Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 10:14 pm BST

PDB ID	:	2Q1E
Title	:	Altered dimer interface decreases stability in an amyloidogenic kappa1 Bence Jones protein.
Authors	:	Thompson, J.R.; Ramirez-Alvarado, M.; Baden, E.M.
Deposited on	:	2007-05-24
Resolution	:	2.55 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

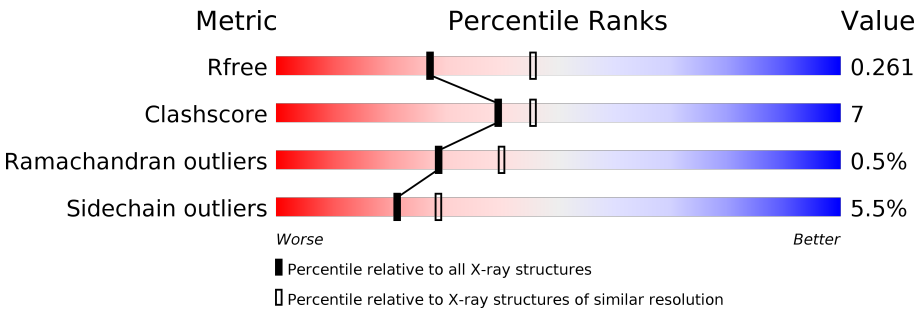
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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%

Mol	Chain	Length	Quality of chain
1	A	109	84% 14% ••
1	B	109	69% 25% 6%
1	C	109	86% 11% •
1	D	109	88% 10% •

2 Entry composition (i)

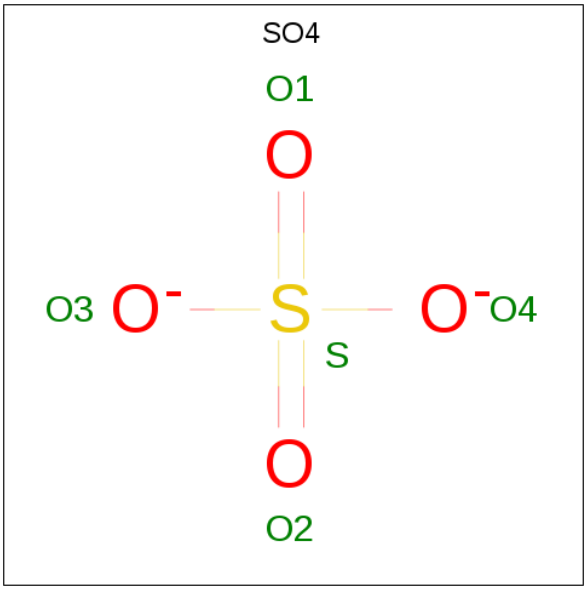
There are 3 unique types of molecules in this entry. The entry contains 3938 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Amyloidogenic immunoglobulin light chain protein AL-09.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	109	858	537	140	178	3	0	2	0
1	B	109	890	555	146	186	3	0	6	0
1	C	109	875	546	142	184	3	0	4	0
1	D	109	867	542	141	181	3	0	3	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

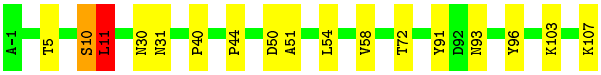
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	123	123	123	0	0
			Total	O		
3	B	60	60	60	0	0
			Total	O		
3	C	91	91	91	0	0
			Total	O		
3	D	169	169	169	0	0

3 Residue-property plots (i)

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.

- Molecule 1: Amyloidogenic immunoglobulin light chain protein AL-09

Chain A:



- Molecule 1: Amyloidogenic immunoglobulin light chain protein AL-09

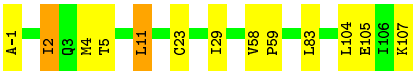
Chain B:

- Molecule 1: Amyloidogenic immunoglobulin light chain protein AL-09

Chain C:

- Molecule 1: Amyloidogenic immunoglobulin light chain protein AL-09

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	176.05Å 176.05Å 176.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.21 – 2.55 35.21 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.21-2.55) 97.9 (35.21-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	6.11 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.206 0.232 , 0.261	Depositor DCC
R_{free} test set	529 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3938	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0480e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.91	0/876	0.88	2/1190 (0.2%)
1	B	0.81	0/907	0.89	2/1228 (0.2%)
1	C	0.84	0/892	0.90	3/1209 (0.2%)
1	D	0.98	1/884 (0.1%)	0.95	2/1198 (0.2%)
All	All	0.89	1/3559 (0.0%)	0.91	9/4825 (0.2%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	105	GLU	CD-OE2	7.05	1.33	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	11	LEU	CA-CB-CG	10.33	139.07	115.30
1	C	11	LEU	CA-CB-CG	8.85	135.66	115.30
1	A	11	LEU	CA-CB-CG	8.52	134.90	115.30
1	C	1	ASP	CB-CG-OD1	8.43	125.89	118.30
1	C	1	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	B	11	LEU	CA-CB-CG	7.61	132.80	115.30
1	D	11	LEU	CB-CG-CD1	-6.43	100.07	111.00
1	B	1	ASP	CB-CG-OD1	6.27	123.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	LEU	CB-CG-CD1	-5.29	102.01	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	-1	ALA	Peptide

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	858	0	823	11	0
1	B	890	0	853	22	0
1	C	875	0	835	13	0
1	D	867	0	832	10	0
2	A	5	0	0	0	0
3	A	123	0	0	3	1
3	B	60	0	0	5	1
3	C	91	0	0	3	0
3	D	169	0	0	3	0
All	All	3938	0	3343	51	1

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 7.

All (51) 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:42:GLN:O	1:D:-1:ALA:CB	2.19	0.90
1:D:5[B]:THR:HG22	3:D:166:HOH:O	1.73	0.88
1:C:42:GLN:O	1:D:-1:ALA:HB2	1.73	0.88
1:B:34:ILE:HD12	1:B:91:TYR:CE1	2.21	0.75
1:C:5[A]:THR:HG22	3:C:160:HOH:O	1.88	0.73
1:A:107:LYS:OXT	3:A:151:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PRO:O	3:A:187:HOH:O	2.07	0.72
1:B:57:GLY:O	3:B:132:HOH:O	2.08	0.72
1:B:5[B]:THR:CG2	3:B:125:HOH:O	2.39	0.71
1:C:106:ILE:O	1:C:107[B]:LYS:HB2	1.93	0.69
1:D:107[B]:LYS:HG2	3:D:253:HOH:O	1.94	0.68
1:B:84:ALA:HB3	1:B:86:TYR:CE2	2.29	0.66
1:A:44:PRO:HG2	1:B:94:LEU:O	1.96	0.64
1:C:42:GLN:C	1:D:-1:ALA:HB2	2.20	0.62
1:B:33:LEU:HD22	1:B:71:PHE:CG	2.38	0.59
1:C:72:THR:HG22	3:C:161:HOH:O	2.04	0.57
1:B:15:VAL:HG23	3:B:144:HOH:O	2.06	0.54
1:B:41:GLY:O	1:B:42:GLN:HB2	2.08	0.54
1:B:34:ILE:HD12	1:B:91:TYR:CD1	2.42	0.54
1:B:34:ILE:HG12	1:B:46:LEU:HD13	1.91	0.53
1:B:5[B]:THR:HG23	3:B:125:HOH:O	2.02	0.53
1:B:40:PRO:O	1:B:41:GLY:O	2.26	0.53
1:C:83:LEU:HB2	1:C:106:ILE:HD12	1.90	0.53
1:B:5[B]:THR:HG22	1:B:24:GLN:HB3	1.91	0.52
1:C:107[A]:LYS:NZ	3:C:153:HOH:O	2.44	0.50
1:B:106:ILE:O	1:B:107[B]:LYS:HB3	2.12	0.50
1:C:42:GLN:O	1:D:-1:ALA:HB3	2.07	0.50
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.94	0.49
1:C:106:ILE:O	1:C:107[A]:LYS:HB2	2.12	0.48
1:A:72:THR:HG22	3:A:140:HOH:O	2.13	0.47
1:B:83:LEU:C	1:B:83:LEU:HD23	2.35	0.47
1:A:30:ASN:HB3	1:A:31[A]:ASN:H	1.55	0.47
1:B:54:LEU:HD11	1:B:62:PHE:O	2.14	0.47
1:B:48:ILE:HG21	1:B:51:ALA:O	2.14	0.46
1:A:30:ASN:HB3	1:A:31[B]:ASN:H	1.52	0.46
1:B:80:PRO:C	1:B:82:ASP:H	2.20	0.44
1:B:48:ILE:CD1	1:B:54:LEU:HD12	2.48	0.43
1:A:10:SER:HB3	1:A:103[B]:LYS:HB3	2.00	0.43
1:D:4:MET:HE3	1:D:23:CYS:SG	2.59	0.43
1:D:2:ILE:HD12	1:D:29:ILE:HG22	2.01	0.42
1:D:58:VAL:HG13	1:D:59:PRO:HD2	2.01	0.42
1:D:107[A]:LYS:HD2	3:D:253:HOH:O	2.19	0.41
1:A:54:LEU:HD11	1:A:58:VAL:HG12	2.01	0.41
1:B:79:GLN:O	1:B:82:ASP:HB2	2.20	0.41
1:B:81:GLU:OE1	3:B:167:HOH:O	2.21	0.41
1:B:36:TYR:CD2	1:B:44:PRO:HB3	2.56	0.41
1:A:11:LEU:C	1:A:11:LEU:HD23	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ILE:HD13	1:C:21:ILE:HG21	1.81	0.41
1:C:4:MET:HE3	1:C:23:CYS:SG	2.60	0.41
1:A:91:TYR:HA	1:A:96:TYR:CD1	2.55	0.40
1:A:50:ASP:O	1:A:51:ALA:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:117:HOH:O	3:B:151:HOH:O[17_455]	2.17	0.03

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	109/109 (100%)	103 (94%)	6 (6%)	0	100 100
1	B	112/109 (103%)	101 (90%)	9 (8%)	2 (2%)	8 10
1	C	110/109 (101%)	103 (94%)	7 (6%)	0	100 100
1	D	109/109 (100%)	103 (94%)	6 (6%)	0	100 100
All	All	440/436 (101%)	410 (93%)	28 (6%)	2 (0%)	29 40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	GLY
1	B	81	GLU

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	A	97/95 (102%)	93 (96%)	4 (4%)	30	41
1	B	101/95 (106%)	91 (90%)	10 (10%)	8	9
1	C	99/95 (104%)	94 (95%)	5 (5%)	24	32
1	D	98/95 (103%)	94 (96%)	4 (4%)	30	41
All	All	395/380 (104%)	372 (94%)	23 (6%)	21	26

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	10	SER
1	A	11	LEU
1	A	93	ASN
1	B	11	LEU
1	B	34	ILE
1	B	38	GLN
1	B	52	SER
1	B	54	LEU
1	B	93	ASN
1	B	104	LEU
1	B	106	ILE
1	B	107[A]	LYS
1	B	107[B]	LYS
1	C	0	THR
1	C	11	LEU
1	C	72	THR
1	C	107[A]	LYS
1	C	107[B]	LYS
1	D	2	ILE
1	D	11	LEU
1	D	83	LEU
1	D	104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	93	ASN
1	C	100	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	501	-	4,4,4	0.19	0	6,6,6	0.05	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.