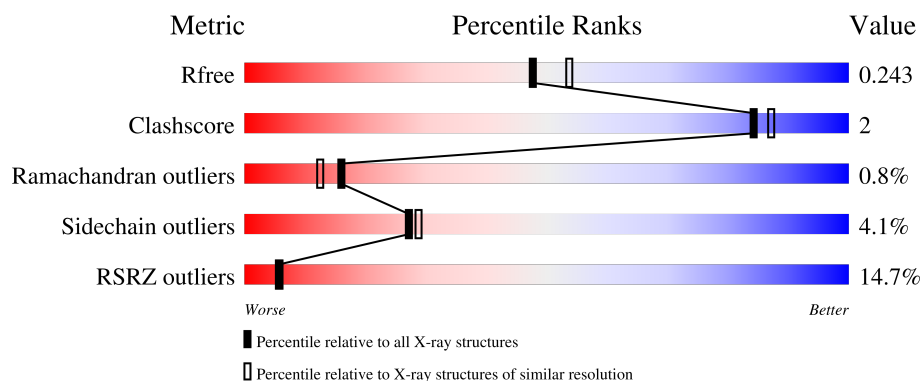
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	H	222	11% 87% 9% .
2	L	214	10% 91% 8% .
3	R	163	20% 58% 10% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4432 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 Fab 3C8 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	1	0
			1603	1013	265	321	4			

- Molecule 2 is a protein called Fab 3C8 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	1	0
			1660	1041	275	338	6			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	110	Total	C	N	O	S	0	0	0
			823	489	158	159	17			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	8	MET	-	initiating methionine	UNP P43489
R	9	GLY	-	expression tag	UNP P43489
R	10	SER	-	expression tag	UNP P43489
R	11	SER	-	expression tag	UNP P43489
R	12	HIS	-	expression tag	UNP P43489
R	13	HIS	-	expression tag	UNP P43489
R	14	HIS	-	expression tag	UNP P43489
R	15	HIS	-	expression tag	UNP P43489
R	16	HIS	-	expression tag	UNP P43489
R	17	HIS	-	expression tag	UNP P43489
R	18	SER	-	expression tag	UNP P43489
R	19	SER	-	expression tag	UNP P43489
R	20	GLY	-	expression tag	UNP P43489
R	21	LEU	-	expression tag	UNP P43489

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Chain	Residue	Modelled	Actual	Comment	Reference
R	22	VAL	-	expression tag	UNP P43489
R	23	PRO	-	expression tag	UNP P43489
R	24	ARG	-	expression tag	UNP P43489
R	25	GLY	-	expression tag	UNP P43489
R	26	SER	-	expression tag	UNP P43489
R	27	HIS	-	expression tag	UNP P43489
R	28	MET	-	expression tag	UNP P43489

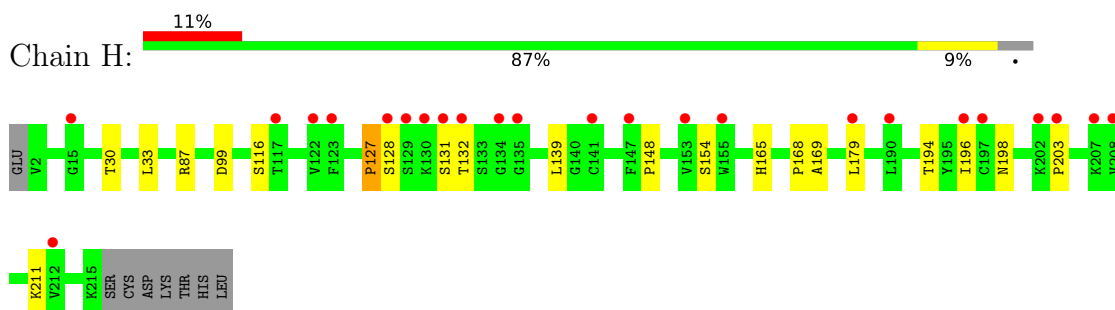
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	119	Total 119	O 119	0	0
4	L	184	Total 184	O 184	0	0
4	R	43	Total 43	O 43	0	0

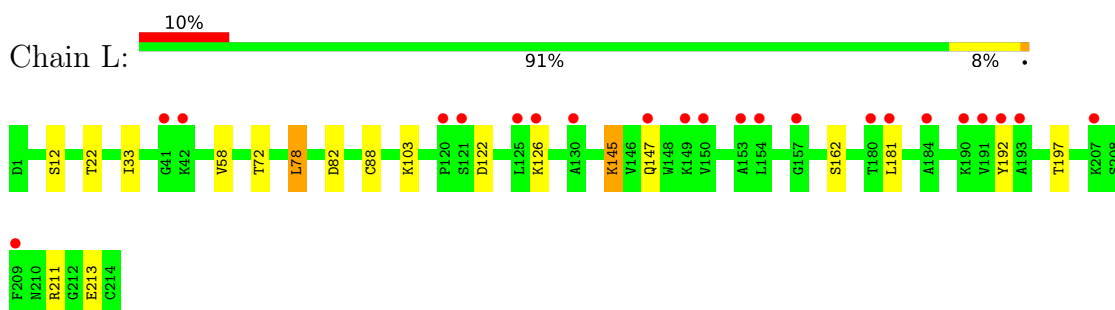
3 Residue-property plots [i](#)

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 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.

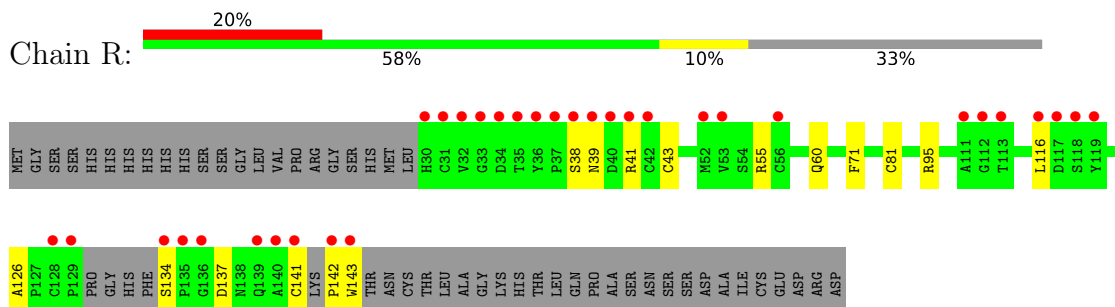
- Molecule 1: Fab 3C8 Heavy Chain



- Molecule 2: Fab 3C8 light chain



- Molecule 3: Tumor necrosis factor receptor superfamily member 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.01Å 117.01Å 118.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.89 – 2.10 47.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.89-2.10) 99.9 (47.89-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.211 , 0.238 0.218 , 0.243	Depositor DCC
R_{free} test set	2429 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.005 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4432	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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	H	0.85	0/1640	1.13	2/2237 (0.1%)
2	L	0.81	0/1699	1.11	1/2305 (0.0%)
3	R	0.85	0/843	1.21	2/1145 (0.2%)
All	All	0.83	0/4182	1.14	5/5687 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	38	SER	CA-C-N	5.88	132.76	121.54
3	R	38	SER	C-N-CA	5.88	132.76	121.54
2	L	58	VAL	N-CA-C	5.09	113.01	108.63
1	H	131	SER	CA-C-N	5.05	131.19	121.54
1	H	131	SER	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	H	1603	0	1581	8	0
2	L	1660	0	1590	8	0
3	R	823	0	754	3	0
4	H	119	0	0	1	0
4	L	184	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	43	0	0	0	0
All	All	4432	0	3925	18	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 (18) 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)
3:R:134:SER:HB2	3:R:141:CYS:HB3	1.59	0.85
3:R:116:LEU:HD21	3:R:126:ALA:HB2	1.80	0.64
1:H:168:PRO:HD2	2:L:162:SER:OG	2.03	0.58
2:L:78:LEU:HD22	2:L:82:ASP:HB2	1.89	0.54
2:L:122:ASP:O	2:L:126:LYS:HG2	2.11	0.49
1:H:194:THR:HG23	1:H:211:LYS:HE3	1.99	0.45
2:L:33:ILE:HD11	2:L:88:CYS:HB2	1.98	0.45
2:L:192:TYR:HD2	4:L:303:HOH:O	2.00	0.44
1:H:127:PRO:HB2	1:H:128:SER:H	1.58	0.43
2:L:145:LYS:HD3	2:L:197:THR:HB	2.00	0.43
1:H:33:LEU:HB2	1:H:99:ASP:HB3	2.01	0.43
1:H:165:HIS:HD2	4:H:411:HOH:O	1.99	0.43
1:H:169:ALA:HA	1:H:179:LEU:HB3	1.99	0.43
2:L:22:THR:HG22	2:L:72:THR:HG22	2.02	0.42
1:H:148:PRO:HD2	1:H:203:PRO:CB	2.50	0.42
2:L:145:LYS:HE2	2:L:147:GLN:HB2	2.02	0.41
1:H:154[B]:SER:OG	1:H:198:ASN:HB2	2.21	0.41
3:R:71:PHE:HB3	3:R:81:CYS:HB3	2.01	0.41

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	H	213/222 (96%)	200 (94%)	12 (6%)	1 (0%)	24	22
2	L	213/214 (100%)	208 (98%)	4 (2%)	1 (0%)	24	22
3	R	106/163 (65%)	102 (96%)	2 (2%)	2 (2%)	6	3
All	All	532/599 (89%)	510 (96%)	18 (3%)	4 (1%)	16	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	R	39	ASN
1	H	127	PRO
2	L	213	GLU
3	R	142	PRO

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	H	181/188 (96%)	175 (97%)	6 (3%)	33	37
2	L	190/189 (100%)	184 (97%)	6 (3%)	34	38
3	R	97/142 (68%)	90 (93%)	7 (7%)	13	11
All	All	468/519 (90%)	449 (96%)	19 (4%)	27	29

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	30	THR
1	H	87	ARG
1	H	116	SER
1	H	132	THR
1	H	139	LEU
1	H	196	ILE
2	L	12	SER
2	L	78	LEU
2	L	103	LYS

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Mol	Chain	Res	Type
2	L	145	LYS
2	L	181	LEU
2	L	211	ARG
3	R	41	ARG
3	R	43	CYS
3	R	55	ARG
3	R	60	GLN
3	R	95	ARG
3	R	137	ASP
3	R	143	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	160	GLN
2	L	210	ASN
3	R	30	HIS
3	R	39	ASN
3	R	50	ASN
3	R	60	GLN
3	R	114	GLN

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

6.1 Protein, DNA and RNA chains

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	H	214/222 (96%)	0.94	24 (11%)	10 10	27, 53, 81, 113	1 (0%)
2	L	214/214 (100%)	0.51	22 (10%)	12 12	19, 43, 75, 110	1 (0%)
3	R	110/163 (67%)	1.35	33 (30%)	1 1	37, 65, 123, 135	0
All	All	538/599 (89%)	0.85	79 (14%)	6 6	19, 51, 102, 135	2 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	132	THR	7.0
3	R	143	TRP	6.0
3	R	129	PRO	5.0
3	R	119	TYR	4.5
3	R	32	VAL	4.5
1	H	129	SER	4.4
2	L	190	LYS	4.1
2	L	157	GLY	3.8
1	H	208	VAL	3.8
1	H	122	VAL	3.7
3	R	42	CYS	3.7
3	R	33	GLY	3.6
3	R	140	ALA	3.5
3	R	37	PRO	3.4
1	H	196	ILE	3.4
3	R	116	LEU	3.4
1	H	212	VAL	3.3
2	L	184	ALA	3.3
2	L	41	GLY	3.3
3	R	142	PRO	3.3
3	R	41	ARG	3.3
3	R	53	VAL	3.2
3	R	117	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	134	GLY	3.2
3	R	135	PRO	3.1
2	L	42	LYS	3.1
2	L	125	LEU	3.0
3	R	134	SER	3.0
1	H	128	SER	2.9
3	R	36	TYR	2.9
3	R	128	CYS	2.9
1	H	123	PHE	2.9
3	R	56	CYS	2.8
2	L	150	VAL	2.8
2	L	126	LYS	2.7
3	R	139	GLN	2.7
2	L	191	VAL	2.7
2	L	153	ALA	2.6
3	R	30	HIS	2.6
1	H	131	SER	2.6
2	L	130	ALA	2.6
3	R	35	THR	2.6
2	L	154	LEU	2.6
1	H	147	PHE	2.6
1	H	141	CYS	2.5
3	R	118	SER	2.5
2	L	147	GLN	2.5
3	R	112	GLY	2.5
1	H	203	PRO	2.4
3	R	111	ALA	2.4
1	H	197	CYS	2.3
1	H	190	LEU	2.3
1	H	202	LYS	2.3
1	H	207	LYS	2.3
2	L	120	PRO	2.3
3	R	31	CYS	2.3
2	L	192	TYR	2.3
2	L	209	PHE	2.2
3	R	113	THR	2.2
3	R	34	ASP	2.2
3	R	40	ASP	2.2
1	H	15	GLY	2.2
1	H	179	LEU	2.2
2	L	121	SER	2.2
3	R	39	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	181	LEU	2.2
3	R	38	SER	2.2
1	H	117	THR	2.1
3	R	52	MET	2.1
1	H	155	TRP	2.1
1	H	153	VAL	2.1
2	L	149	LYS	2.1
2	L	207	LYS	2.1
2	L	193	ALA	2.1
2	L	180	THR	2.0
1	H	130	LYS	2.0
3	R	141	CYS	2.0
1	H	135	GLY	2.0
3	R	136	GLY	2.0

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.