



wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 01:50 PM EDT

PDB ID : 3JAY
EMDB ID: : EMD-6378
Title : Atomic model of transcribing cytoplasmic polyhedrosis virus
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on : 2015-07-06
Resolution : 3.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

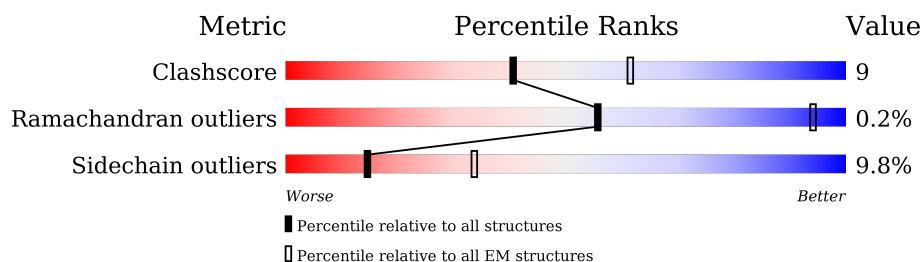
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	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 ≥ 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 [i](#)

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		

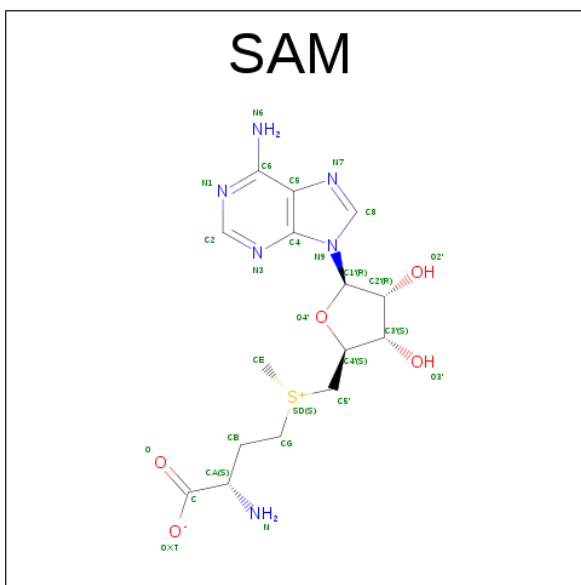
- Molecule 2 is a protein called Capsid protein VP1.

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.

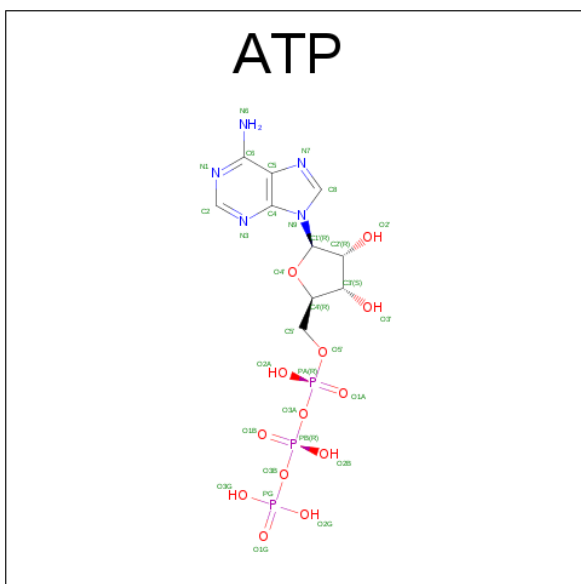
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



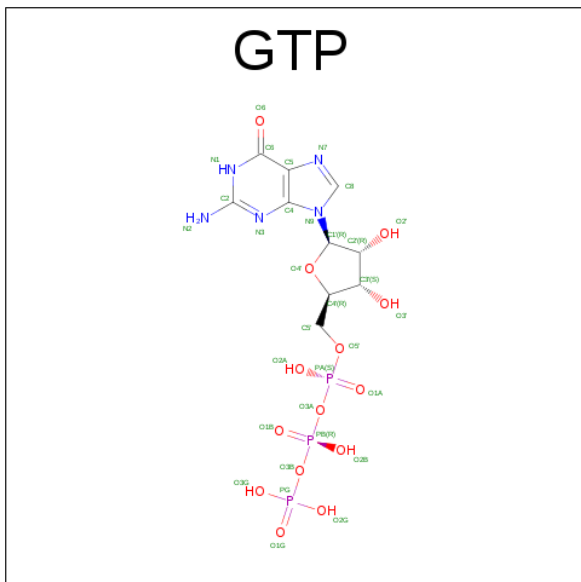
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 54	C 30	N 12	O 10	S 2	0
4	A	1	Total 54	C 30	N 12	O 10	S 2	0

- 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	

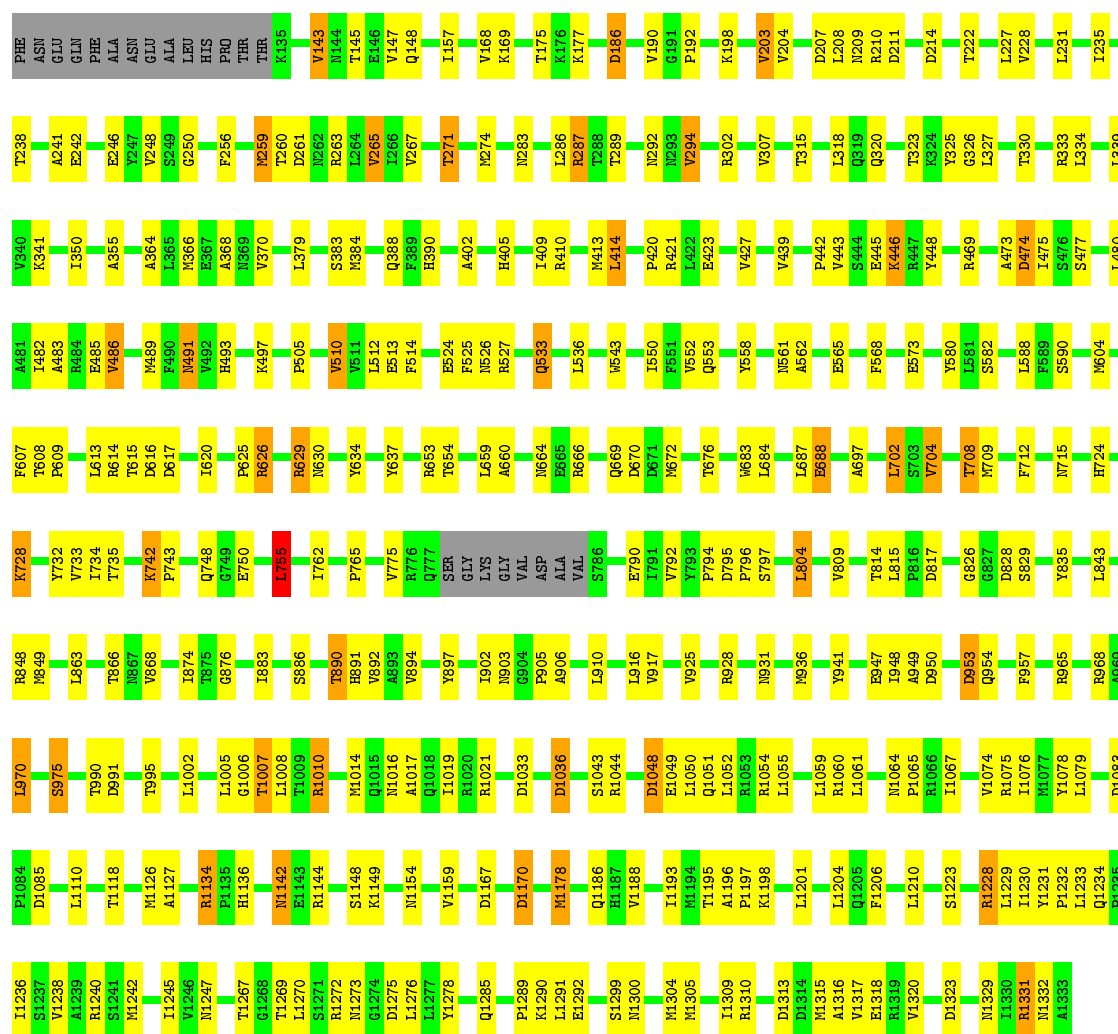
- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

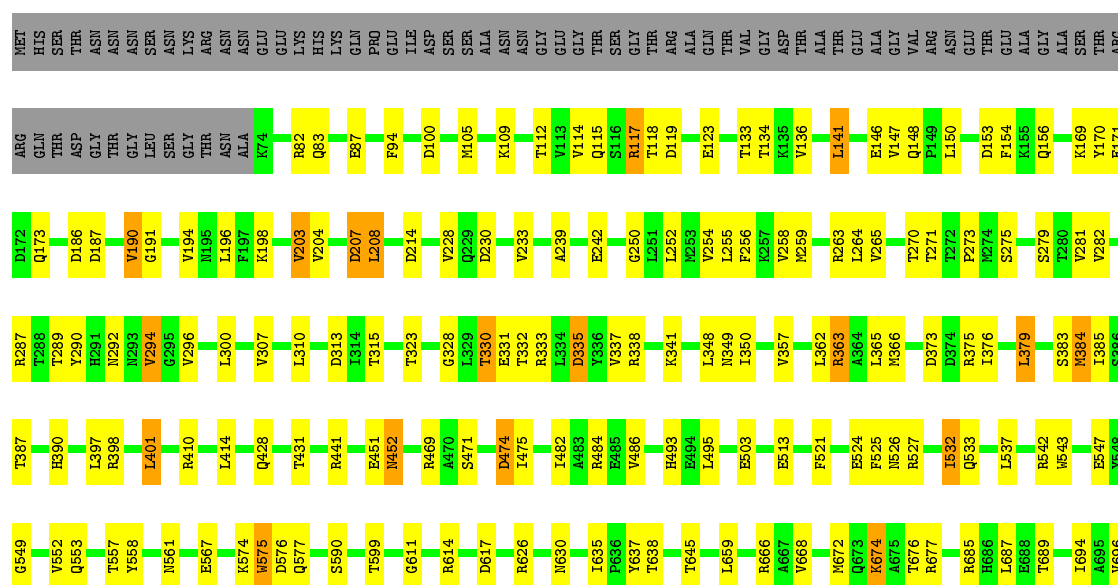
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

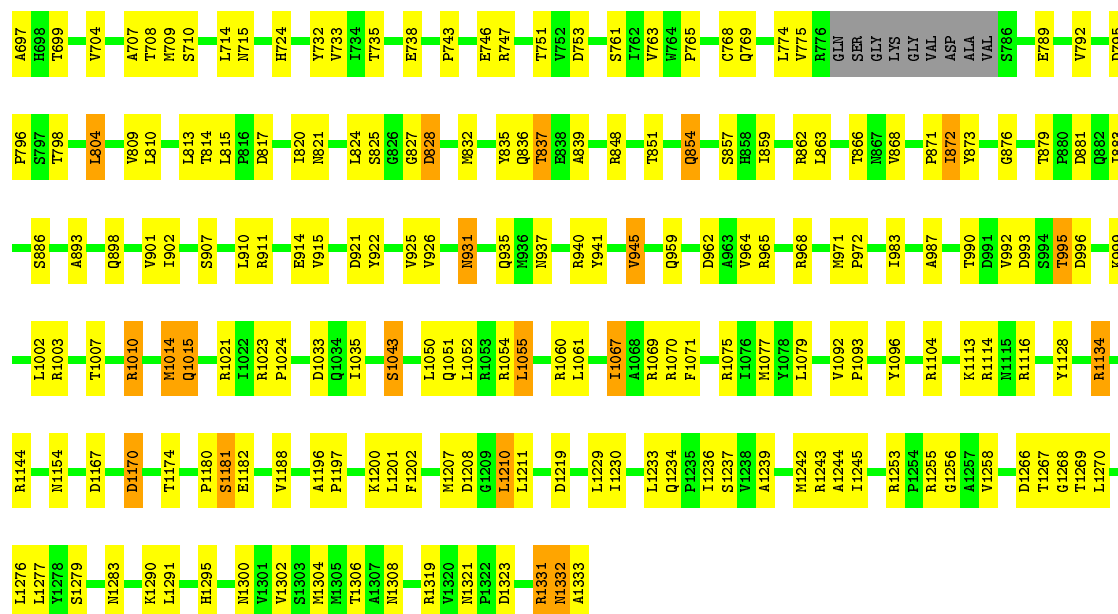
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
7	A	1	1	1	0



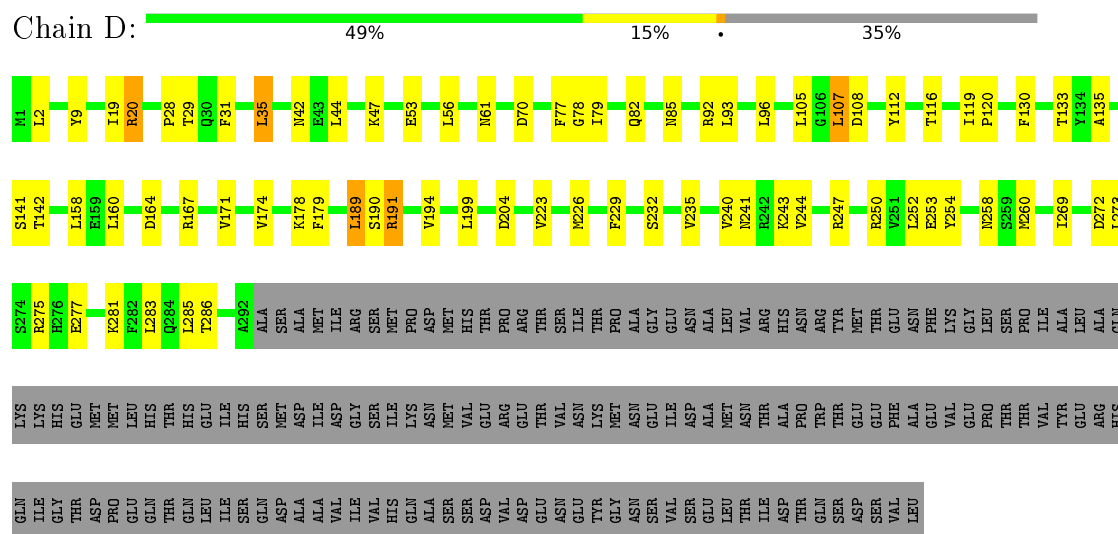
• Molecule 2: Capsid protein VP1

Chain C: 67% 24% 6%

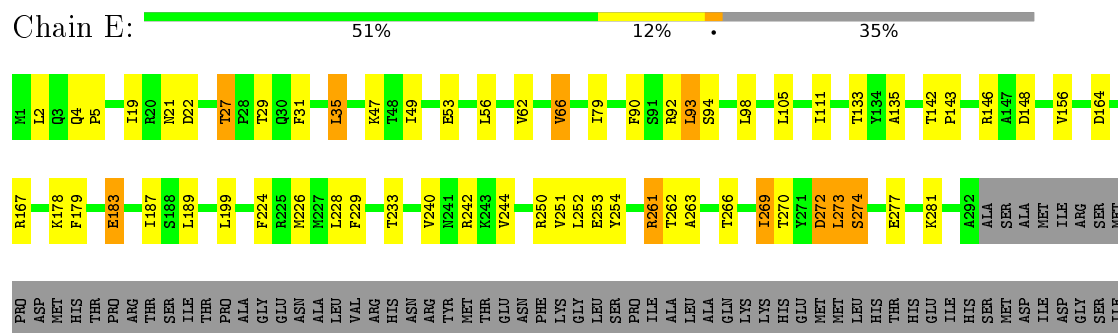




• Molecule 3: Viral structural protein 5



• Molecule 3: Viral structural protein 5



LYS	ASN	GLN
MET	ALA	ALA
VAL	SER	SER
GLU	ASP	VAL
ARG	VAL	ASP
GLU	ASP	GLU
THR	GLU	ASN
VAL	ASN	GLU
ASN	LYS	TYR
LYS	MET	GLY
MET	ASN	ASN
GLU	GLU	SER
ILE	ILE	VAL
ASP	SER	SER
ALA	GLU	GLU
MET	LEU	THR
ASN	THR	ILE
THR	ALA	ASP
ALA	PRO	THR
TRP	GLN	GLN
THR	SER	SER
GLU	ASP	ASP
GLU	SER	SER
PHE	VAL	VAL
ALA	LEU	LEU
GLU	THR	THR
VAL	GLU	GLU
GLU	VAL	THR
PRO	THR	TYR
THR	VAL	GLU
THR	VAL	ARG
TYR	GLU	HIS
GLU	ARG	GLN
ARG	HIS	ILE
HIS	GLN	GLY
GLN	ILE	THR
GLY	THR	ASP
THR	ASP	PRO
ASP	PRO	GLU
GLU	GLU	GLN
GLN	THR	THR
THR	GLN	GLN
LEU	ILE	LEU
ILE	SER	SER
SER	GLN	GLN
GLN	ASP	ALA
ALA	ALA	ALA
VAL	VAL	VAL
ILE	ILE	ILE
VAL	VAL	VAL
VAL	VAL	HIS
HIS		

GLN
ALA
SER
SER
ASP
VAL
ASP
GLU
ASN
GLU
TYR
GLY
ASN
SER
SER
VAL
SER
GLU
LEU
THR
ILE
ASP
THR
GLN
SER
SER
ASP
SER
VAL
LEU

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	41624	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

5.1 Standard geometry

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	0.49	0/11737
2	B	0.33	0/9590	0.57	1/13056 (0.0%)
2	C	0.34	0/10058	0.55	0/13695
3	D	0.31	0/2327	0.53	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.32	0/32921	0.54	1/44814 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	755	LEU	CA-CB-CG	5.35	127.61	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ARG	Sidechain
1	A	46	ARG	Sidechain
1	A	52	ARG	Sidechain

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	8434	0	8399	170	0
2	B	9397	0	9315	190	0
2	C	9857	0	9767	180	0
3	D	2281	0	2282	43	0
3	E	2281	0	2282	31	0
4	A	54	0	44	1	0
5	A	31	0	12	0	0
6	A	32	0	12	1	0
7	A	1	0	0	0	0
All	All	32368	0	32113	589	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 9.

All (589) 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:52:ARG:NH2	1:A:52:ARG:HB2	1.72	1.02
1:A:43:ASN:OD1	1:A:46:ARG:HG2	1.72	0.89
1:A:41:THR:HG23	1:A:50:THR:HG23	1.56	0.88
2:C:383:SER:HB3	2:C:796:PRO:HG3	1.57	0.87
2:C:1134:ARG:NH2	2:C:1154:ASN:OD1	2.12	0.82
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.62	0.81
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.63	0.81
1:A:309:ASN:OD1	1:A:311:GLN:HG2	1.80	0.80
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.65	0.79
1:A:168:ASN:ND2	1:A:173:ASP:OD2	2.16	0.79
1:A:41:THR:CG2	1:A:50:THR:HG23	2.12	0.78
1:A:857:GLN:NE2	1:A:914:GLU:OE1	2.16	0.78
1:A:52:ARG:NH1	1:A:169:SER:OG	2.15	0.78
1:A:797:ARG:NH2	1:A:876:MET:O	2.18	0.77
2:B:1134:ARG:NH2	2:B:1154:ASN:OD1	2.16	0.77
1:A:52:ARG:HB2	1:A:52:ARG:HH21	1.48	0.75
1:A:52:ARG:HB2	1:A:52:ARG:CZ	2.16	0.74
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TYR:O	1:A:317:ARG:NH1	2.21	0.74
2:C:1128:TYR:O	2:C:1134:ARG:NH1	2.20	0.74
2:C:363:ARG:NH1	3:E:183:GLU:OE1	2.21	0.73
2:C:709:MET:O	2:C:715:ASN:ND2	2.21	0.72
2:C:836:GLN:NE2	2:C:940:ARG:O	2.21	0.72
2:C:169:LYS:NZ	2:C:1182:GLU:OE2	2.23	0.72
1:A:12:ARG:NH2	1:A:16:ASP:OD1	2.23	0.71
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.23	0.70
3:E:66:VAL:HG13	3:E:111:ILE:HB	1.74	0.69
2:C:1060:ARG:NH1	2:C:1291:LEU:O	2.26	0.69
1:A:685:PRO:O	1:A:714:ARG:NH2	2.26	0.69
2:C:493:HIS:O	2:C:577:GLN:NE2	2.26	0.69
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.26	0.69
1:A:958:ALA:HB3	1:A:1055:LEU:HB2	1.76	0.68
2:B:950:ASP:OD1	2:B:965:ARG:NH1	2.27	0.68
1:A:502:ASP:HA	1:A:574:ARG:HD3	1.76	0.67
2:B:817:ASP:OD2	2:B:1010:ARG:NH2	2.28	0.67
2:C:1170:ASP:OD1	2:C:1170:ASP:N	2.24	0.67
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.75	0.67
2:B:383:SER:HB3	2:B:796:PRO:HG3	1.77	0.67
3:D:164:ASP:OD1	3:D:167:ARG:NH2	2.28	0.67
2:B:287:ARG:HE	2:B:330:THR:HG22	1.59	0.66
3:E:261:ARG:NH1	3:E:263:ALA:O	2.28	0.66
2:C:313:ASP:OD2	2:C:1253:ARG:NH2	2.28	0.66
2:B:975:SER:HB2	2:C:696:VAL:HG21	1.77	0.66
2:C:1208:ASP:OD1	2:C:1243:ARG:NH2	2.20	0.66
1:A:202:SER:HB2	2:B:630:ASN:HB3	1.79	0.65
1:A:935:PRO:HG2	1:A:938:MET:HG3	1.77	0.65
1:A:662:ILE:HD12	1:A:675:THR:HG21	1.79	0.65
2:B:1273:ASN:ND2	2:B:1275:ASP:OD2	2.28	0.65
2:B:1060:ARG:NH1	2:B:1291:LEU:O	2.30	0.64
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.80	0.64
3:E:79:ILE:HG13	3:E:269:ILE:HG22	1.78	0.64
2:C:190:VAL:HG22	2:C:300:LEU:HB3	1.78	0.64
2:C:87:GLU:OE2	2:C:263:ARG:NH1	2.29	0.64
1:A:964:GLU:HB3	1:A:1049:TYR:HD1	1.62	0.64
2:B:209:ASN:ND2	2:B:211:ASP:OD1	2.32	0.63
2:B:267:VAL:HA	2:B:1304:MET:HE2	1.80	0.63
2:C:746:GLU:OE2	2:C:1010:ARG:NH2	2.25	0.63
3:E:53:GLU:OE2	3:E:281:LYS:NZ	2.31	0.63
2:C:287:ARG:HH11	2:C:330:THR:HB	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:709:MET:O	2:B:715:ASN:ND2	2.32	0.63
2:C:410:ARG:HD3	2:C:1043:SER:HA	1.81	0.63
1:A:285:GLU:HB2	1:A:287:VAL:HG23	1.80	0.63
1:A:213:TRP:HB2	1:A:215:VAL:HG12	1.79	0.63
2:B:1170:ASP:OD1	2:B:1170:ASP:N	2.32	0.62
2:B:480:LEU:HD11	2:B:755:LEU:HD23	1.81	0.62
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.32	0.62
2:C:493:HIS:ND1	2:C:524:GLU:OE2	2.32	0.62
2:B:524:GLU:OE2	2:B:527:ARG:NH1	2.32	0.62
2:C:837:THR:HG21	2:C:911:ARG:HG3	1.82	0.62
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.81	0.62
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.33	0.62
2:C:1174:THR:HG23	2:C:1201:LEU:HD22	1.82	0.62
2:C:704:VAL:O	2:C:708:THR:HG23	2.00	0.62
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.17	0.62
2:B:626:ARG:NH2	2:B:712:PHE:O	2.33	0.61
2:C:146:GLU:O	2:C:148:GLN:NE2	2.31	0.61
2:C:94:PHE:HB3	2:C:105:MET:HG3	1.83	0.61
2:C:697:ALA:HB2	2:C:775:VAL:HG23	1.83	0.61
1:A:856:THR:HG23	1:A:857:GLN:HG2	1.83	0.61
2:C:153:ASP:HB3	2:C:401:LEU:HD22	1.83	0.61
2:C:357:VAL:HG13	2:C:1054:ARG:HD3	1.82	0.61
2:C:441:ARG:NH2	2:C:789:GLU:OE1	2.34	0.60
1:A:697:ILE:HD11	1:A:701:VAL:HG22	1.83	0.60
2:B:483:ALA:HA	2:B:709:MET:HE3	1.83	0.60
2:C:169:LYS:HB2	2:C:203:VAL:HG23	1.84	0.60
2:C:156:GLN:OE1	2:C:1308:ASN:ND2	2.34	0.60
1:A:201:LYS:HD3	3:D:260:MET:HB3	1.82	0.60
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.84	0.60
2:B:1048:ASP:N	2:B:1048:ASP:OD1	2.35	0.60
2:C:848:ARG:HE	2:C:914:GLU:HB3	1.66	0.60
2:B:666:ARG:NH1	2:B:670:ASP:OD2	2.35	0.59
1:A:558:ILE:HG13	1:A:612:PHE:HB2	1.82	0.59
2:B:248:VAL:HG22	2:B:970:LEU:HB3	1.84	0.59
2:B:1289:PRO:HD2	3:D:20:ARG:HD3	1.84	0.59
2:C:825:SER:HA	2:C:1015:GLN:HE21	1.66	0.59
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.02	0.59
1:A:772:TRP:HA	1:A:817:GLY:HA3	1.85	0.59
2:C:795:ASP:OD1	2:C:1319:ARG:NH2	2.35	0.59
1:A:192:VAL:HG21	1:A:347:LEU:HD13	1.85	0.59
2:C:866:THR:HG23	2:C:868:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:ASP:N	2:B:474:ASP:OD1	2.29	0.59
2:B:210:ARG:HH21	2:B:222:THR:HA	1.67	0.58
2:B:439:VAL:HG21	2:B:702:LEU:HD13	1.85	0.58
2:C:987:ALA:HB1	2:C:992:VAL:HG22	1.84	0.58
2:B:168:VAL:HG22	2:B:204:VAL:HG22	1.85	0.58
2:C:1069:ARG:HD2	2:C:1239:ALA:HB2	1.86	0.58
2:C:1236:ILE:HG22	2:C:1237:SER:H	1.68	0.58
2:C:384:MET:HA	2:C:708:THR:HG21	1.85	0.58
2:C:1071:PHE:HD1	2:C:1234:GLN:HE21	1.51	0.58
2:C:996:ASP:HA	2:C:999:LYS:HD2	1.85	0.58
3:E:178:LYS:HB3	3:E:251:VAL:HG22	1.85	0.58
1:A:104:VAL:HG23	1:A:138:PRO:HB2	1.86	0.58
1:A:304:TYR:HA	1:A:307:HIS:HB2	1.86	0.58
2:C:1266:ASP:OD1	2:C:1279:SER:OG	2.22	0.57
2:B:486:VAL:HG21	2:B:709:MET:HB3	1.86	0.57
1:A:14:ALA:HA	1:A:112:ARG:HH22	1.70	0.57
2:B:469:ARG:NH1	2:B:513:GLU:OE2	2.35	0.57
2:B:704:VAL:O	2:B:708:THR:HG22	2.05	0.57
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.38	0.56
2:C:879:THR:HG22	2:C:881:ASP:H	1.70	0.56
2:C:817:ASP:HA	2:C:983:ILE:HG12	1.87	0.56
2:C:214:ASP:OD1	2:C:214:ASP:N	2.39	0.56
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.87	0.56
2:C:379:LEU:HD12	2:C:796:PRO:HB2	1.86	0.56
1:A:39:LEU:HG	1:A:54:LEU:HD21	1.88	0.56
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.33	0.56
2:B:613:LEU:HD13	2:B:634:TYR:HD1	1.70	0.56
2:B:326:GLY:H	2:B:1267:THR:HG21	1.70	0.56
3:D:35:LEU:HD12	3:D:179:PHE:HB3	1.86	0.56
3:D:78:GLY:O	3:D:275:ARG:NH2	2.39	0.56
1:A:373:ILE:HD13	1:A:817:GLY:N	2.20	0.55
1:A:241:GLN:OE1	1:A:258:GLN:NE2	2.38	0.55
1:A:43:ASN:OD1	1:A:46:ARG:CG	2.50	0.55
1:A:916:ASN:N	1:A:955:ASN:O	2.39	0.55
2:B:697:ALA:HB2	2:B:775:VAL:HG23	1.88	0.55
1:A:563:ALA:HB3	1:A:588:GLY:H	1.71	0.55
2:B:1188:VAL:HG21	2:B:1204:LEU:HD23	1.88	0.55
2:C:893:ALA:HB1	2:C:915:VAL:HA	1.89	0.55
2:C:452:ASN:N	2:C:452:ASN:OD1	2.39	0.55
2:C:259:MET:O	2:C:1054:ARG:NH1	2.39	0.55
2:B:573:GLU:OE2	2:C:674:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:ASP:OD1	2:C:338:ARG:NH2	2.40	0.55
2:C:474:ASP:N	2:C:474:ASP:OD1	2.39	0.55
2:C:366:MET:HG2	3:E:266:THR:HG21	1.88	0.54
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.89	0.54
2:C:1077:MET:O	2:C:1229:LEU:HA	2.07	0.54
2:C:732:TYR:OH	2:C:1021:ARG:NH2	2.41	0.54
3:D:112:TYR:CE2	3:D:119:ILE:HG21	2.42	0.54
1:A:681:ALA:O	1:A:1037:SER:HB2	2.07	0.54
1:A:890:LEU:H	1:A:890:LEU:HD23	1.72	0.54
3:D:283:LEU:HA	3:D:286:THR:HG22	1.88	0.54
2:C:171:GLU:OE1	2:C:1181:SER:OG	2.20	0.54
2:B:1126:MET:HE3	3:E:146:ARG:HB3	1.89	0.54
1:A:278:LEU:HD11	1:A:316:TYR:HB2	1.90	0.54
2:B:614:ARG:NH1	2:B:617:ASP:OD1	2.39	0.54
1:A:849:ILE:HD12	1:A:871:VAL:HG12	1.90	0.54
2:C:543:TRP:CD2	2:C:666:ARG:HD3	2.43	0.54
3:E:156:VAL:HG13	3:E:228:LEU:HD22	1.88	0.54
1:A:615:CYS:HB3	1:A:648:VAL:HA	1.90	0.53
2:B:1007:THR:OG1	2:B:1008:LEU:N	2.39	0.53
1:A:887:ILE:HD11	1:A:901:SER:HB2	1.90	0.53
1:A:318:ARG:HG3	3:D:42:ASN:HA	1.90	0.53
2:C:428:GLN:HA	2:C:431:THR:HG22	1.89	0.53
1:A:108:ASP:HB2	1:A:111:LEU:HD22	1.91	0.53
1:A:221:TYR:OH	1:A:230:HIS:ND1	2.30	0.53
2:B:954:GLN:HE21	3:D:240:VAL:HG12	1.73	0.53
2:C:254:VAL:O	2:C:258:VAL:HG12	2.08	0.53
2:B:157:ILE:HG12	2:B:263:ARG:HD2	1.91	0.53
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.89	0.53
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.91	0.53
2:B:256:PHE:HE2	2:B:990:THR:HG21	1.73	0.53
2:B:325:TYR:HA	2:B:1267:THR:HG23	1.90	0.53
2:C:289:THR:O	2:C:328:GLY:HA3	2.09	0.53
2:C:738:GLU:OE2	2:C:857:SER:OG	2.18	0.53
2:B:302:ARG:HD2	2:B:318:LEU:HD12	1.91	0.52
2:C:242:GLU:HB2	2:C:1200:LYS:HE2	1.90	0.52
1:A:41:THR:HG23	1:A:50:THR:CG2	2.35	0.52
1:A:466:LEU:HB3	1:A:470:LEU:HD23	1.91	0.52
2:C:196:LEU:HD23	2:C:296:VAL:HG11	1.91	0.52
1:A:267:THR:HG23	1:A:320:TYR:OH	2.09	0.52
2:B:1331:ARG:HB2	2:B:1332:ASN:HA	1.90	0.52
2:B:169:LYS:HB2	2:B:203:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:558:TYR:HB3	2:B:568:PHE:CD2	2.44	0.52
3:D:253:GLU:HB3	3:D:254:TYR:CE1	2.44	0.52
1:A:573:ARG:NH2	1:A:584:ILE:O	2.39	0.52
2:C:883:ILE:HD13	2:C:910:LEU:HD21	1.91	0.52
2:B:891:HIS:CG	3:D:240:VAL:HG21	2.45	0.52
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.39	0.52
1:A:836:ILE:HD11	1:A:1033:ILE:HG21	1.91	0.52
2:C:383:SER:HB2	2:C:387:THR:HG21	1.92	0.52
1:A:755:ALA:HB2	1:A:781:VAL:HG11	1.92	0.51
2:B:1228:ARG:HG2	2:B:1231:TYR:CZ	2.45	0.51
2:C:414:LEU:HD23	2:C:814:THR:HB	1.92	0.51
1:A:496:CYS:O	1:A:574:ARG:NH1	2.43	0.51
2:B:1005:LEU:HB2	2:B:1006:GLY:HA2	1.91	0.51
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.91	0.51
2:B:491:ASN:OD1	2:B:491:ASN:N	2.41	0.51
2:B:792:VAL:HG12	2:B:794:PRO:HD3	1.91	0.51
1:A:420:VAL:HA	1:A:974:SER:HB2	1.92	0.51
2:C:611:GLY:HA3	2:C:635:ILE:O	2.10	0.51
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.92	0.51
1:A:487:GLN:O	1:A:492:HIS:ND1	2.31	0.51
1:A:205:VAL:HG23	1:A:263:LEU:HB2	1.93	0.51
2:B:903:ASN:HD22	2:B:905:PRO:HG2	1.75	0.51
1:A:372:ARG:HD2	1:A:772:TRP:CE3	2.45	0.51
1:A:918:ILE:HG23	1:A:957:VAL:HG13	1.93	0.51
2:B:1305:MET:HE2	2:B:1309:ILE:HG21	1.93	0.51
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.93	0.51
2:C:851:THR:HG23	2:C:854:GLN:HB2	1.93	0.50
2:C:743:PRO:HB2	2:C:746:GLU:HG2	1.93	0.50
2:B:931:ASN:ND2	2:B:936:MET:O	2.44	0.50
2:C:576:ASP:OD1	2:C:747:ARG:NH2	2.44	0.50
1:A:166:ILE:HG21	1:A:179:TYR:CE1	2.47	0.50
1:A:424:PRO:HG3	1:A:706:TYR:CZ	2.46	0.50
1:A:910:ASN:OD1	1:A:910:ASN:N	2.45	0.50
2:B:1051:GLN:O	2:B:1055:LEU:HB2	2.12	0.50
2:C:233:VAL:HG23	2:C:239:ALA:HB2	1.92	0.50
2:B:370:VAL:HG11	2:B:402:ALA:HB2	1.93	0.50
2:C:668:VAL:HG23	2:C:674:LYS:HD3	1.94	0.50
1:A:290:LEU:HD12	1:A:293:LEU:HD13	1.91	0.50
1:A:472:LEU:HD23	1:A:475:ARG:HH21	1.76	0.50
1:A:943:ILE:HG12	1:A:960:ILE:HG21	1.94	0.50
2:B:287:ARG:NE	2:B:330:THR:HG22	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:HG22	1:A:204:LEU:HG	1.93	0.49
2:B:1289:PRO:HG3	3:D:191:ARG:NH2	2.27	0.49
1:A:143:TYR:CG	1:A:149:ALA:HB2	2.47	0.49
1:A:336:LEU:HG	1:A:348:LEU:HD22	1.94	0.49
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.45	0.49
1:A:636:VAL:HG22	1:A:648:VAL:HG11	1.95	0.49
2:C:114:VAL:HG22	2:C:136:VAL:HG23	1.93	0.49
2:C:672:MET:O	2:C:676:THR:HG23	2.12	0.49
3:D:273:LEU:O	3:D:277:GLU:HG3	2.11	0.49
2:B:558:TYR:CE1	2:B:590:SER:HB3	2.47	0.49
1:A:540:LYS:NZ	1:A:543:GLU:OE2	2.29	0.49
2:B:866:THR:HG23	2:B:868:VAL:HG13	1.94	0.49
2:C:561:ASN:ND2	2:C:567:GLU:OE2	2.44	0.49
1:A:170:ASN:ND2	1:A:173:ASP:OD1	2.45	0.49
2:B:505:PRO:HG2	2:B:672:MET:SD	2.53	0.49
1:A:272:LEU:HA	1:A:275:ILE:HD11	1.95	0.49
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.95	0.49
1:A:374:LYS:HG2	1:A:770:THR:HG22	1.94	0.49
1:A:846:ARG:HB2	1:A:871:VAL:HA	1.95	0.49
1:A:474:TYR:HD1	1:A:499:VAL:HG12	1.77	0.49
1:A:186:ALA:HB2	1:A:195:ILE:HD12	1.94	0.48
1:A:301:SER:HB2	1:A:316:TYR:OH	2.12	0.48
1:A:288:LEU:HD21	1:A:300:LEU:HD22	1.94	0.48
1:A:764:SER:HA	1:A:795:GLU:HG2	1.93	0.48
2:B:514:PHE:HB3	2:B:607:PHE:HE2	1.78	0.48
2:B:876:GLY:HA2	2:B:902:ILE:HA	1.94	0.48
1:A:923:ALA:H	1:A:961:SER:HB3	1.77	0.48
2:C:150:LEU:HD21	2:C:398:ARG:HB3	1.94	0.48
2:C:549:GLY:O	2:C:553:GLN:HB2	2.13	0.48
1:A:688:TYR:HB2	1:A:715:TYR:HB2	1.95	0.48
1:A:427:ASP:HA	1:A:703:PHE:HA	1.96	0.48
1:A:13:VAL:HG22	1:A:213:TRP:CD1	2.48	0.48
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.94	0.48
1:A:658:ILE:O	1:A:662:ILE:HG12	2.14	0.48
1:A:385:HIS:NE2	1:A:803:SER:OG	2.44	0.48
2:C:638:THR:O	2:C:699:THR:HB	2.14	0.48
2:C:810:LEU:HA	2:C:813:LEU:HB3	1.96	0.48
1:A:849:ILE:HG12	1:A:918:ILE:HD13	1.95	0.48
2:B:405:HIS:ND1	2:B:625:PRO:HA	2.28	0.48
2:C:1243:ARG:HD3	2:C:1256:GLY:O	2.14	0.48
2:C:294:VAL:O	2:C:349:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:272:ASP:OD1	3:E:274:SER:OG	2.15	0.48
2:B:826:GLY:HA3	2:B:949:ALA:HB2	1.96	0.48
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.95	0.48
1:A:588:GLY:H	1:A:591:ALA:HB2	1.79	0.48
2:B:1044:ARG:NH1	2:B:1049:GLU:OE2	2.41	0.48
2:B:795:ASP:OD1	2:B:795:ASP:N	2.47	0.48
1:A:739:ASN:HB2	1:A:796:PHE:CE1	2.49	0.48
2:B:890:THR:O	2:B:890:THR:OG1	2.29	0.48
2:C:810:LEU:O	2:C:814:THR:HG23	2.14	0.48
3:E:224:PHE:O	3:E:228:LEU:HG	2.14	0.48
2:C:1211:LEU:HD11	2:C:1244:ALA:HA	1.95	0.47
2:C:207:ASP:OD1	2:C:207:ASP:N	2.47	0.47
2:C:824:LEU:O	2:C:1015:GLN:NE2	2.47	0.47
1:A:552:MET:H	1:A:576:ASN:ND2	2.11	0.47
2:C:1236:ILE:HG22	2:C:1237:SER:N	2.29	0.47
1:A:752:VAL:HG23	1:A:816:LEU:HD21	1.95	0.47
1:A:980:ILE:HG23	1:A:989:VAL:HG12	1.95	0.47
2:B:526:ASN:HB2	2:B:724:HIS:CE1	2.49	0.47
1:A:234:LYS:HA	1:A:234:LYS:HD3	1.72	0.47
2:B:261:ASP:CG	2:B:263:ARG:HE	2.17	0.47
2:B:405:HIS:CE1	2:B:625:PRO:HA	2.50	0.47
2:C:1268:GLY:HA3	2:C:1277:LEU:O	2.14	0.47
2:C:931:ASN:ND2	2:C:931:ASN:O	2.44	0.47
3:D:244:VAL:HG13	3:D:247:ARG:HB2	1.96	0.47
1:A:59:TYR:HB3	6:A:1104:GTP:C6	2.50	0.47
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.97	0.47
1:A:840:MET:HG2	1:A:1024:LEU:HA	1.96	0.47
1:A:40:TYR:OH	1:A:49:HIS:ND1	2.40	0.47
2:B:604:MET:HE1	2:B:607:PHE:CE1	2.50	0.47
2:B:712:PHE:HB2	2:B:715:ASN:ND2	2.30	0.47
2:C:1075:ARG:NH1	2:C:1167:ASP:OD1	2.47	0.47
2:C:186:ASP:OD2	2:C:279:SER:OG	2.18	0.47
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.28	0.47
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.76	0.47
1:A:499:VAL:O	1:A:574:ARG:NH1	2.48	0.47
2:B:241:ALA:HB2	2:B:1197:PRO:HB2	1.97	0.47
2:B:443:VAL:HG22	2:B:445:GLU:H	1.79	0.47
3:E:35:LEU:HD12	3:E:179:PHE:HB3	1.96	0.47
1:A:126:TYR:HA	1:A:131:GLY:HA3	1.96	0.47
2:B:829:SER:HB3	2:B:947:GLU:HA	1.96	0.47
2:C:1210:LEU:HD21	2:C:1255:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:525:PHE:HD2	2:C:724:HIS:CE1	2.33	0.46
2:C:827:GLY:HA3	2:C:964:VAL:HG11	1.97	0.46
2:B:364:ALA:HB2	2:B:1050:LEU:HD21	1.97	0.46
2:C:817:ASP:O	2:C:821:ASN:ND2	2.39	0.46
2:B:1149:LYS:HG3	2:B:1195:THR:HG21	1.98	0.46
1:A:552:MET:HB2	1:A:576:ASN:ND2	2.31	0.46
3:E:178:LYS:HA	3:E:250:ARG:O	2.16	0.46
3:E:62:VAL:HB	3:E:92:ARG:HD3	1.97	0.46
1:A:281:ASN:O	1:A:285:GLU:HG2	2.15	0.46
2:B:207:ASP:N	2:B:207:ASP:OD1	2.47	0.46
2:B:660:ALA:O	2:B:664:ASN:HB2	2.16	0.46
1:A:925:ILE:HD11	1:A:939:GLN:HB3	1.98	0.46
2:B:616:ASP:O	2:B:620:ILE:HG12	2.15	0.46
2:B:863:LEU:HA	2:B:866:THR:HG22	1.98	0.46
2:C:1033:ASP:N	2:C:1033:ASP:OD1	2.46	0.46
2:B:1050:LEU:HA	2:B:1050:LEU:HD23	1.74	0.46
2:C:1128:TYR:HB3	2:C:1134:ARG:HD3	1.98	0.46
2:C:1200:LYS:HE3	2:C:1200:LYS:HB2	1.74	0.46
2:C:141:LEU:HA	2:C:141:LEU:HD12	1.81	0.46
2:B:829:SER:O	2:C:645:THR:HG21	2.16	0.46
2:C:804:LEU:HA	2:C:804:LEU:HD13	1.85	0.46
2:B:368:ALA:HA	3:D:82:GLN:HG3	1.98	0.46
2:C:191:GLY:HA2	2:C:194:VAL:HG22	1.96	0.46
2:C:154:PHE:HE2	2:C:365:LEU:HD13	1.81	0.46
1:A:677:LEU:HD13	1:A:706:TYR:CZ	2.51	0.46
2:B:259:MET:HB2	2:B:1055:LEU:HD23	1.98	0.46
2:B:1118:THR:CG2	2:B:1127:ALA:HB1	2.46	0.46
2:B:1206:PHE:HE2	2:B:1232:PRO:HD3	1.81	0.46
2:C:835:TYR:HA	2:C:941:TYR:HA	1.98	0.46
1:A:409:MET:HE3	1:A:409:MET:HB3	1.65	0.45
2:B:423:GLU:O	2:B:427:VAL:HG23	2.16	0.45
2:B:683:TRP:CH2	2:B:687:LEU:HD11	2.51	0.45
1:A:647:LEU:HD13	1:A:691:TYR:HB3	1.99	0.45
2:B:1228:ARG:HG2	2:B:1231:TYR:CE1	2.51	0.45
2:B:925:VAL:HA	2:B:928:ARG:HD2	1.99	0.45
2:B:897:TYR:CZ	2:B:928:ARG:HG2	2.51	0.45
2:C:674:LYS:HG3	2:C:677:ARG:NH2	2.32	0.45
3:E:142:THR:HA	3:E:143:PRO:HD3	1.84	0.45
1:A:328:MET:HE1	1:A:336:LEU:HD22	1.97	0.45
1:A:449:THR:HG22	1:A:450:SER:H	1.80	0.45
2:C:614:ARG:HG3	2:C:1333:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:876:GLY:HA2	2:C:902:ILE:HA	1.97	0.45
3:E:273:LEU:O	3:E:277:GLU:HG3	2.16	0.45
1:A:226:ASP:HA	1:A:229:ASP:OD2	2.17	0.45
1:A:431:ALA:O	1:A:435:ILE:HG13	2.16	0.45
2:C:828:ASP:OD2	2:C:862:ARG:NH2	2.50	0.45
3:E:148:ASP:N	3:E:148:ASP:OD1	2.50	0.45
1:A:617:ILE:HD12	4:A:1101:SAM:C4	2.46	0.45
1:A:231:PHE:HE2	1:A:262:PRO:HD3	1.82	0.45
2:C:872:ILE:HD12	2:C:886:SER:HB2	1.99	0.45
2:C:337:VAL:HG22	3:E:187:ILE:HG13	1.99	0.45
3:E:253:GLU:HA	3:E:254:TYR:HA	1.58	0.45
3:E:49:ILE:HG13	3:E:49:ILE:H	1.54	0.45
2:B:1206:PHE:CE2	2:B:1232:PRO:HD3	2.51	0.45
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.98	0.45
2:B:1076:ILE:HG22	2:B:1159:VAL:HG21	1.99	0.45
2:B:214:ASP:N	2:B:214:ASP:OD1	2.41	0.45
2:B:493:HIS:ND1	2:B:524:GLU:OE1	2.48	0.45
1:A:712:ILE:HG22	1:A:716:MET:HG3	1.99	0.45
2:B:1085:ASP:N	2:B:1085:ASP:OD1	2.50	0.45
2:C:537:LEU:HD23	2:C:537:LEU:HA	1.76	0.45
3:D:253:GLU:HA	3:D:254:TYR:HA	1.70	0.45
2:B:505:PRO:HA	2:B:543:TRP:CZ2	2.53	0.44
3:D:108:ASP:OD2	3:D:112:TYR:OH	2.18	0.44
1:A:828:TYR:HA	1:A:1032:GLY:O	2.17	0.44
2:B:1075:ARG:NH2	2:B:1167:ASP:OD2	2.31	0.44
2:B:883:ILE:HD13	2:B:910:LEU:HD21	1.98	0.44
2:C:945:VAL:HG21	2:C:962:ASP:OD1	2.17	0.44
1:A:573:ARG:HA	1:A:584:ILE:HD12	1.99	0.44
2:B:334:LEU:HA	2:B:341:LYS:HA	2.00	0.44
2:B:421:ARG:HG2	2:B:750:GLU:CD	2.38	0.44
2:B:653:ARG:HA	2:B:688:GLU:CD	2.37	0.44
2:C:482:ILE:HD13	2:C:521:PHE:HE1	1.82	0.44
2:C:575:TRP:HZ3	2:C:577:GLN:OE1	1.99	0.44
2:B:267:VAL:HG22	2:B:1304:MET:HG3	1.99	0.44
2:B:482:ILE:HD13	2:B:702:LEU:HD11	1.99	0.44
2:C:1114:ARG:HG3	2:C:1116:ARG:HD3	1.99	0.44
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.51	0.44
2:B:1270:LEU:HD12	2:B:1270:LEU:HA	1.75	0.44
2:B:271:THR:HG22	2:B:292:ASN:OD1	2.16	0.44
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	1.99	0.44
2:C:265:VAL:HB	2:C:1304:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:LEU:HD12	2:C:1302:VAL:HG21	1.99	0.44
2:C:451:GLU:HA	2:C:452:ASN:HA	1.58	0.44
1:A:14:ALA:HA	1:A:112:ARG:NH2	2.33	0.44
1:A:375:HIS:CD2	1:A:771:THR:HG23	2.52	0.44
1:A:477:TYR:HA	1:A:482:THR:HG22	1.99	0.44
2:C:617:ASP:OD1	2:C:617:ASP:N	2.51	0.44
2:B:953:ASP:OD1	3:D:243:LYS:HE2	2.18	0.44
1:A:184:TRP:HB3	1:A:195:ILE:HD13	1.99	0.44
3:D:253:GLU:HB3	3:D:254:TYR:CD1	2.53	0.44
3:E:4:GLN:HA	3:E:5:PRO:HD3	1.82	0.44
1:A:511:ILE:HG13	1:A:511:ILE:H	1.64	0.44
2:B:1142:ASN:N	2:B:1142:ASN:OD1	2.51	0.44
2:B:410:ARG:HD3	2:B:1043:SER:HA	1.99	0.44
2:B:894:VAL:HG22	2:B:916:LEU:HB3	1.99	0.44
2:C:170:TYR:CE1	2:C:198:LYS:HG2	2.52	0.44
1:A:285:GLU:O	1:A:366:SER:HB3	2.17	0.44
2:B:379:LEU:O	2:B:383:SER:OG	2.28	0.44
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.98	0.44
2:C:373:ASP:HA	2:C:376:ILE:HG12	2.00	0.44
1:A:199:MET:HG3	1:A:205:VAL:HG21	1.99	0.43
1:A:322:ASP:OD2	1:A:325:THR:OG1	2.30	0.43
1:A:675:THR:HA	1:A:693:TYR:O	2.18	0.43
1:A:90:ASP:OD1	1:A:91:ASN:N	2.51	0.43
2:B:1148:SER:HB2	2:C:390:HIS:CD2	2.53	0.43
2:B:1267:THR:HG22	2:B:1299:SER:HB3	1.99	0.43
2:B:489:MET:HE3	2:B:580:TYR:HE2	1.83	0.43
2:B:414:LEU:HD13	2:B:814:THR:HG21	2.00	0.43
3:D:28:PRO:HG3	3:D:223:VAL:HG22	1.99	0.43
1:A:486:THR:HB	1:A:489:SER:HB3	2.00	0.43
1:A:615:CYS:HB2	1:A:639:CYS:SG	2.58	0.43
2:B:1060:ARG:HA	2:B:1060:ARG:HE	1.83	0.43
2:B:1292:GLU:OE2	3:D:20:ARG:NH1	2.46	0.43
2:B:903:ASN:ND2	2:B:905:PRO:HG2	2.32	0.43
2:C:252:LEU:HA	2:C:252:LEU:HD23	1.83	0.43
2:B:1148:SER:HB2	2:C:390:HIS:CG	2.53	0.43
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.75	0.43
2:B:1313:ASP:N	2:B:1313:ASP:OD1	2.51	0.43
2:B:469:ARG:NE	2:B:513:GLU:OE1	2.51	0.43
2:C:1093:PRO:HB2	2:C:1096:TYR:CE1	2.54	0.43
2:C:341:LYS:HD3	2:C:341:LYS:HA	1.86	0.43
1:A:602:PHE:CG	1:A:608:ILE:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:LYS:HE2	2:B:1178:MET:HE2	2.00	0.43
2:B:835:TYR:CD2	2:B:941:TYR:HB3	2.54	0.43
2:B:1230:ILE:HG13	2:C:119:ASP:HA	2.00	0.43
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	2.01	0.43
2:C:495:LEU:HD13	2:C:532:ILE:HG22	2.01	0.43
2:C:256:PHE:HE2	2:C:990:THR:HG21	1.84	0.43
3:E:27:THR:HB	3:E:29:THR:HG22	1.99	0.43
1:A:271:ARG:O	1:A:275:ILE:HG13	2.19	0.43
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.51	0.43
2:B:1076:ILE:HG23	2:B:1229:LEU:HG	2.01	0.43
2:C:117:ARG:HD2	2:C:117:ARG:HA	1.71	0.43
2:C:674:LYS:HG3	2:C:677:ARG:HH21	1.83	0.43
2:C:968:ARG:HA	2:C:971:MET:HE3	2.01	0.43
3:D:44:LEU:HG	3:D:174:VAL:HG22	2.01	0.43
2:B:608:THR:HA	2:B:609:PRO:HD3	1.88	0.43
3:D:53:GLU:CD	3:D:53:GLU:H	2.22	0.43
1:A:238:ASP:OD2	1:A:259:ARG:NE	2.52	0.43
2:C:1050:LEU:HA	2:C:1050:LEU:HD23	1.65	0.43
2:C:820:ILE:HA	2:C:820:ILE:HD13	1.77	0.43
3:E:93:LEU:HA	3:E:93:LEU:HD23	1.88	0.43
1:A:143:TYR:CD2	1:A:146:PRO:HA	2.54	0.43
1:A:470:LEU:HD13	1:A:470:LEU:HA	1.90	0.43
1:A:532:MET:HA	1:A:535:LEU:HD12	1.99	0.43
2:B:186:ASP:O	2:B:190:VAL:HB	2.19	0.43
2:C:526:ASN:HB2	2:C:724:HIS:CE1	2.53	0.43
1:A:962:PHE:CE1	1:A:1051:PRO:HB2	2.53	0.42
2:B:186:ASP:N	2:B:186:ASP:OD1	2.51	0.42
2:B:355:ALA:HB3	2:B:1276:LEU:HD11	2.01	0.42
2:B:561:ASN:OD1	2:B:562:ALA:N	2.51	0.42
3:D:189:LEU:HD12	3:D:189:LEU:HA	1.81	0.42
3:D:272:ASP:OD1	3:D:273:LEU:N	2.48	0.42
1:A:313:ARG:HD2	1:A:317:ARG:NH1	2.34	0.42
2:B:732:TYR:CE1	2:B:1021:ARG:HG3	2.53	0.42
2:B:1118:THR:HG21	2:B:1127:ALA:HB1	2.00	0.42
2:B:388:GLN:HB2	2:B:1320:VAL:HB	1.99	0.42
2:C:848:ARG:HH21	2:C:914:GLU:HG2	1.84	0.42
3:E:229:PHE:O	3:E:233:THR:HG23	2.19	0.42
2:B:886:SER:O	2:B:890:THR:HG23	2.20	0.42
2:C:1331:ARG:HG3	2:C:1332:ASN:H	1.83	0.42
2:C:993:ASP:OD1	2:C:995:THR:OG1	2.29	0.42
1:A:925:ILE:HG12	1:A:925:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:ALA:O	2:B:910:LEU:HG	2.19	0.42
2:C:1144:ARG:N	2:C:1170:ASP:OD2	2.47	0.42
2:C:558:TYR:CE1	2:C:590:SER:HB3	2.54	0.42
3:D:178:LYS:HA	3:D:250:ARG:O	2.20	0.42
3:D:9:TYR:H	3:D:204:ASP:CG	2.21	0.42
3:D:35:LEU:HD21	3:D:229:PHE:CE1	2.55	0.42
2:C:1181:SER:HG	2:C:1181:SER:H	1.50	0.42
2:C:839:ALA:HB2	2:C:935:GLN:NE2	2.35	0.42
1:A:418:GLY:C	1:A:976:ALA:HB2	2.40	0.42
1:A:586:GLY:O	1:A:587:MET:HG3	2.20	0.42
2:B:1002:LEU:HD23	2:B:1002:LEU:HA	1.71	0.42
2:B:473:ALA:HB2	2:B:765:PRO:HB3	2.01	0.42
1:A:561:LEU:HD11	1:A:602:PHE:HZ	1.85	0.42
3:E:263:ALA:O	3:E:270:THR:HG21	2.19	0.42
1:A:488:GLY:HA3	1:A:549:SER:HA	2.01	0.42
1:A:66:ASP:CG	1:A:122:ARG:HH22	2.23	0.42
2:C:714:LEU:HA	2:C:714:LEU:HD23	1.80	0.42
1:A:415:ASP:N	1:A:415:ASP:OD1	2.52	0.42
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.54	0.42
2:B:477:SER:OG	2:B:762:ILE:HD11	2.20	0.42
2:C:273:PRO:HD3	2:C:290:TYR:HE1	1.84	0.42
2:C:524:GLU:HA	2:C:527:ARG:HD2	2.02	0.42
3:D:77:PHE:HA	3:D:269:ILE:HD13	2.02	0.42
1:A:143:TYR:CE2	1:A:146:PRO:HA	2.55	0.42
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.55	0.42
2:B:265:VAL:HB	2:B:1304:MET:HB3	2.00	0.42
2:B:420:PRO:HG2	2:B:750:GLU:OE1	2.20	0.42
2:C:383:SER:CB	2:C:387:THR:HG21	2.50	0.42
2:C:751:THR:OG1	2:C:753:ASP:OD1	2.33	0.42
1:A:329:THR:HG22	1:A:332:HIS:ND1	2.34	0.41
1:A:717:THR:HB	1:A:1020:SER:HB2	2.01	0.41
2:B:1014:MET:HA	2:B:1017:ALA:HB2	2.02	0.41
2:B:957:PHE:HE1	2:B:1016:ASN:HB3	1.85	0.41
2:B:446:LYS:HB3	2:B:448:TYR:CD2	2.55	0.41
2:B:474:ASP:O	2:B:477:SER:OG	2.23	0.41
2:B:442:PRO:HG2	2:B:475:ILE:HB	2.01	0.41
2:C:208:LEU:HD21	2:C:1067:ILE:HG13	2.02	0.41
2:C:1180:PRO:HA	2:C:1207:MET:SD	2.60	0.41
2:C:574:LYS:NZ	2:C:574:LYS:HB3	2.35	0.41
2:C:707:ALA:O	2:C:710:SER:OG	2.38	0.41
2:C:751:THR:HG22	2:C:1002:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:112:TYR:CZ	3:D:119:ILE:HD13	2.55	0.41
3:D:130:PHE:CZ	3:D:199:LEU:HD22	2.55	0.41
2:B:143:VAL:HG11	2:B:1316:ALA:HB1	2.02	0.41
2:B:525:PHE:HD2	2:B:724:HIS:CE1	2.38	0.41
2:B:536:LEU:HA	2:B:536:LEU:HD23	1.91	0.41
2:B:874:ILE:HD11	2:B:917:VAL:HG13	2.01	0.41
2:C:469:ARG:NE	2:C:513:GLU:OE1	2.53	0.41
3:D:281:LYS:O	3:D:285:LEU:HG	2.20	0.41
1:A:812:VAL:HA	1:A:813:PRO:HA	1.80	0.41
2:B:510:VAL:O	2:B:513:GLU:HB3	2.21	0.41
2:C:1180:PRO:HD3	2:C:1208:ASP:O	2.20	0.41
2:C:547:GLU:OE2	2:C:599:THR:OG1	2.36	0.41
2:C:971:MET:HA	2:C:972:PRO:HD3	1.96	0.41
2:B:1036:ASP:OD1	2:B:1036:ASP:N	2.53	0.41
2:B:1076:ILE:CG2	2:B:1159:VAL:HG21	2.51	0.41
2:B:804:LEU:HA	2:B:804:LEU:HD12	1.80	0.41
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.54	0.41
2:C:332:THR:O	2:C:335:ASP:HB2	2.20	0.41
1:A:944:ARG:HB2	1:A:1006:MET:SD	2.60	0.41
2:B:1064:ASN:HA	2:B:1065:PRO:HD3	1.86	0.41
2:B:1278:TYR:CZ	2:B:1290:LYS:HG2	2.55	0.41
2:C:1197:PRO:HG2	2:C:1200:LYS:HB3	2.02	0.41
2:C:922:TYR:O	2:C:925:VAL:HG23	2.21	0.41
1:A:569:VAL:HG22	1:A:584:ILE:HG22	2.03	0.41
1:A:663:GLU:OE2	1:A:667:GLN:NE2	2.53	0.41
2:B:742:LYS:HB3	2:B:742:LYS:HE2	1.89	0.41
1:A:333:GLN:HG3	1:A:354:ILE:HD12	2.02	0.41
1:A:872:VAL:HA	1:A:873:PRO:HD3	1.96	0.41
2:B:1050:LEU:O	2:B:1054:ARG:HG3	2.21	0.41
2:B:550:ILE:O	2:B:553:GLN:HG3	2.20	0.41
2:B:735:THR:O	2:B:1017:ALA:HA	2.20	0.41
2:B:795:ASP:HA	2:B:796:PRO:HD3	1.96	0.41
1:A:665:LEU:HD21	1:A:694:ILE:HD12	2.03	0.41
2:B:497:LYS:HA	2:B:497:LYS:HD3	1.86	0.41
2:B:235:ILE:HG13	2:C:774:LEU:HD22	2.02	0.41
2:C:926:VAL:HG21	2:C:937:ASN:HA	2.03	0.41
3:D:85:ASN:HB3	3:D:141:SER:HB3	2.02	0.41
2:B:1232:PRO:HB3	2:B:1236:ILE:HD11	2.02	0.41
2:B:948:ILE:HD13	2:B:948:ILE:HA	1.86	0.41
1:A:591:ALA:HB3	1:A:597:ARG:HA	2.02	0.41
1:A:655:GLU:HG2	1:A:712:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:VAL:HG21	2:B:1245:ILE:HG22	2.03	0.41
2:B:390:HIS:HB2	2:B:1318:GLU:HB3	2.02	0.41
2:B:192:PRO:HG3	2:B:294:VAL:HG23	2.03	0.41
2:B:524:GLU:HA	2:B:527:ARG:HD2	2.03	0.41
2:C:385:ILE:HG12	2:C:708:THR:HG22	2.02	0.41
1:A:474:TYR:CD1	1:A:499:VAL:HG12	2.55	0.41
1:A:915:ASN:OD1	1:A:953:ARG:HG3	2.20	0.41
1:A:926:MET:HB2	1:A:995:VAL:HG21	2.03	0.41
2:B:227:LEU:HA	2:B:246:GLU:O	2.21	0.41
2:B:409:ILE:O	2:B:413:MET:HG2	2.21	0.41
2:B:582:SER:O	2:B:728:LYS:HE3	2.21	0.41
2:B:849:MET:HA	2:B:917:VAL:O	2.20	0.41
2:C:1323:ASP:N	2:C:1323:ASP:OD1	2.53	0.41
3:D:190:SER:O	3:D:194:VAL:HG23	2.21	0.41
1:A:67:ARG:NH1	1:A:171:ILE:O	2.47	0.40
1:A:41:THR:HG22	1:A:50:THR:HG23	1.99	0.40
1:A:552:MET:H	1:A:576:ASN:HD21	1.69	0.40
1:A:882:ASP:HB3	1:A:885:THR:OG1	2.22	0.40
2:B:145:THR:OG1	2:B:1317:VAL:HG23	2.21	0.40
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.82	0.40
2:C:471:SER:O	2:C:765:PRO:HG3	2.21	0.40
1:A:1019:PRO:HG2	1:A:1047:ASN:OD1	2.21	0.40
1:A:197:ALA:O	1:A:200:ARG:HG2	2.21	0.40
1:A:379:VAL:HG11	1:A:794:LEU:HG	2.03	0.40
2:C:204:VAL:HB	2:C:1242:MET:HB2	2.04	0.40
1:A:615:CYS:SG	1:A:617:ILE:HG12	2.61	0.40
1:A:881:ILE:HG23	1:A:900:GLN:HB3	2.04	0.40
1:A:919:TYR:HB3	1:A:921:PHE:HE1	1.86	0.40
2:B:1055:LEU:O	2:B:1059:LEU:HG	2.22	0.40
2:B:1289:PRO:HG2	2:B:1292:GLU:HB2	2.03	0.40
2:B:809:VAL:HG11	2:B:1002:LEU:HG	2.04	0.40
3:D:235:VAL:HB	3:D:258:ASN:OD1	2.22	0.40
1:A:154:PHE:CG	1:A:185:HIS:HB2	2.56	0.40
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	2.02	0.40
2:B:863:LEU:O	2:B:866:THR:HG22	2.22	0.40
2:C:1071:PHE:HD1	2:C:1234:GLN:NE2	2.18	0.40
2:C:1269:THR:OG1	2:C:1270:LEU:N	2.54	0.40
2:C:863:LEU:HD13	2:C:871:PRO:HD3	2.03	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 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%)	1009 (96%)	45 (4%)	1 (0%)	56	90
2	B	1187/1333 (89%)	1129 (95%)	55 (5%)	3 (0%)	46	84
2	C	1247/1333 (94%)	1188 (95%)	55 (4%)	4 (0%)	46	84
3	D	290/448 (65%)	279 (96%)	10 (3%)	1 (0%)	46	84
3	E	290/448 (65%)	283 (98%)	7 (2%)	0	100	100
All	All	4069/4620 (88%)	3888 (96%)	172 (4%)	9 (0%)	56	88

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1136	HIS
2	C	769	GLN
2	B	790	GLU
2	B	1310	ARG
2	C	1014	MET
2	C	1331	ARG
3	D	61	ASN
1	A	982	VAL
2	C	901	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 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%)	853 (91%)	89 (9%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1038/1153 (90%)	933 (90%)	105 (10%)	9	34
2	C	1090/1153 (94%)	978 (90%)	112 (10%)	9	33
3	D	240/379 (63%)	220 (92%)	20 (8%)	14	46
3	E	240/379 (63%)	217 (90%)	23 (10%)	10	38
All	All	3550/4007 (89%)	3201 (90%)	349 (10%)	14	36

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	7	ILE
1	A	18	LYS
1	A	50	THR
1	A	52	ARG
1	A	54	LEU
1	A	73	ARG
1	A	76	LEU
1	A	81	LYS
1	A	99	VAL
1	A	102	LEU
1	A	105	ARG
1	A	111	LEU
1	A	112	ARG
1	A	133	LEU
1	A	157	LEU
1	A	160	ASP
1	A	181	VAL
1	A	188	THR
1	A	196	LEU
1	A	199	MET
1	A	222	ARG
1	A	236	LEU
1	A	246	ASP
1	A	255	ARG
1	A	259	ARG
1	A	282	GLU
1	A	290	LEU
1	A	297	LEU
1	A	298	LEU
1	A	303	THR
1	A	306	GLN

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	313	ARG
1	A	317	ARG
1	A	318	ARG
1	A	324	ARG
1	A	329	THR
1	A	348	LEU
1	A	366	SER
1	A	368	THR
1	A	377	LEU
1	A	390	ASP
1	A	415	ASP
1	A	423	THR
1	A	433	GLU
1	A	453	LEU
1	A	466	LEU
1	A	471	SER
1	A	475	ARG
1	A	478	ILE
1	A	487	GLN
1	A	493	LEU
1	A	532	MET
1	A	533	LEU
1	A	556	THR
1	A	569	VAL
1	A	572	LEU
1	A	577	ARG
1	A	582	VAL
1	A	583	ARG
1	A	593	GLU
1	A	639	CYS
1	A	647	LEU
1	A	664	ARG
1	A	665	LEU
1	A	750	VAL
1	A	757	LEU
1	A	763	LYS
1	A	771	THR
1	A	780	LEU
1	A	781	VAL
1	A	783	ILE
1	A	812	VAL

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Mol	Chain	Res	Type
1	A	816	LEU
1	A	861	ILE
1	A	877	LYS
1	A	886	ARG
1	A	890	LEU
1	A	900	GLN
1	A	910	ASN
1	A	925	ILE
1	A	951	LEU
1	A	978	LYS
1	A	982	VAL
1	A	996	ASP
1	A	1018	ARG
1	A	1034	ARG
1	A	1057	ARG
2	B	143	VAL
2	B	147	VAL
2	B	148	GLN
2	B	175	THR
2	B	177	LYS
2	B	186	ASP
2	B	198	LYS
2	B	203	VAL
2	B	208	LEU
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	271	THR
2	B	274	MET
2	B	283	ASN
2	B	286	LEU
2	B	287	ARG
2	B	289	THR
2	B	294	VAL
2	B	315	THR
2	B	320	GLN
2	B	323	THR
2	B	327	LEU
2	B	333	ARG

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Mol	Chain	Res	Type
2	B	339	LEU
2	B	366	MET
2	B	384	MET
2	B	414	LEU
2	B	446	LYS
2	B	474	ASP
2	B	485	GLU
2	B	486	VAL
2	B	491	ASN
2	B	510	VAL
2	B	512	LEU
2	B	533	GLN
2	B	552	VAL
2	B	565	GLU
2	B	615	THR
2	B	626	ARG
2	B	629	ARG
2	B	637	TYR
2	B	654	THR
2	B	659	LEU
2	B	669	GLN
2	B	676	THR
2	B	684	LEU
2	B	688	GLU
2	B	702	LEU
2	B	704	VAL
2	B	708	THR
2	B	728	LYS
2	B	742	LYS
2	B	748	GLN
2	B	755	LEU
2	B	797	SER
2	B	804	LEU
2	B	815	LEU
2	B	828	ASP
2	B	843	LEU
2	B	848	ARG
2	B	890	THR
2	B	892	VAL
2	B	953	ASP
2	B	970	LEU
2	B	975	SER

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Mol	Chain	Res	Type
2	B	991	ASP
2	B	995	THR
2	B	1007	THR
2	B	1010	ARG
2	B	1033	ASP
2	B	1036	ASP
2	B	1048	ASP
2	B	1052	LEU
2	B	1061	LEU
2	B	1067	ILE
2	B	1074	VAL
2	B	1079	LEU
2	B	1083	ASP
2	B	1110	LEU
2	B	1134	ARG
2	B	1142	ASN
2	B	1170	ASP
2	B	1178	MET
2	B	1186	GLN
2	B	1193	ILE
2	B	1198	LYS
2	B	1201	LEU
2	B	1210	LEU
2	B	1223	SER
2	B	1228	ARG
2	B	1233	LEU
2	B	1234	GLN
2	B	1238	VAL
2	B	1240	ARG
2	B	1247	ASN
2	B	1269	THR
2	B	1285	GLN
2	B	1315	MET
2	B	1323	ASP
2	B	1329	ASN
2	B	1331	ARG
2	C	82	ARG
2	C	83	GLN
2	C	109	LYS
2	C	112	THR
2	C	115	GLN
2	C	117	ARG

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Mol	Chain	Res	Type
2	C	118	THR
2	C	133	THR
2	C	134	THR
2	C	141	LEU
2	C	147	VAL
2	C	173	GLN
2	C	187	ASP
2	C	190	VAL
2	C	203	VAL
2	C	207	ASP
2	C	208	LEU
2	C	230	ASP
2	C	255	LEU
2	C	264	LEU
2	C	270	THR
2	C	275	SER
2	C	281	VAL
2	C	282	VAL
2	C	294	VAL
2	C	310	LEU
2	C	315	THR
2	C	323	THR
2	C	330	THR
2	C	331	GLU
2	C	335	ASP
2	C	362	LEU
2	C	363	ARG
2	C	375	ARG
2	C	379	LEU
2	C	384	MET
2	C	397	LEU
2	C	401	LEU
2	C	452	ASN
2	C	474	ASP
2	C	475	ILE
2	C	484	ARG
2	C	486	VAL
2	C	503	GLU
2	C	532	ILE
2	C	533	GLN
2	C	542	ARG
2	C	552	VAL

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Mol	Chain	Res	Type
2	C	557	THR
2	C	575	TRP
2	C	626	ARG
2	C	630	ASN
2	C	637	TYR
2	C	659	LEU
2	C	674	LYS
2	C	685	ARG
2	C	687	LEU
2	C	689	THR
2	C	694	ILE
2	C	735	THR
2	C	761	SER
2	C	763	VAL
2	C	768	CYS
2	C	792	VAL
2	C	798	THR
2	C	804	LEU
2	C	809	VAL
2	C	815	LEU
2	C	828	ASP
2	C	832	MET
2	C	837	THR
2	C	854	GLN
2	C	859	ILE
2	C	872	ILE
2	C	907	SER
2	C	921	ASP
2	C	931	ASN
2	C	945	VAL
2	C	959	GLN
2	C	965	ARG
2	C	995	THR
2	C	1003	ARG
2	C	1007	THR
2	C	1010	ARG
2	C	1014	MET
2	C	1015	GLN
2	C	1035	ILE
2	C	1043	SER
2	C	1052	LEU
2	C	1055	LEU

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Mol	Chain	Res	Type
2	C	1061	LEU
2	C	1067	ILE
2	C	1070	ARG
2	C	1079	LEU
2	C	1104	ARG
2	C	1113	LYS
2	C	1134	ARG
2	C	1170	ASP
2	C	1181	SER
2	C	1188	VAL
2	C	1202	PHE
2	C	1210	LEU
2	C	1219	ASP
2	C	1230	ILE
2	C	1233	LEU
2	C	1258	VAL
2	C	1267	THR
2	C	1283	ASN
2	C	1295	HIS
2	C	1306	THR
2	C	1321	ASN
2	C	1332	ASN
3	D	2	LEU
3	D	20	ARG
3	D	29	THR
3	D	35	LEU
3	D	47	LYS
3	D	92	ARG
3	D	93	LEU
3	D	96	LEU
3	D	107	LEU
3	D	116	THR
3	D	133	THR
3	D	142	THR
3	D	158	LEU
3	D	160	LEU
3	D	171	VAL
3	D	189	LEU
3	D	191	ARG
3	D	226	MET
3	D	232	SER
3	D	252	LEU

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Mol	Chain	Res	Type
3	E	2	LEU
3	E	21	ASN
3	E	27	THR
3	E	35	LEU
3	E	47	LYS
3	E	66	VAL
3	E	93	LEU
3	E	94	SER
3	E	98	LEU
3	E	133	THR
3	E	183	GLU
3	E	189	LEU
3	E	226	MET
3	E	240	VAL
3	E	242	ARG
3	E	244	VAL
3	E	252	LEU
3	E	261	ARG
3	E	262	THR
3	E	269	ILE
3	E	272	ASP
3	E	273	LEU
3	E	274	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	A	241	GLN
1	A	258	GLN
1	A	375	HIS
1	A	576	ASN
2	B	724	HIS
2	B	1138	HIS
2	C	724	HIS
2	C	1015	GLN
2	C	1234	GLN
2	C	1308	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 ⓘ

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	1.03	2 (8%)	15,42,42	3.05	1 (6%)
4	SAM	A	1102	-	23,29,29	1.05	2 (8%)	15,42,42	2.99	1 (6%)
5	ATP	A	1103	-	26,33,33	0.92	1 (3%)	26,52,52	1.80	3 (11%)
6	GTP	A	1104	7	26,34,34	0.97	1 (3%)	29,54,54	1.62	5 (17%)

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	2.28	1.38	1.33
4	A	1102	SAM	C2-N1	2.38	1.38	1.33
5	A	1103	ATP	C5-C4	2.99	1.47	1.40
6	A	1104	GTP	C6-N1	3.16	1.38	1.33
4	A	1101	SAM	C2-N3	3.44	1.38	1.32
4	A	1102	SAM	C2-N3	3.46	1.38	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	SAM	N3-C2-N1	-11.34	119.96	128.87
4	A	1102	SAM	N3-C2-N1	-11.21	120.07	128.87
5	A	1103	ATP	N3-C2-N1	-6.93	123.43	128.87
6	A	1104	GTP	N3-C2-N1	-5.30	120.34	127.56
6	A	1104	GTP	C5-C6-N1	-2.96	119.66	123.52
6	A	1104	GTP	C1'-N9-C4	-2.81	123.67	126.81
5	A	1103	ATP	C2'-C1'-N9	-2.69	106.27	113.47
6	A	1104	GTP	N2-C2-N1	2.06	120.59	117.20
5	A	1103	ATP	O3G-PG-O2G	2.22	115.58	107.44
6	A	1104	GTP	C6-N1-C2	3.35	119.81	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	1	0
6	A	1104	GTP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.