



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:46 PM GMT

PDB ID : 1QKZ
Title : FAB FRAGMENT (MN14C11.6) IN COMPLEX WITH A PEPTIDE ANTIGEN DERIVED FROM NEISSERIA MENINGITIDIS P1.7 SEROSUBTYPE ANTIGEN AND DOMAIN II FROM STREPTOCOCCAL PROTEIN G
Authors : Derrick, J.P.; Feavers, I.; Maiden, M.C.J.
Deposited on : 1999-08-17
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

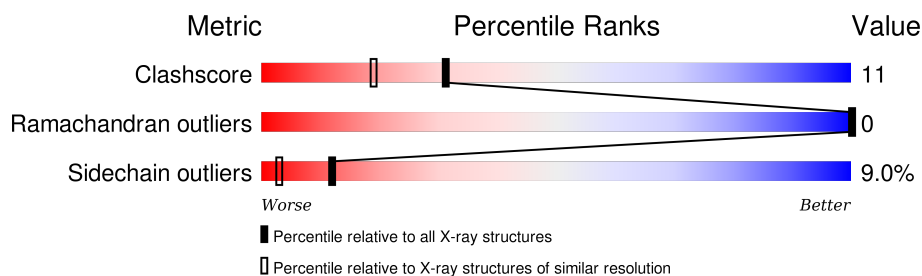
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	64	
2	H	219	
3	L	217	
4	P	10	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4369 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 PROTEIN G-PRIME.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	58	Total	C	N	O	0	0	0
			449	283	71	95			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LYS	GLU	ENGINEERED	UNP Q54181

- Molecule 2 is a protein called ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1670	1057	273	331	9			

- Molecule 3 is a protein called ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1662	1039	284	333	6			

- Molecule 4 is a protein called MAJOR OUTER MEMBRANE PROTEIN P1.16.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	10	Total	C	N	O	0	0	0
			62	35	13	14			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	234	Total 234	O 234	0	0
5	L	221	Total 221	O 221	0	0
5	P	10	Total 10	O 10	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

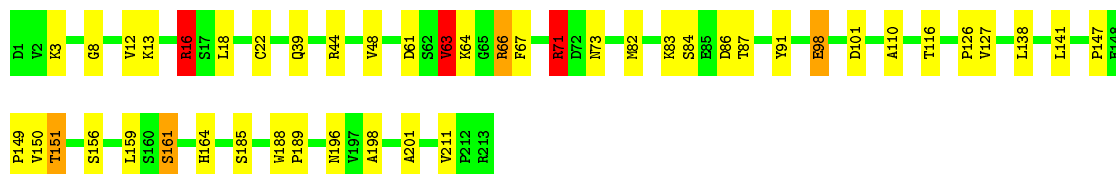
• Molecule 1: PROTEIN G-PRIME

Chain A: 



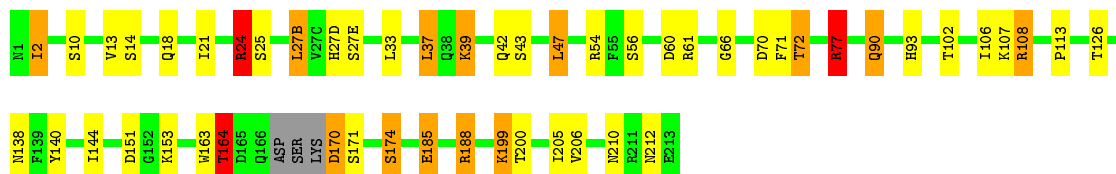
• Molecule 2: ANTIBODY

Chain H: 



• Molecule 3: ANTIBODY

Chain L: 



• Molecule 4: MAJOR OUTER MEMBRANE PROTEIN P1.16

Chain P: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.48 Å 63.10 Å 89.37 Å 90.00° 81.54° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95	Depositor
% Data completeness (in resolution range)	99.0 (10.00-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4369	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.50	0/455	1.16	4/617 (0.6%)
2	H	0.53	0/1714	1.47	10/2338 (0.4%)
3	L	0.51	0/1700	1.22	13/2305 (0.6%)
4	P	0.60	0/61	1.15	0/78
All	All	0.52	0/3930	1.33	27/5338 (0.5%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	71	ARG	CD-NE-CZ	38.33	177.26	123.60
2	H	71	ARG	NE-CZ-NH1	-11.23	114.69	120.30
3	L	54	ARG	NE-CZ-NH2	-7.91	116.34	120.30
3	L	77	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	L	151	ASP	CB-CG-OD1	6.75	124.38	118.30
2	H	66	ARG	NE-CZ-NH2	-6.60	117.00	120.30
3	L	54	ARG	NH1-CZ-NH2	6.44	126.49	119.40
3	L	54	ARG	NE-CZ-NH1	-6.26	117.17	120.30
2	H	71	ARG	NE-CZ-NH2	6.21	123.40	120.30
3	L	170	ASP	CB-CG-OD1	5.99	123.69	118.30
2	H	71	ARG	CG-CD-NE	5.93	124.25	111.80
1	A	38	TYR	CB-CG-CD1	5.80	124.48	121.00
2	H	63	VAL	N-CA-CB	-5.79	98.77	111.50
3	L	54	ARG	CG-CD-NE	-5.72	99.80	111.80
3	L	140	TYR	CB-CG-CD1	5.71	124.42	121.00
2	H	16	ARG	NE-CZ-NH2	-5.57	117.51	120.30
3	L	164	THR	N-CA-CB	-5.56	99.74	110.30
1	A	38	TYR	CB-CG-CD2	-5.38	117.77	121.00
3	L	24	ARG	CD-NE-CZ	5.21	130.90	123.60
2	H	101	ASP	CB-CG-OD1	5.18	122.96	118.30
2	H	86	ASP	CB-CG-OD1	5.14	122.93	118.30
3	L	174	SER	N-CA-CB	5.12	118.19	110.50
3	L	140	TYR	CB-CG-CD2	-5.11	117.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	188	ARG	CD-NE-CZ	5.11	130.76	123.60
1	A	50	TYR	CB-CG-CD2	5.09	124.05	121.00
1	A	50	TYR	CB-CG-CD1	-5.07	117.96	121.00
2	H	150	VAL	N-CA-CB	5.02	122.54	111.50

There are no chirality outliers.

There are no planarity outliers.

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	449	0	441	6	0
2	H	1670	0	1616	30	0
3	L	1662	0	1606	44	0
4	P	62	0	62	4	0
5	A	61	0	0	5	0
5	H	234	0	0	8	0
5	L	221	0	0	12	0
5	P	10	0	0	4	0
All	All	4369	0	3725	81	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 11.

All (81) 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)
3:L:60:ASP:HB2	5:L:2081:HOH:O	1.31	1.25
2:H:161:SER:HB2	5:H:2191:HOH:O	1.33	1.25
4:P:2:ASN:HB2	5:P:2003:HOH:O	1.37	1.22
4:P:2:ASN:CB	5:P:2003:HOH:O	1.90	1.16
4:P:2:ASN:ND2	5:P:2003:HOH:O	1.88	1.03
3:L:37:LEU:HD13	3:L:39:LYS:HE2	1.47	0.96
3:L:2:ILE:HD11	3:L:25:SER:HB2	1.46	0.95
3:L:27(D):HIS:HA	5:L:2039:HOH:O	0.75	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:211:VAL:HG11	5:H:2102:HOH:O	1.67	0.92
2:H:156:SER:H	2:H:196:ASN:HD21	1.14	0.91
2:H:12:VAL:HG13	2:H:16:ARG:HB3	1.55	0.88
3:L:90:GLN:HE22	3:L:93:HIS:H	1.25	0.83
4:P:2:ASN:CG	5:P:2003:HOH:O	1.99	0.76
2:H:12:VAL:CG1	2:H:16:ARG:HB3	2.15	0.75
2:H:161:SER:C	5:H:2191:HOH:O	2.24	0.75
3:L:108:ARG:HG3	3:L:171:SER:HB3	1.67	0.75
2:H:156:SER:H	2:H:196:ASN:ND2	1.87	0.72
3:L:14:SER:HA	5:L:2021:HOH:O	1.93	0.68
3:L:72:THR:HG22	5:L:2101:HOH:O	1.94	0.67
3:L:24:ARG:HG2	3:L:24:ARG:HH11	1.63	0.65
3:L:164:THR:HG22	3:L:174:SER:H	1.63	0.64
3:L:108:ARG:HG3	3:L:171:SER:CB	2.28	0.64
2:H:151:THR:HG22	2:H:198:ALA:HB3	1.81	0.62
1:A:9:LYS:HG2	1:A:22:THR:HG22	1.83	0.61
1:A:60:THR:HG23	5:A:2047:HOH:O	2.01	0.61
3:L:27(B):LEU:HD23	3:L:33:LEU:HB2	1.86	0.57
2:H:12:VAL:HG13	2:H:16:ARG:HD3	1.85	0.57
2:H:126:PRO:HD3	2:H:138:LEU:CD2	2.35	0.56
1:A:47:GLU:HG3	5:A:2015:HOH:O	2.05	0.56
3:L:210:ASN:HD22	3:L:212:ASN:H	1.54	0.56
3:L:170:ASP:O	3:L:171:SER:HB2	2.04	0.56
2:H:98:GLU:HG2	5:H:2126:HOH:O	2.05	0.56
3:L:206:VAL:HG21	5:L:2095:HOH:O	2.06	0.55
3:L:27(D):HIS:CA	5:L:2039:HOH:O	1.64	0.54
3:L:199:LYS:HE2	3:L:199:LYS:O	2.08	0.54
3:L:21:ILE:HG12	3:L:102:THR:HG21	1.90	0.54
5:A:2038:HOH:O	3:L:126:THR:HG22	2.07	0.53
3:L:188:ARG:NH2	5:L:2193:HOH:O	2.42	0.53
3:L:90:GLN:NE2	3:L:93:HIS:H	2.03	0.51
3:L:144:ILE:HG22	3:L:163:TRP:CZ3	2.46	0.50
2:H:66:ARG:NH2	2:H:83:LYS:HE2	2.26	0.50
5:H:2134:HOH:O	3:L:42:GLN:HG2	2.12	0.50
2:H:164:HIS:HE1	3:L:138:ASN:HD21	1.60	0.49
1:A:60:THR:HG21	5:A:2011:HOH:O	2.13	0.49
2:H:211:VAL:HG22	5:H:2231:HOH:O	2.11	0.49
3:L:39:LYS:N	3:L:39:LYS:HE3	2.28	0.48
3:L:113:PRO:HG2	3:L:205:ILE:HD12	1.95	0.48
2:H:164:HIS:HE1	3:L:138:ASN:ND2	2.11	0.48
2:H:61:ASP:HA	2:H:64:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:ILE:HG12	3:L:90:GLN:HG2	1.97	0.47
2:H:8:GLY:O	2:H:18:LEU:HD21	2.15	0.47
2:H:188:TRP:CG	2:H:189:PRO:HA	2.49	0.47
3:L:24:ARG:NH1	3:L:25:SER:O	2.48	0.47
2:H:156:SER:N	2:H:196:ASN:HD21	1.98	0.46
3:L:24:ARG:HG2	3:L:24:ARG:NH1	2.26	0.46
3:L:60:ASP:CA	5:L:2081:HOH:O	2.56	0.46
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.98	0.45
3:L:27(B):LEU:CD2	3:L:33:LEU:HD23	2.47	0.44
3:L:199:LYS:HG3	3:L:200:THR:N	2.32	0.44
2:H:71:ARG:HD3	2:H:73:ASN:OD1	2.17	0.44
3:L:66:GLY:HA3	3:L:71:PHE:HA	1.98	0.44
1:A:5:VAL:CG1	1:A:24:LYS:HB3	2.48	0.44
2:H:13:LYS:HE3	5:H:2014:HOH:O	2.18	0.43
3:L:21:ILE:O	3:L:72:THR:HA	2.18	0.43
3:L:18:GLN:NE2	5:L:2027:HOH:O	2.46	0.43
3:L:61:ARG:HD3	3:L:77:ARG:NH2	2.34	0.43
2:H:61:ASP:OD1	2:H:64:LYS:HE3	2.18	0.43
3:L:60:ASP:CB	5:L:2081:HOH:O	2.15	0.42
2:H:126:PRO:HD3	2:H:138:LEU:HD22	2.01	0.42
2:H:91:TYR:CE1	3:L:43:SER:HB3	2.55	0.42
3:L:27(E):SER:N	5:L:2039:HOH:O	2.50	0.42
2:H:67:PHE:CZ	2:H:82:MET:HE2	2.54	0.42
2:H:147:PRO:HD2	2:H:201:ALA:CB	2.50	0.42
3:L:37:LEU:CD1	3:L:39:LYS:HE2	2.35	0.41
1:A:33:LYS:HE2	5:A:2030:HOH:O	2.20	0.41
2:H:87:THR:HG23	2:H:110:ALA:HA	2.01	0.41
3:L:61:ARG:HH11	3:L:61:ARG:HD2	1.73	0.41
2:H:39:GLN:HA	2:H:44:ARG:O	2.22	0.40
3:L:37:LEU:HB2	3:L:47:LEU:HD22	2.02	0.40
2:H:127:VAL:HA	5:H:2157:HOH:O	2.21	0.40
3:L:185:GLU:HG3	5:L:2187:HOH:O	2.20	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	56/64 (88%)	55 (98%)	1 (2%)	0	100	100
2	H	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
3	L	210/217 (97%)	206 (98%)	4 (2%)	0	100	100
4	P	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	491/510 (96%)	482 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	48/53 (91%)	44 (92%)	4 (8%)	14	4
2	H	188/188 (100%)	173 (92%)	15 (8%)	15	4
3	L	192/195 (98%)	172 (90%)	20 (10%)	9	2
4	P	5/5 (100%)	5 (100%)	0	100	100
All	All	433/441 (98%)	394 (91%)	39 (9%)	12	3

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	13	ASN
1	A	15	LYS
1	A	62	LYS
2	H	3	LYS
2	H	16	ARG
2	H	22	CYS
2	H	48	VAL

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Mol	Chain	Res	Type
2	H	63	VAL
2	H	71	ARG
2	H	84	SER
2	H	98	GLU
2	H	116	THR
2	H	141	LEU
2	H	149	PRO
2	H	151	THR
2	H	159	LEU
2	H	161	SER
2	H	185	SER
3	L	2	ILE
3	L	10	SER
3	L	13	VAL
3	L	24	ARG
3	L	27(B)	LEU
3	L	37	LEU
3	L	39	LYS
3	L	47	LEU
3	L	56	SER
3	L	70	ASP
3	L	72	THR
3	L	77	ARG
3	L	90	GLN
3	L	106	ILE
3	L	107	LYS
3	L	108	ARG
3	L	153	LYS
3	L	164	THR
3	L	185	GLU
3	L	199	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
2	H	105	GLN
2	H	164	HIS
2	H	196	ASN
3	L	18	GLN
3	L	30	ASN
3	L	90	GLN

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Mol	Chain	Res	Type
3	L	138	ASN
3	L	210	ASN

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](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.