WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:15 AM GMT

PDB ID	:	3OCH
Title	:	Chemically Self-assembled Antibody Nanorings (CSANs): Design and Characterization of an Anti-CD3 IgM Biomimetic
Authors	:	Cody, Vivian
Deposited on	:	2010-08-10
Resolution	:	1.79 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 1.79 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.
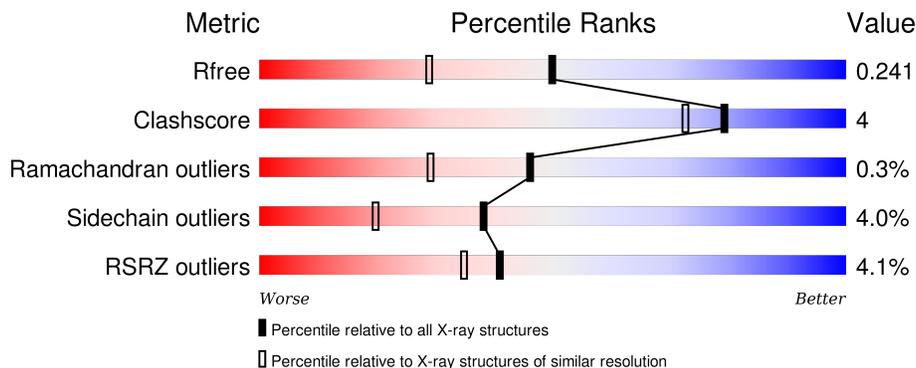
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 <=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	159	
1	B	159	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2744 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 Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total 1267	C 805	N 216	O 239	S 7	0	0	0
1	B	159	Total 1268	C 805	N 216	O 240	S 7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	CONFLICT	UNP P0ABQ4
B	237	ASP	ASN	CONFLICT	UNP P0ABQ4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Cl 2	0	0
2	A	1	Total 1	Cl 1	0	0

- Molecule 3 is (2S,2'S)-5,5'-(NONANE-1,9-DIYLDIIMINO)BIS(2-{[(4-{[(2,4-DIAMINO PTERIDIN-6-YL)METHYL](METHYL)AMINO}PHENYL)CARBONYL]AMINO}-5-O XOPENTANOIC ACID) (NON-PREFERRED NAME) (three-letter code: 2MX) (formula: $C_{49}H_{62}N_{18}O_8$).

2MX
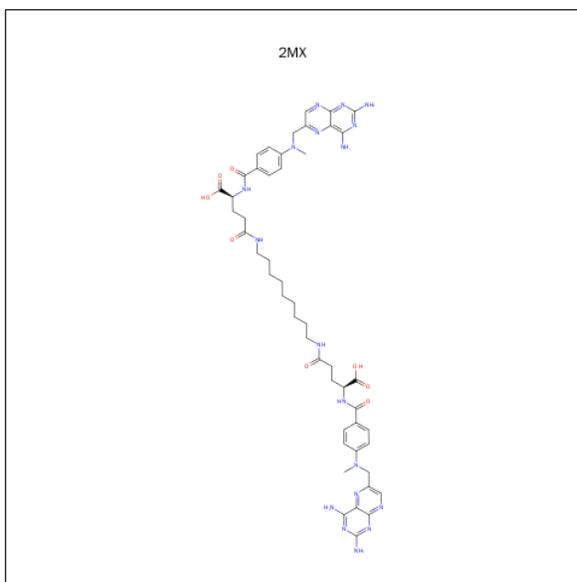
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	75	49	18	8	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	B	2	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	79	79	79	0	0
5	B	50	50	50	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 (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.

- Molecule 1: Dihydrofolate reductase
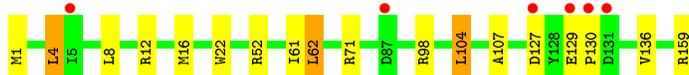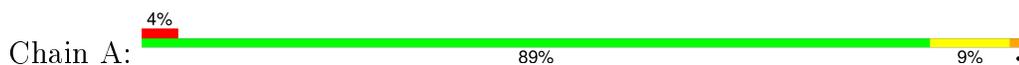
- Molecule 1: Dihydrofolate reductase
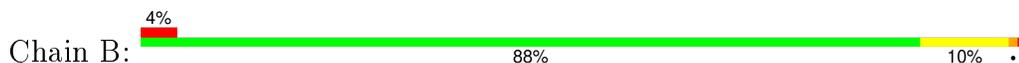
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	91.71Å 91.71Å 73.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.20 – 1.79 23.20 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.8 (23.20-1.79) 98.8 (23.20-1.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	10.10 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.203 , 0.242 0.202 , 0.241	Depositor DCC
R_{free} test set	1663 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 44.5	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 32398 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2744	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 2MX, MN, CL

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	1.15	0/1301	1.22	10/1770 (0.6%)
1	B	1.07	1/1302 (0.1%)	1.01	3/1770 (0.2%)
All	All	1.11	1/2603 (0.0%)	1.12	13/3540 (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
1	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	301	GLU	CD-OE1	5.07	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	NE-CZ-NH1	-16.58	112.01	120.30
1	A	159	ARG	NE-CZ-NH2	14.30	127.45	120.30
1	B	296	GLY	N-CA-C	7.18	131.06	113.10
1	A	104	LEU	CB-CG-CD2	6.94	122.80	111.00
1	A	8	LEU	CB-CG-CD2	6.50	122.06	111.00
1	A	159	ARG	CG-CD-NE	-6.05	99.10	111.80
1	B	261	ILE	CG1-CB-CG2	-6.02	98.16	111.40
1	A	52	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	62	LEU	CB-CG-CD1	5.72	120.72	111.00
1	B	295	GLY	C-N-CA	5.57	133.99	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	CD-NE-CZ	5.34	131.08	123.60
1	A	71	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	4	LEU	CB-CG-CD1	5.20	119.84	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	295	GLY	Mainchain,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	1267	0	1221	4	0
1	B	1268	0	1218	10	0
2	A	1	0	0	0	0
2	B	2	0	0	1	0
3	A	75	0	60	5	0
4	B	2	0	0	0	0
5	A	79	0	0	1	0
5	B	50	0	0	0	0
All	All	2744	0	2499	18	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 4.

All (18) 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:129:GLU:HG3	1:A:130:PRO:HD2	1.25	1.18
3:A:160:2MX:HG	1:B:228:LEU:HB3	1.69	0.73
1:B:261:ILE:HD13	1:B:272:VAL:HG21	1.72	0.72
1:B:261:ILE:HD13	1:B:272:VAL:CG2	2.33	0.59
1:B:308:GLN:HE22	1:B:358:ARG:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:O	1:A:136:VAL:CG1	2.57	0.52
1:B:258:LYS:NZ	1:B:284:ALA:O	2.37	0.52
3:A:160:2MX:CD	5:A:214:HOH:O	2.60	0.49
1:B:212:ARG:NH2	1:B:327:ASP:HA	2.28	0.49
3:A:160:2MX:HAA	3:A:160:2MX:HAT	1.64	0.47
3:A:160:2MX:HGA	3:A:160:2MX:CCD	2.46	0.45
1:A:4:LEU:HD13	1:A:107:ALA:HB2	1.98	0.44
1:B:318:GLU:HA	1:B:318:GLU:OE2	2.17	0.44
1:A:136:VAL:O	1:A:136:VAL:HG12	2.16	0.44
3:A:160:2MX:HAB	3:A:160:2MX:HAV	1.58	0.42
1:B:241:ILE:HD13	1:B:281:ALA:HB1	2.02	0.41
1:B:338:SER:HA	1:B:353:PHE:O	2.21	0.41
1:B:296:GLY:HA3	2:B:366:CL:CL	2.59	0.40

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	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	B	157/159 (99%)	155 (99%)	1 (1%)	1 (1%)	30	14
All	All	314/318 (99%)	309 (98%)	4 (1%)	1 (0%)	46	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	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	136/136 (100%)	127 (93%)	9 (7%)	21	7
1	B	136/136 (100%)	134 (98%)	2 (2%)	72	62
All	All	272/272 (100%)	261 (96%)	11 (4%)	38	20

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	12	ARG
1	A	16	MET
1	A	22	TRP
1	A	61	ILE
1	A	62	LEU
1	A	98	ARG
1	A	104	LEU
1	A	127	ASP
1	B	222	TRP
1	B	320	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	102	GLN
1	A	124	HIS
1	B	308	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)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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	2MX	A	160	-	70,80,80	1.31	7 (10%)	77,109,109	1.94	20 (25%)

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	2MX	A	160	-	-	0/56/64/64	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	160	2MX	CBK-CCU	-2.74	1.49	1.53
3	A	160	2MX	C2-N3	-2.13	1.31	1.35
3	A	160	2MX	C7-N8	2.06	1.35	1.31
3	A	160	2MX	CBG-NBW	2.23	1.51	1.46
3	A	160	2MX	CAX-NBO	2.65	1.36	1.31
3	A	160	2MX	CCK-NBU	2.92	1.38	1.32
3	A	160	2MX	C9-N10	3.93	1.53	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	160	2MX	CAS-CAO-CCL	-4.28	115.81	120.76
3	A	160	2MX	N1-C2-N3	-4.00	121.35	127.44
3	A	160	2MX	NBS-CCG-NBQ	-3.97	121.40	127.44
3	A	160	2MX	CG-CB-CA	-3.61	105.64	112.98
3	A	160	2MX	CG-CD-NE2	-3.44	110.49	116.46
3	A	160	2MX	CAV-CCO-NCW	-3.16	116.90	121.68
3	A	160	2MX	OE1-CD-CG	-2.94	116.91	121.98
3	A	160	2MX	C6-C9-N10	-2.84	108.84	113.78
3	A	160	2MX	CAT-CCN-N10	-2.83	117.38	121.68
3	A	160	2MX	CB-CG-CD	-2.69	106.88	113.27
3	A	160	2MX	CBM-CCK-NBU	-2.36	113.25	117.11
3	A	160	2MX	N2-C2-N3	2.21	120.85	117.20
3	A	160	2MX	NAD-CCG-NBQ	2.55	121.42	117.20
3	A	160	2MX	CCG-NBQ-CCI	2.59	124.89	116.70
3	A	160	2MX	CBM-NCW-CCO	2.74	125.20	119.36
3	A	160	2MX	CAO-CCL-CAP	2.78	122.73	118.60
3	A	160	2MX	CBF-NE2-CD	3.56	129.80	122.79
3	A	160	2MX	CAX-NBO-CCQ	3.58	121.15	116.93
3	A	160	2MX	OE1-CD-NE2	4.82	132.50	122.94
3	A	160	2MX	CBG-NBW-CCA	5.33	133.27	122.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	160	2MX	5	0

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	159/159 (100%)	0.16	6 (3%)	44	38	9, 14, 30, 49	0
1	B	159/159 (100%)	0.32	7 (4%)	38	32	9, 19, 38, 52	0
All	All	318/318 (100%)	0.24	13 (4%)	41	35	9, 17, 36, 52	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	ASP	5.1
1	A	130	PRO	3.8
1	B	327	ASP	3.1
1	A	129	GLU	2.8
1	A	87	ASP	2.8
1	B	268	THR	2.7
1	B	266	PRO	2.5
1	B	287	ASP	2.4
1	B	277	SER	2.4
1	A	5	ILE	2.3
1	B	320	GLU	2.3
1	B	217	GLU	2.2
1	A	127	ASP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

Full wwPDB X-ray Structure Validation Report

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	2MX	A	160	75/75	0.92	0.13	0.38	7,13,51,54	0
2	CL	A	364	1/1	0.99	0.08	-0.67	13,13,13,13	0
2	CL	B	365	1/1	0.99	0.06	-1.14	14,14,14,14	0
2	CL	B	366	1/1	0.98	0.07	-1.29	24,24,24,24	0
4	MN	B	1	1/1	1.00	0.04	-1.93	12,12,12,12	0
4	MN	B	2	1/1	0.97	0.14	-	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.