



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BK0
Title : CRYSTAL STRUCTURE OF THE MAJOR CELERY ALLERGEN API G 1
Authors : Schirmer, T.; Hoffmann-Sommergruber, K.; Breiteneder, H.; Markovic-Housley, Z.
Deposited on : 2005-02-09
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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
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

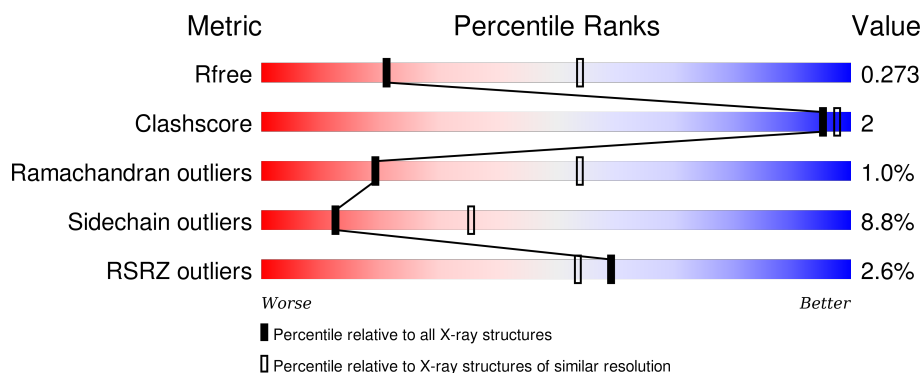
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 $\leq 5\%$. 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	154	<div> <div style="width: 88%;"></div> <div style="width: 10%;"></div> <div style="width: 2%;"></div> </div> <div> <div style="width: 5%;"></div> <div style="width: 81%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div>
1	B	154	<div> <div style="width: 5%;"></div> <div style="width: 81%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div> <div> <div style="width: 81%;"></div> <div style="width: 15%;"></div> <div style="width: 4%;"></div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2280 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 MAJOR ALLERGEN API G 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	31	0	0
			1140	730	181	227	2			
1	B	153	Total	C	N	O	S	54	0	0
			1140	730	181	227	2			

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.

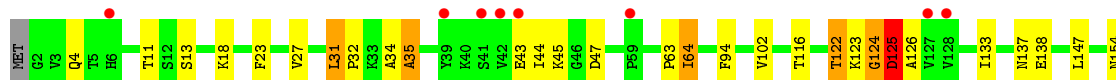
• Molecule 1: MAJOR ALLERGEN API G 1

Chain A:  88% 10% ..



• Molecule 1: MAJOR ALLERGEN API G 1

Chain B:  5% 81% 15% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.88Å 67.95Å 48.00Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 36.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.90) 89.9 (36.96-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.269 0.225 , 0.273	Depositor DCC
R_{free} test set	315 reflections (4.80%)	DCC
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.2	EDS
Estimated twinning fraction	0.040 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 6886 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2280	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	A	1.46	7/1159 (0.6%)	1.06	12/1578 (0.8%)
1	B	2.01	12/1159 (1.0%)	2.20	27/1578 (1.7%)
All	All	1.76	19/2318 (0.8%)	1.73	39/3156 (1.2%)

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	1	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	SER	CB-OG	-40.34	0.89	1.42
1	B	43	GLU	CD-OE2	-35.94	0.86	1.25
1	B	94	PHE	CG-CD2	27.15	1.79	1.38
1	B	124	GLY	C-N	-25.40	0.75	1.34
1	B	94	PHE	CG-CD1	-22.08	1.05	1.38
1	B	44	ILE	CB-CG2	18.76	2.11	1.52
1	B	44	ILE	CB-CG1	15.65	1.97	1.54
1	A	45	LYS	CB-CG	-14.77	1.12	1.52
1	B	4	GLN	CB-CG	-12.37	1.19	1.52
1	A	4	GLN	CB-CG	-12.12	1.19	1.52
1	B	147	LEU	CG-CD1	12.05	1.96	1.51
1	A	130	GLU	CG-CD	-11.69	1.34	1.51
1	B	64	ILE	CA-CB	-11.10	1.29	1.54
1	B	45	LYS	CG-CD	7.86	1.79	1.52
1	B	133	ILE	CB-CG1	7.02	1.73	1.54
1	A	94	PHE	CG-CD2	-6.69	1.28	1.38
1	A	147	LEU	CG-CD1	-6.47	1.27	1.51
1	A	94	PHE	CG-CD1	-5.98	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	LYS	CG-CD	5.89	1.72	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	PHE	CB-CG-CD1	41.24	149.67	120.80
1	B	94	PHE	CB-CG-CD2	-31.67	98.63	120.80
1	B	43	GLU	OE1-CD-OE2	-29.48	87.92	123.30
1	B	124	GLY	C-N-CA	-26.48	55.51	121.70
1	B	124	GLY	CA-C-N	-24.98	62.24	117.20
1	A	94	PHE	CB-CG-CD1	-18.30	107.99	120.80
1	B	44	ILE	CG1-CB-CG2	-16.12	75.94	111.40
1	B	43	GLU	CG-CD-OE2	15.61	149.52	118.30
1	B	126	ALA	C-N-CA	-15.27	83.53	121.70
1	A	147	LEU	CB-CG-CD1	13.22	133.47	111.00
1	A	94	PHE	CD1-CG-CD2	12.99	135.18	118.30
1	B	94	PHE	CG-CD1-CE1	12.52	134.57	120.80
1	A	45	LYS	CA-CB-CG	12.33	140.52	113.40
1	B	126	ALA	O-C-N	11.73	141.47	122.70
1	B	44	ILE	CA-CB-CG2	-11.08	88.75	110.90
1	A	94	PHE	CB-CG-CD2	-10.99	113.11	120.80
1	B	126	ALA	CA-C-N	-10.70	93.65	117.20
1	B	125	ASP	CA-C-N	-10.37	94.38	117.20
1	B	44	ILE	CA-CB-CG1	-9.68	92.62	111.00
1	B	64	ILE	CB-CA-C	9.23	130.07	111.60
1	B	147	LEU	CB-CG-CD1	-8.67	96.26	111.00
1	A	94	PHE	CG-CD1-CE1	-8.48	111.47	120.80
1	A	94	PHE	CG-CD2-CE2	-8.44	111.51	120.80
1	B	45	LYS	CB-CG-CD	-7.94	90.96	111.60
1	B	125	ASP	O-C-N	7.89	135.32	122.70
1	B	4	GLN	CA-CB-CG	6.52	127.75	113.40
1	B	125	ASP	CB-CA-C	6.25	122.89	110.40
1	B	94	PHE	CG-CD2-CE2	-5.92	114.29	120.80
1	A	130	GLU	CB-CG-CD	5.82	129.91	114.20
1	A	130	GLU	CG-CD-OE1	-5.73	106.84	118.30
1	A	130	GLU	CG-CD-OE2	5.70	129.69	118.30
1	B	122	THR	OG1-CB-CG2	5.68	123.07	110.00
1	A	41	SER	CA-CB-OG	5.53	126.14	111.20
1	A	45	LYS	CB-CG-CD	5.46	125.79	111.60
1	B	94	PHE	CD1-CG-CD2	-5.45	111.22	118.30
1	B	133	ILE	CG1-CB-CG2	-5.38	99.56	111.40
1	B	133	ILE	CA-CB-CG1	-5.31	100.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	LYS	CG-CD-CE	-5.10	96.59	111.90
1	B	147	LEU	CD1-CG-CD2	-5.08	95.27	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	64	ILE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	124	GLY	Mainchain,Peptide

5.2 Too-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 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	1140	0	1153	2	0
1	B	1140	0	1152	5	0
All	All	2280	0	2305	7	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 2.

All (7) 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:B:27:VAL:HG23	1:B:31:LEU:HD13	1.76	0.68
1:B:27:VAL:CG2	1:B:31:LEU:HD13	2.36	0.55
1:B:154:ASN:HD22	1:B:154:ASN:N	2.13	0.47
1:A:2:GLY:N	1:A:124:GLY:O	2.48	0.46
1:B:31:LEU:N	1:B:32:PRO:HD2	2.31	0.45
1:A:129:PRO:HD2	1:A:132:ASN:HD22	1.84	0.42
1:B:34:ALA:O	1:B:35:ALA:HB2	2.19	0.42

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	A	151/154 (98%)	144 (95%)	7 (5%)	0	100	100
1	B	151/154 (98%)	141 (93%)	7 (5%)	3 (2%)	9	33
All	All	302/308 (98%)	285 (94%)	14 (5%)	3 (1%)	19	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	ALA
1	B	125	ASP
1	B	63	PRO

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	A	125/126 (99%)	116 (93%)	9 (7%)	18	46
1	B	125/126 (99%)	112 (90%)	13 (10%)	9	26
All	All	250/252 (99%)	228 (91%)	22 (9%)	12	35

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	45	LYS
1	A	47	ASP

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Mol	Chain	Res	Type
1	A	57	THR
1	A	102	VAL
1	A	125	ASP
1	A	131	GLU
1	A	138	GLU
1	A	147	LEU
1	B	11	THR
1	B	13	SER
1	B	23	PHE
1	B	31	LEU
1	B	47	ASP
1	B	64	ILE
1	B	102	VAL
1	B	116	THR
1	B	122	THR
1	B	123	LYS
1	B	125	ASP
1	B	137	ASN
1	B	138	GLU

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

Mol	Chain	Res	Type
1	A	100	ASN
1	A	137	ASN
1	A	139	GLN
1	B	100	ASN
1	B	137	ASN
1	B	139	GLN
1	B	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	A	153/154 (99%)	-0.35	0 100 100	19, 24, 26, 27	10 (6%)
1	B	151/154 (98%)	0.10	8 (5%) 30 23	19, 24, 32, 35	14 (9%)
All	All	304/308 (98%)	-0.13	8 (2%) 59 54	19, 24, 27, 35	24 (7%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	SER	3.8
1	B	128	VAL	3.7
1	B	59	PRO	3.5
1	B	39	TYR	2.9
1	B	6	HIS	2.9
1	B	127	VAL	2.3
1	B	42	VAL	2.3
1	B	43	GLU	2.2

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.