W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:57 AM GMT

PDB ID	:	3QJO
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
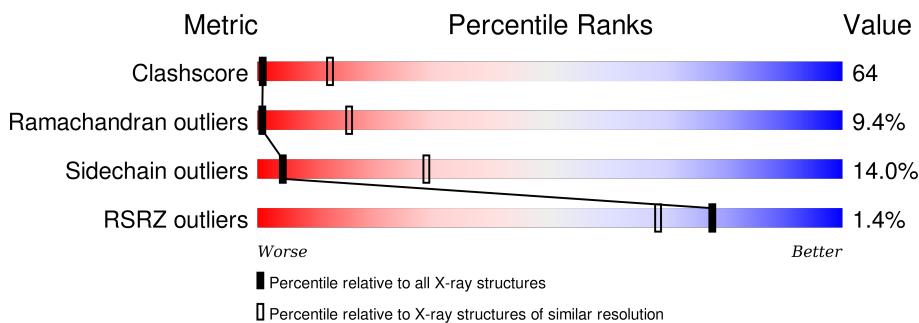
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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

Mol	Chain	Length	Quality of chain
1	A	491	26% 58% 15% •
1	B	491	25% 58% 15% •
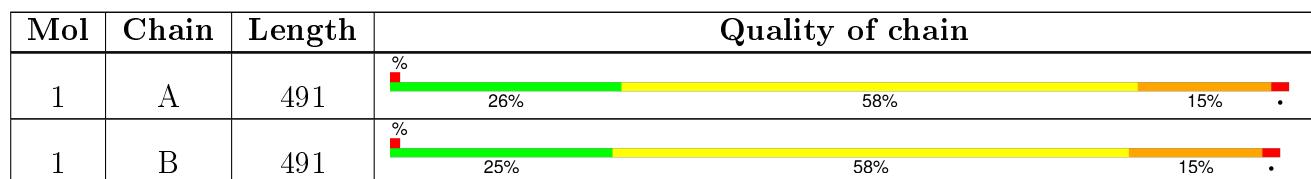
2 Entry composition (i)

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	B	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		

3 Residue-property plots (i)

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

- Molecule 1: Hemocyanin 1
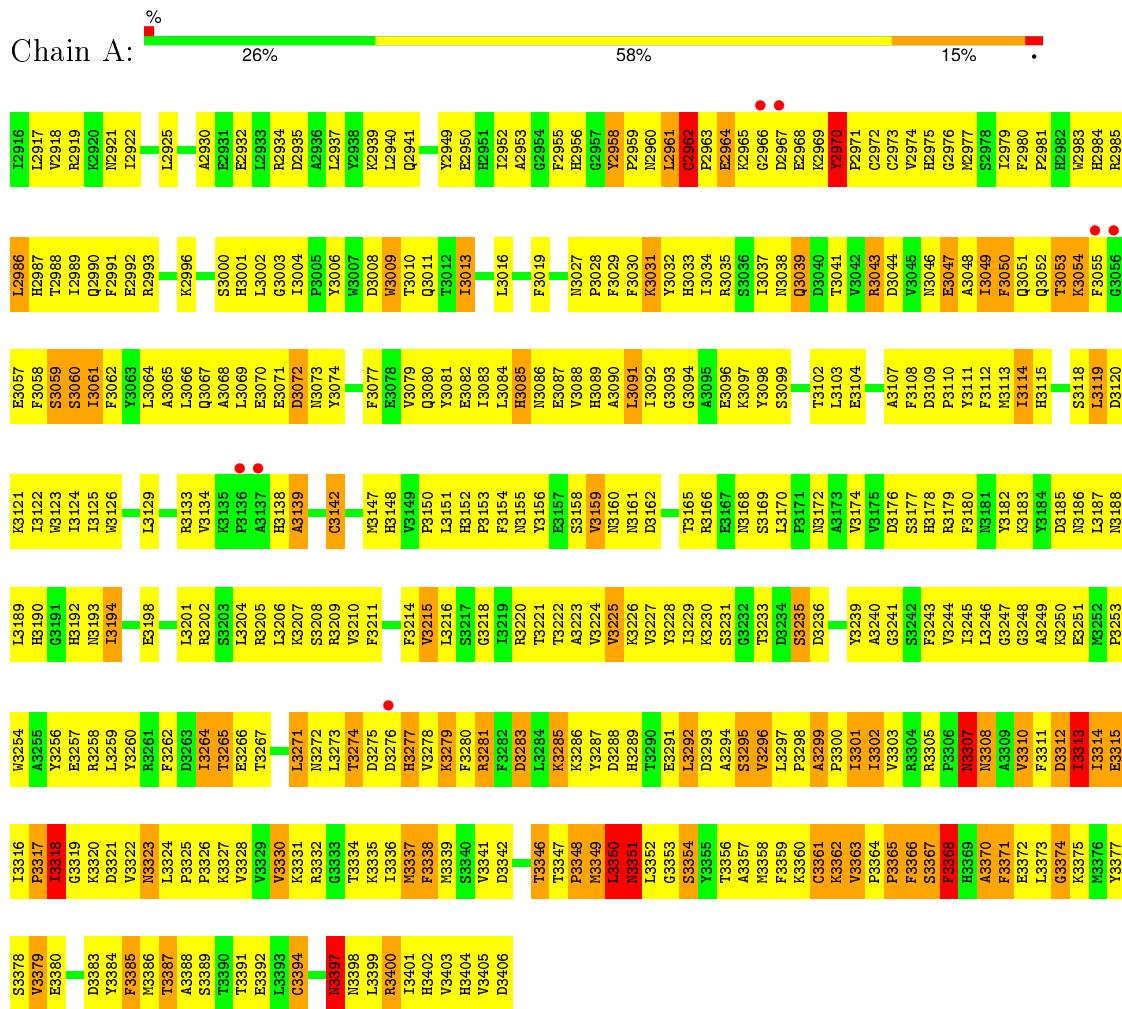
- Molecule 1: Hemocyanin 1
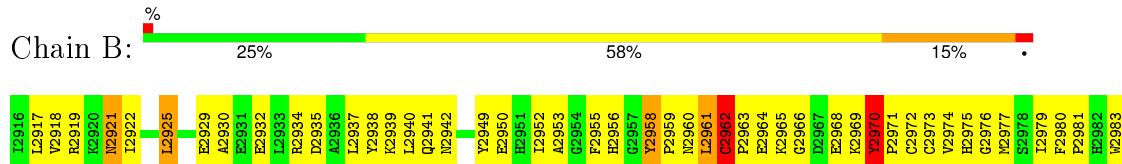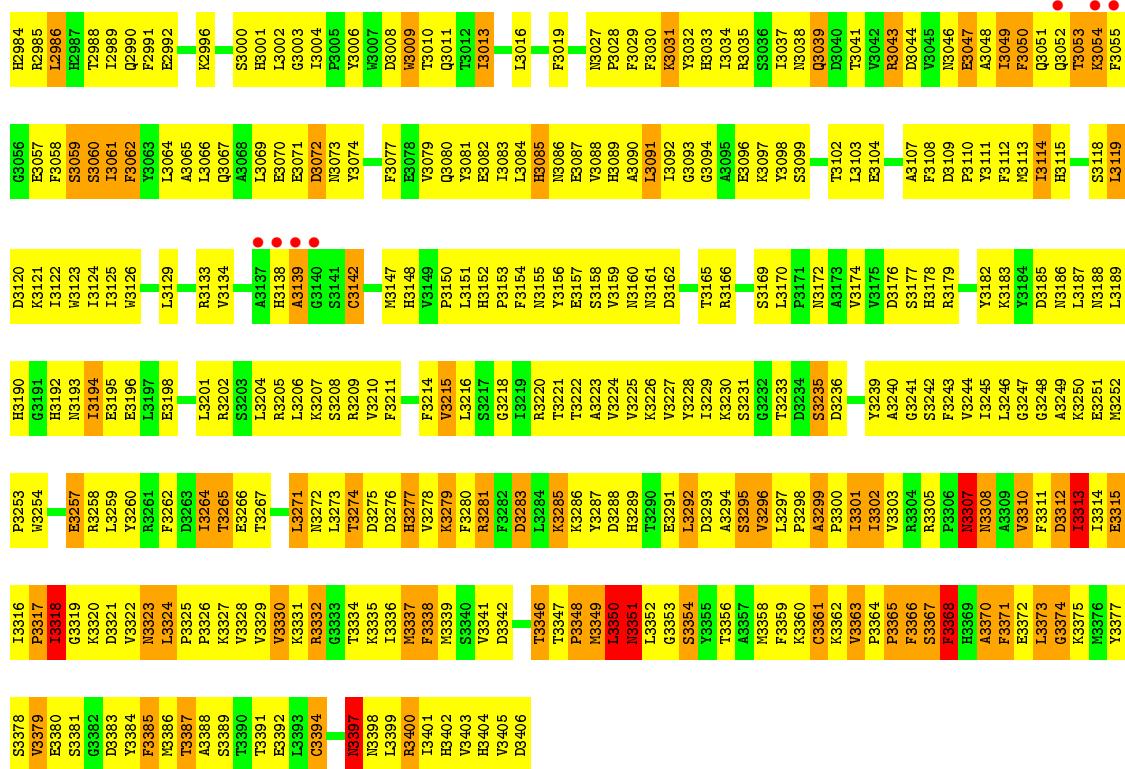
4 Data and refinement statistics (i)

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 0.287 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	122.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 149.9	EDS
Estimated twinning fraction	0.055 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 22294 reflections	Xtriage
F_o,F_c correlation	0.86	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:HA	1:A:3279:LYS:HZ2	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:3316:ILE:HG22	1:B:3339:MET:HG2	1.61	0.81
1:B:3142:CYS:HB2	1:B:3258:ARG:HH22	1.45	0.81
1:B:3215:VAL:HG23	1:B:3298:PRO:HG2	1.60	0.81
1:A:2962:CYS:HB2	1:A:2963:PRO:HD3	1.61	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: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:A:3125:ILE:O	1:A:3129:LEU:HB2	1.82	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:3159:VAL:HG13	1:A:3161:ASN:H	1.47	0.77
1:A:3071:GLU:HG3	1:A:3080:GLN:HG3	1.66	0.77
1:B:3274:THR:HB	1:B:3277:HIS:HB3	1.66	0.77
1:A:3194:ILE:H	1:A:3194:ILE:HD13	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:HE2	1:A:3207:LYS:HA	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:HA	1:B:3207:LYS:HE2	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:3297:LEU:HB2	1:B:3298:PRO:CA	2.19	0.72
1:B:3072:ASP:HB2	1:B:3311:PHE:HE2	1.54	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:3273:LEU:HD22	1:B:3279:LYS:HD2	1.73	0.71
1:B:3227:VAL:HA	1:B:3283:ASP:HB3	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:3208:SER:N	1:B:3307:ASN:HB3	2.06	0.70
1:B:2921:ASN:HD22	1:B:2922:ILE:H	1.37	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: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:3027:ASN:HD22	1:B:3028:PRO:HD2	1.57	0.70
1:B:3204:LEU:HD12	1:B:3204:LEU:H	1.56	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:3027:ASN:HD22	1:A:3028:PRO:HD2	1.57	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:3142:CYS:HB2	1:A:3258:ARG:NH2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3253:PRO:HB3	1:B:3358:MET:HE3	1.75	0.69
1:A:2986:LEU:HD12	1:A:3151:LEU:HD12	1.74	0.69
1:B:3046:ASN:ND2	1:B:3047:GLU:H	1.91	0.69
1:A:3215:VAL:HG22	1:A:3301:ILE:HD11	1.75	0.69
1:A:3058:PHE:CD2	1:A:3062:PHE:HB3	2.28	0.69
1:B:3302:ILE:HD13	1:B:3303:VAL:N	2.08	0.69
1:A:3216:LEU:HD22	1:A:3216:LEU:H	1.58	0.69
1:B:3319:GLY:O	1:B:3320:LYS:HB3	1.93	0.68
1:A:3046:ASN:ND2	1:A:3047:GLU:H	1.91	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: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:3150:PRO:HB2	1:A:3155:ASN:ND2	2.07	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:3285:LYS:HG3	1:B:3292:LEU:CD1	2.24	0.67
1:B:2992:GLU:HA	1:B:3004:ILE:HD11	1.77	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:3302:ILE:C	1:B:3302:ILE:HD13	2.16	0.66
1:B:3318:ILE:HG13	1:B:3339:MET:HG3	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:A:3302:ILE:HD13	1:A:3303:VAL:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3033:HIS:HE1	1:A:3038:ASN:HA	1.60	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:B:3335:LYS:HB2	1:B:3335:LYS:NZ	2.11	0.66
1:B:3320:LYS:HG2	1:B:3342:ASP:OD1	1.95	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: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:3303:VAL:HG12	1:A:3315:GLU:HA	1.78	0.66
1:A:3221:THR:HA	1:A:3248:GLY:HA2	1.75	0.66
1:A:2992:GLU:HA	1:A:3004:ILE:HD11	1.78	0.66
1:A:3301:ILE:HG23	1:A:3317:PRO:HA	1.77	0.65
1:B:3274:THR:H	1:B:3277:HIS:CE1	2.14	0.65
1:B:3058:PHE:CD2	1:B:3062:PHE:HB3	2.31	0.65
1:B:3279:LYS:HZ1	1:B:3280:PHE:H	1.43	0.65
1:A:3103:LEU:HD22	1:A:3247:GLY:HA2	1.78	0.65
1:A:3049:ILE:HG22	1:A:3050:PHE:H	1.61	0.65
1:A:3096:GLU:HB2	1:A:3099:SER:HB3	1.78	0.65
1:B:3301:ILE:HD12	1:B:3301:ILE:H	1.62	0.65
1:B:2986:LEU:HD22	1:B:3154:PHE:CE1	2.31	0.65
1:B:3033:HIS:HE1	1:B:3038:ASN:HA	1.61	0.65
1:A:3350:LEU:HD23	1:A:3351:ASN:N	2.12	0.65
1:A:3228:TYR:O	1:A:3281:ARG:HB2	1.96	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:3054:LYS:HE3	1:B:3190:HIS:NE2	2.12	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: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:A:3038:ASN:CG	1:A:3039:GLN:H	2.00	0.64
1:B:3318:ILE:HG13	1:B:3339:MET:CB	2.28	0.63
1:B:3049:ILE:HG22	1:B:3050:PHE:H	1.64	0.63
1:A:3327:LYS:NZ	1:A:3401:ILE:HG21	2.13	0.63
1:A:3313:ILE:HG22	1:A:3334:THR:HG23	1.80	0.63
1:A:3122:ILE:O	1:A:3125:ILE:HG12	1.99	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: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: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:B:3047:GLU:O	1:B:3049:ILE:HG12	1.99	0.63
1:A:3400:ARG:HD2	1:A:3400:ARG:O	1.99	0.62
1:B:3211:PHE:HB2	1:B:3303:VAL:HG23	1.80	0.62
1:B:3350:LEU:O	1:B:3351:ASN:HB3	1.99	0.62
1:B:3326:PRO:HB3	1:B:3402:HIS:CB	2.26	0.62
1:B:3224:VAL:HG22	1:B:3225:VAL:H	1.64	0.62
1:B:3038:ASN:CG	1:B:3039:GLN:H	2.02	0.62
1:A:3302:ILE:C	1:A:3302:ILE:HD13	2.19	0.62
1:B:3215:VAL:HG23	1:B:3298:PRO:CG	2.28	0.62
1:A:3249:ALA:O	1:A:3250:LYS:HB2	1.98	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:3320:LYS:HD3	1:A:3321:ASP:N	2.14	0.62
1:B:3301:ILE:HD12	1:B:3301:ILE:N	2.15	0.62
1:A:2985:ARG:HD2	1:A:3174:VAL:HG12	1.81	0.62
1:B:2983:TRP:HA	1:B:3151:LEU:HD13	1.81	0.62
1:A:3335:LYS:NZ	1:A:3335:LYS:HB2	2.14	0.62
1:B:3336:ILE:HG22	1:B:3378:SER:HB3	1.82	0.62
1:B:3325:PRO:HB3	1:B:3326:PRO:HD2	1.81	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:3301:ILE:HG23	1:B:3317:PRO:HA	1.82	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: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:3187:LEU:HD23	1:B:3187:LEU:H	1.65	0.61
1:B:3010:THR:HG21	1:B:3189:LEU:HD11	1.83	0.61
1:A:3317:PRO:HB3	1:A:3327:LYS:NZ	2.15	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: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:B:3320:LYS:HD3	1:B:3321:ASP:N	2.17	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:A:3049:ILE:HG22	1:A:3050:PHE:N	2.16	0.60
1:A:3205:ARG:NH1	1:A:3305:ARG:HD3	2.17	0.60
1:A:2979:ILE:HG22	1:A:3147:MET:HG2	1.83	0.60
1:A:3318:ILE:CG2	1:A:3319:GLY:N	2.65	0.60
1:A:3227:VAL:HG21	1:A:3262:PHE:HE2	1.65	0.60
1:A:2985:ARG:O	1:A:2989:ILE:HG23	2.02	0.60
1:B:3310:VAL:HG12	1:B:3311:PHE:N	2.17	0.59
1:B:3225:VAL:HA	1:B:3285:LYS:HA	1.84	0.59
1:B:3285:LYS:HG2	1:B:3294:ALA:HA	1.84	0.59
1:A:3225:VAL:HA	1:A:3285:LYS:HA	1.83	0.59
1:B:3227:VAL:HG21	1:B:3262:PHE:HE2	1.66	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:B:3336:ILE:HG22	1:B:3378:SER:CB	2.33	0.59
1:B:3307:ASN:CG	1:B:3308:ASN:H	2.03	0.59
1:A:3286:LYS:HE3	1:A:3291:GLU:OE2	2.02	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:3320:LYS:HD3	1:A:3321:ASP:H	1.67	0.59
1:A:2986:LEU:HD22	1:A:3154:PHE:CE1	2.37	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: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:3279:LYS:NZ	1:A:3280:PHE:H	2.00	0.58
1:A:3312:ASP:O	1:A:3313:ILE:O	2.21	0.58
1:A:2932:GLU:HG2	1:A:3001:HIS:CB	2.33	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:B:3320:LYS:HD3	1:B:3321:ASP:H	1.69	0.58
1:B:2962:CYS:HB2	1:B:2963:PRO:CD	2.28	0.58
1:A:2973:CYS:SG	1:A:3103:LEU:HD11	2.44	0.58
1:A:3224:VAL:HG22	1:A:3225:VAL:N	2.18	0.58
1:A:3218:GLY:HA2	1:A:3254:TRP:NE1	2.19	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:B:3312:ASP:O	1:B:3313:ILE:O	2.21	0.58
1:B:2950:GLU:HB3	1:B:3035:ARG:NH2	2.18	0.58
1:A:3226:LYS:HD2	1:A:3241:GLY:O	2.04	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: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:3038:ASN:ND2	1:A:3039:GLN:H	2.02	0.57
1:A:2991:PHE:CD2	1:A:3113:MET:HB3	2.38	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:3085:HIS:HB2	1:A:3119:LEU:HG	1.85	0.57
1:B:3384:TYR:O	1:B:3385:PHE:HB2	2.04	0.57
1:B:3055:PHE:HD2	1:B:3192:HIS:HE2	1.53	0.57
1:B:2932:GLU:HG2	1:B:3001:HIS:CB	2.34	0.57
1:A:3187:LEU:H	1:A:3187:LEU:HD23	1.69	0.57
1:A:3350:LEU:HG	1:A:3351:ASN:HD22	1.68	0.57
1:A:3336:ILE:HD12	1:A:3403:VAL:HG11	1.86	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:3336:ILE:HG22	1:A:3378:SER:HB3	1.85	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:2986:LEU:HD13	1:B:3154:PHE:CD1	2.39	0.57
1:A:2917:LEU:HD11	1:A:3002:LEU:C	2.25	0.57
1:B:3205:ARG:HH12	1:B:3305:ARG:NH1	2.03	0.57
1:B:3318:ILE:CG2	1:B:3319:GLY:N	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2985:ARG:O	1:B:2989:ILE:HG23	2.04	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:3325:PRO:CB	1:B:3326:PRO:HD2	2.35	0.57
1:B:3307:ASN:CG	1:B:3308:ASN:N	2.57	0.57
1:B:3049:ILE:HG22	1:B:3050:PHE: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:3051:GLN:HG3	1:A:3052:GLN:N	2.20	0.57
1:A:3330:VAL:HG12	1:A:3331:LYS:H	1.69	0.56
1:A:3120:ASP:O	1:A:3124:ILE:HG12	2.05	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:N	1:B:3312:ASP:OD2	2.38	0.56
1:A:3034:ILE:HB	1:A:3038:ASN:O	2.04	0.56
1:A:3297:LEU:HB2	1:A:3299:ALA:N	2.19	0.56
1:A:3258:ARG:HH11	1:A:3330:VAL:HG21	1.71	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:B:2960:ASN:HB3	1:B:2970:TYR:C	2.25	0.56
1:A:3121:LYS:O	1:A:3125:ILE:HG23	2.06	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:3388:ALA:CB	1:B:3394:CYS:HA	2.35	0.56
1:B:3372:GLU:HG3	1:B:3386:MET:HG2	1.86	0.56
1:B:2991:PHE:CG	1:B:3113:MET:HB3	2.41	0.56
1:A:2921:ASN:ND2	1:A:2922:ILE:H	2.04	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:2991:PHE:CG	1:A:3113:MET:HB3	2.41	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:3224:VAL:HG22	1:B:3225:VAL:N	2.21	0.55
1:B:3037:ILE:HG13	1:B:3037:ILE:O	2.06	0.55
1:A:3336:ILE:HD11	1:A:3403:VAL:HG21	1.87	0.55
1:B:3351:ASN:CB	1:B:3371:PHE:HB3	2.36	0.55
1:A:2917:LEU:HD12	1:A:2918:VAL:N	2.18	0.55
1:B:2992:GLU:HB2	1:B:3004:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3008:ASP:O	1:B:3011:GLN:HG2	2.06	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:B:3301:ILE:HG22	1:B:3315:GLU:OE2	2.05	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:A:3311:PHE:HD2	1:A:3331:LYS:HZ1	1.54	0.55
1:B:3350:LEU:HG	1:B:3351:ASN:HD22	1.71	0.55
1:B:3154:PHE:HA	1:B:3159:VAL:HG21	1.88	0.55
1:B:3312:ASP:O	1:B:3334:THR:HA	2.07	0.55
1:B:3231:SER:OG	1:B:3236:ASP:HB2	2.07	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:B:3350:LEU:HD23	1:B:3351:ASN:O	2.07	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:A:3222:THR:OG1	1:A:3246:LEU:HA	2.06	0.55
1:B:3287:TYR:CG	1:B:3288:ASP:N	2.75	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:3318:ILE:HG13	1:B:3339:MET:CG	2.37	0.54
1:B:3301:ILE:HG21	1:B:3327:LYS:HE3	1.89	0.54
1:B:3223:ALA:HB1	1:B:3286:LYS:O	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:3133:ARG:O	1:A:3134:VAL:HG12	2.07	0.54
1:A:2921:ASN:ND2	1:A:2922:ILE:N	2.56	0.54
1:B:3353:GLY:O	1:B:3354:SER:HB2	2.08	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: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:3348:PRO:HB2	1:A:3389:SER:OG	2.08	0.54
1:A:3013:ILE:O	1:A:3049:ILE:HG23	2.07	0.54
1:A:3210:VAL:O	1:A:3264:ILE:HD13	2.07	0.54
1:A:3039:GLN:HG3	1:A:3098:TYR:CE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3323:ASN:O	1:A:3324:LEU:HB3	2.08	0.54
1:A:3087:GLU:O	1:A:3091:LEU:HD22	2.07	0.54
1:B:3350:LEU:HD21	1:B:3353:GLY:N	2.23	0.54
1:B:3013:ILE:CD1	1:B:3013:ILE:H	2.16	0.54
1:A:3008:ASP:O	1:A:3011:GLN:HG2	2.08	0.54
1:A:3350:LEU:HG	1:A:3351:ASN:ND2	2.23	0.54
1:B:3348:PRO:HB2	1:B:3389:SER:HB3	1.90	0.54
1:B:2992:GLU:HB2	1:B:3004:ILE:CG1	2.38	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:B:3177:SER:C	1:B:3179:ARG:H	2.11	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:A:3030:PHE:C	1:A:3031:LYS:HG2	2.28	0.53
1:B:3258:ARG:HH11	1:B:3330:VAL:HG21	1.73	0.53
1:B:3327:LYS:NZ	1:B:3401:ILE:HG21	2.23	0.53
1:B:3091:LEU:N	1:B:3091:LEU:HD13	2.24	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:A:3229:ILE:HA	1:A:3281:ARG:HB2	1.89	0.53
1:B:3013:ILE:CD1	1:B:3049:ILE:HA	2.35	0.53
1:B:3103:LEU:HD22	1:B:3247:GLY:HA2	1.90	0.53
1:B:3051:GLN:HG3	1:B:3052:GLN:N	2.22	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:B:3281:ARG:O	1:B:3281:ARG:HD2	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:3062:PHE:CE1	1:A:3066:LEU:HD22	2.43	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:A:3013:ILE:HD13	1:A:3049:ILE:HD13	1.90	0.53
1:B:3030:PHE:C	1:B:3031:LYS:HG2	2.27	0.53
1:A:3006:TYR:HE2	1:A:3185:ASP:OD1	1.91	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:3318:ILE:HG13	1:A:3339:MET:CB	2.39	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:2964:GLU:HG2	1:A:3156:TYR:CE1	2.44	0.53
1:B:3038:ASN:ND2	1:B:3039:GLN:H	2.07	0.53
1:A:3138:HIS:CG	1:A:3139:ALA:H	2.27	0.53
1:B:3348:PRO:HB2	1:B:3389:SER:OG	2.09	0.52
1:B:3307:ASN:O	1:B:3308:ASN:C	2.46	0.52
1:B:2930:ALA:HB1	1:B:2934:ARG:NH1	2.24	0.52
1:A:3312:ASP:O	1:A:3334:THR:HA	2.09	0.52
1:B:3062:PHE:CE1	1:B:3066:LEU:HD22	2.45	0.52
1:B:2960:ASN:HB3	1:B:2970:TYR:N	2.24	0.52
1:A:2985:ARG:HH12	1:A:3124:ILE:CD1	2.17	0.52
1:B:3187:LEU:HD23	1:B:3187:LEU:N	2.23	0.52
1:B:3336:ILE:HD12	1:B:3403:VAL:HG11	1.91	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:A:3326:PRO:HG3	1:B:3356:THR:HB	1.91	0.52
1:A:2992:GLU:HB2	1:A:3004:ILE:HG12	1.91	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:3086:ASN:OD1	1:A:3246:LEU:HD22	2.10	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:A:2930:ALA:HB1	1:A:2934:ARG:NH1	2.24	0.52
1:B:3314:ILE:CG2	1:B:3316:ILE:HD11	2.40	0.52
1:A:3305:ARG:HG3	1:A:3313:ILE:CD1	2.39	0.52
1:B:3350:LEU:HG	1:B:3351:ASN:ND2	2.24	0.52
1:A:2919:ARG:NH2	1:A:2989:ILE:HG22	2.25	0.52
1:B:3328:VAL:HG13	1:B:3404:HIS:HB3	1.91	0.52
1:B:2991:PHE:HB2	1:B:3113:MET:SD	2.50	0.52
1:A:2937:LEU:CG	1:A:2941:GLN:HE21	2.21	0.52
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:3223:ALA:HB1	1:A:3286:LYS:O	2.10	0.51
1:A:3111:TYR:O	1:A:3114:ILE:HG13	2.10	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:3037:ILE:O	1:A:3037:ILE:HG13	2.09	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:3317:PRO:CG	1:B:3338:PHE:HA	2.38	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:3348:PRO:HA	1:B:3368:PHE:CZ	2.45	0.51
1:B:3154:PHE:HA	1:B:3159:VAL:CG2	2.40	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:A:2979:ILE:CG2	1:A:3147:MET:HG2	2.41	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:3086:ASN:CG	1:A:3246:LEU:HD13	2.30	0.51
1:A:3351:ASN:CG	1:A:3352:LEU:H	2.14	0.51
1:A:3325:PRO:HA	1:A:3400:ARG:NH2	2.26	0.51
1:A:2937:LEU:HG	1:A:2941:GLN:NE2	2.23	0.51
1:B:3059:SER:O	1:B:3060:SER:HB2	2.11	0.51
1:A:3328:VAL:HG13	1:A:3404:HIS:HB3	1.93	0.51
1:B:3349:MET:O	1:B:3350:LEU:C	2.49	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:B:2985:ARG:HH12	1:B:3124:ILE:CD1	2.17	0.51
1:A:3227:VAL:HG21	1:A:3262:PHE:CE2	2.45	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:3383:ASP:CG	1:A:3402:HIS:HE2	2.14	0.50
1:A:3061:ILE:CG2	1:A:3062:PHE:H	2.07	0.50
1:A:2986:LEU:HD22	1:A:3154:PHE:HE1	1.76	0.50
1:A:2918:VAL:HG23	1:A:3183:LYS:O	2.11	0.50
1:A:3034:ILE:HD13	1:A:3039:GLN:O	2.11	0.50
1:B:3159:VAL:HG13	1:B:3161:ASN:N	2.24	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:3209:ARG:HB2	1:B:3211:PHE:HE1	1.76	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:A:2921:ASN:HD22	1:A:2922:ILE:N	2.07	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:2992:GLU:HB2	1:A:3004:ILE:CG1	2.42	0.50
1:A:2980:PHE:CE2	1:A:3082:GLU:HG3	2.47	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:B:2918:VAL:HG23	1:B:3183:LYS:O	2.11	0.50
1:A:3091:LEU:H	1:A:3091:LEU:HD22	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:3279:LYS:NZ	1:A:3280:PHE:N	2.59	0.50
1:B:3046:ASN:ND2	1:B:3047:GLU:N	2.58	0.50
1:A:3150:PRO:HB2	1:A:3155:ASN:HD22	1.75	0.50
1:A:3198:GLU:HA	1:A:3201:LEU:HD12	1.94	0.49
1:A:3397:ASN:HD22	1:A:3397:ASN:C	2.16	0.49
1:A:3357:ALA:HA	1:B:3325:PRO:CB	2.42	0.49
1:A:3273:LEU:CD2	1:A:3279:LYS:HD2	2.42	0.49
1:A:3091:LEU:HD13	1:A:3091:LEU:N	2.26	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: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:B:3226:LYS:HD2	1:B:3241:GLY:O	2.12	0.49
1:B:3351:ASN:HB2	1:B:3371:PHE:HD2	1.77	0.49
1:B:3325:PRO:HA	1:B:3400:ARG:NH2	2.27	0.49
1:A:3187:LEU:N	1:A:3187:LEU:HD23	2.27	0.49
1:B:3138:HIS:CD2	1:B:3139:ALA:H	2.31	0.49
1:A:3372:GLU:HG3	1:A:3386:MET:HG2	1.94	0.49
1:A:3307:ASN:O	1:A:3308:ASN:C	2.50	0.49
1:A:3351:ASN:HD22	1:A:3351:ASN:N	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:B:3370:ALA:O	1:B:3371:PHE:HB2	2.12	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:A:2991:PHE:HB2	1:A:3113:MET:SD	2.52	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:3209:ARG:HB2	1:A:3211:PHE:HE1	1.78	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:3325:PRO:HA	1:B:3400:ARG:CZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3046:ASN:HD22	1:B:3047:GLU:H	1.61	0.49
1:A:3226:LYS:HE2	1:A:3239:TYR:CD2	2.48	0.49
1:A:3138:HIS:CD2	1:A:3139:ALA:H	2.31	0.49
1:A:3079:VAL:O	1:A:3083:ILE:HG12	2.12	0.49
1:A:3059:SER:O	1:A:3060:SER:HB2	2.13	0.49
1:A:3370:ALA:O	1:A:3371:PHE:HB2	2.12	0.49
1:A:2952:ILE:HD12	1:A:2990:GLN:HG3	1.93	0.49
1:A:3298:PRO:O	1:A:3299:ALA:C	2.51	0.49
1:A:3325:PRO:HA	1:A:3400:ARG:HH22	1.78	0.48
1:B:3387:THR:HG23	1:B:3388:ALA:N	2.27	0.48
1:B:2962:CYS:CB	1:B:2963:PRO:HD3	2.36	0.48
1:A:3154:PHE:HA	1:A:3159:VAL:CG2	2.42	0.48
1:A:2974:VAL:HG13	1:A:2977:MET:HG3	1.94	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: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: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:3214:PHE:HB3	1:A:3216:LEU:CD2	2.43	0.48
1:A:2981:PRO:HB3	1:A:3081:TYR:CE2	2.47	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:3174:VAL:O	1:A:3174:VAL:HG12	2.14	0.48
1:A:3202:ARG:O	1:A:3206:LEU:HG	2.13	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:A:3096:GLU:CB	1:A:3099:SER:HB3	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3098:TYR:CD2	1:A:3098:TYR:N	2.80	0.48
1:B:3350:LEU:CD2	1:B:3351:ASN:H	2.19	0.48
1:B:3225:VAL:HG11	1:B:3243:PHE:CE1	2.49	0.48
1:A:2980:PHE:N	1:A:2981:PRO:HD2	2.29	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:3069:LEU:CD2	1:B:3126:TRP:HB2	2.44	0.47
1:B:3038:ASN:O	1:B:3039:GLN:HB2	2.13	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:3337:MET:CG	1:A:3338:PHE:H	2.27	0.47
1:A:3317:PRO:CG	1:A:3338:PHE:HA	2.41	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:3279:LYS:NZ	1:B:3280:PHE:N	2.62	0.47
1:B:2958:TYR:OH	1:B:3250:LYS:HD3	2.13	0.47
1:A:3368:PHE:O	1:A:3370:ALA:N	2.46	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:B:3363:VAL:HG13	1:B:3391:THR:HG22	1.97	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:3227:VAL:HG23	1:A:3240:ALA:HB3	1.96	0.47
1:A:3214:PHE:HB3	1:A:3216:LEU:HD22	1.96	0.47
1:A:2935:ASP:O	1:A:2939:LYS:HG3	2.14	0.47
1:B:3273:LEU:CD2	1:B:3279:LYS:HD2	2.43	0.47
1:B:2962:CYS:SG	1:B:2970:TYR:O	2.73	0.47
1:A:3159:VAL:CG2	1:A:3160:ASN:H	2.19	0.47
1:B:3311:PHE:HD2	1:B:3331:LYS:HZ1	1.62	0.47
1:A:3280:PHE:CZ	1:A:3300:PRO:HD2	2.49	0.47
1:A:3188:ASN:ND2	1:A:3193:ASN:HA	2.30	0.47
1:A:2958:TYR:CD2	1:A:2959:PRO:HA	2.50	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:3114:ILE:HG13	1:A:3115:HIS:N	2.28	0.47
1:B:3347:THR:N	1:B:3348:PRO:CD	2.76	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:A:3348:PRO:HA	1:A:3368:PHE:HZ	1.80	0.47
1:A:3397:ASN:CG	1:A:3399:LEU:HG	2.35	0.47
1:B:2941:GLN:NE2	1:B:3028:PRO:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2984:HIS:O	1:A:2988:THR:HG22	2.15	0.47
1:B:2919:ARG:NH2	1:B:2989:ILE:HG22	2.29	0.47
1:A:3276:ASP:CG	1:A:3375:LYS:HE2	2.35	0.47
1:B:3202:ARG:O	1:B:3206:LEU:HG	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: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:A:3321:ASP:H	1:A:3397:ASN:CB	2.28	0.46
1:B:3210:VAL:CG1	1:B:3265:THR:HA	2.41	0.46
1:A:3069:LEU:CD2	1:A:3126:TRP:HB2	2.45	0.46
1:B:3170:LEU:HD12	1:B:3172:ASN:HB2	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:3088:VAL:HA	1:A:3091:LEU:HD23	1.97	0.46
1:A:3322:VAL:HG22	1:A:3324:LEU:CD2	2.45	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:A:3121:LYS:HE2	1:A:3186:ASN:O	2.16	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:2980:PHE:CE2	1:B:3082:GLU:HG3	2.50	0.46
1:B:3039:GLN:HG3	1:B:3098:TYR:CE1	2.50	0.46
1:A:3201:LEU:O	1:A:3205:ARG:HG2	2.16	0.46
1:A:3391:THR:O	1:A:3394:CYS:HB3	2.16	0.46
1:B:3302:ILE:HG23	1:B:3316:ILE:HB	1.98	0.46
1:B:2996:LYS:NZ	1:B:3001:HIS:HA	2.31	0.46
1:A:3229:ILE:HG21	1:A:3271:LEU:HD11	1.97	0.46
1:B:3034:ILE:O	1:B:3035:ARG:HB3	2.16	0.46
1:A:2981:PRO:HB2	1:A:3123:TRP:CZ3	2.51	0.46
1:B:3114:ILE:HG13	1:B:3115:HIS:N	2.31	0.46
1:B:3296:VAL:O	1:B:3296:VAL:HG22	2.15	0.46
1:A:3354:SER:HB3	1:A:3358:MET:HB3	1.98	0.46
1:B:3397:ASN:C	1:B:3397:ASN:HD22	2.15	0.46
1:B:3009:TRP:CZ3	1:B:3061:ILE:HD11	2.51	0.46
1:B:2962:CYS:CB	1:B:2963:PRO:CD	2.93	0.46
1:A:2986:LEU:HD11	1:A:3169:SER:HA	1.98	0.46
1:B:2917:LEU:O	1:B:3182:TYR:HA	2.16	0.46
1:B:3307:ASN:O	1:B:3310:VAL:HG22	2.16	0.46
1:B:3090:ALA:O	1:B:3094:GLY:N	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3296:VAL:O	1:A:3296:VAL:HG22	2.15	0.46
1:A:3044:ASP:O	1:A:3094:GLY:HA3	2.16	0.46
1:A:3070:GLU:OE2	1:A:3209:ARG:NH2	2.45	0.46
1:A:3065:ALA:HA	1:A:3084:LEU:HG	1.96	0.46
1:B:2918:VAL:O	1:B:3003:GLY:N	2.43	0.46
1:A:3125:ILE:HG13	1:A:3126:TRP:N	2.31	0.46
1:A:2962:CYS:CB	1:A:2963:PRO:CD	2.94	0.46
1:B:2969:LYS:O	1:B:2970:TYR:CB	2.50	0.46
1:B:3013:ILE:HD13	1:B:3049:ILE:HD13	1.98	0.46
1:A:3210:VAL:CG1	1:A:3265:THR:HA	2.40	0.46
1:B:3096:GLU:CB	1:B:3099:SER:HB3	2.45	0.46
1:A:2950:GLU:HB3	1:A:3032:TYR:OH	2.15	0.46
1:B:3034:ILE:HD13	1:B:3039:GLN:O	2.15	0.46
1:B:3170:LEU:HD13	1:B:3172:ASN:H	1.80	0.46
1:B:2974:VAL:HG13	1:B:2977:MET:HG3	1.98	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:3310:VAL:HG12	1:A:3311:PHE:H	1.80	0.45
1:A:3305:ARG:HG3	1:A:3313:ILE:HD11	1.99	0.45
1:B:3363:VAL:HG23	1:B:3364:PRO:HD2	1.98	0.45
1:A:3058:PHE:HB3	1:A:3062:PHE:CD1	2.52	0.45
1:A:2960:ASN:HB3	1:A:2970:TYR:H	1.81	0.45
1:A:3271:LEU:HD13	1:A:3273:LEU:HD13	1.97	0.45
1:B:2958:TYR:CD2	1:B:2959:PRO:HA	2.51	0.45
1:A:3356:THR:HB	1:B:3326:PRO:CG	2.47	0.45
1:B:3321:ASP:H	1:B:3397:ASN:CB	2.29	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:A:3152:HIS:HD2	1:A:3155:ASN:HD21	1.62	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:A:2917:LEU:O	1:A:3182:TYR:HA	2.17	0.45
1:B:3049:ILE:CG2	1:B:3050:PHE:H	2.23	0.45
1:B:3125:ILE:HG13	1:B:3126:TRP:N	2.31	0.45
1:B:3121:LYS:HE2	1:B:3186:ASN:O	2.16	0.45
1:B:2935:ASP:O	1:B:2939:LYS:HG3	2.15	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:A:3327:LYS:HZ3	1:A:3401:ILE:HG21	1.79	0.45

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3043:ARG:NE	1:A:3109:ASP:OD2	2.50	0.44
1:A:2958:TYR:OH	1:A:3250:LYS:HD3	2.18	0.44
1:A:3170:LEU:HD13	1:A:3172:ASN:H	1.82	0.44
1:A:3029:PHE:O	1:A:3110:PRO:HB2	2.17	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:3348:PRO:HA	1:B:3368:PHE:HZ	1.82	0.44
1:A:2996:LYS:HA	1:A:3000:SER:CB	2.33	0.44
1:B:3205:ARG:HH22	1:B:3305:ARG:NH1	2.16	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: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:B:3159:VAL:C	1:B:3161:ASN:H	2.21	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: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: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:3245:ILE:N	1:A:3245:ILE:HD12	2.32	0.44
1:A:3318:ILE:HG23	1:A:3319:GLY:H	1.83	0.44
1:A:3243:PHE:CE1	1:A:3245:ILE:HD11	2.52	0.44
1:A:3038:ASN:CG	1:A:3039:GLN:N	2.69	0.44
1:B:3107:ALA:HA	1:B:3112:PHE:CD1	2.53	0.44
1:B:3085:HIS:NE2	1:B:3089:HIS:NE2	2.65	0.44
1:B:2930:ALA:CB	1:B:2934:ARG:HH12	2.30	0.44
1:A:3334:THR:HG22	1:A:3335:LYS:N	2.33	0.44
1:B:3314:ILE:HG13	1:B:3335:LYS:HD2	1.99	0.44
1:B:3072:ASP:O	1:B:3073:ASN:HB3	2.18	0.44
1:A:2991:PHE:CD1	1:A:3113:MET:SD	3.11	0.44
1:A:2930:ALA:HB1	1:A:2934:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2965:LYS:HD2	1:A:2965:LYS:HA	1.75	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:3205:ARG:HB3	1:A:3310:VAL:HG21	2.00	0.43
1:A:2960:ASN:OD1	1:A:2971:PRO:HG3	2.18	0.43
1:B:3305:ARG:HG3	1:B:3313:ILE:CD1	2.48	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:A:3185:ASP:OD1	1:A:3185:ASP:N	2.51	0.43
1:A:3054:LYS:HB2	1:A:3190:HIS:NE2	2.33	0.43
1:A:2941:GLN:NE2	1:A:3028:PRO:HB2	2.33	0.43
1:B:3088:VAL:HA	1:B:3091:LEU:HD23	2.00	0.43
1:A:3170:LEU:CD1	1:A:3172:ASN:H	2.31	0.43
1:A:3258:ARG:CD	1:A:3330:VAL:HG21	2.49	0.43
1:B:3271:LEU:HD13	1:B:3273:LEU:HD13	2.00	0.43
1:B:3285:LYS:NZ	1:B:3285:LYS:HB2	2.34	0.43
1:B:3069:LEU:HA	1:B:3126:TRP:HD1	1.82	0.43
1:B:3091:LEU:H	1:B:3091:LEU:HD22	1.83	0.43
1:A:3351:ASN:HB2	1:A:3371:PHE:CD2	2.53	0.43
1:A:3327:LYS:O	1:A:3403:VAL:HA	2.18	0.43
1:A:3129:LEU:HD22	1:A:3133:ARG:NH2	2.33	0.43
1:B:3227:VAL:HG23	1:B:3240:ALA:HB3	2.00	0.43
1:A:3088:VAL:HG11	1:A:3115:HIS:CE1	2.53	0.43
1:A:3215:VAL:HG21	1:A:3324:LEU:CB	2.47	0.43
1:A:3337:MET:HG2	1:A:3338:PHE:H	1.83	0.43
1:B:3368:PHE:O	1:B:3370:ALA:N	2.49	0.43
1:A:3054:LYS:HD3	1:A:3055:PHE:HB2	1.99	0.43
1:B:3176:ASP:HB3	1:B:3179:ARG:HD3	2.01	0.43
1:A:3287:TYR:HB2	1:A:3292:LEU:HD23	2.01	0.43
1:A:2965:LYS:O	1:A:2965:LYS:HG3	2.18	0.43
1:B:2925:LEU:HD23	1:B:2929:GLU:HB2	2.00	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: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:3186:ASN:ND2	1:A:3188:ASN:H	2.16	0.43
1:B:3058:PHE:HB3	1:B:3062:PHE:CD1	2.54	0.43
1:A:2975:HIS:NE2	1:A:2984:HIS:CE1	2.86	0.43
1:B:3205:ARG:NH1	1:B:3305:ARG:HD3	2.33	0.43
1:A:3231:SER:HB3	1:A:3236:ASP:O	2.19	0.43
1:A:3006:TYR:HB2	1:A:3118:SER:HA	2.01	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:B:3354:SER:HB3	1:B:3358:MET:CB	2.49	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:A:3079:VAL:HG13	1:A:3256:TYR:CE2	2.54	0.42
1:A:3335:LYS:HZ3	1:A:3335:LYS:HB2	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: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:3069:LEU:HA	1:A:3126:TRP:CD1	2.54	0.42
1:B:3249:ALA:O	1:B:3250:LYS:CB	2.66	0.42
1:B:3327:LYS:O	1:B:3403:VAL:HA	2.20	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: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:3346:THR:OG1	1:B:3348:PRO:HD3	2.20	0.42
1:B:3325:PRO:CA	1:B:3400:ARG:HH22	2.32	0.42
1:A:2989:ILE:HD11	1:A:3165:THR:HG22	2.00	0.42
1:B:3194:ILE:HG12	1:B:3195:GLU:H	1.83	0.42
1:B:3006:TYR:HB2	1:B:3118:SER:HA	2.00	0.42
1:A:2965:LYS:NZ	1:A:2967:ASP:HB3	2.34	0.42
1:B:2965:LYS:HA	1:B:2965:LYS:HD2	1.69	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:3325:PRO:CA	1:A:3400:ARG:HH22	2.32	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:3159:VAL:HG13	1:A:3161:ASN:N	2.24	0.42
1:B:3222:THR:HA	1:B:3245:ILE:O	2.19	0.42
1:A:3218:GLY:HA2	1:A:3254:TRP:CE2	2.55	0.42
1:B:3059:SER:O	1:B:3060:SER:CB	2.68	0.42
1:B:3029:PHE:O	1:B:3110:PRO:HB2	2.19	0.42
1:A:2990:GLN:NE2	1:A:3165:THR:HG21	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3038:ASN:CG	1:B:3039:GLN:N	2.70	0.42
1:A:3059:SER:O	1:A:3060:SER:CB	2.67	0.42
1:A:3358:MET:HE3	1:B:3253:PRO:HB3	2.02	0.42
1:B:3337:MET:HG2	1:B:3338:PHE:H	1.84	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:A:3248:GLY:O	1:A:3251:GLU:HG2	2.19	0.41
1:A:2956:HIS:HB3	1:A:3107:ALA:HB2	2.02	0.41
1:B:3243:PHE:CE1	1:B:3245:ILE:HD11	2.55	0.41
1:B:3226:LYS:HD2	1:B:3242:SER:HB3	2.02	0.41
1:A:3068:ALA:O	1:A:3077:PHE:HD1	2.03	0.41
1:B:3348:PRO:CB	1:B:3389:SER:HB3	2.49	0.41
1:A:2961:LEU:HB2	1:A:2962:CYS:H	1.60	0.41
1:B:2996:LYS:CA	1:B:3000:SER:HB3	2.36	0.41
1:A:3277:HIS:O	1:A:3279:LYS:N	2.53	0.41
1:B:3245:ILE:N	1:B:3245:ILE:HD12	2.34	0.41
1:A:3081:TYR:CE1	1:A:3119:LEU:HD22	2.56	0.41
1:A:3031:LYS:HB3	1:A:3031:LYS:HE2	1.94	0.41
1:B:3289:HIS:N	1:B:3289:HIS:ND1	2.68	0.41
1:A:3348:PRO:CB	1:A:3389:SER:HB3	2.49	0.41
1:B:3277:HIS:O	1:B:3279:LYS:N	2.53	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:A:3074:TYR:HA	1:A:3077:PHE:HB3	2.02	0.41
1:B:3257:GLU:HG3	1:B:3257:GLU:H	1.48	0.41
1:A:3327:LYS:HZ2	1:A:3401:ILE:HG21	1.83	0.41
1:A:3009:TRP:CZ3	1:A:3061:ILE:HD11	2.54	0.41
1:B:3193:ASN:HB3	1:B:3196:GLU:HG3	2.02	0.41
1:A:3092:ILE:N	1:A:3092:ILE:HD12	2.35	0.41
1:A:3072:ASP:HB2	1:A:3311:PHE:HE2	1.80	0.41
1:B:3350:LEU:HD22	1:B:3387:THR:CB	2.44	0.41
1:A:2983:TRP:HD1	1:A:3151:LEU:HB3	1.85	0.41
1:A:3103:LEU:HD22	1:A:3247:GLY:CA	2.47	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:A:3083:ILE:HG21	1:A:3260:TYR:CZ	2.56	0.41
1:A:3276:ASP:OD1	1:A:3375:LYS:HE2	2.21	0.41
1:A:3364:PRO:HA	1:A:3365:PRO:HD3	1.87	0.41
1:B:3207:LYS:N	1:B:3307:ASN:HB2	2.36	0.41
1:A:3229:ILE:HD13	1:A:3281:ARG:HB3	2.01	0.41
1:B:3185:ASP:N	1:B:3185:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3079:VAL:HG11	1:A:3260:TYR:HA	2.01	0.41
1:B:3220:ARG:HA	1:B:3251:GLU:HG2	2.02	0.41
1:A:3314:ILE:HG13	1:A:3335:LYS:HD2	2.03	0.41
1:B:3391:THR:O	1:B:3394:CYS:HB3	2.20	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:2956:HIS:CD2	1:A:2973:CYS:HB2	2.56	0.41
1:B:2990:GLN:NE2	1:B:3165:THR:HG21	2.36	0.41
1:B:3177:SER:C	1:B:3179:ARG:N	2.73	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:A:3098:TYR:HD2	1:A:3098:TYR:N	2.19	0.41
1:B:3098:TYR:N	1:B:3098:TYR:HD2	2.19	0.41
1:B:3081:TYR:CE1	1:B:3119:LEU:HD22	2.56	0.41
1:B:3081:TYR:CE2	1:B:3119:LEU:HD13	2.56	0.41
1:A:3085:HIS:NE2	1:A:3089:HIS:NE2	2.69	0.41
1:B:3231:SER:HB3	1:B:3236:ASP:O	2.21	0.41
1:A:3090:ALA:O	1:A:3094:GLY:N	2.42	0.41
1:B:3332:ARG:HB3	1:B:3406:ASP:OD1	2.21	0.41
1:A:3397:ASN:HD21	1:A:3399:LEU:HG	1.81	0.41
1:A:3220:ARG:HA	1:A:3251:GLU:HG2	2.03	0.41
1:B:3351:ASN:HB2	1:B:3371:PHE:CD2	2.55	0.41
1:B:3347:THR:OG1	1:B:3374:GLY:N	2.54	0.41
1:A:3049:ILE:CG2	1:A:3050:PHE:H	2.21	0.41
1:A:3264:ILE:H	1:A:3264:ILE:HD13	1.86	0.41
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:3380:GLU:HG2	1:B:3381:SER:N	2.37	0.40
1:A:2990:GLN:NE2	1:A:3160:ASN:ND2	2.69	0.40
1:B:3258:ARG:NH1	1:B:3330:VAL:HG11	2.36	0.40
1:B:3069:LEU:HA	1:B:3126:TRP:CD1	2.55	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:B:2990:GLN:NE2	1:B:3160:ASN:ND2	2.70	0.40
1:A:3289:HIS:ND1	1:A:3289:HIS:N	2.69	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:3365:PRO:O	1:B:3367:SER:N	2.54	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: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:A:2953:ALA:HB1	1:A:3108:PHE:HA	2.01	0.40
1:A:3258:ARG:NH1	1:A:3330:VAL:HG11	2.37	0.40
1:B:3364:PRO:HB2	1:B:3367:SER:HB3	2.04	0.40
1:A:2952:ILE:O	1:A:2987:HIS:HE1	2.03	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:2956:HIS:NE2	1:B:2973:CYS:SG	2.93	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: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
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:B:3157:GLU:OE2	1:B:3157:GLU:HA	2.21	0.40
1:B:3043:ARG:HB3	1:B:3092:ILE:O	2.21	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%)	1	16
1	B	489/491 (100%)	342 (70%)	101 (21%)	46 (9%)	1	16
All	All	978/982 (100%)	683 (70%)	203 (21%)	92 (9%)	1	16

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%)	4	29
1	B	437/437 (100%)	376 (86%)	61 (14%)	4	29
All	All	874/874 (100%)	752 (86%)	122 (14%)	4	29

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

Some 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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	491/491 (100%)	-0.27	7 (1%)	78	68	57, 135, 209, 279	0
1	B	491/491 (100%)	-0.29	7 (1%)	78	68	58, 134, 208, 279	0
All	All	982/982 (100%)	-0.28	14 (1%)	78	68	57, 135, 209, 279	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3055	PHE	4.1
1	B	3054	LYS	3.7
1	B	3055	PHE	3.4
1	B	3052	GLN	3.0
1	A	2967	ASP	2.7
1	A	3137	ALA	2.7
1	B	3138	HIS	2.5
1	A	3136	PRO	2.4
1	A	2966	GLY	2.2
1	B	3137	ALA	2.2
1	B	3140	GLY	2.2
1	B	3139	ALA	2.2
1	A	3276	ASP	2.2
1	A	3056	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	CU	B	3408	1/1	0.98	0.17	-1.06	74,74,74,74	0
2	CU	A	3408	1/1	0.95	0.13	-1.83	86,86,86,86	0
2	CU	B	3407	1/1	0.98	0.15	-2.15	79,79,79,79	0
2	CU	A	3407	1/1	0.96	0.12	-2.31	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.