



## wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 02:31 PM EDT

PDB ID : 3JB3  
EMDB ID: : EMD-6377  
Title : Atomic model of cytoplasmic polyhedrosis virus with SAM, GTP and ATP  
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.  
Deposited on : 2015-07-06  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
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) : rb-20027939

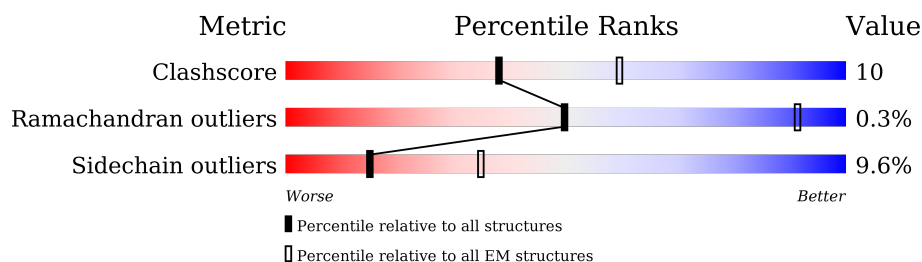
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1058	
2	B	1333	
2	C	1333	
3	D	448	
3	E	448	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32368 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

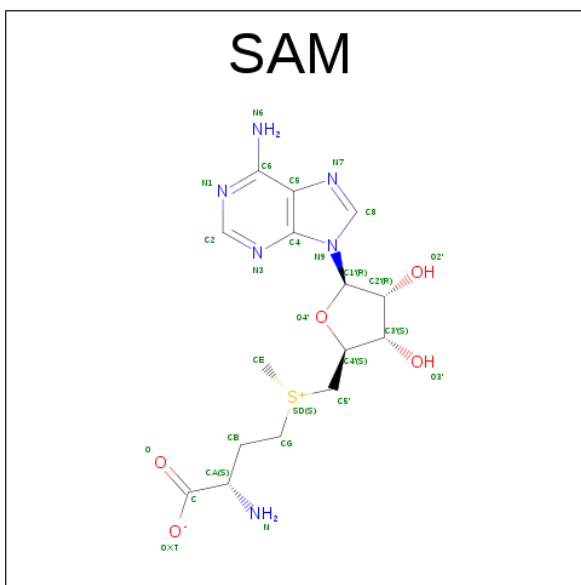
- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1251	Total	C	N	O	S	0	0
			9857	6222	1713	1884	38		

- Molecule 3 is a protein called Viral structural protein 5.

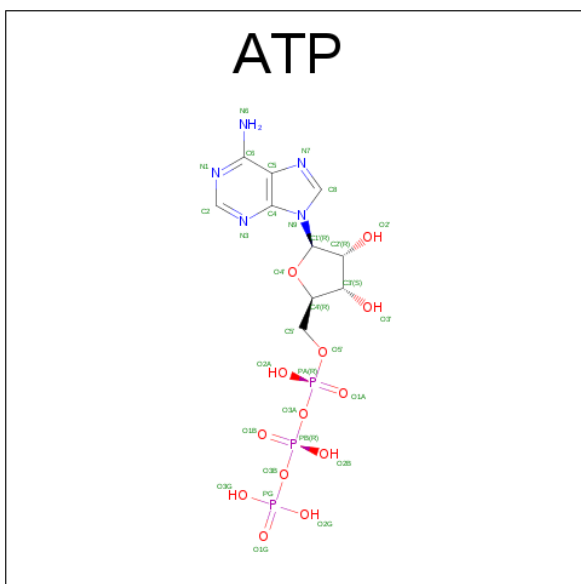
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S).



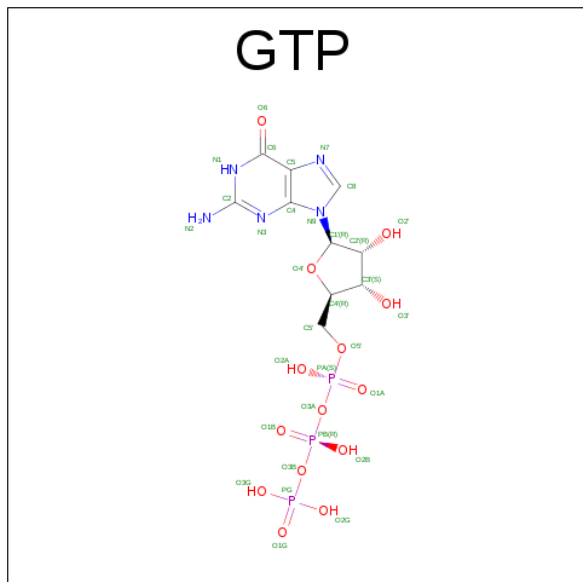
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 54	C 30	N 12	O 10	S 2	0
4	A	1	Total 54	C 30	N 12	O 10	S 2	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

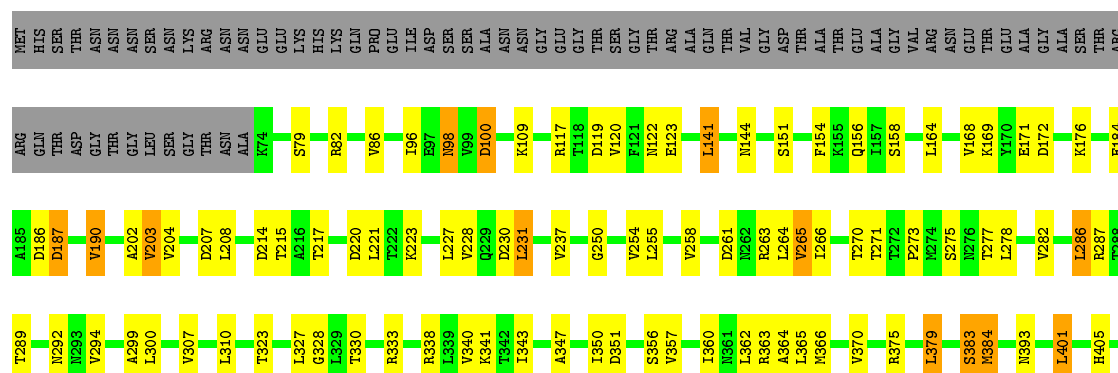


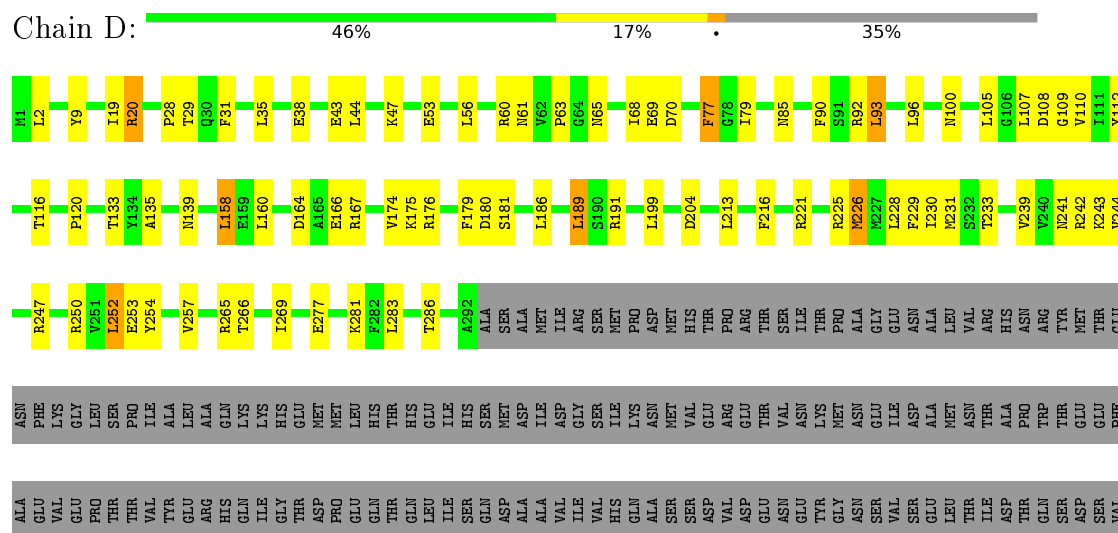
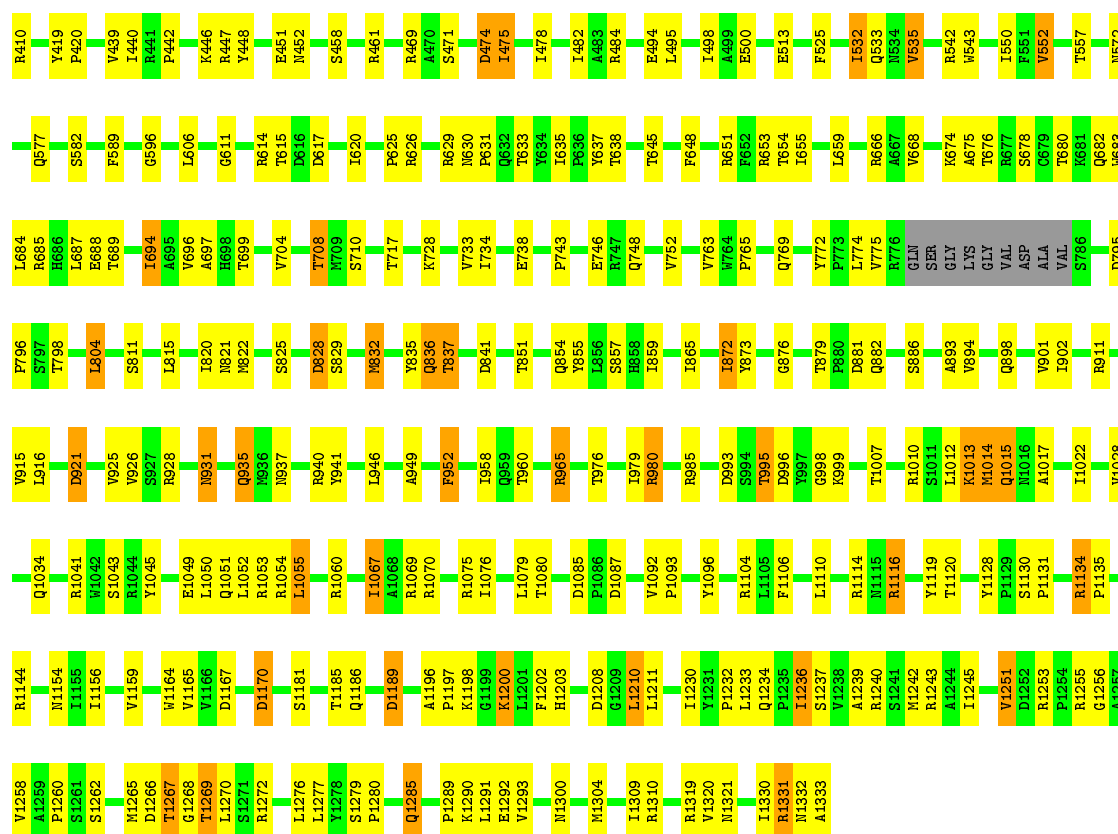
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	32	10	5	14	3	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
7	A	1	1	1	0









GLN	THR	HIS	F282	L160	M1
	THR	HIS	L283	T163	L2
	LEU	GLU	T286	D164	T6
	ILE	ILE			
	SER	HIS	A292	R167	T10
	GLN	SER	ALA		
	ASP	MET	SER	P173	M21
	ALA	ALA	ALA	V174	D22
	ALA	ILE	MET	K175	
	VAL	ASP	ILE		T27
ILE	GLY	ARG	K178	K178	F28
	VAL	SER	F179	D180	T29
	VAL	ILE	MET		Q30
	HIS	ILE	PRO	E183	L35
	GLN	LYS	ASP		
	GLN	ASN	MET		
	ALA	MET	THR	L189	L44
	SER	VAL	HIS		
	ASP	GLU	THR	L199	E53
	VAL	ARG	PRO		
ASP	GLU	GLU	ARG		
	GLU	THR	THR	D204	L56
	ASN	VAL	SER		
	GLU	ASN	ILE	F224	V62
	TYR	LYS	THR	E225	
	GLY	MET	PRO	M226	V66
	ASN	ASN	ALA	M227	V67
	SER	GLU	GLY	L228	I68
	VAL	ILE	GLU	F229	
	SER	ASP	ASN		F90
GLU	GLU	ALA	ALA	T233	S91
	LEU	MET	LEU		R92
	THR	ASN	VAL	N238	L93
	ILE	THR	ARG	V239	
	ASP	ALA	HIS	V240	L96
	THR	PRO	ASN		A97
	GLN	TRP	ARG	V244	L98
	SER	THR	TYR	T245	
	ASP	GLU	MET	K246	T101
	SER	GLU	THR	R247	
VAL	VAL	PHE	GLU	V248	L105
	LEU	ALA	ASN	D249	
		GLU	PHE	R250	T111
		VAL	LYS	V251	
		GLU	GLY	L252	T116
		PRO	LEU	E253	
		THR	SER	Y254	D123
		THR	PRO		P124
		VAL	ILE	T262	
		TYR	ALA	A263	V127
GLU	GLU	LEU	ALA	T266	F130
	ARG	ALA	GLN		
	HIS	HIS	LYS	T270	T133
	GLN	ILE	LYS	D271	A135
	ILE	GLY	HIS	T272	
	THR	THR	GLU	L273	
	ASP	ASP	MET	S274	T142
	PRO	PRO	MET		P143
	GLU	GLU	LEU	V281	
		THR	THR		

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	40898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 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: GTP, MG, ATP, SAM

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  >2	RMSZ	# Z  >2
1	A	0.28	0/8619	0.51	0/11737
2	B	0.34	0/9590	0.56	0/13056
2	C	0.34	0/10058	0.56	0/13695
3	D	0.32	0/2327	0.53	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.32	0/32921	0.54	0/44814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8434	0	8398	175	0
2	B	9397	0	9315	194	0
2	C	9857	0	9767	193	0
3	D	2281	0	2282	47	0
3	E	2281	0	2282	32	0
4	A	54	0	44	3	0
5	A	31	0	12	3	0
6	A	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
All	All	32368	0	32112	624	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 10.

All (624) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:THR:HG22	1:A:271:ARG:HE	1.41	0.83
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.64	0.79
1:A:305:TYR:O	1:A:317:ARG:NH1	2.16	0.78
2:B:1144:ARG:NH1	2:B:1170:ASP:OD1	2.17	0.78
5:A:1103:ATP:H8	5:A:1103:ATP:H5'1	1.50	0.77
1:A:12:ARG:NH2	1:A:16:ASP:OD1	2.18	0.77
2:B:1289:PRO:HD2	3:D:20:ARG:HD3	1.71	0.73
2:C:1144:ARG:NH1	2:C:1170:ASP:OD1	2.21	0.73
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.22	0.72
2:B:626:ARG:NH2	2:B:712:PHE:O	2.23	0.72
1:A:926:MET:HB2	1:A:995:VAL:HG21	1.73	0.71
2:C:494:GLU:HG2	2:C:577:GLN:HG3	1.73	0.71
3:D:176:ARG:HG3	3:D:253:GLU:HB3	1.72	0.71
2:B:248:VAL:HG22	2:B:970:LEU:HB3	1.71	0.71
2:C:1208:ASP:OD1	2:C:1243:ARG:NH2	2.21	0.70
2:C:458:SER:HB3	2:C:675:ALA:HB1	1.72	0.70
1:A:487:GLN:O	1:A:492:HIS:ND1	2.24	0.70
2:C:996:ASP:HA	2:C:999:LYS:HD2	1.75	0.69
1:A:210:SER:O	1:A:255:ARG:NH1	2.25	0.69
2:B:873:TYR:HB3	2:B:898:GLN:HB2	1.74	0.69
2:C:1272:ARG:NH1	3:E:22:ASP:OD2	2.26	0.69
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.75	0.68
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.75	0.68
2:B:746:GLU:OE2	2:C:685:ARG:NH1	2.27	0.68
3:D:239:VAL:HG12	3:D:250:ARG:HD2	1.76	0.68
2:B:1273:ASN:ND2	2:B:1275:ASP:OD2	2.26	0.68
1:A:51:LEU:HD23	1:A:171:ILE:HD11	1.76	0.67
2:B:1226:ASP:OD1	2:C:122:ASN:ND2	2.28	0.67
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.77	0.66
2:C:1240:ARG:HD2	2:C:1243:ARG:HB2	1.78	0.66
2:B:287:ARG:HE	2:B:330:THR:HG22	1.60	0.65
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:ASP:OD1	2:B:965:ARG:NH1	2.30	0.65
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.77	0.65
1:A:662:ILE:HD12	1:A:675:THR:HG21	1.77	0.65
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.78	0.65
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.78	0.65
2:B:1227:MET:HG3	2:C:123:GLU:HG2	1.77	0.65
2:C:829:SER:O	2:C:965:ARG:NH2	2.30	0.64
2:C:653:ARG:HG3	2:C:688:GLU:CD	2.18	0.64
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.79	0.64
3:D:164:ASP:OD1	3:D:167:ARG:NH2	2.31	0.64
1:A:173:ASP:N	1:A:173:ASP:OD1	2.31	0.64
1:A:267:THR:HG21	1:A:271:ARG:HH21	1.63	0.64
1:A:340:ILE:HD11	1:A:348:LEU:HD11	1.79	0.64
2:C:1060:ARG:NH1	2:C:1291:LEU:O	2.30	0.64
2:B:263:ARG:O	2:B:361:ASN:ND2	2.31	0.63
2:B:836:GLN:HE21	2:B:843:LEU:HA	1.63	0.63
2:C:795:ASP:OD1	2:C:1319:ARG:NH2	2.31	0.63
1:A:925:ILE:HG12	1:A:942:LYS:HD2	1.81	0.63
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.30	0.63
1:A:372:ARG:HD3	1:A:823:THR:HG21	1.80	0.63
1:A:27:LYS:NZ	1:A:37:ASP:OD1	2.27	0.63
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.32	0.63
2:B:388:GLN:HB2	2:B:1320:VAL:HB	1.81	0.63
1:A:686:TYR:HA	1:A:714:ARG:HH21	1.64	0.62
2:C:931:ASN:HD22	2:C:931:ASN:H	1.46	0.62
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.18	0.62
2:C:1236:ILE:HG22	2:C:1237:SER:H	1.63	0.62
2:C:879:THR:HG22	2:C:881:ASP:H	1.65	0.62
1:A:411:ILE:HD11	1:A:415:ASP:HB2	1.82	0.62
2:C:1289:PRO:HG2	2:C:1292:GLU:HB2	1.81	0.62
1:A:205:VAL:HG23	1:A:263:LEU:HB2	1.81	0.62
1:A:540:LYS:NZ	1:A:543:GLU:OE2	2.31	0.61
2:C:1134:ARG:NH2	2:C:1154:ASN:OD1	2.30	0.61
2:C:668:VAL:HG23	2:C:674:LYS:HD3	1.81	0.61
1:A:964:GLU:HB3	1:A:1049:TYR:HD1	1.66	0.61
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.34	0.61
3:E:62:VAL:HB	3:E:92:ARG:HD3	1.82	0.61
1:A:714:ARG:NH1	1:A:1044:ASP:OD2	2.34	0.60
1:A:677:LEU:HD23	1:A:711:MET:HB2	1.83	0.60
2:B:235:ILE:HD12	2:C:774:LEU:HD22	1.83	0.60
3:D:283:LEU:HA	3:D:286:THR:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:53:GLU:OE2	3:E:281:LYS:NZ	2.32	0.60
3:D:69:GLU:HG3	3:D:199:LEU:HG	1.83	0.60
3:E:272:ASP:OD1	3:E:274:SER:OG	2.18	0.60
3:D:93:LEU:HD12	3:D:96:LEU:HD12	1.83	0.60
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.36	0.59
2:B:383:SER:HB3	2:B:796:PRO:HG3	1.83	0.59
2:B:1085:ASP:N	2:B:1085:ASP:OD1	2.36	0.59
3:E:180:ASP:OD2	3:E:247:ARG:NH1	2.36	0.59
1:A:212:HIS:ND1	6:A:1104:GTP:O2A	2.33	0.59
1:A:189:MET:HE1	1:A:348:LEU:H	1.68	0.59
1:A:569:VAL:HG22	1:A:584:ILE:HG22	1.85	0.59
3:D:108:ASP:OD2	3:D:112:TYR:OH	2.18	0.59
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.35	0.58
2:C:822:MET:O	2:C:825:SER:OG	2.22	0.58
2:C:1232:PRO:HB3	2:C:1236:ILE:HD11	1.84	0.58
1:A:14:ALA:HA	1:A:112:ARG:NH2	2.18	0.58
1:A:999:VAL:HG13	1:A:1002:ASP:HB2	1.86	0.58
2:C:615:THR:OG1	2:C:1333:ALA:O	2.19	0.58
1:A:227:MET:HG2	1:A:269:VAL:HG21	1.85	0.57
1:A:573:ARG:NH2	1:A:584:ILE:O	2.34	0.57
2:B:439:VAL:HG13	2:B:440:ILE:HG13	1.85	0.57
2:B:1108:SER:O	2:C:393:ASN:ND2	2.34	0.57
2:B:620:ILE:HD11	2:B:631:PRO:HG2	1.87	0.57
1:A:257:ILE:HG21	1:A:326:LEU:HD11	1.87	0.57
2:C:343:ILE:HD13	2:C:362:LEU:HD21	1.87	0.57
2:C:1269:THR:OG1	2:C:1270:LEU:N	2.25	0.57
2:C:851:THR:HG23	2:C:854:GLN:HB2	1.87	0.57
2:C:79:SER:OG	2:C:172:ASP:OD1	2.23	0.56
2:C:439:VAL:HG13	2:C:440:ILE:HG13	1.87	0.56
3:D:77:PHE:HB3	3:D:230:ILE:HG21	1.86	0.56
1:A:41:THR:HG23	1:A:50:THR:HG23	1.86	0.56
1:A:655:GLU:HG2	1:A:712:ILE:HG21	1.88	0.56
1:A:735:LYS:HB2	1:A:738:SER:HB2	1.87	0.56
2:B:524:GLU:HA	2:B:527:ARG:HD2	1.87	0.56
2:C:273:PRO:HB2	2:C:278:LEU:HD11	1.88	0.56
3:D:35:LEU:HD12	3:D:179:PHE:HB3	1.87	0.56
1:A:374:LYS:HG2	1:A:770:THR:HG22	1.88	0.56
2:B:576:ASP:OD2	2:B:747:ARG:NH1	2.36	0.56
2:C:615:THR:H	2:C:1333:ALA:HB1	1.71	0.56
1:A:267:THR:HG23	1:A:320:TYR:OH	2.06	0.56
1:A:697:ILE:HD11	1:A:701:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.87	0.56
2:C:410:ARG:HD3	2:C:1043:SER:HA	1.88	0.55
1:A:474:TYR:HD1	1:A:499:VAL:HG12	1.70	0.55
2:C:746:GLU:OE1	2:C:748:GLN:NE2	2.36	0.55
1:A:213:TRP:HB2	1:A:215:VAL:HG12	1.87	0.55
2:C:366:MET:HG3	3:E:266:THR:HG21	1.88	0.55
2:B:405:HIS:ND1	2:B:625:PRO:HA	2.20	0.55
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.39	0.55
2:B:157:ILE:HG12	2:B:263:ARG:HD2	1.88	0.55
2:B:817:ASP:O	2:B:821:ASN:ND2	2.31	0.55
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.89	0.55
1:A:499:VAL:O	1:A:574:ARG:NH1	2.40	0.55
2:B:287:ARG:NH1	2:B:326:GLY:HA3	2.20	0.55
2:C:865:ILE:HD11	2:C:1041:ARG:HB2	1.89	0.55
2:C:214:ASP:OD1	2:C:215:THR:N	2.39	0.55
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.89	0.55
3:D:166:GLU:OE1	3:D:175:LYS:NZ	2.32	0.55
2:B:704:VAL:HG12	2:B:1330:ILE:HD11	1.88	0.55
3:D:180:ASP:OD1	3:D:247:ARG:NH2	2.40	0.55
2:B:652:PHE:HA	2:B:655:ILE:HD12	1.88	0.54
2:B:1149:LYS:HG3	2:B:1195:THR:HG21	1.89	0.54
2:C:1075:ARG:NH1	2:C:1167:ASP:OD1	2.40	0.54
2:C:795:ASP:O	2:C:798:THR:HG22	2.06	0.54
2:C:993:ASP:OD1	2:C:995:THR:OG1	2.22	0.54
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.88	0.54
2:B:1022:ILE:HG22	2:B:1028:VAL:HG22	1.89	0.54
2:B:626:ARG:NH1	2:B:715:ASN:O	2.40	0.54
2:B:1048:ASP:OD1	2:B:1048:ASP:N	2.40	0.54
1:A:203:THR:HG22	1:A:204:LEU:HG	1.90	0.54
1:A:836:ILE:HD11	1:A:1033:ILE:HG21	1.89	0.54
2:C:265:VAL:HB	2:C:1304:MET:HB3	1.90	0.54
3:E:66:VAL:HG13	3:E:111:ILE:HB	1.88	0.54
2:B:168:VAL:HG22	2:B:204:VAL:HG22	1.88	0.54
2:B:339:LEU:HD11	3:D:63:PRO:HB2	1.90	0.54
1:A:427:ASP:HA	1:A:703:PHE:HA	1.90	0.54
2:B:287:ARG:HH11	2:B:326:GLY:HA3	1.73	0.54
2:C:100:ASP:HB2	2:C:338:ARG:HH22	1.73	0.54
2:C:186:ASP:OD1	2:C:282:VAL:HG21	2.08	0.54
1:A:288:LEU:HD21	1:A:300:LEU:HD22	1.90	0.53
1:A:685:PRO:O	1:A:714:ARG:NH2	2.40	0.53
2:B:1008:LEU:HD11	2:B:1010:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:732:TYR:CE1	2:B:1021:ARG:HG3	2.43	0.53
1:A:409:MET:HE1	1:A:1037:SER:HB3	1.88	0.53
1:A:385:HIS:NE2	1:A:803:SER:OG	2.41	0.53
2:C:347:ALA:HB1	2:C:1267:THR:HG21	1.91	0.53
2:C:926:VAL:HG21	2:C:937:ASN:HA	1.91	0.53
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.90	0.53
2:C:1069:ARG:HD2	2:C:1239:ALA:HB2	1.91	0.53
2:B:271:THR:HG22	2:B:292:ASN:OD1	2.06	0.53
2:C:254:VAL:O	2:C:258:VAL:HG12	2.09	0.53
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.89	0.53
1:A:636:VAL:HG22	1:A:648:VAL:HG11	1.91	0.53
2:B:502:PHE:CE2	2:B:539:PHE:HB2	2.44	0.53
3:D:229:PHE:O	3:D:233:THR:HG23	2.09	0.53
1:A:712:ILE:HG22	1:A:716:MET:HG3	1.91	0.52
2:B:370:VAL:HG22	2:B:400:GLU:O	2.09	0.52
2:C:1266:ASP:OD1	2:C:1279:SER:OG	2.25	0.52
2:B:990:THR:OG1	2:B:990:THR:O	2.24	0.52
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.90	0.52
1:A:764:SER:HA	1:A:795:GLU:HG2	1.91	0.52
2:B:1266:ASP:OD1	2:B:1279:SER:OG	2.24	0.52
2:C:190:VAL:HG23	2:C:300:LEU:HB3	1.91	0.52
2:B:619:ALA:HB2	2:B:711:ASN:HA	1.91	0.52
2:C:471:SER:O	2:C:765:PRO:HG3	2.09	0.52
2:B:705:VAL:HA	2:B:708:THR:HG22	1.90	0.52
2:B:1206:PHE:CE2	2:B:1232:PRO:HD3	2.45	0.52
2:C:614:ARG:HG3	2:C:1333:ALA:HA	1.91	0.52
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.27	0.52
2:C:100:ASP:OD1	2:C:338:ARG:NH2	2.42	0.52
2:C:384:MET:HA	2:C:708:THR:HG21	1.90	0.52
2:C:469:ARG:HH21	2:C:513:GLU:CD	2.13	0.52
2:B:739:GLY:HA2	2:C:653:ARG:HD3	1.92	0.52
3:E:245:THR:OG1	3:E:246:LYS:N	2.41	0.52
1:A:681:ALA:O	1:A:1037:SER:HB2	2.10	0.52
2:B:214:ASP:N	2:B:214:ASP:OD1	2.41	0.52
2:C:383:SER:HB3	2:C:796:PRO:HG3	1.92	0.52
1:A:74:LEU:HD13	1:A:83:ILE:HG21	1.91	0.51
2:B:505:PRO:HG2	2:B:672:MET:SD	2.50	0.51
2:C:498:ILE:HG22	2:C:500:GLU:H	1.74	0.51
2:C:606:LEU:HD22	2:C:655:ILE:HG12	1.92	0.51
3:E:238:ASN:HB3	3:E:253:GLU:HG3	1.92	0.51
1:A:411:ILE:HG23	1:A:469:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1014:MET:HA	2:B:1017:ALA:HB2	1.91	0.51
2:B:512:LEU:HD22	2:B:659:LEU:HD23	1.92	0.51
2:B:759:ASP:OD2	2:B:761:SER:OG	2.27	0.51
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.11	0.51
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.92	0.51
3:E:96:LEU:HA	3:E:101:THR:HG21	1.92	0.51
1:A:807:GLU:OE2	1:A:810:ARG:NH1	2.44	0.51
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.92	0.51
2:B:473:ALA:HB2	2:B:765:PRO:HB3	1.93	0.51
2:B:694:ILE:HG13	2:B:772:TYR:CE1	2.45	0.51
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.32	0.51
2:C:606:LEU:HA	2:C:651:ARG:HH21	1.76	0.51
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.92	0.51
1:A:797:ARG:NH2	1:A:876:MET:O	2.44	0.51
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.93	0.51
2:C:1128:TYR:CZ	2:C:1135:PRO:HD3	2.46	0.51
2:C:208:LEU:HD21	2:C:1067:ILE:HG13	1.93	0.51
2:B:287:ARG:NE	2:B:330:THR:HG22	2.25	0.51
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.92	0.51
1:A:887:ILE:HD11	1:A:901:SER:HB2	1.93	0.51
2:B:1128:TYR:CZ	2:B:1135:PRO:HD3	2.45	0.51
2:B:697:ALA:HB2	2:B:775:VAL:HG23	1.93	0.51
3:D:69:GLU:HB2	3:D:109:GLY:HA3	1.93	0.51
2:C:872:ILE:HD12	2:C:886:SER:HB2	1.92	0.50
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.46	0.50
1:A:846:ARG:HB2	1:A:871:VAL:HA	1.94	0.50
1:A:479:LYS:NZ	1:A:481:ASP:OD2	2.31	0.50
1:A:856:THR:HG22	1:A:916:ASN:HB2	1.94	0.50
2:B:186:ASP:OD2	2:B:279:SER:OG	2.27	0.50
1:A:531:LYS:HD3	1:A:691:TYR:OH	2.12	0.50
2:B:1008:LEU:HG	2:B:1010:ARG:H	1.75	0.50
1:A:674:HIS:HA	1:A:701:VAL:HG21	1.93	0.50
1:A:860:SER:OG	1:A:868:ASP:OD2	2.23	0.50
2:B:267:VAL:HA	2:B:1304:MET:HE2	1.93	0.50
2:B:342:THR:HB	2:B:1309:ILE:HD11	1.94	0.50
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.26	0.50
2:B:873:TYR:HA	2:B:896:LEU:O	2.12	0.50
2:C:171:GLU:OE1	2:C:1181:SER:N	2.33	0.50
3:D:9:TYR:H	3:D:204:ASP:CG	2.14	0.50
1:A:552:MET:H	1:A:576:ASN:ND2	2.09	0.50
2:C:184:GLU:HA	2:C:187:ASP:OD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ALA:HB2	1:A:781:VAL:HG11	1.93	0.50
2:C:828:ASP:OD1	2:C:960:THR:OG1	2.29	0.50
1:A:840:MET:HG2	1:A:1024:LEU:HA	1.93	0.49
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.47	0.49
2:B:742:LYS:HG3	2:B:1012:LEU:HD13	1.93	0.49
2:C:1243:ARG:HD3	2:C:1256:GLY:O	2.12	0.49
1:A:192:VAL:HG22	1:A:216:LEU:HD22	1.94	0.49
1:A:52:ARG:NH2	1:A:169:SER:OG	2.45	0.49
1:A:557:SER:HB3	1:A:583:ARG:HB3	1.94	0.49
2:B:357:VAL:HG23	2:B:1057:VAL:HG11	1.94	0.49
3:E:229:PHE:O	3:E:233:THR:HG23	2.12	0.49
1:A:881:ILE:HG23	1:A:900:GLN:HB3	1.94	0.49
3:D:213:LEU:O	3:D:216:PHE:HB3	2.12	0.49
1:A:12:ARG:O	1:A:12:ARG:NE	2.45	0.49
2:B:186:ASP:O	2:B:190:VAL:HB	2.12	0.49
2:B:360:ILE:HG12	2:B:363:ARG:NH2	2.27	0.49
1:A:665:LEU:HD21	1:A:694:ILE:HD12	1.94	0.49
2:B:1087:ASP:OD2	2:B:1240:ARG:NH2	2.45	0.49
2:C:1268:GLY:HA3	2:C:1277:LEU:O	2.12	0.49
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.93	0.49
1:A:535:LEU:HD22	1:A:647:LEU:HD11	1.95	0.49
2:B:439:VAL:HG23	2:B:701:HIS:CE1	2.47	0.49
3:E:124:PRO:HA	3:E:127:VAL:HG22	1.95	0.49
2:B:265:VAL:HG22	2:B:358:LEU:HD22	1.95	0.49
2:C:976:THR:HA	2:C:979:ILE:HD12	1.95	0.49
6:A:1104:GTP:O1B	6:A:1104:GTP:H5"	2.13	0.49
2:B:157:ILE:HD13	2:B:160:PRO:HB3	1.95	0.49
2:C:474:ASP:N	2:C:474:ASP:OD1	2.45	0.49
2:C:620:ILE:HD11	2:C:631:PRO:HG2	1.95	0.49
2:C:893:ALA:HB1	2:C:915:VAL:HA	1.95	0.49
2:B:153:ASP:OD1	2:B:153:ASP:N	2.42	0.49
2:B:170:TYR:CE1	2:B:198:LYS:HG2	2.47	0.49
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	1.94	0.49
2:C:1043:SER:O	2:C:1045:TYR:N	2.46	0.49
2:B:1051:GLN:O	2:B:1055:LEU:HB2	2.13	0.48
2:B:836:GLN:OE1	2:B:836:GLN:N	2.46	0.48
1:A:26:THR:HG22	1:A:57:PHE:HZ	1.78	0.48
2:C:617:ASP:OD1	2:C:617:ASP:N	2.46	0.48
1:A:943:ILE:HG12	1:A:960:ILE:HG21	1.95	0.48
2:B:997:TYR:O	2:B:1001:THR:HG23	2.13	0.48
2:B:332:THR:HG23	2:B:344:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:VAL:O	2:B:810:LEU:HG	2.13	0.48
2:C:611:GLY:HA3	2:C:635:ILE:O	2.13	0.48
2:C:697:ALA:HB2	2:C:775:VAL:HG23	1.95	0.48
1:A:102:LEU:HD23	1:A:135:VAL:HA	1.96	0.48
2:B:1036:ASP:OD1	2:B:1036:ASP:N	2.46	0.48
2:B:522:PRO:HD2	2:B:636:PRO:HB3	1.94	0.48
2:C:879:THR:HB	2:C:882:GLN:HB2	1.96	0.48
1:A:890:LEU:HD23	1:A:890:LEU:H	1.79	0.48
2:B:737:PRO:HA	2:B:861:GLU:HG2	1.94	0.48
2:C:552:VAL:HG13	2:C:572:ASN:HB2	1.94	0.48
1:A:962:PHE:HB2	1:A:998:LEU:HD23	1.95	0.48
2:B:458:SER:HB3	2:B:676:THR:HG22	1.96	0.48
2:C:704:VAL:O	2:C:708:THR:HG23	2.14	0.48
1:A:202:SER:O	1:A:264:SER:OG	2.17	0.47
2:B:1007:THR:OG1	2:B:1008:LEU:N	2.45	0.47
2:B:1148:SER:HB3	2:B:1151:VAL:HG23	1.96	0.47
2:B:446:LYS:HA	2:B:769:GLN:HB3	1.96	0.47
2:C:821:ASN:OD1	2:C:1014:MET:N	2.46	0.47
2:C:1159:VAL:HA	2:C:1164:TRP:HB2	1.95	0.47
2:C:168:VAL:HG13	2:C:204:VAL:HG22	1.95	0.47
1:A:234:LYS:HA	1:A:234:LYS:HD3	1.59	0.47
1:A:552:MET:H	1:A:576:ASN:HD21	1.62	0.47
1:A:919:TYR:HB3	1:A:921:PHE:HE1	1.79	0.47
2:B:184:GLU:O	2:B:188:ARG:HG3	2.12	0.47
2:C:363:ARG:HH12	3:E:183:GLU:CD	2.17	0.47
2:C:532:ILE:O	2:C:535:VAL:HG23	2.15	0.47
1:A:114:ASN:ND2	1:A:117:LEU:HD22	2.29	0.47
1:A:186:ALA:HB2	1:A:195:ILE:HD12	1.96	0.47
2:B:446:LYS:HB3	2:B:448:TYR:CE2	2.49	0.47
2:B:835:TYR:CD2	2:B:941:TYR:HB3	2.50	0.47
2:C:633:THR:HG21	2:C:710:SER:HB2	1.96	0.47
2:B:612:PHE:CE2	2:B:614:ARG:HB2	2.49	0.47
2:C:738:GLU:OE2	2:C:857:SER:OG	2.21	0.47
2:B:505:PRO:HA	2:B:543:TRP:CZ2	2.50	0.47
2:B:891:HIS:HB3	3:D:242:ARG:HG2	1.96	0.47
2:C:1130:SER:O	2:C:1134:ARG:HD3	2.14	0.47
3:E:44:LEU:HG	3:E:174:VAL:HG22	1.95	0.47
2:B:489:MET:HE1	2:B:580:TYR:HE2	1.78	0.47
2:C:405:HIS:CE1	2:C:625:PRO:HA	2.49	0.47
2:C:1156:ILE:HA	2:C:1156:ILE:HD13	1.82	0.47
3:E:283:LEU:HA	3:E:286:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PRO:HG3	1:A:706:TYR:CZ	2.50	0.47
2:B:462:LEU:HA	2:B:506:SER:HB2	1.97	0.47
3:E:253:GLU:HA	3:E:254:TYR:HA	1.52	0.47
1:A:316:TYR:OH	5:A:1103:ATP:N1	2.31	0.47
1:A:511:LEU:HB3	1:A:171:ILE:HG12	1.96	0.47
2:B:227:LEU:HA	2:B:246:GLU:O	2.15	0.47
2:C:894:VAL:HG22	2:C:916:LEU:HB3	1.97	0.47
2:C:952:PHE:HB3	2:C:958:ILE:HD11	1.97	0.47
2:B:1143:GLU:HG2	2:B:1145:ALA:H	1.80	0.47
2:C:360:ILE:HD11	2:C:1054:ARG:HG2	1.95	0.47
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.96	0.47
3:D:253:GLU:HA	3:D:254:TYR:HA	1.49	0.47
1:A:564:GLU:OE1	4:A:1101:SAM:O3'	2.32	0.46
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.79	0.46
1:A:944:ARG:HB2	1:A:1006:MET:SD	2.55	0.46
2:B:1156:ILE:O	2:B:1159:VAL:HB	2.16	0.46
2:B:561:ASN:HB3	2:B:565:GLU:HG2	1.97	0.46
2:B:585:PHE:CE1	2:B:728:LYS:HD3	2.51	0.46
1:A:420:VAL:HG23	1:A:711:MET:HE1	1.96	0.46
1:A:911:MET:HE2	1:A:946:VAL:HA	1.97	0.46
2:B:719:ASN:OD1	2:B:719:ASN:N	2.38	0.46
2:B:903:ASN:ND2	2:B:905:PRO:HG2	2.31	0.46
2:C:837:THR:HG21	2:C:911:ARG:HG3	1.97	0.46
2:C:231:LEU:HD12	2:C:985:ARG:HG2	1.97	0.46
3:E:10:THR:N	3:E:204:ASP:OD2	2.47	0.46
1:A:563:ALA:HB3	1:A:588:GLY:H	1.80	0.46
1:A:907:ASP:O	1:A:911:MET:HG2	2.15	0.46
1:A:420:VAL:HA	1:A:974:SER:HB2	1.96	0.46
2:B:409:ILE:HD13	2:B:625:PRO:HB2	1.98	0.46
3:D:38:GLU:OE1	3:D:242:ARG:NH1	2.27	0.46
1:A:143:TYR:CG	1:A:149:ALA:HB2	2.50	0.46
1:A:654:SER:O	1:A:658:ILE:HG12	2.16	0.46
2:B:1134:ARG:H	2:B:1134:ARG:HG2	1.36	0.46
2:B:550:ILE:O	2:B:553:GLN:HG3	2.15	0.46
2:B:429:ILE:HG23	2:B:799:THR:HG22	1.98	0.46
2:C:1050:LEU:HD23	2:C:1050:LEU:HA	1.72	0.46
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.39	0.46
2:B:684:LEU:HA	2:B:684:LEU:HD12	1.76	0.46
2:C:442:PRO:HD3	2:C:475:ILE:HG23	1.97	0.46
2:C:683:TRP:CH2	2:C:687:LEU:HD11	2.51	0.46
1:A:133:LEU:HD11	1:A:140:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HH21	1:A:313:ARG:HB3	1.81	0.46
1:A:849:ILE:HG12	1:A:918:ILE:HD13	1.98	0.46
1:A:862:GLY:HA3	1:A:924:VAL:HG11	1.98	0.46
2:B:1055:LEU:O	2:B:1059:LEU:HG	2.15	0.46
3:E:178:LYS:HB3	3:E:251:VAL:HG22	1.97	0.46
1:A:915:ASN:HD21	1:A:954:THR:HG22	1.80	0.46
2:B:157:ILE:HG13	2:B:157:ILE:H	1.61	0.46
2:B:334:LEU:HA	2:B:341:LYS:HA	1.97	0.46
1:A:281:ASN:O	1:A:285:GLU:HG2	2.16	0.45
1:A:39:LEU:HG	1:A:54:LEU:HD21	1.98	0.45
1:A:771:THR:HG22	1:A:783:ILE:HB	1.97	0.45
1:A:919:TYR:HB3	1:A:921:PHE:CE1	2.52	0.45
2:C:1331:ARG:HG3	2:C:1332:ASN:H	1.80	0.45
1:A:271:ARG:O	1:A:275:ILE:HG13	2.15	0.45
2:C:543:TRP:CD2	2:C:666:ARG:HD3	2.50	0.45
1:A:282:GLU:HG2	1:A:282:GLU:H	1.48	0.45
1:A:474:TYR:CD1	1:A:499:VAL:HG12	2.51	0.45
1:A:845:ILE:HD12	1:A:922:ILE:HD11	1.98	0.45
2:C:774:LEU:HA	2:C:774:LEU:HD23	1.67	0.45
1:A:757:LEU:O	1:A:760:SER:OG	2.31	0.45
1:A:74:LEU:HB3	1:A:83:ILE:HD13	1.98	0.45
1:A:923:ALA:H	1:A:961:SER:HB3	1.81	0.45
2:B:897:TYR:CZ	2:B:928:ARG:HG2	2.51	0.45
2:C:495:LEU:HD22	2:C:532:ILE:HG22	1.98	0.45
2:C:979:ILE:HD13	2:C:1013:LYS:HB2	1.97	0.45
3:D:221:ARG:NH2	3:D:225:ARG:HD2	2.32	0.45
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.81	0.45
2:C:1116:ARG:HD2	2:C:1116:ARG:HA	1.83	0.45
2:C:289:THR:O	2:C:328:GLY:HA3	2.16	0.45
2:C:401:LEU:HA	2:C:401:LEU:HD12	1.79	0.45
1:A:552:MET:HB2	1:A:576:ASN:ND2	2.32	0.45
2:C:156:GLN:HB3	2:C:266:ILE:HD13	1.99	0.45
1:A:773:ARG:O	1:A:818:PHE:HA	2.17	0.45
2:B:1075:ARG:HB2	2:B:1233:LEU:HD21	1.99	0.45
2:B:1208:ASP:OD1	2:B:1243:ARG:NH1	2.49	0.45
2:C:1189:ASP:OD1	2:C:1189:ASP:N	2.50	0.45
1:A:658:ILE:O	1:A:662:ILE:HG12	2.17	0.45
2:B:802:GLN:O	2:B:806:VAL:HG23	2.16	0.45
2:B:863:LEU:HA	2:B:866:THR:HG22	1.98	0.45
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.98	0.45
1:A:255:ARG:NH2	6:A:1104:GTP:O1A	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ILE:HG21	1:A:375:HIS:CE1	2.52	0.44
2:B:1002:LEU:HA	2:B:1002:LEU:HD23	1.73	0.44
2:B:883:ILE:HG23	2:B:895:VAL:HG11	1.99	0.44
2:C:1131:PRO:HG3	2:C:1154:ASN:ND2	2.32	0.44
2:C:164:LEU:HD21	2:C:1067:ILE:HD11	2.00	0.44
2:C:446:LYS:HB3	2:C:448:TYR:CE2	2.53	0.44
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.27	0.44
1:A:895:LYS:HA	1:A:895:LYS:HD3	1.84	0.44
2:B:397:LEU:HA	2:B:397:LEU:HD23	1.78	0.44
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.86	0.44
2:C:119:ASP:OD1	2:C:119:ASP:N	2.51	0.44
2:C:286:LEU:HD23	2:C:327:LEU:HD23	1.98	0.44
2:C:525:PHE:HZ	2:C:589:PHE:CE1	2.35	0.44
2:C:1210:LEU:HD21	2:C:1255:ARG:O	2.17	0.44
2:C:223:LYS:NZ	2:C:1203:HIS:HB2	2.33	0.44
2:C:835:TYR:CE2	2:C:941:TYR:HB3	2.53	0.44
1:A:12:ARG:HG3	1:A:213:TRP:CZ2	2.53	0.44
1:A:486:THR:HB	1:A:489:SER:HB3	2.00	0.44
2:B:1240:ARG:HD2	2:B:1243:ARG:HB2	1.99	0.44
2:B:1267:THR:HG22	2:B:1299:SER:OG	2.18	0.44
2:B:209:ASN:ND2	2:B:211:ASP:OD1	2.51	0.44
1:A:918:ILE:HG23	1:A:957:VAL:HG13	1.99	0.44
2:B:1130:SER:O	2:B:1134:ARG:HD3	2.17	0.44
2:B:1087:ASP:OD1	2:B:1237:SER:OG	2.36	0.44
2:C:1243:ARG:HB3	2:C:1258:VAL:HG22	2.00	0.44
2:C:478:ILE:O	2:C:482:ILE:HG12	2.18	0.44
3:E:173:PRO:HG2	3:E:175:LYS:HE3	2.00	0.44
1:A:573:ARG:HA	1:A:584:ILE:HD12	1.99	0.44
2:C:156:GLN:OE1	2:C:1309:ILE:HG12	2.18	0.44
2:C:96:ILE:H	2:C:96:ILE:HG12	1.60	0.44
1:A:849:ILE:HD12	1:A:871:VAL:HG12	1.98	0.44
2:B:828:ASP:HA	2:C:645:THR:HG23	2.00	0.44
2:B:561:ASN:OD1	2:B:562:ALA:N	2.50	0.44
2:B:991:ASP:N	2:B:991:ASP:OD1	2.51	0.44
2:C:820:ILE:HD13	2:C:820:ILE:HA	1.87	0.44
2:C:98:ASN:OD1	2:C:98:ASN:N	2.50	0.44
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.53	0.43
2:B:1053:ARG:HD3	2:B:1053:ARG:HA	1.71	0.43
2:B:286:LEU:HD22	2:B:286:LEU:HA	1.85	0.43
2:C:275:SER:HA	2:C:278:LEU:HD12	1.99	0.43
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:158:LEU:HD13	3:D:158:LEU:HA	1.83	0.43
2:B:1120:THR:OG1	2:B:1120:THR:O	2.33	0.43
2:B:1233:LEU:HD23	2:B:1233:LEU:HA	1.72	0.43
2:B:1309:ILE:HA	2:B:1309:ILE:HD13	1.87	0.43
2:B:489:MET:HE1	2:B:580:TYR:CE2	2.53	0.43
2:C:1114:ARG:HG3	2:C:1116:ARG:HD3	2.00	0.43
2:B:193:THR:HA	2:B:296:VAL:HG13	2.00	0.43
2:B:208:LEU:HD12	2:B:213:PHE:CE2	2.53	0.43
2:B:681:LYS:HG2	2:B:685:ARG:NH1	2.33	0.43
2:C:1211:LEU:HD12	2:C:1211:LEU:HA	1.85	0.43
2:C:1277:LEU:HD23	2:C:1289:PRO:HA	2.00	0.43
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	2.01	0.43
2:C:451:GLU:HA	2:C:452:ASN:HA	1.56	0.43
1:A:540:LYS:O	1:A:543:GLU:HG2	2.18	0.43
2:B:612:PHE:HE2	2:B:614:ARG:HB2	1.83	0.43
2:C:1096:TYR:CE2	2:C:1165:VAL:HG23	2.52	0.43
2:C:475:ILE:H	2:C:475:ILE:HG13	1.52	0.43
5:A:1103:ATP:H5'1	5:A:1103:ATP:C8	2.42	0.43
1:A:373:ILE:HD13	1:A:817:GLY:HA2	2.00	0.43
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.86	0.43
1:A:906:PHE:O	1:A:945:ASN:HB3	2.19	0.43
2:B:1188:VAL:HG11	2:B:1193:ILE:HD13	1.99	0.43
2:B:793:TYR:CE1	2:B:1322:PRO:HG2	2.54	0.43
1:A:353:TYR:OH	3:D:43:GLU:OE1	2.30	0.43
1:A:285:GLU:O	1:A:366:SER:HB3	2.18	0.43
2:B:414:LEU:HD11	2:B:1014:MET:SD	2.59	0.43
2:B:813:LEU:HA	2:B:813:LEU:HD12	1.86	0.43
2:C:356:SER:O	2:C:360:ILE:HG23	2.19	0.43
2:C:980:ARG:HA	2:C:1012:LEU:HD12	2.01	0.43
3:D:65:ASN:HB3	3:D:110:VAL:CG1	2.49	0.43
1:A:591:ALA:HB3	1:A:597:ARG:HA	2.00	0.43
2:C:351:ASP:OD1	2:C:351:ASP:N	2.51	0.43
2:C:851:THR:CG2	2:C:854:GLN:HB2	2.48	0.43
2:C:832:MET:HE3	2:C:946:LEU:HB2	2.00	0.43
1:A:381:GLY:H	1:A:802:THR:HB	1.84	0.43
2:B:620:ILE:HD13	2:B:620:ILE:HA	1.83	0.43
2:C:1049:GLU:O	2:C:1053:ARG:HG2	2.18	0.43
1:A:502:ASP:OD1	1:A:574:ARG:HD3	2.19	0.43
2:B:442:PRO:HG2	2:B:475:ILE:HB	2.00	0.43
2:C:1242:MET:SD	2:C:1260:PRO:HD3	2.59	0.43
2:C:836:GLN:HB2	2:C:940:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1176:GLU:HB2	2:B:1203:HIS:CE1	2.54	0.43
2:B:614:ARG:HD2	2:B:635:ILE:HD11	1.99	0.43
2:C:176:LYS:HA	2:C:176:LYS:HD2	1.86	0.43
2:C:364:ALA:HB2	2:C:1050:LEU:HD21	2.01	0.43
3:D:2:LEU:HA	3:D:2:LEU:HD23	1.91	0.43
1:A:275:ILE:H	1:A:275:ILE:HG13	1.74	0.42
2:C:1015:GLN:H	2:C:1015:GLN:HG3	1.26	0.42
2:C:154:PHE:CE2	2:C:365:LEU:HB2	2.54	0.42
3:E:233:THR:HG22	3:E:252:LEU:HD22	2.01	0.42
3:E:68:ILE:HG12	3:E:93:LEU:HG	1.99	0.42
1:A:204:LEU:HD23	1:A:227:MET:HE2	2.01	0.42
1:A:408:PRO:HB2	1:A:468:PRO:HG2	2.01	0.42
1:A:913:LEU:O	1:A:953:ARG:HD2	2.18	0.42
1:A:913:LEU:O	1:A:953:ARG:NH2	2.50	0.42
2:B:1147:MET:HE3	2:B:1155:ILE:HD12	2.01	0.42
3:D:189:LEU:HD12	3:D:189:LEU:HA	1.84	0.42
1:A:108:ASP:OD1	1:A:108:ASP:N	2.52	0.42
1:A:160:ASP:N	1:A:160:ASP:OD1	2.48	0.42
1:A:234:LYS:HB3	1:A:259:ARG:HA	2.01	0.42
2:B:326:GLY:H	2:B:1267:THR:HG21	1.84	0.42
2:C:1210:LEU:HA	2:C:1210:LEU:HD22	1.88	0.42
2:C:341:LYS:HD3	2:C:341:LYS:HA	1.77	0.42
1:A:14:ALA:HA	1:A:112:ARG:HH22	1.84	0.42
2:B:1314:ASP:N	2:B:1314:ASP:OD1	2.52	0.42
2:B:974:LEU:HD23	2:B:978:GLN:NE2	2.34	0.42
1:A:222:ARG:N	1:A:222:ARG:HD2	2.35	0.42
1:A:644:THR:O	1:A:696:PRO:HD2	2.19	0.42
2:B:459:ALA:HB2	2:B:679:CYS:SG	2.60	0.42
2:C:1200:LYS:NZ	2:C:1200:LYS:HB3	2.33	0.42
2:C:261:ASP:CG	2:C:263:ARG:HE	2.21	0.42
1:A:313:ARG:HD3	1:A:317:ARG:NH1	2.35	0.42
1:A:714:ARG:HD3	1:A:1044:ASP:OD1	2.19	0.42
1:A:916:ASN:N	1:A:955:ASN:O	2.51	0.42
2:B:614:ARG:NH1	2:B:617:ASP:OD1	2.52	0.42
2:B:925:VAL:O	2:B:928:ARG:HB2	2.19	0.42
2:C:1197:PRO:HG2	2:C:1200:LYS:HB2	2.01	0.42
2:C:1280:PRO:HB3	2:C:1285:GLN:O	2.20	0.42
3:D:38:GLU:HB2	3:D:176:ARG:HB3	2.01	0.42
2:B:1277:LEU:O	2:B:1290:LYS:HE3	2.19	0.42
2:C:1106:PHE:CE2	2:C:1119:TYR:HB2	2.54	0.42
1:A:890:LEU:O	1:A:894:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:VAL:HG13	2:B:379:LEU:HD21	2.01	0.42
2:B:483:ALA:O	2:B:487:SER:OG	2.26	0.42
2:B:494:GLU:HG2	2:B:577:GLN:HG3	2.02	0.42
2:B:491:ASN:ND2	2:B:750:GLU:O	2.53	0.42
2:C:648:PHE:HB2	2:C:699:THR:HG21	2.02	0.42
2:C:694:ILE:HG13	2:C:772:TYR:CE1	2.55	0.42
2:C:931:ASN:HD22	2:C:931:ASN:N	2.16	0.42
3:E:123:ASP:HA	3:E:124:PRO:HD3	1.89	0.42
1:A:102:LEU:HA	1:A:102:LEU:HD12	1.80	0.42
1:A:613:ILE:HG13	1:A:643:ALA:HB2	2.00	0.42
1:A:772:TRP:HA	1:A:817:GLY:HA3	2.02	0.42
2:B:691:PHE:O	2:B:695:ALA:HB2	2.20	0.42
1:A:404:SER:HB3	1:A:826:PHE:CD1	2.55	0.42
1:A:882:ASP:HB3	1:A:885:THR:OG1	2.20	0.42
2:B:265:VAL:HB	2:B:1304:MET:HB3	2.02	0.42
2:B:300:LEU:HD23	2:B:300:LEU:HA	1.85	0.42
2:B:451:GLU:O	2:B:452:ASN:HB2	2.20	0.42
2:C:550:ILE:HD13	2:C:596:GLY:HA3	2.02	0.42
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.72	0.42
4:A:1102:SAM:H5'2	4:A:1102:SAM:HB2	1.77	0.41
1:A:238:ASP:OD2	1:A:279:TYR:OH	2.20	0.41
1:A:282:GLU:HG3	1:A:300:LEU:HD11	2.02	0.41
2:B:297:ASN:HA	2:B:298:PRO:HD3	1.92	0.41
2:C:379:LEU:HA	2:C:379:LEU:HD12	1.88	0.41
2:C:876:GLY:HA2	2:C:902:ILE:HA	2.02	0.41
1:A:184:TRP:HB3	1:A:195:ILE:HD13	2.01	0.41
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.87	0.41
2:B:576:ASP:H	2:B:579:LEU:HD12	1.85	0.41
2:B:701:HIS:O	2:B:704:VAL:HG22	2.20	0.41
2:B:949:ALA:O	3:D:243:LYS:HE3	2.20	0.41
2:C:865:ILE:HA	2:C:865:ILE:HD12	1.91	0.41
1:A:7:ILE:HG22	1:A:250:LEU:HD11	2.03	0.41
1:A:616:ASP:OD2	4:A:1101:SAM:N	2.53	0.41
2:B:156:GLN:HB3	2:B:266:ILE:HD11	2.02	0.41
3:D:85:ASN:HD21	3:D:277:GLU:HG3	1.85	0.41
3:D:35:LEU:HD12	3:D:35:LEU:HA	1.82	0.41
2:B:1236:ILE:HG22	2:B:1237:SER:N	2.34	0.41
2:B:231:LEU:HB3	2:B:249:SER:HB2	2.03	0.41
2:B:439:VAL:HG21	2:B:702:LEU:HD13	2.02	0.41
3:D:60:ARG:HE	3:D:60:ARG:HB2	1.74	0.41
1:A:143:TYR:CD1	1:A:146:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:SER:OG	1:A:226:ASP:OD2	2.38	0.41
2:B:608:THR:HA	2:B:609:PRO:HD3	1.80	0.41
2:C:151:SER:O	2:C:1310:ARG:NH2	2.53	0.41
2:C:220:ASP:OD1	2:C:227:LEU:HB2	2.21	0.41
3:E:142:THR:HA	3:E:143:PRO:HD3	1.89	0.41
1:A:755:ALA:N	1:A:756:PRO:HD2	2.35	0.41
2:B:606:LEU:HA	2:B:651:ARG:HH21	1.86	0.41
2:C:1067:ILE:HD12	2:C:1067:ILE:HA	1.87	0.41
2:C:804:LEU:HA	2:C:804:LEU:HD13	1.91	0.41
3:D:44:LEU:HG	3:D:174:VAL:HG22	2.03	0.41
3:D:186:LEU:HD23	3:D:186:LEU:HA	1.76	0.41
1:A:444:LEU:HD11	1:A:449:THR:HG23	2.02	0.41
2:B:774:LEU:HA	2:B:774:LEU:HD23	1.91	0.41
2:B:852:TYR:HB2	2:B:920:PRO:HA	2.03	0.41
2:B:329:LEU:HD11	2:B:344:VAL:HB	2.02	0.41
2:B:1280:PRO:HB3	2:B:1285:GLN:O	2.20	0.41
2:B:373:ASP:O	2:B:376:ILE:HG12	2.21	0.41
2:B:772:TYR:N	2:B:772:TYR:CD1	2.89	0.41
2:C:141:LEU:HA	2:C:141:LEU:HD12	1.73	0.41
3:D:28:PRO:CB	3:D:226:MET:HG3	2.51	0.41
3:D:228:LEU:HA	3:D:231:MET:HE3	2.03	0.41
1:A:43:ASN:O	1:A:47:ARG:N	2.53	0.41
1:A:717:THR:CB	1:A:1020:SER:HB2	2.51	0.41
2:B:1272:ARG:HH12	3:D:69:GLU:HB3	1.86	0.41
2:B:480:LEU:HA	2:B:480:LEU:HD12	1.82	0.41
2:C:1076:ILE:HG22	2:C:1159:VAL:HG11	2.03	0.41
2:C:704:VAL:HA	2:C:1330:ILE:HG21	2.01	0.41
2:C:419:TYR:HA	2:C:420:PRO:HD2	1.94	0.41
2:C:442:PRO:CD	2:C:475:ILE:HG23	2.51	0.41
1:A:445:TYR:CD2	1:A:625:PHE:HB2	2.56	0.41
1:A:967:ILE:HG21	1:A:987:LEU:HD11	2.03	0.41
2:B:231:LEU:HD21	2:B:986:ILE:HG12	2.03	0.41
2:B:659:LEU:HD12	2:B:659:LEU:HA	1.73	0.41
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	2.01	0.41
2:C:582:SER:O	2:C:728:LYS:HE3	2.21	0.41
2:C:678:SER:O	2:C:682:GLN:HG3	2.20	0.41
2:C:835:TYR:HA	2:C:941:TYR:HA	2.02	0.41
3:E:27:THR:O	3:E:30:GLN:HG2	2.20	0.41
2:B:957:PHE:CG	2:B:958:ILE:HG13	2.56	0.40
2:C:1085:ASP:HB2	2:C:1087:ASP:OD1	2.21	0.40
2:C:169:LYS:HB2	2:C:203:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:680:THR:O	2:C:684:LEU:HG	2.21	0.40
3:E:263:ALA:O	3:E:270:THR:HG21	2.21	0.40
1:A:112:ARG:HB3	1:A:143:TYR:CZ	2.57	0.40
2:B:259:MET:HE1	2:B:1047:LEU:HD13	2.03	0.40
2:B:713:MET:HE1	2:B:804:LEU:HD13	2.03	0.40
2:C:287:ARG:O	2:C:289:THR:N	2.53	0.40
2:C:357:VAL:O	2:C:360:ILE:HG12	2.22	0.40
1:A:108:ASP:HB2	1:A:111:LEU:HD22	2.03	0.40
2:B:135:LYS:HA	2:B:135:LYS:HD2	1.82	0.40
2:B:674:LYS:HB2	2:B:674:LYS:HE2	1.91	0.40
2:B:716:PHE:CD1	2:B:717:THR:HG23	2.56	0.40
2:C:998:GLY:HA3	2:C:1012:LEU:HD21	2.04	0.40
1:A:226:ASP:HA	1:A:229:ASP:OD2	2.22	0.40
1:A:278:LEU:HD11	1:A:316:TYR:HB2	2.03	0.40
1:A:883:PRO:HG3	1:A:903:PRO:HA	2.04	0.40
2:C:169:LYS:O	2:C:202:ALA:N	2.53	0.40
2:C:837:THR:O	2:C:935:GLN:HB3	2.21	0.40
3:E:224:PHE:O	3:E:228:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1055/1058 (100%)	1002 (95%)	53 (5%)	0	100	100
2	B	1187/1333 (89%)	1126 (95%)	58 (5%)	3 (0%)	46	80
2	C	1247/1333 (94%)	1191 (96%)	49 (4%)	7 (1%)	30	68
3	D	290/448 (65%)	282 (97%)	6 (2%)	2 (1%)	26	65
3	E	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	46	80
All	All	4069/4620 (88%)	3883 (95%)	173 (4%)	13 (0%)	50	80

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	769	GLN
2	C	1251	VAL
3	D	61	ASN
2	B	1310	ARG
2	C	340	VAL
2	C	1014	MET
3	E	116	THR
2	C	901	VAL
2	C	1331	ARG
2	C	1236	ILE
3	D	244	VAL
2	B	1235	PRO
2	B	1309	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	942/943 (100%)	850 (90%)	92 (10%)	10	36
2	B	1038/1153 (90%)	946 (91%)	92 (9%)	12	42
2	C	1090/1153 (94%)	974 (89%)	116 (11%)	8	31
3	D	240/379 (63%)	221 (92%)	19 (8%)	15	49
3	E	240/379 (63%)	218 (91%)	22 (9%)	11	40
All	All	3550/4007 (89%)	3209 (90%)	341 (10%)	15	37

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	7	ILE
1	A	12	ARG
1	A	31	VAL
1	A	41	THR

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Mol	Chain	Res	Type
1	A	46	ARG
1	A	47	ARG
1	A	50	THR
1	A	54	LEU
1	A	65	THR
1	A	76	LEU
1	A	81	LYS
1	A	89	ILE
1	A	99	VAL
1	A	102	LEU
1	A	105	ARG
1	A	108	ASP
1	A	111	LEU
1	A	130	VAL
1	A	153	VAL
1	A	157	LEU
1	A	173	ASP
1	A	177	THR
1	A	190	THR
1	A	196	LEU
1	A	199	MET
1	A	202	SER
1	A	203	THR
1	A	222	ARG
1	A	236	LEU
1	A	242	LYS
1	A	255	ARG
1	A	264	SER
1	A	282	GLU
1	A	284	THR
1	A	297	LEU
1	A	298	LEU
1	A	313	ARG
1	A	345	ASN
1	A	348	LEU
1	A	352	THR
1	A	368	THR
1	A	377	LEU
1	A	378	THR
1	A	423	THR
1	A	449	THR
1	A	464	ASP

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Mol	Chain	Res	Type
1	A	466	LEU
1	A	475	ARG
1	A	493	LEU
1	A	503	ILE
1	A	532	MET
1	A	561	LEU
1	A	565	ARG
1	A	569	VAL
1	A	583	ARG
1	A	592	VAL
1	A	593	GLU
1	A	595	ASN
1	A	628	MET
1	A	633	ILE
1	A	647	LEU
1	A	664	ARG
1	A	665	LEU
1	A	716	MET
1	A	719	VAL
1	A	737	HIS
1	A	745	LEU
1	A	750	VAL
1	A	757	LEU
1	A	763	LYS
1	A	781	VAL
1	A	783	ILE
1	A	792	ILE
1	A	797	ARG
1	A	812	VAL
1	A	816	LEU
1	A	833	VAL
1	A	861	ILE
1	A	886	ARG
1	A	890	LEU
1	A	915	ASN
1	A	924	VAL
1	A	925	ILE
1	A	953	ARG
1	A	978	LYS
1	A	980	ILE
1	A	982	VAL
1	A	996	ASP

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Mol	Chain	Res	Type
1	A	1018	ARG
1	A	1025	ILE
1	A	1034	ARG
2	B	143	VAL
2	B	147	VAL
2	B	186	ASP
2	B	198	LYS
2	B	203	VAL
2	B	231	LEU
2	B	238	THR
2	B	242	GLU
2	B	259	MET
2	B	260	THR
2	B	265	VAL
2	B	270	THR
2	B	271	THR
2	B	274	MET
2	B	283	ASN
2	B	286	LEU
2	B	289	THR
2	B	294	VAL
2	B	315	THR
2	B	320	GLN
2	B	323	THR
2	B	339	LEU
2	B	366	MET
2	B	414	LEU
2	B	431	THR
2	B	447	ARG
2	B	486	VAL
2	B	512	LEU
2	B	533	GLN
2	B	552	VAL
2	B	615	THR
2	B	637	TYR
2	B	638	THR
2	B	659	LEU
2	B	674	LYS
2	B	684	LEU
2	B	685	ARG
2	B	687	LEU
2	B	689	THR

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Mol	Chain	Res	Type
2	B	694	ILE
2	B	702	LEU
2	B	736	SER
2	B	742	LYS
2	B	748	GLN
2	B	750	GLU
2	B	753	ASP
2	B	756	THR
2	B	788	MET
2	B	799	THR
2	B	804	LEU
2	B	815	LEU
2	B	837	THR
2	B	890	THR
2	B	925	VAL
2	B	937	ASN
2	B	951	ILE
2	B	953	ASP
2	B	968	ARG
2	B	970	LEU
2	B	976	THR
2	B	988	GLN
2	B	990	THR
2	B	991	ASP
2	B	995	THR
2	B	1007	THR
2	B	1036	ASP
2	B	1041	ARG
2	B	1048	ASP
2	B	1052	LEU
2	B	1070	ARG
2	B	1074	VAL
2	B	1079	LEU
2	B	1085	ASP
2	B	1108	SER
2	B	1110	LEU
2	B	1120	THR
2	B	1134	ARG
2	B	1170	ASP
2	B	1174	THR
2	B	1178	MET
2	B	1186	GLN

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Mol	Chain	Res	Type
2	B	1198	LYS
2	B	1210	LEU
2	B	1223	SER
2	B	1247	ASN
2	B	1305	MET
2	B	1310	ARG
2	B	1314	ASP
2	B	1315	MET
2	B	1317	VAL
2	B	1329	ASN
2	B	1331	ARG
2	C	82	ARG
2	C	86	VAL
2	C	98	ASN
2	C	100	ASP
2	C	109	LYS
2	C	117	ARG
2	C	120	VAL
2	C	141	LEU
2	C	144	ASN
2	C	158	SER
2	C	187	ASP
2	C	190	VAL
2	C	203	VAL
2	C	207	ASP
2	C	217	THR
2	C	221	LEU
2	C	230	ASP
2	C	231	LEU
2	C	237	VAL
2	C	255	LEU
2	C	264	LEU
2	C	265	VAL
2	C	270	THR
2	C	277	THR
2	C	286	LEU
2	C	294	VAL
2	C	310	LEU
2	C	323	THR
2	C	330	THR
2	C	370	VAL
2	C	375	ARG

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Mol	Chain	Res	Type
2	C	379	LEU
2	C	383	SER
2	C	384	MET
2	C	401	LEU
2	C	447	ARG
2	C	474	ASP
2	C	475	ILE
2	C	484	ARG
2	C	532	ILE
2	C	533	GLN
2	C	535	VAL
2	C	542	ARG
2	C	552	VAL
2	C	557	THR
2	C	626	ARG
2	C	629	ARG
2	C	630	ASN
2	C	637	TYR
2	C	638	THR
2	C	654	THR
2	C	659	LEU
2	C	689	THR
2	C	694	ILE
2	C	696	VAL
2	C	708	THR
2	C	717	THR
2	C	752	VAL
2	C	763	VAL
2	C	804	LEU
2	C	811	SER
2	C	815	LEU
2	C	828	ASP
2	C	832	MET
2	C	836	GLN
2	C	837	THR
2	C	841	ASP
2	C	855	TYR
2	C	859	ILE
2	C	872	ILE
2	C	921	ASP
2	C	925	VAL
2	C	931	ASN

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Mol	Chain	Res	Type
2	C	935	GLN
2	C	952	PHE
2	C	965	ARG
2	C	980	ARG
2	C	995	THR
2	C	1007	THR
2	C	1010	ARG
2	C	1013	LYS
2	C	1015	GLN
2	C	1022	ILE
2	C	1028	VAL
2	C	1034	GLN
2	C	1052	LEU
2	C	1055	LEU
2	C	1067	ILE
2	C	1070	ARG
2	C	1079	LEU
2	C	1080	THR
2	C	1104	ARG
2	C	1110	LEU
2	C	1116	ARG
2	C	1120	THR
2	C	1134	ARG
2	C	1170	ASP
2	C	1185	THR
2	C	1186	GLN
2	C	1189	ASP
2	C	1198	LYS
2	C	1200	LYS
2	C	1202	PHE
2	C	1210	LEU
2	C	1230	ILE
2	C	1233	LEU
2	C	1234	GLN
2	C	1251	VAL
2	C	1253	ARG
2	C	1262	SER
2	C	1267	THR
2	C	1269	THR
2	C	1285	GLN
2	C	1293	VAL
2	C	1320	VAL

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Mol	Chain	Res	Type
2	C	1321	ASN
3	D	20	ARG
3	D	29	THR
3	D	47	LYS
3	D	77	PHE
3	D	92	ARG
3	D	93	LEU
3	D	100	ASN
3	D	116	THR
3	D	133	THR
3	D	139	ASN
3	D	158	LEU
3	D	160	LEU
3	D	181	SER
3	D	189	LEU
3	D	191	ARG
3	D	226	MET
3	D	252	LEU
3	D	257	VAL
3	D	265	ARG
3	E	1	MET
3	E	2	LEU
3	E	6	THR
3	E	21	ASN
3	E	29	THR
3	E	35	LEU
3	E	66	VAL
3	E	93	LEU
3	E	98	LEU
3	E	130	PHE
3	E	133	THR
3	E	160	LEU
3	E	163	THR
3	E	189	LEU
3	E	226	MET
3	E	240	VAL
3	E	244	VAL
3	E	247	ARG
3	E	249	ASP
3	E	252	LEU
3	E	262	THR
3	E	272	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	576	ASN
1	A	837	HIS
2	B	430	ASN
2	B	1138	HIS
2	C	931	ASN
3	D	85	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
4	SAM	A	1101	-	23,29,29	1.05	2 (8%)	15,42,42	3.05	2 (13%)
4	SAM	A	1102	-	23,29,29	1.07	2 (8%)	15,42,42	2.98	1 (6%)
5	ATP	A	1103	-	26,33,33	0.93	1 (3%)	26,52,52	1.71	5 (19%)
6	GTP	A	1104	7	26,34,34	0.93	1 (3%)	29,54,54	1.59	4 (13%)

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
4	SAM	A	1101	-	-	0/8/33/33	0/3/3/3
4	SAM	A	1102	-	-	0/8/33/33	0/3/3/3
5	ATP	A	1103	-	-	0/18/38/38	0/3/3/3
6	GTP	A	1104	7	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	SAM	C2-N1	2.40	1.38	1.33
4	A	1102	SAM	C2-N1	2.42	1.38	1.33
5	A	1103	ATP	C5-C4	3.01	1.47	1.40
6	A	1104	GTP	C6-N1	3.04	1.38	1.33
4	A	1102	SAM	C2-N3	3.50	1.38	1.32
4	A	1101	SAM	C2-N3	3.62	1.38	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	SAM	N3-C2-N1	-11.27	120.02	128.87
4	A	1102	SAM	N3-C2-N1	-11.00	120.23	128.87
5	A	1103	ATP	N3-C2-N1	-6.11	124.07	128.87
6	A	1104	GTP	N3-C2-N1	-5.42	120.18	127.56
6	A	1104	GTP	C5-C6-N1	-2.93	119.69	123.52
5	A	1103	ATP	C2'-C1'-N9	-2.62	106.46	113.47
6	A	1104	GTP	C1'-N9-C4	-2.53	123.98	126.81
5	A	1103	ATP	O3G-PG-O2G	2.07	115.04	107.44
5	A	1103	ATP	C4'-O4'-C1'	2.11	111.88	109.64
5	A	1103	ATP	N6-C6-N1	2.14	122.10	118.52
4	A	1101	SAM	O4'-C1'-N9	2.44	112.71	108.11
6	A	1104	GTP	C6-N1-C2	3.34	119.79	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	2	0
4	A	1102	SAM	1	0
5	A	1103	ATP	3	0
6	A	1104	GTP	3	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.