



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:43 PM GMT

PDB ID : 1PSK
Title : THE CRYSTAL STRUCTURE OF AN FAB FRAGMENT THAT BINDS TO
THE MELANOMA-ASSOCIATED GD2 GANGLIOSIDE
Authors : Pichla, S.L.; Murali, R.; Burnett, R.M.
Deposited on : 1997-03-03
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

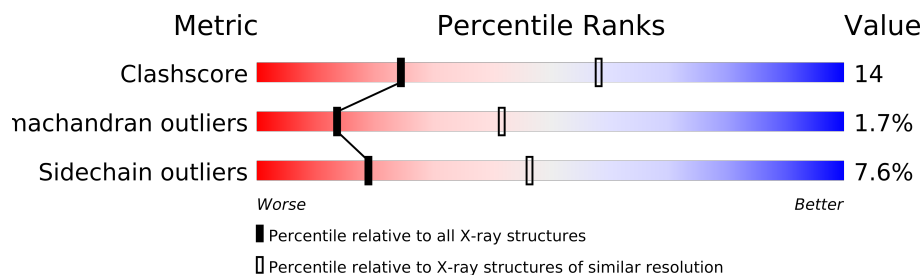
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	213	
2	H	209	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3885 atoms, of which 725 are hydrogens and 0 are deuterium.

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 ANTIBODY.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	213	Total	C	H	N	O	S	0	0	0
			2015	1016	385	274	332	8			

- Molecule 2 is a protein called ANTIBODY.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	198	Total	C	H	N	O	S	0	0	0
			1836	946	340	244	300	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	14	PRO	THR	CONFLICT	EMBL Y11590
H	24	THR	ALA	CONFLICT	EMBL Y11590
H	28	THR	SER	CONFLICT	EMBL Y11590
H	31	LYS	SER	CONFLICT	EMBL Y11590
H	33	THR	TYR	CONFLICT	EMBL Y11590
H	35	HIS	TYR	CONFLICT	EMBL Y11590
H	50	ASP	TYR	CONFLICT	EMBL Y11590
H	52	ASN	SER	CONFLICT	EMBL Y11590
H	53	PRO	CYS	CONFLICT	EMBL Y11590
H	54	ASN	TYR	CONFLICT	EMBL Y11590
H	57	GLY	ALA	CONFLICT	EMBL Y11590
H	59	ASN	THR	CONFLICT	EMBL Y11590
H	62	GLN	ARG	CONFLICT	EMBL Y11590
H	67	THR	LYS	CONFLICT	EMBL Y11590
H	70	LEU	PHE	CONFLICT	EMBL Y11590
H	73	HIS	ASP	CONFLICT	EMBL Y11590
H	74	LYS	THR	CONFLICT	EMBL Y11590
H	77	THR	SER	CONFLICT	EMBL Y11590
H	82	GLU	GLN	CONFLICT	EMBL Y11590
H	83	LEU	PHE	CONFLICT	EMBL Y11590

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Chain	Residue	Modelled	Actual	Comment	Reference
H	84	ARG	ASN	CONFLICT	EMBL Y11590
H	?	-	ALA	DELETION	EMBL Y11590
H	?	-	ARG	DELETION	EMBL Y11590
H	?	-	HIS	DELETION	EMBL Y11590
H	97	THR	TYR	CONFLICT	EMBL Y11590
H	98	SER	TYR	CONFLICT	EMBL Y11590
H	99	LYS	GLY	CONFLICT	EMBL Y11590
H	?	-	PRO	DELETION	EMBL Y11590
H	101	PHE	LEU	CONFLICT	EMBL Y11590
H	136	ALA	SER	CONFLICT	EMBL Y11590

- Molecule 3 is water.

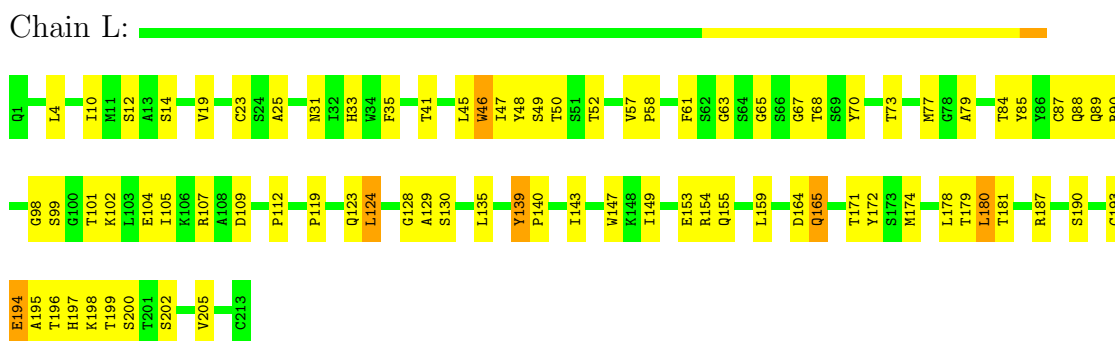
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	13	Total O 13 13	0	0
3	L	21	Total O 21 21	0	0

3 Residue-property plots

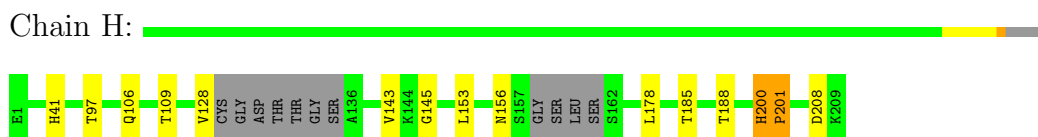
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: ANTIBODY



• Molecule 2: ANTIBODY



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	37.60Å 94.10Å 67.40Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	96.0 (8.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.204 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3885	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	L	0.46	0/1669	0.72	0/2265
2	H	0.46	0/1534	0.87	3/2095 (0.1%)
All	All	0.46	0/3203	0.79	3/4360 (0.1%)

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	L	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	200	HIS	C-N-CD	-17.65	81.76	120.60
2	H	200	HIS	N-CA-C	6.20	127.75	111.00
2	H	145	GLY	N-CA-C	5.33	126.43	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	139	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1630	385	1183	43	0
2	H	1496	340	0	0	0
3	H	13	0	0	0	0
3	L	21	0	0	0	0
All	All	3160	725	1183	43	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (43) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:139:TYR:HB2	1:L:171:THR:HG22	1.64	0.78
1:L:23:CYS:HG	1:L:87:CYS:HG	0.77	0.76
1:L:10:ILE:HD12	1:L:102:LYS:HD3	1.72	0.72
1:L:65:GLY:HA3	1:L:70:TYR:HA	1.71	0.72
1:L:119:PRO:HG3	1:L:129:ALA:HB1	1.78	0.66
1:L:109:ASP:HA	1:L:139:TYR:O	2.02	0.60
1:L:154:ARG:HG2	1:L:178:LEU:HD11	1.84	0.60
1:L:149:ILE:HD11	1:L:178:LEU:HD21	1.85	0.59
1:L:200:SER:HB3	1:L:202:SER:O	2.04	0.56
1:L:197:HIS:HD2	1:L:199:THR:OG1	1.89	0.55
1:L:112:PRO:HG3	1:L:143:ILE:HD11	1.90	0.54
1:L:45:LEU:HD11	1:L:48:TYR:HB3	1.91	0.52
1:L:35:PHE:O	1:L:85:TYR:HA	2.08	0.52
1:L:129:ALA:O	1:L:180:LEU:HD12	2.10	0.51
1:L:12:SER:HA	1:L:104:GLU:O	2.10	0.51
1:L:107:ARG:HG3	1:L:139:TYR:CG	2.46	0.51
1:L:50:THR:O	1:L:63:GLY:HA3	2.12	0.50
1:L:84:THR:HA	1:L:101:THR:O	2.13	0.49
1:L:79:ALA:HA	1:L:105:ILE:CD1	2.42	0.49
1:L:107:ARG:HG3	1:L:139:TYR:CD2	2.50	0.47
1:L:147:TRP:O	1:L:153:GLU:HA	2.15	0.47
1:L:135:LEU:CD2	1:L:195:ALA:HB2	2.46	0.46
1:L:165:GLN:HB2	1:L:172:TYR:CE1	2.51	0.45
1:L:130:SER:HB3	1:L:179:THR:HG23	1.99	0.45
1:L:31:ASN:HB3	1:L:49:SER:HA	1.98	0.45
1:L:194:GLU:HB3	1:L:205:VAL:HG22	1.99	0.45
1:L:23:CYS:HG	1:L:87:CYS:CB	2.24	0.44
1:L:4:LEU:O	1:L:98:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:79:ALA:HA	1:L:105:ILE:HD11	2.00	0.43
1:L:23:CYS:SG	1:L:87:CYS:CB	3.06	0.43
1:L:124:LEU:HD12	1:L:124:LEU:HA	1.83	0.42
1:L:140:PRO:HG3	1:L:198:LYS:HD2	2.01	0.42
1:L:140:PRO:O	1:L:197:HIS:HE1	2.03	0.41
1:L:4:LEU:HD23	1:L:25:ALA:HA	2.03	0.41
1:L:47:ILE:HG23	1:L:52:THR:O	2.19	0.41
1:L:58:PRO:HD2	1:L:61:PHE:CE2	2.56	0.41
1:L:88:GLN:HG2	1:L:89:GLN:N	2.36	0.41
1:L:46:TRP:O	1:L:57:VAL:HG21	2.21	0.41
1:L:123:GLN:HG2	1:L:128:GLY:O	2.21	0.40
1:L:33:HIS:CD2	1:L:90:ARG:NH2	2.90	0.40
1:L:193:CYS:O	1:L:193:CYS:SG	2.80	0.40
1:L:58:PRO:HD2	1:L:61:PHE:CD2	2.56	0.40
1:L:19:VAL:O	1:L:73:THR:HA	2.21	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	L	211/213 (99%)	201 (95%)	7 (3%)	3 (1%)	16	49
2	H	192/209 (92%)	171 (89%)	17 (9%)	4 (2%)	11	33
All	All	403/422 (96%)	372 (92%)	24 (6%)	7 (2%)	14	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	41	HIS
2	H	200	HIS
2	H	201	PRO
1	L	187	ARG
2	H	156	ASN

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Mol	Chain	Res	Type
1	L	67	GLY
1	L	165	GLN

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	L	186/186 (100%)	170 (91%)	16 (9%)	15	40
2	H	170/182 (93%)	159 (94%)	11 (6%)	24	57
All	All	356/368 (97%)	329 (92%)	27 (8%)	19	46

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14	SER
1	L	41	THR
1	L	46	TRP
1	L	68	THR
1	L	77	MET
1	L	99	SER
1	L	124	LEU
1	L	155	GLN
1	L	159	LEU
1	L	164	ASP
1	L	174	MET
1	L	180	LEU
1	L	181	THR
1	L	190	SER
1	L	194	GLU
1	L	196	THR
2	H	97	THR
2	H	106	GLN
2	H	109	THR
2	H	128	VAL
2	H	143	VAL
2	H	153	LEU
2	H	178	LEU

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Mol	Chain	Res	Type
2	H	185	THR
2	H	188	THR
2	H	201	PRO
2	H	208	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	88	GLN
1	L	189	ASN
1	L	197	HIS
1	L	209	ASN
1	L	211	ASN
2	H	55	ASN
2	H	197	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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