Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 03:53 pm GMT

PDB ID	:	2FUN
Title	:	alternative p35-caspase-8 complex
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Deposited on	:	2006-01-27
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

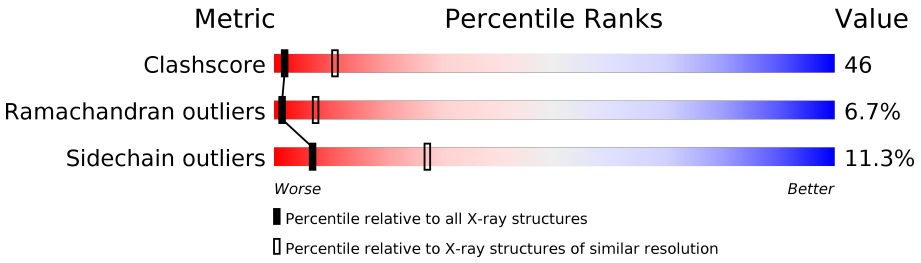
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	298	36% 49% 12%
1	C	298	35% 51% 11%
2	B	258	35% 51% 8% 6%
2	D	258	28% 51% 14% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8713 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 Early 35 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2406	1541	393	461	11			
1	C	293	Total	C	N	O	S	0	0	0
			2406	1541	393	461	11			

- Molecule 2 is a protein called caspase-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1945	1228	333	368	16			
2	D	241	Total	C	N	O	S	0	0	0
			1930	1221	331	362	16			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	4	Total	O	0	0
			4	4		
3	C	9	Total	O	0	0
			9	9		
3	D	3	Total	O	0	0
			3	3		

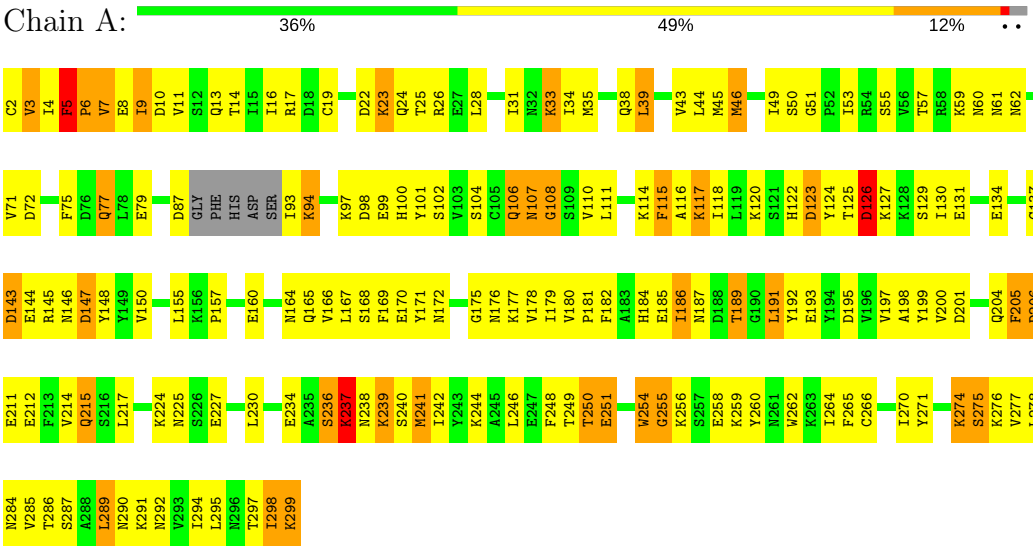
3 Residue-property plots (i)

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

Note EDS was not executed.

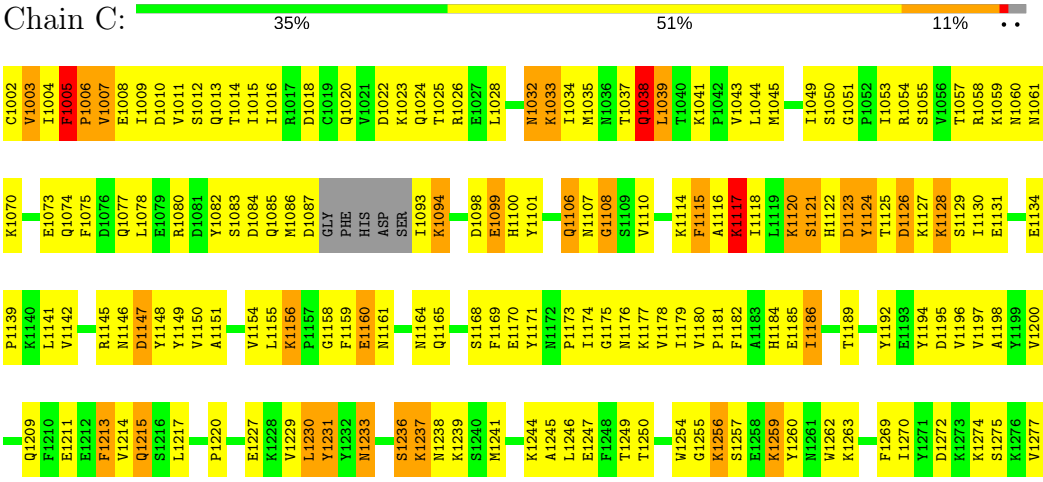
• Molecule 1: Early 35 kDa protein

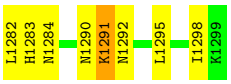
Chain A:



• Molecule 1: Early 35 kDa protein

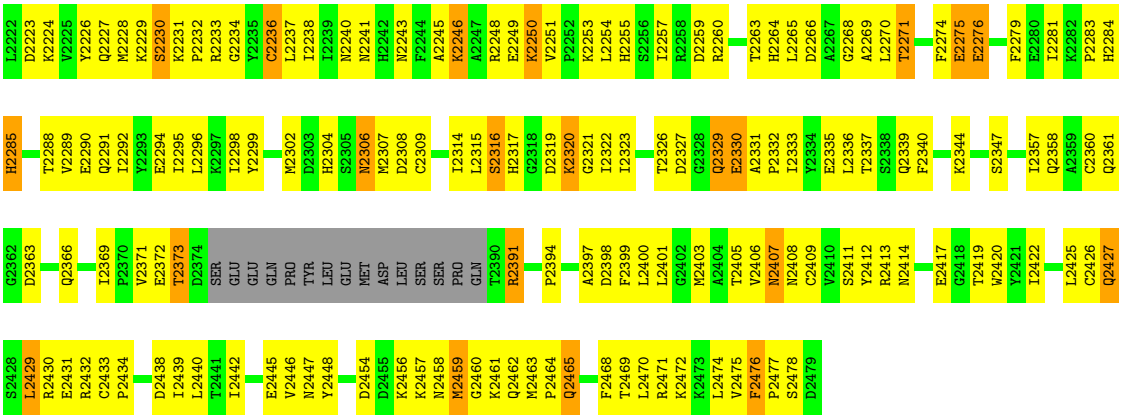
Chain C:





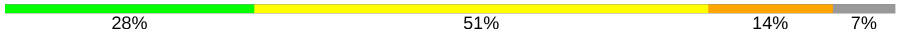
• Molecule 2: caspase-8

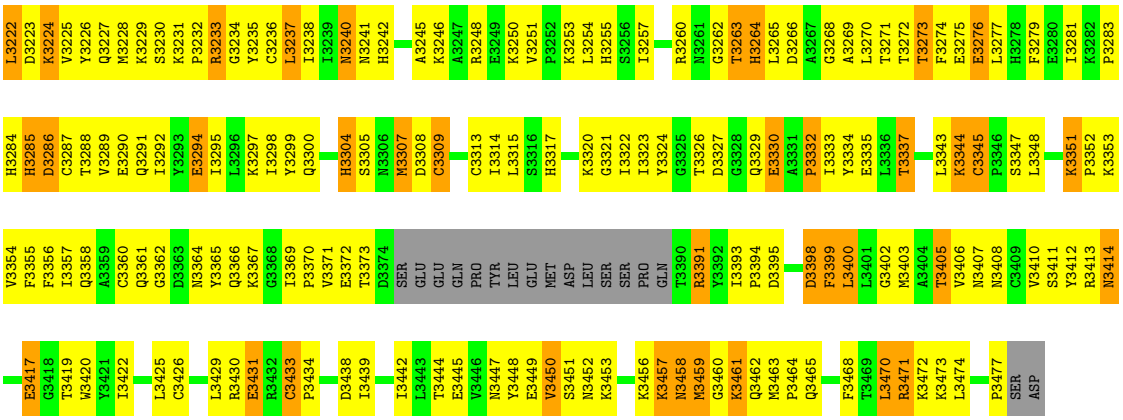
Chain B:



• Molecule 2: caspase-8

Chain D:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	99.97Å 117.34Å 346.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (24.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8713	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/2454	0.65	0/3307
1	C	0.40	0/2454	0.66	0/3307
2	B	0.37	0/1987	0.60	0/2682
2	D	0.34	0/1972	0.56	0/2663
All	All	0.38	0/8867	0.62	0/11959

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2406	0	2389	219	0
1	C	2406	0	2389	210	0
2	B	1945	0	1915	168	0
2	D	1930	0	1906	211	0
3	A	10	0	0	3	0
3	B	4	0	0	2	0
3	C	9	0	0	3	0
3	D	3	0	0	1	0
All	All	8713	0	8599	796	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 46.

All (796) 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:1039:LEU:HD12	1:C:1043:VAL:HG21	1.33	1.10
2:D:3273:THR:HG23	2:D:3430:ARG:HB3	1.32	1.10
2:B:2231:LYS:HB2	2:B:2232:PRO:HD3	1.34	1.08
2:D:3393:ILE:HG12	2:D:3471:ARG:HH22	1.13	1.07
1:A:104:SER:HB2	1:A:120:LYS:HD2	1.36	1.07
2:D:3456:LYS:HE2	2:D:3456:LYS:HA	1.38	1.02
2:D:3391:ARG:HH11	2:D:3391:ARG:HB3	1.21	1.01
1:C:1184:HIS:H	1:C:1290:ASN:ND2	1.59	1.00
2:B:2228:MET:HE2	2:B:2476:PHE:HD1	1.26	1.00
1:C:1049:ILE:HD11	1:C:1151:ALA:HB2	1.45	0.99
1:A:38:GLN:HA	1:A:160:GLU:HG3	1.41	0.98
1:A:227:GLU:HB2	1:A:246:LEU:HD21	1.44	0.97
1:C:1184:HIS:N	1:C:1290:ASN:HD21	1.62	0.97
1:A:60:ASN:HD21	1:A:62:ASN:HD22	1.01	0.97
1:C:1013:GLN:HG3	1:C:1014:THR:H	1.33	0.94
2:D:3271:THR:HG22	2:D:3281:ILE:HG21	1.49	0.94
2:D:3270:LEU:HD21	2:D:3422:ILE:HG23	1.50	0.93
1:C:1018:ASP:HB3	1:C:1200:VAL:HG12	1.51	0.92
1:A:33:LYS:HD2	1:A:33:LYS:H	1.35	0.90
1:C:1061:ASN:HD21	1:C:1165:GLN:HG2	1.37	0.89
2:D:3260:ARG:HH22	2:D:3263:THR:HG23	1.39	0.87
2:D:3288:THR:HG22	2:D:3326:THR:HB	1.55	0.87
1:A:60:ASN:HD21	1:A:62:ASN:ND2	1.73	0.87
1:C:1035:MET:HG2	1:C:1155:LEU:HD21	1.58	0.86
1:A:241:MET:HG2	1:A:270:ILE:HG23	1.58	0.85
2:B:2357:ILE:HD12	2:B:2403:MET:HE1	1.55	0.85
1:C:1032:ASN:HD22	1:C:1032:ASN:C	1.79	0.85
1:A:39:LEU:H	1:A:39:LEU:HD22	1.42	0.85
1:A:34:ILE:H	1:A:34:ILE:HD12	1.42	0.84
2:D:3233:ARG:NH2	2:D:3477:PRO:HG2	1.91	0.84
2:B:2224:LYS:HG3	2:B:2472:LYS:HD3	1.60	0.83
1:C:1038:GLN:HA	1:C:1160:GLU:HG2	1.59	0.83
1:C:1259:LYS:HD2	1:C:1259:LYS:H	1.43	0.82
2:D:3391:ARG:NH1	2:D:3391:ARG:HB3	1.94	0.82
2:B:2413:ARG:HG3	2:B:2419:THR:HG22	1.59	0.82
2:D:3393:ILE:HG12	2:D:3471:ARG:NH2	1.95	0.82
2:B:2251:VAL:HG13	2:B:2254:LEU:HB2	1.61	0.81
2:D:3222:LEU:HG	2:D:3223:ASP:H	1.45	0.80
1:A:104:SER:CB	1:A:120:LYS:HD2	2.12	0.80
1:C:1281:LYS:HE2	1:C:1283:HIS:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3315:LEU:HD23	2:D:3358:GLN:HB3	1.64	0.80
1:A:53:ILE:O	1:A:94:LYS:HE3	1.82	0.79
1:A:60:ASN:ND2	1:A:62:ASN:HD22	1.79	0.79
1:A:214:VAL:HG21	1:A:242:ILE:HG22	1.62	0.79
2:B:2266:ASP:HB3	2:B:2422:ILE:HG21	1.62	0.79
2:B:2414:ASN:HD22	2:B:2417:GLU:H	1.32	0.78
2:D:3393:ILE:HG23	2:D:3394:PRO:HD2	1.65	0.78
1:A:106:GLN:NE2	1:A:106:GLN:H	1.81	0.78
2:D:3274:PHE:O	2:D:3279:PHE:HB2	1.84	0.78
2:D:3333:ILE:HD12	2:D:3334:TYR:H	1.48	0.78
2:D:3270:LEU:HD23	2:D:3426:CYS:SG	2.24	0.78
2:D:3238:ILE:HA	2:D:3313:CYS:SG	2.24	0.77
2:B:2271:THR:HG22	2:B:2281:ILE:HG21	1.67	0.77
1:C:1004:ILE:HD11	2:D:3253:LYS:HD2	1.66	0.77
1:A:207:GLY:O	1:A:211:GLU:HG3	1.84	0.77
1:A:237:LYS:HG2	1:A:238:ASN:H	1.47	0.77
2:B:2260:ARG:NH2	2:B:2263:THR:HG23	1.99	0.77
1:A:204:GLN:HE21	1:A:205:PHE:H	1.32	0.77
1:A:118:ILE:HG12	1:A:122:HIS:HB3	1.67	0.77
2:B:2274:PHE:O	2:B:2279:PHE:HB2	1.85	0.76
1:C:1038:GLN:HA	1:C:1160:GLU:CG	2.15	0.76
2:D:3354:VAL:HG13	2:D:3400:LEU:HB3	1.66	0.76
1:C:1039:LEU:HD22	1:C:1039:LEU:H	1.50	0.76
2:B:2372:GLU:O	2:B:2373:THR:HG23	1.86	0.76
2:B:2439:ILE:HD11	2:B:2476:PHE:CE2	2.20	0.76
2:B:2291:GLN:O	2:B:2295:ILE:HG13	1.85	0.76
1:A:87:ASP:OD1	2:B:2260:ARG:HD2	1.86	0.75
2:B:2228:MET:HE2	2:B:2476:PHE:CD1	2.15	0.75
2:B:2323:ILE:HD11	2:B:2357:ILE:HD13	1.69	0.75
1:A:195:ASP:OD1	1:A:283:HIS:HD2	1.69	0.75
2:D:3227:GLN:O	2:D:3308:ASP:HB3	1.86	0.75
2:B:2240:ASN:OD1	2:B:2263:THR:HG22	1.87	0.75
2:D:3270:LEU:HD21	2:D:3422:ILE:CG2	2.16	0.75
1:A:179:ILE:HG13	1:A:294:ILE:HG13	1.69	0.74
2:B:2425:LEU:O	2:B:2429:LEU:HB2	1.87	0.74
1:A:241:MET:CG	1:A:270:ILE:HG23	2.18	0.74
1:A:35:MET:HE2	1:A:167:LEU:HD12	1.69	0.74
1:C:1053:ILE:HD13	1:C:1169:PHE:HD2	1.52	0.74
2:D:3260:ARG:HH12	2:D:3263:THR:HG21	1.51	0.74
1:A:99:GLU:HG3	1:A:100:HIS:N	2.02	0.74
1:C:1061:ASN:ND2	1:C:1165:GLN:HG2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1145:ARG:O	1:C:1147:ASP:N	2.19	0.74
1:C:1114:LYS:O	1:C:1117:LYS:HG3	1.88	0.73
1:A:118:ILE:O	1:A:118:ILE:HG23	1.86	0.73
2:D:3323:ILE:O	2:D:3323:ILE:HG13	1.88	0.73
2:B:2394:PRO:HG2	2:B:2397:ALA:HB2	1.70	0.73
1:A:60:ASN:ND2	1:A:62:ASN:HB2	2.03	0.73
2:B:2339:GLN:HE21	2:B:2344:LYS:NZ	1.86	0.73
2:D:3447:ASN:ND2	2:D:3464:PRO:HB2	2.03	0.73
2:D:3304:HIS:H	2:D:3347:SER:HB2	1.53	0.73
1:A:211:GLU:O	1:A:215:GLN:HB2	1.87	0.73
2:D:3246:LYS:HE2	2:D:3246:LYS:HA	1.69	0.72
2:B:2248:ARG:HD3	2:B:2257:ILE:O	1.90	0.72
1:C:1125:THR:HB	1:C:1129:SER:HB3	1.70	0.72
2:D:3393:ILE:CG1	2:D:3471:ARG:HH22	1.99	0.72
1:C:1032:ASN:ND2	1:C:1035:MET:H	1.88	0.72
1:C:1120:LYS:H	1:C:1120:LYS:HD2	1.55	0.72
1:A:17:ARG:HG3	1:A:199:TYR:HD1	1.55	0.71
1:A:99:GLU:HG3	1:A:100:HIS:H	1.54	0.71
2:B:2260:ARG:HH21	2:B:2263:THR:HG23	1.55	0.71
1:C:1041:LYS:HE3	1:C:1124:TYR:HE2	1.56	0.71
1:A:289:LEU:HD22	1:A:291:LYS:HG2	1.73	0.71
2:B:2432:ARG:HH11	2:B:2432:ARG:HG3	1.56	0.71
2:B:2227:GLN:O	2:B:2308:ASP:HB3	1.91	0.71
2:D:3276:GLU:HG2	2:D:3277:LEU:N	2.05	0.71
2:B:2332:PRO:HB2	2:B:2335:GLU:HG3	1.73	0.70
1:A:127:LYS:O	1:A:131:GLU:HB2	1.92	0.70
1:A:130:ILE:HD12	1:A:131:GLU:N	2.06	0.70
1:A:180:VAL:HG21	1:A:200:VAL:HG11	1.71	0.70
1:A:61:ASN:HD21	1:A:165:GLN:CG	2.04	0.70
1:A:237:LYS:CG	1:A:238:ASN:H	2.04	0.70
2:D:3333:ILE:HD12	2:D:3334:TYR:N	2.06	0.70
2:D:3369:ILE:HG23	2:D:3370:PRO:HD2	1.74	0.70
1:A:250:THR:HG21	3:B:4019:HOH:O	1.91	0.70
2:B:2314:ILE:HG21	2:B:2323:ILE:HG21	1.73	0.70
1:C:1160:GLU:H	1:C:1160:GLU:CD	1.95	0.70
1:C:1227:GLU:HB2	1:C:1246:LEU:HD21	1.73	0.70
2:D:3314:ILE:HG21	2:D:3323:ILE:HD12	1.73	0.69
2:D:3248:ARG:HD3	2:D:3257:ILE:O	1.93	0.69
1:C:1082:TYR:CE2	1:C:1260:TYR:HB3	2.27	0.69
1:C:1013:GLN:CG	1:C:1014:THR:H	2.02	0.69
1:A:186:ILE:HA	1:A:192:TYR:OH	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LYS:HG2	1:A:238:ASN:N	2.07	0.69
2:D:3234:GLY:HA2	2:D:3307:MET:SD	2.33	0.69
2:D:3344:LYS:HA	2:D:3344:LYS:HE3	1.74	0.69
1:A:102:SER:HB3	1:A:120:LYS:NZ	2.09	0.68
1:A:187:ASN:OD1	1:A:189:THR:HG23	1.93	0.68
2:B:2241:ASN:HB2	2:B:2316:SER:HB2	1.76	0.68
1:C:1106:GLN:H	1:C:1106:GLN:NE2	1.91	0.68
2:B:2231:LYS:HB2	2:B:2232:PRO:CD	2.17	0.68
2:D:3288:THR:HB	2:D:3327:ASP:OD1	1.94	0.68
1:A:35:MET:CE	1:A:167:LEU:HD12	2.22	0.68
1:C:1281:LYS:HE2	1:C:1283:HIS:CB	2.23	0.68
2:D:3226:TYR:CD1	2:D:3352:PRO:HD3	2.29	0.68
1:A:53:ILE:HD12	1:A:169:PHE:HB3	1.74	0.68
1:A:59:LYS:O	1:A:164:ASN:HA	1.93	0.68
2:B:2306:ASN:HB2	2:B:2307:MET:HE3	1.75	0.68
2:D:3334:TYR:HB3	2:D:3335:GLU:OE2	1.94	0.68
1:C:1145:ARG:C	1:C:1147:ASP:H	1.97	0.68
1:A:38:GLN:HA	1:A:160:GLU:CG	2.21	0.67
1:C:1130:ILE:HD12	1:C:1134:GLU:OE1	1.95	0.67
1:A:179:ILE:HG22	1:A:179:ILE:O	1.94	0.67
2:D:3356:PHE:C	2:D:3357:ILE:HD12	2.14	0.67
1:A:274:LYS:O	1:A:276:LYS:HG2	1.94	0.67
1:C:1122:HIS:CE1	1:C:1125:THR:HG21	2.30	0.67
2:D:3289:VAL:HG23	2:D:3290:GLU:OE2	1.95	0.67
1:C:1061:ASN:HD21	1:C:1165:GLN:CG	2.08	0.66
1:C:1211:GLU:O	1:C:1215:GLN:HB2	1.95	0.66
1:C:1032:ASN:HD21	1:C:1035:MET:H	1.43	0.66
1:C:1034:ILE:HG21	1:C:1043:VAL:HG11	1.78	0.66
1:A:225:ASN:HD22	1:A:225:ASN:H	1.44	0.66
1:C:1259:LYS:CD	1:C:1259:LYS:H	2.09	0.66
1:A:87:ASP:HB3	2:B:2317:HIS:HA	1.77	0.66
2:D:3371:VAL:HG13	2:D:3373:THR:H	1.61	0.66
2:D:3393:ILE:HG23	2:D:3394:PRO:CD	2.26	0.66
1:A:16:ILE:HD11	1:A:182:PHE:HE1	1.61	0.66
2:B:2290:GLU:O	2:B:2294:GLU:HG3	1.94	0.66
2:D:3413:ARG:HG3	2:D:3419:THR:HG22	1.77	0.65
2:D:3260:ARG:HH22	2:D:3263:THR:CG2	2.08	0.65
1:C:1041:LYS:HE3	1:C:1124:TYR:CE2	2.31	0.65
2:B:2407:ASN:ND2	2:B:2408:ASN:H	1.95	0.65
2:B:2431:GLU:O	2:B:2434:PRO:HD2	1.96	0.65
2:D:3260:ARG:NH2	2:D:3263:THR:HG23	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:CG2	1:A:200:VAL:HG11	2.26	0.65
2:B:2339:GLN:HE21	2:B:2344:LYS:HZ2	1.43	0.65
1:A:17:ARG:HH12	1:A:66:ARG:HH21	1.43	0.65
2:D:3289:VAL:HG23	2:D:3290:GLU:CD	2.16	0.65
2:B:2248:ARG:HG3	2:B:2257:ILE:HG22	1.78	0.65
2:B:2294:GLU:O	2:B:2298:ILE:HG13	1.97	0.65
1:A:61:ASN:HD21	1:A:165:GLN:HG2	1.60	0.64
1:C:1050:SER:HB3	1:C:1177:LYS:O	1.97	0.64
2:D:3321:GLY:N	2:D:3361:GLN:HE22	1.95	0.64
2:D:3366:GLN:N	3:D:4021:HOH:O	2.31	0.64
1:A:39:LEU:HD22	1:A:39:LEU:N	2.13	0.64
2:D:3351:LYS:HB3	2:D:3351:LYS:NZ	2.12	0.64
2:D:3426:CYS:O	2:D:3430:ARG:HG2	1.98	0.64
2:B:2251:VAL:CG2	2:B:2254:LEU:HD13	2.27	0.64
1:C:1032:ASN:HD21	1:C:1035:MET:HG3	1.63	0.64
1:A:53:ILE:HD13	1:A:171:TYR:HB3	1.80	0.64
1:C:1074:GLN:HG3	1:C:1279:TYR:CD2	2.33	0.64
1:A:204:GLN:HE21	1:A:205:PHE:N	1.96	0.64
2:B:2251:VAL:HG21	2:B:2254:LEU:HD13	1.80	0.64
1:C:1180:VAL:HG22	1:C:1200:VAL:HG11	1.80	0.64
1:A:125:THR:O	1:A:129:SER:HB3	1.98	0.64
2:D:3289:VAL:HG22	2:D:3327:ASP:OD1	1.98	0.64
1:C:1127:LYS:O	1:C:1131:GLU:HB2	1.98	0.63
2:D:3335:GLU:OE2	2:D:3335:GLU:N	2.31	0.63
1:C:1050:SER:OG	1:C:1178:VAL:HA	1.98	0.63
1:C:1274:LYS:HG3	1:C:1275:SER:H	1.64	0.63
1:A:198:ALA:HB3	1:A:280:VAL:HB	1.80	0.63
2:B:2321:GLY:HA2	2:B:2361:GLN:HE22	1.63	0.63
2:D:3304:HIS:CD2	2:D:3348:LEU:HD21	2.34	0.63
2:B:2357:ILE:HB	2:B:2403:MET:CE	2.28	0.63
1:A:145:ARG:O	1:A:147:ASP:N	2.32	0.63
2:D:3227:GLN:O	2:D:3228:MET:HG3	1.98	0.63
2:B:2413:ARG:HG3	2:B:2419:THR:CG2	2.29	0.63
1:C:1118:ILE:HA	1:C:1120:LYS:CD	2.29	0.63
2:D:3308:ASP:O	2:D:3309:CYS:HB2	1.98	0.62
2:D:3442:ILE:HA	2:D:3445:GLU:OE1	1.99	0.62
1:C:1125:THR:HB	1:C:1129:SER:CB	2.29	0.62
2:D:3251:VAL:HG11	2:D:3254:LEU:HD12	1.80	0.62
1:A:122:HIS:CE1	1:A:125:THR:HG21	2.35	0.62
1:C:1171:TYR:O	1:C:1173:PRO:HD3	1.98	0.62
2:D:3236:CYS:SG	2:D:3274:PHE:CD2	2.92	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3288:THR:CG2	2:D:3326:THR:HB	2.27	0.62
1:A:50:SER:OG	1:A:178:VAL:HA	1.99	0.62
2:B:2322:ILE:C	2:B:2322:ILE:HD12	2.20	0.62
2:B:2413:ARG:CG	2:B:2419:THR:HG22	2.30	0.62
2:B:2398:ASP:HA	2:B:2470:LEU:HD23	1.82	0.62
1:A:123:ASP:O	1:A:126:ASP:N	2.31	0.61
1:A:251:GLU:OE1	1:A:251:GLU:N	2.32	0.61
1:C:1078:LEU:HD11	1:C:1270:ILE:HD11	1.82	0.61
2:D:3314:ILE:HG21	2:D:3323:ILE:CD1	2.29	0.61
1:A:98:ASP:OD1	1:A:99:GLU:N	2.34	0.61
1:C:1200:VAL:HG23	1:C:1278:LEU:HB3	1.80	0.61
1:A:160:GLU:HB2	3:A:4006:HOH:O	1.99	0.61
1:A:31:ILE:HG12	1:A:166:VAL:HG22	1.80	0.61
2:D:3231:LYS:HB2	2:D:3232:PRO:HD3	1.82	0.61
2:D:3345:CYS:SG	2:D:3348:LEU:HD12	2.41	0.61
2:B:2292:ILE:HA	2:B:2295:ILE:HD12	1.83	0.61
2:D:3288:THR:O	2:D:3292:ILE:HG13	1.99	0.61
2:D:3400:LEU:HG	2:D:3439:ILE:HD13	1.83	0.61
1:A:2:CYS:O	1:A:3:VAL:HB	2.00	0.61
1:C:1230:LEU:HD11	1:C:1247:GLU:HG3	1.81	0.61
2:D:3231:LYS:HB2	2:D:3232:PRO:CD	2.31	0.60
1:A:264:ILE:HG13	1:A:265:PHE:CD2	2.36	0.60
1:A:4:ILE:O	1:A:4:ILE:HG22	2.00	0.60
1:C:1026:ARG:HG3	1:C:1173:PRO:HG2	1.83	0.60
2:D:3228:MET:HA	2:D:3308:ASP:HB2	1.83	0.60
1:A:179:ILE:N	1:A:179:ILE:HD12	2.16	0.60
1:A:164:ASN:N	1:A:164:ASN:HD22	1.98	0.60
1:A:200:VAL:CG2	1:A:278:LEU:HB3	2.31	0.60
2:B:2406:VAL:HG13	2:B:2463:MET:O	2.01	0.60
1:C:1007:VAL:HA	1:C:1011:VAL:HG21	1.84	0.60
1:C:1074:GLN:HG3	1:C:1279:TYR:CE2	2.37	0.60
2:B:2231:LYS:CB	2:B:2232:PRO:HD3	2.23	0.60
2:D:3233:ARG:HH22	2:D:3477:PRO:HG2	1.66	0.60
1:A:68:LYS:O	1:A:72:ASP:HB2	2.01	0.60
1:A:8:GLU:HG3	1:A:9:ILE:N	2.15	0.60
2:B:2296:LEU:HD22	2:B:2340:PHE:CZ	2.36	0.60
1:C:1059:LYS:O	1:C:1164:ASN:HA	2.00	0.60
2:B:2248:ARG:HA	2:B:2254:LEU:O	2.02	0.60
2:D:3321:GLY:H	2:D:3361:GLN:NE2	2.00	0.60
1:A:214:VAL:HG12	1:A:244:LYS:HG3	1.83	0.60
1:A:93:ILE:O	1:A:94:LYS:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:N	1:A:33:LYS:HD2	2.12	0.59
2:B:2251:VAL:CG1	2:B:2254:LEU:HB2	2.31	0.59
1:A:125:THR:HB	1:A:129:SER:HB3	1.84	0.59
2:B:2414:ASN:ND2	2:B:2417:GLU:H	1.99	0.59
1:C:1037:THR:O	1:C:1039:LEU:HD22	2.01	0.59
1:C:1211:GLU:HG3	1:C:1231:TYR:OH	2.02	0.59
2:D:3226:TYR:HD2	2:D:3473:LYS:O	1.85	0.59
2:D:3290:GLU:H	2:D:3290:GLU:CD	2.06	0.59
2:D:3448:TYR:O	2:D:3451:SER:HB2	2.02	0.59
1:C:1008:GLU:H	1:C:1011:VAL:HG23	1.67	0.59
1:A:13:GLN:HG3	1:A:14:THR:H	1.67	0.59
1:A:16:ILE:HD11	1:A:182:PHE:CE1	2.37	0.59
1:A:118:ILE:CG2	1:A:118:ILE:O	2.50	0.59
2:B:2257:ILE:HD11	2:B:2317:HIS:ND1	2.17	0.59
2:B:2289:VAL:HG13	2:B:2331:ALA:HB2	1.85	0.59
2:B:2371:VAL:HG22	2:B:2373:THR:OG1	2.03	0.59
1:C:1184:HIS:CD2	1:C:1194:TYR:CE2	2.90	0.59
2:D:3352:PRO:HG3	2:D:3474:LEU:CD1	2.32	0.59
1:A:114:LYS:O	1:A:117:LYS:HD3	2.02	0.59
2:B:2358:GLN:HE21	2:B:2419:THR:CB	2.15	0.59
2:B:2412:TYR:N	2:B:2462:GLN:OE1	2.35	0.59
1:A:39:LEU:HD23	1:A:157:PRO:HA	1.84	0.59
2:D:3348:LEU:HA	2:D:3351:LYS:HD2	1.85	0.58
1:A:71:VAL:HG11	1:A:197:VAL:HG13	1.85	0.58
2:B:2366:GLN:NE2	2:B:2409:CYS:SG	2.75	0.58
2:D:3367:LYS:HD2	2:D:3367:LYS:N	2.18	0.58
2:B:2319:ASP:O	2:B:2322:ILE:HG13	2.04	0.58
2:D:3352:PRO:HG3	2:D:3474:LEU:HD13	1.84	0.58
1:A:200:VAL:HG22	1:A:278:LEU:HB3	1.86	0.58
2:B:2391:ARG:HD3	2:B:2391:ARG:H	1.69	0.58
1:C:1291:LYS:HD3	1:C:1292:ASN:O	2.03	0.58
2:D:3276:GLU:HG2	2:D:3277:LEU:HG	1.85	0.58
1:A:77:GLN:HE22	1:A:239:LYS:NZ	2.01	0.58
2:B:2281:ILE:HG22	2:B:2283:PRO:HD3	1.85	0.58
2:D:3254:LEU:HD11	2:D:3324:TYR:CE1	2.38	0.58
1:A:138:LEU:N	1:A:139:PRO:HD2	2.18	0.58
1:A:195:ASP:OD1	1:A:283:HIS:CD2	2.55	0.58
1:A:224:LYS:O	1:A:227:GLU:HG2	2.04	0.58
2:D:3398:ASP:HA	2:D:3470:LEU:HA	1.85	0.58
1:A:134:GLU:O	1:A:139:PRO:HD3	2.04	0.58
1:A:61:ASN:OD1	1:A:164:ASN:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2236:CYS:O	2:B:2238:ILE:HG13	2.04	0.58
2:D:3233:ARG:NH1	2:D:3477:PRO:HD2	2.18	0.58
2:D:3291:GLN:O	2:D:3295:ILE:HG13	2.04	0.58
2:D:3321:GLY:H	2:D:3361:GLN:HE22	1.52	0.58
2:D:3473:LYS:HE2	2:D:3473:LYS:HA	1.85	0.57
2:B:2463:MET:HE2	2:B:2464:PRO:N	2.19	0.57
1:A:97:LYS:NZ	1:A:97:LYS:HB2	2.19	0.57
2:B:2299:TYR:HA	2:B:2302:MET:HE3	1.87	0.57
2:B:2288:THR:HG22	2:B:2326:THR:HB	1.86	0.57
1:C:1004:ILE:O	1:C:1004:ILE:HG22	2.04	0.57
2:B:2407:ASN:HD22	2:B:2408:ASN:H	1.53	0.57
1:C:1100:HIS:O	1:C:1156:LYS:HB2	2.04	0.57
2:D:3236:CYS:SG	2:D:3274:PHE:HD2	2.28	0.57
1:C:1013:GLN:CG	1:C:1014:THR:N	2.67	0.57
1:A:182:PHE:CZ	1:A:280:VAL:HG11	2.40	0.57
1:C:1016:ILE:HD13	1:C:1181:PRO:HG2	1.85	0.57
2:D:3351:LYS:O	2:D:3353:LYS:HD3	2.05	0.56
2:B:2413:ARG:NH1	2:B:2413:ARG:HB3	2.20	0.56
2:D:3251:VAL:HG13	2:D:3254:LEU:HB2	1.86	0.56
1:C:1214:VAL:O	1:C:1244:LYS:NZ	2.34	0.56
1:C:1082:TYR:HE2	1:C:1260:TYR:HB3	1.70	0.56
1:A:299:LYS:HD2	1:A:299:LYS:OXT	2.05	0.56
2:B:2251:VAL:HG11	2:B:2254:LEU:HD22	1.88	0.56
1:C:1099:GLU:OE1	1:C:1099:GLU:N	2.37	0.56
1:C:1184:HIS:H	1:C:1290:ASN:HD21	0.77	0.56
1:A:22:ASP:OD1	1:A:23:LYS:N	2.39	0.56
2:D:3400:LEU:HD22	2:D:3468:PHE:HB3	1.87	0.56
1:A:123:ASP:C	1:A:125:THR:H	2.09	0.56
1:C:1176:ASN:N	1:C:1176:ASN:HD22	2.04	0.56
1:A:185:GLU:O	1:A:186:ILE:C	2.43	0.55
2:D:3355:PHE:O	2:D:3402:GLY:N	2.34	0.55
2:D:3237:LEU:HD11	2:D:3299:TYR:CD2	2.41	0.55
1:A:125:THR:HB	1:A:129:SER:CB	2.37	0.55
2:B:2260:ARG:HA	2:B:2413:ARG:NH2	2.22	0.55
1:A:260:TYR:O	1:A:262:TRP:HD1	1.88	0.55
2:B:2248:ARG:HG2	2:B:2255:HIS:O	2.07	0.55
2:B:2289:VAL:HG23	2:B:2327:ASP:OD1	2.06	0.55
1:A:181:PRO:HA	1:A:292:ASN:OD1	2.06	0.55
1:C:1130:ILE:HD12	1:C:1130:ILE:C	2.27	0.55
2:D:3226:TYR:HA	2:D:3472:LYS:NZ	2.21	0.55
1:A:87:ASP:C	2:B:2360:CYS:SG	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1192:TYR:CD1	1:C:1290:ASN:HB2	2.42	0.54
1:A:123:ASP:O	1:A:125:THR:N	2.41	0.54
2:B:2284:HIS:O	2:B:2285:HIS:O	2.25	0.54
2:B:2304:HIS:H	2:B:2347:SER:HB3	1.71	0.54
1:C:1274:LYS:HG3	1:C:1275:SER:N	2.23	0.54
1:A:38:GLN:CA	1:A:160:GLU:HG3	2.27	0.54
2:D:3222:LEU:HD23	2:D:3222:LEU:N	2.23	0.54
2:D:3245:ALA:HA	2:D:3248:ARG:HH21	1.73	0.54
2:D:3321:GLY:O	2:D:3333:ILE:HG13	2.06	0.54
1:A:230:LEU:HD12	1:A:230:LEU:N	2.23	0.54
1:A:33:LYS:CD	1:A:33:LYS:H	2.05	0.54
2:B:2233:ARG:NH2	2:B:2477:PRO:O	2.41	0.54
1:C:1115:PHE:CE1	1:C:1138:LEU:HD13	2.42	0.54
1:C:1014:THR:HB	1:C:1196:VAL:HG23	1.89	0.54
1:C:1237:LYS:HG3	1:C:1238:ASN:H	1.73	0.54
2:D:3433:CYS:N	2:D:3434:PRO:CD	2.71	0.54
1:C:1084:ASP:OD2	2:D:3414:ASN:ND2	2.41	0.54
2:D:3343:LEU:HG	2:D:3344:LYS:H	1.73	0.54
1:C:1230:LEU:H	1:C:1230:LEU:HD12	1.73	0.53
2:B:2320:LYS:O	2:B:2322:ILE:HG23	2.08	0.53
1:C:1127:LYS:HG3	1:C:1128:LYS:N	2.23	0.53
2:D:3233:ARG:NH2	2:D:3477:PRO:CG	2.67	0.53
2:B:2264:HIS:CE1	2:B:2265:LEU:HG	2.43	0.53
2:B:2391:ARG:CD	2:B:2391:ARG:H	2.22	0.53
1:C:1032:ASN:ND2	1:C:1035:MET:HG3	2.23	0.53
1:A:225:ASN:ND2	1:A:225:ASN:H	2.06	0.53
2:B:2226:TYR:CE1	2:B:2472:LYS:HG3	2.44	0.53
2:D:3248:ARG:HG2	2:D:3255:HIS:O	2.08	0.53
2:B:2447:ASN:ND2	2:B:2464:PRO:HB2	2.24	0.53
1:C:1281:LYS:O	1:C:1282:LEU:HD23	2.09	0.53
1:A:209:GLN:HG3	1:A:291:LYS:HZ1	1.74	0.53
2:B:2243:ASN:O	2:B:2326:THR:HG23	2.09	0.53
1:C:1039:LEU:CD1	1:C:1043:VAL:HG21	2.23	0.53
1:A:275:SER:O	1:A:276:LYS:HB2	2.08	0.53
1:C:1050:SER:CB	1:C:1177:LYS:O	2.57	0.53
2:B:2253:LYS:HG3	2:B:2254:LEU:CD1	2.39	0.53
2:B:2371:VAL:HG13	2:B:2372:GLU:N	2.24	0.53
2:B:2358:GLN:NE2	2:B:2419:THR:HB	2.24	0.53
2:B:2275:GLU:OE2	2:B:2275:GLU:HA	2.09	0.52
2:B:2248:ARG:NH2	2:B:2259:ASP:OD1	2.41	0.52
2:D:3345:CYS:HB3	2:D:3348:LEU:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:O	1:A:134:GLU:OE1	2.27	0.52
2:B:2319:ASP:O	2:B:2320:LYS:C	2.47	0.52
1:A:102:SER:HB3	1:A:120:LYS:HZ1	1.73	0.52
1:C:1032:ASN:ND2	1:C:1032:ASN:C	2.52	0.52
2:D:3248:ARG:HA	2:D:3254:LEU:O	2.10	0.52
1:C:1007:VAL:HA	1:C:1011:VAL:CG2	2.40	0.52
1:C:1049:ILE:CD1	1:C:1053:ILE:HD11	2.40	0.52
2:D:3420:TRP:N	2:D:3420:TRP:CD1	2.75	0.52
1:A:44:LEU:HD23	1:A:45:MET:N	2.25	0.52
2:D:3240:ASN:HD22	2:D:3241:ASN:N	2.08	0.52
2:B:2268:GLY:HA2	2:B:2271:THR:OG1	2.10	0.52
2:B:2369:ILE:O	2:B:2369:ILE:HD12	2.09	0.52
1:C:1098:ASP:OD1	1:C:1099:GLU:N	2.43	0.52
2:D:3236:CYS:HG	2:D:3274:PHE:HD2	1.45	0.52
2:D:3313:CYS:C	2:D:3314:ILE:HD12	2.30	0.52
1:A:237:LYS:CG	1:A:238:ASN:N	2.67	0.52
2:D:3238:ILE:HG23	2:D:3313:CYS:SG	2.50	0.52
2:D:3240:ASN:C	2:D:3240:ASN:HD22	2.14	0.52
2:D:3242:HIS:HB3	2:D:3286:ASP:OD2	2.09	0.52
2:D:3225:VAL:HG22	2:D:3473:LYS:HB2	1.91	0.52
1:A:164:ASN:ND2	1:A:164:ASN:N	2.58	0.51
2:B:2260:ARG:HD3	2:B:2316:SER:HA	1.92	0.51
1:C:1013:GLN:HG3	1:C:1014:THR:N	2.12	0.51
2:D:3240:ASN:HD21	2:D:3263:THR:HB	1.74	0.51
2:D:3344:LYS:CE	2:D:3344:LYS:HA	2.41	0.51
1:A:108:GLY:HA2	1:A:150:VAL:HG23	1.91	0.51
2:D:3233:ARG:HH22	2:D:3477:PRO:CG	2.23	0.51
2:B:2266:ASP:OD1	2:B:2419:THR:HG23	2.09	0.51
1:A:7:VAL:HB	1:A:11:VAL:HG11	1.92	0.51
2:D:3265:LEU:O	2:D:3269:ALA:HB2	2.11	0.51
1:C:1180:VAL:HG12	1:C:1182:PHE:CE1	2.45	0.51
2:B:2358:GLN:HE21	2:B:2419:THR:HB	1.76	0.51
1:C:1002:CYS:N	2:D:3257:ILE:HG22	2.26	0.51
2:D:3450:VAL:HG12	2:D:3462:GLN:O	2.11	0.51
1:C:1073:GLU:HG3	1:C:1074:GLN:N	2.26	0.51
2:D:3413:ARG:HA	2:D:3419:THR:HA	1.92	0.51
2:D:3452:ASN:O	2:D:3453:LYS:C	2.49	0.51
1:A:176:ASN:N	1:A:176:ASN:HD22	2.08	0.51
1:A:236:SER:HB3	1:A:237:LYS:NZ	2.26	0.51
2:B:2234:GLY:HA3	2:B:2309:CYS:O	2.11	0.51
2:B:2369:ILE:C	2:B:2369:ILE:HD12	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3304:HIS:CG	2:D:3348:LEU:HD21	2.46	0.51
1:A:75:PHE:CZ	1:A:270:ILE:HG13	2.46	0.50
2:B:2420:TRP:CD1	2:B:2420:TRP:N	2.76	0.50
1:C:1082:TYR:HB2	1:C:1262:TRP:CZ2	2.46	0.50
1:C:1118:ILE:HA	1:C:1120:LYS:HD2	1.93	0.50
2:B:2288:THR:OG1	2:B:2291:GLN:NE2	2.39	0.50
1:A:102:SER:HB3	1:A:120:LYS:HZ2	1.75	0.50
1:A:176:ASN:N	1:A:176:ASN:ND2	2.59	0.50
1:A:184:HIS:HE1	1:A:193:GLU:O	1.94	0.50
1:A:3:VAL:HG23	3:B:4001:HOH:O	2.10	0.50
2:D:3456:LYS:CA	2:D:3456:LYS:HE2	2.25	0.50
2:B:2246:LYS:HD3	2:B:2250:LYS:HE3	1.93	0.50
2:D:3224:LYS:O	2:D:3225:VAL:HG23	2.11	0.50
1:A:4:ILE:C	1:A:6:PRO:HD2	2.31	0.50
1:C:1123:ASP:O	1:C:1125:THR:N	2.45	0.50
1:C:1141:LEU:HD13	1:C:1150:VAL:HG11	1.92	0.50
2:D:3245:ALA:CA	2:D:3248:ARG:HH21	2.25	0.50
2:D:3358:GLN:HB2	2:D:3422:ILE:HD11	1.92	0.50
1:A:5:PHE:N	1:A:6:PRO:CD	2.75	0.50
1:C:1160:GLU:N	1:C:1160:GLU:CD	2.65	0.50
2:B:2357:ILE:CD1	2:B:2403:MET:HE1	2.34	0.50
2:D:3281:ILE:HG22	2:D:3283:PRO:HD3	1.93	0.50
1:A:284:ASN:HB2	3:A:4014:HOH:O	2.11	0.50
2:B:2357:ILE:HB	2:B:2403:MET:HE1	1.94	0.50
1:C:1106:GLN:N	1:C:1106:GLN:NE2	2.58	0.50
1:C:1206:ASP:HA	3:C:4017:HOH:O	2.11	0.50
2:B:2229:LYS:O	2:B:2230:SER:C	2.50	0.49
1:C:1130:ILE:HD12	1:C:1131:GLU:N	2.27	0.49
1:C:1138:LEU:HB3	1:C:1139:PRO:HD3	1.94	0.49
1:A:115:PHE:CE1	1:A:138:LEU:HD13	2.47	0.49
1:C:1012:SER:HB3	1:C:1033:LYS:HA	1.94	0.49
1:C:1269:PHE:CD1	1:C:1269:PHE:N	2.80	0.49
1:C:1118:ILE:CD1	1:C:1123:ASP:HB3	2.42	0.49
1:A:79:GLU:HG2	1:A:266:CYS:SG	2.53	0.49
1:A:8:GLU:O	1:A:11:VAL:HG12	2.13	0.49
1:C:1185:GLU:O	1:C:1186:ILE:C	2.50	0.49
1:C:1004:ILE:CD1	2:D:3253:LYS:HD2	2.40	0.49
2:D:3298:ILE:C	2:D:3300:GLN:H	2.16	0.49
1:C:1075:PHE:CE2	1:C:1281:LYS:HB3	2.48	0.49
1:A:237:LYS:N	1:A:237:LYS:HD2	2.27	0.49
1:C:1106:GLN:H	1:C:1106:GLN:HE21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3264:HIS:HD2	2:D:3265:LEU:H	1.61	0.49
1:C:1064:ARG:HG2	1:C:1064:ARG:HH11	1.77	0.49
1:C:1256:LYS:HD3	1:C:1257:SER:H	1.76	0.49
2:D:3266:ASP:O	2:D:3270:LEU:HG	2.12	0.49
1:A:106:GLN:NE2	1:A:106:GLN:N	2.56	0.49
1:A:17:ARG:HG3	1:A:199:TYR:CD1	2.43	0.49
2:B:2314:ILE:CG2	2:B:2323:ILE:HG21	2.41	0.49
1:C:1120:LYS:HD2	1:C:1120:LYS:N	2.26	0.49
1:C:1192:TYR:CE1	1:C:1290:ASN:HB2	2.48	0.49
2:D:3393:ILE:HG23	2:D:3394:PRO:N	2.28	0.49
2:B:2439:ILE:HD11	2:B:2476:PHE:CZ	2.48	0.48
1:C:1020:GLN:HB2	1:C:1026:ARG:NH1	2.28	0.48
1:C:1028:LEU:O	1:C:1168:SER:HA	2.13	0.48
1:C:1114:LYS:O	1:C:1116:ALA:N	2.46	0.48
2:D:3305:SER:C	2:D:3307:MET:H	2.17	0.48
2:D:3345:CYS:CB	2:D:3348:LEU:HD12	2.42	0.48
2:B:2275:GLU:OE2	2:B:2281:ILE:HG12	2.12	0.48
2:B:2333:ILE:O	2:B:2337:THR:HG22	2.12	0.48
1:C:1236:SER:OG	1:C:1237:LYS:N	2.46	0.48
2:D:3251:VAL:HG22	2:D:3254:LEU:H	1.77	0.48
2:B:2240:ASN:OD1	2:B:2263:THR:CG2	2.60	0.48
1:A:137:CYS:C	1:A:139:PRO:HD2	2.34	0.48
1:A:39:LEU:H	1:A:39:LEU:CD2	2.20	0.48
1:C:1007:VAL:CA	1:C:1011:VAL:HG21	2.42	0.48
2:D:3251:VAL:CG1	2:D:3254:LEU:HB2	2.43	0.48
1:C:1145:ARG:C	1:C:1147:ASP:N	2.66	0.48
2:B:2270:LEU:HD23	2:B:2426:CYS:SG	2.52	0.48
1:C:1200:VAL:CG2	1:C:1278:LEU:HB3	2.43	0.48
2:D:3439:ILE:HG22	2:D:3474:LEU:HB3	1.96	0.48
2:B:2432:ARG:NH1	2:B:2445:GLU:OE1	2.46	0.48
1:C:1159:PHE:HE2	1:C:1165:GLN:HA	1.78	0.48
1:C:1083:SER:HB2	2:D:3457:LYS:HD2	1.96	0.48
1:A:51:GLY:HA3	1:A:172:ASN:O	2.13	0.48
1:C:1184:HIS:CD2	1:C:1194:TYR:HE2	2.31	0.48
1:A:44:LEU:HD23	1:A:44:LEU:C	2.34	0.47
1:C:1236:SER:HB3	1:C:1239:LYS:HB2	1.95	0.47
1:C:1272:ASP:OD1	1:C:1274:LYS:HG2	2.14	0.47
2:B:2228:MET:CE	2:B:2233:ARG:HD2	2.44	0.47
1:C:1118:ILE:HA	1:C:1120:LYS:CE	2.44	0.47
1:C:1275:SER:OG	1:C:1277:VAL:HG23	2.14	0.47
2:D:3364:ASN:HB3	2:D:3408:ASN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2245:ALA:O	2:B:2249:GLU:HG3	2.13	0.47
1:C:1002:CYS:O	1:C:1003:VAL:HB	2.14	0.47
1:C:1279:TYR:CD1	1:C:1279:TYR:N	2.82	0.47
2:D:3372:GLU:O	2:D:3372:GLU:HG2	2.14	0.47
2:D:3262:GLY:HA2	2:D:3264:HIS:NE2	2.29	0.47
2:D:3273:THR:CG2	2:D:3430:ARG:HB3	2.24	0.47
1:A:111:LEU:CD2	1:A:150:VAL:HG11	2.44	0.47
1:C:1118:ILE:HA	1:C:1120:LYS:NZ	2.29	0.47
1:C:1108:GLY:H	1:C:1149:TYR:HA	1.79	0.47
2:D:3322:ILE:HD12	2:D:3330:GLU:HB3	1.96	0.47
1:A:60:ASN:HA	1:A:164:ASN:ND2	2.30	0.47
2:D:3322:ILE:HG22	2:D:3332:PRO:HA	1.97	0.47
1:A:117:LYS:H	1:A:117:LYS:HD2	1.80	0.47
1:C:1038:GLN:HA	1:C:1160:GLU:HG3	1.94	0.47
1:C:1159:PHE:CE2	1:C:1165:GLN:HA	2.49	0.47
2:D:3237:LEU:HD21	2:D:3299:TYR:CD1	2.50	0.47
2:D:3300:GLN:O	2:D:3345:CYS:SG	2.67	0.47
1:A:249:THR:CG2	1:A:259:LYS:HB2	2.44	0.47
2:B:2241:ASN:CB	2:B:2316:SER:HB2	2.43	0.47
1:C:1085:GLN:NE2	3:C:4013:HOH:O	2.47	0.47
1:A:87:ASP:HB2	2:B:2360:CYS:SG	2.55	0.47
2:D:3367:LYS:HD2	2:D:3367:LYS:H	1.80	0.47
2:B:2260:ARG:HH21	2:B:2263:THR:CG2	2.25	0.47
2:B:2458:ASN:O	2:B:2460:GLY:N	2.48	0.47
1:C:1039:LEU:CD2	1:C:1039:LEU:H	2.24	0.47
1:C:1186:ILE:O	1:C:1186:ILE:HG22	2.14	0.47
2:B:2413:ARG:CB	2:B:2419:THR:HG22	2.45	0.46
1:C:1130:ILE:O	1:C:1134:GLU:OE1	2.32	0.46
1:A:184:HIS:N	1:A:290:ASN:OD1	2.42	0.46
1:C:1093:ILE:N	3:C:4022:HOH:O	2.48	0.46
1:A:178:VAL:C	1:A:179:ILE:HD12	2.35	0.46
1:A:264:ILE:HG13	1:A:265:PHE:HD2	1.80	0.46
1:C:1061:ASN:C	1:C:1063:LEU:N	2.68	0.46
1:C:1213:PHE:CD2	1:C:1291:LYS:HE2	2.50	0.46
1:C:1230:LEU:H	1:C:1230:LEU:CD1	2.26	0.46
2:D:3365:TYR:HE1	2:D:3412:TYR:OH	1.98	0.46
2:B:2336:LEU:O	2:B:2339:GLN:HB2	2.15	0.46
1:C:1060:ASN:OD1	1:C:1062:ASN:HB3	2.16	0.46
1:C:1114:LYS:O	1:C:1115:PHE:C	2.53	0.46
1:C:1220:PRO:O	1:C:1246:LEU:HD12	2.15	0.46
2:D:3260:ARG:HA	2:D:3413:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2427:GLN:HB3	2:B:2427:GLN:HE21	1.52	0.46
2:D:3233:ARG:HH12	2:D:3477:PRO:HD2	1.80	0.46
1:C:1087:ASP:HA	2:D:3317:HIS:ND1	2.30	0.46
2:D:3371:VAL:HG13	2:D:3373:THR:N	2.28	0.46
2:D:3447:ASN:HD22	2:D:3464:PRO:HB2	1.77	0.46
2:D:3289:VAL:HG23	2:D:3290:GLU:OE1	2.14	0.46
2:D:3297:LYS:HB2	2:D:3297:LYS:NZ	2.31	0.46
2:D:3357:ILE:HD12	2:D:3357:ILE:N	2.30	0.46
2:B:2316:SER:OG	2:B:2317:HIS:N	2.47	0.46
2:B:2433:CYS:N	2:B:2434:PRO:CD	2.79	0.46
2:B:2440:LEU:HD21	2:B:2468:PHE:CZ	2.51	0.46
1:C:1035:MET:HG2	1:C:1155:LEU:CD2	2.35	0.46
1:A:57:THR:HG23	3:A:4018:HOH:O	2.15	0.46
2:B:2296:LEU:HD22	2:B:2340:PHE:CE1	2.50	0.46
1:C:1137:CYS:SG	1:C:1185:GLU:HG2	2.55	0.46
1:C:1175:GLY:O	1:C:1176:ASN:HB2	2.15	0.46
2:D:3320:LYS:HG2	2:D:3408:ASN:ND2	2.31	0.46
1:A:278:LEU:HD22	1:A:295:LEU:HD21	1.98	0.46
2:B:2339:GLN:NE2	2:B:2344:LYS:NZ	2.62	0.46
2:B:2432:ARG:HH11	2:B:2432:ARG:CG	2.25	0.46
1:C:1158:GLY:O	1:C:1161:ASN:HB2	2.16	0.46
2:D:3431:GLU:O	2:D:3434:PRO:HD2	2.16	0.46
2:D:3447:ASN:HD21	2:D:3464:PRO:HB2	1.79	0.46
1:A:114:LYS:O	1:A:115:PHE:C	2.53	0.46
1:A:227:GLU:HB2	1:A:246:LEU:CD2	2.32	0.46
1:A:93:ILE:O	1:A:93:ILE:HG13	2.16	0.46
2:D:3289:VAL:HG23	2:D:3290:GLU:H	1.80	0.46
2:D:3289:VAL:HG22	2:D:3327:ASP:CG	2.35	0.46
1:A:39:LEU:CD2	1:A:157:PRO:HA	2.46	0.45
2:D:3264:HIS:CD2	2:D:3265:LEU:HG	2.51	0.45
1:A:248:PHE:O	1:A:248:PHE:CD1	2.68	0.45
1:A:34:ILE:HG21	1:A:43:VAL:HG21	1.98	0.45
2:B:2251:VAL:O	2:B:2251:VAL:HG13	2.16	0.45
2:B:2429:LEU:CD2	2:B:2433:CYS:SG	3.05	0.45
2:D:3227:GLN:HE21	2:D:3229:LYS:H	1.64	0.45
2:D:3240:ASN:C	2:D:3240:ASN:ND2	2.70	0.45
1:A:13:GLN:NE2	1:A:68:LYS:NZ	2.64	0.45
1:A:179:ILE:HG13	1:A:294:ILE:CG1	2.44	0.45
1:A:217:LEU:HB3	1:A:285:VAL:HG21	1.98	0.45
2:B:2432:ARG:NH1	2:B:2432:ARG:HG3	2.27	0.45
1:C:1106:GLN:HB3	1:C:1110:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3304:HIS:H	2:D:3347:SER:CB	2.25	0.45
1:C:1206:ASP:OD2	1:C:1209:GLN:HB3	2.17	0.45
2:D:3425:LEU:O	2:D:3429:LEU:HB3	2.17	0.45
1:A:277:VAL:HG12	1:A:278:LEU:N	2.32	0.45
1:A:4:ILE:C	1:A:6:PRO:CD	2.84	0.45
1:C:1120:LYS:O	1:C:1121:SER:HB3	2.15	0.45
1:A:254:TRP:O	1:A:255:GLY:O	2.34	0.45
2:B:2260:ARG:HD3	2:B:2317:HIS:HD2	1.82	0.45
1:C:1015:ILE:HG13	1:C:1064:ARG:HG3	1.99	0.45
1:C:1114:LYS:HB3	1:C:1117:LYS:CG	2.47	0.45
1:C:1245:ALA:HB1	1:C:1263:LYS:HG3	1.98	0.45
2:D:3450:VAL:HG11	2:D:3462:GLN:HG2	1.98	0.45
1:A:114:LYS:O	1:A:116:ALA:N	2.49	0.45
1:A:50:SER:HA	1:A:179:ILE:HD13	1.99	0.45
1:A:43:VAL:CG1	1:A:155:LEU:HB2	2.47	0.45
2:B:2295:ILE:HA	2:B:2298:ILE:HD12	1.99	0.45
2:B:2398:ASP:OD2	2:B:2471:ARG:NH1	2.50	0.45
1:C:1058:ARG:HG3	1:C:1101:TYR:HE2	1.81	0.45
1:C:1107:ASN:O	1:C:1110:VAL:HG12	2.17	0.45
1:C:1272:ASP:OD1	1:C:1274:LYS:CG	2.64	0.45
1:C:1278:LEU:HD22	1:C:1295:LEU:HD11	1.99	0.45
2:D:3236:CYS:SG	2:D:3279:PHE:HB3	2.57	0.45
1:A:24:GLN:HG2	1:A:24:GLN:O	2.17	0.45
2:B:2251:VAL:HG22	2:B:2254:LEU:HD13	1.97	0.45
1:C:1093:ILE:O	1:C:1094:LYS:HB2	2.16	0.45
2:D:3348:LEU:O	2:D:3351:LYS:HG2	2.17	0.45
2:D:3320:LYS:HG2	2:D:3408:ASN:HD21	1.82	0.45
1:A:227:GLU:CB	1:A:246:LEU:HD21	2.33	0.44
2:B:2454:ASP:OD2	2:B:2460:GLY:O	2.35	0.44
1:C:1016:ILE:O	1:C:1198:ALA:HA	2.16	0.44
2:D:3266:ASP:OD2	2:D:3422:ILE:HB	2.18	0.44
2:B:2329:GLN:NE2	2:B:2330:GLU:N	2.64	0.44
2:D:3403:MET:HB2	2:D:3465:GLN:O	2.17	0.44
2:D:3407:ASN:O	2:D:3408:ASN:HB2	2.17	0.44
1:A:192:TYR:O	1:A:286:THR:HG23	2.17	0.44
1:A:34:ILE:H	1:A:34:ILE:CD1	2.19	0.44
1:A:71:VAL:HG11	1:A:197:VAL:CG1	2.47	0.44
2:B:2275:GLU:OE2	2:B:2281:ILE:CG1	2.65	0.44
2:D:3406:VAL:HG13	2:D:3463:MET:O	2.17	0.44
1:A:61:ASN:HD21	1:A:165:GLN:HG3	1.77	0.44
2:B:2243:ASN:HA	2:B:2259:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2407:ASN:O	2:B:2408:ASN:HB2	2.18	0.44
1:C:1250:THR:O	1:C:1259:LYS:HA	2.18	0.44
2:D:3294:GLU:HA	2:D:3297:LYS:HB3	2.00	0.44
1:C:1125:THR:O	1:C:1129:SER:HB3	2.17	0.44
1:C:1127:LYS:HA	1:C:1130:ILE:HG13	1.98	0.44
1:C:1195:ASP:OD1	1:C:1283:HIS:ND1	2.40	0.44
1:A:55:SER:OG	1:A:170:GLU:HB3	2.17	0.44
1:A:22:ASP:OD2	1:A:25:THR:HB	2.18	0.44
2:B:2271:THR:O	2:B:2275:GLU:HB2	2.16	0.44
2:B:2400:LEU:HD21	2:B:2439:ILE:HG21	2.00	0.44
2:B:2361:GLN:HB3	2:B:2407:ASN:HD22	1.83	0.44
1:A:115:PHE:CD1	1:A:138:LEU:HD22	2.53	0.44
1:A:31:ILE:CD1	1:A:166:VAL:HG22	2.47	0.44
1:C:1049:ILE:HD11	1:C:1053:ILE:HD11	1.99	0.44
2:D:3226:TYR:CD2	2:D:3473:LYS:O	2.68	0.44
2:B:2266:ASP:HA	2:B:2269:ALA:HB3	2.00	0.44
1:C:1044:LEU:HD23	1:C:1045:MET:N	2.33	0.44
1:C:1231:TYR:CD2	1:C:1231:TYR:C	2.90	0.43
1:A:106:GLN:CD	1:A:106:GLN:N	2.71	0.43
1:A:117:LYS:H	1:A:117:LYS:CD	2.30	0.43
1:A:120:LYS:HB3	1:A:120:LYS:HE3	1.83	0.43
1:A:19:CYS:HA	1:A:201:ASP:OD2	2.18	0.43
1:A:205:PHE:CG	1:A:206:ASP:N	2.86	0.43
1:A:214:VAL:CG1	1:A:244:LYS:HG3	2.47	0.43
1:A:39:LEU:CD2	1:A:39:LEU:N	2.78	0.43
1:C:1070:LYS:O	1:C:1073:GLU:HG2	2.17	0.43
1:C:1283:HIS:O	1:C:1284:ASN:HB2	2.18	0.43
2:D:3248:ARG:HG3	2:D:3257:ILE:CG1	2.48	0.43
2:D:3268:GLY:O	2:D:3272:THR:HG23	2.19	0.43
2:D:3284:HIS:CD2	2:D:3295:ILE:HD13	2.53	0.43
2:D:3413:ARG:HB3	2:D:3413:ARG:NH1	2.33	0.43
1:A:145:ARG:C	1:A:147:ASP:H	2.21	0.43
1:A:28:LEU:O	1:A:168:SER:HA	2.17	0.43
1:A:260:TYR:O	1:A:262:TRP:CD1	2.71	0.43
1:C:1120:LYS:CG	1:C:1154:VAL:HG21	2.48	0.43
2:D:3417:GLU:HG2	2:D:3417:GLU:H	1.40	0.43
1:A:115:PHE:O	1:A:116:ALA:C	2.55	0.43
2:B:2442:ILE:O	2:B:2446:VAL:HG23	2.18	0.43
2:B:2463:MET:C	2:B:2463:MET:HE2	2.39	0.43
1:C:1117:LYS:O	1:C:1117:LYS:CE	2.66	0.43
1:C:1123:ASP:C	1:C:1125:THR:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1086:MET:HG2	2:D:3412:TYR:CD1	2.53	0.43
1:A:107:ASN:HB3	1:A:110:VAL:HG23	1.99	0.43
1:A:123:ASP:C	1:A:125:THR:N	2.72	0.43
1:A:39:LEU:O	1:A:39:LEU:HD23	2.18	0.43
2:B:2429:LEU:O	2:B:2431:GLU:N	2.51	0.43
1:C:1217:LEU:HD11	1:C:1282:LEU:HD22	1.99	0.43
2:B:2230:SER:O	2:B:2231:LYS:C	2.57	0.43
1:C:1145:ARG:NH2	1:C:1177:LYS:HZ1	2.17	0.43
1:C:1179:ILE:O	1:C:1181:PRO:HD3	2.19	0.43
2:D:3289:VAL:HG11	2:D:3329:GLN:O	2.19	0.43
1:A:125:THR:O	1:A:126:ASP:O	2.35	0.43
1:A:26:ARG:HB2	1:A:171:TYR:CE1	2.54	0.43
2:B:2260:ARG:NE	2:B:2316:SER:HA	2.33	0.43
1:C:1106:GLN:NE2	1:C:1150:VAL:O	2.51	0.43
2:D:3412:TYR:N	2:D:3462:GLN:OE1	2.52	0.43
2:D:3365:TYR:CE1	2:D:3412:TYR:OH	2.70	0.43
1:A:8:GLU:CG	1:A:9:ILE:N	2.78	0.43
2:B:2400:LEU:HD12	2:B:2401:LEU:N	2.33	0.43
2:B:2440:LEU:HA	2:B:2440:LEU:HD12	1.69	0.43
1:C:1259:LYS:HD2	1:C:1259:LYS:N	2.21	0.43
1:C:1281:LYS:CE	1:C:1283:HIS:HB2	2.42	0.43
1:C:1220:PRO:HG3	1:C:1284:ASN:O	2.18	0.43
2:B:2469:THR:O	2:B:2469:THR:OG1	2.36	0.43
1:C:1118:ILE:HA	1:C:1120:LYS:HZ2	1.82	0.43
1:A:143:ASP:O	1:A:145:ARG:N	2.51	0.43
1:C:1254:TRP:CZ2	2:D:3453:LYS:HD3	2.53	0.43
2:D:3351:LYS:HB3	2:D:3351:LYS:HZ3	1.83	0.43
1:C:1118:ILE:C	1:C:1120:LYS:HD2	2.39	0.42
1:C:1123:ASP:C	1:C:1125:THR:N	2.72	0.42
1:C:1184:HIS:HD2	1:C:1194:TYR:CE2	2.35	0.42
2:D:3274:PHE:HB2	2:D:3281:ILE:HD11	2.01	0.42
1:C:1229:VAL:O	1:C:1229:VAL:HG12	2.19	0.42
2:D:3229:LYS:O	2:D:3230:SER:C	2.57	0.42
1:A:49:ILE:HD13	1:A:53:ILE:HD11	2.01	0.42
1:A:118:ILE:HA	1:A:118:ILE:HD12	1.85	0.42
1:A:9:ILE:HG22	1:A:9:ILE:O	2.19	0.42
2:D:3323:ILE:CG1	2:D:3323:ILE:O	2.63	0.42
2:D:3461:LYS:HB3	2:D:3461:LYS:HZ2	1.84	0.42
1:A:254:TRP:HB2	1:A:255:GLY:H	1.48	0.42
2:B:2438:ASP:HA	2:B:2474:LEU:O	2.20	0.42
2:D:3238:ILE:HD12	2:D:3271:THR:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3264:HIS:HD2	2:D:3265:LEU:N	2.17	0.42
1:A:140:LYS:HE2	1:A:290:ASN:O	2.18	0.42
2:B:2323:ILE:HD11	2:B:2357:ILE:CG2	2.49	0.42
1:C:1006:PRO:HB2	1:C:1007:VAL:H	1.62	0.42
1:C:1118:ILE:CA	1:C:1120:LYS:HD2	2.50	0.42
2:D:3241:ASN:O	2:D:3260:ARG:NH1	2.53	0.42
2:D:3257:ILE:O	2:D:3257:ILE:HG13	2.18	0.42
2:D:3294:GLU:OE2	2:D:3298:ILE:HG12	2.20	0.42
2:D:3299:TYR:N	2:D:3299:TYR:CD1	2.88	0.42
2:D:3414:ASN:HB3	2:D:3417:GLU:HG3	2.00	0.42
1:A:31:ILE:CG1	1:A:166:VAL:HG22	2.46	0.42
1:A:234:GLU:HB2	1:A:241:MET:HE3	2.02	0.42
2:B:2366:GLN:HB3	2:B:2461:LYS:O	2.20	0.42
1:C:1075:PHE:CZ	1:C:1281:LYS:HB3	2.54	0.42
1:A:101:TYR:C	1:A:101:TYR:CD1	2.93	0.42
1:A:77:GLN:HE22	1:A:239:LYS:HZ3	1.65	0.42
1:C:1093:ILE:HG23	1:C:1093:ILE:O	2.18	0.42
1:C:1201:ASP:O	1:C:1202:SER:HB2	2.20	0.42
2:B:2275:GLU:CA	2:B:2275:GLU:OE2	2.67	0.42
1:C:1004:ILE:C	1:C:1006:PRO:HD2	2.40	0.42
2:D:3411:SER:HA	2:D:3462:GLN:OE1	2.19	0.42
2:B:2419:THR:OG1	2:B:2422:ILE:HB	2.19	0.42
1:C:1011:VAL:HG12	1:C:1064:ARG:NH2	2.35	0.42
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.79	0.41
1:A:240:SER:OG	1:A:271:TYR:HB3	2.19	0.41
1:A:44:LEU:HD21	1:A:46:MET:SD	2.60	0.41
2:D:3438:ASP:OD1	2:D:3473:LYS:HE2	2.20	0.41
1:A:50:SER:CB	1:A:177:LYS:O	2.68	0.41
1:C:1080:ARG:HH11	1:C:1080:ARG:HG3	1.86	0.41
1:A:11:VAL:O	1:A:11:VAL:HG13	2.20	0.41
2:B:2226:TYR:HE2	2:B:2470:LEU:HD22	1.84	0.41
1:C:1005:PHE:N	1:C:1006:PRO:CD	2.84	0.41
1:A:250:THR:O	1:A:260:TYR:N	2.53	0.41
1:A:2:CYS:O	1:A:3:VAL:CB	2.64	0.41
1:C:1051:GLY:HA2	1:C:1174:ILE:HG12	2.02	0.41
1:C:1176:ASN:ND2	1:C:1176:ASN:N	2.69	0.41
2:D:3226:TYR:HA	2:D:3472:LYS:CE	2.50	0.41
2:D:3458:ASN:O	2:D:3460:GLY:N	2.53	0.41
1:A:175:GLY:O	1:A:177:LYS:HD2	2.21	0.41
1:A:50:SER:HB3	1:A:177:LYS:O	2.20	0.41
2:D:3233:ARG:CZ	2:D:3477:PRO:HD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PHE:HZ	1:A:280:VAL:HG11	1.85	0.41
2:B:2228:MET:HG3	2:B:2475:VAL:O	2.20	0.41
2:D:3343:LEU:CG	2:D:3344:LYS:H	2.34	0.41
1:A:179:ILE:O	1:A:181:PRO:HD3	2.20	0.41
2:B:2403:MET:HB2	2:B:2465:GLN:O	2.21	0.41
2:B:2431:GLU:C	2:B:2434:PRO:HD2	2.41	0.41
1:C:1135:LYS:HE3	1:C:1135:LYS:HB2	1.86	0.41
1:C:1269:PHE:CD2	1:C:1280:VAL:HG22	2.56	0.41
1:C:1099:GLU:CD	1:C:1099:GLU:H	2.23	0.41
1:C:1099:GLU:CD	1:C:1099:GLU:N	2.74	0.41
1:C:1159:PHE:HE2	1:C:1165:GLN:CA	2.34	0.41
2:D:3314:ILE:CG2	2:D:3323:ILE:HD12	2.47	0.41
2:B:2248:ARG:HG3	2:B:2257:ILE:CG2	2.49	0.41
2:B:2432:ARG:NH1	2:B:2432:ARG:CG	2.81	0.41
2:B:2411:SER:HA	2:B:2462:GLN:OE1	2.20	0.41
1:C:1064:ARG:HG2	1:C:1064:ARG:NH1	2.35	0.41
1:C:1054:ARG:NH1	1:C:1170:GLU:OE1	2.53	0.41
2:B:2238:ILE:HD11	2:B:2281:ILE:HD12	2.03	0.41
2:B:2241:ASN:HB2	2:B:2315:LEU:O	2.21	0.41
2:D:3226:TYR:HA	2:D:3472:LYS:HE3	2.02	0.41
1:A:297:THR:O	1:A:298:ILE:C	2.60	0.41
1:A:77:GLN:HE22	1:A:239:LYS:HZ1	1.68	0.41
2:B:2265:LEU:O	2:B:2269:ALA:HB2	2.20	0.41
2:B:2407:ASN:ND2	2:B:2408:ASN:N	2.66	0.41
2:D:3337:THR:O	2:D:3399:PHE:CZ	2.74	0.41
2:D:3405:THR:OG1	2:D:3406:VAL:N	2.54	0.41
1:A:127:LYS:NZ	1:A:127:LYS:CB	2.84	0.40
1:A:230:LEU:N	1:A:230:LEU:CD1	2.84	0.40
1:A:297:THR:O	1:A:299:LYS:N	2.54	0.40
2:B:2445:GLU:O	2:B:2448:TYR:HB3	2.21	0.40
1:C:1231:TYR:OH	1:C:1233:ASN:ND2	2.54	0.40
2:D:3343:LEU:HD12	2:D:3344:LYS:N	2.36	0.40
2:D:3400:LEU:HG	2:D:3439:ILE:CD1	2.49	0.40
1:A:107:ASN:O	1:A:108:GLY:C	2.59	0.40
1:A:102:SER:CB	1:A:120:LYS:NZ	2.82	0.40
1:A:201:ASP:C	1:A:201:ASP:OD2	2.60	0.40
1:A:217:LEU:HD23	1:A:287:SER:HB2	2.04	0.40
2:B:2260:ARG:CD	2:B:2316:SER:HA	2.51	0.40
1:C:1061:ASN:C	1:C:1063:LEU:H	2.23	0.40
1:C:1291:LYS:HD2	1:C:1291:LYS:C	2.41	0.40
2:D:3369:ILE:N	2:D:3369:ILE:HD12	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:HG21	1:A:259:LYS:HE2	2.04	0.40
2:B:2254:LEU:N	2:B:2254:LEU:HD12	2.36	0.40
2:B:2260:ARG:HG2	2:B:2317:HIS:NE2	2.37	0.40
2:B:2276:GLU:O	2:B:2478:SER:HB2	2.22	0.40
2:D:3224:LYS:O	2:D:3224:LYS:HD2	2.22	0.40
2:D:3283:PRO:O	2:D:3284:HIS:ND1	2.55	0.40
1:C:1022:ASP:OD2	1:C:1025:THR:HB	2.20	0.40
1:C:1114:LYS:HB3	1:C:1117:LYS:HG3	2.02	0.40
1:C:1196:VAL:HG22	1:C:1197:VAL:N	2.37	0.40
1:C:1246:LEU:C	1:C:1246:LEU:HD23	2.42	0.40
2:D:3322:ILE:HG22	2:D:3332:PRO:HG3	2.02	0.40
2:D:3371:VAL:HG13	2:D:3372:GLU:N	2.37	0.40
2:D:3362:GLY:O	2:D:3410:VAL:HG12	2.22	0.40
1:A:118:ILE:CG1	1:A:122:HIS:HB3	2.46	0.40
1:A:241:MET:HE3	1:A:241:MET:H	1.86	0.40
2:B:2260:ARG:NH1	2:B:2413:ARG:HD3	2.36	0.40
1:C:1024:GLN:HG2	1:C:1024:GLN:O	2.22	0.40
2:D:3399:PHE:O	2:D:3468:PHE:HA	2.22	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	289/298 (97%)	218 (75%)	44 (15%)	27 (9%)	1 4
1	C	289/298 (97%)	221 (76%)	45 (16%)	23 (8%)	1 5
2	B	239/258 (93%)	193 (81%)	36 (15%)	10 (4%)	3 18
2	D	237/258 (92%)	181 (76%)	45 (19%)	11 (5%)	3 16
All	All	1054/1112 (95%)	813 (77%)	170 (16%)	71 (7%)	1 7

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	94	LYS
1	A	108	GLY
1	A	115	PHE
1	A	126	ASP
1	A	146	ASN
1	A	186	ILE
1	A	255	GLY
1	A	298	ILE
2	B	2250	LYS
2	B	2285	HIS
2	B	2459	MET
1	C	1003	VAL
1	C	1007	VAL
1	C	1094	LYS
1	C	1115	PHE
1	C	1146	ASN
1	C	1186	ILE
2	D	3233	ARG
2	D	3250	LYS
2	D	3285	HIS
1	A	7	VAL
1	A	124	TYR
1	A	144	GLU
1	A	147	ASP
1	A	236	SER
1	A	256	LYS
1	A	275	SER
2	B	2320	LYS
2	B	2457	LYS
1	C	1006	PRO
1	C	1038	GLN
1	C	1108	GLY
1	C	1124	TYR
1	C	1255	GLY
1	C	1256	LYS
2	D	3237	LEU
2	D	3309	CYS
2	D	3457	LYS
2	D	3459	MET
1	A	205	PHE
2	B	2230	SER
2	B	2430	ARG

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Mol	Chain	Res	Type
2	B	2456	LYS
1	C	1023	LYS
2	D	3330	GLU
2	D	3449	GLU
1	A	6	PRO
1	A	10	ASP
1	A	23	LYS
1	A	117	LYS
1	A	148	TYR
1	A	206	ASP
1	A	237	LYS
1	A	274	LYS
2	B	2237	LEU
2	B	2373	THR
1	C	1010	ASP
1	C	1148	TYR
1	C	1236	SER
1	A	5	PHE
1	C	1005	PHE
1	C	1126	ASP
1	C	1147	ASP
1	C	1117	LYS
1	C	1121	SER
1	A	9	ILE
1	C	1298	ILE
2	D	3332	PRO
1	C	1009	ILE
2	D	3450	VAL

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	276/280 (99%)	252 (91%)	24 (9%)	12 41
1	C	276/280 (99%)	245 (89%)	31 (11%)	7 28
2	B	218/233 (94%)	198 (91%)	20 (9%)	11 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	216/233 (93%)	180 (83%)	36 (17%)	2 13
All	All	986/1026 (96%)	875 (89%)	111 (11%)	7 27

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	33	LYS
1	A	39	LEU
1	A	46	MET
1	A	77	GLN
1	A	106	GLN
1	A	107	ASN
1	A	123	ASP
1	A	126	ASP
1	A	143	ASP
1	A	189	THR
1	A	191	LEU
1	A	208	GLU
1	A	212	GLU
1	A	215	GLN
1	A	237	LYS
1	A	239	LYS
1	A	241	MET
1	A	250	THR
1	A	251	GLU
1	A	254	TRP
1	A	258	GLU
1	A	289	LEU
1	A	299	LYS
2	B	2223	ASP
2	B	2236	CYS
2	B	2246	LYS
2	B	2271	THR
2	B	2275	GLU
2	B	2276	GLU
2	B	2306	ASN
2	B	2316	SER
2	B	2329	GLN
2	B	2330	GLU
2	B	2363	ASP
2	B	2391	ARG

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Mol	Chain	Res	Type
2	B	2399	PHE
2	B	2405	THR
2	B	2407	ASN
2	B	2427	GLN
2	B	2429	LEU
2	B	2459	MET
2	B	2465	GLN
2	B	2476	PHE
1	C	1005	PHE
1	C	1032	ASN
1	C	1033	LYS
1	C	1038	GLN
1	C	1039	LEU
1	C	1055	SER
1	C	1057	THR
1	C	1062	ASN
1	C	1077	GLN
1	C	1099	GLU
1	C	1106	GLN
1	C	1117	LYS
1	C	1120	LYS
1	C	1123	ASP
1	C	1126	ASP
1	C	1128	LYS
1	C	1142	VAL
1	C	1156	LYS
1	C	1160	GLU
1	C	1189	THR
1	C	1213	PHE
1	C	1215	GLN
1	C	1230	LEU
1	C	1231	TYR
1	C	1233	ASN
1	C	1237	LYS
1	C	1241	MET
1	C	1249	THR
1	C	1259	LYS
1	C	1279	TYR
1	C	1291	LYS
2	D	3222	LEU
2	D	3224	LYS
2	D	3235	TYR

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Mol	Chain	Res	Type
2	D	3240	ASN
2	D	3263	THR
2	D	3264	HIS
2	D	3273	THR
2	D	3275	GLU
2	D	3276	GLU
2	D	3285	HIS
2	D	3286	ASP
2	D	3287	CYS
2	D	3294	GLU
2	D	3304	HIS
2	D	3307	MET
2	D	3337	THR
2	D	3344	LYS
2	D	3345	CYS
2	D	3351	LYS
2	D	3360	CYS
2	D	3391	ARG
2	D	3395	ASP
2	D	3398	ASP
2	D	3399	PHE
2	D	3400	LEU
2	D	3405	THR
2	D	3414	ASN
2	D	3417	GLU
2	D	3431	GLU
2	D	3433	CYS
2	D	3444	THR
2	D	3458	ASN
2	D	3459	MET
2	D	3461	LYS
2	D	3470	LEU
2	D	3471	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	60	ASN
1	A	77	GLN
1	A	85	GLN
1	A	100	HIS

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Mol	Chain	Res	Type
1	A	106	GLN
1	A	107	ASN
1	A	122	HIS
1	A	164	ASN
1	A	172	ASN
1	A	176	ASN
1	A	184	HIS
1	A	204	GLN
1	A	225	ASN
1	A	283	HIS
2	B	2291	GLN
2	B	2329	GLN
2	B	2339	GLN
2	B	2361	GLN
2	B	2366	GLN
2	B	2407	ASN
2	B	2414	ASN
2	B	2427	GLN
2	B	2447	ASN
2	B	2458	ASN
2	B	2465	GLN
1	C	1032	ASN
1	C	1048	ASN
1	C	1074	GLN
1	C	1106	GLN
1	C	1165	GLN
1	C	1172	ASN
1	C	1233	ASN
1	C	1238	ASN
1	C	1284	ASN
1	C	1290	ASN
2	D	3227	GLN
2	D	3240	ASN
2	D	3241	ASN
2	D	3264	HIS
2	D	3291	GLN
2	D	3306	ASN
2	D	3361	GLN
2	D	3408	ASN
2	D	3414	ASN
2	D	3447	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.