wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:52 PM GMT

PDB ID	:	1MIM
Title	:	IGG FAB FRAGMENT (CD25-BINDING)
Authors	:	Mikol, V.
Deposited on	:	1995-12-04
Resolution	:	2.60 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 (1)) were used in the production of this report:

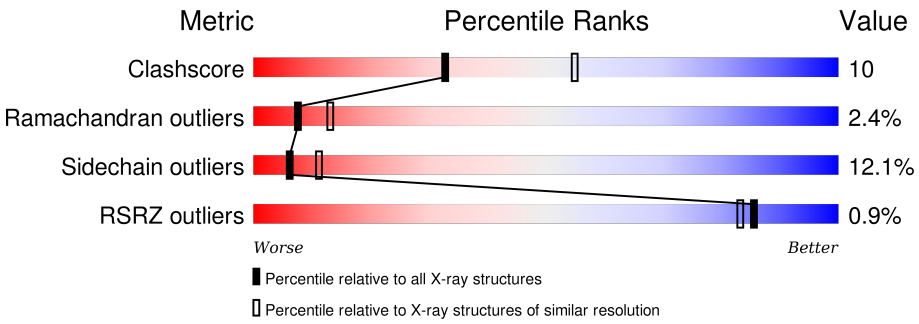
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	L	210	70% 24% • •
2	H	215	2% 62% 31% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3303 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 CHIMERIC SDZ CHI621.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	210	1604	996	271	329	8	0	0	0

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	4	SER	LEU	CONFLICT	UNP P01834
L	10	ILE	THR	CONFLICT	UNP P01834
L	11	MET	LEU	CONFLICT	UNP P01834
L	13	ALA	LEU	CONFLICT	UNP P01834
L	18	LYS	ARG	CONFLICT	UNP P01834
L	19	VAL	ALA	CONFLICT	UNP P01834
L	21	MET	LEU	CONFLICT	UNP P01834
L	22	THR	SER	CONFLICT	UNP P01834
L	24	SER	ARG	CONFLICT	UNP P01834
L	?	-	GLN	DELETION	UNP P01834
L	28	SER	VAL	CONFLICT	UNP P01834
L	29	ARG	GLY	CONFLICT	UNP P01834
L	32	MET	LEU	CONFLICT	UNP P01834
L	33	GLN	ALA	CONFLICT	UNP P01834
L	41	THR	GLN	CONFLICT	UNP P01834
L	42	SER	ALA	CONFLICT	UNP P01834
L	44	LYS	ARG	CONFLICT	UNP P01834
L	45	ARG	PRO	CONFLICT	UNP P01834
L	46	TRP	LEU	CONFLICT	UNP P01834
L	50	THR	ALA	CONFLICT	UNP P01834
L	52	LYS	ASN	CONFLICT	UNP P01834
L	53	LEU	ARG	CONFLICT	UNP P01834
L	55	SER	THR	CONFLICT	UNP P01834
L	57	VAL	ILE	CONFLICT	UNP P01834
L	69	SER	ASP	CONFLICT	UNP P01834
L	70	TYR	PHE	CONFLICT	UNP P01834
L	71	SER	THR	CONFLICT	UNP P01834

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Chain	Residue	Modelled	Actual	Comment	Reference
L	77	MET	LEU	CONFLICT	UNP P01834
L	79	ALA	PRO	CONFLICT	UNP P01834
L	82	ALA	PHE	CONFLICT	UNP P01834
L	84	THR	VAL	CONFLICT	UNP P01834
L	88	HIS	GLN	CONFLICT	UNP P01834
L	89	GLN	HIS	CONFLICT	UNP P01834
L	?	-	ASP	DELETION	UNP P01834
L	?	-	ASN	DELETION	UNP P01834
L	?	-	TRP	DELETION	UNP P01834
L	?	-	PRO	DELETION	UNP P01834
L	91	SER	PRO	CONFLICT	UNP P01834
L	92	SER	GLY	CONFLICT	UNP P01834
L	93	TYR	ALA	CONFLICT	UNP P01834
L	101	LEU	VAL	CONFLICT	UNP P01834

- Molecule 2 is a protein called CHIMERIC SDZ CHI621.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	215	1630	1032	270	321	7	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	-	INSERTION	GB 9857755
H	17	LYS	ARG	CONFLICT	GB 9857755
H	29	ARG	SER	CONFLICT	GB 9857755
H	32	MET	LEU	CONFLICT	GB 9857755
H	48	ALA	GLY	CONFLICT	GB 9857755
H	54	SER	ARG	CONFLICT	GB 9857755
H	57	SER	ARG	CONFLICT	GB 9857755
H	59	ASN	THR	CONFLICT	GB 9857755
H	61	LYS	ARG	CONFLICT	GB 9857755
H	63	GLU	LYS	CONFLICT	GB 9857755
H	64	GLY	ASP	CONFLICT	GB 9857755
H	75	SER	ASN	CONFLICT	GB 9857755
H	86	HIS	ASN	CONFLICT	GB 9857755
H	96	ARG	ILE	CONFLICT	GB 9857755
H	97	ASP	ILE	CONFLICT	GB 9857755
H	99	GLY	PHE	CONFLICT	GB 9857755
H	100	TYR	ASP	CONFLICT	GB 9857755
H	102	PHE	ALA	CONFLICT	GB 9857755

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ILE	DELETION	GB 9857755
H	?	-	MET	DELETION	GB 9857755
H	?	-	ASP	DELETION	GB 9857755
H	?	-	TYR	DELETION	GB 9857755
H	111	LEU	VAL	CONFLICT	GB 9857755
H	115	SER	THR	CONFLICT	GB 9857755
H	129	SER	CYS	CONFLICT	GB 9857755
H	131	LYS	ARG	CONFLICT	GB 9857755
H	135	GLY	GLU	CONFLICT	GB 9857755
H	136	GLY	SER	CONFLICT	GB 9857755
H	190	SER	ASN	CONFLICT	GB 9857755
H	191	LEU	PHE	CONFLICT	GB 9857755
H	197	ILE	THR	CONFLICT	GB 9857755
H	201	ASN	ASP	CONFLICT	GB 9857755
H	212	ARG	THR	CONFLICT	GB 9857755

- Molecule 3 is water.

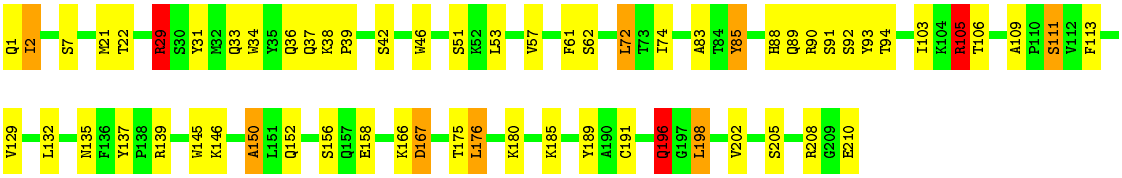
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	H	35	35	35	0	0
			Total	O		
3	L	34	34	34	0	0

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.

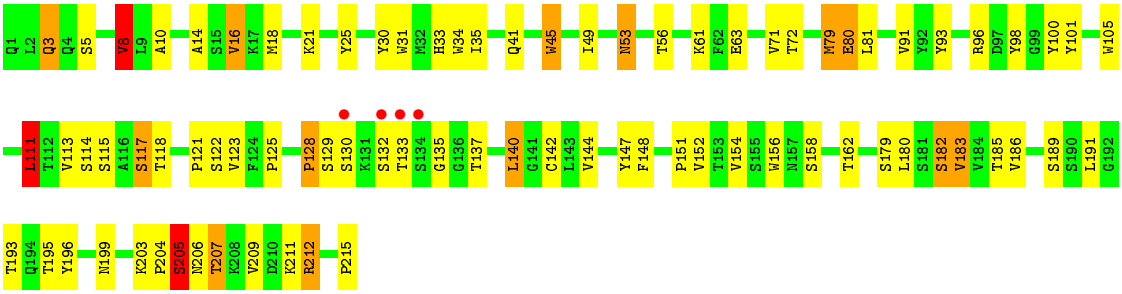
- Molecule 1: CHIMERIC SDZ CHI621

Chain L:



- Molecule 2: CHIMERIC SDZ CHI621

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.58Å 59.76Å 102.09Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 14.94 – 2.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 82.8 (14.94-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 2.48Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 76.4	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 14331 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3303	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[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)

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	1.00	0/1639	1.78	30/2220 (1.4%)
2	H	0.94	0/1675	1.77	38/2281 (1.7%)
All	All	0.97	0/3314	1.78	68/4501 (1.5%)

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.

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	46	TRP	CD1-CG-CD2	10.50	114.70	106.30
1	L	208	ARG	NE-CZ-NH2	-10.09	115.26	120.30
1	L	145	TRP	CD1-CG-CD2	10.02	114.31	106.30
2	H	45	TRP	CD1-CG-CD2	9.00	113.50	106.30
2	H	31	TRP	CD1-CG-CD2	8.98	113.48	106.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	189	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	1604	0	1550	30	0
2	H	1630	0	1575	40	0
3	H	35	0	0	7	0
3	L	34	0	0	9	0
All	All	3303	0	3125	66	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 10.

The worst 5 of 66 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)
2:H:33:HIS:HD2	2:H:45:TRP:HE1	1.22	0.85
1:L:129:VAL:HA	3:L:237:HOH:O	1.80	0.81
1:L:38:LYS:HD3	1:L:83:ALA:HB2	1.66	0.77
2:H:158:SER:H	2:H:199:ASN:HD21	1.37	0.72
2:H:204:PRO:HB2	3:H:220:HOH:O	1.90	0.70

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	208/210 (99%)	194 (93%)	10 (5%)	4 (2%)	10 19
2	H	213/215 (99%)	189 (89%)	18 (8%)	6 (3%)	6 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	421/425 (99%)	383 (91%)	28 (7%)	10 (2%)	7 13

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	167	ASP
2	H	130	SER
2	H	205	SER
1	L	135	ASN
1	L	196	GLN

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	182/182 (100%)	163 (90%)	19 (10%)	9 16
2	H	181/181 (100%)	156 (86%)	25 (14%)	4 7
All	All	363/363 (100%)	319 (88%)	44 (12%)	6 11

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	3	GLN
2	H	72	THR
2	H	193	THR
2	H	8	VAL
2	H	41	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	33	GLN
1	L	196	GLN
2	H	33	HIS

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Mol	Chain	Res	Type
2	H	199	ASN
2	H	201	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 (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	L	210/210 (100%)	-0.92	0 100 100	4, 28, 58, 92	0
2	H	215/215 (100%)	-0.74	4 (1%) 70 64	5, 29, 58, 104	0
All	All	425/425 (100%)	-0.83	4 (0%) 85 83	4, 28, 58, 104	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	134	SER	5.8
2	H	133	THR	4.8
2	H	132	SER	3.4
2	H	130	SER	2.0

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.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.