wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2024 – 10:04 AM EDT

PDB ID	:	1D0G
Title	:	CRYSTAL STRUCTURE OF DEATH RECEPTOR 5 (DR5) BOUND TO APO2L/TRAIL
Authors	:	Hymowitz, S.G.; Christinger, H.W.; Fuh, G.; O'Connell, M.P.; Kelley, R.F.; Ashkenazi, A.; de Vos, A.M.
Deposited on	:	1999-09-09
Resolution	:	2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

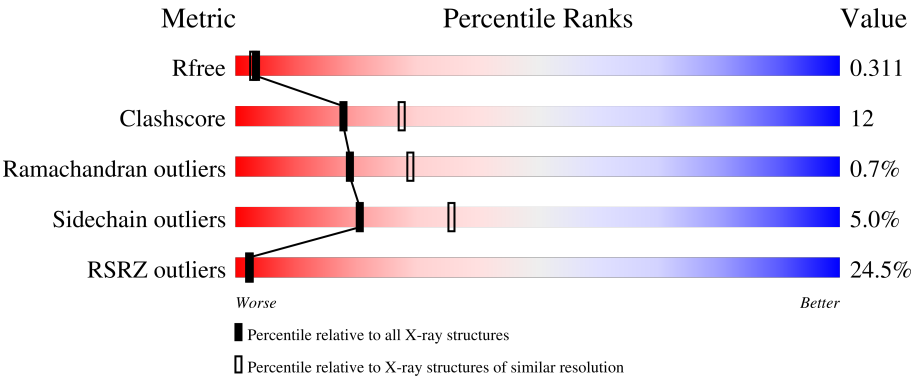
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	R	130	11% 58% 24% • 17%
1	S	130	42% 65% 17% • 15%
1	T	130	25% 55% 26% • 15%
2	A	168	16% 67% 20% • 10%
2	B	168	24% 67% 22% • 10%
2	D	168	14% 69% 19% •• 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6576 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 DEATH RECEPTOR-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	108	Total	C	N	O	S	0	0	0
			833	498	150	169	16			
1	S	110	Total	C	N	O	S	0	0	0
			849	506	152	175	16			
1	T	110	Total	C	N	O	S	0	0	0
			849	506	152	175	16			

- Molecule 2 is a protein called APOPTOSIS-2 LIGAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	151	Total	C	N	O	S	8	1	0
			1253	800	216	233	4			
2	B	151	Total	C	N	O	S	16	1	0
			1253	800	216	233	4			
2	D	151	Total	C	N	O	S	16	1	0
			1253	800	216	233	4			

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

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

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

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

- Molecule 5 is water.

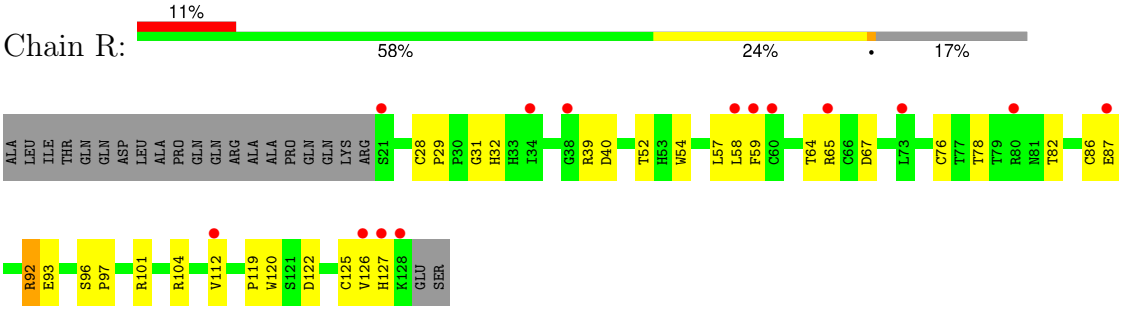
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	40	Total O 40 40	0	0
5	S	39	Total O 39 39	0	0
5	T	26	Total O 26 26	0	0
5	A	71	Total O 71 71	0	0
5	B	58	Total O 58 58	0	0
5	D	50	Total O 50 50	0	0

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. 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.

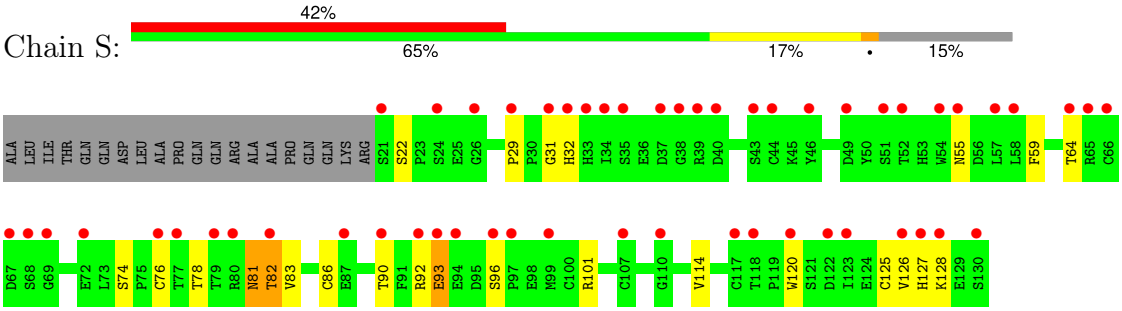
• Molecule 1: DEATH RECEPTOR-5

Chain R:



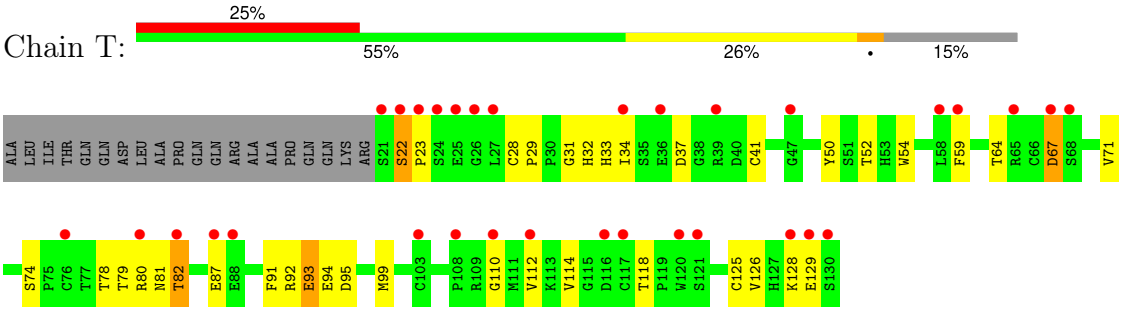
• Molecule 1: DEATH RECEPTOR-5

Chain S:



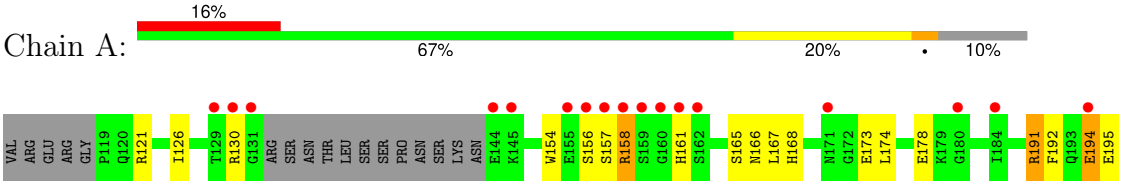
• Molecule 1: DEATH RECEPTOR-5

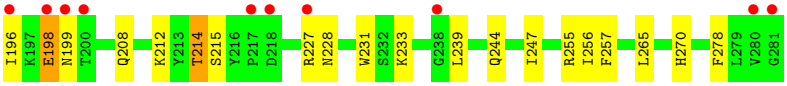
Chain T:



• Molecule 2: APOPTOSIS-2 LIGAND

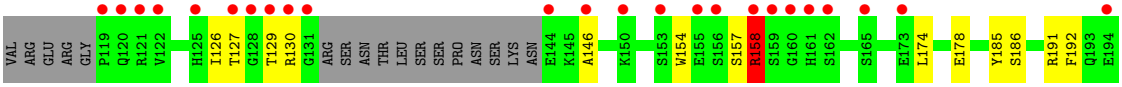
Chain A:

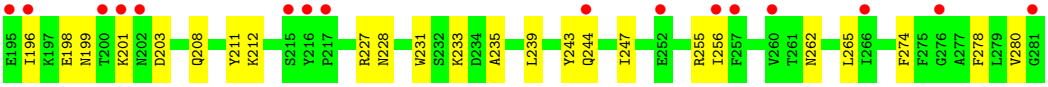




• Molecule 2: APOPTOSIS-2 LIGAND

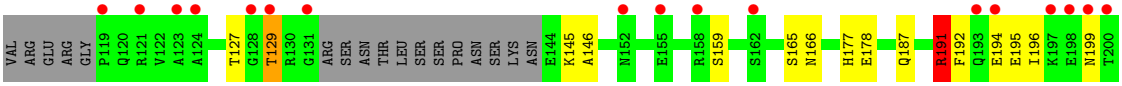
Chain B:

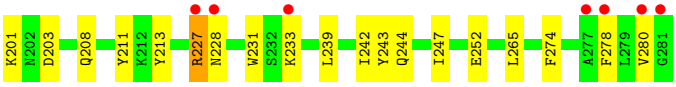




• Molecule 2: APOPTOSIS-2 LIGAND

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.82Å 111.02Å 130.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.40) 99.5 (30.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.88 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.222 , 0.267 0.282 , 0.311	Depositor DCC
R_{free} test set	3794 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6576	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, ZN

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	R	0.55	0/851	0.82	0/1150
1	S	0.51	0/867	0.77	0/1170
1	T	0.53	0/867	0.83	1/1170 (0.1%)
2	A	0.85	4/1288 (0.3%)	0.86	2/1729 (0.1%)
2	B	0.68	0/1288	0.90	4/1729 (0.2%)
2	D	0.64	0/1288	0.86	2/1729 (0.1%)
All	All	0.66	4/6449 (0.1%)	0.85	9/8677 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	198	GLU	CG-CD	13.26	1.71	1.51
2	A	198	GLU	CD-OE1	9.97	1.36	1.25
2	A	198	GLU	CD-OE2	6.88	1.33	1.25
2	A	194	GLU	CB-CG	-5.27	1.42	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	158	ARG	NE-CZ-NH2	-9.43	115.59	120.30
2	B	158	ARG	CG-CD-NE	6.93	126.36	111.80
2	B	158	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	T	129	GLU	N-CA-C	-6.62	93.14	111.00
2	D	191	ARG	NE-CZ-NH1	5.57	123.09	120.30

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	R	833	0	755	25	0
1	S	849	0	766	19	0
1	T	849	0	766	27	0
2	A	1253	0	1204	37	0
2	B	1253	0	1204	34	0
2	D	1253	0	1204	31	0
3	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	71	0	0	3	0
5	B	58	0	0	0	0
5	D	50	0	0	4	0
5	R	40	0	0	0	0
5	S	39	0	0	1	0
5	T	26	0	0	0	0
All	All	6576	0	5899	146	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 12.

The worst 5 of 146 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)
2:B:158:ARG:N	2:B:158:ARG:HD3	1.75	1.01
2:A:192:PHE:CD1	2:A:194:GLU:HG2	1.97	1.00
2:B:158:ARG:HD3	2:B:158:ARG:H	1.31	0.93
1:R:67:ASP:HB3	2:A:130:ARG:HH12	1.49	0.77
1:T:28:CYS:SG	1:T:34:ILE:HG22	2.26	0.76

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	R	106/130 (82%)	104 (98%)	2 (2%)	0	100	100
1	S	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
1	T	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
2	A	148/168 (88%)	138 (93%)	8 (5%)	2 (1%)	9	13
2	B	148/168 (88%)	140 (95%)	6 (4%)	2 (1%)	9	13
2	D	148/168 (88%)	137 (93%)	10 (7%)	1 (1%)	19	29
All	All	766/894 (86%)	731 (95%)	30 (4%)	5 (1%)	19	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	157	SER
2	B	198	GLU
2	A	198	GLU
2	B	196	ILE
2	D	196	ILE

5.3.2 Protein sidechains (i)

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	R	99/117 (85%)	94 (95%)	5 (5%)	20	35
1	S	101/117 (86%)	96 (95%)	5 (5%)	20	36
1	T	101/117 (86%)	95 (94%)	6 (6%)	16	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	134/149 (90%)	126 (94%)	8 (6%)	16 27
2	B	134/149 (90%)	130 (97%)	4 (3%)	36 57
2	D	134/149 (90%)	126 (94%)	8 (6%)	16 27
All	All	703/798 (88%)	667 (95%)	36 (5%)	20 35

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	145	LYS
2	D	233	LYS
2	D	178	GLU
2	D	213	TYR
1	T	67	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	208	GLN
2	B	270	HIS
2	A	208	GLN
2	B	228	ASN
1	T	127	HIS

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

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

Warning: The R factor obtained from EDS is 0.2878,which does not match the depositor's R factor of 0.222. Please interpret the results in this section carefully.

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, 95^{th} 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	R	108/130 (83%)	1.05	14 (12%)	9	7	32, 49, 78, 97	0
1	S	110/130 (84%)	2.12	54 (49%)	0	0	29, 47, 81, 96	0
1	T	110/130 (84%)	1.61	32 (29%)	1	1	34, 48, 84, 97	0
2	A	151/168 (89%)	1.29	27 (17%)	4	4	21, 38, 81, 92	3 (1%)
2	B	151/168 (89%)	1.61	40 (26%)	2	2	21, 34, 74, 98	5 (3%)
2	D	151/168 (89%)	1.05	24 (15%)	6	5	21, 38, 76, 95	5 (3%)
All	All	781/894 (87%)	1.43	191 (24%)	2	2	21, 43, 81, 98	13 (1%)

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	131	GLY	5.5
2	D	131	GLY	5.5
1	T	130	SER	4.9
1	T	110	GLY	4.9
2	D	198	GLU	4.9

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

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, 95^{th} 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	300	1/1	0.94	0.11	44,44,44,44	0
4	CL	B	400	1/1	0.96	0.06	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.