wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:35 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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

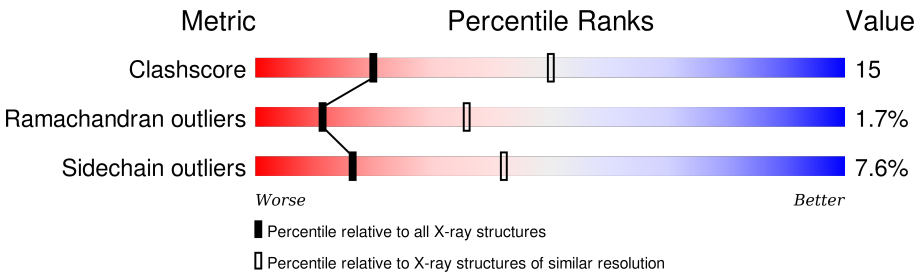
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	213	61% 36% •
2	H	209	65% 26% • • 5%

2 Entry composition (i)

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
			Total	C	H	N	O	S			
1	L	213	2015	1016	385	274	332	8	0	0	0

- Molecule 2 is a protein called ANTIBODY.

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

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
			Total	O		
3	H	13	13	13	0	0
			Total	O		
3	L	21	21	21	0	0

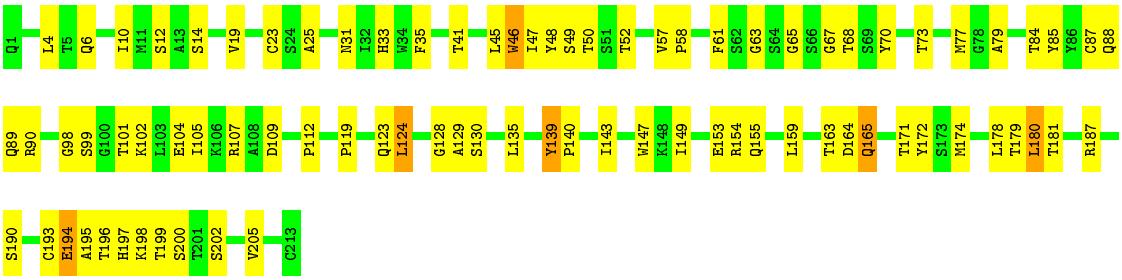
3 Residue-property plots (i)

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.

Note EDS was not executed.

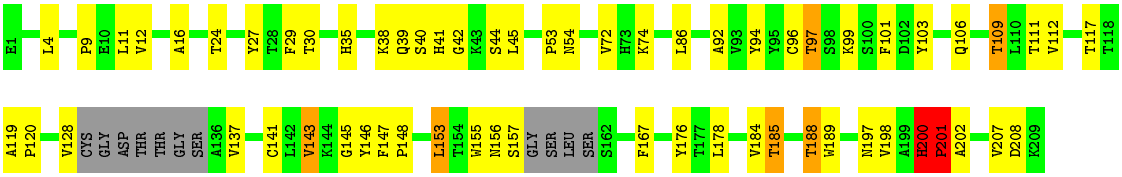
- Molecule 1: ANTIBODY

Chain L:



- Molecule 2: ANTIBODY

Chain H:



4 Data and refinement statistics (i)

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 (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(^{o})	Ideal(^{o})
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	45	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	89	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.

The worst 5 of 89 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: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

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%)	14 42
2	H	192/209 (92%)	171 (89%)	17 (9%)	4 (2%)	9 29
All	All	403/422 (96%)	372 (92%)	24 (6%)	7 (2%)	11 36

5 of 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

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	L	186/186 (100%)	170 (91%)	16 (9%)	13 36
2	H	170/182 (93%)	159 (94%)	11 (6%)	21 52
All	All	356/368 (97%)	329 (92%)	27 (8%)	16 42

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	181	THR
1	L	196	THR
2	H	188	THR
1	L	190	SER
1	L	77	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	197	HIS
2	H	197	ASN
1	L	209	ASN
1	L	189	ASN
2	H	3	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)

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.