



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:17 PM GMT

PDB ID : 1OBU
Title : APOCRUSTACYANIN C1 CRYSTALS GROWN IN SPACE AND EARTH
USING VAPOUR DIFFUSION GEOMETRY
Authors : Habash, J.; Boggon, T.J.; Raftery, J.; Chayen, N.E.; Zagalsky, P.F.; Helliwell,
J.R.
Deposited on : 2003-01-31
Resolution : 2.00 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

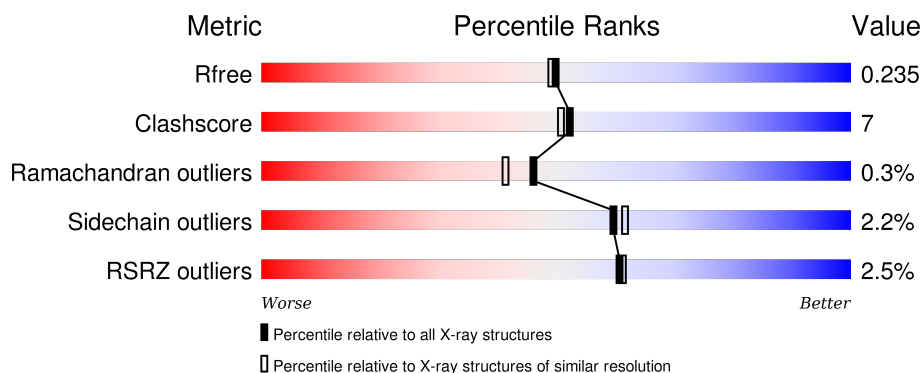
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	181	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	B	181	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>..</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3059 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 CRUSTACYANIN C1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1461	935	239	281	6			
1	B	180	Total	C	N	O	S	0	0	0
			1452	931	238	277	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GLU	LYS	CONFLICT	UNP P80029
B	66	GLU	LYS	CONFLICT	UNP P80029

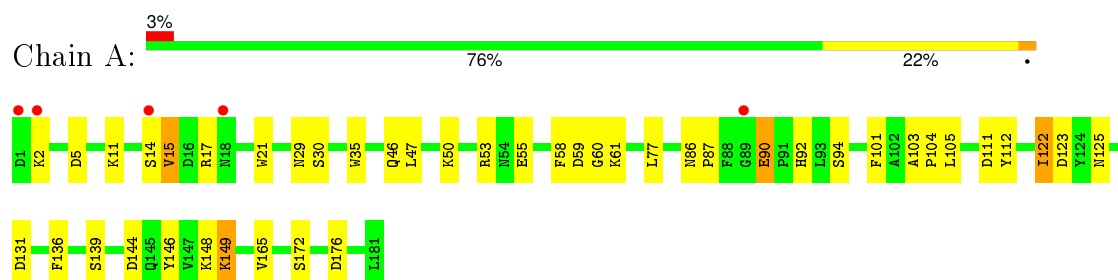
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	76	Total	O	0	0
			76	76		
2	B	70	Total	O	0	0
			70	70		

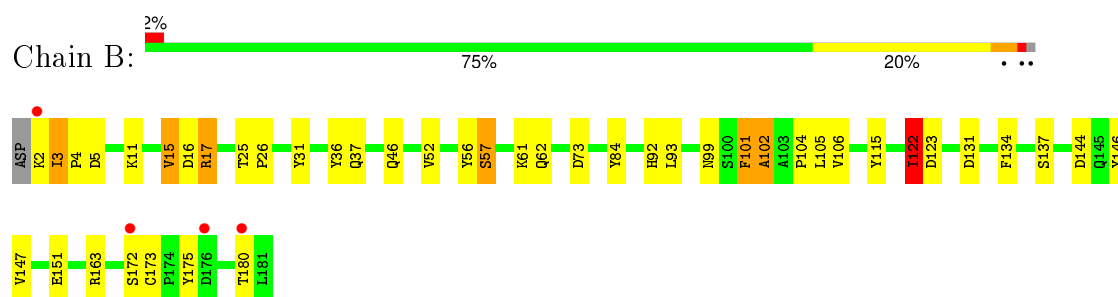
3 Residue-property plots [i](#)

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: CRUSTACYANIN C1 SUBUNIT



• Molecule 1: CRUSTACYANIN C1 SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.02Å 81.03Å 110.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.94 – 2.00 24.27 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (65.94-2.00) 99.3 (24.27-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.227 0.186 , 0.235	Depositor DCC
R_{free} test set	1326 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26054 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3059	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% 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	1.65	13/1501 (0.9%)	1.34	12/2038 (0.6%)
1	B	1.66	18/1492 (1.2%)	1.37	12/2026 (0.6%)
All	All	1.66	31/2993 (1.0%)	1.35	24/4064 (0.6%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	VAL	CB-CG1	-10.51	1.30	1.52
1	A	35	TRP	CB-CG	9.58	1.67	1.50
1	A	30	SER	CB-OG	9.30	1.54	1.42
1	A	35	TRP	CE3-CZ3	-8.01	1.24	1.38
1	A	149	LYS	CD-CE	7.73	1.70	1.51
1	A	136	PHE	CG-CD2	7.62	1.50	1.38
1	B	106	VAL	CB-CG1	-7.57	1.36	1.52
1	B	146	TYR	CE1-CZ	-7.13	1.29	1.38
1	B	172	SER	CB-OG	7.10	1.51	1.42
1	A	90	GLU	CD-OE2	7.10	1.33	1.25
1	B	122	ILE	CB-CG2	-7.09	1.30	1.52
1	B	57	SER	CB-OG	-7.06	1.33	1.42
1	A	53	ARG	CZ-NH2	-6.20	1.25	1.33
1	B	115	TYR	CD2-CE2	-6.17	1.30	1.39
1	B	175	TYR	CE2-CZ	6.17	1.46	1.38
1	A	165	VAL	CB-CG1	-6.10	1.40	1.52
1	B	52	VAL	CB-CG2	6.09	1.65	1.52
1	A	11	LYS	CD-CE	5.94	1.66	1.51
1	B	137	SER	CB-OG	5.80	1.49	1.42
1	B	84	TYR	CB-CG	5.73	1.60	1.51
1	B	102	ALA	CA-CB	-5.71	1.40	1.52
1	B	101	PHE	CB-CG	-5.65	1.41	1.51
1	A	21	TRP	CB-CG	-5.57	1.40	1.50
1	B	31	TYR	CE2-CZ	-5.36	1.31	1.38
1	B	56	TYR	CE2-CZ	-5.34	1.31	1.38
1	A	94	SER	CB-OG	-5.25	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	LEU	CA-CB	-5.12	1.42	1.53
1	B	173	CYS	CB-SG	-5.10	1.73	1.81
1	B	36	TYR	CE1-CZ	-5.05	1.31	1.38
1	A	55	GLU	CD-OE2	-5.05	1.20	1.25
1	A	139	SER	CA-CB	5.04	1.60	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ARG	NE-CZ-NH1	12.24	126.42	120.30
1	B	5	ASP	CB-CG-OD1	9.66	126.99	118.30
1	B	122	ILE	CG1-CB-CG2	-9.66	90.16	111.40
1	B	163	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	176	ASP	CB-CG-OD2	8.15	125.63	118.30
1	A	111	ASP	CB-CG-OD2	8.09	125.58	118.30
1	B	131	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	122	ILE	CG1-CB-CG2	-7.28	95.38	111.40
1	B	73	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	123	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	5	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	163	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	144	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	123	ASP	OD1-CG-OD2	-5.88	112.12	123.30
1	B	16	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	131	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	123	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	134	PHE	CB-CG-CD2	-5.38	117.03	120.80
1	A	105	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	131	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	131	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	105	LEU	CA-CB-CG	-5.17	103.41	115.30
1	A	112	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	A	53	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1461	0	1383	21	0
1	B	1452	0	1376	21	0
2	A	76	0	0	4	0
2	B	70	0	0	1	0
All	All	3059	0	2759	38	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 7.

All (38) 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:A:59:ASP:OD1	1:A:61:LYS:HG2	1.84	0.77
1:A:17:ARG:HH11	1:A:92:HIS:HD2	1.37	0.72
1:A:144:ASP:HB3	1:A:148:LYS:NZ	2.08	0.68
1:A:125:ASN:O	2:A:2056:HOH:O	2.14	0.66
1:B:17:ARG:HH11	1:B:92:HIS:HD2	1.48	0.61
1:B:37:GLN:HE22	1:B:46:GLN:HE21	1.51	0.58
1:B:61:LYS:HE3	1:B:62:GLN:NE2	2.22	0.55
1:B:15:VAL:CG1	1:B:15:VAL:O	2.55	0.54
1:A:144:ASP:HB3	1:A:148:LYS:HZ2	1.72	0.53
1:B:122:ILE:HD12	1:B:123:ASP:N	2.24	0.53
1:A:58:PHE:CE2	1:A:60:GLY:HA2	2.44	0.52
1:A:144:ASP:HB3	1:A:148:LYS:HZ1	1.74	0.51
1:B:122:ILE:O	1:B:122:ILE:HG23	2.09	0.51
1:A:146:TYR:HA	1:A:149:LYS:HD2	1.93	0.50
1:B:11:LYS:NZ	1:B:123:ASP:OD2	2.42	0.50
1:B:147:VAL:O	1:B:151:GLU:HG3	2.12	0.50
1:A:14:SER:O	1:A:15:VAL:O	2.30	0.50
1:A:103:ALA:HB1	1:A:104:PRO:HD2	1.94	0.49
1:B:101:PHE:N	1:B:101:PHE:CD2	2.80	0.49
1:A:77:LEU:HD12	2:A:2039:HOH:O	2.16	0.46
1:A:90:GLU:OE1	1:B:99:ASN:ND2	2.48	0.46
1:A:46:GLN:HE21	1:A:47:LEU:N	2.13	0.46
1:A:29:ASN:HB2	2:A:2010:HOH:O	2.16	0.46
1:A:17:ARG:HH11	1:A:92:HIS:CD2	2.26	0.45
1:B:92:HIS:CE1	1:B:104:PRO:HB3	2.51	0.44
1:B:3:ILE:HA	1:B:4:PRO:HD3	1.58	0.43
1:B:25:THR:N	1:B:26:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HG	2:B:2041:HOH:O	2.19	0.43
1:B:15:VAL:HG13	1:B:15:VAL:O	2.19	0.43
1:A:86:ASN:HA	1:A:87:PRO:HD3	1.99	0.42
1:B:17:ARG:HH11	1:B:92:HIS:CD2	2.35	0.42
1:A:122:ILE:HD13	1:B:101:PHE:CD2	2.54	0.41
1:A:14:SER:O	1:A:15:VAL:HB	2.21	0.41
1:B:3:ILE:HD13	1:B:3:ILE:HG21	1.82	0.40
1:A:101:PHE:HB2	1:B:102:ALA:O	2.20	0.40
1:B:122:ILE:HD12	1:B:123:ASP:H	1.84	0.40
1:A:122:ILE:HD13	1:B:101:PHE:HD2	1.86	0.40
1:A:50:LYS:NZ	2:A:2026:HOH:O	2.33	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	A	179/181 (99%)	172 (96%)	6 (3%)	1 (1%)	30	22
1	B	178/181 (98%)	171 (96%)	7 (4%)	0	100	100
All	All	357/362 (99%)	343 (96%)	13 (4%)	1 (0%)	46	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	VAL

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	A	160/160 (100%)	158 (99%)	2 (1%)	76	79
1	B	159/160 (99%)	154 (97%)	5 (3%)	47	46
All	All	319/320 (100%)	312 (98%)	7 (2%)	60	62

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	172	SER
1	B	2	LYS
1	B	3	ILE
1	B	57	SER
1	B	122	ILE
1	B	180	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	75	ASN
1	A	92	HIS
1	B	37	GLN
1	B	62	GLN
1	B	92	HIS
1	B	99	ASN
1	B	141	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	181/181 (100%)	-0.02	5 (2%) 56 57	11, 19, 34, 51	0
1	B	180/181 (99%)	-0.17	4 (2%) 65 66	8, 17, 36, 56	0
All	All	361/362 (99%)	-0.09	9 (2%) 61 61	8, 18, 35, 56	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	THR	3.7
1	B	2	LYS	3.6
1	A	2	LYS	3.3
1	A	1	ASP	3.2
1	B	172	SER	2.5
1	A	14	SER	2.5
1	A	89	GLY	2.4
1	A	18	ASN	2.1
1	B	176	ASP	2.1

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.