Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:11 AM GMT

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	:	2009-12-27
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:

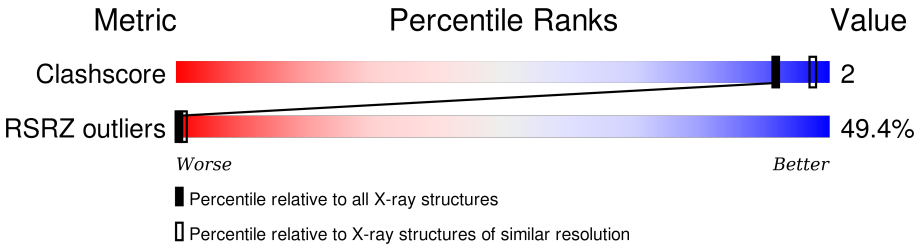
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	102246	1052 (4.40-3.60)
RSRZ outliers	91569	1013 (4.42-3.56)

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	A	491	44% 97%
1	B	491	52% 96%

2 Entry composition (i)

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.

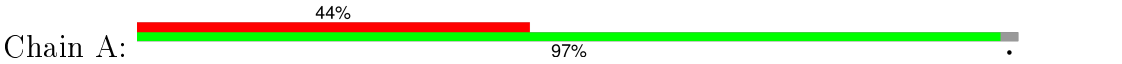
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	479	Total	C	0	0	479
			479	479			
1	B	475	Total	C	0	0	475
			475	475			

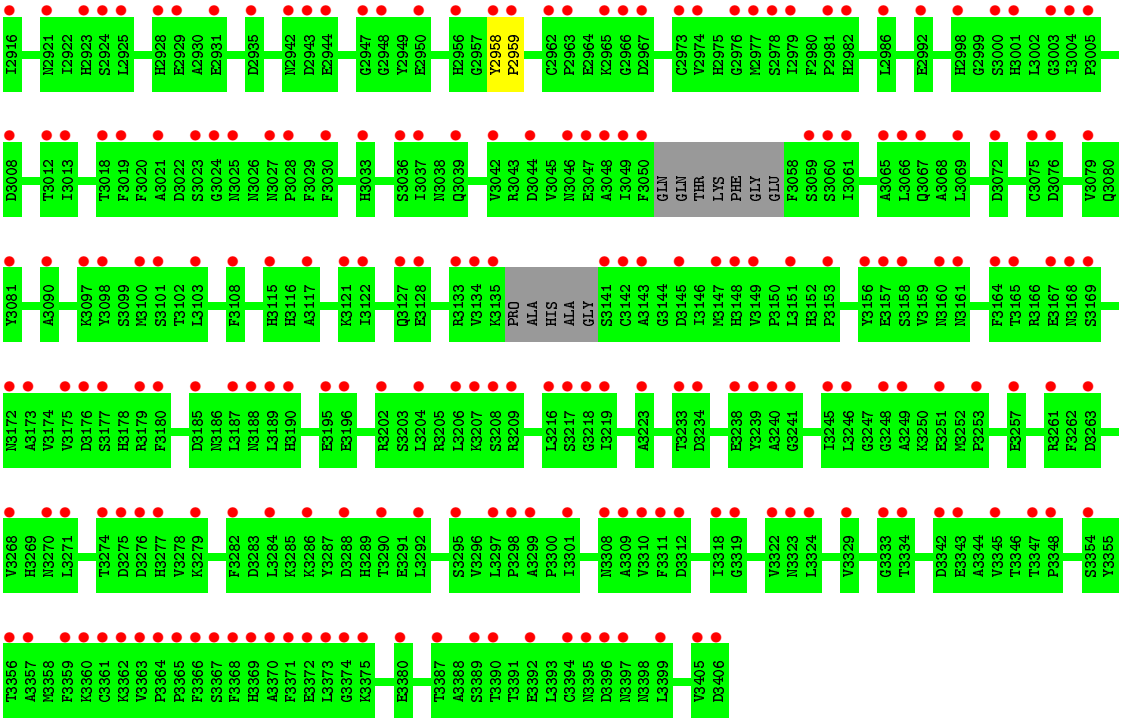
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Hemocyanin 1

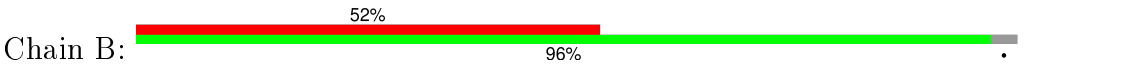
Chain A:

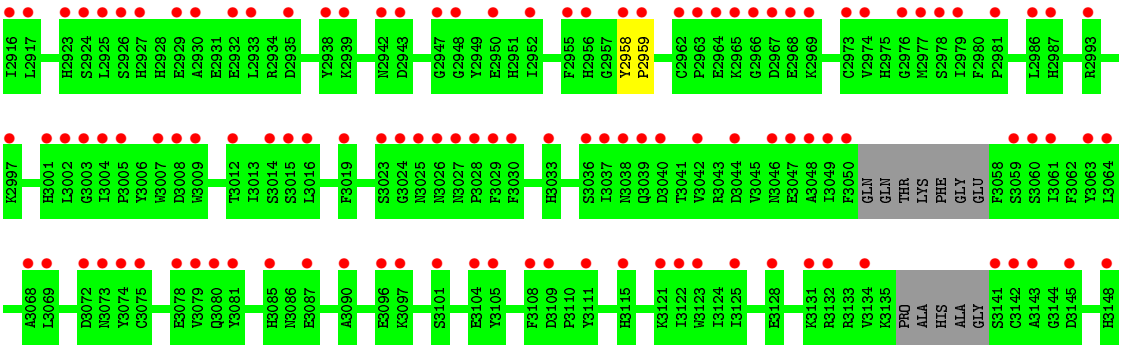


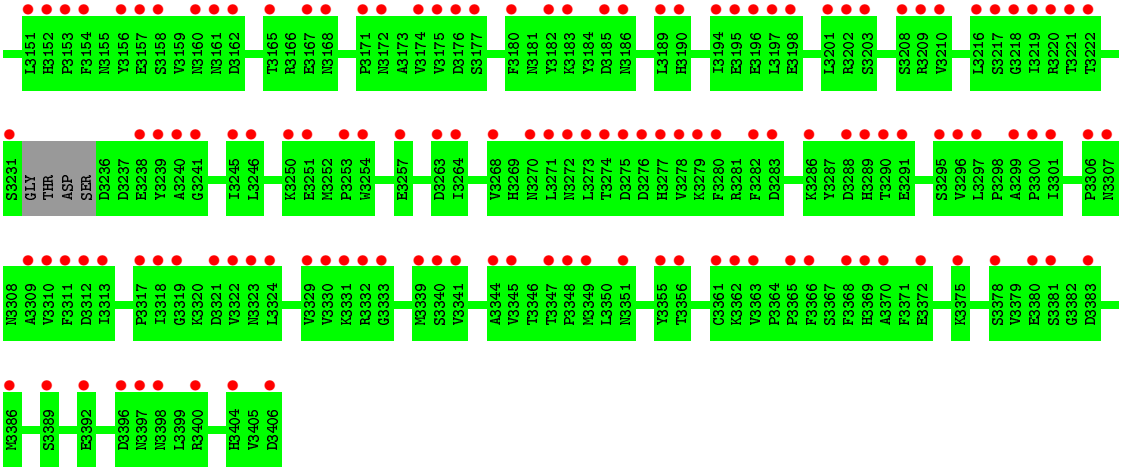


- Molecule 1: Hemocyanin 1

Chain B:






L3151 H3152 P3153 F3154 N3155 Y3156 E3157 S3158 V3159 N3160 N3161 D3162
T3165 R3166 E3167 N3168
P3171 N3172 A3173 V3174 V3175 D3176 S3177
F3180 N3181 Y3182 K3183 Y3184 D3185 M3186
L3189 H3190
I3194 E3195 E3196 L3197 E3198
L3201 R3202 S3203
S3208 R3209 V3210
L3216 S3217 G3218 I3219 R3220 T3221 T3222
S3231 GLY THR ASP SER D3236 D3237 E3238 Y3239 A3240 G3241
I3245 L3246
K3250 E3251 M3252 P3253 W3254
E3257
D3263 I3264
V3268 H3269 N3270 L3271 N3272 L3273 T3274 D3275 D3276 H3277 V3278 K3279 F3280 R3281 F3282 D3283
K3286 Y3287 D3288 H3289 T3290 E3291
S3295 V3296 L3297 P3298 A3299 P3300 I3301
P3306 N3307
N3308 A3309 V3310 F3311 D3312 I3313
P3317 I3318 G3319 K3320 D3321 V3322 N3323 L3324
V3329 V3330 K3331 R3332 G3333
M3339 S3340 V3341
A3344 V3345 T3346 T3347 P3348 M3349 L3350 N3351
Y3355 T3356
C3361 K3362 V3363 P3364 P3365 F3366 S3367 F3368 H3369 A3370 F3371 E3372
K3375
S3378 V3379 E3380 S3381 G3382 D3383
M3386
S3389
E3392
D3396 N3397 N3398 L3399 R3400
H3404 V3405 D3406

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.73 (at 3.98Å)	Xtriage
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available) 0.485 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	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
Estimated twinning fraction	0.055 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 22294 reflections	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.*

[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

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).

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

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

5.3.1 Protein backbone

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

5.3.2 Protein sidechains

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

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	2.90	218 (45%)	0	1	0, 0, 0, 0	0
1	B	475/491 (96%)	3.11	253 (53%)	0	1	0, 0, 0, 0	0
All	All	954/982 (97%)	3.00	471 (49%)	0	1	0, 0, 0, 0	0

All (471) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2916	ILE	26.7
1	B	3196	GLU	25.2
1	A	3012	THR	23.0
1	B	3380	GLU	22.6
1	B	2967	ASP	19.9
1	B	3075	CYS	19.9
1	A	3405	VAL	18.4
1	A	3274	THR	17.7
1	B	3048	ALA	17.6
1	B	3012	THR	17.3
1	B	3274	THR	14.7
1	A	3370	ALA	14.4
1	B	3097	LYS	14.1
1	A	3374	GLY	14.0
1	B	3001	HIS	13.4
1	B	3180	PHE	13.3
1	A	3168	ASN	13.3
1	A	3312	ASP	13.1
1	A	3001	HIS	12.9
1	B	3003	GLY	12.7
1	B	3073	ASN	12.4
1	B	3363	VAL	12.2
1	B	3142	CYS	11.7
1	B	3246	LEU	11.4

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Mol	Chain	Res	Type	RSRZ
1	A	3406	ASP	11.3
1	A	2963	PRO	11.1
1	B	3356	THR	11.1
1	A	3246	LEU	10.9
1	B	3217	SER	10.9
1	A	2916	ILE	10.8
1	A	3216	LEU	10.8
1	B	3362	LYS	10.6
1	A	2967	ASP	10.6
1	A	3069	LEU	10.6
1	A	3075	CYS	10.5
1	A	3319	GLY	10.5
1	B	3275	ASP	10.3
1	A	3318	ILE	10.3
1	B	3208	SER	10.3
1	A	2976	GLY	10.3
1	A	3368	PHE	10.2
1	B	3168	ASN	10.2
1	B	3272	ASN	10.0
1	A	3373	LEU	9.6
1	A	3363	VAL	9.6
1	B	3074	TYR	9.6
1	B	2981	PRO	9.4
1	B	3036	SER	9.4
1	B	2997	LYS	9.3
1	B	3050	PHE	9.2
1	A	3299	ALA	9.2
1	A	3275	ASP	9.1
1	B	3312	ASP	9.0
1	B	3160	ASN	9.0
1	B	2947	GLY	9.0
1	A	3048	ALA	8.9
1	A	3395	ASN	8.9
1	B	3108	PHE	8.9
1	B	3186	ASN	8.8
1	B	3288	ASP	8.7
1	B	3321	ASP	8.5
1	A	2973	CYS	8.5
1	B	3381	SER	8.4
1	A	2925	LEU	8.3
1	A	3049	ILE	8.3
1	A	3301	ILE	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	3044	ASP	8.2
1	A	3158	SER	8.2
1	B	2924	SER	8.2
1	B	3323	ASN	8.1
1	B	2963	PRO	8.1
1	B	2959	PRO	8.0
1	A	3028	PRO	8.0
1	A	3324	LEU	7.9
1	B	3306	PRO	7.9
1	A	3149	VAL	7.8
1	A	3387	THR	7.7
1	A	3310	VAL	7.7
1	B	3241	GLY	7.6
1	A	2947	GLY	7.5
1	B	3263	ASP	7.5
1	B	3158	SER	7.5
1	B	3069	LEU	7.5
1	A	3295	SER	7.5
1	A	3375	LYS	7.5
1	A	2978	SER	7.5
1	B	3162	ASP	7.4
1	B	3219	ILE	7.4
1	A	3284	LEU	7.4
1	A	3347	THR	7.3
1	A	3323	ASN	7.3
1	B	3190	HIS	7.3
1	A	3141	SER	7.3
1	B	3257	GLU	7.3
1	A	2944	GLU	7.3
1	A	3390	THR	7.2
1	B	3004	ILE	7.2
1	B	3081	TYR	7.1
1	A	3345	VAL	7.1
1	A	3365	PRO	7.1
1	A	3369	HIS	7.1
1	A	2962	CYS	7.0
1	B	3123	TRP	7.0
1	A	3059	SER	6.9
1	B	3177	SER	6.9
1	B	3072	ASP	6.9
1	B	3141	SER	6.9
1	A	3276	ASP	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	3024	GLY	6.8
1	A	3354	SER	6.7
1	B	3375	LYS	6.7
1	A	3050	PHE	6.7
1	B	3240	ALA	6.6
1	A	3081	TYR	6.6
1	A	3151	LEU	6.6
1	B	3218	GLY	6.6
1	A	3217	SER	6.6
1	B	2976	GLY	6.5
1	A	3219	ILE	6.4
1	A	3127	GLN	6.4
1	B	2932	GLU	6.4
1	B	3049	ILE	6.3
1	A	3389	SER	6.3
1	A	3176	ASP	6.3
1	A	3065	ALA	6.2
1	A	3000	SER	6.2
1	A	3195	GLU	6.2
1	A	3046	ASN	6.2
1	A	3380	GLU	6.1
1	A	3360	LYS	6.1
1	B	3348	PRO	6.1
1	A	2966	GLY	6.1
1	B	3156	TYR	6.0
1	A	3239	TYR	6.0
1	A	3282	PHE	6.0
1	B	3028	PRO	6.0
1	A	3165	THR	6.0
1	A	3348	PRO	6.0
1	B	3365	PRO	5.9
1	B	3157	GLU	5.9
1	A	2923	HIS	5.9
1	A	3172	ASN	5.9
1	A	3097	LYS	5.9
1	A	2943	ASP	5.8
1	B	3044	ASP	5.8
1	B	3145	ASP	5.8
1	B	3295	SER	5.8
1	A	3067	GLN	5.8
1	B	3345	VAL	5.7
1	B	3291	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	2942	ASN	5.7
1	B	3222	THR	5.7
1	B	3372	GLU	5.7
1	A	3160	ASN	5.7
1	A	3024	GLY	5.7
1	A	3241	GLY	5.7
1	B	3333	GLY	5.7
1	B	3176	ASP	5.6
1	A	3366	PHE	5.6
1	B	2943	ASP	5.6
1	A	2935	ASP	5.6
1	A	3013	ILE	5.5
1	B	3194	ILE	5.5
1	B	3167	GLU	5.5
1	A	3018	THR	5.5
1	B	2968	GLU	5.5
1	A	3322	VAL	5.5
1	A	3286	LYS	5.4
1	A	3196	GLU	5.4
1	A	3133	ARG	5.4
1	B	2973	CYS	5.4
1	A	2942	ASN	5.3
1	B	3115	HIS	5.3
1	B	3101	SER	5.3
1	A	3253	PRO	5.3
1	B	3025	ASN	5.3
1	A	3117	ALA	5.3
1	A	3204	LEU	5.2
1	A	3072	ASP	5.2
1	B	3331	LYS	5.2
1	B	3318	ILE	5.1
1	A	2950	GLU	5.1
1	A	3036	SER	5.1
1	A	3288	ASP	5.1
1	B	3019	PHE	5.0
1	A	3019	PHE	5.0
1	A	3364	PRO	5.0
1	A	3308	ASN	5.0
1	A	3257	GLU	5.0
1	A	3037	ILE	5.0
1	A	3251	GLU	5.0
1	B	2966	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	2929	GLU	4.9
1	B	3347	THR	4.9
1	A	3279	LYS	4.9
1	B	3183	LYS	4.9
1	A	3025	ASN	4.9
1	A	2959	PRO	4.9
1	A	3234	ASP	4.9
1	B	3042	VAL	4.8
1	A	3342	ASP	4.8
1	B	3309	ALA	4.8
1	A	3180	PHE	4.7
1	A	2924	SER	4.7
1	A	3245	ILE	4.7
1	B	3279	LYS	4.7
1	B	3404	HIS	4.6
1	A	3362	LYS	4.6
1	B	3369	HIS	4.6
1	A	3359	PHE	4.6
1	B	2935	ASP	4.6
1	A	3218	GLY	4.5
1	B	3277	HIS	4.5
1	B	2939	LYS	4.5
1	B	3216	LEU	4.5
1	B	3171	PRO	4.5
1	A	3066	LEU	4.4
1	B	3002	LEU	4.4
1	A	3394	CYS	4.4
1	A	3233	THR	4.4
1	A	3128	GLU	4.4
1	B	2925	LEU	4.4
1	A	3027	ASN	4.3
1	A	3372	GLU	4.3
1	B	3027	ASN	4.3
1	B	3406	ASP	4.3
1	A	3021	ALA	4.3
1	A	3334	THR	4.3
1	B	3324	LEU	4.3
1	A	3311	PHE	4.3
1	A	2981	PRO	4.3
1	A	3361	CYS	4.2
1	A	2998	HIS	4.2
1	B	3197	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	3297	LEU	4.2
1	A	2977	MET	4.2
1	B	3319	GLY	4.2
1	A	3270	ASN	4.1
1	B	3087	GLU	4.1
1	A	3187	LEU	4.1
1	B	3313	ILE	4.1
1	A	3079	VAL	4.1
1	B	2979	ILE	4.1
1	B	3396	ASP	4.1
1	A	3147	MET	4.1
1	B	3366	PHE	4.1
1	B	2930	ALA	4.1
1	B	3239	TYR	4.0
1	A	3090	ALA	4.0
1	A	3039	GLN	4.0
1	B	3151	LEU	4.0
1	A	3003	GLY	4.0
1	A	3396	ASP	4.0
1	B	3264	ILE	4.0
1	B	3182	TYR	4.0
1	A	2965	LYS	3.9
1	B	2965	LYS	3.9
1	B	3231	SER	3.9
1	B	2958	TYR	3.9
1	B	3361	CYS	3.9
1	A	3189	LEU	3.9
1	B	3251	GLU	3.9
1	B	3329	VAL	3.9
1	B	3175	VAL	3.9
1	A	3004	ILE	3.9
1	A	3277	HIS	3.8
1	A	3005	PRO	3.8
1	A	3103	LEU	3.8
1	A	3333	GLY	3.8
1	B	2962	CYS	3.8
1	B	3030	PHE	3.8
1	B	3278	VAL	3.8
1	B	3307	ASN	3.8
1	B	3016	LEU	3.8
1	A	2982	HIS	3.7
1	B	3007	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	2992	GLU	3.7
1	A	3033	HIS	3.7
1	A	3098	TYR	3.7
1	B	2950	GLU	3.7
1	B	3253	PRO	3.7
1	B	3330	VAL	3.7
1	A	3392	GLU	3.7
1	A	3371	PHE	3.7
1	A	3268	VAL	3.7
1	B	3392	GLU	3.7
1	B	3283	ASP	3.7
1	B	3195	GLU	3.7
1	B	3172	ASN	3.7
1	B	3154	PHE	3.7
1	B	3290	THR	3.7
1	B	3143	ALA	3.6
1	B	3220	ARG	3.6
1	B	2964	GLU	3.6
1	B	3221	THR	3.6
1	B	2978	SER	3.6
1	A	3177	SER	3.6
1	A	2931	GLU	3.5
1	A	3100	MET	3.5
1	B	3121	LYS	3.5
1	B	2955	PHE	3.5
1	B	3322	VAL	3.5
1	A	3023	SER	3.5
1	A	3076	ASP	3.5
1	A	3169	SER	3.5
1	B	3080	GLN	3.4
1	A	3108	PHE	3.4
1	B	3047	GLU	3.4
1	B	3398	ASN	3.4
1	B	2987	HIS	3.4
1	B	3033	HIS	3.4
1	B	3046	ASN	3.4
1	B	3104	GLU	3.4
1	B	3014	SER	3.4
1	B	3039	GLN	3.4
1	B	3332	ARG	3.4
1	B	3310	VAL	3.4
1	A	3190	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	3105	TYR	3.3
1	A	3047	GLU	3.3
1	B	3128	GLU	3.3
1	A	3356	THR	3.3
1	B	3271	LEU	3.3
1	B	3238	GLU	3.3
1	B	3125	ILE	3.3
1	A	3161	ASN	3.3
1	B	3202	ARG	3.2
1	A	3042	VAL	3.2
1	A	3167	GLU	3.2
1	A	3208	SER	3.2
1	A	2928	HIS	3.2
1	A	3142	CYS	3.2
1	B	3026	ASN	3.2
1	A	3397	ASN	3.2
1	A	2979	ILE	3.2
1	B	3245	ILE	3.2
1	A	3329	VAL	3.1
1	B	3297	LEU	3.1
1	B	3008	ASP	3.1
1	B	3040	ASP	3.1
1	B	3400	ARG	3.1
1	B	3185	ASP	3.1
1	B	3301	ILE	3.1
1	A	3179	ARG	3.0
1	B	3268	VAL	3.0
1	B	3189	LEU	3.0
1	B	3289	HIS	3.0
1	A	3061	ILE	3.0
1	B	3090	ALA	3.0
1	A	3157	GLU	3.0
1	B	3397	ASN	3.0
1	A	3030	PHE	3.0
1	B	2923	HIS	3.0
1	B	3250	LYS	2.9
1	A	3292	LEU	2.9
1	A	3223	ALA	2.9
1	A	2956	HIS	2.9
1	A	3148	HIS	2.9
1	A	3134	VAL	2.9
1	A	3101	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	3254	TRP	2.9
1	A	3202	ARG	2.9
1	A	3238	GLU	2.9
1	B	3300	PRO	2.9
1	B	3368	PHE	2.8
1	B	2929	GLU	2.8
1	B	3174	VAL	2.8
1	B	3005	PRO	2.8
1	B	3023	SER	2.8
1	A	2948	GLY	2.8
1	B	3060	SER	2.8
1	A	3298	PRO	2.8
1	A	3121	LYS	2.8
1	A	3261	ARG	2.8
1	B	2986	LEU	2.8
1	B	3068	ALA	2.7
1	B	3286	LYS	2.7
1	B	2948	GLY	2.7
1	A	3357	ALA	2.7
1	B	3299	ALA	2.7
1	B	3009	TRP	2.7
1	B	3389	SER	2.7
1	A	2921	ASN	2.7
1	B	3280	PHE	2.7
1	B	3131	LYS	2.7
1	B	2927	HIS	2.7
1	B	3341	VAL	2.7
1	A	3115	HIS	2.7
1	A	2958	TYR	2.7
1	B	3096	GLU	2.7
1	A	3153	PRO	2.7
1	A	3309	ALA	2.6
1	A	3175	VAL	2.6
1	B	3015	SER	2.6
1	A	3145	ASP	2.6
1	B	3344	ALA	2.6
1	B	3148	HIS	2.6
1	B	3349	MET	2.6
1	B	3109	ASP	2.6
1	B	2917	LEU	2.6
1	B	2956	HIS	2.6
1	A	3164	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	3198	GLU	2.5
1	A	3122	ILE	2.5
1	B	3063	TYR	2.5
1	A	3206	LEU	2.5
1	B	3340	SER	2.5
1	B	3029	PHE	2.5
1	B	3209	ARG	2.5
1	B	2969	LYS	2.5
1	B	3085	HIS	2.5
1	A	3156	TYR	2.5
1	B	3111	TYR	2.5
1	B	3276	ASP	2.5
1	B	3370	ALA	2.4
1	B	3132	ARG	2.4
1	B	3161	ASN	2.4
1	A	2974	VAL	2.4
1	B	2938	TYR	2.4
1	B	3270	ASN	2.4
1	B	3311	PHE	2.4
1	A	3263	ASP	2.4
1	B	3355	TYR	2.3
1	B	3386	MET	2.3
1	A	3207	LYS	2.3
1	B	3282	PHE	2.3
1	A	3240	ALA	2.3
1	B	3122	ILE	2.3
1	A	3367	SER	2.3
1	A	3399	LEU	2.3
1	A	3248	GLY	2.3
1	A	2986	LEU	2.3
1	A	3185	ASP	2.3
1	A	3008	ASP	2.3
1	B	3351	ASN	2.3
1	B	3059	SER	2.2
1	A	3343	GLU	2.2
1	A	3271	LEU	2.2
1	B	3383	ASP	2.2
1	A	3173	ALA	2.2
1	B	2993	ARG	2.2
1	B	3273	LEU	2.2
1	B	3152	HIS	2.2
1	B	3079	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2952	ILE	2.2
1	B	3078	GLU	2.2
1	B	3038	ASN	2.2
1	B	3210	VAL	2.2
1	B	3201	LEU	2.2
1	A	3143	ALA	2.2
1	B	2926	SER	2.2
1	A	3060	SER	2.1
1	B	3064	LEU	2.1
1	A	3209	ARG	2.1
1	A	3135	LYS	2.1
1	B	3165	THR	2.1
1	B	3378	SER	2.1
1	A	3188	ASN	2.1
1	B	3203	SER	2.1
1	B	3339	MET	2.1
1	A	3290	THR	2.1
1	B	2974	VAL	2.1
1	B	3153	PRO	2.1
1	B	3317	PRO	2.1
1	B	2977	MET	2.1
1	B	3037	ILE	2.1
1	B	3134	VAL	2.0
1	A	3249	ALA	2.0
1	B	3296	VAL	2.0
1	B	3061	ILE	2.0
1	B	2933	LEU	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.