



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 02:49 PM BST

PDB ID : 6AL5
Title : COMPLEX BETWEEN CD19 (N138Q MUTANT) AND B43 FAB
Authors : Teplyakov, A.; Obmolova, G.; Gilliland, G.L.
Deposited on : 2017-08-07
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

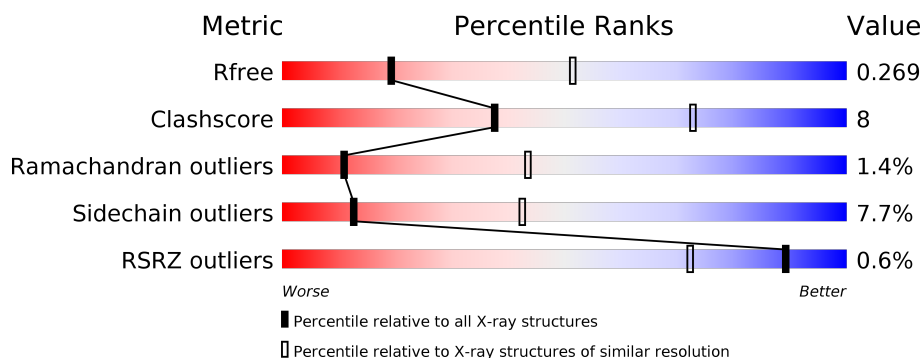
1 Overall quality at a glance

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	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 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 $\leq 5\%$. 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	265	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>•</div> <div>12%</div> </div> </div>
2	L	218	<div> <div>81%</div> <div>17%</div> <div>•</div> </div>
3	H	233	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>•</div> <div>5%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5063 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 B-lymphocyte antigen CD19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1710	1107	301	291	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLN	ASN	engineered mutation	UNP P15391
A	278	GLY	-	expression tag	UNP P15391
A	279	SER	-	expression tag	UNP P15391
A	280	HIS	-	expression tag	UNP P15391
A	281	HIS	-	expression tag	UNP P15391
A	282	HIS	-	expression tag	UNP P15391
A	283	HIS	-	expression tag	UNP P15391
A	284	HIS	-	expression tag	UNP P15391
A	285	HIS	-	expression tag	UNP P15391

- Molecule 2 is a protein called B43 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1651	1035	272	340	4			

- Molecule 3 is a protein called B43 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	222	Total	C	N	O	S	0	0	0
			1672	1054	276	334	8			

There are 6 discrepancies between the modelled and reference sequences:

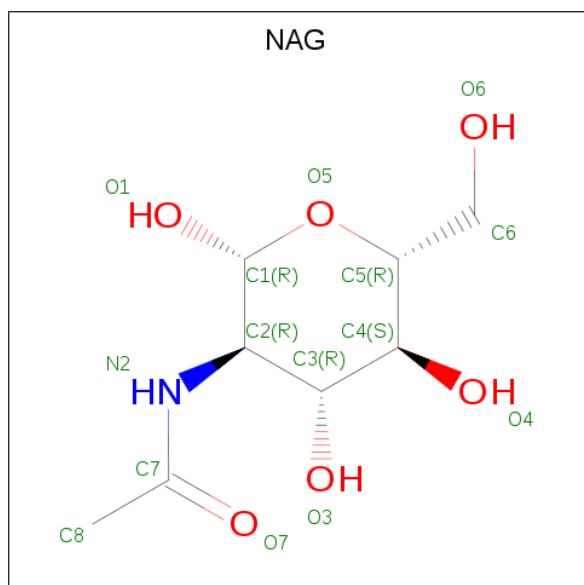
Chain	Residue	Modelled	Actual	Comment	Reference
H	228	HIS	-	expression tag	UNP A8K008

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	229	HIS	-	expression tag	UNP A8K008
H	230	HIS	-	expression tag	UNP A8K008
H	231	HIS	-	expression tag	UNP A8K008
H	232	HIS	-	expression tag	UNP A8K008
H	233	HIS	-	expression tag	UNP A8K008

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	O	0	0
			1	1		
5	H	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.80Å 92.35Å 146.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-3.00) 99.7 (29.93-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.189 , 0.263 0.192 , 0.269	Depositor DCC
R_{free} test set	930 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5063	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PCA, NAG

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	0.40	0/1768	0.58	0/2425
2	L	0.36	0/1688	0.56	0/2298
3	H	0.36	0/1707	0.56	0/2332
All	All	0.37	0/5163	0.57	0/7055

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 [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	1710	0	1565	36	0
2	L	1651	0	1571	16	0
3	H	1672	0	1595	28	0
4	A	28	0	26	0	0
5	H	1	0	0	0	0
5	L	1	0	0	0	0
All	All	5063	0	4757	76	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 8.

The worst 5 of 76 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:218:HIS:HD2	1:A:220:LYS:H	1.04	0.96
3:H:99:ARG:HD3	3:H:109:TYR:HB2	1.52	0.90
3:H:161:VAL:CG2	3:H:189:LEU:CD2	2.64	0.75
1:A:218:HIS:CD2	1:A:220:LYS:H	1.97	0.74
3:H:161:VAL:CG2	3:H:189:LEU:HD21	2.18	0.74

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	226/265 (85%)	195 (86%)	24 (11%)	7 (3%)	4	23
2	L	215/218 (99%)	203 (94%)	11 (5%)	1 (0%)	29	68
3	H	218/233 (94%)	208 (95%)	9 (4%)	1 (0%)	29	68
All	All	659/716 (92%)	606 (92%)	44 (7%)	9 (1%)	11	43

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	105	LYS
1	A	203	PRO
1	A	236	ALA
1	A	264	GLY

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	163/228 (72%)	146 (90%)	17 (10%)	7	27
2	L	186/192 (97%)	172 (92%)	14 (8%)	13	43
3	H	183/197 (93%)	173 (94%)	10 (6%)	21	57
All	All	532/617 (86%)	491 (92%)	41 (8%)	13	42

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	64	SER
2	L	114	VAL
3	H	190	SER
2	L	77	LEU
2	L	112	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	142	ASN
2	L	202	HIS
2	L	156	ASN
1	A	218	HIS
2	L	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
3	PCA	H	1	3	7,8,9	0.60	0	9,10,12	1.03	0
4	NAG	A	902	1	14,14,15	0.49	0	17,19,21	1.44	3 (17%)
4	NAG	A	901	1	14,14,15	0.77	1 (7%)	17,19,21	1.57	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	H	1	3	-	0/0/11/13	0/1/1/1
4	NAG	A	902	1	-	2/6/23/26	0/1/1/1
4	NAG	A	901	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	NAG	C1-C2	2.18	1.55	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	NAG	C1-O5-C5	3.24	116.59	112.19
4	A	901	NAG	C2-N2-C7	3.21	127.47	122.90
4	A	901	NAG	O5-C5-C6	2.53	111.18	107.20
4	A	902	NAG	C2-N2-C7	2.38	126.30	122.90
4	A	901	NAG	C8-C7-N2	2.37	120.12	116.10

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	NAG	C8-C7-N2-C2
4	A	902	NAG	O7-C7-N2-C2
4	A	901	NAG	C8-C7-N2-C2
4	A	901	NAG	O7-C7-N2-C2
4	A	901	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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
4	NAG	A	902	1	14,14,15	0.49	0	17,19,21	1.44	3 (17%)
4	NAG	A	901	1	14,14,15	0.77	1 (7%)	17,19,21	1.57	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	902	1	-	2/6/23/26	0/1/1/1
4	NAG	A	901	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	NAG	C1-C2	2.18	1.55	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	NAG	C1-O5-C5	3.24	116.59	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	NAG	C2-N2-C7	3.21	127.47	122.90
4	A	901	NAG	O5-C5-C6	2.53	111.18	107.20
4	A	902	NAG	C2-N2-C7	2.38	126.30	122.90
4	A	901	NAG	C8-C7-N2	2.37	120.12	116.10

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	NAG	C8-C7-N2-C2
4	A	902	NAG	O7-C7-N2-C2
4	A	901	NAG	C8-C7-N2-C2
4	A	901	NAG	O7-C7-N2-C2
4	A	901	NAG	C4-C5-C6-O6

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](#)

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	234/265 (88%)	-0.44	2 (0%) 84 63	39, 64, 101, 131	0
2	L	217/218 (99%)	-0.37	0 100 100	40, 62, 84, 96	0
3	H	221/233 (94%)	-0.38	2 (0%) 84 63	37, 56, 91, 125	0
All	All	672/716 (93%)	-0.40	4 (0%) 89 72	37, 61, 93, 131	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	PRO	4.3
3	H	227	CYS	3.3
3	H	202	THR	2.8
1	A	265	ASN	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [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
4	NAG	A	901	14/15	0.67	0.32	115,126,138,142	0
4	NAG	A	902	14/15	0.87	0.22	76,89,94,95	0
3	PCA	H	1	8/9	0.90	0.27	69,77,84,94	0

6.3 Carbohydrates [i](#)

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
4	NAG	A	901	14/15	0.67	0.32	115,126,138,142	0
4	NAG	A	902	14/15	0.87	0.22	76,89,94,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.