W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 19, 2023 – 01:58 AM EDT

PDB ID	:	5CIR
Title	:	Crystal structure of death receptor 4 (DR4; TNFFRSF10A) bound to TRAIL (TNFSF10)
Authors	:	Sheriff, S.
Deposited on	:	2015-07-13
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

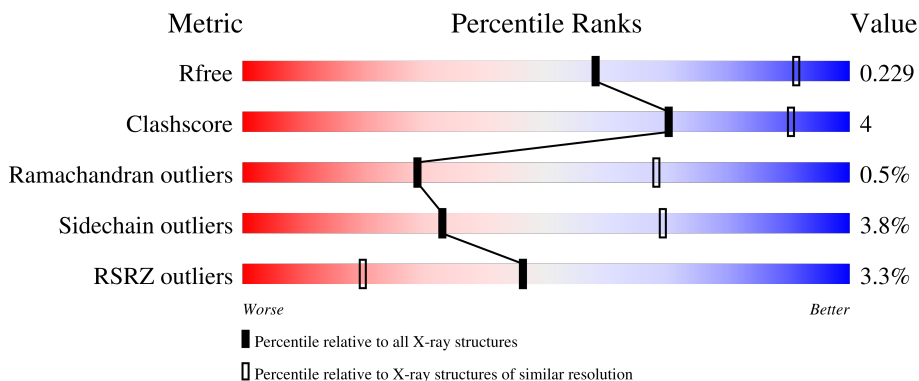|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.00 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.
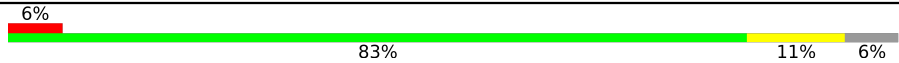
Metric	Percentile Ranks	Value
Rfree		0.229
Clashscore		4
Ramachandran outliers		0.5%
Sidechain outliers		3.8%
RSRZ outliers		3.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	169	% — 79% 9% · 12%
1	B	169	2% — 81% 8% · 11%
1	D	169	% — 79% 9% · 11%
2	E	108	8% — 82% 11% · 6%
2	F	108	4% — 80% 11% · 9%

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Mol	Chain	Length	Quality of chain
2	G	108	

6%

83% 11% 6%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5611 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 ligand superfamily member 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1183	764	201	214	4			
1	B	151	Total	C	N	O	S	0	0	0
			1181	765	193	219	4			
1	D	150	Total	C	N	O	S	0	0	0
			1178	763	193	218	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	MET	-	initiating methionine	UNP P50591
B	113	MET	-	initiating methionine	UNP P50591
D	113	MET	-	initiating methionine	UNP P50591

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	102	Total	C	N	O	S	0	0	0
			687	409	126	136	16			
2	F	98	Total	C	N	O	S	0	0	0
			674	398	126	135	15			
2	G	102	Total	C	N	O	S	0	0	0
			698	417	127	138	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	141	ARG	HIS	variant	UNP O00220
E	209	THR	ARG	variant	UNP O00220
F	141	ARG	HIS	variant	UNP O00220
F	209	THR	ARG	variant	UNP O00220
G	141	ARG	HIS	variant	UNP O00220

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Chain	Residue	Modelled	Actual	Comment	Reference
G	209	THR	ARG	variant	UNP O00220

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	O 2	0	0
5	D	4	Total 4	O 4	0	0
5	E	1	Total 1	O 1	0	0
5	F	1	Total 1	O 1	0	0

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.
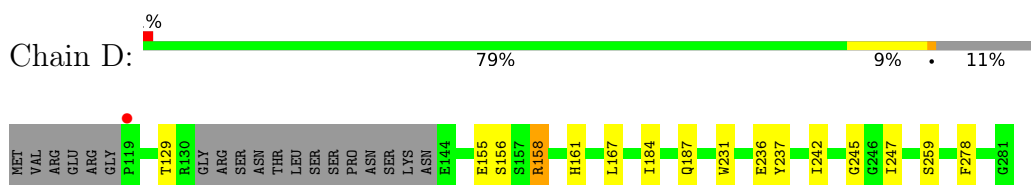
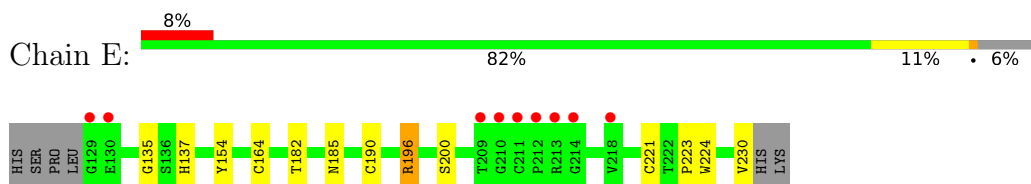• Molecule 1: Tumor necrosis factor ligand superfamily member 10
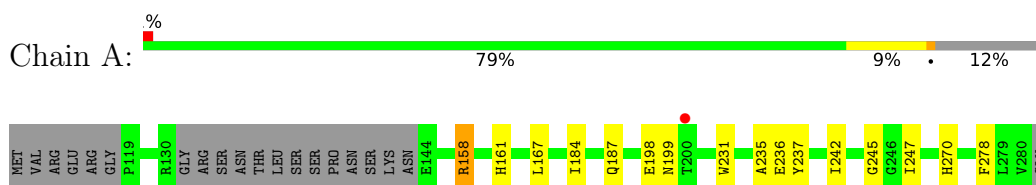
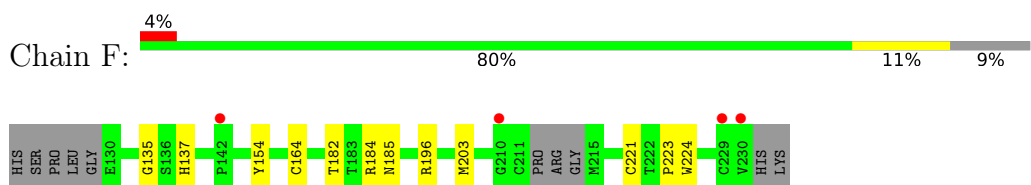• Molecule 1: Tumor necrosis factor ligand superfamily member 10
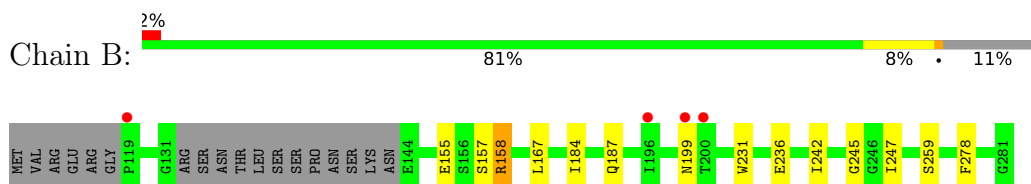
• Molecule 1: Tumor necrosis factor ligand superfamily member 10

• Molecule 2: Tumor necrosis factor receptor superfamily member 10A

• Molecule 2: Tumor necrosis factor receptor superfamily member 10A

• Molecule 2: Tumor necrosis factor receptor superfamily member 10A

Chain G:

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.60Å 87.60Å 107.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.60 – 3.00 27.60 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.60-3.00) 98.5 (27.60-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.86 (at 3.00Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5	Depositor
R, R_{free}	0.177 , 0.216 0.183 , 0.229	Depositor DCC
R_{free} test set	1058 reflections (6.34%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5611	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: ZN, CL

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	0.53	0/1214	0.72	0/1637
1	B	0.54	0/1212	0.72	0/1636
1	D	0.53	0/1209	0.73	0/1630
2	E	0.48	0/700	0.73	0/955
2	F	0.48	0/685	0.70	0/932
2	G	0.48	0/711	0.73	0/970
All	All	0.51	0/5731	0.72	0/7760

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	1183	0	1101	12	0
1	B	1181	0	1072	9	0
1	D	1178	0	1073	11	0
2	E	687	0	576	7	0
2	F	674	0	563	6	0
2	G	698	0	600	6	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	B	2	0	0	0	0
5	D	4	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	5611	0	4985	38	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 4.

The worst 5 of 38 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:247:ILE:HD11	1:B:278:PHE:HD2	1.52	0.75
1:B:247:ILE:HD11	1:D:278:PHE:HD2	1.58	0.68
1:A:247:ILE:HD11	1:B:278:PHE:CD2	2.35	0.61
1:A:278:PHE:HD2	1:D:247:ILE:HD11	1.65	0.60
1:B:157:SER:O	1:B:158:ARG:HB3	2.05	0.57

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	145/169 (86%)	137 (94%)	6 (4%)	2 (1%)	11	43
1	B	147/169 (87%)	139 (95%)	7 (5%)	1 (1%)	22	60
1	D	146/169 (86%)	140 (96%)	6 (4%)	0	100	100
2	E	100/108 (93%)	98 (98%)	2 (2%)	0	100	100
2	F	94/108 (87%)	92 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	100/108 (93%)	95 (95%)	4 (4%)	1 (1%)	15	53
All	All	732/831 (88%)	701 (96%)	27 (4%)	4 (0%)	29	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
2	G	217	LYS
1	A	198	GLU
1	B	199	ASN

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	117/150 (78%)	115 (98%)	2 (2%)	60	85
1	B	113/150 (75%)	109 (96%)	4 (4%)	36	71
1	D	112/150 (75%)	106 (95%)	6 (5%)	22	57
2	E	68/94 (72%)	65 (96%)	3 (4%)	28	65
2	F	68/94 (72%)	65 (96%)	3 (4%)	28	65
2	G	72/94 (77%)	69 (96%)	3 (4%)	30	66
All	All	550/732 (75%)	529 (96%)	21 (4%)	33	69

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	230	VAL
2	F	221	CYS
2	G	230	VAL
2	G	196	ARG
2	F	196	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	253	ASN
1	D	193	GLN
2	F	137	HIS
2	F	146	ASN
2	G	146	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

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 ⓘ

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 ⓘ

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	149/169 (88%)	-0.43	1 (0%)	87	69	17, 36, 74, 108	0
1	B	151/169 (89%)	-0.42	4 (2%)	56	27	11, 29, 74, 94	0
1	D	150/169 (88%)	-0.50	1 (0%)	87	69	15, 33, 65, 76	0
2	E	102/108 (94%)	0.17	9 (8%)	10	3	27, 50, 91, 100	0
2	F	98/108 (90%)	-0.03	4 (4%)	37	14	19, 39, 89, 114	0
2	G	102/108 (94%)	0.14	6 (5%)	22	7	28, 55, 86, 102	0
All	All	752/831 (90%)	-0.23	25 (3%)	46	20	11, 39, 86, 114	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	142	PRO	5.8
2	G	142	PRO	5.5
2	F	229	CYS	4.6
2	E	213	ARG	4.0
2	E	214	GLY	3.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides 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($Å^2$)	Q<0.9
3	ZN	A	301	1/1	0.99	0.11	37,37,37,37	0
4	CL	B	301	1/1	0.99	0.14	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.