



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:51 am BST

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 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

<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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

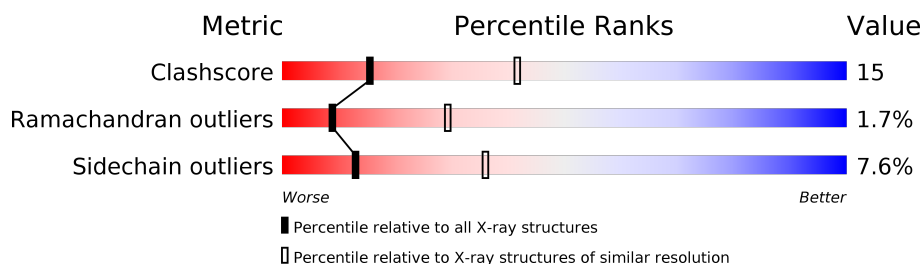
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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 $\leq 5\%$.

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 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 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.

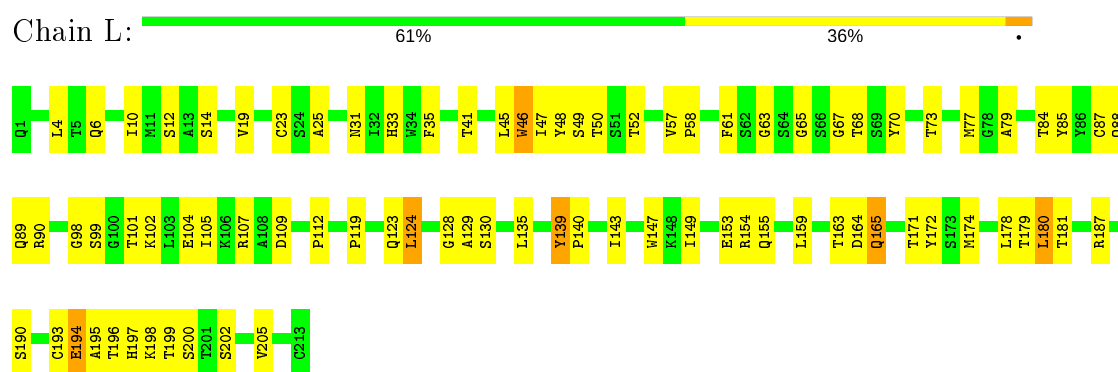
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	21	Total O 21 21	0	0
3	H	13	Total O 13 13	0	0

3 Residue-property plots [i](#)

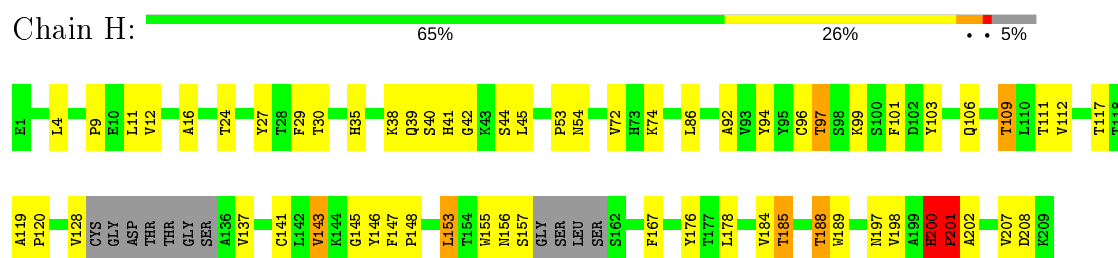
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

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 is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.60 Å 94.10 Å 67.40 Å 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 [i](#)

5.1 Standard geometry [i](#)

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 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	L	1630	385	1568	46	0
2	H	1496	340	1441	45	0
3	H	13	0	0	0	0
3	L	21	0	0	0	0
All	All	3160	725	3009	90	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 15.

All (90) 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:L:23:CYS:SG	1:L:87:CYS:SG	2.53	0.97
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
2:H:197:ASN:HD22	2:H:207:VAL:HG12	1.50	0.74
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
2:H:97:THR:CG2	2:H:101:PHE:HA	2.26	0.65
2:H:146:TYR:HB2	2:H:201:PRO:HB3	1.81	0.62
2:H:29:PHE:HE2	2:H:74:LYS:HA	1.64	0.61
2:H:30:THR:HG21	2:H:74:LYS:HE3	1.82	0.60
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
2:H:97:THR:HG22	2:H:101:PHE:HA	1.83	0.59
2:H:137:VAL:HG13	2:H:184:VAL:HG13	1.87	0.57
2:H:200:HIS:O	2:H:202:ALA:N	2.38	0.56
2:H:40:SER:HB3	2:H:44:SER:HB2	1.87	0.56
1:L:200:SER:HB3	1:L:202:SER:O	2.04	0.56
2:H:30:THR:CG2	2:H:54:ASN:HB2	2.35	0.56
1:L:197:HIS:HD2	1:L:199:THR:OG1	1.89	0.55
2:H:16:ALA:O	2:H:86:LEU:HD12	2.07	0.55
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.88	0.54
1:L:112:PRO:HG3	1:L:143:ILE:HD11	1.90	0.54
2:H:120:PRO:HB2	2:H:143:VAL:HG23	1.90	0.53
2:H:4:LEU:HG	2:H:24:THR:HG22	1.90	0.53
2:H:29:PHE:CE2	2:H:74:LYS:HA	2.43	0.52
1:L:45:LEU:HD11	1:L:48:TYR:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:PRO:HD3	2:H:201:PRO:HB2	1.90	0.52
1:L:35:PHE:O	1:L:85:TYR:HA	2.08	0.52
2:H:30:THR:HG21	2:H:54:ASN:HB2	1.91	0.52
2:H:153:LEU:HD22	2:H:198:VAL:HG22	1.92	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
2:H:155:TRP:O	2:H:157:SER:N	2.44	0.50
1:L:50:THR:O	1:L:63:GLY:HA3	2.12	0.50
2:H:97:THR:HG21	2:H:101:PHE:HA	1.92	0.49
1:L:163:THR:HG23	2:H:167:PHE:CD2	2.48	0.49
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
2:H:38:LYS:HG3	2:H:94:TYR:CE1	2.47	0.48
2:H:29:PHE:HZ	2:H:72:VAL:CG2	2.26	0.48
1:L:107:ARG:HG3	1:L:139:TYR:CD2	2.50	0.47
2:H:120:PRO:HD3	2:H:201:PRO:CB	2.45	0.47
1:L:147:TRP:O	1:L:153:GLU:HA	2.15	0.47
2:H:137:VAL:CG1	2:H:184:VAL:HG13	2.46	0.46
2:H:12:VAL:O	2:H:112:VAL:HA	2.15	0.46
1:L:135:LEU:CD2	1:L:195:ALA:HB2	2.46	0.46
2:H:137:VAL:HG21	2:H:189:TRP:CE3	2.50	0.46
2:H:30:THR:HA	2:H:53:PRO:HB2	1.98	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
2:H:38:LYS:HG3	2:H:94:TYR:HE1	1.81	0.45
1:L:194:GLU:HB3	1:L:205:VAL:HG22	1.99	0.45
2:H:35:HIS:O	2:H:96:CYS:HA	2.17	0.44
1:L:23:CYS:HG	1:L:87:CYS:CB	2.24	0.44
2:H:141:CYS:HB2	2:H:155:TRP:CH2	2.52	0.44
1:L:4:LEU:O	1:L:98:GLY:HA2	2.17	0.44
2:H:40:SER:O	2:H:42:GLY:N	2.51	0.44
1:L:79:ALA:HA	1:L:105:ILE:HD11	2.00	0.43
2:H:185:THR:HG22	2:H:188:THR:OG1	2.19	0.43
1:L:23:CYS:SG	1:L:87:CYS:CB	3.06	0.43
2:H:184:VAL:HG22	2:H:185:THR:N	2.34	0.43
2:H:24:THR:HB	2:H:27:TYR:HE1	1.83	0.42
2:H:9:PRO:HA	2:H:109:THR:O	2.18	0.42
2:H:11:LEU:HA	2:H:111:THR:O	2.19	0.42
2:H:39:GLN:O	2:H:92:ALA:HB1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:LEU:HD12	1:L:124:LEU:HA	1.83	0.42
2:H:147:PHE:O	2:H:176:TYR:CE1	2.73	0.42
2:H:117:THR:HA	2:H:148:PRO:HD3	2.02	0.42
2:H:30:THR:HG22	2:H:54:ASN:HB2	2.01	0.42
2:H:38:LYS:O	2:H:45:LEU:HA	2.20	0.42
2:H:29:PHE:HZ	2:H:72:VAL:HG22	1.84	0.42
1:L:140:PRO:HG3	1:L:198:LYS:HD2	2.01	0.42
2:H:99:LYS:HB2	2:H:103:TYR:CE2	2.56	0.41
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
2:H:119:ALA:HB2	2:H:202:ALA:HB3	2.03	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:6:GLN:HE21	1:L:6:GLN:HB3	1.70	0.40
1:L:193:CYS:SG	1:L:193:CYS:O	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 [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	L	211/213 (99%)	201 (95%)	7 (3%)	3 (1%)	11	34
2	H	192/209 (92%)	171 (89%)	17 (9%)	4 (2%)	7	23
All	All	403/422 (96%)	372 (92%)	24 (6%)	7 (2%)	9	29

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
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%)	10	30
2	H	170/182 (93%)	159 (94%)	11 (6%)	17	44
All	All	356/368 (97%)	329 (92%)	27 (8%)	13	36

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

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Mol	Chain	Res	Type
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
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 (6) 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
2	H	3	GLN
2	H	197	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

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.