



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7P3I / pdb_00007p3i
Title : Crystal structure of human CD40/TNFRSF5 in complex with the anti-CD40 DARPin protein
Authors : Malvezzi, F.; Mangold, S.; Hospodarsch, T.; Reichen, C.; Iss, C.; Lammens, A.; Krapp, S.; Domke, C.
Deposited on : 2021-07-07
Resolution : 2.29 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

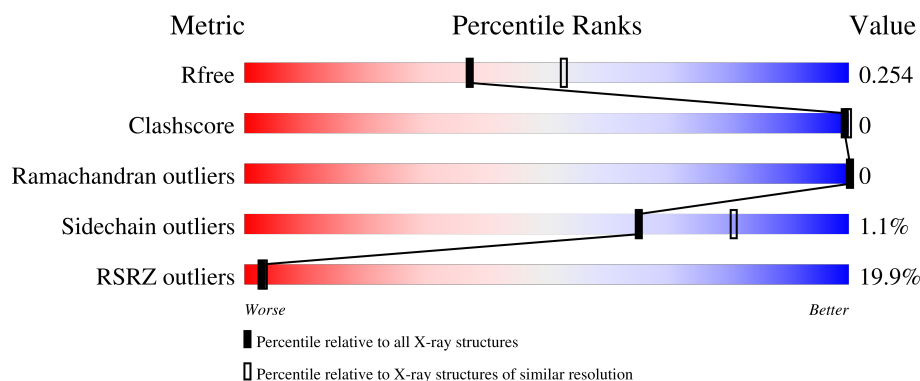
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	177	2% 92% 5%
1	C	177	7% 90% 7%
2	B	159	4% 96% .
2	D	159	67% 97% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5104 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 Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	11	0	0
			1282	780	219	263	20			
1	C	165	Total	C	N	O	S	55	1	0
			1267	771	217	259	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	LEU	-	expression tag	UNP P25942
A	195	VAL	-	expression tag	UNP P25942
A	196	PRO	-	expression tag	UNP P25942
A	197	ARG	-	expression tag	UNP P25942
C	194	LEU	-	expression tag	UNP P25942
C	195	VAL	-	expression tag	UNP P25942
C	196	PRO	-	expression tag	UNP P25942
C	197	ARG	-	expression tag	UNP P25942

- Molecule 2 is a protein called Darpin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	22	0	0
			1180	742	215	223			
2	D	156	Total	C	N	O	172	0	0
			1165	734	212	219			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total 78	O 78	0	0
4	B	76	Total 76	O 76	0	0
4	C	49	Total 49	O 49	0	0
4	D	5	Total 5	O 5	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.67Å 59.56Å 81.84Å 90.00° 106.99° 90.00°	Depositor
Resolution (Å)	92.61 – 2.29 92.61 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.8 (92.61-2.29) 97.8 (92.61-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.220 , 0.253 0.223 , 0.254	Depositor DCC
R_{free} test set	1962 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5104	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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

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

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	0.90	1/1310 (0.1%)	0.99	1/1779 (0.1%)
1	C	0.86	1/1294 (0.1%)	0.95	1/1757 (0.1%)
2	B	1.03	3/1199 (0.3%)	1.23	4/1625 (0.2%)
2	D	0.94	0/1184	1.10	1/1605 (0.1%)
All	All	0.93	5/4987 (0.1%)	1.07	7/6766 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	169	THR	CB-OG1	-7.81	1.31	1.43
1	A	25	ALA	CA-C	6.21	1.61	1.52
2	B	29	GLU	CG-CD	-5.67	1.37	1.52
2	B	12	SER	N-CA	5.08	1.52	1.46
2	B	37	GLY	C-N	5.00	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	GLY	CA-C-O	5.67	126.77	119.68
2	D	160	ASP	CA-CB-CG	5.67	118.27	112.60
2	B	61	GLU	CB-CG-CD	5.51	121.96	112.60
1	C	173	VAL	CA-CB-CG2	5.45	119.66	110.40
2	B	29	GLU	CB-CG-CD	5.17	121.39	112.60
2	B	37	GLY	O-C-N	-5.14	116.32	122.33
1	A	73	ARG	CB-CA-C	-5.03	103.34	111.28

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	A	1282	0	1173	0	0
1	C	1267	0	1160	1	0
2	B	1180	0	1193	0	0
2	D	1165	0	1180	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	78	0	0	0	0
4	B	76	0	0	0	0
4	C	49	0	0	0	0
4	D	5	0	0	0	0
All	All	5104	0	4706	1	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 0.

All (1) 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:C:29:LYS:HA	1:C:40:LEU:HD12	2.03	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	A	166/177 (94%)	165 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	164/177 (93%)	164 (100%)	0	0	100	100
2	B	157/159 (99%)	157 (100%)	0	0	100	100
2	D	154/159 (97%)	154 (100%)	0	0	100	100
All	All	641/672 (95%)	640 (100%)	1 (0%)	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	152/161 (94%)	149 (98%)	3 (2%)	48	67
1	C	150/161 (93%)	149 (99%)	1 (1%)	76	87
2	B	116/116 (100%)	114 (98%)	2 (2%)	53	72
2	D	115/116 (99%)	115 (100%)	0	100	100
All	All	533/554 (96%)	527 (99%)	6 (1%)	65	81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	36	GLN
1	A	68	LEU
2	B	32	GLU
2	B	152	LEU
1	C	68	LEU

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	42	GLN
1	C	36	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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	168/177 (94%)	0.30	4 (2%) 59 62	34, 56, 80, 116	6 (3%)
1	C	165/177 (93%)	0.67	13 (7%) 18 20	36, 61, 88, 109	21 (12%)
2	B	159/159 (100%)	0.30	6 (3%) 44 46	35, 52, 72, 84	11 (6%)
2	D	156/159 (98%)	2.83	106 (67%) 0 0	39, 101, 160, 182	55 (35%)
All	All	648/672 (96%)	1.00	129 (19%) 3 3	34, 61, 131, 182	93 (14%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	18	LEU	6.9
2	D	19	LEU	6.7
2	D	51	LEU	6.2
2	D	28	ASP	5.6
2	D	27	LEU	5.4
2	D	128	ILE	5.4
2	D	63	VAL	5.2
2	D	121	ALA	5.1
1	C	54	PHE	5.0
2	D	168	ALA	5.0
2	D	98	VAL	5.0
2	D	117	LEU	4.9
2	D	69	ALA	4.9
2	D	30	VAL	4.9
2	D	150	ALA	4.7
2	D	55	ALA	4.7
2	D	114	TRP	4.7
2	D	97	GLU	4.7
1	C	189	GLN	4.6
2	D	62	ILE	4.6
2	D	65	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	48	PHE	4.5
2	D	22	ALA	4.4
2	D	14	LEU	4.4
2	D	60	LEU	4.3
2	D	131	ILE	4.3
2	D	108	ALA	4.3
2	D	26	GLN	4.3
2	D	135	ALA	4.2
2	D	50	PRO	4.2
2	D	88	ALA	4.2
2	D	102	ALA	4.2
2	D	95	ILE	4.1
2	D	64	GLU	4.1
2	D	101	LYS	4.0
2	D	84	LEU	3.9
1	C	55	THR	3.9
2	D	122	TRP	3.9
2	D	106	VAL	3.7
2	D	54	ALA	3.7
2	D	40	VAL	3.7
2	D	141	ALA	3.6
2	D	53	ILE	3.6
2	D	157	GLY	3.6
2	D	61	GLU	3.4
2	D	93	LEU	3.4
2	D	15	GLY	3.4
2	D	21	ALA	3.3
2	D	38	ALA	3.3
2	D	20	GLN	3.3
2	D	109	LYS	3.3
2	D	75	ALA	3.3
2	D	96	VAL	3.3
2	D	139	VAL	3.3
2	B	11	GLY	3.3
2	D	49	THR	3.3
2	D	17	LYS	3.2
2	D	132	LEU	3.2
2	D	104	ALA	3.2
1	A	23	PRO	3.2
1	C	169	THR	3.2
2	D	45	THR	3.1
2	D	68	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	56	GLU	3.1
2	D	36	ALA	3.1
2	D	44	ASP	3.0
1	C	25	ALA	3.0
2	D	34	LEU	3.0
2	D	100	LEU	3.0
2	D	83	PRO	3.0
2	D	78	VAL	3.0
2	D	29	GLU	3.0
2	D	46	TRP	3.0
2	D	66	LEU	2.9
2	D	52	HIS	2.9
1	A	24	THR	2.9
2	D	33	LEU	2.9
2	D	67	LEU	2.9
2	D	140	ASN	2.9
2	D	89	HIS	2.8
2	B	12	SER	2.8
2	D	130	GLU	2.8
2	D	87	ALA	2.8
2	D	85	HIS	2.8
2	D	99	LEU	2.8
2	D	24	ALA	2.7
1	C	158	PHE	2.7
1	C	171	ASP	2.7
2	D	79	GLN	2.7
2	D	156	ALA	2.6
2	B	145	SER	2.6
2	D	13	ASP	2.5
2	D	142	GLN	2.5
2	D	31	ARG	2.5
2	D	81	ARG	2.5
1	C	32	LEU	2.5
1	C	59	CYS	2.4
2	D	164	VAL	2.4
2	D	35	LYS	2.4
2	D	160	ASP	2.4
2	D	161	ILE	2.4
2	D	47	GLY	2.4
1	A	34	ASN	2.3
1	C	48	VAL	2.3
2	D	127	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	23	ARG	2.3
2	D	119	LEU	2.3
1	A	186	CYS	2.3
2	D	165	LEU	2.2
2	D	80	GLY	2.2
2	B	97	GLU	2.2
2	D	42	ALA	2.2
2	D	86	ILE	2.2
2	D	113	GLY	2.2
2	B	65	VAL	2.1
2	D	73	VAL	2.1
2	D	145	SER	2.1
2	D	118	HIS	2.1
2	D	136	GLY	2.1
2	D	43	LYS	2.1
2	D	126	LEU	2.1
2	D	111	PHE	2.1
2	B	94	GLU	2.1
1	C	37	CYS	2.0
2	D	71	ALA	2.0
2	D	74	ASN	2.0
1	C	173	VAL	2.0
1	C	70[A]	THR	2.0
2	D	57	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	C	201	1/1	0.87	0.09	51,51,51,51	0
3	NA	A	201	1/1	0.88	0.09	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.