



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 08:10 PM EDT

PDB ID : 3L6W
Title : Structure of the collar functional unit (KLH1-H) of keyhole limpet hemocyanin
Authors : Jaenicke, E.; Buechler, K.; Markl, J.; Decker, H.; Barends, T.R.M.
Deposited on : unknown
Resolution : 4.00 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

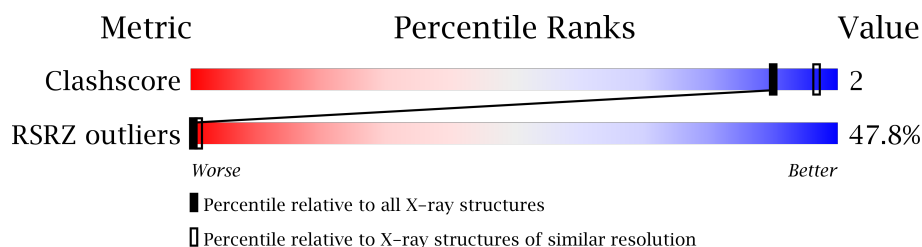
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

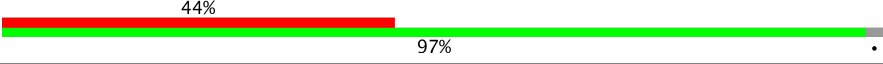
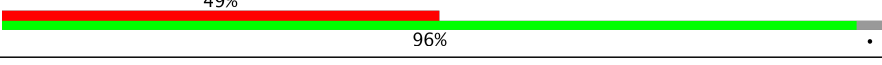
The reported resolution of this entry is 4.00 Å.

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	112137	1187 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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 $\leq 5\%$. 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 is only 1 type of molecule in this entry. The entry contains 954 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	479	Total	C	0	0	479
			479	479			
1	B	475	Total	C	0	0	475
			475	475			

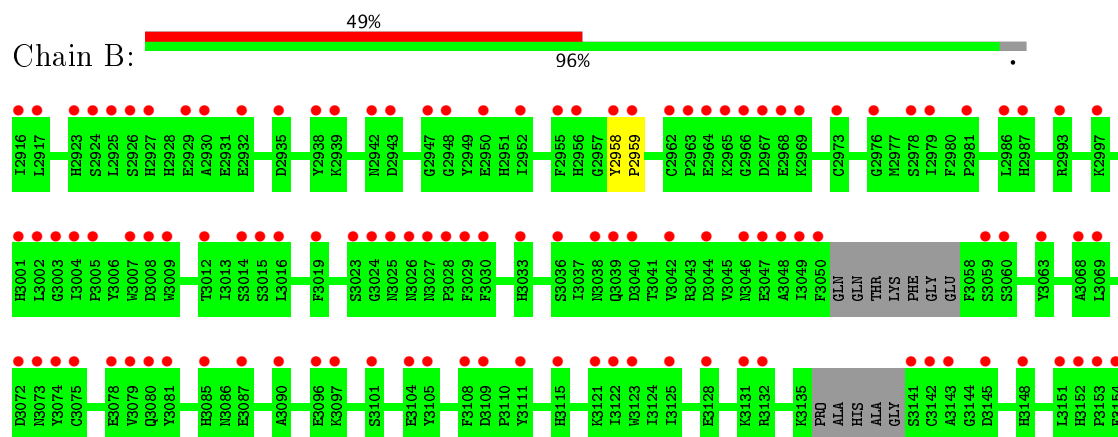
3 Residue-property plots [i](#)

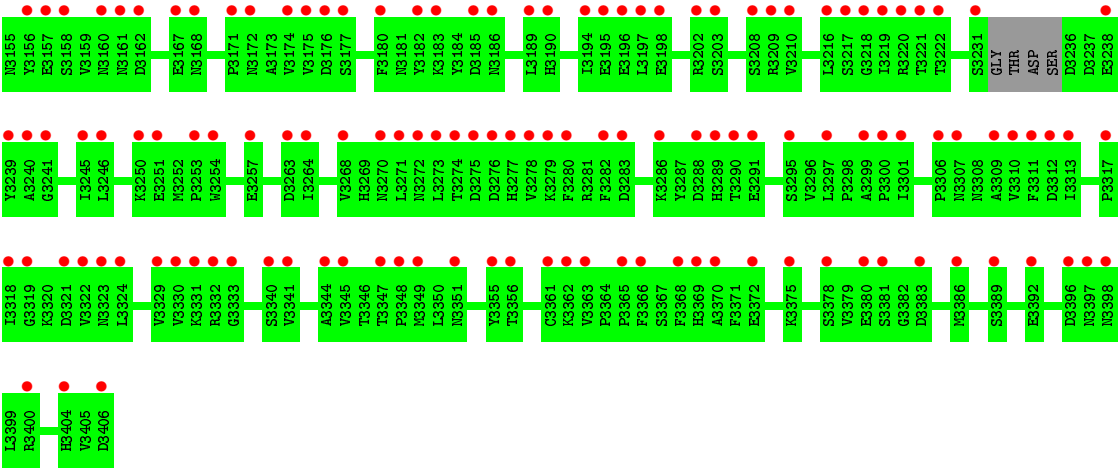
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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





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)	(Not available) – 4.00 29.58 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00) 100.0 (29.58-4.00)	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		Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	122.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 49.8	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	0.65	EDS
Total number of atoms	954	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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 [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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 [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	A	479	0	0	1	0
1	B	475	0	0	1	0
All	All	954	0	0	2	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 (2) 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:2958:TYR:CA	1:B:2959:PRO:CA	2.94	0.46
1:A:2958:TYR:CA	1:A:2959:PRO:CA	2.94	0.46

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

6.1 Protein, DNA and RNA chains

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	479/491 (97%)	2.73	214 (44%) 0 1	0, 0, 0, 0	0
1	B	475/491 (96%)	2.94	242 (50%) 0 1	0, 0, 0, 0	0
All	All	954/982 (97%)	2.83	456 (47%) 0 1	0, 0, 0, 0	0

All (456) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2916	ILE	25.1
1	B	3196	GLU	24.3
1	B	3380	GLU	21.8
1	A	3012	THR	21.7
1	B	3075	CYS	19.7
1	B	2967	ASP	19.1
1	A	3405	VAL	17.5
1	A	3274	THR	16.8
1	B	3012	THR	16.3
1	B	3048	ALA	16.2
1	B	3097	LYS	13.9
1	B	3274	THR	13.9
1	A	3374	GLY	13.3
1	A	3370	ALA	13.2
1	A	3168	ASN	13.0
1	B	3001	HIS	12.8
1	B	3180	PHE	12.6
1	A	3312	ASP	12.6
1	A	3001	HIS	12.3
1	B	3073	ASN	12.1
1	B	3003	GLY	12.1
1	B	3363	VAL	11.6
1	B	3142	CYS	11.5
1	A	3406	ASP	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	2963	PRO	10.8
1	B	3246	LEU	10.7
1	B	3217	SER	10.5
1	B	3362	LYS	10.5
1	B	3356	THR	10.4
1	A	3075	CYS	10.4
1	A	3246	LEU	10.2
1	A	2967	ASP	10.2
1	A	2916	ILE	10.1
1	A	3216	LEU	10.1
1	A	3319	GLY	10.0
1	B	3168	ASN	9.9
1	B	3208	SER	9.9
1	A	3069	LEU	9.9
1	B	3275	ASP	9.9
1	B	3272	ASN	9.8
1	A	2976	GLY	9.8
1	A	3368	PHE	9.7
1	A	3318	ILE	9.7
1	B	2981	PRO	9.2
1	B	2997	LYS	9.1
1	A	3363	VAL	9.1
1	B	3036	SER	9.0
1	A	3373	LEU	9.0
1	B	3074	TYR	8.8
1	B	3160	ASN	8.8
1	B	3050	PHE	8.7
1	A	3275	ASP	8.7
1	A	3395	ASN	8.7
1	B	3312	ASP	8.6
1	B	3186	ASN	8.5
1	B	2947	GLY	8.5
1	A	3299	ALA	8.5
1	B	3108	PHE	8.4
1	A	2973	CYS	8.4
1	B	3288	ASP	8.3
1	A	3048	ALA	8.2
1	B	3321	ASP	8.2
1	B	3381	SER	8.1
1	B	3323	ASN	7.9
1	B	2963	PRO	7.9
1	A	3158	SER	7.9

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Mol	Chain	Res	Type	RSRZ
1	B	2924	SER	7.8
1	B	2959	PRO	7.8
1	A	3044	ASP	7.8
1	A	3028	PRO	7.8
1	A	2925	LEU	7.8
1	A	3049	ILE	7.7
1	A	3301	ILE	7.7
1	B	3306	PRO	7.7
1	A	3324	LEU	7.4
1	A	3149	VAL	7.4
1	A	3375	LYS	7.3
1	A	3387	THR	7.3
1	A	3310	VAL	7.3
1	B	3158	SER	7.2
1	B	3241	GLY	7.2
1	B	3263	ASP	7.2
1	A	3295	SER	7.2
1	A	2978	SER	7.2
1	A	2947	GLY	7.1
1	A	3323	ASN	7.1
1	B	3162	ASP	7.1
1	A	3141	SER	7.0
1	B	3069	LEU	7.0
1	B	3257	GLU	7.0
1	A	2944	GLU	7.0
1	A	2962	CYS	6.9
1	B	3219	ILE	6.9
1	B	3190	HIS	6.9
1	A	3284	LEU	6.9
1	A	3347	THR	6.9
1	A	3365	PRO	6.9
1	A	3390	THR	6.8
1	A	3345	VAL	6.7
1	A	3369	HIS	6.7
1	B	3004	ILE	6.7
1	A	3059	SER	6.7
1	B	3177	SER	6.7
1	B	3141	SER	6.6
1	B	3072	ASP	6.6
1	B	3375	LYS	6.6
1	A	3276	ASP	6.5
1	B	3081	TYR	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	3354	SER	6.5
1	B	3024	GLY	6.5
1	B	3123	TRP	6.5
1	A	3050	PHE	6.3
1	A	3217	SER	6.3
1	B	3218	GLY	6.2
1	A	3127	GLN	6.2
1	A	3151	LEU	6.1
1	B	2932	GLU	6.1
1	B	2976	GLY	6.1
1	A	3389	SER	6.1
1	B	3240	ALA	6.1
1	A	3081	TYR	6.0
1	A	3219	ILE	6.0
1	A	3046	ASN	6.0
1	A	3360	LYS	6.0
1	A	3176	ASP	6.0
1	A	3000	SER	6.0
1	B	3348	PRO	5.9
1	A	3195	GLU	5.9
1	B	3049	ILE	5.9
1	A	3380	GLU	5.9
1	B	3028	PRO	5.9
1	A	3348	PRO	5.8
1	B	3365	PRO	5.8
1	A	2966	GLY	5.8
1	A	3097	LYS	5.8
1	A	3172	ASN	5.7
1	A	3282	PHE	5.7
1	A	3065	ALA	5.7
1	B	3157	GLU	5.7
1	A	3165	THR	5.6
1	A	2923	HIS	5.6
1	A	2943	ASP	5.6
1	B	3044	ASP	5.6
1	B	2942	ASN	5.6
1	B	3295	SER	5.5
1	B	3145	ASP	5.5
1	A	3067	GLN	5.5
1	B	3156	TYR	5.5
1	A	3239	TYR	5.5
1	A	3160	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	3291	GLU	5.5
1	B	3372	GLU	5.5
1	B	3345	VAL	5.4
1	B	3176	ASP	5.4
1	A	3024	GLY	5.4
1	B	3222	THR	5.4
1	A	3241	GLY	5.4
1	B	3333	GLY	5.4
1	B	2943	ASP	5.3
1	A	2935	ASP	5.3
1	A	3286	LYS	5.3
1	A	3366	PHE	5.3
1	B	2973	CYS	5.3
1	B	3167	GLU	5.3
1	B	2968	GLU	5.2
1	A	3133	ARG	5.2
1	A	3196	GLU	5.2
1	A	3322	VAL	5.2
1	A	2942	ASN	5.2
1	A	3253	PRO	5.2
1	A	3018	THR	5.2
1	B	3025	ASN	5.1
1	A	3013	ILE	5.1
1	B	3194	ILE	5.1
1	B	3101	SER	5.1
1	B	3331	LYS	5.1
1	B	3115	HIS	5.0
1	A	3072	ASP	5.0
1	A	3036	SER	4.9
1	A	2950	GLU	4.9
1	A	3364	PRO	4.9
1	A	3288	ASP	4.9
1	A	3308	ASN	4.9
1	A	3204	LEU	4.8
1	A	3279	LYS	4.8
1	B	3183	LYS	4.8
1	A	3117	ALA	4.8
1	A	3257	GLU	4.8
1	B	3318	ILE	4.8
1	A	3251	GLU	4.8
1	A	2959	PRO	4.7
1	B	3019	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	3019	PHE	4.7
1	A	3025	ASN	4.7
1	A	2929	GLU	4.7
1	B	2966	GLY	4.7
1	A	3037	ILE	4.6
1	A	3234	ASP	4.6
1	B	3347	THR	4.6
1	B	3279	LYS	4.6
1	A	3342	ASP	4.6
1	B	3042	VAL	4.6
1	A	2924	SER	4.6
1	A	3362	LYS	4.5
1	A	3180	PHE	4.5
1	B	2939	LYS	4.4
1	A	3245	ILE	4.4
1	B	3404	HIS	4.4
1	B	3171	PRO	4.4
1	B	3309	ALA	4.4
1	B	3369	HIS	4.4
1	B	2935	ASP	4.3
1	A	3359	PHE	4.3
1	A	3394	CYS	4.3
1	A	3218	GLY	4.3
1	B	3277	HIS	4.3
1	A	3027	ASN	4.2
1	B	3027	ASN	4.2
1	A	3128	GLU	4.2
1	B	3216	LEU	4.2
1	A	3361	CYS	4.2
1	A	2981	PRO	4.1
1	A	3372	GLU	4.1
1	A	3066	LEU	4.1
1	A	3233	THR	4.1
1	B	3406	ASP	4.1
1	B	3002	LEU	4.1
1	B	2925	LEU	4.1
1	A	3311	PHE	4.0
1	A	3334	THR	4.0
1	A	3270	ASN	4.0
1	B	3324	LEU	4.0
1	A	2998	HIS	4.0
1	B	3087	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	2977	MET	3.9
1	B	3319	GLY	3.9
1	A	3021	ALA	3.9
1	B	3396	ASP	3.9
1	B	3197	LEU	3.9
1	A	3079	VAL	3.9
1	A	3297	LEU	3.9
1	A	2965	LYS	3.8
1	A	3039	GLN	3.8
1	A	3147	MET	3.8
1	A	3187	LEU	3.8
1	B	2965	LYS	3.8
1	B	3361	CYS	3.8
1	B	3313	ILE	3.8
1	B	3366	PHE	3.8
1	B	2979	ILE	3.8
1	A	3396	ASP	3.8
1	A	3003	GLY	3.8
1	B	3231	SER	3.7
1	A	3005	PRO	3.7
1	B	3151	LEU	3.7
1	B	2962	CYS	3.7
1	B	2930	ALA	3.7
1	B	3251	GLU	3.7
1	B	3264	ILE	3.7
1	B	3239	TYR	3.7
1	A	3090	ALA	3.7
1	B	3329	VAL	3.6
1	B	3175	VAL	3.6
1	B	3307	ASN	3.6
1	A	3277	HIS	3.6
1	B	3253	PRO	3.6
1	A	3189	LEU	3.6
1	A	3333	GLY	3.6
1	B	3182	TYR	3.6
1	A	3004	ILE	3.6
1	A	2992	GLU	3.6
1	B	3172	ASN	3.5
1	A	3103	LEU	3.5
1	B	2950	GLU	3.5
1	B	2958	TYR	3.5
1	A	3392	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	3278	VAL	3.5
1	B	3030	PHE	3.5
1	A	2982	HIS	3.5
1	B	3392	GLU	3.5
1	A	3033	HIS	3.5
1	B	3283	ASP	3.5
1	B	3330	VAL	3.5
1	B	3195	GLU	3.5
1	B	3220	ARG	3.5
1	A	3268	VAL	3.5
1	B	3016	LEU	3.5
1	A	3371	PHE	3.5
1	B	3121	LYS	3.4
1	B	2964	GLU	3.4
1	B	3007	TRP	3.4
1	B	3154	PHE	3.4
1	B	2978	SER	3.4
1	A	3177	SER	3.4
1	B	3290	THR	3.4
1	A	3098	TYR	3.4
1	A	2931	GLU	3.4
1	B	3221	THR	3.3
1	A	3023	SER	3.3
1	A	3169	SER	3.3
1	A	3100	MET	3.3
1	B	3398	ASN	3.3
1	B	3143	ALA	3.3
1	A	3076	ASP	3.3
1	B	3046	ASN	3.3
1	B	3080	GLN	3.3
1	B	3322	VAL	3.3
1	B	2955	PHE	3.3
1	B	3047	GLU	3.3
1	B	3332	ARG	3.2
1	B	3014	SER	3.2
1	B	3039	GLN	3.2
1	B	3104	GLU	3.2
1	A	3108	PHE	3.2
1	B	2987	HIS	3.2
1	B	3033	HIS	3.2
1	B	3310	VAL	3.2
1	A	3047	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	3128	GLU	3.2
1	A	3161	ASN	3.1
1	A	3190	HIS	3.1
1	A	3142	CYS	3.1
1	B	3202	ARG	3.1
1	B	3238	GLU	3.1
1	A	3208	SER	3.1
1	A	3167	GLU	3.1
1	B	3026	ASN	3.1
1	A	3356	THR	3.1
1	A	3397	ASN	3.1
1	A	3042	VAL	3.1
1	B	3271	LEU	3.0
1	B	3125	ILE	3.0
1	A	2928	HIS	3.0
1	B	3105	TYR	3.0
1	B	3400	ARG	3.0
1	B	3008	ASP	3.0
1	A	3329	VAL	2.9
1	B	3040	ASP	2.9
1	A	2979	ILE	2.9
1	B	3245	ILE	2.9
1	A	3179	ARG	2.9
1	B	3185	ASP	2.9
1	B	3297	LEU	2.9
1	B	3250	LYS	2.9
1	B	3397	ASN	2.9
1	B	3268	VAL	2.8
1	B	3301	ILE	2.8
1	A	3157	GLU	2.8
1	B	3289	HIS	2.8
1	B	3189	LEU	2.8
1	B	3300	PRO	2.8
1	B	2923	HIS	2.8
1	A	3061	ILE	2.8
1	A	3030	PHE	2.8
1	A	3202	ARG	2.7
1	B	3005	PRO	2.7
1	A	2956	HIS	2.7
1	A	3101	SER	2.7
1	A	3148	HIS	2.7
1	A	3238	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	3298	PRO	2.7
1	A	3292	LEU	2.7
1	A	3121	LYS	2.7
1	A	3134	VAL	2.7
1	B	3090	ALA	2.7
1	B	2929	GLU	2.7
1	B	3023	SER	2.7
1	B	3286	LYS	2.7
1	B	3060	SER	2.7
1	B	3368	PHE	2.7
1	B	3174	VAL	2.7
1	A	3261	ARG	2.6
1	A	3223	ALA	2.6
1	A	2948	GLY	2.6
1	B	3131	LYS	2.6
1	B	3254	TRP	2.6
1	A	2921	ASN	2.6
1	A	3153	PRO	2.6
1	B	3389	SER	2.6
1	B	2948	GLY	2.6
1	B	2986	LEU	2.5
1	B	3015	SER	2.5
1	B	3096	GLU	2.5
1	B	3341	VAL	2.5
1	B	2927	HIS	2.5
1	B	3280	PHE	2.5
1	A	3115	HIS	2.5
1	A	3175	VAL	2.5
1	B	3068	ALA	2.5
1	A	3145	ASP	2.5
1	B	3009	TRP	2.5
1	B	3109	ASP	2.5
1	A	3357	ALA	2.4
1	B	3148	HIS	2.4
1	B	3349	MET	2.4
1	B	3299	ALA	2.4
1	B	2969	LYS	2.4
1	B	3198	GLU	2.4
1	B	2956	HIS	2.4
1	A	3309	ALA	2.4
1	A	2958	TYR	2.4
1	B	3340	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	3209	ARG	2.4
1	B	2917	LEU	2.4
1	A	3164	PHE	2.4
1	B	3344	ALA	2.3
1	B	3161	ASN	2.3
1	B	3276	ASP	2.3
1	B	3029	PHE	2.3
1	A	3122	ILE	2.3
1	B	3132	ARG	2.3
1	B	3085	HIS	2.3
1	A	3206	LEU	2.3
1	B	3270	ASN	2.3
1	A	2974	VAL	2.3
1	A	3207	LYS	2.3
1	B	3063	TYR	2.2
1	A	3263	ASP	2.2
1	B	3311	PHE	2.2
1	A	3156	TYR	2.2
1	B	3111	TYR	2.2
1	B	3370	ALA	2.2
1	A	3367	SER	2.2
1	B	3351	ASN	2.2
1	B	3386	MET	2.2
1	B	2938	TYR	2.2
1	A	3185	ASP	2.2
1	A	3008	ASP	2.1
1	B	3282	PHE	2.1
1	A	3248	GLY	2.1
1	B	3059	SER	2.1
1	B	3122	ILE	2.1
1	A	3343	GLU	2.1
1	B	2993	ARG	2.1
1	A	3399	LEU	2.1
1	B	3383	ASP	2.1
1	B	3038	ASN	2.1
1	B	3355	TYR	2.1
1	A	2986	LEU	2.1
1	A	3135	LYS	2.1
1	A	3240	ALA	2.1
1	B	3078	GLU	2.1
1	B	3079	VAL	2.1
1	B	3152	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2926	SER	2.1
1	A	3209	ARG	2.0
1	A	3271	LEU	2.0
1	A	3060	SER	2.0
1	B	3210	VAL	2.0
1	A	3188	ASN	2.0
1	B	3273	LEU	2.0
1	B	3378	SER	2.0
1	B	3153	PRO	2.0
1	B	2952	ILE	2.0
1	B	3317	PRO	2.0
1	B	3203	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.