



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:35 AM UTC

PDB ID : 1ALY / pdb_00001aly
Title : CRYSTAL STRUCTURE OF HUMAN CD40 LIGAND
Authors : Karpusas, M.; Hsu, Y.M.; Thomas, D.
Deposited on : 1997-06-05
Resolution : 2.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

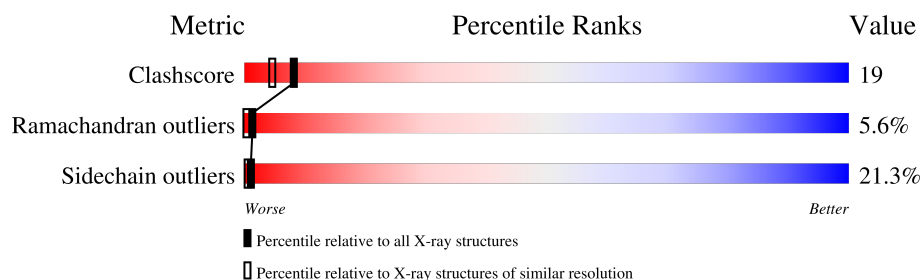
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	146	37% 39% 15% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1566 atoms, of which 389 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 CD40 LIGAND.

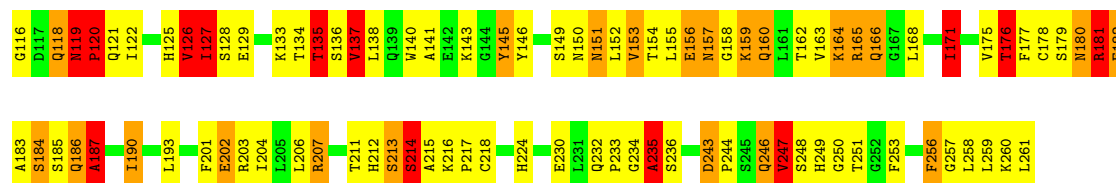
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	146	Total	C	H	N	O	S	0	0	0
			1374	701	261	195	213	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	64	Total	H	O	0	0
			192	128	64		

Note EDS was not executed.

Chain A: 37% 39% 15% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	77.17Å 77.17Å 90.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.50 – 2.00	Depositor
% Data completeness (in resolution range)	82.3 (7.50-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.223 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1566	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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	A	1.33	4/1136 (0.4%)	2.40	74/1538 (4.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	HIS	CG-ND1	-5.79	1.31	1.38
1	A	135	THR	CA-CB	5.63	1.60	1.53
1	A	125	HIS	CG-CD2	5.54	1.42	1.35
1	A	224	HIS	ND1-CE1	5.01	1.37	1.32

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PHE	N-CA-C	11.94	127.03	111.75
1	A	156	GLU	CA-C-N	-10.42	108.56	122.42
1	A	156	GLU	C-N-CA	-10.42	108.56	122.42
1	A	260	LYS	CA-C-N	-10.35	103.07	121.70
1	A	260	LYS	C-N-CA	-10.35	103.07	121.70
1	A	235	ALA	CA-C-N	9.74	140.46	122.74
1	A	235	ALA	C-N-CA	9.74	140.46	122.74
1	A	186	GLN	N-CA-C	9.52	126.58	114.31
1	A	203	ARG	CA-C-N	-7.92	112.15	122.37
1	A	203	ARG	C-N-CA	-7.92	112.15	122.37
1	A	151	ASN	N-CA-C	7.89	122.34	112.87
1	A	128	SER	N-CA-C	7.88	121.65	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	GLN	CA-C-N	-7.38	110.65	121.71
1	A	246	GLN	C-N-CA	-7.38	110.65	121.71
1	A	207	ARG	CD-NE-CZ	-7.31	114.17	124.40
1	A	256	PHE	CA-CB-CG	7.28	121.08	113.80
1	A	120	PRO	N-CA-C	7.26	127.42	112.47
1	A	157	ASN	CA-CB-CG	-7.24	105.36	112.60
1	A	201	PHE	CA-CB-CG	-7.07	106.73	113.80
1	A	129	GLU	CB-CG-CD	-6.97	100.75	112.60
1	A	181	ARG	CB-CG-CD	6.93	127.25	111.30
1	A	129	GLU	N-CA-C	6.86	120.48	108.75
1	A	184	SER	CB-CA-C	-6.66	102.49	111.88
1	A	126	VAL	CA-CB-CG1	6.65	121.71	110.40
1	A	181	ARG	N-CA-CB	-6.56	99.40	110.49
1	A	178	CYS	CA-C-N	-6.54	111.12	122.37
1	A	178	CYS	C-N-CA	-6.54	111.12	122.37
1	A	177	PHE	CA-C-N	-6.53	113.79	123.00
1	A	177	PHE	C-N-CA	-6.53	113.79	123.00
1	A	248	SER	N-CA-C	6.32	118.46	108.67
1	A	137	VAL	N-CA-C	6.28	117.15	109.30
1	A	154	THR	CA-C-O	6.26	128.33	121.06
1	A	149	SER	N-CA-C	6.18	120.43	113.01
1	A	175	VAL	CA-C-N	-6.18	112.14	122.64
1	A	175	VAL	C-N-CA	-6.18	112.14	122.64
1	A	243	ASP	CA-CB-CG	-6.15	106.45	112.60
1	A	166	GLN	CB-CG-CD	-6.11	102.21	112.60
1	A	213	SER	N-CA-C	6.10	123.80	110.80
1	A	180	ASN	CA-C-O	6.07	127.05	120.43
1	A	179	SER	N-CA-C	6.02	119.29	109.06
1	A	127	ILE	CA-C-N	-5.90	112.33	120.71
1	A	127	ILE	C-N-CA	-5.90	112.33	120.71
1	A	171	ILE	CB-CA-C	5.90	119.42	110.62
1	A	202	GLU	N-CA-CB	5.86	120.40	110.49
1	A	247	VAL	N-CA-C	5.86	117.18	109.21
1	A	119	ASN	CA-C-N	5.83	127.13	119.84
1	A	119	ASN	C-N-CA	5.83	127.13	119.84
1	A	183	ALA	N-CA-C	5.81	118.49	111.40
1	A	249	HIS	N-CA-C	5.80	120.16	111.81
1	A	184	SER	N-CA-CB	5.67	117.60	110.45
1	A	164	LYS	CA-C-O	5.67	126.06	119.32
1	A	145	TYR	N-CA-C	5.61	122.74	110.80
1	A	243	ASP	N-CA-C	5.60	118.75	109.79
1	A	182	GLU	N-CA-C	5.49	118.02	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	159	LYS	N-CA-CB	5.40	119.68	110.50
1	A	211	THR	CA-C-N	-5.34	111.79	120.71
1	A	211	THR	C-N-CA	-5.34	111.79	120.71
1	A	187	ALA	N-CA-C	5.33	125.93	111.00
1	A	138	LEU	N-CA-C	5.31	117.93	110.23
1	A	249	HIS	CA-CB-CG	-5.29	108.51	113.80
1	A	256	PHE	CA-C-N	-5.26	113.09	120.56
1	A	256	PHE	C-N-CA	-5.26	113.09	120.56
1	A	150	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	165	ARG	CA-C-N	-5.19	110.42	121.32
1	A	165	ARG	C-N-CA	-5.19	110.42	121.32
1	A	145	TYR	CA-CB-CG	-5.18	104.58	113.90
1	A	162	THR	N-CA-C	5.16	117.14	108.73
1	A	176	THR	CA-CB-OG1	5.15	117.33	109.60
1	A	260	LYS	N-CA-C	5.12	117.72	110.10
1	A	125	HIS	CA-CB-CG	-5.11	108.69	113.80
1	A	121	GLN	N-CA-CB	-5.04	101.97	110.49
1	A	159	LYS	CA-CB-CG	5.04	124.19	114.10
1	A	243	ASP	CB-CA-C	-5.03	104.62	111.21

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	PRO	Peptide
1	A	134	THR	Peptide
1	A	135	THR	Peptide
1	A	145	TYR	Sidechain
1	A	146	TYR	Sidechain
1	A	165	ARG	Sidechain
1	A	234	GLY	Peptide
1	A	235	ALA	Peptide

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	1113	261	1100	43	0
2	A	64	128	0	1	0
All	All	1177	389	1100	43	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 19.

All (43) 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:135:THR:HB	1:A:136:SER:HA	1.70	0.73
1:A:171:ILE:HD12	1:A:257:GLY:O	1.94	0.68
1:A:140:TRP:H	1:A:159:LYS:HG3	1.59	0.66
1:A:127:ILE:HD13	1:A:143:LYS:O	1.97	0.63
1:A:235:ALA:HB1	1:A:236:SER:HA	1.80	0.63
1:A:181:ARG:HG3	1:A:212:HIS:O	2.01	0.61
1:A:186:GLN:N	1:A:187:ALA:HA	2.15	0.60
1:A:176:THR:HG23	1:A:253:PHE:O	2.02	0.60
1:A:163:VAL:H	1:A:235:ALA:HB2	1.69	0.58
1:A:152:LEU:HA	1:A:164:LYS:HD2	1.85	0.57
1:A:156:GLU:O	1:A:158:GLY:HA3	2.03	0.57
1:A:181:ARG:HD3	1:A:216:LYS:O	2.06	0.56
1:A:186:GLN:H	1:A:187:ALA:HA	1.70	0.55
1:A:181:ARG:HG3	1:A:212:HIS:C	2.33	0.53
1:A:244:PRO:HA	1:A:247:VAL:HG13	1.90	0.53
1:A:116:GLY:N	1:A:119:ASN:OD1	2.42	0.52
1:A:180:ASN:HD22	1:A:217:PRO:HA	1.75	0.52
1:A:180:ASN:ND2	1:A:217:PRO:HA	2.25	0.51
1:A:181:ARG:HB3	1:A:214:SER:HA	1.93	0.51
1:A:181:ARG:HB3	1:A:214:SER:N	2.25	0.51
1:A:166:GLN:HB3	1:A:233:PRO:HD3	1.92	0.51
1:A:135:THR:HG22	1:A:137:VAL:O	2.11	0.50
1:A:190:ILE:HD11	1:A:207:ARG:HE	1.78	0.49
1:A:153:VAL:HG11	1:A:258:LEU:HD11	1.95	0.48
1:A:163:VAL:H	1:A:235:ALA:CB	2.27	0.48
1:A:232:GLN:NE2	1:A:232:GLN:HA	2.30	0.47
1:A:180:ASN:OD1	1:A:182:GLU:N	2.48	0.46
1:A:182:GLU:HB2	1:A:215:ALA:HB1	1.97	0.46
1:A:214:SER:HA	1:A:215:ALA:HA	1.59	0.45
1:A:181:ARG:HG2	1:A:216:LYS:HB2	1.97	0.45
1:A:181:ARG:H	1:A:181:ARG:CD	2.31	0.44
1:A:126:VAL:HG13	1:A:140:TRP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLN:HE21	1:A:160:GLN:HB3	1.60	0.43
1:A:250:GLY:HA2	1:A:253:PHE:HB2	2.01	0.43
1:A:122:ILE:HD13	2:A:537:HOH:O	2.18	0.42
1:A:250:GLY:HA2	1:A:253:PHE:H	1.83	0.42
1:A:157:ASN:HA	1:A:159:LYS:HA	2.02	0.42
1:A:157:ASN:ND2	1:A:159:LYS:HE3	2.35	0.41
1:A:181:ARG:HB3	1:A:213:SER:C	2.46	0.41
1:A:126:VAL:HG22	1:A:141:ALA:O	2.20	0.41
1:A:244:PRO:O	1:A:247:VAL:HG13	2.21	0.41
1:A:243:ASP:HB3	1:A:246:GLN:OE1	2.21	0.41
1:A:171:ILE:HD11	1:A:256:PHE:HE1	1.86	0.40

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	144/146 (99%)	126 (88%)	10 (7%)	8 (6%)	1 0

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	218	CYS
1	A	235	ALA
1	A	120	PRO
1	A	119	ASN
1	A	202	GLU
1	A	214	SER
1	A	187	ALA

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	122/122 (100%)	96 (79%)	26 (21%)	1 0

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	119	ASN
1	A	126	VAL
1	A	127	ILE
1	A	133	LYS
1	A	137	VAL
1	A	151	ASN
1	A	153	VAL
1	A	155	LEU
1	A	160	GLN
1	A	168	LEU
1	A	171	ILE
1	A	176	THR
1	A	181	ARG
1	A	184	SER
1	A	185	SER
1	A	190	ILE
1	A	193	LEU
1	A	204	ILE
1	A	206	LEU
1	A	214	SER
1	A	230	GLU
1	A	247	VAL
1	A	251	THR
1	A	259	LEU
1	A	261	LEU

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	119	ASN
1	A	151	ASN
1	A	160	GLN
1	A	212	HIS
1	A	220	GLN
1	A	232	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.