



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:58 PM UTC

PDB ID : 3QJO / pdb_00003qjo
Title : Refined Structure of the functional unit (KLH1-H) of keyhole limpet hemo-
cyanin
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Deposited on : 2011-01-30
Resolution : 4.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

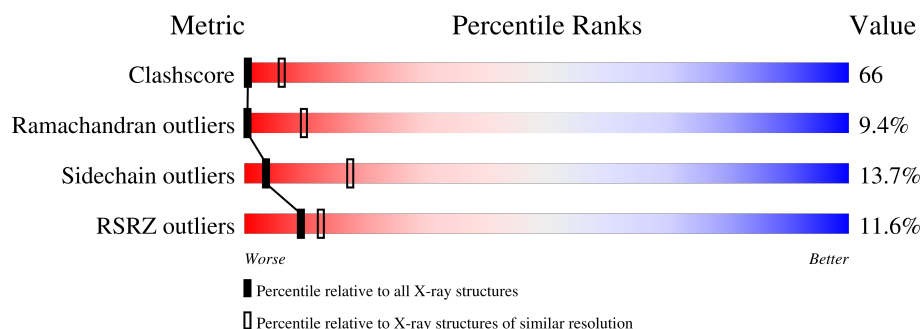
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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))
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 of 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 $\leq 5\%$. 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	491	
1	B	491	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7994 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 Hemocyanin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3995	2558	683	736	18			
1	B	491	Total	C	N	O	S	0	0	0
			3995	2558	683	736	18			

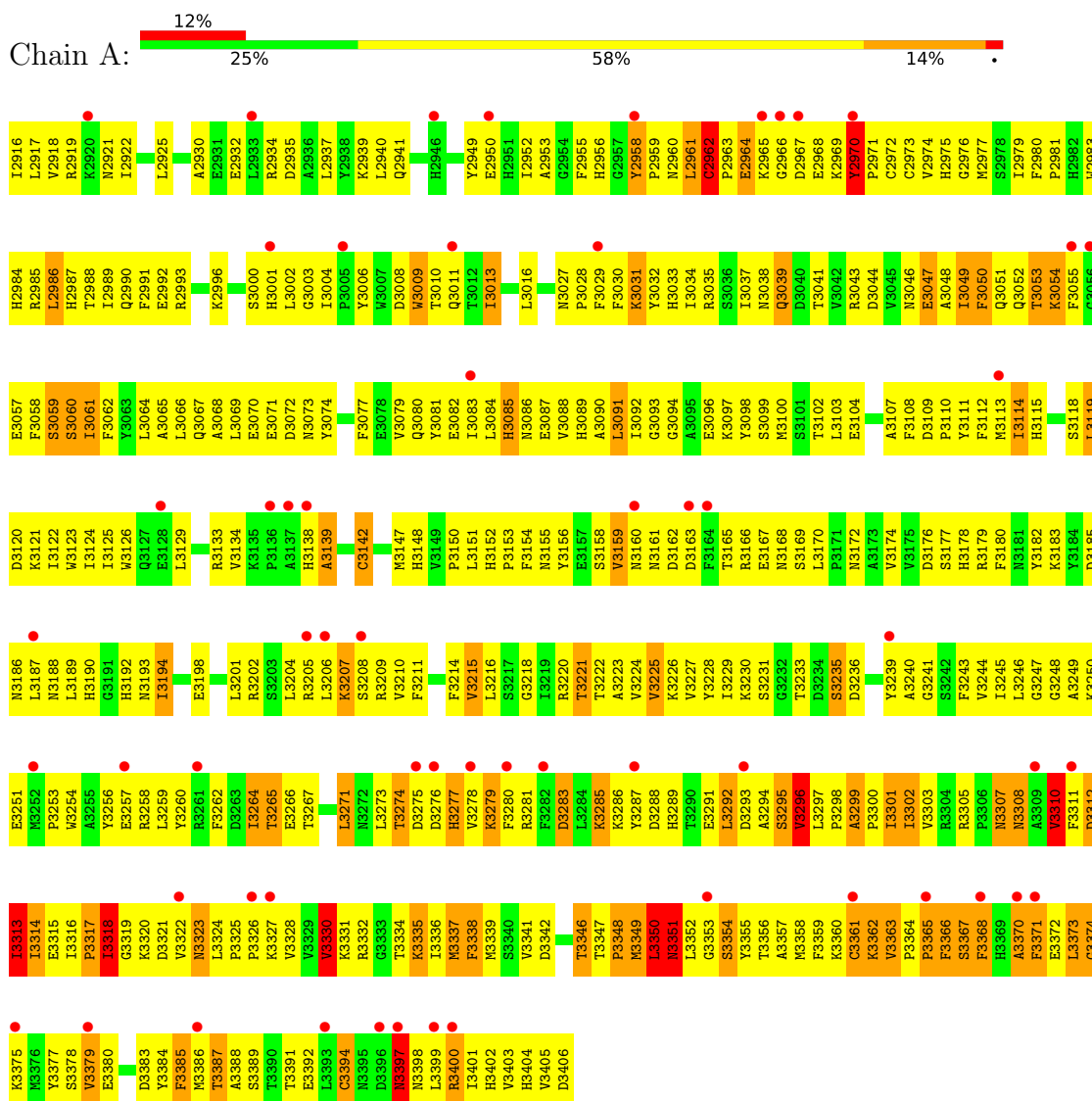
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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: Hemocyanin 1



• Molecule 1: Hemocyanin 1



E3372	F3311	G3248	D3185	S3118	T3063	H2984	I2916
L3373	D3312	A3249	N3186	L3119	K3054	R2985	L2917
G3374	I3313	K3250	N3187	L3120	F3055	L2986	R2918
K3375	I3314	E3251	N3188	K3121	G3056	T2987	V2919
E3376	E3315	P3252	N3189	K3122	F3057	T2988	K2920
K3377	I3316	P3253	N3190	K3123	F3058	T2989	N2921
S3378	P3317	W3254	N3191	K3124	S3059	T2990	L2922
I3318	I3318	E3257	N3192	I3125	S3060	T2991	L2925
K3319	K3320	R3258	N3193	W3126	F3062	E2992	E2929
K3320	D3321	L3259	E3195	L3129	L3064	A2930	A2930
V3322	V3322	Y3260	E3196	R3133	Y3063	E2931	E2932
N3323	N3323	F3261	L3197	V3134	A3065	E2933	E2933
L3324	L3324	F3262	E3198	R3147	L3066	R2934	R2934
P3325	P3325	D3263	L3201	A3137	A3068	I3004	I2935
P3326	P3326	T3264	R3202	H3138	L3069	F3005	A2936
K3327	K3327	T3265	S3203	H3139	E3070	L2937	L2937
V3328	V3328	E3266	S3204	A3139	E3071	Y3006	A2938
V3329	V3329	T3267	L3204	G3140	D3072	K3007	Y2939
V3330	V3330	L3271	R3205	S3141	N3073	D3008	K2939
K3331	K3331	N3272	L3206	C3142	Y3074	W3009	L2940
R3332	R3332	L3273	S3207	M3147	F3077	T3011	Q2941
G3333	G3333	D3274	R3209	H3148	E3078	T3012	N2942
T3334	T3334	D3275	V3210	V3149	Q3080	I3013	Y2949
K3335	K3335	D3276	F3211	P3150	V3079	L3016	E2950
I3336	I3336	H3277	F3214	L3151	Q3081	P3017	H2951
M3337	M3337	V3278	N3214	H3152	E3082	T3018	L2952
F3338	F3338	K3279	V3215	P3153	I3083	G2954	A2953
M3339	M3339	F3280	L3216	F3154	L3084	F2955	F2955
S3340	S3340	R3281	S3217	N3155	H3085	R2956	R2956
V3341	V3341	F3282	G3218	Y3156	N3086	G2957	Y2958
D3342	D3342	D3283	L3219	S3157	E3087	P2959	P2959
V3345	V3345	L3284	R3220	S3158	H3088	N2960	L2961
T3347	T3347	K3285	T3221	N3159	F3028	C2962	C2962
P3348	P3348	K3286	T3222	N3160	F3029	E2964	E2964
M3349	M3349	Y3287	A3223	N3161	A3090	K2965	K2965
L3350	L3350	D3288	V3224	D3162	L3091	G2966	G2966
L3351	L3351	H3289	V3225	D3163	I3092	D2967	D2967
L3352	L3352	E3291	V3227	F3164	G3093	E2968	E2968
G3353	G3353	L3292	Y3228	T3165	G3094	K2969	K2969
S3354	S3354	D3293	I3229	R3166	A3095	Y2970	Y2970
Y3355	Y3355	A3294	K3230	S3169	E3096	C2971	C2971
T3356	T3356	S3295	S3231	L3170	K3097	C2972	C2972
A3357	A3357	V3296	G3232	P3171	Y3098	C2973	C2973
M3358	M3358	L3297	T3233	N3172	S3099	V2974	V2974
F3359	F3359	P3298	D3234	A3173	T3102	H2975	H2975
K3360	K3360	A3299	S3235	N3174	L3103	G2976	G2976
C3361	C3361	P3300	D3236	V3175	E3104	M2977	M2977
K3362	K3362	I3301	Y3239	V3176	A3107	L2978	L2978
V3363	V3363	I3302	A3240	S3177	F3108	F2980	F2980
P3364	P3364	V3303	G3241	H3178	D3109	P2981	P2981
P3365	P3365	K3304	S3242	R3179	P3110	H2982	H2982
F3366	F3366	F3305	F3243	F3180	F3111	W2983	W2983
S3367	S3367	P3306	V3244	N3181	F3112		
F3368	F3368	N3307	L3245	K3182	M3113		
H3369	H3369	N3308	L3246	K3183	I3114		
A3370	A3370	V3310	G3247	Y3184	H3115		
F3371	F3371						

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	251.02Å 251.02Å 251.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 30.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-4.00) 99.7 (30.00-4.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.293 0.269 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	122.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 157.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7994	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU

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	0.28	0/4110	0.73	0/5575
1	B	0.28	0/4110	0.72	0/5575
All	All	0.28	0/8220	0.73	0/11150

There are no bond length outliers.

There are no bond angle outliers.

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	3995	0	3831	524	0
1	B	3995	0	3831	518	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	7994	0	7662	1033	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 66.

The worst 5 of 1033 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:3318:ILE:HA	1:A:3339:MET:HB2	1.35	1.08
1:B:3318:ILE:HA	1:B:3339:MET:HB2	1.36	1.06
1:A:3061:ILE:HG23	1:A:3062:PHE:H	1.24	1.03
1:B:3061:ILE:HG23	1:B:3062:PHE:H	1.23	1.00
1:A:3253:PRO:HB3	1:B:3358:MET:HE3	1.44	0.98

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	489/491 (100%)	341 (70%)	102 (21%)	46 (9%)	0	10
1	B	489/491 (100%)	342 (70%)	101 (21%)	46 (9%)	0	10
All	All	978/982 (100%)	683 (70%)	203 (21%)	92 (9%)	0	10

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2962	CYS
1	A	2970	TYR
1	A	3061	ILE
1	A	3139	ALA
1	A	3158	SER

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	437/437 (100%)	376 (86%)	61 (14%)	3	17
1	B	437/437 (100%)	378 (86%)	59 (14%)	4	18
All	All	874/874 (100%)	754 (86%)	120 (14%)	3	17

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3387	THR
1	B	3349	MET
1	B	3031	LYS
1	B	3338	PHE
1	B	3394	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3026	ASN
1	B	3115	HIS
1	B	3027	ASN
1	B	3046	ASN
1	B	3155	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	491/491 (100%)	0.94	58 (11%) 9 12	57, 135, 209, 279	0
1	B	491/491 (100%)	0.97	56 (11%) 10 13	58, 134, 208, 279	0
All	All	982/982 (100%)	0.96	114 (11%) 9 12	57, 135, 209, 279	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3276	ASP	4.9
1	B	3160	ASN	4.8
1	B	3138	HIS	4.5
1	A	3257	GLU	4.1
1	B	3139	ALA	4.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	A	3408	1/1	0.95	0.08	86,86,86,86	0
2	CU	A	3407	1/1	0.98	0.09	79,79,79,79	0
2	CU	B	3407	1/1	0.99	0.07	79,79,79,79	0
2	CU	B	3408	1/1	1.00	0.10	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.