Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:42 pm BST

PDB ID	:	1ALY
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)

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

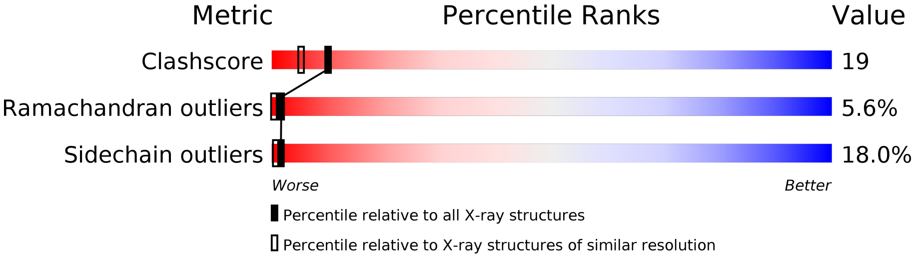
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	146	

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
			Total	C	H	N	O	S			
1	A	146	1374	701	261	195	213	4	0	0	0

- Molecule 2 is water.

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

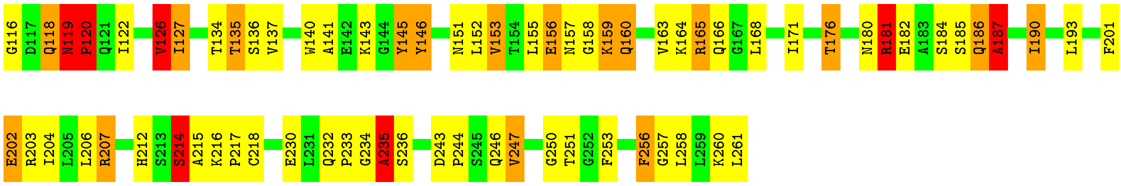
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

- Molecule 1: CD40 LIGAND

Chain A:



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	1.02	0/1136	1.82	23/1538 (1.5%)

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

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	A	146	TYR	CB-CG-CD2	-9.21	115.48	121.00
1	A	165	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	145	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	235	ALA	C-N-CA	7.50	140.46	121.70
1	A	260	LYS	C-N-CA	-7.45	103.07	121.70
1	A	256	PHE	CB-CG-CD2	-7.38	115.63	120.80
1	A	126	VAL	CA-CB-CG1	7.21	121.71	110.90
1	A	203	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	145	TYR	CG-CD1-CE1	-6.77	115.88	121.30
1	A	207	ARG	CD-NE-CZ	-6.74	114.17	123.60
1	A	181	ARG	N-CA-CB	-6.22	99.40	110.60
1	A	181	ARG	CB-CG-CD	6.02	127.25	111.60
1	A	201	PHE	N-CA-C	5.94	127.03	111.00
1	A	120	PRO	N-CA-C	5.89	127.42	112.10
1	A	186	GLN	N-CA-C	5.77	126.58	111.00
1	A	207	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	187	ALA	N-CA-C	5.53	125.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	GLU	N-CA-CB	5.44	120.40	110.60
1	A	145	TYR	CG-CD2-CE2	-5.28	117.08	121.30
1	A	156	GLU	C-N-CA	-5.25	108.56	121.70
1	A	146	TYR	CD1-CG-CD2	5.12	123.54	117.90
1	A	159	LYS	N-CA-CB	5.05	119.68	110.60

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	42	0
2	A	64	128	0	1	0
All	All	1177	389	1100	42	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 (42) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:181:ARG:HG3	1:A:212:HIS:C	2.33	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:CD	1:A:181:ARG:H	2.31	0.44
1:A:126:VAL:HG13	1:A:140:TRP:HB3	2.00	0.44
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: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 ⓘ

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	144/146 (99%)	126 (88%)	10 (7%)	8 (6%)	2 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%)	100 (82%)	22 (18%)	1 1

All (22) 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

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Mol	Chain	Res	Type
1	A	127	ILE
1	A	151	ASN
1	A	153	VAL
1	A	155	LEU
1	A	160	GLN
1	A	168	LEU
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	261	LEU

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

Mol	Chain	Res	Type
1	A	119	ASN
1	A	151	ASN
1	A	160	GLN
1	A	186	GLN
1	A	212	HIS
1	A	220	GLN
1	A	232	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.