



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 3QJO / pdb_00003qjo
Title : Refined Structure of the functional unit (KLH1-H) of keyhole limpet hemo-
cyanin
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

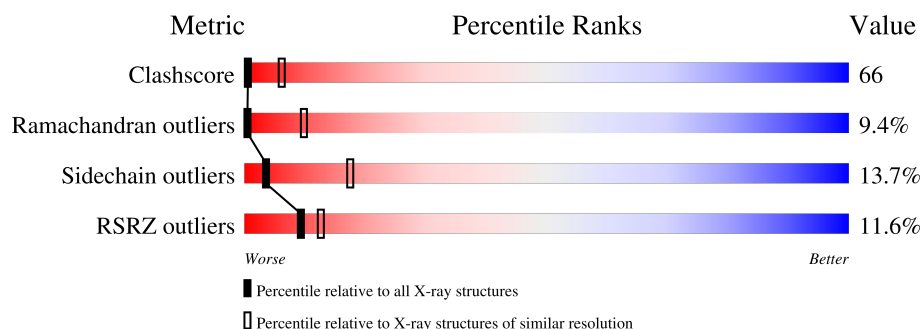
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	
1	B	491	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7994 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemocyanin 1.

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

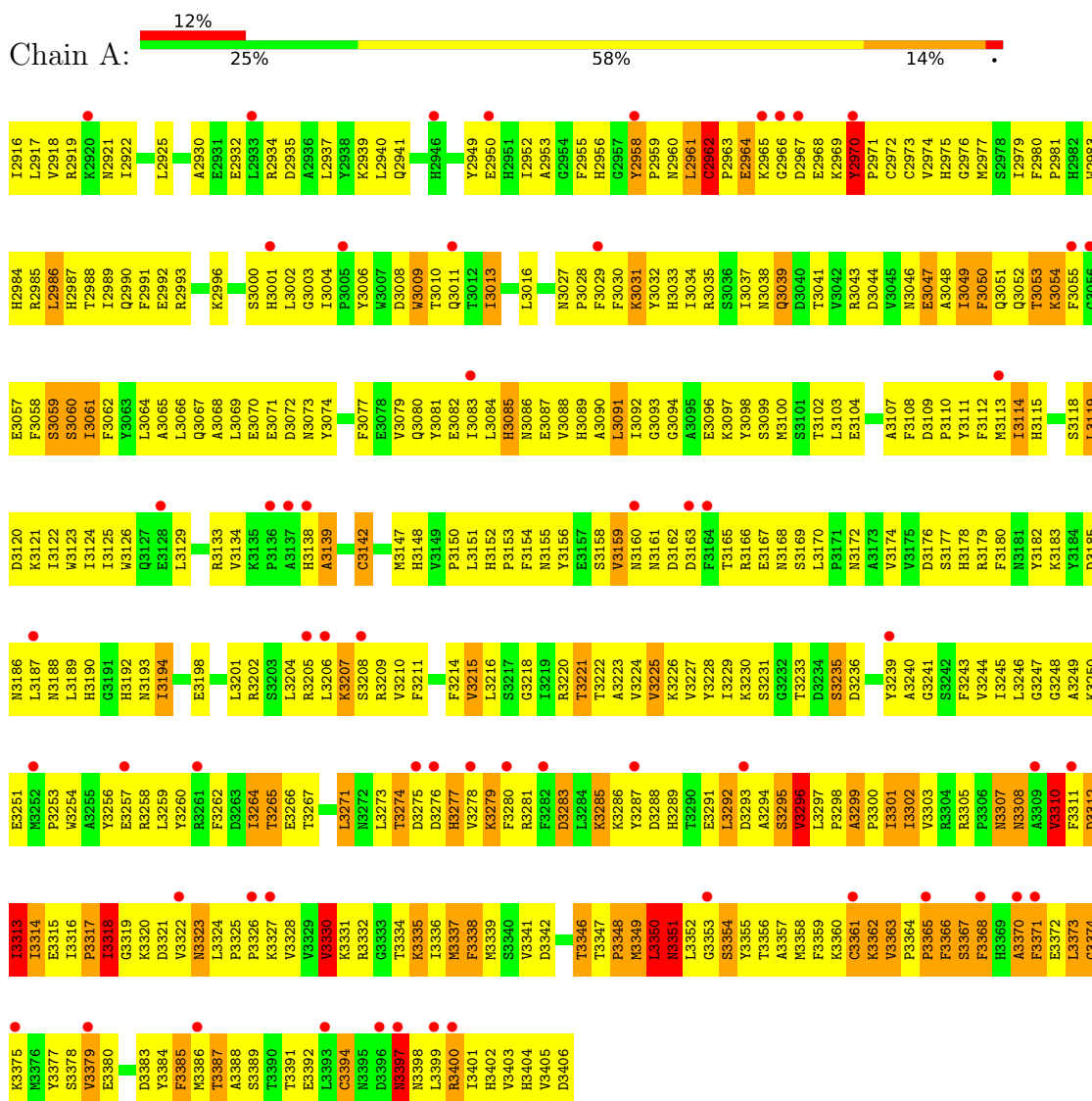
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Hemocyanin 1



• Molecule 1: Hemocyanin 1



E3372	F3311	G3248	D3185	S3118	H2984	L2916
L3373	D3312	A3249	N3186	L3119	R2985	L2917
G3374	I3313	K3250	N3187	D3120	L2986	R2918
K3375	E3314	E3251	N3188	K3121	T2987	R2919
N3376	E3315	P3252	L3189	L3122	E3057	K2920
N3377	L3316	P3253	N3190	L3123	F3058	N2921
S3378	P3317	W3254	G3191	L3124	S3059	L2922
L3379	I3318	E3257	N3192	I3125	S3060	L2925
E3380	K3319	R3258	N3193	W3126	F3062	E2929
S3381	K3320	L3259	L3194	L3129	Y3063	A2930
G3382	D3321	E3260	E3195	R3133	A3065	A2931
D3383	V3322	F3261	E3196	V3134	L3066	E2932
Y3384	N3323	F3262	L3197	E3198	Q3067	L2933
F3385	L3324	D3263	L3201		A3068	R2934
M3386	P3325	I3264	R3202		L3069	I3004
T3387	P3326	T3265	S3203	A3137	E3070	A2936
A3388	K3327	E3266	S3204	H3138	E3071	L2937
S3389	V3328	T3267	L3204	A3139	Y3066	Y2938
T3390	V3329		R3205	G3140	D3072	K2939
T3391	W3330	L3271	L3206	S3141	N3073	L2940
E3392	R3331	N3272	K3207	C3142	Y3074	Q2941
L3393	G3332	L3273	S3208		F3077	N2942
C3394	G3333	D3274	R3209	H3147	E3078	Y2949
	T3334	T3275	V3210	H3148	Q3080	H2950
	K3335	D3276	F3211	V3149	Y3081	L2952
	L3336	H3277	F3214	P3150	I3013	A2953
	M3337	V3278	L3215	H3152	P3017	G2954
	F3338	K3279	V3216	P3155	T3018	F2955
	M3339	F3280	L3217	N3156	G3024	R2956
	S3340	R3281	S3218	Y3157	H3025	G2957
	V3341	F3282	L3219	S3158	N3026	Y2958
	D3342	D3283	R3220	T3221	N3027	P2959
		K3284	T3222	A3223	F3028	N2960
		L3285	V3224	N3160	F3029	L2961
		K3286	V3225	N3161	K3031	C2962
		D3287	K3226	D3162	I3092	P2963
		H3288	Y3227	F3164	G3093	E2964
		T3289	V3227	T3165	L3034	K2965
		E3291	L3292	R3166	R3035	G2966
		D3293	K3293		S3036	D2967
		A3294	K3294		I3037	E2968
		S3295	S3231	S3169	N3038	K2969
		W3296	G3232	L3170	Q3039	Y2970
		L3297	T3233	P3171	D3040	P2971
		P3298	D3234	N3172	T3041	C2972
		A3299	S3235	A3173	Y3042	C2973
		P3300	D3236	V3174	R3043	V2974
		I3301		V3175	D3044	H2975
		L3302	Y3239	D3176	V3045	G2976
		V3303	A3240	S3177	N3046	M2977
		K3304	G3241	H3178	E3047	L2978
		F3305	S3242	R3179	A3048	I2979
		P3306	F3243	F3180	I3049	F2980
		N3307	V3244	N3181	F3050	P2981
		N3308	L3245	Y3182	I3114	H2982
		A3309	L3246	K3183	Q3052	W2983
		V3310	G3247	Y3184		

4 Data and refinement statistics

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/4110	0.73	0/5575
1	B	0.28	0/4110	0.72	0/5575
All	All	0.28	0/8220	0.73	0/11150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3995	0	3831	524	0
1	B	3995	0	3831	518	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	7994	0	7662	1033	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 66.

All (1033) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3318:ILE:HA	1:A:3339:MET:HB2	1.35	1.08
1:B:3318:ILE:HA	1:B:3339:MET:HB2	1.36	1.06
1:A:3061:ILE:HG23	1:A:3062:PHE:H	1.24	1.03
1:B:3061:ILE:HG23	1:B:3062:PHE:H	1.23	1.00
1:A:3253:PRO:HB3	1:B:3358:MET:HE3	1.44	0.98
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: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

Continued on next page...

Continued from previous page...

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: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:A:3307:ASN:CG	1:A:3308:ASN:H	1.87	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:A:3279:LYS:HZ2	1:A:3279:LYS:HA	1.49	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: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:B:3279:LYS:HZ1	1:B:3280:PHE:H	1.34	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:A:3279:LYS:HZ1	1:A:3280:PHE:H	1.35	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3207:LYS:HE2	1:B:3207:LYS:HA	1.71	0.73
1:B:3279:LYS:HZ2	1:B:3279:LYS:HA	1.53	0.73
1:A:3086:ASN:HB3	1:A:3244:VAL:HG13	1.71	0.72
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: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:3302:ILE:C	1:B:3302:ILE:HD13	2.16	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:A:3038:ASN:CG	1:A:3039:GLN:H	2.00	0.70
1:A:3327:LYS:HZ3	1:A:3401:ILE:HG21	1.57	0.70
1:B:3061:ILE:HG23	1:B:3062:PHE:N	2.01	0.70
1:B:3160:ASN:HD22	1:B:3162:ASP:HB2	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:3142:CYS:HB2	1:A:3258:ARG:NH2	2.08	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:3038:ASN:CG	1:B:3039:GLN:H	2.02	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:3302:ILE:HD13	1:A:3302:ILE:C	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:3318:ILE:HG13	1:A:3339:MET:HG3	1.78	0.64
1:B:3307:ASN:CG	1:B:3308:ASN:H	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:3249:ALA:O	1:A:3250:LYS:HB2	1.98	0.62
1:A:3318:ILE:HG23	1:A:3319:GLY:N	2.13	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:3307:ASN:CG	1:B:3308:ASN:N	2.57	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:2917:LEU:HD11	1:A:3002:LEU:C	2.25	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:2960:ASN:HB3	1:B:2970:TYR:C	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3159:VAL:HG22	1:A:3160:ASN:N	2.14	0.61
1:B:2917:LEU:HD11	1:B:3002:LEU:C	2.26	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:A:3139:ALA:C	1:A:3147:MET:HE1	2.25	0.61
1:B:2961:LEU:O	1:B:2963:PRO:HD2	2.01	0.61
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:3318:ILE:HG23	1:B:3319:GLY:N	2.14	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:2960:ASN:HB3	1:A:2970:TYR:C	2.26	0.59
1:A:3225:VAL:HA	1:A:3285:LYS:HA	1.83	0.59
1:B:3139:ALA:C	1:B:3147:MET:HE1	2.26	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:3365:PRO:C	1:A:3367:SER:H	2.11	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: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:B:3359:PHE:C	1:B:3361:CYS:H	2.11	0.59
1:A:2961:LEU:O	1:A:2963:PRO:HD2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:3286:LYS:HE3	1:B:3291:GLU:OE2	2.03	0.58
1:A:3030:PHE:C	1:A:3031:LYS:HG2	2.28	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:B:3086:ASN:CG	1:B:3246:LEU:HD13	2.29	0.58
1:A:2950:GLU:HB3	1:A:3035:ARG:NH2	2.18	0.58
1:B:3177:SER:C	1:B:3179:ARG:H	2.11	0.58
1:B:3365:PRO:C	1:B:3367:SER:H	2.10	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:3307:ASN:O	1:B:3308:ASN:C	2.46	0.57
1:A:3336:ILE:HG22	1:A:3378:SER:HB3	1.85	0.57
1:A:3359:PHE:C	1:A:3361:CYS:H	2.13	0.57
1:B:2986:LEU:HD13	1:B:3154:PHE:CD1	2.39	0.57
1:B:3030:PHE:C	1:B:3031:LYS:HG2	2.27	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
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:3325:PRO:CB	1:B:3326:PRO:HD2	2.35	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:3086:ASN:CG	1:A:3246:LEU:HD13	2.30	0.56
1:B:3351:ASN:CG	1:B:3352:LEU:H	2.12	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: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:3215:VAL:HG21	1:B:3324:LEU:HB2	1.86	0.56
1:A:3051:GLN:HG3	1:A:3052:GLN:N	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:3351:ASN:CG	1:A:3352:LEU:H	2.14	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:B:3224:VAL:HG22	1:B:3225:VAL:N	2.21	0.55
1:B:3349:MET:O	1:B:3350:LEU:C	2.49	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:A:3349:MET:O	1:A:3350:LEU:C	2.49	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
1:B:3351:ASN:CG	1:B:3352:LEU:N	2.64	0.55
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:3383:ASP:CG	1:A:3402:HIS:HE2	2.14	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:3177:SER:C	1:A:3179:ARG:H	2.12	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:3013:ILE:CD1	1:A:3049:ILE:HA	2.36	0.55
1:B:3037:ILE:HG13	1:B:3037:ILE:O	2.06	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:3397:ASN:HD22	1:A:3397:ASN:C	2.16	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: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
1:B:3298:PRO:O	1:B:3299:ALA:C	2.50	0.54
1:A:3087:GLU:O	1:A:3091:LEU:HD22	2.07	0.54
1:A:3008:ASP:O	1:A:3011:GLN:HG2	2.08	0.54
1:A:3307:ASN:O	1:A:3308:ASN:C	2.50	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:B:3383:ASP:CG	1:B:3402:HIS:HE2	2.16	0.54
1:B:3397:ASN:HD22	1:B:3397:ASN:C	2.15	0.54
1:A:3349:MET:HE1	1:A:3399:LEU:HB3	1.89	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:A:3335:LYS:HB2	1:A:3335:LYS:HZ2	1.73	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:3281:ARG:HD2	1:A:3281:ARG:O	2.08	0.53
1:A:3298:PRO:O	1:A:3299:ALA:C	2.51	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:3318:ILE:HG13	1:A:3339:MET:CB	2.39	0.53
1:B:3341:VAL:O	1:B:3342:ASP:HB3	2.06	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:A:3341:VAL:O	1:A:3342:ASP:HB3	2.08	0.52
1:B:2930:ALA:HB1	1:B:2934:ARG:NH1	2.24	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: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:3287:TYR:CG	1:A:3288:ASP:N	2.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:3351:ASN:CG	1:A:3352:LEU:N	2.65	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:3276:ASP:CG	1:A:3375:LYS:HE2	2.35	0.51
1:A:3350:LEU:CB	1:A:3387:THR:HG22	2.40	0.51
1:A:3397:ASN:CG	1:A:3399:LEU:HG	2.35	0.51
1:A:3323:ASN:O	1:A:3324:LEU:HB3	2.08	0.51
1:A:3350:LEU:HD21	1:A:3353:GLY:N	2.25	0.51
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: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: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:HG2	1:B:3364:PRO:HD3	1.92	0.51
1:A:3279:LYS:HZ1	1:A:3280:PHE:N	2.06	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:A:3207:LYS:N	1:A:3307:ASN:HB2	2.26	0.51
1:B:2976:GLY:HA3	1:B:3254:TRP:CE3	2.46	0.51
1:B:2979:ILE:CG2	1:B:3147:MET:HG2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:B:3226:LYS:HE2	1:B:3239:TYR:CD2	2.47	0.49
1:B:3397:ASN:CG	1:B:3399:LEU:HG	2.37	0.49
1:A:3358:MET:HE3	1:B:3253:PRO:HB3	1.93	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: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:3351:ASN:N	1:A:3351:ASN:HD22	2.09	0.49
1:B:3279:LYS:HZ1	1:B:3280:PHE:N	2.08	0.49
1:B:3297:LEU:HB2	1:B:3298:PRO:C	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3350:LEU:CB	1:B:3387:THR:HG22	2.41	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: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
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:3279:LYS:NZ	1:A:3280:PHE:N	2.59	0.49
1:A:3297:LEU:HB2	1:A:3298:PRO:C	2.38	0.49
1:B:3276:ASP:CG	1:B:3375:LYS:HE2	2.37	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:3370:ALA:O	1:A:3371:PHE:HB2	2.12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3327:LYS:HZ3	1:A:3401:ILE:CG2	2.24	0.48
1:B:3159:VAL:C	1:B:3161:ASN:H	2.21	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
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:A:3349:MET:HE2	1:A:3387:THR:C	2.39	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:B:3349:MET:HE1	1:B:3399:LEU:HD22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:3348:PRO:HA	1:A:3368:PHE:HZ	1.80	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:3317:PRO:HD2	1:B:3337:MET:C	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3277:HIS:ND1	1:A:3277:HIS:C	2.73	0.46
1:A:3354:SER:HB3	1:A:3358:MET:HB3	1.98	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
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:A:3317:PRO:HB3	1:A:3327:LYS:HZ2	1.80	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:B:3349:MET:HE1	1:B:3399:LEU:HB3	1.98	0.46
1:A:2960:ASN:HB3	1:A:2970:TYR:H	1.81	0.45
1:A:2990:GLN:CD	1:A:3165:THR:HG21	2.41	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:3038:ASN:CG	1:B:3039:GLN:N	2.70	0.45
1:B:3363:VAL:HG23	1:B:3364:PRO:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3356:THR:HB	1:B:3326:PRO:CG	2.47	0.45
1:A:3365:PRO:C	1:A:3367:SER:N	2.74	0.45
1:B:2990:GLN:CD	1:B:3165:THR:HG21	2.42	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:3177:SER:C	1:A:3179:ARG:N	2.75	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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3277:HIS:ND1	1:B:3277:HIS:C	2.74	0.45
1:A:2956:HIS:HB2	1:A:2983:TRP:HH2	1.82	0.45
1:A:3072:ASP:O	1:A:3073:ASN:HB3	2.17	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:B:3317:PRO:HB3	1:B:3327:LYS:HZ1	1.79	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: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
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: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: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:B:3162:ASP:O	1:B:3163:ASP:C	2.60	0.44
1:A:3245:ILE:N	1:A:3245:ILE:HD12	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:3331:LYS:O	1:B:3332:ARG:C	2.61	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
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:A:3355:TYR:O	1:A:3356:THR:C	2.60	0.43
1:B:2962:CYS:O	1:B:2963:PRO:C	2.61	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:3084:LEU:C	1:B:3084:LEU:HD13	2.43	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:3084:LEU:HD13	1:A:3084:LEU:C	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3358:MET:HE1	1:A:3362:LYS:HB3	2.00	0.43
1:B:3177:SER:C	1:B:3179:ARG:N	2.73	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:3279:LYS:HA	1:B:3279:LYS:NZ	2.29	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:3311:PHE:HD2	1:A:3331:LYS:NZ	2.16	0.43
1:A:3405:VAL:O	1:A:3406:ASP:HB2	2.19	0.43
1:B:3275:ASP:CG	1:B:3276:ASP:N	2.76	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:3038:ASN:CG	1:A:3039:GLN:N	2.69	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
1:A:3159:VAL:C	1:A:3161:ASN:H	2.26	0.43
1:A:3279:LYS:HA	1:A:3279:LYS:NZ	2.27	0.43
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:B:3159:VAL:C	1:B:3161:ASN:N	2.77	0.43
1:A:3079:VAL:HG13	1:A:3256:TYR:CE2	2.54	0.42
1:A:3167:GLU:C	1:A:3169:SER:H	2.27	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:B:3355:TYR:O	1:B:3356:THR:C	2.60	0.42
1:A:2962:CYS:O	1:A:2963:PRO:C	2.61	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:3331:LYS:O	1:A:3332:ARG:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:3302:ILE:CD1	1:A:3302:ILE:C	2.88	0.42
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2996:LYS:CA	1:B:3000:SER:HB3	2.36	0.41
1:B:3111:TYR:O	1:B:3112:PHE:C	2.63	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:B:3327:LYS:HZ3	1:B:3401:ILE:HG21	1.84	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:3275:ASP:CG	1:A:3276:ASP:N	2.78	0.41
1:A:3378:SER:OG	1:A:3379:VAL:N	2.49	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: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
1:B:3207:LYS:N	1:B:3307:ASN:HB2	2.36	0.41
1:B:3339:MET:C	1:B:3341:VAL:H	2.29	0.41
1:B:3024:GLY:C	1:B:3026:ASN:N	2.79	0.41
1:B:3359:PHE:C	1:B:3361:CYS:N	2.77	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: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:3111:TYR:O	1:A:3112:PHE:C	2.64	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:2991:PHE:CE2	1:B:3113:MET:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:3339:MET:C	1:A:3341:VAL:H	2.28	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: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:B:3060:SER:O	1:B:3061:ILE:C	2.64	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:3162:ASP:O	1:A:3163:ASP:C	2.63	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
1:B:3046:ASN:O	1:B:3047:GLU:C	2.64	0.40
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3347:THR:OG1	1:A:3374:GLY:N	2.55	0.40
1:A:3349:MET:HE1	1:A:3399:LEU:HD22	2.04	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:3222:THR:HG1	1:B:3246:LEU:HA	1.87	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	10
1	B	489/491 (100%)	342 (70%)	101 (21%)	46 (9%)	0	10
All	All	978/982 (100%)	683 (70%)	203 (21%)	92 (9%)	0	10

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2962	CYS
1	A	2970	TYR
1	A	3061	ILE
1	A	3139	ALA
1	A	3158	SER
1	A	3235	SER
1	A	3265	THR
1	A	3278	VAL
1	A	3295	SER
1	A	3296	VAL
1	A	3307	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/437 (100%)	376 (86%)	61 (14%)	3	17
1	B	437/437 (100%)	378 (86%)	59 (14%)	4	18
All	All	874/874 (100%)	754 (86%)	120 (14%)	3	17

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2916	ILE
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	3031	LYS
1	A	3047	GLU
1	A	3050	PHE
1	A	3054	LYS
1	A	3057	GLU
1	A	3059	SER
1	A	3085	HIS
1	A	3091	LEU
1	A	3100	MET
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	3207	LYS
1	A	3215	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3221	THR
1	A	3225	VAL
1	A	3235	SER
1	A	3257	GLU
1	A	3264	ILE
1	A	3271	LEU
1	A	3274	THR
1	A	3277	HIS
1	A	3279	LYS
1	A	3283	ASP
1	A	3285	LYS
1	A	3292	LEU
1	A	3296	VAL
1	A	3301	ILE
1	A	3302	ILE
1	A	3310	VAL
1	A	3312	ASP
1	A	3313	ILE
1	A	3314	ILE
1	A	3318	ILE
1	A	3323	ASN
1	A	3330	VAL
1	A	3335	LYS
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	3373	LEU
1	A	3387	THR
1	A	3392	GLU
1	A	3394	CYS
1	A	3397	ASN
1	B	2916	ILE
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3013	ILE
1	B	3016	LEU
1	B	3031	LYS
1	B	3047	GLU
1	B	3050	PHE
1	B	3054	LYS
1	B	3057	GLU
1	B	3059	SER
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	3207	LYS
1	B	3215	VAL
1	B	3221	THR
1	B	3225	VAL
1	B	3235	SER
1	B	3257	GLU
1	B	3264	ILE
1	B	3271	LEU
1	B	3274	THR
1	B	3277	HIS
1	B	3279	LYS
1	B	3283	ASP
1	B	3285	LYS
1	B	3292	LEU
1	B	3296	VAL
1	B	3301	ILE
1	B	3302	ILE
1	B	3312	ASP
1	B	3313	ILE
1	B	3314	ILE
1	B	3318	ILE
1	B	3323	ASN
1	B	3330	VAL
1	B	3335	LYS
1	B	3338	PHE
1	B	3349	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3350	LEU
1	B	3351	ASN
1	B	3360	LYS
1	B	3363	VAL
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 (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2921	ASN
1	A	2941	GLN
1	A	2982	HIS
1	A	2987	HIS
1	A	2990	GLN
1	A	3026	ASN
1	A	3027	ASN
1	A	3033	HIS
1	A	3038	ASN
1	A	3046	ASN
1	A	3067	GLN
1	A	3080	GLN
1	A	3115	HIS
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	3269	HIS
1	A	3272	ASN
1	A	3308	ASN
1	A	3397	ASN
1	B	2921	ASN
1	B	2941	GLN
1	B	2982	HIS
1	B	2990	GLN
1	B	3026	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3027	ASN
1	B	3033	HIS
1	B	3038	ASN
1	B	3046	ASN
1	B	3067	GLN
1	B	3080	GLN
1	B	3115	HIS
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	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	491/491 (100%)	0.94	58 (11%) 9 12	57, 135, 209, 279	0
1	B	491/491 (100%)	0.97	56 (11%) 10 13	58, 134, 208, 279	0
All	All	982/982 (100%)	0.96	114 (11%) 9 12	57, 135, 209, 279	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3276	ASP	4.9
1	B	3160	ASN	4.8
1	B	3138	HIS	4.5
1	A	3257	GLU	4.1
1	B	3139	ALA	4.0
1	B	3140	GLY	3.9
1	A	3055	PHE	3.9
1	B	3137	ALA	3.7
1	B	3205	ARG	3.7
1	B	3327	LYS	3.6
1	B	2991	PHE	3.5
1	B	3055	PHE	3.5
1	B	3356	THR	3.5
1	A	3239	TYR	3.4
1	A	3397	ASN	3.4
1	B	3187	LEU	3.2
1	A	3056	GLY	3.2
1	B	2965	LYS	3.2
1	B	3358	MET	3.1
1	A	3282	PHE	3.1
1	A	3322	VAL	3.1
1	B	3371	PHE	3.1
1	B	3386	MET	3.1
1	A	3001	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	3029	PHE	3.0
1	B	3379	VAL	2.9
1	A	3400	ARG	2.9
1	B	3355	TYR	2.9
1	A	3208	SER	2.8
1	B	3311	PHE	2.8
1	A	3393	LEU	2.8
1	A	3136	PRO	2.8
1	A	3252	MET	2.8
1	B	3322	VAL	2.7
1	A	3138	HIS	2.7
1	B	3060	SER	2.7
1	A	3327	LYS	2.7
1	B	3180	PHE	2.7
1	B	3370	ALA	2.7
1	A	3160	ASN	2.7
1	B	3276	ASP	2.6
1	A	2958	TYR	2.6
1	B	2942	ASN	2.6
1	B	3309	ALA	2.6
1	A	2967	ASP	2.5
1	B	3398	ASN	2.5
1	B	3159	VAL	2.5
1	B	2970	TYR	2.5
1	A	3163	ASP	2.5
1	A	3113	MET	2.5
1	B	3345	VAL	2.5
1	B	2968	GLU	2.5
1	B	3164	PHE	2.5
1	A	2920	LYS	2.4
1	A	2933	LEU	2.4
1	B	3377	TYR	2.4
1	B	3257	GLU	2.4
1	B	3353	GLY	2.4
1	B	3326	PRO	2.4
1	A	3375	LYS	2.4
1	A	3128	GLU	2.4
1	A	3371	PHE	2.4
1	A	3386	MET	2.4
1	B	2958	TYR	2.4
1	A	3353	GLY	2.4
1	B	3029	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	3361	CYS	2.4
1	A	3164	PHE	2.3
1	A	3370	ALA	2.3
1	A	3137	ALA	2.3
1	A	3379	VAL	2.3
1	A	2946	HIS	2.3
1	A	3368	PHE	2.3
1	B	3380	GLU	2.3
1	A	2970	TYR	2.3
1	A	3280	PHE	2.3
1	B	3080	GLN	2.3
1	B	2967	ASP	2.3
1	A	2966	GLY	2.3
1	B	3266	GLU	2.2
1	B	3189	LEU	2.2
1	B	3287	TYR	2.2
1	A	3206	LEU	2.2
1	B	3260	TYR	2.2
1	A	2950	GLU	2.2
1	A	3396	ASP	2.2
1	A	3399	LEU	2.2
1	B	3397	ASN	2.2
1	B	3206	LEU	2.2
1	A	3011	GLN	2.2
1	A	3083	ILE	2.1
1	B	3114	ILE	2.1
1	A	3205	ARG	2.1
1	B	3113	MET	2.1
1	A	3326	PRO	2.1
1	A	3287	TYR	2.1
1	B	3001	HIS	2.1
1	B	3340	SER	2.1
1	A	3309	ALA	2.1
1	A	2965	LYS	2.1
1	B	2950	GLU	2.1
1	A	3005	PRO	2.1
1	A	3311	PHE	2.1
1	A	3365	PRO	2.1
1	A	3261	ARG	2.1
1	A	3293	ASP	2.1
1	B	3018	THR	2.1
1	B	3005	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	3278	VAL	2.1
1	A	3187	LEU	2.0
1	B	3362	LYS	2.0
1	B	3056	GLY	2.0
1	A	3275	ASP	2.0
1	B	3282	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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

6.5 Other polymers [i](#)

There are no such residues in this entry.