wwPDB X-ray Structure Validation Summary Report (i)

Dec 8, 2023 – 04:36 am GMT

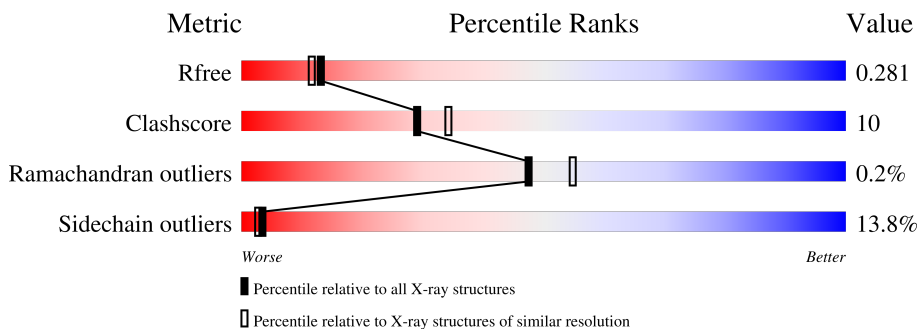|		
PDB ID	:	1UWX
Title	:	P1.2 serosubtype antigen derived from N. meningitidis PorA in complex with Fab fragment
Authors	:	Tzitzilonis, C.; Prince, S.M.; Collins, R.F.; Maiden, M.C.J.; Feavers, I.M.; Derrick, J.P.
Deposited on	:	2004-02-12
Resolution	:	2.20 Å(reported)

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 2.20 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	Percentile Ranks	Value
Rfree		0.281
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		13.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

❘ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	63	78% 13% • 8%
1	B	63	79% 11% 5% 5%
2	H	225	74% 18% • •
2	M	225	75% 16% 5% •
3	K	213	77% 17% 5%
3	L	213	74% 20% • •
4	P	13	62% 23% 8% 8%

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Mol	Chain	Length	Quality of chain
4	Q	13	85% 15%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8120 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 441	C 277	N 70	O 94	0	0	1
1	B	60	Total 466	C 293	N 73	O 100	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LYS	GLU	engineered mutation	UNP Q54181
B	24	LYS	GLU	engineered mutation	UNP Q54181

- Molecule 2 is a protein called ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total 1686	C 1083	N 270	O 327	S 6	0	0	0
2	M	218	Total 1686	C 1083	N 270	O 327	S 6	0	0	0

- Molecule 3 is a protein called ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	212	Total 1616	C 1015	N 268	O 327	S 6	0	0	1
3	L	212	Total 1616	C 1015	N 268	O 327	S 6	0	0	1

- Molecule 4 is a protein called CLASS 1 OUTER MEMBRANE PROTEIN VARIABLE RE-GION 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	13	Total 107	C 68	N 19	O 20	0	0	0
4	Q	13	Total 107	C 68	N 19	O 20	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total 41	O 41	0	0
5	B	29	Total 29	O 29	0	0
5	H	103	Total 103	O 103	0	0
5	K	45	Total 45	O 45	0	0
5	L	94	Total 94	O 94	0	0
5	M	73	Total 73	O 73	0	0
5	P	7	Total 7	O 7	0	0
5	Q	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
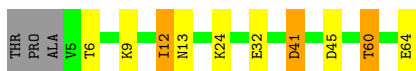
- Molecule 1: PROTEIN G-PRIME

Chain A:

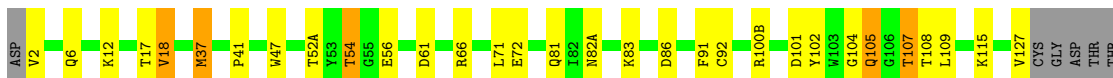- Molecule 1: PROTEIN G-PRIME

Chain B:

- Molecule 2: ANTIBODY

Chain H:

- Molecule 2: ANTIBODY

Chain M:

- Molecule 3: ANTIBODY

Chain K:

G3 I4 V5 M6 T7 Q8 T9 P10 Q13 V21 T24 C25 L26 I31 L35 A36 W37 K41 K44 S45 L49 D58 R63 S69 K72 F73 S74 F75 S79 L80 Q81 D84 Q92 T97 K105 L106 E106A I107 K108 R109 K143

N146 D152 G153 K154 Q157 N158 L161 W164 T165 D166 S169 K170 D171 D185 N191 S192 V207 N213 GLU

• Molecule 3: ANTIBODY

Chain L:

74%　　　　　　　　　20%

G3 I4 V5 M6 T7 Q8 T9 Q13 V21 T24 C25 L26 I31 L35 A36 W37 K44 S45 L49 D58 R63 S69 K72 F73 S74 F75 S79 L80 Q81 D84 Q92 P95B Y96 T97 K105 L106 E106A I107 K108 R109 A110 D111 L137

N138 N139 K143 N146 D152 G153 K154 Q157 N158 L161 D166 Q167 D168 S169 K170 D171 L182 D185 R189 H190 N191 S192 A197 V207 N213 GLU

• Molecule 4: CLASS 1 OUTER MEMBRANE PROTEIN VARIABLE REGION 2

Chain P:

62%　　　　　　　　　23%　　　　8%　　　8%

H1 F2 V3 K8 T12 L13

• Molecule 4: CLASS 1 OUTER MEMBRANE PROTEIN VARIABLE REGION 2

Chain Q:

85%　　　　　　　　　15%

H1 Q10 L13

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.43Å 110.57Å 138.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-2.20) 77.7 (20.89-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.223 , 0.265 0.264 , 0.281	Depositor DCC
R_{free} test set	2487 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.6	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8120	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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 35.20 % 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 6.0577e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

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	0.99	2/447 (0.4%)	1.03	2/608 (0.3%)
1	B	0.85	2/473 (0.4%)	0.97	3/641 (0.5%)
2	H	0.79	1/1736 (0.1%)	0.91	8/2366 (0.3%)
2	M	0.73	1/1736 (0.1%)	0.92	9/2366 (0.4%)
3	K	0.62	0/1653	0.87	6/2245 (0.3%)
3	L	0.73	0/1653	0.89	10/2245 (0.4%)
4	P	0.70	0/110	1.07	1/148 (0.7%)
4	Q	0.62	0/110	0.75	0/148
All	All	0.74	6/7918 (0.1%)	0.91	39/10767 (0.4%)

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
2	M	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CD-OE2	-6.12	1.19	1.25
1	B	32	GLU	CD-OE2	-6.05	1.19	1.25
1	A	32	GLU	CD-OE1	-5.74	1.19	1.25
1	B	32	GLU	CD-OE1	-5.47	1.19	1.25
2	H	211	GLU	CD-OE2	-5.10	1.20	1.25

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	213	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	32	GLU	OE1-CD-OE2	-8.41	113.21	123.30
3	K	164	TRP	CA-CB-CG	8.21	129.30	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	213	ARG	NE-CZ-NH2	8.16	124.38	120.30
3	L	166	ASP	CB-CG-OD2	7.95	125.45	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	213	ARG	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	441	0	428	8	0
1	B	466	0	454	8	0
2	H	1686	0	1623	41	0
2	M	1686	0	1623	44	0
3	K	1616	0	1566	20	0
3	L	1616	0	1566	25	0
4	P	107	0	108	5	0
4	Q	107	0	108	0	0
5	A	41	0	0	6	0
5	B	29	0	0	6	0
5	H	103	0	0	7	0
5	K	45	0	0	9	1
5	L	94	0	0	9	1
5	M	73	0	0	8	0
5	P	7	0	0	1	0
5	Q	3	0	0	0	0
All	All	8120	0	7476	146	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 10.

The worst 5 of 146 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:B:12:ILE:HG21	5:B:2017:HOH:O	1.07	1.25
1:A:13:ASN:HB3	5:A:2006:HOH:O	1.47	1.13
2:M:171:GLN:HG2	2:M:172:SER:N	1.67	1.05
2:H:171:GLN:HG2	2:H:172:SER:N	1.69	1.01
2:H:171:GLN:HG2	2:H:172:SER:H	1.23	1.00

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)
5:K:2045:HOH:O	5:L:2019:HOH:O[2_655]	2.17	0.03

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	56/63 (89%)	55 (98%)	1 (2%)	0	100	100
1	B	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
2	H	214/225 (95%)	209 (98%)	4 (2%)	1 (0%)	29	31
2	M	214/225 (95%)	207 (97%)	6 (3%)	1 (0%)	29	31
3	K	210/213 (99%)	205 (98%)	5 (2%)	0	100	100
3	L	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
4	P	11/13 (85%)	11 (100%)	0	0	100	100
4	Q	11/13 (85%)	11 (100%)	0	0	100	100
All	All	984/1028 (96%)	958 (97%)	24 (2%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	41	PRO

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Mol	Chain	Res	Type
2	M	41	PRO

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	47/52 (90%)	44 (94%)	3 (6%)	17	20
1	B	50/52 (96%)	47 (94%)	3 (6%)	19	22
2	H	186/191 (97%)	168 (90%)	18 (10%)	8	7
2	M	186/191 (97%)	166 (89%)	20 (11%)	6	6
3	K	183/185 (99%)	146 (80%)	37 (20%)	1	1
3	L	183/185 (99%)	150 (82%)	33 (18%)	1	1
4	P	13/13 (100%)	10 (77%)	3 (23%)	1	0
4	Q	13/13 (100%)	11 (85%)	2 (15%)	2	2
All	All	861/882 (98%)	742 (86%)	119 (14%)	3	3

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	170	LYS
2	M	186	SER
3	L	44	LYS
2	M	177	LEU
4	Q	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	82(A)	ASN
2	M	196	ASN
2	M	164	HIS
3	K	211	ASN

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Mol	Chain	Res	Type
2	M	6	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 monosaccharides 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 ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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

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

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

6.3   Carbohydrates ⓘ

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

6.4   Ligands ⓘ

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

6.5   Other polymers ⓘ

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