Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 08:50 PM EDT

PDB ID	:	3QJO
Title	:	Refined Structure of the functional unit (KLH1-H) of keyhole limpet hemocyanin
Authors	:	Jaenicke, E.; Buchler, K.; Decker, H.; Markl, J.; Schroder, G.F.
Deposited on	:	2011-01-30
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
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:

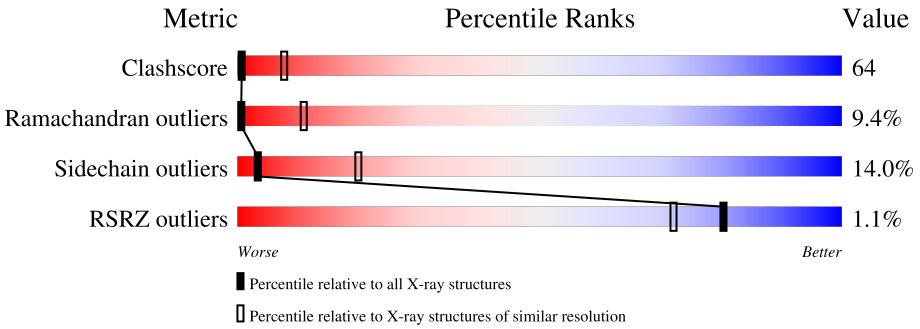
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 <=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	% 26% 58% 15% ·
1	B	491	% 25% 58% 15% ·

2 Entry composition (i)

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 (three-letter code: CU) (formula: Cu).

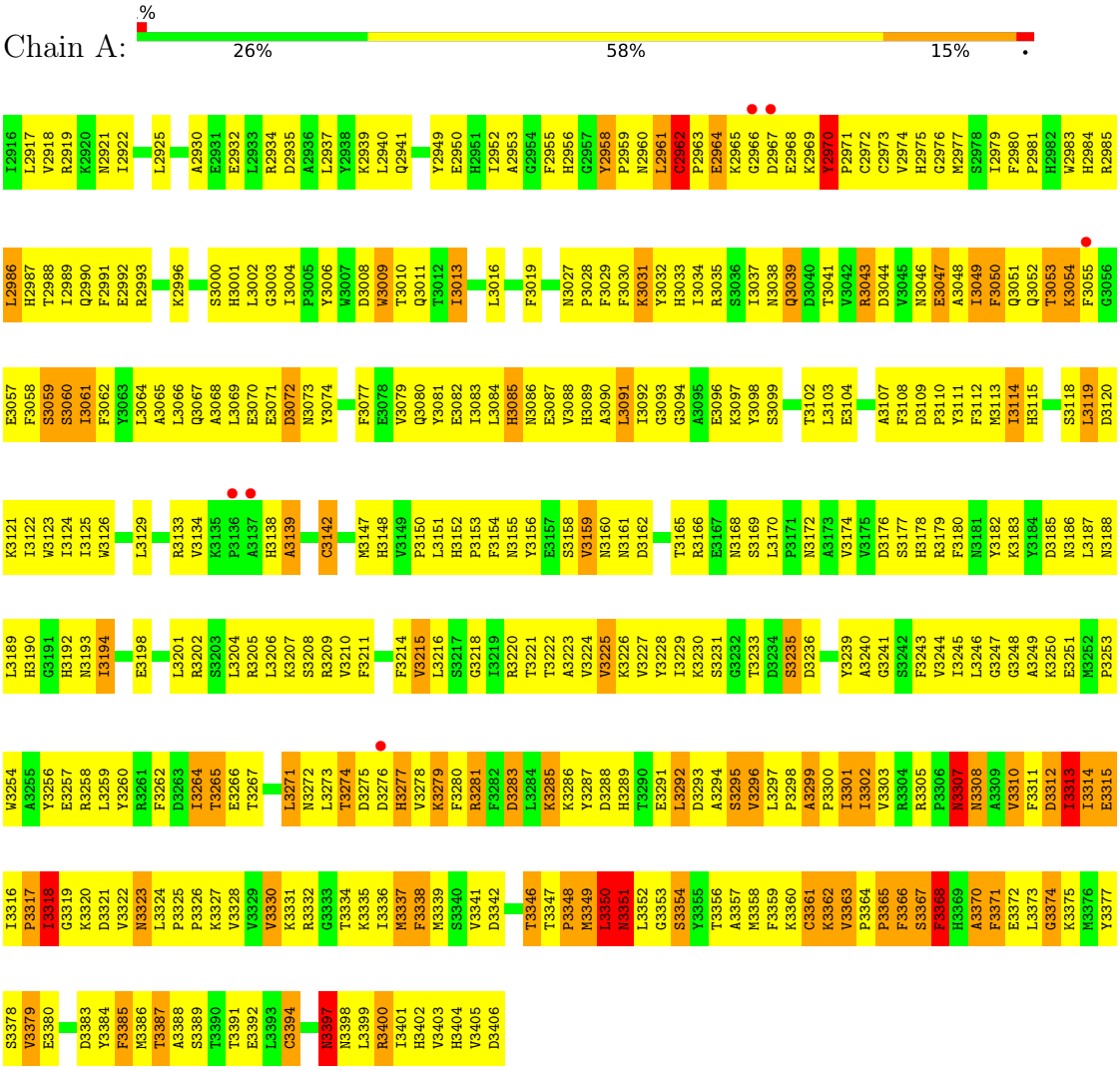
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

3 Residue-property plots (i)

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.

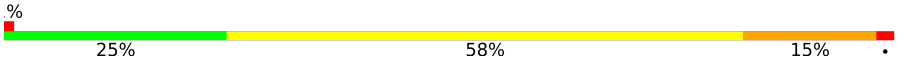
• Molecule 1: Hemocyanin 1

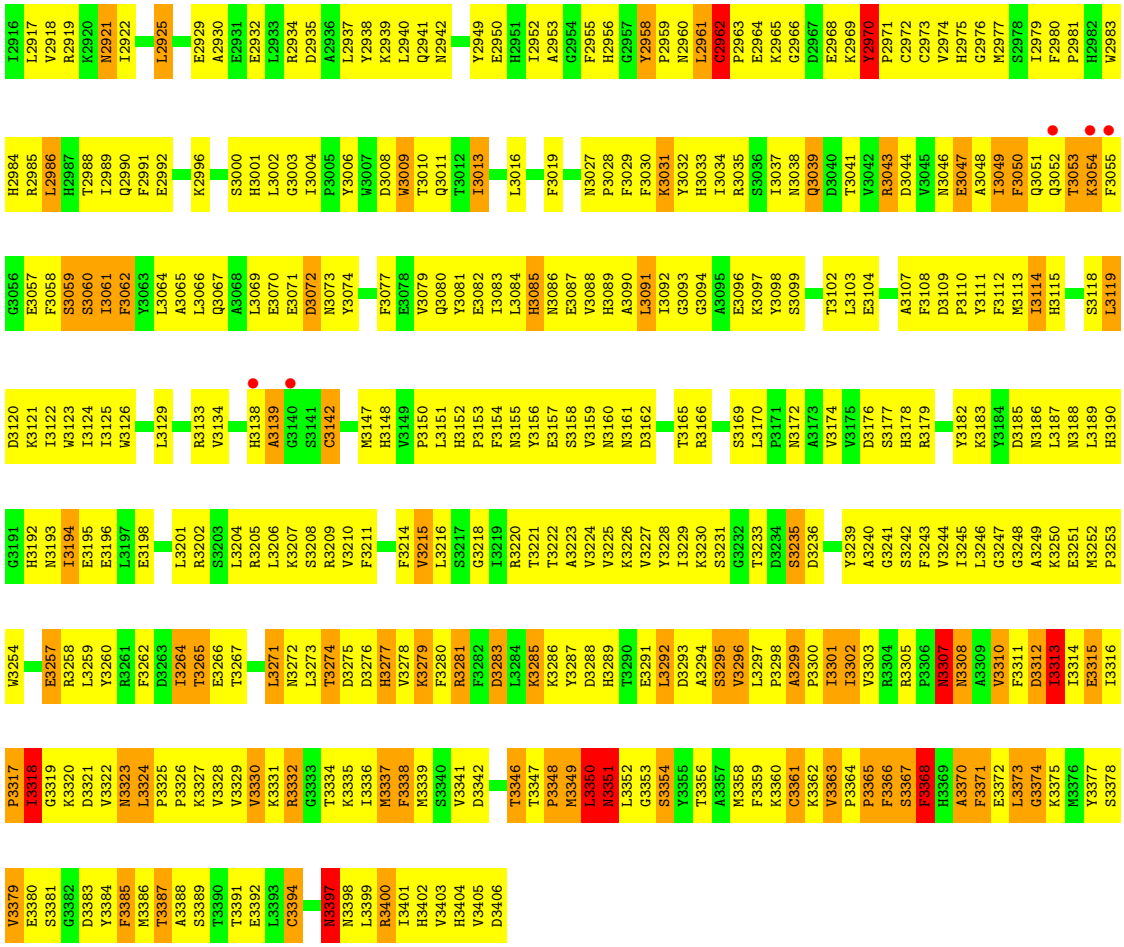
Chain A:



• Molecule 1: Hemocyanin 1

Chain B:




I2916 L2917 V2918 R2919 K2920 N2921 I2922 L2925 E2929 A2930 E2931 E2932 L2933 R2934 D2935 A2936 L2937 Y2938 K2939 L2940 Q2941 N2942 Y2949 E2950 H2951 I2952 A2953 G2954 F2955 H2956 G2957 Y2958 P2959 N2960 L2961 C2962 P2963 E2964 K2965 G2966 D2967 E2968 K2969 Y2970 P2971 C2972 C2973 V2974 H2975 G2976 M2977 S2978 I2979 F2980 P2981 H2982 W2983
H2984 R2985 L2986 H2987 T2988 I2989 Q2990 F2991 E2992 K2996 S3000 H3001 L3002 G3003 I3004 P3005 Y3006 W3007 D3008 W3009 T3010 Q3011 T3012 I3013 L3016 F3019 N3027 P3028 F3029 F3030 K3031 Y3032 H3033 I3034 R3035 S3036 I3037 N3038 Q3039 D3040 T3041 V3042 R3043 D3044 V3045 N3046 E3047 A3048 I3049 F3050 Q3051 Q3052 T3053 K3054 F3055
G3056 E3057 F3058 S3059 S3060 I3061 F3062 Y3063 L3064 A3065 L3066 Q3067 A3068 L3069 E3070 E3071 D3072 N3073 Y3074 F3077 E3078 V3079 Q3080 Y3081 E3082 I3083 L3084 H3085 N3086 E3087 V3088 H3089 A3090 L3091 I3092 G3093 G3094 A3095 E3096 K3097 Y3098 S3099 T3102 L3103 E3104 A3107 F3108 D3109 P3110 Y3111 F3112 M3113 I3114 H3115 S3118 L3119
D3120 K3121 I3122 W3123 I3124 I3125 W3126 L3129 R3133 V3134 H3138 A3139 G3140 S3141 C3142 M3147 H3148 V3149 P3150 L3151 H3152 P3153 F3154 N3155 Y3156 E3157 S3158 V3159 N3160 N3161 D3162 T3165 R3166 S3169 L3170 P3171 N3172 A3173 V3174 V3175 D3176 S3177 H3178 R3179 Y3182 K3183 Y3184 D3185 N3186 L3187 N3188 L3189 H3190
G3191 H3192 N3193 I3194 E3195 E3196 L3197 E3198 L3201 R3202 S3203 L3204 R3205 L3206 K3207 S3208 R3209 V3210 F3211 F3214 V3215 L3216 S3217 G3218 I3219 R3220 T3221 T3222 A3223 V3224 V3225 K3226 V3227 Y3228 I3229 K3230 S3231 G3232 T3233 D3234 S3235 D3236 Y3239 A3240 G3241 S3242 F3243 V3244 I3245 L3246 G3247 G3248 A3249 K3250 E3251 M3252 P3253
W3254 E3257 R3258 L3259 Y3260 R3261 F3262 D3263 I3264 T3265 E3266 T3267 L3271 N3272 L3273 T3274 D3275 D3276 H3277 V3278 K3279 F3280 R3281 F3282 D3283 L3284 K3285 K3286 Y3287 D3288 H3289 T3290 E3291 L3292 D3293 A3294 S3295 V3296 L3297 P3298 A3299 P3300 I3301 I3302 V3303 R3304 R3305 P3306 N3307 N3308 A3309 V3310 F3311 D3312 I3313 I3314 E3315 I3316
P3317 I3318 G3319 K3320 D3321 V3322 N3323 L3324 P3325 P3326 K3327 V3328 V3329 V3330 K3331 R3332 G3333 T3334 K3335 I3336 M3337 F3338 M3339 S3340 V3341 D3342 T3346 T3347 P3348 M3349 L3350 N3351 L3352 G3353 S3354 Y3355 T3356 A3357 M3358 F3359 K3360 C3361 K3362 V3363 P3364 P3365 F3366 S3367 F3368 H3369 A3370 F3371 E3372 L3373 G3374 K3375 M3376 Y3377 S3378
V3379 E3380 S3381 G3382 D3383 Y3384 F3385 M3386 T3387 A3388 S3389 T3390 T3391 E3392 L3393 C3394 N3397 N3398 L3399 R3400 I3401 H3402 V3403 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)	30.00 – 4.00 29.58 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-4.00) 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	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)	0.24 , 149.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/4110	0.46	0/5575
1	B	0.26	0/4110	0.46	0/5575
All	All	0.26	0/8220	0.46	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	510	0
1	B	3995	0	3831	502	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	7994	0	7662	1000	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 64.

All (1000) 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:B:3326:PRO:HB3	1:B:3402:HIS:HB3	1.44	0.96
1:A:2969:LYS:O	1:A:2970:TYR:HB2	1.66	0.95
1:A:2996:LYS:HA	1:A:3000:SER:HB3	1.46	0.95
1:A:3064:LEU:HB2	1:A:3084:LEU:HD23	1.49	0.93
1:B:2969:LYS:O	1:B:2970:TYR:HB2	1.66	0.93
1:B:2996:LYS:HA	1:B:3000:SER:HB3	1.51	0.92
1:B:2940:LEU:HG	1:B:2949:TYR:HB2	1.49	0.92
1:A:3316:ILE:HG22	1:A:3339:MET:HG2	1.52	0.91
1:B:3064:LEU:HB2	1:B:3084:LEU:HD23	1.52	0.90
1:A:3159:VAL:HG22	1:A:3160:ASN:H	1.36	0.90
1:A:2940:LEU:HG	1:A:2949:TYR:HB2	1.52	0.88
1:A:3328:VAL:HG12	1:A:3330:VAL:HG22	1.54	0.88
1:A:3326:PRO:HB3	1:A:3402:HIS:HB3	1.56	0.88
1:A:3275:ASP:HB2	1:A:3302:ILE:HD11	1.57	0.87
1:B:2985:ARG:HH12	1:B:3124:ILE:HD11	1.40	0.86
1:B:3350:LEU:HD23	1:B:3351:ASN:H	1.41	0.86
1:B:2917:LEU:HD12	1:B:2918:VAL:H	1.41	0.85
1:A:3350:LEU:HD23	1:A:3351:ASN:H	1.42	0.85
1:A:2985:ARG:HH12	1:A:3124:ILE:HD11	1.41	0.84
1:B:3328:VAL:HG12	1:B:3330:VAL:HG22	1.58	0.84
1:A:2917:LEU:HD12	1:A:2918:VAL:H	1.43	0.84
1:B:2962:CYS:HB2	1:B:2963:PRO:HD3	1.60	0.84
1:B:3159:VAL:HG22	1:B:3160:ASN:H	1.43	0.84
1:B:3275:ASP:HB2	1:B:3302:ILE:HD11	1.61	0.83
1:A:2985:ARG:HH22	1:A:3124:ILE:HD13	1.44	0.83
1:A:3279:LYS:HZ2	1:A:3279:LYS:HA	1.43	0.82
1:B:3320:LYS:H	1:B:3399:LEU:HD21	1.45	0.82
1:B:3013:ILE:HD13	1:B:3049:ILE:HA	1.60	0.82
1:B:3317:PRO:HG2	1:B:3338:PHE:HA	1.62	0.82
1:B:3142:CYS:HB2	1:B:3258:ARG:HH22	1.45	0.81
1:B:3316:ILE:HG22	1:B:3339:MET:HG2	1.61	0.81
1:A:2962:CYS:HB2	1:A:2963:PRO:HD3	1.61	0.81
1:B:3215:VAL:HG23	1:B:3298:PRO:HG2	1.60	0.81
1:A:3275:ASP:HB2	1:A:3302:ILE:CD1	2.11	0.81
1:A:3013:ILE:HD13	1:A:3049:ILE:HA	1.62	0.80
1:A:3142:CYS:HB2	1:A:3258:ARG:HH22	1.45	0.80
1:B:3325:PRO:HA	1:B:3400:ARG:HH12	1.46	0.80
1:A:3320:LYS:HA	1:A:3397:ASN:OD1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2937:LEU:HG	1:B:2941:GLN:HE21	1.47	0.79
1:B:3210:VAL:HG12	1:B:3265:THR:HA	1.62	0.79
1:B:3279:LYS:HZ2	1:B:3279:LYS:HA	1.47	0.79
1:B:3320:LYS:HA	1:B:3397:ASN:OD1	1.83	0.79
1:A:3210:VAL:HG12	1:A:3265:THR:HA	1.65	0.79
1:A:3125:ILE:O	1:A:3129:LEU:HB2	1.82	0.78
1:B:3159:VAL:HG13	1:B:3161:ASN:H	1.48	0.78
1:B:3310:VAL:HG12	1:B:3311:PHE:H	1.47	0.78
1:B:2985:ARG:HH22	1:B:3124:ILE:HD13	1.47	0.78
1:A:3320:LYS:H	1:A:3399:LEU:HD21	1.46	0.78
1:B:3350:LEU:HD22	1:B:3387:THR:HB	1.65	0.78
1:A:3215:VAL:HG23	1:A:3298:PRO:HG2	1.64	0.78
1:A:3325:PRO:HA	1:A:3400:ARG:HH12	1.48	0.77
1:A:3071:GLU:HG3	1:A:3080:GLN:HG3	1.66	0.77
1:A:3159:VAL:HG13	1:A:3161:ASN:H	1.47	0.77
1:B:3274:THR:HB	1:B:3277:HIS:HB3	1.66	0.77
1:A:3194:ILE:HD13	1:A:3194:ILE:H	1.50	0.77
1:A:3208:SER:N	1:A:3307:ASN:HB3	2.00	0.76
1:B:3086:ASN:HB3	1:B:3244:VAL:HG13	1.67	0.76
1:B:3072:ASP:HB2	1:B:3311:PHE:CE2	2.21	0.76
1:B:3125:ILE:O	1:B:3129:LEU:HB2	1.84	0.76
1:A:3317:PRO:HG2	1:A:3338:PHE:HA	1.66	0.76
1:B:3275:ASP:HB2	1:B:3302:ILE:CD1	2.15	0.76
1:A:3207:LYS:HA	1:A:3207:LYS:HE2	1.68	0.75
1:A:3307:ASN:CG	1:A:3308:ASN:H	1.87	0.75
1:B:2986:LEU:O	1:B:2989:ILE:HG13	1.86	0.75
1:A:3350:LEU:HD22	1:A:3387:THR:HB	1.68	0.75
1:A:3061:ILE:HG23	1:A:3062:PHE:N	2.02	0.75
1:A:3258:ARG:NH1	1:A:3330:VAL:HG21	2.02	0.75
1:A:3302:ILE:HD12	1:A:3316:ILE:HD13	1.69	0.74
1:A:3325:PRO:HA	1:A:3400:ARG:NH1	2.03	0.74
1:A:3274:THR:HB	1:A:3277:HIS:HB3	1.69	0.74
1:B:3305:ARG:CZ	1:B:3313:ILE:HD11	2.17	0.74
1:B:3325:PRO:HA	1:B:3400:ARG:NH1	2.03	0.74
1:A:3227:VAL:HA	1:A:3283:ASP:HB3	1.67	0.74
1:A:3397:ASN:ND2	1:A:3399:LEU:HG	2.03	0.73
1:B:3318:ILE:HG13	1:B:3339:MET:HB2	1.69	0.73
1:A:2986:LEU:O	1:A:2989:ILE:HG13	1.87	0.73
1:B:3297:LEU:HB2	1:B:3298:PRO:HA	1.70	0.73
1:B:3207:LYS:HE2	1:B:3207:LYS:HA	1.71	0.73
1:A:3086:ASN:HB3	1:A:3244:VAL:HG13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3347:THR:N	1:A:3348:PRO:HD3	2.03	0.72
1:B:3347:THR:N	1:B:3348:PRO:HD3	2.04	0.72
1:B:3397:ASN:HD22	1:B:3398:ASN:N	1.87	0.72
1:A:3297:LEU:HB2	1:A:3298:PRO:HA	1.71	0.72
1:A:2937:LEU:HG	1:A:2941:GLN:HE21	1.53	0.72
1:B:3013:ILE:HD12	1:B:3013:ILE:H	1.55	0.72
1:A:3097:LYS:O	1:A:3102:THR:HG21	1.89	0.72
1:A:3273:LEU:HD22	1:A:3279:LYS:HD2	1.71	0.72
1:B:3097:LYS:O	1:B:3102:THR:HG21	1.89	0.72
1:B:3072:ASP:HB2	1:B:3311:PHE:HE2	1.54	0.72
1:B:3297:LEU:HB2	1:B:3298:PRO:CA	2.19	0.72
1:A:3274:THR:H	1:A:3277:HIS:CE1	2.07	0.71
1:B:3071:GLU:HG3	1:B:3080:GLN:HG3	1.70	0.71
1:A:3348:PRO:HB2	1:A:3389:SER:CB	2.21	0.71
1:B:3061:ILE:HG23	1:B:3062:PHE:N	2.01	0.71
1:B:3194:ILE:HD13	1:B:3194:ILE:H	1.55	0.71
1:B:3227:VAL:HA	1:B:3283:ASP:HB3	1.73	0.71
1:B:3273:LEU:HD22	1:B:3279:LYS:HD2	1.73	0.71
1:B:2955:PHE:HE2	1:B:3159:VAL:HG23	1.55	0.71
1:A:3305:ARG:CZ	1:A:3313:ILE:HD11	2.20	0.70
1:A:3048:ALA:O	1:A:3049:ILE:HD13	1.92	0.70
1:A:3297:LEU:HB2	1:A:3298:PRO:CA	2.21	0.70
1:B:3228:TYR:O	1:B:3281:ARG:HB2	1.91	0.70
1:B:3397:ASN:ND2	1:B:3399:LEU:HG	2.06	0.70
1:B:2921:ASN:HD22	1:B:2922:ILE:H	1.37	0.70
1:B:3208:SER:N	1:B:3307:ASN:HB3	2.06	0.70
1:A:3397:ASN:HD22	1:A:3398:ASN:N	1.89	0.70
1:A:3319:GLY:O	1:A:3320:LYS:HB3	1.91	0.70
1:B:3302:ILE:HD12	1:B:3316:ILE:HD13	1.73	0.70
1:B:3027:ASN:HD22	1:B:3028:PRO:HD2	1.57	0.70
1:B:3338:PHE:HE1	1:B:3374:GLY:HA2	1.55	0.70
1:B:3348:PRO:HB2	1:B:3389:SER:CB	2.22	0.70
1:B:3204:LEU:HD12	1:B:3204:LEU:H	1.56	0.70
1:A:3027:ASN:HD22	1:A:3028:PRO:HD2	1.57	0.70
1:B:3160:ASN:HD22	1:B:3162:ASP:HB2	1.57	0.70
1:B:3258:ARG:NH1	1:B:3330:VAL:HG21	2.06	0.70
1:A:3301:ILE:HD12	1:A:3301:ILE:H	1.57	0.69
1:A:3204:LEU:HD12	1:A:3204:LEU:H	1.56	0.69
1:B:3221:THR:HA	1:B:3248:GLY:HA2	1.75	0.69
1:A:3336:ILE:O	1:A:3377:TYR:HA	1.92	0.69
1:A:2986:LEU:HD12	1:A:3151:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3142:CYS:HB2	1:A:3258:ARG:NH2	2.08	0.69
1:A:3253:PRO:HB3	1:B:3358:MET:HE3	1.75	0.69
1:B:3046:ASN:ND2	1:B:3047:GLU:H	1.91	0.69
1:A:3058:PHE:CD2	1:A:3062:PHE:HB3	2.28	0.69
1:A:3215:VAL:HG22	1:A:3301:ILE:HD11	1.75	0.69
1:A:3216:LEU:HD22	1:A:3216:LEU:H	1.58	0.69
1:B:3302:ILE:HD13	1:B:3303:VAL:N	2.08	0.69
1:A:3046:ASN:ND2	1:A:3047:GLU:H	1.91	0.68
1:B:3319:GLY:O	1:B:3320:LYS:HB3	1.93	0.68
1:A:3338:PHE:HE1	1:A:3374:GLY:HA2	1.56	0.68
1:B:3142:CYS:HB2	1:B:3258:ARG:NH2	2.08	0.68
1:A:3150:PRO:HB2	1:A:3155:ASN:ND2	2.07	0.68
1:A:3380:GLU:HB3	1:A:3384:TYR:OH	1.92	0.68
1:B:3215:VAL:HG22	1:B:3301:ILE:HD11	1.74	0.68
1:A:3320:LYS:HG2	1:A:3342:ASP:OD1	1.92	0.68
1:B:3318:ILE:HA	1:B:3339:MET:CB	2.21	0.68
1:A:3307:ASN:CG	1:A:3308:ASN:N	2.47	0.68
1:B:3336:ILE:O	1:B:3377:TYR:HA	1.94	0.68
1:A:3013:ILE:HD12	1:A:3013:ILE:H	1.58	0.68
1:B:3150:PRO:HB2	1:B:3155:ASN:ND2	2.09	0.68
1:A:2955:PHE:HE2	1:A:3159:VAL:HG23	1.58	0.68
1:A:3285:LYS:HE3	1:A:3292:LEU:HD13	1.74	0.68
1:A:3302:ILE:CD1	1:A:3316:ILE:HD13	2.24	0.67
1:A:3160:ASN:HD22	1:A:3162:ASP:HB2	1.58	0.67
1:A:3072:ASP:HB2	1:A:3311:PHE:CE2	2.30	0.67
1:B:3318:ILE:HG22	1:B:3322:VAL:HB	1.76	0.67
1:B:3285:LYS:HE3	1:B:3292:LEU:HD13	1.75	0.67
1:A:3350:LEU:HB3	1:A:3387:THR:HG22	1.75	0.67
1:B:2986:LEU:HD12	1:B:3151:LEU:HD12	1.76	0.67
1:B:2992:GLU:HA	1:B:3004:ILE:HD11	1.77	0.67
1:B:3285:LYS:HG3	1:B:3292:LEU:CD1	2.24	0.67
1:B:3380:GLU:HB3	1:B:3384:TYR:OH	1.95	0.67
1:B:3350:LEU:HD23	1:B:3351:ASN:N	2.09	0.67
1:A:3285:LYS:HG3	1:A:3292:LEU:CD1	2.25	0.66
1:A:2972:CYS:CB	1:A:3153:PRO:HD3	2.26	0.66
1:B:3096:GLU:HB2	1:B:3099:SER:HB3	1.77	0.66
1:B:2972:CYS:CB	1:B:3153:PRO:HD3	2.26	0.66
1:B:3302:ILE:HD13	1:B:3302:ILE:C	2.16	0.66
1:B:3313:ILE:HG22	1:B:3334:THR:HG23	1.75	0.66
1:B:3318:ILE:HG13	1:B:3339:MET:HG3	1.77	0.66
1:A:3033:HIS:HE1	1:A:3038:ASN:HA	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3302:ILE:HD13	1:A:3303:VAL:N	2.10	0.66
1:B:3216:LEU:H	1:B:3216:LEU:HD22	1.59	0.66
1:B:3218:GLY:HA2	1:B:3254:TRP:NE1	2.11	0.66
1:A:3224:VAL:HG22	1:A:3225:VAL:H	1.61	0.66
1:B:2966:GLY:O	1:B:2968:GLU:HG2	1.95	0.66
1:B:3320:LYS:HG2	1:B:3342:ASP:OD1	1.95	0.66
1:B:3335:LYS:HB2	1:B:3335:LYS:NZ	2.11	0.66
1:B:3350:LEU:HB3	1:B:3387:THR:HG22	1.78	0.66
1:A:3318:ILE:HA	1:A:3339:MET:CB	2.21	0.66
1:A:2992:GLU:HA	1:A:3004:ILE:HD11	1.78	0.66
1:A:3221:THR:HA	1:A:3248:GLY:HA2	1.75	0.66
1:A:3303:VAL:HG12	1:A:3315:GLU:HA	1.78	0.66
1:A:3301:ILE:HG23	1:A:3317:PRO:HA	1.77	0.65
1:B:3058:PHE:CD2	1:B:3062:PHE:HB3	2.31	0.65
1:B:3274:THR:H	1:B:3277:HIS:CE1	2.14	0.65
1:B:3279:LYS:HZ1	1:B:3280:PHE:H	1.43	0.65
1:A:3049:ILE:HG22	1:A:3050:PHE:H	1.61	0.65
1:A:3103:LEU:HD22	1:A:3247:GLY:HA2	1.78	0.65
1:A:3096:GLU:HB2	1:A:3099:SER:HB3	1.78	0.65
1:B:2986:LEU:HD22	1:B:3154:PHE:CE1	2.31	0.65
1:B:3301:ILE:HD12	1:B:3301:ILE:H	1.62	0.65
1:B:3033:HIS:HE1	1:B:3038:ASN:HA	1.61	0.65
1:A:3228:TYR:O	1:A:3281:ARG:HB2	1.96	0.65
1:A:3350:LEU:HD23	1:A:3351:ASN:N	2.12	0.65
1:A:3041:THR:HG21	1:A:3109:ASP:HA	1.79	0.64
1:A:3279:LYS:HZ1	1:A:3280:PHE:H	1.45	0.64
1:A:3318:ILE:HG23	1:A:3319:GLY:N	2.13	0.64
1:A:2921:ASN:HD22	1:A:2922:ILE:H	1.45	0.64
1:B:2973:CYS:SG	1:B:3103:LEU:HD11	2.38	0.64
1:B:3041:THR:HG21	1:B:3109:ASP:HA	1.78	0.64
1:B:3054:LYS:HE3	1:B:3190:HIS:NE2	2.12	0.64
1:A:3301:ILE:HD12	1:A:3301:ILE:N	2.13	0.64
1:A:3325:PRO:HB3	1:A:3326:PRO:HD2	1.80	0.64
1:A:3038:ASN:CG	1:A:3039:GLN:H	2.00	0.64
1:A:3318:ILE:HG13	1:A:3339:MET:HG3	1.78	0.64
1:B:3049:ILE:HG22	1:B:3050:PHE:H	1.64	0.63
1:B:3318:ILE:HG13	1:B:3339:MET:CB	2.28	0.63
1:A:3122:ILE:O	1:A:3125:ILE:HG12	1.99	0.63
1:A:3313:ILE:HG22	1:A:3334:THR:HG23	1.80	0.63
1:A:3327:LYS:NZ	1:A:3401:ILE:HG21	2.13	0.63
1:A:3350:LEU:O	1:A:3351:ASN:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3271:LEU:HB2	1:B:3273:LEU:CD1	2.28	0.63
1:A:2972:CYS:HB3	1:A:3153:PRO:HD3	1.81	0.63
1:A:3271:LEU:HB2	1:A:3273:LEU:CD1	2.29	0.63
1:A:3318:ILE:HG22	1:A:3322:VAL:HB	1.80	0.63
1:B:3318:ILE:HG23	1:B:3319:GLY:N	2.14	0.63
1:B:3047:GLU:O	1:B:3049:ILE:HG12	1.99	0.63
1:A:3400:ARG:O	1:A:3400:ARG:HD2	1.99	0.62
1:B:3211:PHE:HB2	1:B:3303:VAL:HG23	1.80	0.62
1:B:3224:VAL:HG22	1:B:3225:VAL:H	1.64	0.62
1:B:3326:PRO:HB3	1:B:3402:HIS:CB	2.26	0.62
1:B:3350:LEU:O	1:B:3351:ASN:HB3	1.99	0.62
1:B:3038:ASN:CG	1:B:3039:GLN:H	2.02	0.62
1:A:3249:ALA:O	1:A:3250:LYS:HB2	1.98	0.62
1:A:3302:ILE:HD13	1:A:3302:ILE:C	2.19	0.62
1:B:3215:VAL:HG23	1:B:3298:PRO:CG	2.28	0.62
1:B:3122:ILE:O	1:B:3125:ILE:HG12	1.98	0.62
1:B:3249:ALA:O	1:B:3250:LYS:HB2	1.98	0.62
1:A:2985:ARG:HD2	1:A:3174:VAL:HG12	1.81	0.62
1:A:3320:LYS:HD3	1:A:3321:ASP:N	2.14	0.62
1:B:2983:TRP:HA	1:B:3151:LEU:HD13	1.81	0.62
1:B:3301:ILE:HD12	1:B:3301:ILE:N	2.15	0.62
1:A:3335:LYS:HB2	1:A:3335:LYS:NZ	2.14	0.62
1:B:3325:PRO:HB3	1:B:3326:PRO:HD2	1.81	0.62
1:B:3336:ILE:HG22	1:B:3378:SER:HB3	1.82	0.62
1:A:3307:ASN:O	1:A:3310:VAL:HG22	2.00	0.62
1:A:3318:ILE:HG13	1:A:3339:MET:HB2	1.81	0.61
1:B:3013:ILE:O	1:B:3049:ILE:HG23	2.00	0.61
1:B:2972:CYS:HB3	1:B:3153:PRO:HD3	1.81	0.61
1:B:2985:ARG:HD2	1:B:3174:VAL:HG12	1.81	0.61
1:B:3301:ILE:HG23	1:B:3317:PRO:HA	1.82	0.61
1:A:3054:LYS:HE3	1:A:3190:HIS:NE2	2.15	0.61
1:A:3356:THR:HA	1:A:3359:PHE:CD2	2.36	0.61
1:B:3010:THR:HG21	1:B:3189:LEU:HD11	1.83	0.61
1:B:3187:LEU:HD23	1:B:3187:LEU:H	1.65	0.61
1:A:2966:GLY:O	1:A:2968:GLU:HG2	2.00	0.61
1:A:3010:THR:HG21	1:A:3189:LEU:HD11	1.82	0.61
1:A:3317:PRO:HB3	1:A:3327:LYS:NZ	2.15	0.61
1:A:3159:VAL:HG22	1:A:3160:ASN:N	2.14	0.61
1:A:2985:ARG:NH1	1:A:3177:SER:HB3	2.16	0.61
1:A:3187:LEU:HD11	1:A:3194:ILE:HD12	1.83	0.61
1:B:2961:LEU:O	1:B:2963:PRO:HD2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3400:ARG:HD2	1:B:3400:ARG:O	2.01	0.61
1:A:3205:ARG:HH12	1:A:3305:ARG:NH1	1.98	0.61
1:B:3279:LYS:NZ	1:B:3280:PHE:H	1.99	0.61
1:B:3048:ALA:O	1:B:3049:ILE:HD13	1.99	0.60
1:B:2991:PHE:CD2	1:B:3113:MET:HB3	2.36	0.60
1:A:2962:CYS:HB2	1:A:2963:PRO:CD	2.30	0.60
1:B:2921:ASN:HD22	1:B:2922:ILE:N	1.99	0.60
1:B:3320:LYS:HD3	1:B:3321:ASP:N	2.17	0.60
1:A:3049:ILE:HG22	1:A:3050:PHE:N	2.16	0.60
1:A:2979:ILE:HG22	1:A:3147:MET:HG2	1.83	0.60
1:A:3205:ARG:NH1	1:A:3305:ARG:HD3	2.17	0.60
1:A:3227:VAL:HG21	1:A:3262:PHE:HE2	1.65	0.60
1:A:3318:ILE:CG2	1:A:3319:GLY:N	2.65	0.60
1:A:2985:ARG:O	1:A:2989:ILE:HG23	2.02	0.60
1:A:3225:VAL:HA	1:A:3285:LYS:HA	1.83	0.59
1:B:3225:VAL:HA	1:B:3285:LYS:HA	1.84	0.59
1:B:3227:VAL:HG21	1:B:3262:PHE:HE2	1.66	0.59
1:B:3285:LYS:HG2	1:B:3294:ALA:HA	1.84	0.59
1:B:3310:VAL:HG12	1:B:3311:PHE:N	2.17	0.59
1:A:3013:ILE:O	1:A:3049:ILE:HD12	2.03	0.59
1:A:3259:LEU:HD21	1:A:3301:ILE:HD13	1.85	0.59
1:B:2979:ILE:HG22	1:B:3147:MET:HG2	1.84	0.59
1:A:3215:VAL:HG23	1:A:3298:PRO:CG	2.33	0.59
1:A:3286:LYS:HE3	1:A:3291:GLU:OE2	2.02	0.59
1:B:3307:ASN:CG	1:B:3308:ASN:H	2.03	0.59
1:B:3336:ILE:HG22	1:B:3378:SER:CB	2.33	0.59
1:B:3259:LEU:HD21	1:B:3301:ILE:HD13	1.84	0.59
1:B:3317:PRO:HB3	1:B:3327:LYS:NZ	2.16	0.59
1:A:2986:LEU:HD22	1:A:3154:PHE:CE1	2.37	0.59
1:A:3320:LYS:HD3	1:A:3321:ASP:H	1.67	0.59
1:A:2961:LEU:O	1:A:2963:PRO:HD2	2.02	0.59
1:B:3085:HIS:HB2	1:B:3119:LEU:HG	1.85	0.59
1:A:2932:GLU:HG2	1:A:3001:HIS:HB2	1.84	0.58
1:A:2983:TRP:HA	1:A:3151:LEU:HD13	1.83	0.58
1:B:3133:ARG:O	1:B:3134:VAL:HG12	2.03	0.58
1:A:3279:LYS:NZ	1:A:3280:PHE:H	2.00	0.58
1:A:3302:ILE:HG23	1:A:3316:ILE:HB	1.83	0.58
1:A:3388:ALA:HB2	1:A:3394:CYS:HA	1.85	0.58
1:A:2932:GLU:HG2	1:A:3001:HIS:CB	2.33	0.58
1:A:3312:ASP:O	1:A:3313:ILE:O	2.21	0.58
1:B:2921:ASN:ND2	1:B:2922:ILE:N	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3286:LYS:HE3	1:B:3291:GLU:OE2	2.03	0.58
1:A:3047:GLU:O	1:A:3049:ILE:HG12	2.04	0.58
1:B:3006:TYR:HE2	1:B:3185:ASP:OD1	1.86	0.58
1:A:2950:GLU:HB3	1:A:3035:ARG:NH2	2.18	0.58
1:A:2973:CYS:SG	1:A:3103:LEU:HD11	2.44	0.58
1:A:3218:GLY:HA2	1:A:3254:TRP:NE1	2.19	0.58
1:A:3224:VAL:HG22	1:A:3225:VAL:N	2.18	0.58
1:B:2962:CYS:HB2	1:B:2963:PRO:CD	2.28	0.58
1:B:3320:LYS:HD3	1:B:3321:ASP:H	1.69	0.58
1:A:3325:PRO:CB	1:A:3326:PRO:HD2	2.34	0.58
1:A:3350:LEU:HD21	1:A:3353:GLY:CA	2.34	0.58
1:B:2921:ASN:ND2	1:B:2922:ILE:H	2.01	0.58
1:A:3053:THR:O	1:A:3058:PHE:HA	2.04	0.58
1:A:3226:LYS:HD2	1:A:3241:GLY:O	2.04	0.58
1:B:2950:GLU:HB3	1:B:3035:ARG:NH2	2.18	0.58
1:B:3312:ASP:O	1:B:3313:ILE:O	2.21	0.58
1:A:3215:VAL:HG21	1:A:3324:LEU:HB2	1.86	0.58
1:B:2932:GLU:HG2	1:B:3001:HIS:HB2	1.85	0.58
1:B:2937:LEU:CG	1:B:2941:GLN:HE21	2.16	0.58
1:A:2991:PHE:CD2	1:A:3113:MET:HB3	2.38	0.57
1:A:3038:ASN:ND2	1:A:3039:GLN:H	2.02	0.57
1:B:3302:ILE:CD1	1:B:3316:ILE:HD13	2.34	0.57
1:B:3388:ALA:HB2	1:B:3394:CYS:HA	1.85	0.57
1:A:3085:HIS:HB2	1:A:3119:LEU:HG	1.85	0.57
1:A:3384:TYR:O	1:A:3385:PHE:HB2	2.03	0.57
1:B:3356:THR:HA	1:B:3359:PHE:CD2	2.40	0.57
1:A:3187:LEU:H	1:A:3187:LEU:HD23	1.69	0.57
1:B:2932:GLU:HG2	1:B:3001:HIS:CB	2.34	0.57
1:B:3055:PHE:HD2	1:B:3192:HIS:HE2	1.53	0.57
1:B:3384:TYR:O	1:B:3385:PHE:HB2	2.04	0.57
1:A:3336:ILE:HD12	1:A:3403:VAL:HG11	1.86	0.57
1:A:3350:LEU:HG	1:A:3351:ASN:HD22	1.68	0.57
1:B:2917:LEU:HD12	1:B:2918:VAL:N	2.16	0.57
1:B:2964:GLU:HG2	1:B:3156:TYR:CE1	2.40	0.57
1:A:2917:LEU:HD11	1:A:3002:LEU:C	2.25	0.57
1:A:3336:ILE:HG22	1:A:3378:SER:HB3	1.85	0.57
1:B:2986:LEU:HD13	1:B:3154:PHE:CD1	2.39	0.57
1:B:3053:THR:O	1:B:3058:PHE:HA	2.04	0.57
1:B:3061:ILE:CG2	1:B:3062:PHE:H	2.06	0.57
1:B:3205:ARG:HH12	1:B:3305:ARG:NH1	2.03	0.57
1:B:2985:ARG:O	1:B:2989:ILE:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3318:ILE:CG2	1:B:3319:GLY:N	2.68	0.57
1:A:3211:PHE:HB2	1:A:3303:VAL:HG23	1.87	0.57
1:A:3353:GLY:O	1:A:3354:SER:HB2	2.05	0.57
1:B:3049:ILE:HG22	1:B:3050:PHE:N	2.20	0.57
1:B:3307:ASN:CG	1:B:3308:ASN:N	2.57	0.57
1:B:3325:PRO:CB	1:B:3326:PRO:HD2	2.35	0.57
1:A:3051:GLN:HG3	1:A:3052:GLN:N	2.20	0.57
1:A:3314:ILE:CG2	1:A:3316:ILE:HD11	2.35	0.57
1:A:3388:ALA:CB	1:A:3394:CYS:HA	2.35	0.57
1:B:3303:VAL:HG12	1:B:3315:GLU:HA	1.85	0.57
1:B:3350:LEU:HD21	1:B:3353:GLY:CA	2.34	0.57
1:A:3120:ASP:O	1:A:3124:ILE:HG12	2.05	0.56
1:A:3330:VAL:HG12	1:A:3331:LYS:H	1.69	0.56
1:A:3034:ILE:HB	1:A:3038:ASN:O	2.04	0.56
1:A:3055:PHE:HD2	1:A:3192:HIS:HE2	1.52	0.56
1:B:2917:LEU:HD11	1:B:3002:LEU:C	2.26	0.56
1:B:3312:ASP:OD2	1:B:3312:ASP:N	2.38	0.56
1:A:3121:LYS:O	1:A:3125:ILE:HG23	2.06	0.56
1:A:3258:ARG:HH11	1:A:3330:VAL:HG21	1.71	0.56
1:A:3297:LEU:HB2	1:A:3299:ALA:N	2.19	0.56
1:A:3336:ILE:HG22	1:A:3378:SER:CB	2.36	0.56
1:B:2960:ASN:HB3	1:B:2970:TYR:C	2.25	0.56
1:B:3215:VAL:HG21	1:B:3324:LEU:HB2	1.86	0.56
1:A:3348:PRO:HB2	1:A:3389:SER:HB3	1.87	0.56
1:B:3121:LYS:O	1:B:3125:ILE:HG23	2.06	0.56
1:B:3372:GLU:HG3	1:B:3386:MET:HG2	1.86	0.56
1:B:3388:ALA:CB	1:B:3394:CYS:HA	2.35	0.56
1:A:2921:ASN:ND2	1:A:2922:ILE:H	2.04	0.56
1:B:2991:PHE:CG	1:B:3113:MET:HB3	2.41	0.56
1:A:2991:PHE:CG	1:A:3113:MET:HB3	2.41	0.56
1:B:3323:ASN:O	1:B:3324:LEU:HB3	2.05	0.56
1:B:3341:VAL:O	1:B:3342:ASP:HB3	2.06	0.56
1:A:3285:LYS:HG2	1:A:3294:ALA:HA	1.87	0.56
1:B:3087:GLU:O	1:B:3091:LEU:HD22	2.05	0.56
1:A:3317:PRO:HB3	1:A:3327:LYS:HZ1	1.70	0.55
1:B:3037:ILE:HG13	1:B:3037:ILE:O	2.06	0.55
1:B:3224:VAL:HG22	1:B:3225:VAL:N	2.21	0.55
1:A:2917:LEU:HD12	1:A:2918:VAL:N	2.18	0.55
1:A:3336:ILE:HD11	1:A:3403:VAL:HG21	1.87	0.55
1:B:2992:GLU:HB2	1:B:3004:ILE:HG12	1.88	0.55
1:B:3008:ASP:O	1:B:3011:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3351:ASN:CB	1:B:3371:PHE:HB3	2.36	0.55
1:A:2986:LEU:HD13	1:A:3154:PHE:CD1	2.41	0.55
1:A:3013:ILE:H	1:A:3013:ILE:CD1	2.18	0.55
1:B:3187:LEU:HD11	1:B:3194:ILE:HD12	1.88	0.55
1:A:2962:CYS:CB	1:A:2963:PRO:HD3	2.36	0.55
1:A:3266:GLU:HG3	1:A:3267:THR:N	2.21	0.55
1:B:3301:ILE:HG22	1:B:3315:GLU:OE2	2.05	0.55
1:A:3311:PHE:HD2	1:A:3331:LYS:HZ1	1.54	0.55
1:B:3154:PHE:HA	1:B:3159:VAL:HG21	1.88	0.55
1:B:3231:SER:OG	1:B:3236:ASP:HB2	2.07	0.55
1:B:3312:ASP:O	1:B:3334:THR:HA	2.07	0.55
1:B:3350:LEU:HG	1:B:3351:ASN:HD22	1.71	0.55
1:A:2960:ASN:HB3	1:A:2970:TYR:C	2.26	0.55
1:A:3221:THR:HA	1:A:3248:GLY:CA	2.37	0.55
1:A:3222:THR:OG1	1:A:3246:LEU:HA	2.06	0.55
1:B:2986:LEU:HD22	1:B:3154:PHE:HE1	1.70	0.55
1:B:3120:ASP:O	1:B:3124:ILE:HG12	2.07	0.55
1:B:3287:TYR:CG	1:B:3288:ASP:N	2.75	0.55
1:B:3350:LEU:HD23	1:B:3351:ASN:O	2.07	0.55
1:B:3330:VAL:HG12	1:B:3331:LYS:H	1.72	0.55
1:A:3365:PRO:C	1:A:3367:SER:H	2.11	0.55
1:B:3365:PRO:C	1:B:3367:SER:H	2.10	0.55
1:A:3013:ILE:CD1	1:A:3049:ILE:HA	2.36	0.55
1:A:3287:TYR:CG	1:A:3288:ASP:N	2.75	0.55
1:B:3221:THR:HA	1:B:3248:GLY:CA	2.36	0.54
1:B:3223:ALA:HB1	1:B:3286:LYS:O	2.07	0.54
1:B:3301:ILE:HG21	1:B:3327:LYS:HE3	1.89	0.54
1:B:3318:ILE:HG13	1:B:3339:MET:CG	2.37	0.54
1:A:2921:ASN:ND2	1:A:2922:ILE:N	2.56	0.54
1:A:3133:ARG:O	1:A:3134:VAL:HG12	2.07	0.54
1:B:2937:LEU:HG	1:B:2941:GLN:NE2	2.20	0.54
1:B:3013:ILE:O	1:B:3049:ILE:HD12	2.07	0.54
1:A:2976:GLY:HA3	1:A:3254:TRP:CE3	2.42	0.54
1:A:3231:SER:OG	1:A:3236:ASP:HB2	2.07	0.54
1:B:3353:GLY:O	1:B:3354:SER:HB2	2.08	0.54
1:A:3350:LEU:HD23	1:A:3351:ASN:O	2.07	0.54
1:B:3359:PHE:C	1:B:3361:CYS:H	2.11	0.54
1:A:3013:ILE:O	1:A:3049:ILE:HG23	2.07	0.54
1:A:3039:GLN:HG3	1:A:3098:TYR:CE1	2.41	0.54
1:A:3210:VAL:O	1:A:3264:ILE:HD13	2.07	0.54
1:A:3348:PRO:HB2	1:A:3389:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3087:GLU:O	1:A:3091:LEU:HD22	2.07	0.54
1:A:3323:ASN:O	1:A:3324:LEU:HB3	2.08	0.54
1:A:3008:ASP:O	1:A:3011:GLN:HG2	2.08	0.54
1:B:3013:ILE:H	1:B:3013:ILE:CD1	2.16	0.54
1:B:3350:LEU:HD21	1:B:3353:GLY:N	2.23	0.54
1:A:3350:LEU:HG	1:A:3351:ASN:ND2	2.23	0.54
1:B:2992:GLU:HB2	1:B:3004:ILE:CG1	2.38	0.54
1:B:3348:PRO:HB2	1:B:3389:SER:HB3	1.90	0.54
1:B:3298:PRO:HB2	1:B:3323:ASN:O	2.08	0.54
1:B:3328:VAL:CG1	1:B:3330:VAL:HG22	2.36	0.54
1:A:3030:PHE:C	1:A:3031:LYS:HG2	2.28	0.53
1:A:3281:ARG:HD2	1:A:3281:ARG:O	2.08	0.53
1:B:3086:ASN:CG	1:B:3246:LEU:HD13	2.29	0.53
1:B:3177:SER:C	1:B:3179:ARG:H	2.11	0.53
1:B:3258:ARG:HH11	1:B:3330:VAL:HG21	1.73	0.53
1:B:3091:LEU:HD13	1:B:3091:LEU:N	2.24	0.53
1:B:3327:LYS:NZ	1:B:3401:ILE:HG21	2.23	0.53
1:A:3229:ILE:HA	1:A:3281:ARG:HB2	1.89	0.53
1:A:3348:PRO:HA	1:A:3368:PHE:CZ	2.44	0.53
1:B:2985:ARG:NH1	1:B:3177:SER:HB3	2.22	0.53
1:B:3013:ILE:CD1	1:B:3049:ILE:HA	2.35	0.53
1:B:3051:GLN:HG3	1:B:3052:GLN:N	2.22	0.53
1:B:3103:LEU:HD22	1:B:3247:GLY:HA2	1.90	0.53
1:A:3298:PRO:HB2	1:A:3323:ASN:O	2.09	0.53
1:A:3351:ASN:CB	1:A:3371:PHE:HB3	2.38	0.53
1:B:3350:LEU:O	1:B:3351:ASN:CB	2.56	0.53
1:A:3062:PHE:CE1	1:A:3066:LEU:HD22	2.43	0.53
1:B:3281:ARG:HD2	1:B:3281:ARG:O	2.08	0.53
1:B:3297:LEU:HB2	1:B:3299:ALA:N	2.23	0.53
1:B:3348:PRO:HD2	1:B:3389:SER:OG	2.09	0.53
1:A:3006:TYR:HE2	1:A:3185:ASP:OD1	1.91	0.53
1:A:3013:ILE:HD13	1:A:3049:ILE:HD13	1.90	0.53
1:A:3341:VAL:O	1:A:3342:ASP:HB3	2.08	0.53
1:A:3350:LEU:O	1:A:3351:ASN:CB	2.57	0.53
1:B:2960:ASN:CB	1:B:2970:TYR:H	2.21	0.53
1:B:3030:PHE:C	1:B:3031:LYS:HG2	2.27	0.53
1:B:3138:HIS:CG	1:B:3139:ALA:H	2.27	0.53
1:B:2960:ASN:HB3	1:B:2970:TYR:H	1.74	0.53
1:B:3214:PHE:HB3	1:B:3216:LEU:CD2	2.39	0.53
1:A:2964:GLU:HG2	1:A:3156:TYR:CE1	2.44	0.53
1:A:2972:CYS:SG	1:A:3153:PRO:HD3	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3318:ILE:HG13	1:A:3339:MET:CB	2.39	0.53
1:A:3138:HIS:CG	1:A:3139:ALA:H	2.27	0.53
1:B:3038:ASN:ND2	1:B:3039:GLN:H	2.07	0.53
1:B:2930:ALA:HB1	1:B:2934:ARG:NH1	2.24	0.52
1:B:3307:ASN:O	1:B:3308:ASN:C	2.46	0.52
1:B:3348:PRO:HB2	1:B:3389:SER:OG	2.09	0.52
1:A:2985:ARG:HH12	1:A:3124:ILE:CD1	2.17	0.52
1:A:3312:ASP:O	1:A:3334:THR:HA	2.09	0.52
1:B:2960:ASN:HB3	1:B:2970:TYR:N	2.24	0.52
1:B:3062:PHE:CE1	1:B:3066:LEU:HD22	2.45	0.52
1:B:3187:LEU:HD23	1:B:3187:LEU:N	2.23	0.52
1:A:3359:PHE:C	1:A:3361:CYS:H	2.13	0.52
1:B:3214:PHE:HB3	1:B:3216:LEU:HD22	1.91	0.52
1:B:3266:GLU:HG3	1:B:3267:THR:N	2.25	0.52
1:B:3336:ILE:HD12	1:B:3403:VAL:HG11	1.91	0.52
1:A:2992:GLU:HB2	1:A:3004:ILE:HG12	1.91	0.52
1:A:3326:PRO:HG3	1:B:3356:THR:HB	1.91	0.52
1:A:3086:ASN:OD1	1:A:3246:LEU:HD22	2.10	0.52
1:A:3301:ILE:CG2	1:A:3317:PRO:HA	2.39	0.52
1:A:3351:ASN:HB2	1:A:3371:PHE:HD2	1.74	0.52
1:B:3086:ASN:OD1	1:B:3246:LEU:HD22	2.09	0.52
1:A:2930:ALA:HB1	1:A:2934:ARG:NH1	2.24	0.52
1:A:3301:ILE:HG22	1:A:3315:GLU:OE2	2.10	0.52
1:A:3328:VAL:CG1	1:A:3330:VAL:HG22	2.33	0.52
1:B:2960:ASN:HB2	1:B:2969:LYS:HB3	1.91	0.52
1:B:2996:LYS:HA	1:B:3000:SER:CB	2.34	0.52
1:B:3314:ILE:CG2	1:B:3316:ILE:HD11	2.40	0.52
1:A:2919:ARG:NH2	1:A:2989:ILE:HG22	2.25	0.52
1:A:3305:ARG:HG3	1:A:3313:ILE:CD1	2.39	0.52
1:B:2991:PHE:HB2	1:B:3113:MET:SD	2.50	0.52
1:B:3328:VAL:HG13	1:B:3404:HIS:HB3	1.91	0.52
1:B:3350:LEU:HG	1:B:3351:ASN:ND2	2.24	0.52
1:A:2937:LEU:CG	1:A:2941:GLN:HE21	2.21	0.52
1:A:3111:TYR:O	1:A:3114:ILE:HG13	2.10	0.51
1:A:3223:ALA:HB1	1:A:3286:LYS:O	2.10	0.51
1:B:2972:CYS:SG	1:B:3153:PRO:HD3	2.50	0.51
1:B:3079:VAL:O	1:B:3083:ILE:HG12	2.11	0.51
1:A:3037:ILE:HG13	1:A:3037:ILE:O	2.09	0.51
1:A:3350:LEU:CB	1:A:3387:THR:HG22	2.40	0.51
1:B:3351:ASN:CG	1:B:3352:LEU:H	2.12	0.51
1:A:3350:LEU:HD21	1:A:3353:GLY:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3387:THR:HG23	1:A:3388:ALA:N	2.24	0.51
1:B:3159:VAL:HG22	1:B:3160:ASN:N	2.19	0.51
1:B:3227:VAL:HG21	1:B:3262:PHE:CE2	2.44	0.51
1:B:3317:PRO:CG	1:B:3338:PHE:HA	2.38	0.51
1:A:2979:ILE:CG2	1:A:3147:MET:HG2	2.41	0.51
1:A:3230:LYS:O	1:A:3271:LEU:HD22	2.10	0.51
1:A:3285:LYS:HB2	1:A:3285:LYS:NZ	2.25	0.51
1:B:3154:PHE:HA	1:B:3159:VAL:CG2	2.40	0.51
1:B:3348:PRO:HA	1:B:3368:PHE:CZ	2.45	0.51
1:A:3348:PRO:HD2	1:A:3389:SER:OG	2.11	0.51
1:A:3086:ASN:CG	1:A:3246:LEU:HD13	2.30	0.51
1:B:3285:LYS:HG3	1:B:3292:LEU:HD13	1.92	0.51
1:A:2937:LEU:HG	1:A:2941:GLN:NE2	2.23	0.51
1:A:3325:PRO:HA	1:A:3400:ARG:NH2	2.26	0.51
1:A:3351:ASN:CG	1:A:3352:LEU:H	2.14	0.51
1:B:3059:SER:O	1:B:3060:SER:HB2	2.11	0.51
1:A:3227:VAL:HG21	1:A:3262:PHE:CE2	2.45	0.51
1:A:3253:PRO:HB3	1:B:3358:MET:CE	2.39	0.51
1:A:3253:PRO:HG2	1:B:3364:PRO:HD3	1.92	0.51
1:A:3328:VAL:HG13	1:A:3404:HIS:HB3	1.93	0.51
1:B:2985:ARG:HH12	1:B:3124:ILE:CD1	2.17	0.51
1:B:3349:MET:O	1:B:3350:LEU:C	2.49	0.51
1:A:3207:LYS:N	1:A:3307:ASN:HB2	2.26	0.51
1:A:3349:MET:O	1:A:3350:LEU:C	2.49	0.51
1:B:2976:GLY:HA3	1:B:3254:TRP:CE3	2.46	0.51
1:A:3177:SER:C	1:A:3179:ARG:H	2.12	0.51
1:B:2979:ILE:CG2	1:B:3147:MET:HG2	2.41	0.51
1:A:3325:PRO:HA	1:A:3400:ARG:CZ	2.40	0.50
1:B:3354:SER:HB3	1:B:3358:MET:HB3	1.92	0.50
1:A:2918:VAL:HG23	1:A:3183:LYS:O	2.11	0.50
1:A:2986:LEU:HD22	1:A:3154:PHE:HE1	1.76	0.50
1:A:3034:ILE:HD13	1:A:3039:GLN:O	2.11	0.50
1:A:3061:ILE:CG2	1:A:3062:PHE:H	2.07	0.50
1:A:3383:ASP:CG	1:A:3402:HIS:HE2	2.14	0.50
1:B:2950:GLU:HB3	1:B:3032:TYR:OH	2.11	0.50
1:B:3111:TYR:O	1:B:3114:ILE:HG13	2.11	0.50
1:B:3159:VAL:HG13	1:B:3161:ASN:N	2.24	0.50
1:A:2921:ASN:HD22	1:A:2922:ILE:N	2.07	0.50
1:A:3046:ASN:ND2	1:A:3047:GLU:N	2.59	0.50
1:B:3198:GLU:HA	1:B:3201:LEU:HD12	1.92	0.50
1:B:3209:ARG:HB2	1:B:3211:PHE:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2962:CYS:HA	1:A:3153:PRO:HB3	1.94	0.50
1:A:2980:PHE:CE2	1:A:3082:GLU:HG3	2.47	0.50
1:A:2992:GLU:HB2	1:A:3004:ILE:CG1	2.42	0.50
1:A:3091:LEU:HD22	1:A:3091:LEU:H	1.77	0.50
1:B:2918:VAL:HG23	1:B:3183:LYS:O	2.11	0.50
1:B:3335:LYS:HB2	1:B:3335:LYS:HZ2	1.77	0.50
1:B:3351:ASN:CG	1:B:3352:LEU:N	2.64	0.50
1:A:3279:LYS:NZ	1:A:3280:PHE:N	2.59	0.50
1:A:3295:SER:O	1:A:3297:LEU:N	2.45	0.50
1:B:3351:ASN:N	1:B:3351:ASN:HD22	2.10	0.50
1:A:3150:PRO:HB2	1:A:3155:ASN:HD22	1.75	0.50
1:B:3046:ASN:ND2	1:B:3047:GLU:N	2.58	0.50
1:A:3091:LEU:N	1:A:3091:LEU:HD13	2.26	0.49
1:A:3198:GLU:HA	1:A:3201:LEU:HD12	1.94	0.49
1:A:3273:LEU:CD2	1:A:3279:LYS:HD2	2.42	0.49
1:A:3357:ALA:HA	1:B:3325:PRO:CB	2.42	0.49
1:A:3397:ASN:HD22	1:A:3397:ASN:C	2.16	0.49
1:B:3226:LYS:HE2	1:B:3239:TYR:CD2	2.47	0.49
1:B:3210:VAL:O	1:B:3264:ILE:HD13	2.12	0.49
1:B:3226:LYS:HD2	1:B:3241:GLY:O	2.12	0.49
1:B:3298:PRO:O	1:B:3299:ALA:C	2.50	0.49
1:B:3336:ILE:HD11	1:B:3403:VAL:HG21	1.93	0.49
1:A:3187:LEU:HD23	1:A:3187:LEU:N	2.27	0.49
1:A:3372:GLU:HG3	1:A:3386:MET:HG2	1.94	0.49
1:B:3138:HIS:CD2	1:B:3139:ALA:H	2.31	0.49
1:B:3325:PRO:HA	1:B:3400:ARG:NH2	2.27	0.49
1:B:3351:ASN:HB2	1:B:3371:PHE:HD2	1.77	0.49
1:A:3307:ASN:O	1:A:3308:ASN:C	2.50	0.49
1:A:3351:ASN:N	1:A:3351:ASN:HD22	2.09	0.49
1:B:3350:LEU:CB	1:B:3387:THR:HG22	2.41	0.49
1:B:3383:ASP:CG	1:B:3402:HIS:HE2	2.16	0.49
1:A:2991:PHE:HB2	1:A:3113:MET:SD	2.52	0.49
1:A:3154:PHE:HA	1:A:3159:VAL:HG21	1.94	0.49
1:B:2981:PRO:HB3	1:B:3081:TYR:CE2	2.47	0.49
1:B:3370:ALA:O	1:B:3371:PHE:HB2	2.12	0.49
1:A:3220:ARG:NH2	1:B:3358:MET:HE1	2.28	0.49
1:B:3352:LEU:HA	1:B:3385:PHE:HB3	1.94	0.49
1:A:3059:SER:O	1:A:3060:SER:HB2	2.13	0.49
1:A:3079:VAL:O	1:A:3083:ILE:HG12	2.12	0.49
1:A:3138:HIS:CD2	1:A:3139:ALA:H	2.31	0.49
1:A:3209:ARG:HB2	1:A:3211:PHE:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3226:LYS:HE2	1:A:3239:TYR:CD2	2.48	0.49
1:A:3312:ASP:N	1:A:3312:ASP:OD2	2.45	0.49
1:A:3318:ILE:HG13	1:A:3339:MET:CG	2.43	0.49
1:B:3046:ASN:HD22	1:B:3047:GLU:H	1.61	0.49
1:B:3325:PRO:HA	1:B:3400:ARG:CZ	2.42	0.49
1:A:2952:ILE:HD12	1:A:2990:GLN:HG3	1.93	0.49
1:A:3370:ALA:O	1:A:3371:PHE:HB2	2.12	0.49
1:A:3298:PRO:O	1:A:3299:ALA:C	2.51	0.49
1:A:2974:VAL:HG13	1:A:2977:MET:HG3	1.94	0.48
1:A:3154:PHE:HA	1:A:3159:VAL:CG2	2.42	0.48
1:A:3325:PRO:HA	1:A:3400:ARG:HH22	1.78	0.48
1:B:2962:CYS:CB	1:B:2963:PRO:HD3	2.36	0.48
1:B:3387:THR:HG23	1:B:3388:ALA:N	2.27	0.48
1:A:2996:LYS:CA	1:A:3000:SER:HB3	2.32	0.48
1:A:3034:ILE:O	1:A:3035:ARG:HB3	2.14	0.48
1:A:2960:ASN:CB	1:A:2970:TYR:H	2.26	0.48
1:A:2962:CYS:SG	1:A:2970:TYR:O	2.71	0.48
1:A:2981:PRO:HB3	1:A:3081:TYR:CE2	2.47	0.48
1:A:3214:PHE:HB3	1:A:3216:LEU:CD2	2.43	0.48
1:A:3347:THR:OG1	1:A:3374:GLY:HA2	2.13	0.48
1:B:3230:LYS:O	1:B:3271:LEU:HD22	2.13	0.48
1:B:3338:PHE:CE1	1:B:3374:GLY:HA2	2.43	0.48
1:A:3174:VAL:HG12	1:A:3174:VAL:O	2.14	0.48
1:A:3202:ARG:O	1:A:3206:LEU:HG	2.13	0.48
1:A:3301:ILE:HG21	1:A:3327:LYS:HE3	1.95	0.48
1:B:3280:PHE:CZ	1:B:3300:PRO:HD2	2.49	0.48
1:B:3322:VAL:HG22	1:B:3324:LEU:CD2	2.43	0.48
1:B:3325:PRO:HA	1:B:3400:ARG:HH22	1.79	0.48
1:A:3096:GLU:CB	1:A:3099:SER:HB3	2.43	0.48
1:A:3351:ASN:CG	1:A:3352:LEU:N	2.65	0.48
1:B:3295:SER:O	1:B:3297:LEU:N	2.46	0.48
1:B:3378:SER:OG	1:B:3379:VAL:N	2.45	0.48
1:B:3229:ILE:HG21	1:B:3271:LEU:HD11	1.96	0.48
1:B:2962:CYS:HA	1:B:3153:PRO:HB3	1.95	0.48
1:B:3218:GLY:HA2	1:B:3254:TRP:CE2	2.48	0.48
1:B:2917:LEU:HD11	1:B:3003:GLY:N	2.28	0.48
1:B:3034:ILE:HB	1:B:3038:ASN:O	2.14	0.48
1:B:3098:TYR:N	1:B:3098:TYR:CD2	2.80	0.48
1:A:3098:TYR:N	1:A:3098:TYR:CD2	2.80	0.48
1:A:3347:THR:N	1:A:3348:PRO:CD	2.75	0.48
1:A:3357:ALA:HA	1:B:3325:PRO:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3152:HIS:HD2	1:B:3155:ASN:HD21	1.61	0.48
1:A:2980:PHE:N	1:A:2981:PRO:HD2	2.29	0.48
1:B:3225:VAL:HG11	1:B:3243:PHE:CE1	2.49	0.48
1:B:3350:LEU:CD2	1:B:3351:ASN:H	2.19	0.48
1:A:2960:ASN:HB2	1:A:2969:LYS:HB3	1.96	0.47
1:B:2985:ARG:HH22	1:B:3124:ILE:CD1	2.24	0.47
1:B:3038:ASN:O	1:B:3039:GLN:HB2	2.13	0.47
1:B:3069:LEU:CD2	1:B:3126:TRP:HB2	2.44	0.47
1:A:2956:HIS:NE2	1:A:2973:CYS:SG	2.85	0.47
1:A:3285:LYS:HG3	1:A:3292:LEU:HD13	1.95	0.47
1:A:3317:PRO:CG	1:A:3338:PHE:HA	2.41	0.47
1:A:3337:MET:CG	1:A:3338:PHE:H	2.27	0.47
1:B:3215:VAL:HG21	1:B:3324:LEU:CB	2.44	0.47
1:A:3335:LYS:HG3	1:A:3377:TYR:HB2	1.96	0.47
1:B:2958:TYR:OH	1:B:3250:LYS:HD3	2.13	0.47
1:B:3279:LYS:NZ	1:B:3280:PHE:N	2.62	0.47
1:A:2935:ASP:O	1:A:2939:LYS:HG3	2.14	0.47
1:A:2960:ASN:HB3	1:A:2970:TYR:O	2.14	0.47
1:A:2985:ARG:HH22	1:A:3124:ILE:CD1	2.20	0.47
1:A:3214:PHE:HB3	1:A:3216:LEU:HD22	1.96	0.47
1:A:3227:VAL:HG23	1:A:3240:ALA:HB3	1.96	0.47
1:A:3352:LEU:HA	1:A:3385:PHE:HB3	1.97	0.47
1:A:3363:VAL:HG13	1:A:3391:THR:HG22	1.95	0.47
1:A:3368:PHE:O	1:A:3370:ALA:N	2.46	0.47
1:B:3363:VAL:HG13	1:B:3391:THR:HG22	1.97	0.47
1:B:3273:LEU:CD2	1:B:3279:LYS:HD2	2.43	0.47
1:A:2958:TYR:CD2	1:A:2959:PRO:HA	2.50	0.47
1:A:3114:ILE:HG13	1:A:3115:HIS:N	2.28	0.47
1:A:3159:VAL:CG2	1:A:3160:ASN:H	2.19	0.47
1:A:3188:ASN:ND2	1:A:3193:ASN:HA	2.30	0.47
1:A:3280:PHE:CZ	1:A:3300:PRO:HD2	2.49	0.47
1:B:2962:CYS:SG	1:B:2970:TYR:O	2.73	0.47
1:B:2980:PHE:N	1:B:2981:PRO:HD2	2.30	0.47
1:B:2981:PRO:HB2	1:B:3123:TRP:CZ3	2.50	0.47
1:B:3311:PHE:HD2	1:B:3331:LYS:HZ1	1.62	0.47
1:A:3356:THR:HB	1:B:3326:PRO:HG3	1.96	0.47
1:B:2956:HIS:HB3	1:B:3107:ALA:HB2	1.96	0.47
1:B:3347:THR:N	1:B:3348:PRO:CD	2.76	0.47
1:A:2984:HIS:O	1:A:2988:THR:HG22	2.15	0.47
1:A:3276:ASP:CG	1:A:3375:LYS:HE2	2.35	0.47
1:A:3348:PRO:HA	1:A:3368:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3397:ASN:CG	1:A:3399:LEU:HG	2.35	0.47
1:B:2919:ARG:NH2	1:B:2989:ILE:HG22	2.29	0.47
1:B:2941:GLN:NE2	1:B:3028:PRO:HB2	2.30	0.47
1:B:3202:ARG:O	1:B:3206:LEU:HG	2.14	0.47
1:A:2960:ASN:HB3	1:A:2970:TYR:N	2.30	0.47
1:B:3174:VAL:HG12	1:B:3174:VAL:O	2.14	0.47
1:B:3229:ILE:HA	1:B:3281:ARG:HB2	1.96	0.47
1:B:3337:MET:CG	1:B:3338:PHE:H	2.28	0.47
1:A:3069:LEU:CD2	1:A:3126:TRP:HB2	2.45	0.46
1:A:3321:ASP:H	1:A:3397:ASN:CB	2.28	0.46
1:B:3170:LEU:HD12	1:B:3172:ASN:HB2	1.97	0.46
1:B:3210:VAL:CG1	1:B:3265:THR:HA	2.41	0.46
1:A:3088:VAL:HA	1:A:3091:LEU:HD23	1.97	0.46
1:B:3070:GLU:OE2	1:B:3209:ARG:NH2	2.45	0.46
1:B:3318:ILE:CA	1:B:3339:MET:HB2	2.27	0.46
1:A:3121:LYS:HE2	1:A:3186:ASN:O	2.16	0.46
1:A:3322:VAL:HG22	1:A:3324:LEU:CD2	2.45	0.46
1:B:2980:PHE:CE2	1:B:3082:GLU:HG3	2.50	0.46
1:B:3067:GLN:O	1:B:3071:GLU:HG2	2.15	0.46
1:B:3150:PRO:HB2	1:B:3155:ASN:HD22	1.77	0.46
1:B:3248:GLY:O	1:B:3251:GLU:HG2	2.15	0.46
1:B:3363:VAL:HG13	1:B:3391:THR:CG2	2.46	0.46
1:B:3366:PHE:O	1:B:3368:PHE:N	2.49	0.46
1:B:3039:GLN:HG3	1:B:3098:TYR:CE1	2.50	0.46
1:A:2981:PRO:HB2	1:A:3123:TRP:CZ3	2.51	0.46
1:A:3201:LEU:O	1:A:3205:ARG:HG2	2.16	0.46
1:A:3229:ILE:HG21	1:A:3271:LEU:HD11	1.97	0.46
1:A:3391:THR:O	1:A:3394:CYS:HB3	2.16	0.46
1:B:2996:LYS:NZ	1:B:3001:HIS:HA	2.31	0.46
1:B:3034:ILE:O	1:B:3035:ARG:HB3	2.16	0.46
1:B:3114:ILE:HG13	1:B:3115:HIS:N	2.31	0.46
1:B:3296:VAL:HG22	1:B:3296:VAL:O	2.15	0.46
1:B:3302:ILE:HG23	1:B:3316:ILE:HB	1.98	0.46
1:A:3354:SER:HB3	1:A:3358:MET:HB3	1.98	0.46
1:B:3397:ASN:HD22	1:B:3397:ASN:C	2.15	0.46
1:A:2986:LEU:HD11	1:A:3169:SER:HA	1.98	0.46
1:A:3044:ASP:O	1:A:3094:GLY:HA3	2.16	0.46
1:A:3296:VAL:O	1:A:3296:VAL:HG22	2.15	0.46
1:B:2917:LEU:O	1:B:3182:TYR:HA	2.16	0.46
1:B:2962:CYS:CB	1:B:2963:PRO:CD	2.93	0.46
1:B:3009:TRP:CZ3	1:B:3061:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3090:ALA:O	1:B:3094:GLY:N	2.41	0.46
1:B:3307:ASN:O	1:B:3310:VAL:HG22	2.16	0.46
1:A:3065:ALA:HA	1:A:3084:LEU:HG	1.96	0.46
1:A:3070:GLU:OE2	1:A:3209:ARG:NH2	2.45	0.46
1:A:3125:ILE:HG13	1:A:3126:TRP:N	2.31	0.46
1:B:2918:VAL:O	1:B:3003:GLY:N	2.43	0.46
1:A:2950:GLU:HB3	1:A:3032:TYR:OH	2.15	0.46
1:A:2962:CYS:CB	1:A:2963:PRO:CD	2.94	0.46
1:A:3210:VAL:CG1	1:A:3265:THR:HA	2.40	0.46
1:B:2969:LYS:O	1:B:2970:TYR:CB	2.50	0.46
1:B:2974:VAL:HG13	1:B:2977:MET:HG3	1.98	0.46
1:B:3013:ILE:HD13	1:B:3049:ILE:HD13	1.98	0.46
1:B:3034:ILE:HD13	1:B:3039:GLN:O	2.15	0.46
1:B:3096:GLU:CB	1:B:3099:SER:HB3	2.45	0.46
1:B:3170:LEU:HD13	1:B:3172:ASN:H	1.80	0.46
1:A:3358:MET:CE	1:A:3362:LYS:HB3	2.46	0.46
1:A:3363:VAL:HG13	1:A:3391:THR:CG2	2.46	0.46
1:A:2960:ASN:HB3	1:A:2970:TYR:H	1.81	0.45
1:A:3058:PHE:HB3	1:A:3062:PHE:CD1	2.52	0.45
1:A:3271:LEU:HD13	1:A:3273:LEU:HD13	1.97	0.45
1:A:3305:ARG:HG3	1:A:3313:ILE:HD11	1.99	0.45
1:A:3310:VAL:HG12	1:A:3311:PHE:H	1.80	0.45
1:B:2958:TYR:CD2	1:B:2959:PRO:HA	2.51	0.45
1:B:3363:VAL:HG23	1:B:3364:PRO:HD2	1.98	0.45
1:A:3356:THR:HB	1:B:3326:PRO:CG	2.47	0.45
1:A:3152:HIS:HD2	1:A:3155:ASN:HD21	1.62	0.45
1:B:2989:ILE:HD11	1:B:3165:THR:HG22	1.96	0.45
1:B:3129:LEU:HD22	1:B:3133:ARG:NH2	2.32	0.45
1:B:3201:LEU:O	1:B:3205:ARG:HG2	2.15	0.45
1:B:3305:ARG:NH1	1:B:3313:ILE:HD11	2.32	0.45
1:B:3321:ASP:H	1:B:3397:ASN:CB	2.29	0.45
1:A:2917:LEU:O	1:A:3182:TYR:HA	2.17	0.45
1:A:3258:ARG:CZ	1:A:3330:VAL:HG21	2.45	0.45
1:A:3338:PHE:CE1	1:A:3374:GLY:HA2	2.44	0.45
1:B:2935:ASP:O	1:B:2939:LYS:HG3	2.15	0.45
1:B:3049:ILE:CG2	1:B:3050:PHE:H	2.23	0.45
1:B:3121:LYS:HE2	1:B:3186:ASN:O	2.16	0.45
1:B:3125:ILE:HG13	1:B:3126:TRP:N	2.31	0.45
1:A:3327:LYS:HZ3	1:A:3401:ILE:HG21	1.79	0.45
1:A:3363:VAL:HG23	1:A:3364:PRO:HD2	1.99	0.45
1:A:3373:LEU:O	1:A:3374:GLY:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2938:TYR:CZ	1:B:2942:ASN:ND2	2.85	0.45
1:B:2980:PHE:HD1	1:B:2981:PRO:HD3	1.82	0.45
1:B:3054:LYS:HB2	1:B:3190:HIS:NE2	2.32	0.45
1:B:3405:VAL:O	1:B:3406:ASP:HB2	2.16	0.45
1:A:2980:PHE:HD1	1:A:2981:PRO:HD3	1.82	0.45
1:B:2960:ASN:HB3	1:B:2970:TYR:O	2.16	0.45
1:B:3186:ASN:ND2	1:B:3188:ASN:H	2.14	0.45
1:A:3134:VAL:HG13	1:A:3134:VAL:O	2.15	0.45
1:A:3357:ALA:HA	1:B:3325:PRO:HB3	1.99	0.45
1:B:3054:LYS:HD3	1:B:3055:PHE:HB2	1.99	0.45
1:B:3274:THR:HB	1:B:3277:HIS:CB	2.44	0.45
1:B:3276:ASP:OD1	1:B:3375:LYS:HE2	2.17	0.45
1:B:3397:ASN:CG	1:B:3399:LEU:HG	2.37	0.45
1:A:2930:ALA:CB	1:A:2934:ARG:HH12	2.30	0.45
1:A:3038:ASN:O	1:A:3039:GLN:HB2	2.17	0.45
1:A:3072:ASP:O	1:A:3073:ASN:HB3	2.17	0.45
1:B:2930:ALA:HB1	1:B:2934:ARG:HH12	1.81	0.45
1:B:3088:VAL:HG11	1:B:3115:HIS:CE1	2.52	0.45
1:B:3170:LEU:CD1	1:B:3172:ASN:H	2.30	0.45
1:B:3347:THR:OG1	1:B:3374:GLY:HA2	2.17	0.45
1:A:3107:ALA:HA	1:A:3112:PHE:CD1	2.52	0.45
1:A:3205:ARG:HH22	1:A:3305:ARG:NH1	2.13	0.45
1:A:3366:PHE:O	1:A:3368:PHE:N	2.50	0.45
1:B:3222:THR:OG1	1:B:3246:LEU:HA	2.16	0.45
1:A:2956:HIS:HB2	1:A:2983:TRP:HH2	1.82	0.45
1:A:3324:LEU:HA	1:A:3325:PRO:HD3	1.84	0.45
1:B:3054:LYS:HA	1:B:3058:PHE:HD1	1.82	0.45
1:A:2917:LEU:HD11	1:A:3003:GLY:N	2.32	0.44
1:A:3054:LYS:HA	1:A:3058:PHE:HD1	1.82	0.44
1:A:3274:THR:HB	1:A:3277:HIS:CB	2.45	0.44
1:A:3305:ARG:NH1	1:A:3313:ILE:HD11	2.31	0.44
1:B:3093:GLY:CA	1:B:3099:SER:HB2	2.47	0.44
1:B:3188:ASN:ND2	1:B:3193:ASN:HA	2.31	0.44
1:B:3297:LEU:HB2	1:B:3298:PRO:C	2.37	0.44
1:B:3311:PHE:HD2	1:B:3331:LYS:NZ	2.15	0.44
1:B:3318:ILE:CG1	1:B:3339:MET:HB2	2.42	0.44
1:A:2958:TYR:OH	1:A:3250:LYS:HD3	2.18	0.44
1:A:3029:PHE:O	1:A:3110:PRO:HB2	2.17	0.44
1:A:3043:ARG:NE	1:A:3109:ASP:OD2	2.50	0.44
1:A:3067:GLN:O	1:A:3071:GLU:HG2	2.17	0.44
1:A:3069:LEU:HA	1:A:3126:TRP:HD1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3170:LEU:HD13	1:A:3172:ASN:H	1.82	0.44
1:A:3187:LEU:CD1	1:A:3194:ILE:HD12	2.45	0.44
1:A:3222:THR:HA	1:A:3245:ILE:O	2.17	0.44
1:A:3350:LEU:CD2	1:A:3351:ASN:H	2.19	0.44
1:B:2983:TRP:HD1	1:B:3151:LEU:HB3	1.82	0.44
1:B:2986:LEU:HD11	1:B:3169:SER:HA	1.99	0.44
1:A:2996:LYS:HA	1:A:3000:SER:CB	2.33	0.44
1:A:3093:GLY:CA	1:A:3099:SER:HB2	2.47	0.44
1:A:3170:LEU:HD12	1:A:3172:ASN:HB2	1.99	0.44
1:A:3364:PRO:HB2	1:A:3367:SER:HB3	1.99	0.44
1:A:3378:SER:OG	1:A:3379:VAL:N	2.49	0.44
1:B:3205:ARG:HH22	1:B:3305:ARG:NH1	2.16	0.44
1:B:3348:PRO:HA	1:B:3368:PHE:HZ	1.82	0.44
1:B:2956:HIS:CD2	1:B:2973:CYS:HB2	2.53	0.44
1:B:2973:CYS:SG	1:B:2975:HIS:CD2	3.11	0.44
1:B:3159:VAL:C	1:B:3161:ASN:H	2.21	0.44
1:B:3327:LYS:HZ3	1:B:3401:ILE:HG21	1.81	0.44
1:B:3335:LYS:HG3	1:B:3377:TYR:HB2	2.00	0.44
1:A:3297:LEU:CB	1:A:3298:PRO:CA	2.94	0.44
1:A:3324:LEU:HD21	1:A:3401:ILE:HG12	1.98	0.44
1:A:3326:PRO:HB3	1:A:3402:HIS:CB	2.36	0.44
1:A:3346:THR:OG1	1:A:3348:PRO:HD3	2.18	0.44
1:B:3336:ILE:HG12	1:B:3337:MET:N	2.32	0.44
1:A:3297:LEU:HB2	1:A:3298:PRO:C	2.38	0.44
1:B:3276:ASP:CG	1:B:3375:LYS:HE2	2.37	0.44
1:A:3245:ILE:N	1:A:3245:ILE:HD12	2.32	0.44
1:B:2960:ASN:OD1	1:B:2971:PRO:HG3	2.18	0.44
1:B:3065:ALA:HA	1:B:3084:LEU:HG	1.99	0.44
1:B:3134:VAL:HG13	1:B:3134:VAL:O	2.17	0.44
1:B:3329:VAL:HG21	1:B:3334:THR:HG21	1.98	0.44
1:A:3038:ASN:CG	1:A:3039:GLN:N	2.69	0.44
1:A:3243:PHE:CE1	1:A:3245:ILE:HD11	2.52	0.44
1:A:3318:ILE:HG23	1:A:3319:GLY:H	1.83	0.44
1:B:2930:ALA:CB	1:B:2934:ARG:HH12	2.30	0.44
1:B:3085:HIS:NE2	1:B:3089:HIS:NE2	2.65	0.44
1:B:3107:ALA:HA	1:B:3112:PHE:CD1	2.53	0.44
1:A:2930:ALA:HB1	1:A:2934:ARG:HH12	1.82	0.44
1:A:2965:LYS:HD2	1:A:2965:LYS:HA	1.75	0.44
1:A:2991:PHE:CD1	1:A:3113:MET:SD	3.11	0.44
1:A:3334:THR:HG22	1:A:3335:LYS:N	2.33	0.44
1:B:3072:ASP:O	1:B:3073:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3314:ILE:HG13	1:B:3335:LYS:HD2	1.99	0.44
1:A:3046:ASN:HD22	1:A:3047:GLU:H	1.64	0.43
1:B:3329:VAL:CG2	1:B:3334:THR:HG21	2.48	0.43
1:A:2960:ASN:OD1	1:A:2971:PRO:HG3	2.18	0.43
1:A:3185:ASP:OD1	1:A:3185:ASP:N	2.51	0.43
1:A:3205:ARG:HB3	1:A:3310:VAL:HG21	2.00	0.43
1:A:3225:VAL:HG11	1:A:3243:PHE:CE1	2.53	0.43
1:B:3079:VAL:HG11	1:B:3260:TYR:HA	2.00	0.43
1:B:3305:ARG:HG3	1:B:3313:ILE:CD1	2.48	0.43
1:A:2941:GLN:NE2	1:A:3028:PRO:HB2	2.33	0.43
1:A:3054:LYS:HB2	1:A:3190:HIS:NE2	2.33	0.43
1:A:3170:LEU:CD1	1:A:3172:ASN:H	2.31	0.43
1:B:3088:VAL:HA	1:B:3091:LEU:HD23	2.00	0.43
1:A:3258:ARG:CD	1:A:3330:VAL:HG21	2.49	0.43
1:B:3069:LEU:HA	1:B:3126:TRP:HD1	1.82	0.43
1:B:3091:LEU:HD22	1:B:3091:LEU:H	1.83	0.43
1:B:3271:LEU:HD13	1:B:3273:LEU:HD13	2.00	0.43
1:B:3285:LYS:HB2	1:B:3285:LYS:NZ	2.34	0.43
1:A:3088:VAL:HG11	1:A:3115:HIS:CE1	2.53	0.43
1:A:3129:LEU:HD22	1:A:3133:ARG:NH2	2.33	0.43
1:A:3327:LYS:O	1:A:3403:VAL:HA	2.18	0.43
1:A:3351:ASN:HB2	1:A:3371:PHE:CD2	2.53	0.43
1:B:3227:VAL:HG23	1:B:3240:ALA:HB3	2.00	0.43
1:A:2965:LYS:HG3	1:A:2965:LYS:O	2.18	0.43
1:A:3054:LYS:HD3	1:A:3055:PHE:HB2	1.99	0.43
1:A:3215:VAL:HG21	1:A:3324:LEU:CB	2.47	0.43
1:A:3287:TYR:HB2	1:A:3292:LEU:HD23	2.01	0.43
1:A:3337:MET:HG2	1:A:3338:PHE:H	1.83	0.43
1:B:2925:LEU:HD23	1:B:2929:GLU:HB2	2.00	0.43
1:B:3176:ASP:HB3	1:B:3179:ARG:HD3	2.01	0.43
1:B:3368:PHE:O	1:B:3370:ALA:N	2.49	0.43
1:A:3330:VAL:CG1	1:A:3331:LYS:H	2.30	0.43
1:B:3214:PHE:HB2	1:B:3260:TYR:HB3	2.00	0.43
1:A:3186:ASN:ND2	1:A:3188:ASN:H	2.16	0.43
1:A:3405:VAL:O	1:A:3406:ASP:HB2	2.19	0.43
1:B:3373:LEU:O	1:B:3374:GLY:O	2.37	0.43
1:A:2975:HIS:NE2	1:A:2984:HIS:CE1	2.86	0.43
1:A:3006:TYR:HB2	1:A:3118:SER:HA	2.01	0.43
1:A:3231:SER:HB3	1:A:3236:ASP:O	2.19	0.43
1:B:3058:PHE:HB3	1:B:3062:PHE:CD1	2.54	0.43
1:B:3205:ARG:NH1	1:B:3305:ARG:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2991:PHE:CE2	1:B:3004:ILE:HD12	2.53	0.43
1:B:3074:TYR:HA	1:B:3077:PHE:HB3	2.01	0.43
1:A:3079:VAL:HG13	1:A:3256:TYR:CE2	2.54	0.42
1:B:2952:ILE:HD12	1:B:2990:GLN:HG3	1.99	0.42
1:B:3187:LEU:CD1	1:B:3194:ILE:HD12	2.49	0.42
1:B:3354:SER:HB3	1:B:3358:MET:CB	2.49	0.42
1:A:3069:LEU:HA	1:A:3126:TRP:CD1	2.54	0.42
1:A:3165:THR:OG1	1:A:3166:ARG:N	2.52	0.42
1:A:3168:ASN:HB3	1:A:3179:ARG:NH2	2.34	0.42
1:A:3335:LYS:HB2	1:A:3335:LYS:HZ3	1.82	0.42
1:A:3358:MET:HE1	1:B:3220:ARG:NH2	2.34	0.42
1:B:3317:PRO:HD2	1:B:3337:MET:C	2.39	0.42
1:B:3249:ALA:O	1:B:3250:LYS:CB	2.66	0.42
1:A:3249:ALA:O	1:A:3250:LYS:CB	2.66	0.42
1:B:2984:HIS:O	1:B:2988:THR:HG22	2.19	0.42
1:B:3327:LYS:O	1:B:3403:VAL:HA	2.20	0.42
1:A:2965:LYS:NZ	1:A:2967:ASP:HB3	2.34	0.42
1:A:2989:ILE:HD11	1:A:3165:THR:HG22	2.00	0.42
1:B:2965:LYS:HD2	1:B:2965:LYS:HA	1.69	0.42
1:B:3006:TYR:HB2	1:B:3118:SER:HA	2.00	0.42
1:B:3194:ILE:HG12	1:B:3195:GLU:H	1.83	0.42
1:B:3252:MET:HA	1:B:3253:PRO:HD3	1.94	0.42
1:B:3299:ALA:HA	1:B:3300:PRO:HD2	1.93	0.42
1:B:3319:GLY:N	1:B:3339:MET:O	2.52	0.42
1:B:3325:PRO:CA	1:B:3400:ARG:HH22	2.32	0.42
1:B:3346:THR:OG1	1:B:3348:PRO:HD3	2.20	0.42
1:A:3311:PHE:HD2	1:A:3331:LYS:NZ	2.16	0.42
1:B:3165:THR:OG1	1:B:3166:ARG:N	2.52	0.42
1:A:3319:GLY:N	1:A:3339:MET:O	2.53	0.42
1:A:3404:HIS:ND1	1:A:3405:VAL:N	2.67	0.42
1:A:3159:VAL:HG13	1:A:3161:ASN:N	2.24	0.42
1:A:3218:GLY:HA2	1:A:3254:TRP:CE2	2.55	0.42
1:A:3325:PRO:CA	1:A:3400:ARG:HH22	2.32	0.42
1:B:3029:PHE:O	1:B:3110:PRO:HB2	2.19	0.42
1:B:3059:SER:O	1:B:3060:SER:CB	2.68	0.42
1:B:3222:THR:HA	1:B:3245:ILE:O	2.19	0.42
1:B:3317:PRO:HB3	1:B:3327:LYS:HZ1	1.82	0.42
1:B:3346:THR:HB	1:B:3347:THR:H	1.69	0.42
1:A:2990:GLN:NE2	1:A:3165:THR:HG21	2.35	0.42
1:A:3059:SER:O	1:A:3060:SER:CB	2.67	0.42
1:B:3038:ASN:CG	1:B:3039:GLN:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3258:ARG:CD	1:B:3330:VAL:HG21	2.48	0.42
1:B:3307:ASN:O	1:B:3308:ASN:O	2.38	0.42
1:A:2996:LYS:NZ	1:A:3001:HIS:HA	2.34	0.42
1:A:3358:MET:HE3	1:B:3253:PRO:HB3	2.02	0.42
1:B:2941:GLN:HA	1:B:2949:TYR:HB3	2.02	0.42
1:B:3337:MET:HG2	1:B:3338:PHE:H	1.84	0.42
1:A:2956:HIS:HB3	1:A:3107:ALA:HB2	2.02	0.41
1:A:3068:ALA:O	1:A:3077:PHE:HD1	2.03	0.41
1:A:3248:GLY:O	1:A:3251:GLU:HG2	2.19	0.41
1:B:3226:LYS:HD2	1:B:3242:SER:HB3	2.02	0.41
1:B:3243:PHE:CE1	1:B:3245:ILE:HD11	2.55	0.41
1:A:2961:LEU:HB2	1:A:2962:CYS:H	1.60	0.41
1:A:3031:LYS:HE2	1:A:3031:LYS:HB3	1.94	0.41
1:A:3081:TYR:CE1	1:A:3119:LEU:HD22	2.56	0.41
1:A:3277:HIS:O	1:A:3279:LYS:N	2.53	0.41
1:B:2996:LYS:CA	1:B:3000:SER:HB3	2.36	0.41
1:B:3245:ILE:HD12	1:B:3245:ILE:N	2.34	0.41
1:B:3289:HIS:ND1	1:B:3289:HIS:N	2.68	0.41
1:B:3348:PRO:CB	1:B:3389:SER:HB3	2.49	0.41
1:A:3348:PRO:CB	1:A:3389:SER:HB3	2.49	0.41
1:A:3074:TYR:HA	1:A:3077:PHE:HB3	2.02	0.41
1:A:3176:ASP:HB3	1:A:3179:ARG:HD3	2.02	0.41
1:A:3277:HIS:ND1	1:A:3277:HIS:C	2.73	0.41
1:B:3257:GLU:H	1:B:3257:GLU:HG3	1.48	0.41
1:B:3277:HIS:O	1:B:3279:LYS:N	2.53	0.41
1:A:3009:TRP:CZ3	1:A:3061:ILE:HD11	2.54	0.41
1:A:3092:ILE:HD12	1:A:3092:ILE:N	2.35	0.41
1:A:3327:LYS:HZ2	1:A:3401:ILE:HG21	1.83	0.41
1:B:3193:ASN:HB3	1:B:3196:GLU:HG3	2.02	0.41
1:A:2983:TRP:HD1	1:A:3151:LEU:HB3	1.85	0.41
1:A:3072:ASP:HB2	1:A:3311:PHE:HE2	1.80	0.41
1:A:3083:ILE:HG21	1:A:3260:TYR:CZ	2.56	0.41
1:A:3103:LEU:HD22	1:A:3247:GLY:CA	2.47	0.41
1:A:3276:ASP:OD1	1:A:3375:LYS:HE2	2.21	0.41
1:B:3044:ASP:O	1:B:3094:GLY:HA3	2.20	0.41
1:B:3091:LEU:HD13	1:B:3091:LEU:H	1.85	0.41
1:B:3350:LEU:HD22	1:B:3387:THR:CB	2.44	0.41
1:A:3079:VAL:HG11	1:A:3260:TYR:HA	2.01	0.41
1:A:3229:ILE:HD13	1:A:3281:ARG:HB3	2.01	0.41
1:A:3364:PRO:HA	1:A:3365:PRO:HD3	1.87	0.41
1:B:3185:ASP:OD1	1:B:3185:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3207:LYS:N	1:B:3307:ASN:HB2	2.36	0.41
1:A:2956:HIS:CD2	1:A:2973:CYS:HB2	2.56	0.41
1:A:2973:CYS:SG	1:A:2975:HIS:CD2	3.14	0.41
1:A:2990:GLN:CD	1:A:3165:THR:HG21	2.41	0.41
1:A:3085:HIS:NE2	1:A:3089:HIS:NE2	2.69	0.41
1:A:3090:ALA:O	1:A:3094:GLY:N	2.42	0.41
1:A:3098:TYR:N	1:A:3098:TYR:HD2	2.19	0.41
1:A:3314:ILE:HG13	1:A:3335:LYS:HD2	2.03	0.41
1:B:2990:GLN:NE2	1:B:3165:THR:HG21	2.36	0.41
1:B:2990:GLN:CD	1:B:3165:THR:HG21	2.42	0.41
1:B:2991:PHE:CE2	1:B:3113:MET:HB3	2.56	0.41
1:B:3081:TYR:CE2	1:B:3119:LEU:HD13	2.56	0.41
1:B:3081:TYR:CE1	1:B:3119:LEU:HD22	2.56	0.41
1:B:3098:TYR:N	1:B:3098:TYR:HD2	2.19	0.41
1:B:3177:SER:C	1:B:3179:ARG:N	2.73	0.41
1:B:3220:ARG:HA	1:B:3251:GLU:HG2	2.02	0.41
1:B:3231:SER:HB3	1:B:3236:ASP:O	2.21	0.41
1:B:3332:ARG:HB3	1:B:3406:ASP:OD1	2.21	0.41
1:B:3391:THR:O	1:B:3394:CYS:HB3	2.20	0.41
1:A:3049:ILE:CG2	1:A:3050:PHE:H	2.21	0.41
1:A:3220:ARG:HA	1:A:3251:GLU:HG2	2.03	0.41
1:A:3264:ILE:HD13	1:A:3264:ILE:H	1.86	0.41
1:A:3397:ASN:HD21	1:A:3399:LEU:HG	1.81	0.41
1:B:3347:THR:OG1	1:B:3374:GLY:N	2.54	0.41
1:B:3351:ASN:HB2	1:B:3371:PHE:CD2	2.55	0.41
1:A:2990:GLN:NE2	1:A:3160:ASN:ND2	2.69	0.40
1:A:3314:ILE:HG13	1:A:3335:LYS:HB3	2.03	0.40
1:A:3335:LYS:CG	1:A:3377:TYR:HB2	2.51	0.40
1:B:3069:LEU:HA	1:B:3126:TRP:CD1	2.55	0.40
1:B:3258:ARG:NH1	1:B:3330:VAL:HG11	2.36	0.40
1:B:3380:GLU:HG2	1:B:3381:SER:N	2.37	0.40
1:A:2985:ARG:HG3	1:A:3120:ASP:OD2	2.21	0.40
1:A:3177:SER:C	1:A:3179:ARG:N	2.75	0.40
1:A:3289:HIS:ND1	1:A:3289:HIS:N	2.69	0.40
1:B:2990:GLN:NE2	1:B:3160:ASN:ND2	2.70	0.40
1:A:2953:ALA:HB1	1:A:3108:PHE:HA	2.01	0.40
1:A:2989:ILE:HD13	1:A:3180:PHE:HD1	1.86	0.40
1:A:3279:LYS:HZ1	1:A:3280:PHE:N	2.16	0.40
1:A:3330:VAL:HG12	1:A:3331:LYS:N	2.35	0.40
1:A:3336:ILE:HG22	1:A:3378:SER:HB2	2.04	0.40
1:B:2953:ALA:HB1	1:B:3108:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3365:PRO:O	1:B:3367:SER:N	2.54	0.40
1:A:2952:ILE:O	1:A:2987:HIS:HE1	2.03	0.40
1:A:3258:ARG:NH1	1:A:3330:VAL:HG11	2.37	0.40
1:B:2956:HIS:NE2	1:B:2973:CYS:SG	2.93	0.40
1:B:2986:LEU:HD22	1:B:3154:PHE:CD1	2.56	0.40
1:B:3044:ASP:HB2	1:B:3096:GLU:HG2	2.04	0.40
1:B:3364:PRO:HB2	1:B:3367:SER:HB3	2.04	0.40
1:A:2989:ILE:O	1:A:2993:ARG:HG3	2.22	0.40
1:A:3083:ILE:HG21	1:A:3260:TYR:CE2	2.56	0.40
1:A:3336:ILE:HG12	1:A:3337:MET:N	2.37	0.40
1:A:3347:THR:OG1	1:A:3374:GLY:N	2.55	0.40
1:B:3043:ARG:HB3	1:B:3092:ILE:O	2.21	0.40
1:B:3157:GLU:OE2	1:B:3157:GLU:HA	2.21	0.40
1:B:3281:ARG:CD	1:B:3300:PRO:HG3	2.51	0.40
1:B:3336:ILE:HG22	1:B:3378:SER:HB2	2.02	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	489/491 (100%)	341 (70%)	102 (21%)	46 (9%)	0	11
1	B	489/491 (100%)	342 (70%)	101 (21%)	46 (9%)	0	11
All	All	978/982 (100%)	683 (70%)	203 (21%)	92 (9%)	0	11

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2962	CYS
1	A	2970	TYR
1	A	3061	ILE

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Mol	Chain	Res	Type
1	A	3139	ALA
1	A	3158	SER
1	A	3235	SER
1	A	3265	THR
1	A	3278	VAL
1	A	3295	SER
1	A	3296	VAL
1	A	3307	ASN
1	A	3313	ILE
1	A	3317	PRO
1	A	3350	LEU
1	A	3351	ASN
1	A	3354	SER
1	A	3371	PHE
1	A	3379	VAL
1	A	3397	ASN
1	B	2962	CYS
1	B	2970	TYR
1	B	3061	ILE
1	B	3139	ALA
1	B	3158	SER
1	B	3235	SER
1	B	3278	VAL
1	B	3295	SER
1	B	3296	VAL
1	B	3313	ILE
1	B	3317	PRO
1	B	3350	LEU
1	B	3351	ASN
1	B	3354	SER
1	B	3371	PHE
1	B	3379	VAL
1	B	3397	ASN
1	A	3049	ILE
1	A	3299	ALA
1	A	3330	VAL
1	A	3346	THR
1	A	3367	SER
1	A	3374	GLY
1	A	3385	PHE
1	B	3049	ILE
1	B	3265	THR

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Mol	Chain	Res	Type
1	B	3299	ALA
1	B	3307	ASN
1	B	3308	ASN
1	B	3330	VAL
1	B	3346	THR
1	B	3362	LYS
1	B	3367	SER
1	B	3374	GLY
1	A	3060	SER
1	A	3233	THR
1	A	3308	ASN
1	A	3348	PRO
1	A	3361	CYS
1	A	3362	LYS
1	A	3370	ALA
1	A	3400	ARG
1	B	3060	SER
1	B	3178	HIS
1	B	3233	THR
1	B	3293	ASP
1	B	3348	PRO
1	B	3361	CYS
1	B	3385	PHE
1	B	3400	ARG
1	A	3039	GLN
1	A	3053	THR
1	A	3178	HIS
1	A	3293	ASP
1	A	3318	ILE
1	B	3039	GLN
1	B	3053	THR
1	A	2964	GLU
1	A	3310	VAL
1	A	3337	MET
1	A	3365	PRO
1	A	3366	PHE
1	B	3062	PHE
1	B	3310	VAL
1	B	3337	MET
1	B	3365	PRO
1	B	3366	PHE
1	B	3368	PHE

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Mol	Chain	Res	Type
1	B	3370	ALA
1	A	3368	PHE
1	B	3318	ILE
1	A	3159	VAL
1	B	3324	LEU

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 20
1	B	437/437 (100%)	376 (86%)	61 (14%)	3 20
All	All	874/874 (100%)	752 (86%)	122 (14%)	3 20

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2925	LEU
1	A	2958	TYR
1	A	2961	LEU
1	A	2962	CYS
1	A	2970	TYR
1	A	2986	LEU
1	A	3009	TRP
1	A	3013	ILE
1	A	3016	LEU
1	A	3019	PHE
1	A	3031	LYS
1	A	3043	ARG
1	A	3047	GLU
1	A	3050	PHE
1	A	3054	LYS
1	A	3057	GLU
1	A	3059	SER
1	A	3072	ASP

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Mol	Chain	Res	Type
1	A	3085	HIS
1	A	3091	LEU
1	A	3104	GLU
1	A	3114	ILE
1	A	3119	LEU
1	A	3142	CYS
1	A	3148	HIS
1	A	3194	ILE
1	A	3215	VAL
1	A	3225	VAL
1	A	3235	SER
1	A	3257	GLU
1	A	3264	ILE
1	A	3271	LEU
1	A	3272	ASN
1	A	3274	THR
1	A	3277	HIS
1	A	3279	LYS
1	A	3281	ARG
1	A	3283	ASP
1	A	3285	LYS
1	A	3292	LEU
1	A	3301	ILE
1	A	3302	ILE
1	A	3307	ASN
1	A	3312	ASP
1	A	3313	ILE
1	A	3314	ILE
1	A	3315	GLU
1	A	3318	ILE
1	A	3323	ASN
1	A	3332	ARG
1	A	3338	PHE
1	A	3349	MET
1	A	3350	LEU
1	A	3351	ASN
1	A	3360	LYS
1	A	3363	VAL
1	A	3368	PHE
1	A	3387	THR
1	A	3392	GLU
1	A	3394	CYS

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Mol	Chain	Res	Type
1	A	3397	ASN
1	B	2921	ASN
1	B	2925	LEU
1	B	2958	TYR
1	B	2961	LEU
1	B	2962	CYS
1	B	2970	TYR
1	B	2986	LEU
1	B	3009	TRP
1	B	3013	ILE
1	B	3016	LEU
1	B	3019	PHE
1	B	3031	LYS
1	B	3043	ARG
1	B	3047	GLU
1	B	3050	PHE
1	B	3054	LYS
1	B	3057	GLU
1	B	3059	SER
1	B	3072	ASP
1	B	3085	HIS
1	B	3091	LEU
1	B	3104	GLU
1	B	3114	ILE
1	B	3119	LEU
1	B	3142	CYS
1	B	3148	HIS
1	B	3194	ILE
1	B	3215	VAL
1	B	3235	SER
1	B	3257	GLU
1	B	3264	ILE
1	B	3271	LEU
1	B	3272	ASN
1	B	3274	THR
1	B	3277	HIS
1	B	3279	LYS
1	B	3281	ARG
1	B	3283	ASP
1	B	3285	LYS
1	B	3292	LEU
1	B	3301	ILE

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Mol	Chain	Res	Type
1	B	3302	ILE
1	B	3307	ASN
1	B	3312	ASP
1	B	3313	ILE
1	B	3315	GLU
1	B	3318	ILE
1	B	3323	ASN
1	B	3332	ARG
1	B	3338	PHE
1	B	3349	MET
1	B	3350	LEU
1	B	3351	ASN
1	B	3360	LYS
1	B	3363	VAL
1	B	3368	PHE
1	B	3373	LEU
1	B	3387	THR
1	B	3392	GLU
1	B	3394	CYS
1	B	3397	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2921	ASN
1	A	2941	GLN
1	A	2990	GLN
1	A	3026	ASN
1	A	3027	ASN
1	A	3046	ASN
1	A	3067	GLN
1	A	3152	HIS
1	A	3155	ASN
1	A	3160	ASN
1	A	3161	ASN
1	A	3168	ASN
1	A	3186	ASN
1	A	3188	ASN
1	A	3272	ASN
1	A	3308	ASN
1	A	3397	ASN
1	B	2921	ASN

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Mol	Chain	Res	Type
1	B	2941	GLN
1	B	2942	ASN
1	B	2990	GLN
1	B	3026	ASN
1	B	3027	ASN
1	B	3046	ASN
1	B	3067	GLN
1	B	3152	HIS
1	B	3155	ASN
1	B	3160	ASN
1	B	3161	ASN
1	B	3168	ASN
1	B	3186	ASN
1	B	3188	ASN
1	B	3272	ASN
1	B	3308	ASN
1	B	3323	ASN
1	B	3351	ASN
1	B	3369	HIS
1	B	3397	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 monosaccharides 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

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	491/491 (100%)	-0.30	6 (1%)	79	70	57, 135, 209, 279	0
1	B	491/491 (100%)	-0.32	5 (1%)	82	74	58, 134, 208, 279	0
All	All	982/982 (100%)	-0.31	11 (1%)	80	72	57, 135, 209, 279	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3055	PHE	3.8
1	B	3054	LYS	3.6
1	B	3055	PHE	3.2
1	B	3052	GLN	2.9
1	A	2967	ASP	2.6
1	A	3137	ALA	2.4
1	A	3136	PRO	2.4
1	B	3138	HIS	2.3
1	A	2966	GLY	2.1
1	B	3140	GLY	2.1
1	A	3276	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	CU	A	3408	1/1	0.95	0.13	86,86,86,86	0
2	CU	A	3407	1/1	0.96	0.13	79,79,79,79	0
2	CU	B	3407	1/1	0.98	0.15	79,79,79,79	0
2	CU	B	3408	1/1	0.98	0.17	74,74,74,74	0

6.5 Other polymers

There are no such residues in this entry.