



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:35 PM GMT

PDB ID : 1KY4
Title : S-Adenosylhomocysteine hydrolase refined with noncrystallographic restraints
Authors : Takata, Y.; Takusagawa, F.
Deposited on : 2002-02-03
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

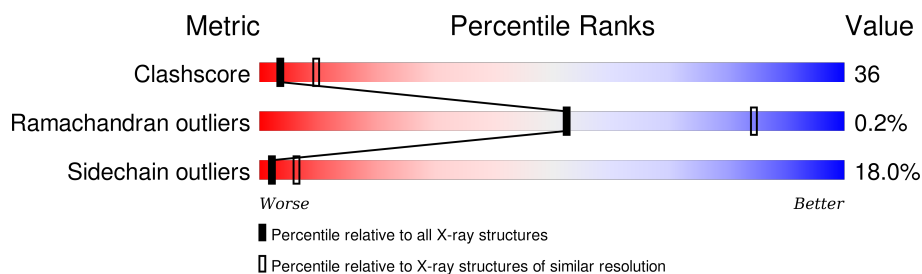
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	
1	B	431	
1	C	431	
1	D	431	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13650 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 S-adenosylhomocysteine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3302	2098	568	611	25			
1	B	428	Total	C	N	O	S	0	0	0
			3302	2098	568	611	25			
1	C	428	Total	C	N	O	S	0	0	0
			3302	2098	568	611	25			
1	D	428	Total	C	N	O	S	0	0	0
			3302	2098	568	611	25			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

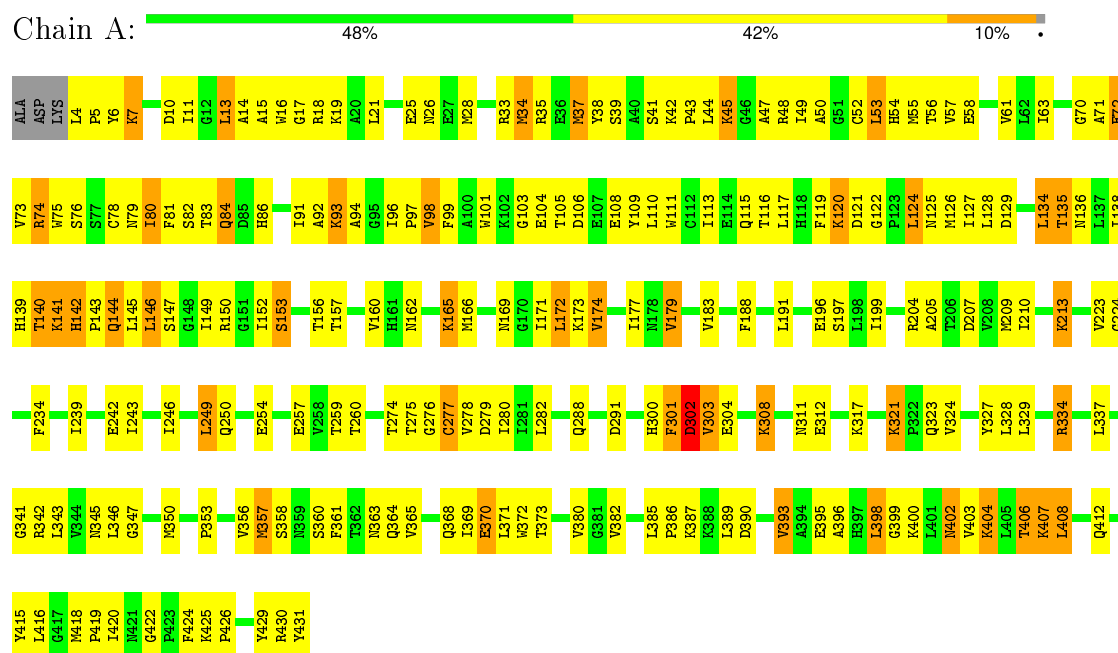
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	75	Total	O	0	0
			75	75		
3	C	60	Total	O	0	0
			60	60		
3	D	63	Total	O	0	0
			63	63		

3 Residue-property plots

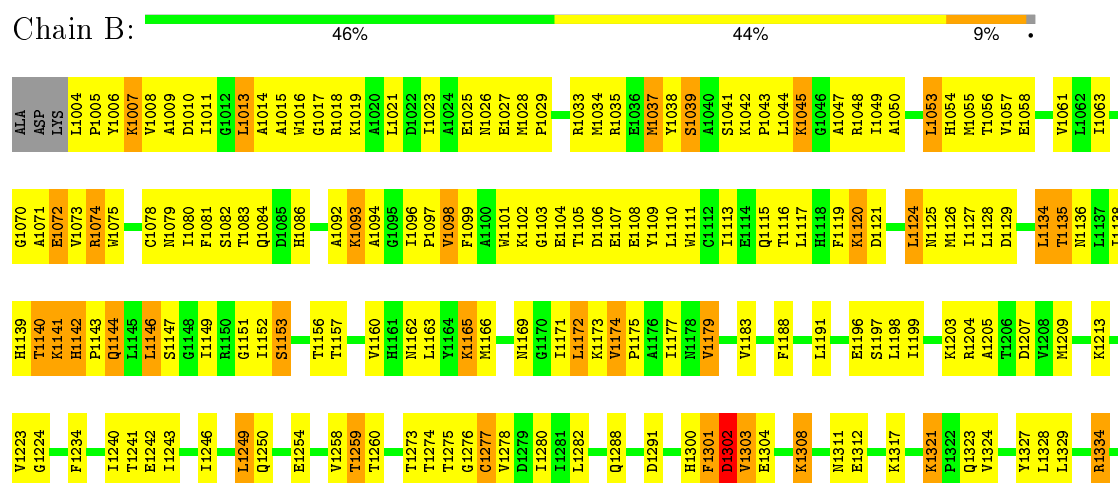
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: S-adenosylhomocysteine hydrolase



• Molecule 1: S-adenosylhomocysteine hydrolase





N3402	Q3412	Y3415	Y3429
V3403		L3416	R3430
K3404		G3417	Y3431
L3405		M3418	
T3406		P3419	
K3407		I3420	
L3408		N3421	
T3409		G3422	
		F3423	
		F3424	
		K3425	
		P3426	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.76 Å 134.48 Å 102.26 Å 90.00° 114.35° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.228 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13650	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

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: NAD

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	0.37	0/3367	0.63	1/4557 (0.0%)
1	B	0.37	0/3367	0.62	1/4557 (0.0%)
1	C	0.37	0/3367	0.62	1/4557 (0.0%)
1	D	0.37	0/3367	0.62	1/4557 (0.0%)
All	All	0.37	0/13468	0.62	4/18228 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3302	ASP	N-CA-C	5.47	125.76	111.00
1	A	302	ASP	N-CA-C	5.31	125.33	111.00
1	C	2302	ASP	N-CA-C	5.06	124.67	111.00
1	B	1302	ASP	N-CA-C	5.01	124.53	111.00

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	3302	0	3324	253	0
1	B	3302	0	3324	268	0
1	C	3302	0	3324	259	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3302	0	3324	266	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
3	A	68	0	0	2	0
3	B	75	0	0	8	0
3	C	60	0	0	2	0
3	D	63	0	0	10	0
All	All	13650	0	13400	968	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 36.

All (968) 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:C:2430:ARG:HB3	1:D:3430:ARG:HB3	1.25	1.15
1:A:430:ARG:HB3	1:B:1430:ARG:HB3	1.29	1.15
1:D:3370:GLU:HG3	1:D:3389:LEU:HD11	1.41	1.03
1:A:370:GLU:HG3	1:A:389:LEU:HD11	1.41	1.03
1:C:2370:GLU:HG3	1:C:2389:LEU:HD11	1.39	1.01
1:B:1370:GLU:HG3	1:B:1389:LEU:HD11	1.40	1.01
1:D:3275:THR:HG21	1:D:3280:ILE:HD11	1.47	0.97
1:A:275:THR:HG22	1:A:277:CYS:H	1.29	0.96
1:D:3143:PRO:HA	1:D:3146:LEU:HD23	1.45	0.96
1:C:2275:THR:HG22	1:C:2277:CYS:H	1.30	0.95
1:D:3275:THR:HG22	1:D:3277:CYS:H	1.29	0.95
1:A:143:PRO:HA	1:A:146:LEU:HD23	1.50	0.94
1:A:277:CYS:HB2	1:B:1416:LEU:HD21	1.51	0.93
1:C:2143:PRO:HA	1:C:2146:LEU:HD23	1.50	0.92
1:B:1275:THR:HG21	1:B:1280:ILE:HD11	1.52	0.92
1:B:1143:PRO:HA	1:B:1146:LEU:HD23	1.53	0.91
1:A:275:THR:HG21	1:A:280:ILE:HD11	1.53	0.90
1:B:1275:THR:HG22	1:B:1277:CYS:H	1.37	0.89
1:D:3275:THR:HG22	1:D:3277:CYS:N	1.88	0.88
1:A:275:THR:HG22	1:A:277:CYS:N	1.89	0.88
1:C:2275:THR:HG21	1:C:2280:ILE:HD11	1.56	0.87
1:C:2275:THR:HG22	1:C:2277:CYS:N	1.90	0.86
1:B:1057:VAL:H	1:B:1084:GLN:NE2	1.74	0.85
1:C:2057:VAL:H	1:C:2084:GLN:NE2	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1275:THR:HG22	1:B:1277:CYS:N	1.93	0.84
1:D:3321:LYS:HD3	1:D:3324:VAL:HG21	1.60	0.83
1:B:1010:ASP:HB3	1:B:1013:LEU:HD22	1.60	0.83
1:A:57:VAL:H	1:A:84:GLN:NE2	1.77	0.83
1:A:407:LYS:HE2	1:A:420:ILE:HG22	1.59	0.82
1:D:3057:VAL:H	1:D:3084:GLN:NE2	1.77	0.82
1:A:321:LYS:HD3	1:A:324:VAL:HG21	1.62	0.82
1:A:243:ILE:HG21	1:B:1408:LEU:HD13	1.59	0.82
1:C:2416:LEU:HD21	1:D:3277:CYS:HB2	1.62	0.82
1:D:3407:LYS:HE2	1:D:3420:ILE:HG22	1.60	0.82
1:A:224:GLY:N	1:A:274:THR:HG21	1.93	0.82
1:B:1105:THR:OG1	1:B:1108:GLU:HG3	1.80	0.81
1:D:3105:THR:OG1	1:D:3108:GLU:HG3	1.80	0.81
1:C:2105:THR:OG1	1:C:2108:GLU:HG3	1.81	0.80
1:D:3224:GLY:N	1:D:3274:THR:HG21	1.95	0.80
1:D:3120:LYS:HD2	1:D:3121:ASP:N	1.96	0.80
1:C:2010:ASP:HB3	1:C:2013:LEU:HD22	1.63	0.80
1:A:105:THR:OG1	1:A:108:GLU:HG3	1.81	0.80
1:D:3127:ILE:HD12	1:D:3149:ILE:HG21	1.64	0.79
1:C:2275:THR:CG2	1:C:2277:CYS:HB3	2.12	0.79
1:A:79:ASN:HB3	1:A:82:SER:OG	1.83	0.79
1:A:275:THR:CG2	1:A:277:CYS:HB3	2.11	0.79
1:A:120:LYS:HD2	1:A:121:ASP:N	1.97	0.79
1:B:1321:LYS:HD3	1:B:1324:VAL:HG21	1.65	0.79
1:D:3275:THR:CG2	1:D:3277:CYS:HB3	2.12	0.79
1:C:2021:LEU:O	1:C:2025:GLU:HG3	1.84	0.78
1:D:3018:ARG:HH21	1:D:3093:LYS:HZ1	1.31	0.78
1:C:2321:LYS:HD3	1:C:2324:VAL:HG21	1.66	0.78
1:D:3079:ASN:HB3	1:D:3082:SER:OG	1.85	0.77
1:B:1224:GLY:N	1:B:1274:THR:HG21	1.99	0.77
1:C:2127:ILE:HD12	1:C:2149:ILE:HG21	1.66	0.77
1:D:3018:ARG:HH21	1:D:3093:LYS:NZ	1.81	0.77
1:C:2129:ASP:OD2	1:C:2135:THR:HG23	1.85	0.77
1:A:125:ASN:O	1:A:126:MET:HE2	1.85	0.76
1:D:3010:ASP:HB3	1:D:3013:LEU:HD22	1.64	0.76
1:B:1275:THR:CG2	1:B:1277:CYS:HB3	2.15	0.76
1:A:10:ASP:HB3	1:A:13:LEU:HD22	1.65	0.76
1:C:2408:LEU:HD13	1:D:3243:ILE:HG21	1.67	0.76
1:A:416:LEU:HD21	1:B:1277:CYS:HB2	1.66	0.76
1:A:224:GLY:H	1:A:274:THR:HG21	1.49	0.76
1:D:3021:LEU:O	1:D:3025:GLU:HG3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2224:GLY:N	1:C:2274:THR:HG21	2.01	0.75
1:B:1120:LYS:HD2	1:B:1121:ASP:N	2.01	0.75
1:A:127:ILE:HD12	1:A:149:ILE:HG21	1.68	0.75
1:A:21:LEU:O	1:A:25:GLU:HG3	1.85	0.75
1:C:2407:LYS:HE2	1:C:2420:ILE:HG22	1.67	0.75
1:A:275:THR:HB	1:A:304:GLU:OE1	1.86	0.75
1:C:2079:ASN:HB3	1:C:2082:SER:OG	1.87	0.74
1:B:1407:LYS:HE2	1:B:1420:ILE:HG22	1.67	0.74
1:A:129:ASP:OD2	1:A:135:THR:HG23	1.87	0.74
1:A:18:ARG:HH21	1:A:93:LYS:NZ	1.83	0.74
1:C:2120:LYS:HD2	1:C:2121:ASP:N	2.01	0.74
1:D:3129:ASP:OD2	1:D:3135:THR:HG23	1.88	0.74
1:D:3224:GLY:H	1:D:3274:THR:HG21	1.53	0.73
1:B:1021:LEU:O	1:B:1025:GLU:HG3	1.88	0.73
1:C:2204:ARG:HH12	1:C:2350:MET:HG2	1.52	0.72
1:C:2028:MET:HE3	1:C:2357:MET:HB3	1.70	0.72
1:A:120:LYS:HD2	1:A:121:ASP:H	1.53	0.72
1:C:2125:ASN:O	1:C:2126:MET:HE2	1.90	0.72
1:D:3166:MET:HA	1:D:3171:ILE:HD12	1.70	0.72
1:B:1079:ASN:HB3	1:B:1082:SER:OG	1.90	0.71
1:C:2277:CYS:HB2	1:D:3416:LEU:HD21	1.72	0.71
1:B:1177:ILE:HG13	1:B:1371:LEU:HD21	1.72	0.71
1:D:3007:LYS:HB3	1:D:3101:TRP:HZ3	1.56	0.71
1:C:2018:ARG:HH21	1:C:2093:LYS:NZ	1.87	0.71
1:A:204:ARG:HH12	1:A:350:MET:HG2	1.56	0.71
1:D:3120:LYS:HD2	1:D:3121:ASP:H	1.53	0.71
1:C:2328:LEU:HD12	1:C:2329:LEU:N	2.06	0.71
1:B:1127:ILE:HD12	1:B:1149:ILE:HG21	1.73	0.71
1:D:3275:THR:HB	1:D:3304:GLU:OE1	1.90	0.70
1:A:343:LEU:HD12	1:A:346:LEU:HD12	1.73	0.70
1:A:7:LYS:HB3	1:A:101:TRP:HZ3	1.56	0.70
1:B:1129:ASP:OD2	1:B:1135:THR:HG23	1.92	0.70
1:B:1276:GLY:HA2	1:B:1300:HIS:HB2	1.72	0.70
1:B:1120:LYS:HD2	1:B:1121:ASP:H	1.56	0.70
1:C:2035:ARG:O	1:C:2039:SER:HB3	1.91	0.70
1:C:2370:GLU:HG3	1:C:2389:LEU:CD1	2.19	0.70
1:B:1275:THR:HB	1:B:1304:GLU:OE1	1.91	0.70
1:B:1018:ARG:HH21	1:B:1093:LYS:NZ	1.89	0.69
1:B:1021:LEU:HD23	1:B:1057:VAL:HG13	1.74	0.69
1:A:223:VAL:HB	1:A:274:THR:HG23	1.73	0.69
1:C:2430:ARG:CB	1:D:3430:ARG:HB3	2.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2172:LEU:HD13	1:C:2380:VAL:HG12	1.74	0.69
1:D:3343:LEU:HD12	1:D:3346:LEU:HD12	1.75	0.69
1:B:1166:MET:HA	1:B:1171:ILE:HD12	1.72	0.69
1:D:3028:MET:HE3	1:D:3357:MET:HB3	1.75	0.69
1:A:127:ILE:HG12	1:A:134:LEU:HD13	1.73	0.68
1:B:1126:MET:HE1	1:B:1372:TRP:HE3	1.59	0.68
1:C:2045:LYS:HA	1:C:2070:GLY:O	1.93	0.68
1:C:2143:PRO:HA	1:C:2146:LEU:CD2	2.24	0.68
1:D:3223:VAL:HB	1:D:3274:THR:HG23	1.75	0.68
1:C:2224:GLY:H	1:C:2274:THR:HG21	1.57	0.68
1:A:14:ALA:HB1	1:A:93:LYS:HD3	1.76	0.68
1:C:2007:LYS:HB3	1:C:2101:TRP:HZ3	1.57	0.68
1:A:28:MET:HE3	1:A:357:MET:HB3	1.76	0.68
1:A:188:PHE:CE2	1:B:1249:LEU:HD21	2.28	0.68
1:D:3204:ARG:HH12	1:D:3350:MET:HG2	1.59	0.68
1:C:2141:LYS:HB2	1:C:2142:HIS:ND1	2.09	0.68
1:B:1224:GLY:H	1:B:1274:THR:HG21	1.57	0.68
1:D:3125:ASN:O	1:D:3126:MET:HE2	1.94	0.68
1:C:2120:LYS:HD2	1:C:2121:ASP:H	1.59	0.67
1:A:166:MET:HA	1:A:171:ILE:HD12	1.75	0.67
1:A:188:PHE:HE2	1:B:1249:LEU:HD21	1.58	0.67
1:B:1028:MET:HE3	1:B:1357:MET:HB3	1.74	0.67
1:B:1172:LEU:HD13	1:B:1380:VAL:HG12	1.77	0.67
1:C:2126:MET:HE1	1:C:2372:TRP:HE3	1.59	0.67
1:D:3177:ILE:HG13	1:D:3371:LEU:HD21	1.77	0.67
1:A:177:ILE:HG13	1:A:371:LEU:HD21	1.77	0.67
1:A:276:GLY:HA2	1:A:300:HIS:HB2	1.75	0.67
1:A:196:GLU:HG3	1:C:2209:MET:HE2	1.77	0.67
1:B:1370:GLU:HG3	1:B:1389:LEU:CD1	2.23	0.66
1:B:1209:MET:HE2	1:D:3196:GLU:HG3	1.77	0.66
1:A:45:LYS:HA	1:A:70:GLY:O	1.95	0.66
1:D:3276:GLY:HA2	1:D:3300:HIS:HB2	1.76	0.66
1:B:1007:LYS:HB3	1:B:1101:TRP:HZ3	1.59	0.66
1:C:2127:ILE:HG12	1:C:2134:LEU:HD13	1.76	0.66
1:B:1057:VAL:H	1:B:1084:GLN:HE22	1.44	0.66
1:B:1127:ILE:HG12	1:B:1134:LEU:HD13	1.77	0.66
1:D:3014:ALA:HB1	1:D:3093:LYS:HD3	1.78	0.66
1:D:3111:TRP:O	1:D:3115:GLN:HG2	1.95	0.66
1:A:328:LEU:HD12	1:A:329:LEU:N	2.11	0.66
1:C:2074:ARG:HD3	1:C:2116:THR:HA	1.78	0.65
1:B:1385:LEU:HD12	1:B:1386:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2276:GLY:HA2	1:C:2300:HIS:HB2	1.77	0.65
1:A:172:LEU:HD13	1:A:380:VAL:HG12	1.79	0.65
1:B:1074:ARG:HD3	1:B:1116:THR:HA	1.78	0.65
1:D:3127:ILE:HG12	1:D:3134:LEU:HD13	1.78	0.65
1:D:3045:LYS:HA	1:D:3070:GLY:O	1.97	0.65
1:C:2430:ARG:HB3	1:D:3430:ARG:CB	2.15	0.65
1:C:2223:VAL:HB	1:C:2274:THR:HG23	1.77	0.65
1:B:1343:LEU:HD12	1:B:1346:LEU:HD12	1.76	0.65
1:C:2021:LEU:HD23	1:C:2057:VAL:HG13	1.79	0.65
1:C:2301:PHE:CE1	1:C:2342:ARG:HB3	2.32	0.65
1:D:3172:LEU:HD13	1:D:3380:VAL:HG12	1.79	0.65
1:A:408:LEU:HD13	1:B:1243:ILE:HG21	1.80	0.64
1:B:1033:ARG:O	1:B:1037:MET:HG2	1.96	0.64
1:C:2275:THR:HB	1:C:2304:GLU:OE1	1.97	0.64
1:A:165:LYS:HD3	1:A:166:MET:N	2.13	0.64
1:D:3035:ARG:O	1:D:3039:SER:HB3	1.97	0.64
1:A:136:ASN:O	1:A:140:THR:HG23	1.97	0.64
1:D:3301:PHE:CE1	1:D:3342:ARG:HB3	2.32	0.64
1:B:1045:LYS:HA	1:B:1070:GLY:O	1.98	0.64
1:B:1204:ARG:HH12	1:B:1350:MET:HG2	1.61	0.64
1:C:2033:ARG:O	1:C:2037:MET:HG2	1.96	0.64
1:D:3385:LEU:HD12	1:D:3386:PRO:HD2	1.80	0.64
1:C:2057:VAL:H	1:C:2084:GLN:HE22	1.45	0.64
1:A:74:ARG:HD3	1:A:116:THR:HA	1.80	0.64
1:B:1223:VAL:HB	1:B:1274:THR:HG23	1.78	0.64
1:C:2080:ILE:HG22	1:C:2104:GLU:HB2	1.78	0.64
1:D:3048:ARG:HD2	1:D:3119:PHE:CG	2.33	0.64
1:A:141:LYS:HB2	1:A:142:HIS:ND1	2.13	0.64
1:B:1035:ARG:O	1:B:1039:SER:HB3	1.97	0.64
1:A:57:VAL:H	1:A:84:GLN:HE22	1.45	0.63
1:B:1328:LEU:HD12	1:B:1329:LEU:N	2.13	0.63
1:B:1141:LYS:HB2	1:B:1142:HIS:ND1	2.13	0.63
1:D:3075:TRP:HB3	1:D:3098:VAL:HG12	1.81	0.63
1:D:3165:LYS:HD3	1:D:3166:MET:N	2.14	0.63
1:A:278:VAL:HG13	1:B:1415:TYR:CE2	2.33	0.63
1:A:5:PRO:HA	3:A:5226:HOH:O	1.98	0.63
1:A:275:THR:HG22	1:A:277:CYS:HB3	1.80	0.63
1:D:3141:LYS:HB2	1:D:3142:HIS:ND1	2.14	0.63
1:A:48:ARG:HD2	1:A:119:PHE:CG	2.34	0.63
1:A:139:HIS:HA	1:A:146:LEU:HD21	1.81	0.63
1:D:3419:PRO:HB2	1:D:3422:GLY:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2141:LYS:HB2	1:C:2142:HIS:CE1	2.34	0.63
1:C:2075:TRP:HB3	1:C:2098:VAL:HG12	1.81	0.63
1:C:2243:ILE:HG21	1:D:3408:LEU:HD13	1.80	0.63
1:B:1125:ASN:O	1:B:1126:MET:HE2	1.99	0.63
1:C:2177:ILE:HG13	1:C:2371:LEU:HD21	1.81	0.63
1:A:21:LEU:HD23	1:A:57:VAL:HG13	1.81	0.63
1:C:2014:ALA:HB1	1:C:2093:LYS:HD3	1.80	0.62
1:D:3092:ALA:HA	1:D:3096:ILE:O	1.99	0.62
1:A:35:ARG:O	1:A:39:SER:HB3	1.99	0.62
1:C:2142:HIS:N	1:C:2143:PRO:HD3	2.14	0.62
1:A:143:PRO:HA	1:A:146:LEU:CD2	2.26	0.62
1:C:2058:GLU:HG2	1:C:2357:MET:HG2	1.82	0.62
1:B:1301:PHE:CE1	1:B:1342:ARG:HB3	2.35	0.62
1:D:3143:PRO:HA	1:D:3146:LEU:CD2	2.26	0.62
1:B:1165:LYS:HD3	1:B:1166:MET:N	2.15	0.62
1:A:18:ARG:HH21	1:A:93:LYS:HZ1	1.47	0.62
1:D:3033:ARG:O	1:D:3037:MET:HG2	2.00	0.62
1:D:3308:LYS:NZ	1:D:3311:ASN:HD22	1.98	0.62
1:A:419:PRO:HB2	1:A:422:GLY:H	1.64	0.62
1:A:134:LEU:O	1:A:138:ILE:HD13	2.00	0.62
1:D:3057:VAL:H	1:D:3084:GLN:HE22	1.47	0.62
1:A:365:VAL:O	1:A:369:ILE:HG13	2.00	0.62
1:A:142:HIS:N	1:A:143:PRO:HD3	2.14	0.62
1:B:1275:THR:HG22	1:B:1277:CYS:HB3	1.81	0.62
1:C:2048:ARG:HD2	1:C:2119:PHE:CG	2.35	0.62
1:B:1419:PRO:HG2	1:B:1422:GLY:HA3	1.81	0.61
1:B:1048:ARG:HD2	1:B:1119:PHE:CG	2.35	0.61
1:D:3328:LEU:HD12	1:D:3329:LEU:N	2.15	0.61
1:A:75:TRP:HB3	1:A:98:VAL:HG12	1.83	0.61
1:C:2166:MET:HA	1:C:2171:ILE:HD12	1.81	0.61
1:B:1142:HIS:N	1:B:1143:PRO:HD3	2.15	0.61
1:A:111:TRP:O	1:A:115:GLN:HG2	2.00	0.61
1:B:1111:TRP:O	1:B:1115:GLN:HG2	2.00	0.61
1:D:3275:THR:HG22	1:D:3277:CYS:HB3	1.83	0.61
1:D:3142:HIS:N	1:D:3143:PRO:HD3	2.15	0.61
1:B:1058:GLU:HG2	1:B:1357:MET:HG2	1.81	0.61
1:B:1014:ALA:HB1	1:B:1093:LYS:HD3	1.81	0.61
1:B:1406:THR:CG2	3:B:5082:HOH:O	2.47	0.61
1:A:183:VAL:HG12	1:B:1430:ARG:CZ	2.30	0.61
1:B:1419:PRO:HB2	1:B:1422:GLY:H	1.64	0.61
1:D:3074:ARG:HD3	1:D:3116:THR:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3169:ASN:HB2	1:D:3171:ILE:HG13	1.82	0.61
1:C:2165:LYS:HD3	1:C:2166:MET:N	2.16	0.61
1:C:2139:HIS:HA	1:C:2146:LEU:HD21	1.83	0.61
1:C:2343:LEU:HD12	1:C:2346:LEU:HD12	1.81	0.61
1:A:406:THR:HG21	3:B:5114:HOH:O	2.01	0.61
1:B:1246:ILE:O	1:B:1250:GLN:HG3	2.01	0.60
1:D:3117:LEU:HD21	1:D:3138:ILE:HD11	1.81	0.60
1:B:1425:LYS:HD2	1:B:1429:TYR:CE2	2.35	0.60
1:B:1353:PRO:O	1:B:1356:VAL:HG13	2.00	0.60
1:B:1169:ASN:HB2	1:B:1171:ILE:HG13	1.82	0.60
1:D:3301:PHE:HE1	1:D:3342:ARG:HB3	1.64	0.60
1:D:3117:LEU:CD2	1:D:3138:ILE:HD11	2.32	0.60
1:A:279:ASP:OD2	1:B:1411:LYS:HE3	2.01	0.60
1:C:2169:ASN:HB2	1:C:2171:ILE:HG13	1.83	0.60
1:A:92:ALA:HA	1:A:96:ILE:O	2.02	0.60
1:B:1075:TRP:HB3	1:B:1098:VAL:HG12	1.83	0.60
1:D:3134:LEU:O	1:D:3138:ILE:HD13	2.01	0.60
1:D:3080:ILE:HG22	1:D:3104:GLU:HB2	1.83	0.59
1:A:126:MET:HE1	1:A:372:TRP:HE3	1.67	0.59
1:D:3407:LYS:CE	1:D:3420:ILE:HG22	2.31	0.59
1:C:2111:TRP:O	1:C:2115:GLN:HG2	2.02	0.59
1:D:3419:PRO:HG2	1:D:3422:GLY:HA3	1.84	0.59
1:D:3169:ASN:HB2	1:D:3171:ILE:CD1	2.33	0.59
1:D:3126:MET:HE1	1:D:3372:TRP:HE3	1.67	0.59
1:A:209:MET:HE2	1:C:2196:GLU:HG3	1.83	0.59
1:B:1143:PRO:HA	1:B:1146:LEU:CD2	2.28	0.59
1:A:301:PHE:CE1	1:A:342:ARG:HB3	2.37	0.59
1:B:1081:PHE:CD1	1:B:1103:GLY:HA2	2.38	0.59
1:C:2419:PRO:HB2	1:C:2422:GLY:H	1.66	0.59
1:B:1139:HIS:HA	1:B:1146:LEU:HD21	1.85	0.59
1:A:425:LYS:HD2	1:A:429:TYR:CE2	2.38	0.59
1:D:3409:THR:HB	3:D:5139:HOH:O	2.03	0.59
1:C:2136:ASN:O	1:C:2140:THR:HG23	2.03	0.59
1:D:3021:LEU:HD23	1:D:3057:VAL:HG13	1.85	0.59
1:B:1308:LYS:HD2	1:B:1312:GLU:OE2	2.02	0.59
1:D:3139:HIS:HA	1:D:3146:LEU:HD21	1.85	0.59
1:D:3232:ARG:HD3	3:D:5394:HOH:O	2.02	0.59
1:A:370:GLU:HG3	1:A:389:LEU:CD1	2.23	0.58
1:A:105:THR:HG23	1:A:108:GLU:CD	2.23	0.58
1:C:2018:ARG:HH21	1:C:2093:LYS:HZ1	1.48	0.58
1:C:2353:PRO:O	1:C:2356:VAL:HG13	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1127:ILE:HG23	1:B:1134:LEU:CD1	2.33	0.58
1:D:3370:GLU:HG3	1:D:3389:LEU:CD1	2.23	0.58
1:C:2275:THR:HG22	1:C:2277:CYS:HB3	1.84	0.58
1:C:2301:PHE:HE1	1:C:2342:ARG:HB3	1.66	0.58
1:C:2419:PRO:HG2	1:C:2422:GLY:HA3	1.84	0.58
1:A:260:THR:HG22	1:B:1406:THR:HG22	1.85	0.58
1:C:2308:LYS:HD2	1:C:2312:GLU:OE2	2.03	0.58
1:A:291:ASP:OD2	1:A:334:ARG:NH1	2.36	0.58
1:B:1141:LYS:HB2	1:B:1142:HIS:CE1	2.39	0.58
1:A:243:ILE:HG21	1:B:1408:LEU:CD1	2.32	0.58
1:C:2399:GLY:C	1:C:2402:ASN:H	2.06	0.58
1:A:277:CYS:HB2	1:B:1416:LEU:CD2	2.30	0.58
1:A:33:ARG:O	1:A:37:MET:HG2	2.04	0.58
1:C:2183:VAL:HG12	1:D:3430:ARG:CZ	2.34	0.58
1:A:156:THR:O	1:A:160:VAL:HG23	2.04	0.58
1:A:431:TYR:CD1	1:A:431:TYR:N	2.72	0.58
1:B:1105:THR:HG23	1:B:1108:GLU:CD	2.24	0.58
1:B:1156:THR:O	1:B:1160:VAL:HG23	2.03	0.58
1:C:2425:LYS:HD2	1:C:2429:TYR:CE2	2.38	0.58
1:A:139:HIS:O	1:A:143:PRO:HG3	2.03	0.57
1:A:169:ASN:HB2	1:A:171:ILE:HG13	1.86	0.57
1:B:1406:THR:HG23	3:B:5082:HOH:O	2.04	0.57
1:A:431:TYR:HD1	1:A:431:TYR:H	1.51	0.57
1:C:2152:ILE:HG13	1:C:2174:VAL:HG22	1.85	0.57
1:D:3319:ASN:HB2	3:D:5377:HOH:O	2.04	0.57
1:D:3425:LYS:HD2	1:D:3429:TYR:CE2	2.39	0.57
1:A:55:MET:HE2	1:A:75:TRP:CD1	2.39	0.57
1:C:2156:THR:O	1:C:2160:VAL:HG23	2.04	0.57
1:C:2117:LEU:HD21	1:C:2138:ILE:HD11	1.85	0.57
1:A:80:ILE:HG22	1:A:104:GLU:HB2	1.85	0.57
1:D:3058:GLU:HG2	1:D:3357:MET:HG2	1.85	0.57
1:C:2300:HIS:HD2	1:C:2303:VAL:CG2	2.17	0.57
1:D:3431:TYR:N	1:D:3431:TYR:CD1	2.72	0.57
1:C:2105:THR:HG23	1:C:2108:GLU:CD	2.25	0.57
1:C:2007:LYS:HB3	1:C:2101:TRP:CZ3	2.38	0.57
1:A:117:LEU:HD21	1:A:138:ILE:HD11	1.86	0.57
1:D:3308:LYS:HD2	1:D:3312:GLU:OE2	2.05	0.57
1:B:1136:ASN:O	1:B:1140:THR:HG23	2.05	0.57
1:C:2127:ILE:HG23	1:C:2134:LEU:CD1	2.34	0.57
1:B:1209:MET:HE3	1:D:3356:VAL:HG12	1.85	0.57
1:B:1426:PRO:HD2	1:B:1429:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD12	1:A:386:PRO:HD2	1.87	0.56
1:D:3127:ILE:HG23	1:D:3134:LEU:CD1	2.35	0.56
1:A:426:PRO:HD2	1:A:429:TYR:HB2	1.87	0.56
1:C:2246:ILE:O	1:C:2250:GLN:HG3	2.05	0.56
1:C:2430:ARG:CZ	1:D:3183:VAL:HG12	2.35	0.56
1:A:169:ASN:HB2	1:A:171:ILE:CD1	2.35	0.56
1:D:3204:ARG:NH1	1:D:3350:MET:HG2	2.20	0.56
1:B:1301:PHE:HE1	1:B:1342:ARG:HB3	1.68	0.56
1:B:1399:GLY:C	1:B:1402:ASN:H	2.07	0.56
1:B:1369:ILE:O	1:B:1373:THR:HB	2.05	0.56
1:C:2079:ASN:HB3	1:C:2082:SER:HG	1.69	0.56
1:C:2081:PHE:CD1	1:C:2103:GLY:HA2	2.41	0.56
1:A:7:LYS:HB3	1:A:101:TRP:CZ3	2.38	0.56
1:D:3007:LYS:HB3	1:D:3101:TRP:CZ3	2.38	0.56
1:C:2249:LEU:HD21	1:D:3188:PHE:CE2	2.40	0.56
1:D:3105:THR:HG23	1:D:3108:GLU:CD	2.26	0.56
1:C:2007:LYS:HG3	1:C:2111:TRP:CH2	2.41	0.56
1:D:3142:HIS:N	1:D:3143:PRO:CD	2.69	0.56
1:A:117:LEU:CD2	1:A:138:ILE:HD11	2.36	0.56
1:B:1117:LEU:CD2	1:B:1138:ILE:HD11	2.36	0.55
1:C:2092:ALA:HA	1:C:2096:ILE:O	2.04	0.55
1:C:2204:ARG:NH1	1:C:2350:MET:HG2	2.20	0.55
1:C:2411:LYS:HE3	1:D:3279:ASP:OD2	2.07	0.55
1:C:2117:LEU:CD2	1:C:2138:ILE:HD11	2.36	0.55
1:D:3016:TRP:CE3	1:D:3086:HIS:HB3	2.41	0.55
1:B:1079:ASN:HB3	1:B:1082:SER:HG	1.71	0.55
1:A:430:ARG:HB3	1:B:1430:ARG:CB	2.20	0.55
1:D:3057:VAL:O	1:D:3061:VAL:HG23	2.07	0.55
1:C:2142:HIS:ND1	1:C:2142:HIS:N	2.54	0.55
1:B:1152:ILE:HG13	1:B:1174:VAL:HG22	1.87	0.55
1:B:1365:VAL:O	1:B:1369:ILE:HG13	2.06	0.55
1:B:1179:VAL:CG2	1:B:1363:ASN:HB3	2.37	0.55
1:D:3431:TYR:H	1:D:3431:TYR:HD1	1.53	0.55
1:A:141:LYS:HB2	1:A:142:HIS:CE1	2.41	0.55
1:A:369:ILE:O	1:A:373:THR:HB	2.07	0.55
1:A:204:ARG:NH1	1:A:350:MET:HG2	2.20	0.55
1:B:1007:LYS:HB3	1:B:1101:TRP:CZ3	2.41	0.55
1:C:2249:LEU:HD21	1:D:3188:PHE:HE2	1.71	0.55
1:A:308:LYS:NZ	1:A:311:ASN:HD22	2.04	0.55
1:D:3141:LYS:HB2	1:D:3142:HIS:CE1	2.41	0.55
1:D:3326:ARG:HD3	3:D:5214:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3156:THR:O	1:D:3160:VAL:HG23	2.07	0.55
1:C:2431:TYR:N	1:C:2431:TYR:CD1	2.72	0.55
1:B:1169:ASN:HB2	1:B:1171:ILE:CD1	2.37	0.55
1:A:17:GLY:HA3	1:A:86:HIS:O	2.06	0.55
1:D:3153:SER:HB2	1:D:3368:GLN:NE2	2.22	0.55
1:D:3152:ILE:HG13	1:D:3174:VAL:HG22	1.89	0.55
1:D:3426:PRO:HD2	1:D:3429:TYR:HB2	1.89	0.55
1:B:1199:ILE:HD12	1:B:1234:PHE:CD2	2.41	0.55
1:B:1300:HIS:HD2	1:B:1303:VAL:CG2	2.20	0.54
1:D:3369:ILE:O	1:D:3373:THR:HB	2.07	0.54
1:A:57:VAL:O	1:A:61:VAL:HG23	2.07	0.54
1:A:356:VAL:HG12	1:C:2209:MET:HE3	1.89	0.54
1:A:142:HIS:N	1:A:143:PRO:CD	2.71	0.54
1:A:152:ILE:HD11	1:A:174:VAL:HG13	1.89	0.54
1:C:2142:HIS:N	1:C:2143:PRO:CD	2.71	0.54
1:B:1134:LEU:O	1:B:1138:ILE:HD13	2.07	0.54
1:C:2126:MET:CE	1:C:2372:TRP:HE3	2.20	0.54
1:B:1146:LEU:HA	1:B:1149:ILE:HD12	1.89	0.54
1:B:1018:ARG:HH21	1:B:1093:LYS:HZ1	1.53	0.54
1:A:63:ILE:HG23	1:A:73:VAL:HG11	1.90	0.54
1:C:2385:LEU:HD12	1:C:2386:PRO:HD2	1.89	0.54
1:A:301:PHE:HE1	1:A:342:ARG:HB3	1.69	0.54
1:B:1431:TYR:CD1	1:B:1431:TYR:N	2.73	0.54
1:D:3138:ILE:HG22	1:D:3146:LEU:HD22	1.88	0.54
1:A:152:ILE:HG13	1:A:174:VAL:HG22	1.90	0.54
1:B:1117:LEU:HD21	1:B:1138:ILE:HD11	1.89	0.54
1:B:1142:HIS:N	1:B:1142:HIS:ND1	2.55	0.54
1:C:2426:PRO:HD2	1:C:2429:TYR:HB2	1.90	0.54
1:A:386:PRO:HG2	1:A:389:LEU:HD12	1.88	0.54
1:D:3291:ASP:OD2	1:D:3334:ARG:NH1	2.41	0.54
1:C:2369:ILE:O	1:C:2373:THR:HB	2.08	0.54
1:A:415:TYR:CD2	1:B:1278:VAL:HG13	2.43	0.54
1:A:153:SER:HB2	1:A:368:GLN:NE2	2.23	0.54
1:C:2057:VAL:O	1:C:2061:VAL:HG23	2.08	0.54
1:B:1017:GLY:HA3	1:B:1086:HIS:O	2.08	0.54
1:A:278:VAL:HG13	1:B:1415:TYR:CD2	2.43	0.54
1:A:152:ILE:HG22	1:A:153:SER:N	2.23	0.53
1:B:1142:HIS:N	1:B:1143:PRO:CD	2.71	0.53
1:A:79:ASN:HB3	1:A:82:SER:HG	1.74	0.53
1:A:142:HIS:ND1	1:A:142:HIS:N	2.56	0.53
1:A:11:ILE:O	1:A:11:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2431:TYR:HD1	1:C:2431:TYR:H	1.54	0.53
1:C:2169:ASN:HB2	1:C:2171:ILE:CD1	2.39	0.53
1:C:2017:GLY:HA3	1:C:2086:HIS:O	2.08	0.53
1:C:2016:TRP:CE3	1:C:2086:HIS:HB3	2.42	0.53
1:B:1126:MET:CE	1:B:1372:TRP:HE3	2.21	0.53
1:B:1196:GLU:HG3	1:D:3209:MET:HE2	1.89	0.53
1:A:430:ARG:CB	1:B:1430:ARG:HB3	2.21	0.53
1:C:2274:THR:O	1:C:2274:THR:HG22	2.09	0.53
1:A:430:ARG:CZ	1:B:1183:VAL:HG12	2.39	0.53
1:D:3420:ILE:N	3:D:5231:HOH:O	2.41	0.53
1:A:105:THR:HG1	1:A:108:GLU:HG3	1.71	0.53
1:C:2074:ARG:HG3	1:C:2097:PRO:HG2	1.90	0.53
1:D:3081:PHE:CD1	1:D:3103:GLY:HA2	2.42	0.53
1:B:1092:ALA:HA	1:B:1096:ILE:O	2.08	0.53
1:D:3105:THR:HG23	1:D:3108:GLU:OE1	2.08	0.53
1:C:2152:ILE:HG22	1:C:2153:SER:N	2.24	0.53
1:B:1152:ILE:HG22	1:B:1153:SER:N	2.24	0.53
1:A:58:GLU:HG2	1:A:357:MET:HG2	1.91	0.53
1:D:3047:ALA:HA	1:D:3125:ASN:HD21	1.74	0.53
3:B:5213:HOH:O	1:D:3353:PRO:HG3	2.09	0.53
1:D:3399:GLY:C	1:D:3402:ASN:H	2.11	0.53
1:D:3300:HIS:HD2	1:D:3303:VAL:CG2	2.22	0.52
1:B:1431:TYR:H	1:B:1431:TYR:HD1	1.55	0.52
1:C:2365:VAL:O	1:C:2369:ILE:HG13	2.09	0.52
1:B:1419:PRO:HB2	1:B:1422:GLY:N	2.25	0.52
1:A:399:GLY:C	1:A:402:ASN:H	2.12	0.52
1:B:1039:SER:O	1:B:1042:LYS:HE2	2.10	0.52
1:B:1004:LEU:HD23	1:B:1005:PRO:HD2	1.91	0.52
1:C:2146:LEU:HA	1:C:2149:ILE:HD12	1.91	0.52
1:D:3152:ILE:HD11	1:D:3174:VAL:HG13	1.91	0.52
1:D:3353:PRO:O	1:D:3356:VAL:HG13	2.10	0.52
1:B:1049:ILE:HB	1:B:1073:VAL:HG22	1.91	0.52
1:A:249:LEU:HD21	1:B:1188:PHE:HE2	1.75	0.52
1:A:16:TRP:CE3	1:A:86:HIS:HB3	2.45	0.52
1:A:81:PHE:CD1	1:A:103:GLY:HA2	2.44	0.52
1:C:2259:THR:HA	1:D:3404:LYS:HB2	1.92	0.52
1:C:2139:HIS:O	1:C:2143:PRO:HG3	2.09	0.52
1:A:343:LEU:CD1	1:A:346:LEU:HD12	2.38	0.52
1:D:3033:ARG:HD2	1:D:3396:ALA:HA	1.91	0.52
1:A:416:LEU:CD2	1:B:1277:CYS:HB2	2.38	0.51
1:A:274:THR:HG22	1:A:274:THR:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2408:LEU:CD1	1:D:3243:ILE:HG21	2.37	0.51
1:B:1127:ILE:HG23	1:B:1134:LEU:HD12	1.92	0.51
1:B:1105:THR:HG1	1:B:1108:GLU:HG3	1.75	0.51
1:A:28:MET:HA	1:A:358:SER:HB2	1.92	0.51
1:D:3386:PRO:HG2	1:D:3389:LEU:HD12	1.92	0.51
1:A:300:HIS:HD2	1:A:303:VAL:CG2	2.23	0.51
1:A:196:GLU:HG3	1:C:2209:MET:CE	2.39	0.51
1:D:3063:ILE:HG23	1:D:3073:VAL:HG11	1.93	0.51
1:D:3419:PRO:HB2	1:D:3422:GLY:N	2.25	0.51
1:D:3142:HIS:ND1	1:D:3142:HIS:N	2.58	0.51
1:A:249:LEU:HD21	1:B:1188:PHE:CE2	2.46	0.51
1:D:3053:LEU:O	1:D:3054:HIS:C	2.47	0.51
1:B:1209:MET:CE	1:D:3356:VAL:HG12	2.40	0.51
1:A:33:ARG:HD2	1:A:396:ALA:HA	1.92	0.51
1:B:1080:ILE:HG22	1:B:1104:GLU:HB2	1.92	0.51
1:D:3079:ASN:HB3	1:D:3082:SER:HG	1.76	0.51
1:B:1053:LEU:O	1:B:1054:HIS:C	2.48	0.51
1:D:3152:ILE:HG22	1:D:3153:SER:N	2.25	0.51
1:B:1007:LYS:HG3	1:B:1111:TRP:CH2	2.46	0.51
1:D:3143:PRO:O	1:D:3146:LEU:HB2	2.11	0.51
1:A:419:PRO:HB2	1:A:422:GLY:N	2.26	0.51
1:B:1356:VAL:HG12	1:D:3209:MET:HE3	1.92	0.51
1:A:105:THR:HG23	1:A:108:GLU:OE1	2.11	0.51
1:C:2099:PHE:CZ	1:C:2115:GLN:HB3	2.46	0.51
1:A:39:SER:O	1:A:42:LYS:HE2	2.11	0.51
1:B:1056:THR:HA	1:B:1084:GLN:HB2	1.92	0.50
1:B:1204:ARG:NH1	1:B:1350:MET:HG2	2.25	0.50
1:D:3048:ARG:HD2	1:D:3119:PHE:CB	2.40	0.50
1:A:308:LYS:HD2	1:A:312:GLU:OE2	2.11	0.50
1:D:3011:ILE:O	1:D:3011:ILE:HG13	2.11	0.50
1:C:2093:LYS:HE2	1:C:2094:ALA:N	2.25	0.50
1:D:3045:LYS:HE3	1:D:3045:LYS:O	2.11	0.50
1:A:146:LEU:HG	1:A:173:LYS:HG3	1.93	0.50
1:B:1169:ASN:HD22	1:B:1171:ILE:HD11	1.77	0.50
1:D:3274:THR:O	1:D:3274:THR:HG22	2.10	0.50
1:D:3017:GLY:HA3	1:D:3086:HIS:O	2.10	0.50
1:C:2049:ILE:HB	1:C:2073:VAL:HG22	1.93	0.50
1:B:1419:PRO:HB2	1:B:1422:GLY:HA3	1.93	0.50
1:C:2179:VAL:CG2	1:C:2363:ASN:HB3	2.41	0.50
1:C:2055:MET:O	1:C:2084:GLN:N	2.37	0.50
1:A:53:LEU:O	1:A:54:HIS:C	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3343:LEU:CD1	1:D:3346:LEU:HD12	2.40	0.50
1:B:1074:ARG:HG3	1:B:1097:PRO:HG2	1.92	0.50
1:C:2093:LYS:HE2	1:C:2093:LYS:C	2.32	0.50
1:D:3317:LYS:HD2	1:D:3327:TYR:CE2	2.46	0.50
1:B:1016:TRP:CE3	1:B:1086:HIS:HB3	2.46	0.50
1:A:407:LYS:CE	1:A:420:ILE:HG22	2.34	0.50
1:D:3386:PRO:HG2	1:D:3389:LEU:CD1	2.41	0.50
1:B:1057:VAL:O	1:B:1061:VAL:HG23	2.11	0.50
1:C:2056:THR:HA	1:C:2084:GLN:HB2	1.92	0.50
1:C:2028:MET:HA	1:C:2358:SER:HB2	1.93	0.50
1:D:3028:MET:HA	1:D:3358:SER:HB2	1.94	0.50
1:B:1011:ILE:HG13	1:B:1011:ILE:O	2.11	0.50
1:D:3146:LEU:HA	1:D:3149:ILE:HD12	1.94	0.50
1:C:2134:LEU:O	1:C:2138:ILE:HD13	2.11	0.50
1:D:3365:VAL:O	1:D:3369:ILE:HG13	2.12	0.50
1:A:75:TRP:HH2	1:A:128:LEU:HD13	1.76	0.50
1:A:56:THR:HA	1:A:84:GLN:HB2	1.94	0.50
1:D:3054:HIS:HB3	1:D:3082:SER:HB2	1.94	0.50
1:C:2111:TRP:NE1	1:C:2115:GLN:NE2	2.60	0.50
1:B:1197:SER:HB2	1:B:1345:ASN:HB2	1.92	0.50
1:D:3136:ASN:O	1:D:3140:THR:HG23	2.11	0.49
1:B:1048:ARG:HD2	1:B:1119:PHE:CB	2.42	0.49
1:A:199:ILE:HD12	1:A:234:PHE:CD2	2.47	0.49
1:A:386:PRO:HG2	1:A:389:LEU:CD1	2.42	0.49
1:B:1386:PRO:HG2	1:B:1389:LEU:CD1	2.42	0.49
1:B:1386:PRO:HG2	1:B:1389:LEU:HD12	1.93	0.49
1:A:138:ILE:HG22	1:A:146:LEU:HD22	1.93	0.49
1:B:1407:LYS:CE	1:B:1420:ILE:HG22	2.37	0.49
1:C:2048:ARG:HB3	1:C:2119:PHE:CE2	2.47	0.49
1:A:127:ILE:HG23	1:A:134:LEU:CD1	2.42	0.49
1:D:3038:TYR:HB3	1:D:3043:PRO:HG3	1.95	0.49
1:D:3127:ILE:HG23	1:D:3134:LEU:HD12	1.94	0.49
1:C:2146:LEU:HG	1:C:2173:LYS:HG3	1.94	0.49
1:C:2055:MET:HE2	1:C:2075:TRP:CD1	2.48	0.49
1:D:3055:MET:HE2	1:D:3075:TRP:CD1	2.47	0.49
1:D:3056:THR:HA	1:D:3084:GLN:HB2	1.95	0.49
1:A:353:PRO:O	1:A:356:VAL:HG13	2.13	0.49
1:D:3048:ARG:HA	1:D:3072:GLU:HB2	1.95	0.49
1:D:3406:THR:HG23	3:D:5319:HOH:O	2.12	0.49
1:C:2127:ILE:HG23	1:C:2134:LEU:HD12	1.94	0.49
1:C:2407:LYS:CE	1:C:2420:ILE:HG22	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2063:ILE:HG23	1:C:2073:VAL:HG11	1.93	0.49
1:B:1105:THR:HG23	1:B:1108:GLU:OE1	2.13	0.49
1:A:343:LEU:HD12	1:A:346:LEU:CD1	2.40	0.49
1:B:1093:LYS:HE2	1:B:1094:ALA:N	2.27	0.49
1:D:3343:LEU:HD12	1:D:3346:LEU:CD1	2.41	0.49
1:C:2153:SER:HB2	1:C:2368:GLN:NE2	2.27	0.49
1:B:1274:THR:O	1:B:1274:THR:HG22	2.13	0.49
1:A:18:ARG:HH21	1:A:93:LYS:HZ3	1.59	0.49
1:A:419:PRO:HG2	1:A:422:GLY:HA3	1.95	0.49
1:D:3139:HIS:O	1:D:3143:PRO:HG3	2.12	0.49
1:D:3126:MET:CE	1:D:3372:TRP:HE3	2.26	0.49
1:C:2048:ARG:HD2	1:C:2119:PHE:CB	2.43	0.49
1:C:2308:LYS:NZ	1:C:2311:ASN:HD22	2.09	0.49
1:C:2152:ILE:O	1:C:2371:LEU:HD11	2.13	0.48
1:A:93:LYS:HE2	1:A:94:ALA:N	2.28	0.48
1:A:350:MET:HG3	1:C:2207:ASP:OD2	2.13	0.48
1:B:1301:PHE:CD1	1:B:1343:LEU:HG	2.48	0.48
1:D:3038:TYR:HB3	1:D:3043:PRO:CG	2.43	0.48
1:B:1075:TRP:HH2	1:B:1128:LEU:HD13	1.78	0.48
1:A:54:HIS:HB3	1:A:82:SER:HB2	1.95	0.48
1:D:3049:ILE:HD12	1:D:3071:ALA:HB1	1.96	0.48
1:D:3015:ALA:O	1:D:3019:LYS:HG2	2.14	0.48
1:C:2291:ASP:OD2	1:C:2334:ARG:NH1	2.45	0.48
1:B:1055:MET:O	1:B:1084:GLN:N	2.38	0.48
1:A:47:ALA:HA	1:A:125:ASN:HD21	1.78	0.48
1:D:3007:LYS:HG3	1:D:3111:TRP:CH2	2.49	0.48
1:A:323:GLN:HG3	1:A:347:GLY:O	2.14	0.48
1:D:3246:ILE:O	1:D:3250:GLN:HG3	2.12	0.48
1:A:239:ILE:HG23	1:A:257:GLU:HG2	1.95	0.48
1:B:1146:LEU:HG	1:B:1173:LYS:HG3	1.95	0.48
1:B:1152:ILE:O	1:B:1371:LEU:HD11	2.14	0.48
1:A:209:MET:HB2	1:C:2353:PRO:HB2	1.95	0.48
1:C:2424:PHE:C	1:C:2425:LYS:HG2	2.33	0.48
1:A:395:GLU:HA	1:A:398:LEU:HD22	1.95	0.48
1:C:2419:PRO:HB2	1:C:2422:GLY:N	2.29	0.48
1:A:127:ILE:HG21	1:A:135:THR:HG22	1.96	0.48
1:D:3093:LYS:HE2	1:D:3094:ALA:N	2.29	0.48
1:C:2054:HIS:CE1	1:C:2078:CYS:SG	3.07	0.48
1:D:3126:MET:HE1	1:D:3150:ARG:HB3	1.95	0.48
1:B:1081:PHE:CE1	1:B:1103:GLY:HA2	2.49	0.48
1:C:2188:PHE:HE2	1:D:3249:LEU:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1138:ILE:HG22	1:B:1146:LEU:HD22	1.96	0.48
1:B:1028:MET:HA	1:B:1358:SER:HB2	1.96	0.48
1:D:3169:ASN:HD22	1:D:3171:ILE:HD11	1.79	0.48
1:A:48:ARG:HD2	1:A:119:PHE:CB	2.43	0.48
1:C:2048:ARG:HA	1:C:2072:GLU:HB2	1.94	0.48
1:D:3179:VAL:CG2	1:D:3363:ASN:HB3	2.43	0.48
1:A:360:SER:O	1:A:363:ASN:HB2	2.13	0.48
1:D:3109:TYR:CZ	1:D:3113:ILE:HD11	2.48	0.48
1:B:1015:ALA:O	1:B:1019:LYS:HG2	2.14	0.48
1:B:1171:ILE:O	1:B:1173:LYS:HG2	2.14	0.47
1:B:1343:LEU:HD12	1:B:1346:LEU:CD1	2.41	0.47
1:B:1317:LYS:HD2	1:B:1327:TYR:CE2	2.49	0.47
1:A:404:LYS:HB2	1:B:1259:THR:HA	1.96	0.47
1:D:3199:ILE:HD12	1:D:3234:PHE:CD2	2.49	0.47
1:C:2075:TRP:HH2	1:C:2128:LEU:HD13	1.79	0.47
1:A:209:MET:CE	1:C:2196:GLU:HG3	2.44	0.47
1:D:3006:TYR:CD1	1:D:3006:TYR:C	2.87	0.47
1:B:1038:TYR:HB3	1:B:1043:PRO:HG3	1.95	0.47
1:D:3117:LEU:HD13	1:D:3142:HIS:CD2	2.49	0.47
1:B:1093:LYS:C	1:B:1093:LYS:HE2	2.35	0.47
1:A:38:TYR:HB3	1:A:43:PRO:HG3	1.97	0.47
1:D:3171:ILE:O	1:D:3173:LYS:HG2	2.15	0.47
1:C:2301:PHE:CD1	1:C:2343:LEU:HG	2.49	0.47
1:D:3424:PHE:C	1:D:3425:LYS:HG2	2.35	0.47
1:C:2277:CYS:SG	1:D:3412:GLN:HB3	2.54	0.47
1:B:1057:VAL:HG23	1:B:1084:GLN:NE2	2.29	0.47
1:A:126:MET:CE	1:A:372:TRP:HE3	2.27	0.47
1:B:1099:PHE:CZ	1:B:1115:GLN:HB3	2.50	0.47
1:B:1038:TYR:HB3	1:B:1043:PRO:CG	2.45	0.47
1:A:6:TYR:CD1	1:A:6:TYR:C	2.87	0.47
1:A:146:LEU:HA	1:A:149:ILE:HD12	1.96	0.47
1:D:3075:TRP:HH2	1:D:3128:LEU:HD13	1.78	0.47
1:C:2386:PRO:HG2	1:C:2389:LEU:HD12	1.95	0.47
1:A:416:LEU:HD11	1:B:1277:CYS:HB2	1.96	0.47
1:B:1055:MET:HE2	1:B:1075:TRP:CD1	2.49	0.47
1:D:3093:LYS:HE2	1:D:3093:LYS:C	2.34	0.47
1:A:13:LEU:HB3	1:A:86:HIS:HA	1.96	0.47
1:A:49:ILE:HB	1:A:73:VAL:HG22	1.97	0.47
1:C:2197:SER:HB2	1:C:2345:ASN:HB2	1.95	0.47
1:C:2006:TYR:C	1:C:2006:TYR:CD1	2.88	0.47
1:C:2004:LEU:HD23	1:C:2005:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3169:ASN:HB2	1:D:3171:ILE:CG1	2.43	0.47
1:D:3034:MET:HG3	1:D:3365:VAL:HG11	1.97	0.47
1:C:2117:LEU:HD13	1:C:2142:HIS:CD2	2.50	0.47
1:D:3055:MET:O	1:D:3084:GLN:N	2.40	0.47
1:D:3105:THR:HG1	1:D:3108:GLU:HG3	1.78	0.47
1:B:1033:ARG:HD2	1:B:1396:ALA:HA	1.97	0.47
1:D:3142:HIS:HB3	1:D:3145:LEU:CD1	2.45	0.47
1:B:1117:LEU:HD13	1:B:1142:HIS:CD2	2.50	0.47
1:A:7:LYS:HG3	1:A:111:TRP:CH2	2.50	0.47
1:A:74:ARG:CD	1:A:116:THR:HA	2.44	0.47
1:C:2015:ALA:O	1:C:2019:LYS:HG2	2.15	0.47
1:D:3398:LEU:HG	1:D:3403:VAL:HG11	1.97	0.47
1:B:1209:MET:CE	1:D:3196:GLU:HG3	2.44	0.46
1:C:2361:PHE:O	1:C:2364:GLN:HB2	2.15	0.46
1:B:1139:HIS:O	1:B:1143:PRO:HG3	2.14	0.46
1:D:3119:PHE:N	1:D:3122:GLY:O	2.40	0.46
1:C:2057:VAL:H	1:C:2084:GLN:HE21	1.60	0.46
1:A:56:THR:HB	1:A:84:GLN:NE2	2.30	0.46
1:D:3056:THR:HB	1:D:3084:GLN:NE2	2.30	0.46
1:B:1274:THR:HG22	3:B:5145:HOH:O	2.14	0.46
1:A:38:TYR:HB3	1:A:43:PRO:CG	2.46	0.46
1:D:3398:LEU:HG	1:D:3403:VAL:CG1	2.45	0.46
1:C:2278:VAL:HG13	1:D:3415:TYR:CD2	2.50	0.46
1:A:93:LYS:C	1:A:93:LYS:HE2	2.35	0.46
1:A:398:LEU:HG	1:A:403:VAL:CG1	2.46	0.46
1:C:2273:THR:HB	1:C:2304:GLU:OE1	2.16	0.46
1:B:1047:ALA:HA	1:B:1125:ASN:HD21	1.81	0.46
1:C:2171:ILE:O	1:C:2173:LYS:HG2	2.16	0.46
1:B:1169:ASN:HB2	1:B:1171:ILE:CG1	2.45	0.46
1:A:207:ASP:OD2	1:C:2350:MET:HG3	2.16	0.46
1:D:3039:SER:O	1:D:3042:LYS:HE2	2.15	0.46
1:C:2353:PRO:HD2	1:C:2356:VAL:CG1	2.45	0.46
1:A:209:MET:HE3	1:C:2356:VAL:HG12	1.97	0.46
1:B:1291:ASP:OD2	1:B:1334:ARG:NH1	2.48	0.46
1:A:143:PRO:O	1:A:146:LEU:HB2	2.16	0.46
1:B:1407:LYS:HE2	1:B:1421:ASN:OD1	2.16	0.46
1:D:3081:PHE:O	1:D:3102:LYS:HG3	2.15	0.46
1:C:2188:PHE:CE2	1:D:3249:LEU:HD21	2.51	0.46
1:D:3395:GLU:HG2	3:D:5043:HOH:O	2.15	0.46
1:C:2386:PRO:HG2	1:C:2389:LEU:CD1	2.45	0.46
1:C:2407:LYS:HE2	1:C:2421:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:ASP:OD2	1:D:3350:MET:HG3	2.16	0.46
1:A:179:VAL:CG2	1:A:363:ASN:HB3	2.44	0.46
1:C:2011:ILE:O	1:C:2011:ILE:HG13	2.15	0.46
1:B:1006:TYR:C	1:B:1006:TYR:CD1	2.89	0.46
1:C:2013:LEU:HB3	1:C:2086:HIS:HA	1.98	0.46
1:A:126:MET:HE1	1:A:150:ARG:HB3	1.98	0.46
1:A:406:THR:HG22	1:B:1260:THR:HG22	1.98	0.46
1:A:398:LEU:HG	1:A:403:VAL:HG11	1.98	0.46
1:B:1240:ILE:HG22	1:B:1241:THR:N	2.31	0.46
1:D:3004:LEU:HD23	1:D:3005:PRO:HD2	1.98	0.46
1:B:1126:MET:CE	1:B:1372:TRP:CE3	2.99	0.45
1:A:45:LYS:O	1:A:45:LYS:HE3	2.16	0.45
1:A:48:ARG:HB3	1:A:119:PHE:CE2	2.51	0.45
1:B:1323:GLN:HG3	1:B:1347:GLY:O	2.16	0.45
1:C:2199:ILE:HD12	1:C:2234:PHE:CD2	2.50	0.45
1:A:250:GLN:OE1	1:B:1431:TYR:HB3	2.17	0.45
1:B:1141:LYS:C	1:B:1142:HIS:ND1	2.69	0.45
1:C:2126:MET:CE	1:C:2372:TRP:CE3	2.99	0.45
1:D:3049:ILE:HB	1:D:3073:VAL:HG22	1.98	0.45
1:C:2323:GLN:HG3	1:C:2347:GLY:O	2.16	0.45
1:A:412:GLN:HB3	1:B:1277:CYS:SG	2.57	0.45
1:A:209:MET:CE	1:C:2356:VAL:HG12	2.47	0.45
1:B:1361:PHE:O	1:B:1364:GLN:HB2	2.16	0.45
1:D:3013:LEU:HB3	1:D:3086:HIS:HA	1.97	0.45
1:B:1074:ARG:CD	1:B:1116:THR:HA	2.45	0.45
1:B:1048:ARG:HA	1:B:1072:GLU:HB2	1.96	0.45
1:B:1424:PHE:C	1:B:1425:LYS:HG2	2.36	0.45
1:D:3069:LEU:HD23	1:D:3369:ILE:HD11	1.98	0.45
1:A:15:ALA:O	1:A:19:LYS:HG2	2.17	0.45
1:D:3124:LEU:HG	1:D:3124:LEU:O	2.16	0.45
1:C:2138:ILE:HG22	1:C:2146:LEU:HD22	1.99	0.45
1:B:1054:HIS:HB3	1:B:1082:SER:HB2	1.99	0.45
1:D:3152:ILE:O	1:D:3371:LEU:HD11	2.17	0.45
1:B:1419:PRO:HB2	1:B:1422:GLY:CA	2.47	0.45
1:B:1063:ILE:HG23	1:B:1073:VAL:HG11	1.97	0.45
1:C:2419:PRO:HB2	1:C:2422:GLY:HA3	1.98	0.45
1:C:2109:TYR:CZ	1:C:2113:ILE:HD11	2.52	0.45
1:D:3137:LEU:HD23	1:D:3138:ILE:HD12	1.99	0.45
1:A:223:VAL:HG23	2:A:432:NAD:O1N	2.17	0.45
1:B:1018:ARG:HH21	1:B:1093:LYS:HZ3	1.64	0.45
1:D:3074:ARG:HG3	1:D:3097:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3127:ILE:HG21	1:D:3135:THR:HG22	1.99	0.45
1:C:2141:LYS:C	1:C:2142:HIS:ND1	2.70	0.45
1:C:2140:THR:OG1	1:C:2141:LYS:HG2	2.16	0.45
1:C:2056:THR:HB	1:C:2084:GLN:NE2	2.31	0.45
1:C:2047:ALA:HA	1:C:2125:ASN:HD21	1.81	0.45
1:C:2050:ALA:HB3	1:C:2124:LEU:HD13	1.99	0.45
1:C:2074:ARG:CD	1:C:2116:THR:HA	2.45	0.45
1:C:2360:SER:O	1:C:2363:ASN:HB2	2.15	0.45
1:A:430:ARG:O	1:A:431:TYR:O	2.34	0.45
1:B:1013:LEU:HB3	1:B:1086:HIS:HA	1.99	0.45
1:A:99:PHE:CZ	1:A:115:GLN:HB3	2.52	0.45
1:C:2045:LYS:O	1:C:2045:LYS:HE3	2.17	0.45
1:A:209:MET:CE	1:C:2353:PRO:HG2	2.46	0.45
1:B:1364:GLN:HA	1:B:1364:GLN:OE1	2.17	0.45
1:C:2053:LEU:O	1:C:2054:HIS:C	2.55	0.45
1:B:1111:TRP:NE1	1:B:1115:GLN:NE2	2.65	0.45
1:B:1353:PRO:HD2	1:B:1356:VAL:HG11	1.97	0.45
1:B:1019:LYS:O	1:B:1023:ILE:HG13	2.17	0.45
1:A:124:LEU:O	1:A:124:LEU:HG	2.16	0.45
1:C:2169:ASN:HB2	1:C:2171:ILE:CG1	2.46	0.45
1:A:224:GLY:CA	1:A:274:THR:HG21	2.46	0.45
1:A:356:VAL:HG12	1:C:2209:MET:CE	2.47	0.45
1:C:2328:LEU:HD12	1:C:2329:LEU:H	1.78	0.44
1:A:301:PHE:CD1	1:A:343:LEU:HG	2.52	0.44
1:B:1353:PRO:HG2	1:D:3209:MET:HE2	1.99	0.44
1:C:2081:PHE:CE1	1:C:2103:GLY:HA2	2.52	0.44
1:D:3361:PHE:O	1:D:3364:GLN:HB2	2.17	0.44
1:C:2381:GLY:O	1:C:2383:HIS:CD2	2.70	0.44
1:C:2398:LEU:HG	1:C:2403:VAL:HG11	1.99	0.44
1:C:2406:THR:HG22	1:D:3260:THR:HG22	1.97	0.44
1:A:127:ILE:HG23	1:A:134:LEU:HD12	2.00	0.44
1:B:1179:VAL:HG21	1:B:1363:ASN:HB3	2.00	0.44
1:B:1004:LEU:HA	1:B:1004:LEU:HD23	1.86	0.44
1:D:3146:LEU:HG	1:D:3173:LYS:HG3	1.99	0.44
1:D:3224:GLY:CA	1:D:3274:THR:HG21	2.47	0.44
1:C:2044:LEU:HD21	1:C:2369:ILE:HA	1.99	0.44
1:B:1343:LEU:CD1	1:B:1346:LEU:HD12	2.47	0.44
1:C:2033:ARG:HD2	1:C:2396:ALA:HA	1.98	0.44
1:B:1049:ILE:HD12	1:B:1071:ALA:HB1	1.99	0.44
1:C:2175:PRO:HA	1:C:2381:GLY:H	1.82	0.44
1:D:3210:ILE:O	1:D:3213:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2105:THR:HG23	1:C:2108:GLU:OE1	2.17	0.44
1:B:1350:MET:HG3	1:D:3207:ASP:OD2	2.17	0.44
1:C:2353:PRO:HD2	1:C:2356:VAL:HG11	1.98	0.44
1:C:2406:THR:HG21	3:D:5108:HOH:O	2.16	0.44
1:B:1398:LEU:HG	1:B:1403:VAL:HG11	2.00	0.44
1:C:2038:TYR:HB3	1:C:2043:PRO:CG	2.48	0.44
1:D:3105:THR:C	1:D:3107:GLU:N	2.69	0.44
1:D:3010:ASP:O	1:D:3013:LEU:HB2	2.17	0.44
1:C:2034:MET:HG3	1:C:2365:VAL:HG11	1.99	0.44
1:C:2124:LEU:HD12	1:C:2126:MET:O	2.18	0.44
1:B:1152:ILE:HD11	1:B:1174:VAL:HG13	1.99	0.44
1:C:2152:ILE:HD11	1:C:2174:VAL:HG13	1.99	0.44
1:B:1144:GLN:HE21	1:B:1144:GLN:HB2	1.56	0.44
1:B:1430:ARG:O	1:B:1431:TYR:O	2.35	0.44
1:D:3056:THR:HB	1:D:3084:GLN:HE22	1.83	0.44
1:D:3360:SER:O	1:D:3363:ASN:HB2	2.17	0.44
1:A:17:GLY:HA2	1:A:86:HIS:CD2	2.52	0.44
1:A:419:PRO:HB2	1:A:422:GLY:HA3	1.98	0.44
1:C:2119:PHE:N	1:C:2119:PHE:CD1	2.86	0.44
1:C:2038:TYR:HB3	1:C:2043:PRO:HG3	1.98	0.44
1:D:3175:PRO:HA	1:D:3381:GLY:H	1.82	0.44
1:C:2205:ALA:HB1	1:C:2324:VAL:HG22	2.00	0.44
1:D:3048:ARG:HD2	1:D:3119:PHE:HB2	1.99	0.44
1:C:2274:THR:CG2	1:C:2274:THR:O	2.65	0.44
1:B:1301:PHE:CE1	1:B:1343:LEU:HG	2.52	0.44
1:A:48:ARG:HA	1:A:72:GLU:HB2	2.00	0.44
1:B:1273:THR:HB	1:B:1304:GLU:OE1	2.18	0.43
1:B:1057:VAL:N	1:B:1084:GLN:NE2	2.56	0.43
1:D:3172:LEU:CD1	1:D:3380:VAL:HG12	2.48	0.43
1:D:3419:PRO:HB2	1:D:3422:GLY:HA3	1.99	0.43
1:B:1353:PRO:HD2	1:B:1356:VAL:CG1	2.47	0.43
1:A:50:ALA:HB3	1:A:124:LEU:HD13	1.99	0.43
1:C:2317:LYS:HD2	1:C:2327:TYR:CE2	2.53	0.43
1:D:3239:ILE:HG23	1:D:3257:GLU:HG2	2.00	0.43
1:A:56:THR:HB	1:A:84:GLN:HE22	1.84	0.43
1:A:278:VAL:HG13	1:B:1415:TYR:CZ	2.52	0.43
1:B:1419:PRO:CG	1:B:1422:GLY:HA3	2.47	0.43
1:B:1356:VAL:HG12	1:D:3209:MET:CE	2.48	0.43
1:C:2144:GLN:HB2	1:C:2144:GLN:HE21	1.53	0.43
1:C:2389:LEU:O	1:C:2393:VAL:HG12	2.18	0.43
1:D:3141:LYS:C	1:D:3142:HIS:ND1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:C	1:A:142:HIS:ND1	2.72	0.43
1:B:1048:ARG:HD2	1:B:1119:PHE:HB2	2.01	0.43
1:A:209:MET:HE2	1:C:2353:PRO:HG2	1.99	0.43
1:C:2302:ASP:HA	1:C:2341:GLY:O	2.17	0.43
1:B:1308:LYS:NZ	1:B:1311:ASN:HD22	2.16	0.43
1:B:1395:GLU:HA	1:B:1398:LEU:HD22	2.01	0.43
1:A:183:VAL:HG21	1:B:1246:ILE:HG21	1.99	0.43
1:A:117:LEU:HD13	1:A:142:HIS:CD2	2.53	0.43
1:B:1056:THR:HB	1:B:1084:GLN:NE2	2.33	0.43
1:C:2018:ARG:HH21	1:C:2093:LYS:HZ3	1.64	0.43
1:A:74:ARG:HG3	1:A:97:PRO:HG2	2.01	0.43
1:D:3049:ILE:N	1:D:3072:GLU:O	2.49	0.43
1:B:1398:LEU:HG	1:B:1403:VAL:CG1	2.47	0.43
1:A:55:MET:O	1:A:84:GLN:N	2.43	0.43
1:C:2054:HIS:HB3	1:C:2082:SER:HB2	2.01	0.43
1:D:3099:PHE:CZ	1:D:3115:GLN:HB3	2.54	0.43
1:A:74:ARG:NE	3:A:5107:HOH:O	2.49	0.43
1:D:3308:LYS:HZ2	1:D:3311:ASN:HD22	1.66	0.43
1:C:2027:GLU:C	1:C:2029:PRO:HD3	2.39	0.43
1:A:246:ILE:O	1:A:250:GLN:HG3	2.18	0.43
1:B:1057:VAL:H	1:B:1084:GLN:HE21	1.62	0.43
1:D:3048:ARG:HB3	1:D:3119:PHE:CE2	2.53	0.43
1:B:1196:GLU:HG3	1:D:3209:MET:CE	2.49	0.43
1:A:424:PHE:C	1:A:425:LYS:HG2	2.39	0.43
1:C:2291:ASP:OD1	1:C:2334:ARG:HD3	2.18	0.43
1:C:2300:HIS:HD2	1:C:2303:VAL:HG21	1.83	0.43
1:C:2151:GLY:HA3	1:C:2371:LEU:HD13	2.00	0.43
1:C:2049:ILE:HD12	1:C:2071:ALA:HB1	2.00	0.43
1:D:3074:ARG:CD	1:D:3116:THR:HA	2.47	0.43
1:B:1081:PHE:O	1:B:1102:LYS:HG3	2.18	0.43
1:D:3199:ILE:HG13	3:D:5064:HOH:O	2.18	0.43
1:B:1127:ILE:HG23	1:B:1134:LEU:HD13	1.99	0.43
1:A:274:THR:CG2	1:A:274:THR:O	2.66	0.43
1:A:204:ARG:HH12	1:A:350:MET:CG	2.29	0.43
1:C:2364:GLN:OE1	1:C:2364:GLN:HA	2.19	0.43
1:D:3038:TYR:HB3	1:D:3043:PRO:CD	2.49	0.43
1:D:3197:SER:HB2	1:D:3345:ASN:HB2	2.00	0.43
1:C:2127:ILE:HG23	1:C:2134:LEU:HD13	1.99	0.42
1:B:1044:LEU:HD21	1:B:1369:ILE:HA	2.01	0.42
1:B:1360:SER:O	1:B:1363:ASN:HB2	2.18	0.42
1:B:1153:SER:HB2	1:B:1368:GLN:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2328:LEU:HD12	1:C:2328:LEU:C	2.37	0.42
1:A:353:PRO:HD2	1:A:356:VAL:CG1	2.49	0.42
1:B:1302:ASP:HA	1:B:1341:GLY:O	2.18	0.42
1:D:3081:PHE:CE1	1:D:3103:GLY:HA2	2.54	0.42
1:A:38:TYR:HB3	1:A:43:PRO:CD	2.49	0.42
1:A:361:PHE:O	1:A:364:GLN:HB2	2.20	0.42
1:B:1027:GLU:C	1:B:1029:PRO:HD3	2.39	0.42
1:B:1105:THR:C	1:B:1107:GLU:N	2.73	0.42
1:A:74:ARG:CG	1:A:116:THR:HA	2.50	0.42
1:D:3373:THR:O	1:D:3373:THR:CG2	2.67	0.42
1:A:49:ILE:HD12	1:A:71:ALA:HB1	2.01	0.42
1:C:2240:ILE:HG22	1:C:2241:THR:N	2.34	0.42
1:A:210:ILE:O	1:A:213:LYS:HB2	2.19	0.42
1:C:2430:ARG:O	1:C:2431:TYR:O	2.37	0.42
1:D:3054:HIS:HB3	1:D:3082:SER:CB	2.50	0.42
1:C:2007:LYS:HG3	1:C:2111:TRP:HH2	1.84	0.42
1:C:2199:ILE:HG21	1:C:2234:PHE:CE2	2.54	0.42
1:A:144:GLN:HB2	1:A:144:GLN:HE21	1.54	0.42
1:C:2382:VAL:HG22	1:C:2382:VAL:O	2.19	0.42
1:C:2210:ILE:O	1:C:2213:LYS:HB2	2.20	0.42
1:A:246:ILE:HG21	1:B:1183:VAL:HG21	2.01	0.42
1:B:1274:THR:CG2	3:B:5145:HOH:O	2.68	0.42
1:B:1050:ALA:HB3	1:B:1124:LEU:HD13	2.02	0.42
1:C:2343:LEU:HD12	1:C:2346:LEU:CD1	2.47	0.42
1:B:1406:THR:HG22	3:B:5082:HOH:O	2.16	0.42
1:A:81:PHE:CE1	1:A:103:GLY:HA2	2.55	0.42
1:B:1179:VAL:HG22	1:B:1363:ASN:HB3	2.00	0.42
1:C:2385:LEU:O	1:C:2386:PRO:C	2.57	0.42
1:A:169:ASN:HB2	1:A:171:ILE:CG1	2.47	0.42
1:B:1140:THR:OG1	1:B:1141:LYS:HG2	2.19	0.42
1:A:44:LEU:HD21	1:A:369:ILE:HA	2.01	0.42
1:B:1151:GLY:HA3	1:B:1371:LEU:HD13	2.01	0.42
1:C:2334:ARG:N	1:C:2334:ARG:HD3	2.34	0.42
1:C:2019:LYS:O	1:C:2023:ILE:HG13	2.19	0.42
1:C:2199:ILE:HB	3:C:5292:HOH:O	2.20	0.42
1:D:3385:LEU:O	1:D:3386:PRO:C	2.56	0.42
1:D:3127:ILE:HG23	1:D:3134:LEU:HD13	2.00	0.42
1:A:138:ILE:HD12	1:A:138:ILE:N	2.35	0.42
1:C:2143:PRO:O	1:C:2146:LEU:HB2	2.20	0.42
1:C:2017:GLY:HA2	1:C:2086:HIS:CD2	2.54	0.42
1:C:2093:LYS:HG2	1:C:2093:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3119:PHE:N	1:D:3119:PHE:CD1	2.88	0.42
1:C:2048:ARG:HD2	1:C:2119:PHE:HB2	2.02	0.42
1:C:2179:VAL:HG22	1:C:2363:ASN:HB3	2.02	0.42
1:C:2004:LEU:HD23	1:C:2004:LEU:HA	1.88	0.42
1:B:1175:PRO:HA	1:B:1381:GLY:H	1.85	0.42
1:D:3382:VAL:O	1:D:3382:VAL:HG22	2.20	0.42
1:C:2275:THR:CG2	1:C:2277:CYS:H	2.17	0.42
1:B:1010:ASP:O	1:B:1013:LEU:HB2	2.20	0.42
1:C:2010:ASP:O	1:C:2013:LEU:HB2	2.20	0.42
1:A:54:HIS:CE1	1:A:78:CYS:SG	3.12	0.42
1:B:1044:LEU:HA	1:B:1372:TRP:CD1	2.55	0.42
1:C:2301:PHE:CE1	1:C:2343:LEU:HG	2.54	0.42
1:A:119:PHE:N	1:A:122:GLY:O	2.44	0.42
1:B:1381:GLY:O	1:B:1383:HIS:CD2	2.72	0.42
1:C:2008:VAL:HG12	1:C:2009:ALA:N	2.35	0.42
1:D:3323:GLN:HG3	1:D:3347:GLY:O	2.20	0.42
1:D:3140:THR:OG1	1:D:3141:LYS:HG2	2.20	0.42
1:D:3031:LEU:O	1:D:3034:MET:HB2	2.20	0.42
1:C:2057:VAL:N	1:C:2084:GLN:NE2	2.56	0.41
1:D:3301:PHE:CD1	1:D:3343:LEU:HG	2.55	0.41
1:A:119:PHE:N	1:A:119:PHE:CD1	2.88	0.41
1:A:419:PRO:HB2	1:A:422:GLY:CA	2.50	0.41
1:C:2398:LEU:HG	1:C:2403:VAL:CG1	2.49	0.41
1:C:2240:ILE:O	1:C:2258:VAL:HA	2.20	0.41
1:B:1165:LYS:HZ3	1:B:1166:MET:HG2	1.85	0.41
1:D:3054:HIS:CE1	1:D:3078:CYS:SG	3.13	0.41
1:A:34:MET:HG3	1:A:365:VAL:HG11	2.02	0.41
1:B:1120:LYS:HG3	1:B:1120:LYS:H	1.64	0.41
1:B:1054:HIS:HB3	1:B:1082:SER:CB	2.50	0.41
1:C:2049:ILE:N	1:C:2072:GLU:O	2.52	0.41
1:A:390:ASP:O	1:A:393:VAL:HG13	2.20	0.41
1:C:2277:CYS:SG	1:C:2278:VAL:N	2.93	0.41
1:B:1143:PRO:O	1:B:1146:LEU:HB2	2.20	0.41
1:D:3057:VAL:H	1:D:3084:GLN:HE21	1.62	0.41
1:B:1054:HIS:CE1	1:B:1078:CYS:SG	3.13	0.41
1:D:3111:TRP:NE1	1:D:3115:GLN:NE2	2.67	0.41
1:B:1124:LEU:HD12	1:B:1126:MET:O	2.20	0.41
1:A:389:LEU:O	1:A:393:VAL:HG12	2.21	0.41
1:A:276:GLY:H	1:A:304:GLU:CD	2.23	0.41
1:A:276:GLY:N	1:A:304:GLU:OE2	2.49	0.41
1:A:142:HIS:HB3	1:A:145:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3017:GLY:HA2	1:D:3086:HIS:CD2	2.55	0.41
1:B:1197:SER:O	1:B:1198:LEU:C	2.59	0.41
1:B:1334:ARG:HD3	1:B:1334:ARG:N	2.36	0.41
1:B:1385:LEU:O	1:B:1386:PRO:C	2.58	0.41
1:D:3276:GLY:H	1:D:3304:GLU:CD	2.22	0.41
1:C:2044:LEU:HA	1:C:2372:TRP:CD1	2.56	0.41
1:C:2125:ASN:ND2	1:C:2372:TRP:CZ3	2.89	0.41
1:A:403:VAL:HG22	1:B:1258:VAL:HB	2.01	0.41
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.86	0.41
1:A:317:LYS:HD2	1:A:327:TYR:CE2	2.56	0.41
1:D:3062:LEU:O	1:D:3065:THR:HB	2.19	0.41
1:C:2415:TYR:CE2	1:D:3278:VAL:HG13	2.54	0.41
1:A:171:ILE:O	1:A:173:LYS:HG2	2.21	0.41
1:C:2138:ILE:N	1:C:2138:ILE:HD12	2.35	0.41
1:C:2146:LEU:HD13	1:C:2146:LEU:HA	1.84	0.41
1:D:3205:ALA:HB1	1:D:3324:VAL:HG22	2.03	0.41
1:A:57:VAL:H	1:A:84:GLN:HE21	1.63	0.41
1:D:3204:ARG:HH12	1:D:3350:MET:CG	2.30	0.41
1:D:3199:ILE:CG1	3:D:5064:HOH:O	2.69	0.41
1:A:197:SER:HB2	1:A:345:ASN:HB2	2.01	0.41
1:D:3169:ASN:HD22	1:D:3171:ILE:CD1	2.34	0.41
1:D:3044:LEU:HA	1:D:3372:TRP:CD1	2.56	0.41
3:C:5105:HOH:O	1:D:3406:THR:HG21	2.19	0.41
1:D:3313:ASN:N	1:D:3313:ASN:ND2	2.69	0.41
1:D:3409:THR:OG1	1:D:3412:GLN:HG3	2.21	0.41
1:B:1017:GLY:HA2	1:B:1086:HIS:CD2	2.55	0.41
1:D:3057:VAL:N	1:D:3084:GLN:NE2	2.58	0.41
1:B:1205:ALA:HB1	1:B:1324:VAL:HG22	2.03	0.41
1:C:2223:VAL:HG23	2:C:2432:NAD:O1N	2.20	0.41
1:D:3419:PRO:HB2	1:D:3422:GLY:CA	2.51	0.41
1:B:1049:ILE:N	1:B:1072:GLU:O	2.52	0.41
1:D:3430:ARG:O	1:D:3431:TYR:O	2.38	0.41
1:A:152:ILE:O	1:A:371:LEU:HD11	2.21	0.41
1:D:3105:THR:C	1:D:3107:GLU:H	2.23	0.41
1:C:2204:ARG:HH12	1:C:2350:MET:CG	2.28	0.41
1:A:328:LEU:HD12	1:A:329:LEU:H	1.83	0.41
1:B:1301:PHE:O	1:B:1302:ASP:OD1	2.38	0.41
1:B:1119:PHE:CD1	1:B:1119:PHE:N	2.89	0.41
1:B:1353:PRO:HG2	1:D:3209:MET:CE	2.50	0.41
1:D:3279:ASP:HA	1:D:3282:LEU:HD11	2.01	0.41
1:B:1038:TYR:HB3	1:B:1043:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2197:SER:O	1:C:2198:LEU:C	2.60	0.41
1:C:2406:THR:HG23	1:D:3242:GLU:O	2.21	0.41
1:B:1008:VAL:HG12	1:B:1009:ALA:N	2.35	0.41
1:A:416:LEU:CG	1:B:1277:CYS:HB2	2.51	0.41
1:C:2057:VAL:HG23	1:C:2084:GLN:NE2	2.35	0.41
1:B:1224:GLY:CA	1:B:1274:THR:HG21	2.51	0.41
1:B:1203:LYS:O	1:B:1207:ASP:N	2.54	0.41
1:D:3300:HIS:HD2	1:D:3303:VAL:HG21	1.86	0.40
1:D:3407:LYS:HE2	1:D:3421:ASN:OD1	2.22	0.40
1:D:3274:THR:O	1:D:3274:THR:CG2	2.68	0.40
1:C:2343:LEU:CD1	1:C:2346:LEU:HD12	2.51	0.40
1:B:1109:TYR:CZ	1:B:1113:ILE:HD11	2.57	0.40
1:B:1382:VAL:O	1:B:1382:VAL:HG22	2.21	0.40
1:D:3052:CYS:HA	1:D:3076:SER:O	2.21	0.40
1:A:21:LEU:CD2	1:A:57:VAL:HG13	2.50	0.40
1:D:3092:ALA:HB2	1:D:3098:VAL:HG23	2.02	0.40
1:A:93:LYS:O	1:A:93:LYS:HG2	2.20	0.40
1:D:3146:LEU:HD13	1:D:3146:LEU:HA	1.85	0.40
1:C:2169:ASN:HD22	1:C:2171:ILE:HD11	1.87	0.40
1:B:1165:LYS:NZ	1:B:1166:MET:HG2	2.36	0.40
1:B:1021:LEU:CD2	1:B:1057:VAL:HG13	2.47	0.40
1:D:3010:ASP:CB	1:D:3013:LEU:HD22	2.45	0.40
1:A:80:ILE:HD12	1:A:81:PHE:CE2	2.55	0.40
1:A:109:TYR:CZ	1:A:113:ILE:HD11	2.56	0.40
1:D:3144:GLN:HB2	1:D:3144:GLN:HE21	1.57	0.40
1:C:2416:LEU:CD2	1:D:3277:CYS:HB2	2.42	0.40
1:A:146:LEU:HA	1:A:146:LEU:HD13	1.84	0.40
1:A:57:VAL:N	1:A:84:GLN:NE2	2.57	0.40
1:A:205:ALA:HB1	1:A:324:VAL:HG22	2.04	0.40
1:A:44:LEU:HA	1:A:372:TRP:CD1	2.57	0.40
1:B:1199:ILE:HG13	3:B:5143:HOH:O	2.21	0.40
1:D:3179:VAL:HG22	1:D:3363:ASN:HB3	2.02	0.40
1:C:2052:CYS:HA	1:C:2076:SER:O	2.22	0.40
1:A:127:ILE:CG2	1:A:152:ILE:HG23	2.51	0.40
1:D:3057:VAL:O	1:D:3060:ALA:HB3	2.22	0.40
1:B:1328:LEU:HD12	1:B:1329:LEU:H	1.82	0.40
1:B:1240:ILE:O	1:B:1258:VAL:HA	2.22	0.40
1:D:3050:ALA:HB3	1:D:3124:LEU:HD13	2.03	0.40
1:D:3364:GLN:HA	1:D:3364:GLN:OE1	2.21	0.40
1:A:302:ASP:HA	1:A:341:GLY:O	2.21	0.40
1:A:91:ILE:HA	1:A:91:ILE:HD13	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:HA	1:A:76:SER: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	426/431 (99%)	409 (96%)	16 (4%)	1 (0%)	52	84
1	B	426/431 (99%)	407 (96%)	18 (4%)	1 (0%)	52	84
1	C	426/431 (99%)	410 (96%)	15 (4%)	1 (0%)	52	84
1	D	426/431 (99%)	408 (96%)	17 (4%)	1 (0%)	52	84
All	All	1704/1724 (99%)	1634 (96%)	66 (4%)	4 (0%)	52	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ASP
1	B	1302	ASP
1	C	2302	ASP
1	D	3302	ASP

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	351/353 (99%)	288 (82%)	63 (18%)	2	6
1	B	351/353 (99%)	288 (82%)	63 (18%)	2	6
1	C	351/353 (99%)	287 (82%)	64 (18%)	2	6
1	D	351/353 (99%)	288 (82%)	63 (18%)	2	6
All	All	1404/1412 (99%)	1151 (82%)	253 (18%)	2	6

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	13	LEU
1	A	26	ASN
1	A	34	MET
1	A	37	MET
1	A	41	SER
1	A	45	LYS
1	A	53	LEU
1	A	72	GLU
1	A	74	ARG
1	A	80	ILE
1	A	83	THR
1	A	84	GLN
1	A	93	LYS
1	A	98	VAL
1	A	106	ASP
1	A	110	LEU
1	A	120	LYS
1	A	124	LEU
1	A	134	LEU
1	A	135	THR
1	A	140	THR
1	A	141	LYS
1	A	142	HIS
1	A	144	GLN
1	A	146	LEU
1	A	147	SER
1	A	153	SER
1	A	157	THR
1	A	162	ASN
1	A	165	LYS
1	A	172	LEU
1	A	174	VAL

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Mol	Chain	Res	Type
1	A	179	VAL
1	A	191	LEU
1	A	213	LYS
1	A	242	GLU
1	A	249	LEU
1	A	254	GLU
1	A	259	THR
1	A	277	CYS
1	A	282	LEU
1	A	288	GLN
1	A	301	PHE
1	A	302	ASP
1	A	303	VAL
1	A	308	LYS
1	A	321	LYS
1	A	334	ARG
1	A	337	LEU
1	A	357	MET
1	A	370	GLU
1	A	382	VAL
1	A	387	LYS
1	A	393	VAL
1	A	398	LEU
1	A	400	LYS
1	A	402	ASN
1	A	404	LYS
1	A	406	THR
1	A	407	LYS
1	A	408	LEU
1	A	418	MET
1	B	1007	LYS
1	B	1013	LEU
1	B	1026	ASN
1	B	1034	MET
1	B	1037	MET
1	B	1039	SER
1	B	1041	SER
1	B	1045	LYS
1	B	1053	LEU
1	B	1072	GLU
1	B	1074	ARG
1	B	1083	THR

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Mol	Chain	Res	Type
1	B	1093	LYS
1	B	1098	VAL
1	B	1106	ASP
1	B	1110	LEU
1	B	1120	LYS
1	B	1124	LEU
1	B	1134	LEU
1	B	1135	THR
1	B	1140	THR
1	B	1141	LYS
1	B	1142	HIS
1	B	1144	GLN
1	B	1146	LEU
1	B	1147	SER
1	B	1153	SER
1	B	1157	THR
1	B	1162	ASN
1	B	1163	LEU
1	B	1165	LYS
1	B	1172	LEU
1	B	1174	VAL
1	B	1179	VAL
1	B	1191	LEU
1	B	1213	LYS
1	B	1242	GLU
1	B	1249	LEU
1	B	1254	GLU
1	B	1259	THR
1	B	1277	CYS
1	B	1282	LEU
1	B	1288	GLN
1	B	1301	PHE
1	B	1302	ASP
1	B	1303	VAL
1	B	1308	LYS
1	B	1321	LYS
1	B	1334	ARG
1	B	1337	LEU
1	B	1357	MET
1	B	1370	GLU
1	B	1382	VAL
1	B	1387	LYS

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Mol	Chain	Res	Type
1	B	1393	VAL
1	B	1398	LEU
1	B	1400	LYS
1	B	1402	ASN
1	B	1404	LYS
1	B	1406	THR
1	B	1407	LYS
1	B	1408	LEU
1	B	1418	MET
1	C	2007	LYS
1	C	2013	LEU
1	C	2026	ASN
1	C	2034	MET
1	C	2037	MET
1	C	2039	SER
1	C	2041	SER
1	C	2045	LYS
1	C	2053	LEU
1	C	2072	GLU
1	C	2074	ARG
1	C	2080	ILE
1	C	2083	THR
1	C	2084	GLN
1	C	2093	LYS
1	C	2098	VAL
1	C	2106	ASP
1	C	2110	LEU
1	C	2120	LYS
1	C	2124	LEU
1	C	2134	LEU
1	C	2135	THR
1	C	2140	THR
1	C	2141	LYS
1	C	2142	HIS
1	C	2144	GLN
1	C	2146	LEU
1	C	2147	SER
1	C	2153	SER
1	C	2157	THR
1	C	2162	ASN
1	C	2163	LEU
1	C	2165	LYS

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Mol	Chain	Res	Type
1	C	2172	LEU
1	C	2174	VAL
1	C	2179	VAL
1	C	2191	LEU
1	C	2213	LYS
1	C	2249	LEU
1	C	2254	GLU
1	C	2259	THR
1	C	2277	CYS
1	C	2282	LEU
1	C	2288	GLN
1	C	2301	PHE
1	C	2302	ASP
1	C	2303	VAL
1	C	2308	LYS
1	C	2321	LYS
1	C	2334	ARG
1	C	2337	LEU
1	C	2357	MET
1	C	2370	GLU
1	C	2382	VAL
1	C	2387	LYS
1	C	2393	VAL
1	C	2398	LEU
1	C	2400	LYS
1	C	2402	ASN
1	C	2404	LYS
1	C	2406	THR
1	C	2407	LYS
1	C	2408	LEU
1	C	2418	MET
1	D	3007	LYS
1	D	3013	LEU
1	D	3026	ASN
1	D	3034	MET
1	D	3037	MET
1	D	3041	SER
1	D	3045	LYS
1	D	3053	LEU
1	D	3072	GLU
1	D	3074	ARG
1	D	3080	ILE

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Mol	Chain	Res	Type
1	D	3083	THR
1	D	3084	GLN
1	D	3093	LYS
1	D	3098	VAL
1	D	3106	ASP
1	D	3110	LEU
1	D	3120	LYS
1	D	3124	LEU
1	D	3134	LEU
1	D	3135	THR
1	D	3140	THR
1	D	3141	LYS
1	D	3142	HIS
1	D	3144	GLN
1	D	3146	LEU
1	D	3147	SER
1	D	3153	SER
1	D	3157	THR
1	D	3162	ASN
1	D	3165	LYS
1	D	3172	LEU
1	D	3174	VAL
1	D	3179	VAL
1	D	3191	LEU
1	D	3213	LYS
1	D	3242	GLU
1	D	3249	LEU
1	D	3254	GLU
1	D	3259	THR
1	D	3277	CYS
1	D	3282	LEU
1	D	3288	GLN
1	D	3301	PHE
1	D	3302	ASP
1	D	3303	VAL
1	D	3308	LYS
1	D	3321	LYS
1	D	3334	ARG
1	D	3337	LEU
1	D	3357	MET
1	D	3370	GLU
1	D	3382	VAL

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Mol	Chain	Res	Type
1	D	3387	LYS
1	D	3393	VAL
1	D	3398	LEU
1	D	3400	LYS
1	D	3402	ASN
1	D	3404	LYS
1	D	3406	THR
1	D	3407	LYS
1	D	3408	LEU
1	D	3418	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	115	GLN
1	A	136	ASN
1	A	144	GLN
1	A	169	ASN
1	A	300	HIS
1	A	311	ASN
1	A	359	ASN
1	A	402	ASN
1	B	1084	GLN
1	B	1115	GLN
1	B	1136	ASN
1	B	1144	GLN
1	B	1162	ASN
1	B	1169	ASN
1	B	1300	HIS
1	B	1311	ASN
1	C	2084	GLN
1	C	2115	GLN
1	C	2136	ASN
1	C	2144	GLN
1	C	2169	ASN
1	C	2300	HIS
1	C	2311	ASN
1	D	3084	GLN
1	D	3115	GLN
1	D	3136	ASN
1	D	3144	GLN

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Mol	Chain	Res	Type
1	D	3169	ASN
1	D	3300	HIS
1	D	3311	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	432	-	38,48,48	1.99	7 (18%)	47,73,73	2.50	12 (25%)
2	NAD	B	1432	-	38,48,48	2.08	7 (18%)	47,73,73	2.53	12 (25%)
2	NAD	C	2432	-	38,48,48	2.08	7 (18%)	47,73,73	2.46	11 (23%)
2	NAD	D	3432	-	38,48,48	2.08	6 (15%)	47,73,73	2.46	11 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	432	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1432	-	-	0/22/62/62	0/5/5/5
2	NAD	C	2432	-	-	0/22/62/62	0/5/5/5
2	NAD	D	3432	-	-	0/22/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	432	NAD	O4B-C1B	-4.78	1.35	1.41
2	D	3432	NAD	O4B-C1B	-4.67	1.35	1.41
2	C	2432	NAD	O4B-C1B	-4.52	1.35	1.41
2	B	1432	NAD	O4B-C1B	-3.91	1.36	1.41
2	A	432	NAD	C6N-C5N	-2.20	1.33	1.38
2	A	432	NAD	C7N-N7N	2.05	1.37	1.33
2	C	2432	NAD	C2A-N1A	2.13	1.38	1.33
2	B	1432	NAD	C2A-N1A	2.22	1.38	1.33
2	D	3432	NAD	C7N-N7N	2.30	1.37	1.33
2	C	2432	NAD	C7N-N7N	2.35	1.37	1.33
2	B	1432	NAD	C7N-N7N	2.47	1.38	1.33
2	D	3432	NAD	C6N-N1N	3.32	1.44	1.35
2	C	2432	NAD	C6N-N1N	3.41	1.44	1.35
2	A	432	NAD	C6N-N1N	3.47	1.44	1.35
2	B	1432	NAD	C6N-N1N	3.54	1.44	1.35
2	A	432	NAD	C2N-C3N	5.08	1.46	1.39
2	A	432	NAD	C4N-C3N	5.12	1.48	1.39
2	C	2432	NAD	C4N-C3N	5.22	1.48	1.39
2	D	3432	NAD	C4N-C3N	5.37	1.48	1.39
2	B	1432	NAD	C4N-C3N	5.41	1.48	1.39
2	C	2432	NAD	C2N-C3N	5.64	1.47	1.39
2	B	1432	NAD	C2N-C3N	5.67	1.47	1.39
2	D	3432	NAD	C2N-C3N	6.14	1.48	1.39
2	A	432	NAD	C5N-C4N	6.20	1.51	1.38
2	D	3432	NAD	C5N-C4N	6.22	1.51	1.38
2	B	1432	NAD	C5N-C4N	6.71	1.52	1.38
2	C	2432	NAD	C5N-C4N	6.80	1.52	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1432	NAD	O3-PN-O5D	-9.40	77.99	102.94
2	A	432	NAD	O3-PN-O5D	-9.26	78.36	102.94
2	D	3432	NAD	O3-PN-O5D	-9.19	78.56	102.94
2	C	2432	NAD	O3-PN-O5D	-8.97	79.13	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	432	NAD	O5D-PN-O1N	-7.07	82.16	109.62
2	C	2432	NAD	O5D-PN-O1N	-7.04	82.29	109.62
2	D	3432	NAD	O5D-PN-O1N	-6.96	82.59	109.62
2	B	1432	NAD	O5D-PN-O1N	-6.86	82.97	109.62
2	B	1432	NAD	O7N-C7N-C3N	-5.97	113.07	119.59
2	C	2432	NAD	O7N-C7N-C3N	-5.80	113.25	119.59
2	A	432	NAD	O7N-C7N-C3N	-5.80	113.25	119.59
2	D	3432	NAD	O7N-C7N-C3N	-5.28	113.82	119.59
2	B	1432	NAD	PN-O3-PA	-4.15	121.08	132.73
2	A	432	NAD	PN-O3-PA	-4.14	121.10	132.73
2	D	3432	NAD	PN-O3-PA	-3.95	121.64	132.73
2	C	2432	NAD	PN-O3-PA	-3.77	122.14	132.73
2	D	3432	NAD	O2N-PN-O5D	-3.46	91.00	108.46
2	C	2432	NAD	O2N-PN-O5D	-3.45	91.09	108.46
2	B	1432	NAD	O2N-PN-O5D	-3.44	91.09	108.46
2	B	1432	NAD	C5N-C4N-C3N	-3.39	116.07	120.33
2	D	3432	NAD	C5N-C4N-C3N	-3.37	116.10	120.33
2	C	2432	NAD	C5N-C4N-C3N	-3.27	116.22	120.33
2	A	432	NAD	O2N-PN-O5D	-3.22	92.22	108.46
2	A	432	NAD	C5N-C4N-C3N	-3.09	116.45	120.33
2	B	1432	NAD	N3A-C2A-N1A	-2.38	127.07	128.89
2	A	432	NAD	N3A-C2A-N1A	-2.36	127.09	128.89
2	A	432	NAD	O5B-C5B-C4B	-2.34	100.49	109.12
2	C	2432	NAD	N3A-C2A-N1A	-2.29	127.14	128.89
2	D	3432	NAD	O5B-C5B-C4B	-2.26	100.77	109.12
2	B	1432	NAD	O5B-C5B-C4B	-2.26	100.80	109.12
2	C	2432	NAD	O5B-C5B-C4B	-2.24	100.85	109.12
2	C	2432	NAD	C5N-C6N-N1N	2.18	124.24	120.47
2	B	1432	NAD	O4D-C1D-N1N	2.21	110.55	108.13
2	B	1432	NAD	C5N-C6N-N1N	2.25	124.36	120.47
2	A	432	NAD	C5N-C6N-N1N	2.25	124.37	120.47
2	D	3432	NAD	C5N-C6N-N1N	2.39	124.61	120.47
2	C	2432	NAD	C4A-C5A-N7A	2.43	111.72	109.48
2	D	3432	NAD	C4A-C5A-N7A	2.46	111.74	109.48
2	A	432	NAD	O4D-C1D-N1N	2.46	110.84	108.13
2	B	1432	NAD	C4A-C5A-N7A	2.52	111.80	109.48
2	A	432	NAD	C4A-C5A-N7A	2.60	111.87	109.48
2	D	3432	NAD	O4D-C1D-N1N	2.92	111.34	108.13
2	D	3432	NAD	C3N-C7N-N7N	5.80	124.16	117.82
2	C	2432	NAD	C3N-C7N-N7N	6.09	124.48	117.82
2	B	1432	NAD	C3N-C7N-N7N	6.20	124.61	117.82
2	A	432	NAD	C3N-C7N-N7N	6.21	124.61	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	432	NAD	1	0
2	C	2432	NAD	1	0

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.