



## wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 01:56 PM EDT

PDB ID : 3JAZ  
EMDB ID: : EMD-6371  
Title : Atomic model of cytoplasmic polyhedrosis virus with 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 : unknown  
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

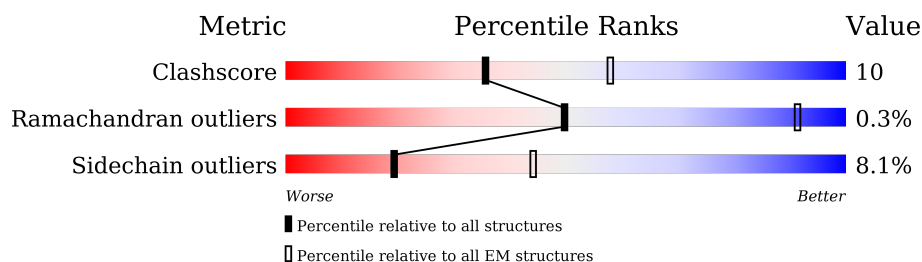
# 1 Overall quality at a glance

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	68% 28% .
2	B	1333	63% 24% . 11%
2	C	1333	69% 23% . 6%
3	D	448	45% 17% . 35%
3	E	448	46% 17% . 35%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32244 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	1250	Total	C	N	O	S	0	0
			9851	6219	1712	1882	38		

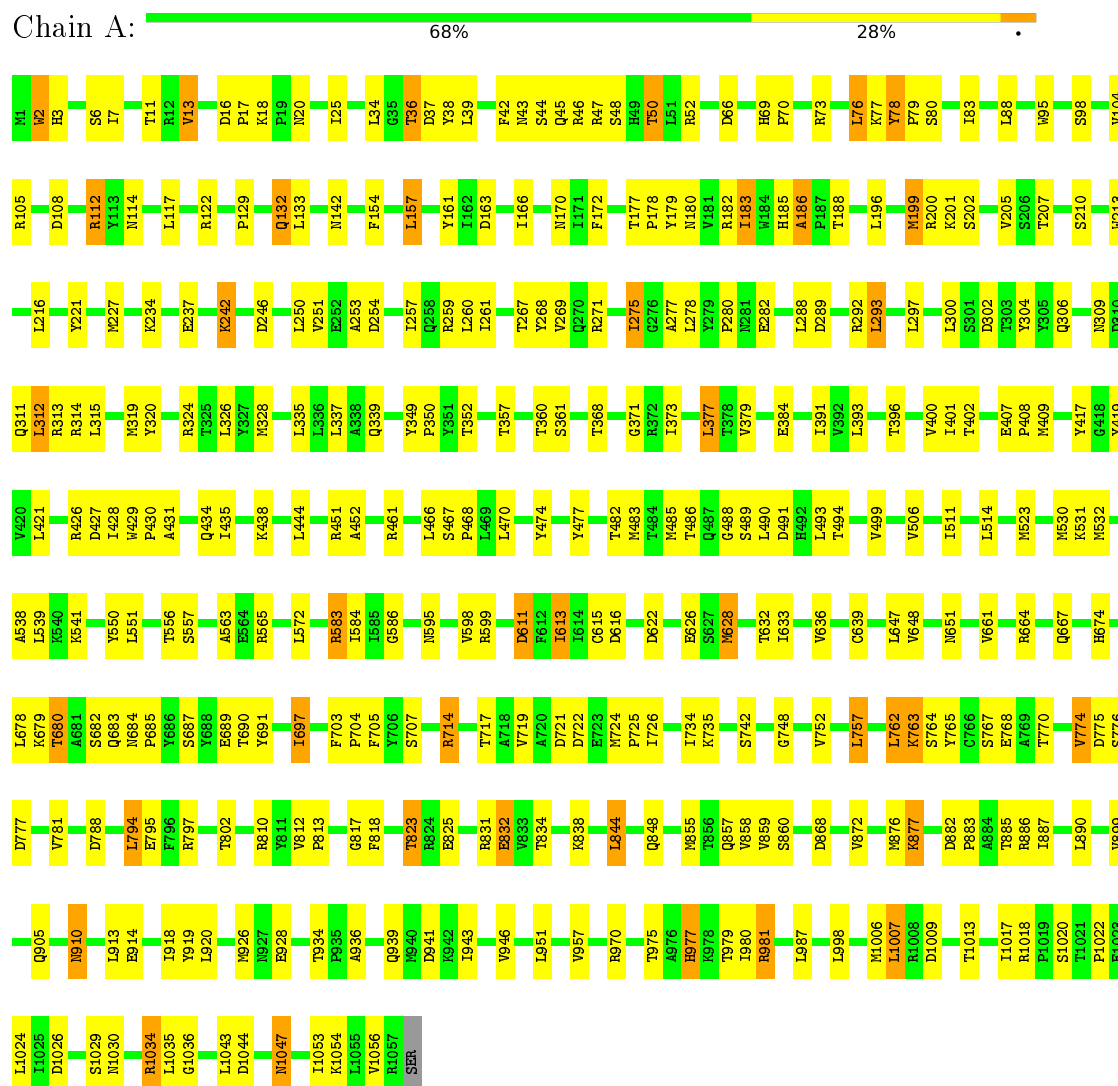
- Molecule 3 is a protein called Viral structural protein 5.

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		

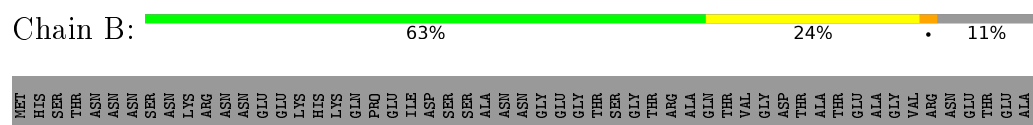
### 3 Residue-property plots

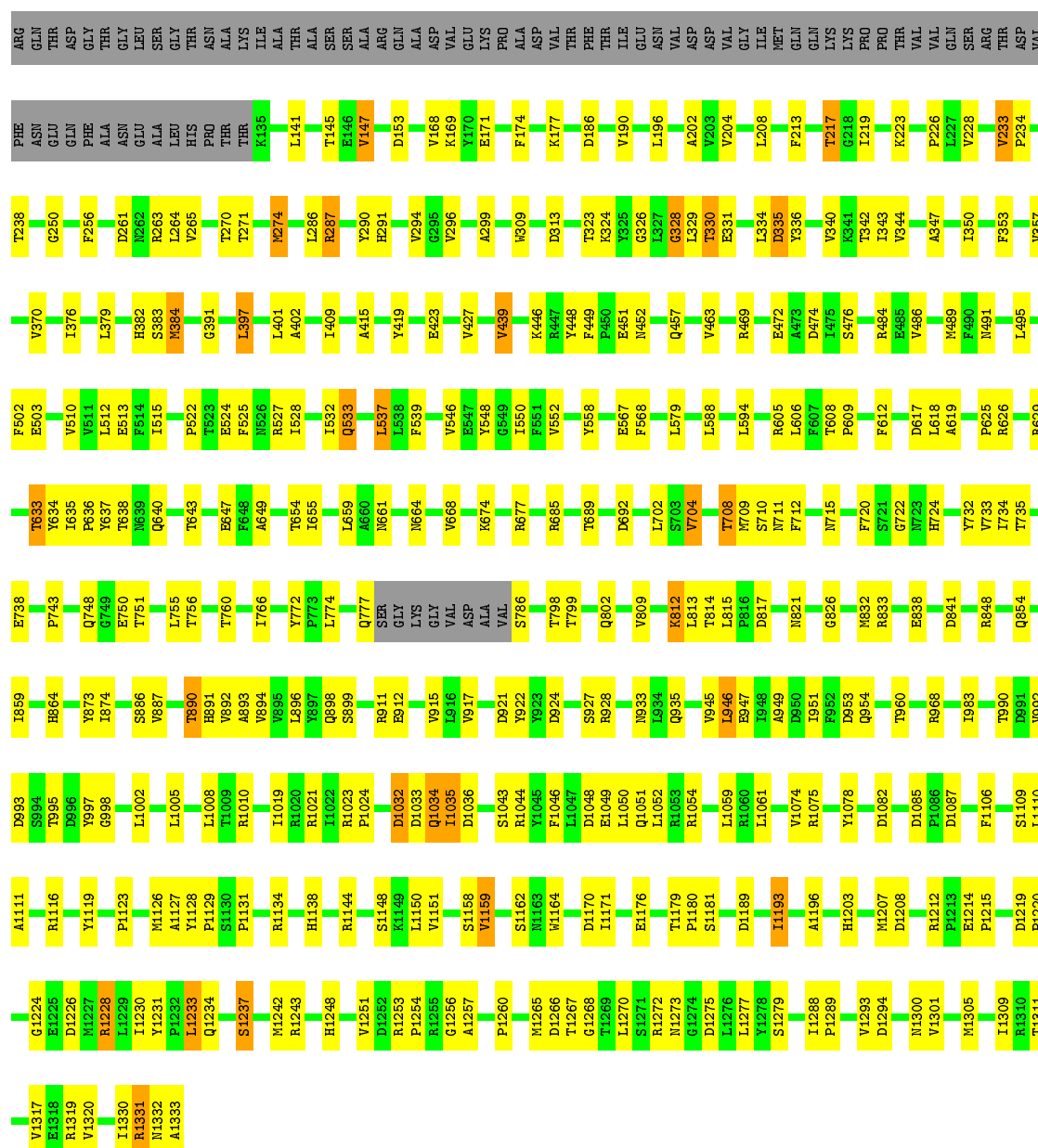
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

#### • Molecule 1: Structural protein VP3



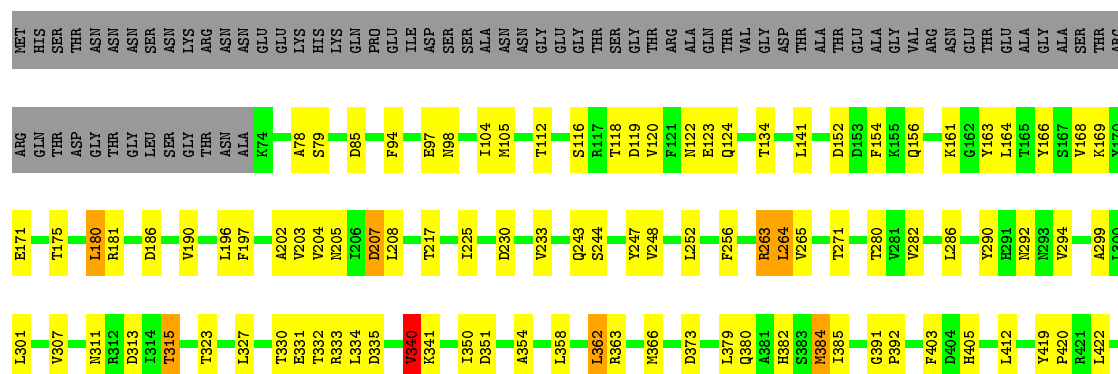
#### • Molecule 2: Capsid protein VP1

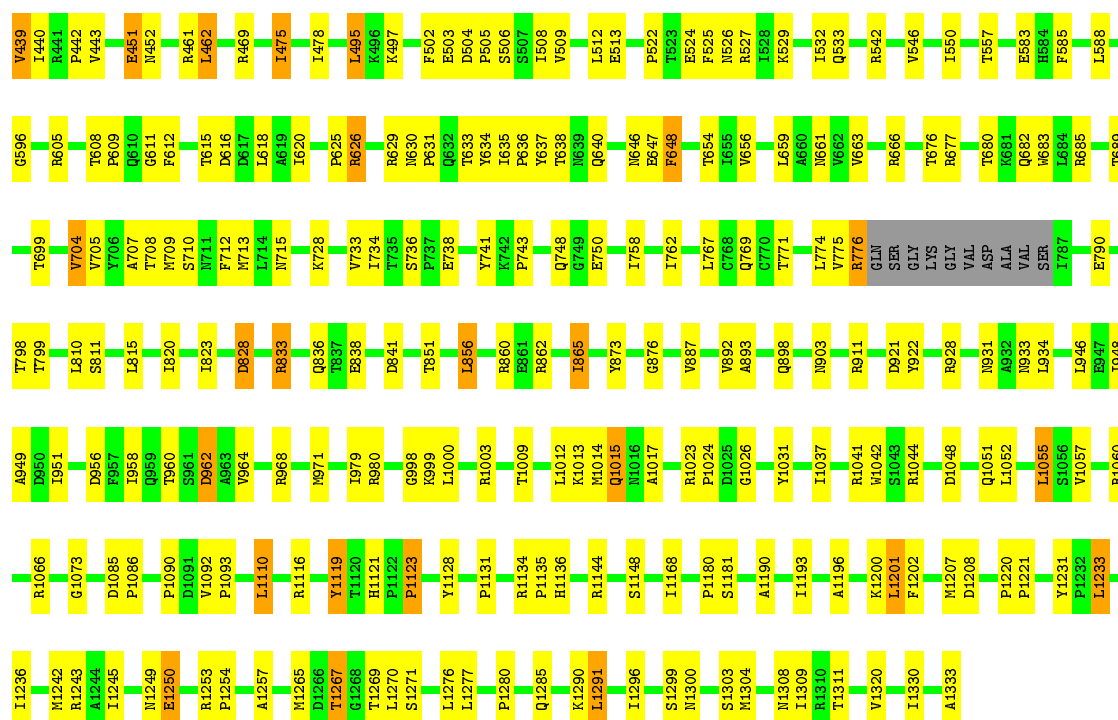




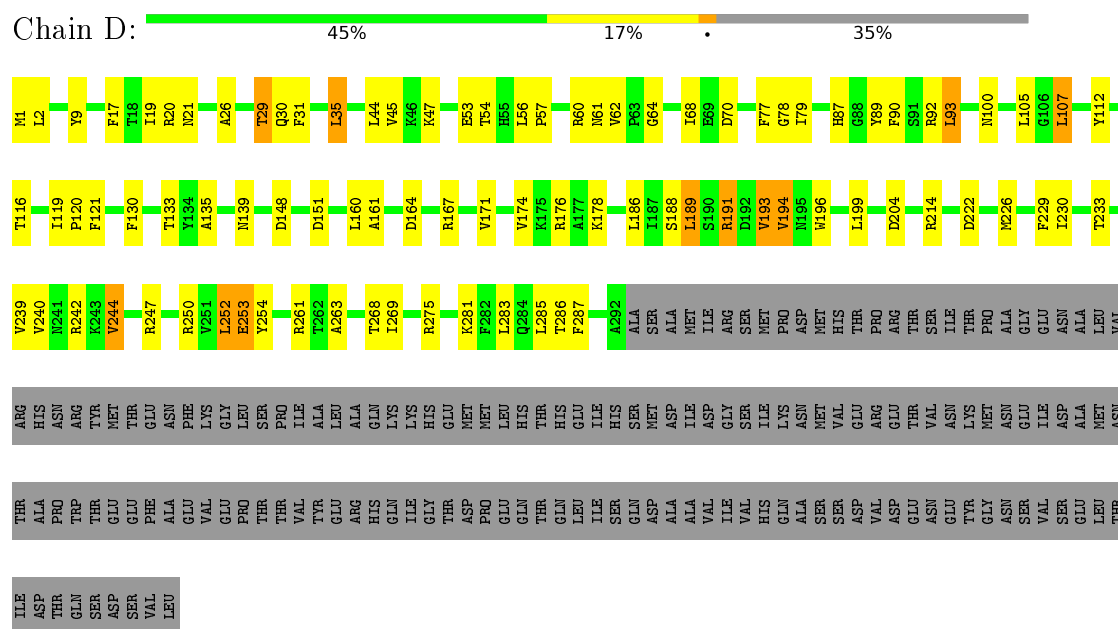
### • Molecule 2: Capsid protein VP1

Chain C:  69% 23% 6%

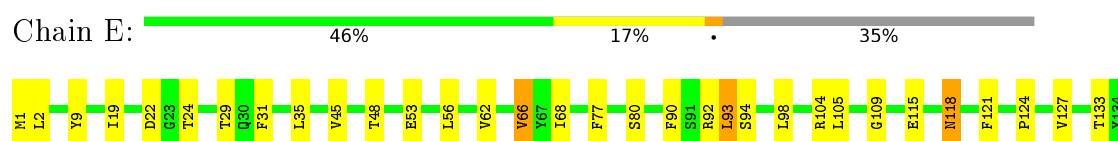




### • Molecule 3: Viral structural protein 5



### • Molecule 3: Viral structural protein 5



GLN SER ASP SER VAL LEU	TRP	ARG	R250	A135
	GLU	TYR	V251	K136
	GLU	MET	L252	L137
	GLU	THR	R253	G138
	PHE	GLU		N139
	ALA	ASN	R258	
	GLU	PHE	S259	T142
	VAL	LYS	R260	L146
	GLU	GLY	R261	A147
	PRO	LEU	T262	D148
THR VAL GLU ARG HIS GLN ILE GLY THR ASP PRO GLU GLN THR VAL GLU ASP GLU GLU ASN GLU TYR GLY VAL SER GLU LEU THR ILE ASP THR	THR	SER	A263	
	THR	PRO		D151
	VAL	ILE	T266	
	GLU	ALA		L158
	THR	LEU	D272	E159
	ARG	ALA	L273	L160
	HIS	GLN	S274	
	GLN	LYS		D164
	ILE	LYS	R277	
	GLY	HIS		R167
ASP PRO GLU GLN THR GLN GLN LEU ILE SER GLN ASP ALA ALA VAL ILE VAL HIS GLN ALA SER SER ASP VAL GLU ASN GLU TYR GLY VAL SER GLU LEU THR ILE ASP THR	ASP	MET	K281	
	PRO	MET	T282	
	GLU	LEU	L283	V171
	GLN	L285	Q284	
	THR	THR	T286	R176
	GLN	HIS	F287	A177
	LEU	GLU	T288	
	ILE	ILE		S181
	SER	HIS	K292	D180
	GLN	SER	ALA	W182
ASP ALA ALA VAL ILE VAL HIS GLN ALA SER SER ASP VAL GLU ASN GLU TYR GLY VAL SER GLU LEU THR ILE ASP THR	ASP	MET	G183	
	ALA	ASP	ALA	S185
	ALA	ILE	MET	
	VAL	ASP	ILE	L189
	ILE	GLY	ARG	
	VAL	ILE	SER	V194
	HIS	ILE	MET	
	GLN	LYS	PRO	L199
	ALA	ASN	ASP	D204
	SER	MET	MET	
ASP VAL GLU ASN GLU TYR GLY VAL SER GLU LEU THR ILE ASP THR	SER	HIS		R221
	ASP	THR		
	VAL	ARG	PRO	F224
	ASP	GLU	ARG	R225
	GLU	THR	THR	M226
	ASN	VAL	SER	M227
	GLU	ASN	ILE	L228
	TYR	LYS	THR	F229
	GLY	MET	PRO	
	ASN	ASN	ALA	T233
VAL SER GLU LEU THR ILE ASP THR	VAL	ILE	GLY	
	SER	GLU	GLY	
	GLU	ASP	ASN	V239
	LEU	ALA	ALA	V240
	THR	MET	LEU	
	ILE	ASN	VAL	V244
	THR	THR	ARG	
	ASP	ALA	HIS	R247
	THR	PRO	ASN	

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	19447	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

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	0.29	0/8619	0.52	3/11737 (0.0%)
2	B	0.34	0/9590	0.55	1/13056 (0.0%)
2	C	0.33	0/10052	0.56	0/13687
3	D	0.33	0/2327	0.55	0/3163
3	E	0.31	0/2327	0.53	0/3163
All	All	0.32	0/32915	0.55	4/44806 (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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ALA	C-N-CD	-8.47	101.96	120.60
1	A	186	ALA	C-N-CA	5.95	146.99	122.00
1	A	78	TYR	C-N-CD	-5.78	107.88	120.60
2	B	274	MET	CG-SD-CE	5.07	108.32	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	328	GLY	Peptide

## 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	184	0
2	B	9397	0	9315	209	0
2	C	9851	0	9762	195	0
3	D	2281	0	2282	53	0
3	E	2281	0	2282	48	0
All	All	32244	0	32040	660	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 (660) 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)
2:B:812:LYS:NZ	2:B:812:LYS:HB3	1.55	1.12
2:B:812:LYS:NZ	2:B:812:LYS:CB	2.12	1.11
2:B:812:LYS:HZ3	2:B:812:LYS:HB3	0.95	1.10
1:A:277:ALA:HB3	1:A:319:MET:HE1	1.54	0.89
2:B:812:LYS:CB	2:B:812:LYS:HZ2	1.86	0.88
2:B:328:GLY:H	2:B:347:ALA:HB3	1.41	0.85
1:A:797:ARG:NH2	1:A:876:MET:O	2.09	0.85
2:B:812:LYS:HZ2	2:B:812:LYS:HB2	1.44	0.82
2:C:363:ARG:NH1	3:E:183:GLU:OE1	2.14	0.81
2:C:1116:ARG:HG2	2:C:1116:ARG:HH11	1.47	0.79
1:A:685:PRO:O	1:A:714:ARG:NH2	2.19	0.76
2:B:376:ILE:HD11	2:B:1317:VAL:HG11	1.69	0.75
1:A:680:THR:HG22	1:A:683:GLN:HG3	1.69	0.75
3:E:77:PHE:HB2	3:E:194:VAL:HG23	1.69	0.75
2:B:484:ARG:NE	2:B:524:GLU:OE2	2.19	0.74
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.69	0.74
2:C:161:LYS:O	2:C:263:ARG:NH2	2.20	0.74
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.20	0.74
2:C:815:LEU:HD11	2:C:1051:GLN:HE22	1.53	0.74
2:B:1208:ASP:OD1	2:B:1243:ARG:NH2	2.20	0.73
2:C:1208:ASP:OD1	2:C:1243:ARG:NH2	2.21	0.73
1:A:752:VAL:HG12	1:A:781:VAL:HG23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HG2	1:A:324:ARG:HE	1.52	0.73
2:C:384:MET:HA	2:C:708:THR:HG21	1.71	0.73
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.21	0.72
2:C:887:VAL:HG22	2:C:893:ALA:HA	1.70	0.72
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.71	0.72
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.23	0.72
2:B:1131:PRO:O	2:B:1162:SER:OG	2.07	0.72
1:A:563:ALA:O	1:A:565:ARG:NH1	2.23	0.72
3:E:283:LEU:HA	3:E:286:THR:HG22	1.72	0.72
2:C:1057:VAL:HG22	2:C:1291:LEU:HD21	1.72	0.71
2:C:841:ASP:OD2	2:C:911:ARG:NH2	2.24	0.71
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.72	0.71
2:C:156:GLN:NE2	2:C:1308:ASN:OD1	2.26	0.69
2:B:469:ARG:NH1	2:B:472:GLU:OE1	2.27	0.68
2:B:921:ASP:OD1	2:B:928:ARG:NH2	2.26	0.68
1:A:408:PRO:HB2	1:A:468:PRO:HG3	1.75	0.68
1:A:680:THR:HG23	1:A:682:SER:H	1.59	0.67
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.27	0.67
1:A:489:SER:OG	1:A:491:ASP:OD1	2.10	0.67
1:A:66:ASP:OD1	1:A:122:ARG:NH2	2.27	0.67
1:A:326:LEU:HB3	1:A:352:THR:HG22	1.74	0.67
2:B:1021:ARG:NE	2:B:1036:ASP:OD1	2.28	0.67
2:B:817:ASP:HA	2:B:983:ILE:HG12	1.77	0.66
3:E:164:ASP:OD2	3:E:167:ARG:NH2	2.28	0.66
2:B:841:ASP:OD1	2:B:911:ARG:NH2	2.27	0.66
2:C:366:MET:HG2	3:E:266:THR:HG21	1.77	0.66
1:A:36:THR:OG1	1:A:37:ASP:N	2.27	0.66
1:A:674:HIS:HB2	1:A:697:ILE:HD12	1.78	0.66
2:B:1254:PRO:HG2	2:B:1257:ALA:HB2	1.77	0.66
1:A:242:LYS:NZ	1:A:246:ASP:OD2	2.26	0.65
3:D:193:VAL:HG11	3:D:230:ILE:HG13	1.79	0.65
1:A:13:VAL:HG23	1:A:213:TRP:CD1	2.31	0.65
2:B:1331:ARG:HH11	2:B:1331:ARG:HB3	1.62	0.64
1:A:427:ASP:HA	1:A:703:PHE:HA	1.80	0.64
3:E:272:ASP:OD2	3:E:274:SER:OG	2.14	0.64
3:D:164:ASP:OD1	3:D:167:ARG:NH2	2.30	0.64
2:B:1085:ASP:OD2	2:B:1243:ARG:NH2	2.31	0.64
2:C:1254:PRO:HG2	2:C:1257:ALA:HB2	1.80	0.64
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.80	0.63
2:C:169:LYS:O	2:C:202:ALA:N	2.31	0.63
2:C:462:LEU:HD13	2:C:680:THR:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:OE1	1:A:810:ARG:NH2	2.31	0.63
3:E:180:ASP:OD1	3:E:247:ARG:NH1	2.32	0.63
2:B:1023:ARG:HG2	2:B:1024:PRO:HD2	1.79	0.62
2:C:313:ASP:OD2	2:C:1253:ARG:NH2	2.31	0.62
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.16	0.62
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.32	0.62
2:B:750:GLU:OE1	2:C:452:ASN:ND2	2.33	0.62
2:B:1228:ARG:HG2	2:B:1231:TYR:CZ	2.35	0.62
2:B:921:ASP:O	2:B:928:ARG:NH1	2.32	0.61
2:B:1048:ASP:HB3	2:B:1051:GLN:HG3	1.80	0.61
2:C:626:ARG:NH2	2:C:712:PHE:O	2.26	0.61
3:D:112:TYR:CE2	3:D:119:ILE:HG21	2.36	0.61
1:A:419:TYR:HE1	1:A:421:LEU:HD23	1.65	0.61
2:C:615:THR:H	2:C:1333:ALA:HA	1.64	0.61
2:C:163:TYR:N	2:C:351:ASP:OD2	2.32	0.61
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.83	0.61
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.81	0.61
2:C:78:ALA:HB2	2:C:1181:SER:HB2	1.81	0.61
2:C:443:VAL:HB	2:C:771:THR:HG23	1.81	0.61
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.26	0.61
1:A:161:TYR:CE2	2:B:1333:ALA:HB1	2.36	0.61
1:A:477:TYR:HA	1:A:482:THR:HG22	1.82	0.61
2:C:704:VAL:O	2:C:708:THR:HG23	2.00	0.61
2:C:709:MET:O	2:C:715:ASN:ND2	2.34	0.61
2:B:1144:ARG:NH1	2:B:1170:ASP:OD1	2.34	0.60
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.18	0.60
2:B:992:VAL:HG12	2:B:992:VAL:O	2.01	0.60
2:B:709:MET:O	2:B:715:ASN:ND2	2.33	0.60
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.34	0.60
2:B:1126:MET:HE1	3:E:146:ARG:HB3	1.83	0.60
2:B:626:ARG:NH2	2:B:712:PHE:O	2.34	0.60
3:D:261:ARG:NH1	3:D:263:ALA:O	2.35	0.60
3:E:148:ASP:OD1	3:E:151:ASP:N	2.32	0.60
1:A:409:MET:HE1	1:A:1036:GLY:HA2	1.83	0.60
1:A:288:LEU:HD22	1:A:368:THR:HG22	1.84	0.59
2:B:384:MET:HA	2:B:708:THR:HG21	1.84	0.59
1:A:129:PRO:HB2	2:B:1332:ASN:HD22	1.67	0.59
1:A:227:MET:HG2	1:A:269:VAL:HG21	1.84	0.59
1:A:957:VAL:HG22	1:A:1056:VAL:HG23	1.85	0.59
2:B:342:THR:OG1	2:B:343:ILE:N	2.36	0.59
1:A:47:ARG:NH1	1:A:80:SER:OG	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:ASP:OD1	1:A:1030:ASN:ND2	2.35	0.59
2:B:640:GLN:OE1	2:B:647:GLU:N	2.33	0.58
1:A:114:ASN:ND2	1:A:117:LEU:HB2	2.17	0.58
1:A:848:GLN:OE1	1:A:1054:LYS:NZ	2.35	0.58
2:B:335:ASP:OD1	2:B:340:VAL:N	2.33	0.58
2:B:891:HIS:CG	3:D:240:VAL:HG21	2.38	0.58
1:A:234:LYS:NZ	1:A:237:GLU:OE2	2.37	0.58
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.86	0.58
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.86	0.57
2:B:226:PRO:HB2	2:B:250:GLY:HA3	1.85	0.57
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	1.86	0.57
1:A:129:PRO:HG2	2:B:1332:ASN:HB2	1.85	0.57
2:B:537:LEU:HD13	2:B:548:TYR:HE1	1.69	0.57
1:A:292:ARG:NH1	1:A:777:ASP:OD1	2.35	0.57
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.86	0.57
2:B:528:ILE:HG13	2:B:532:ILE:HD12	1.85	0.57
2:C:1119:TYR:HH	2:C:1121:HIS:HD1	1.51	0.57
2:C:207:ASP:OD1	2:C:207:ASP:N	2.37	0.57
2:C:533:GLN:HG3	2:C:588:LEU:HD12	1.85	0.57
2:C:741:TYR:OH	2:C:1026:GLY:O	2.21	0.57
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.87	0.57
2:B:704:VAL:O	2:B:708:THR:HG23	2.05	0.57
2:C:171:GLU:OE2	2:C:1181:SER:OG	2.23	0.57
2:C:550:ILE:HD13	2:C:596:GLY:HA3	1.87	0.57
2:C:244:SER:HA	2:C:1201:LEU:HD22	1.85	0.56
1:A:651:ASN:HA	1:A:689:GLU:HG3	1.88	0.56
2:C:104:ILE:HG12	2:C:1311:THR:HG23	1.88	0.56
2:B:1032:ASP:HB3	2:B:1035:ILE:HG23	1.87	0.56
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.69	0.56
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.87	0.56
1:A:687:SER:OG	1:A:689:GLU:OE1	2.21	0.56
1:A:163:ASP:OD1	1:A:182:ARG:NE	2.32	0.56
1:A:257:ILE:HG21	1:A:326:LEU:HD11	1.87	0.56
2:B:606:LEU:HD13	2:B:655:ILE:HG23	1.88	0.56
1:A:565:ARG:NH2	1:A:616:ASP:OD2	2.37	0.56
2:C:838:GLU:OE1	2:C:933:ASN:ND2	2.39	0.56
2:C:931:ASN:HB3	2:C:934:LEU:HD23	1.87	0.56
3:E:45:VAL:HA	3:E:171:VAL:HG12	1.87	0.56
2:B:147:VAL:HG22	2:B:379:LEU:HD11	1.88	0.55
1:A:36:THR:OG1	1:A:37:ASP:OD1	2.24	0.55
1:A:541:LYS:HD3	1:A:550:TYR:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:THR:HG21	2:B:710:SER:HB3	1.87	0.55
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.89	0.55
1:A:714:ARG:NH1	1:A:1044:ASP:OD1	2.40	0.55
2:B:1171:ILE:HD11	2:B:1193:ILE:HG23	1.88	0.55
2:B:474:ASP:OD2	2:B:476:SER:OG	2.24	0.55
2:C:469:ARG:NE	2:C:513:GLU:OE1	2.39	0.55
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.88	0.55
2:B:873:TYR:HB3	2:B:898:GLN:HB2	1.88	0.55
2:C:1048:ASP:HB3	2:C:1051:GLN:HG3	1.88	0.55
2:B:1127:ALA:O	3:E:146:ARG:NH2	2.39	0.55
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.89	0.55
2:C:180:LEU:HD12	2:C:181:ARG:H	1.72	0.54
2:B:1109:SER:HB2	3:E:262:THR:HG21	1.88	0.54
2:C:1128:TYR:CZ	2:C:1135:PRO:HD3	2.42	0.54
2:C:203:VAL:HG12	2:C:1243:ARG:HG3	1.89	0.54
2:C:230:ASP:HA	2:C:233:VAL:HG11	1.89	0.54
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.40	0.54
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.88	0.54
1:A:78:TYR:CE2	1:A:83:ILE:HA	2.42	0.54
2:B:1273:ASN:ND2	2:B:1275:ASP:OD1	2.35	0.54
1:A:664:ARG:HD2	1:A:667:GLN:HE21	1.72	0.54
1:A:928:GLU:HG2	1:A:934:THR:HG22	1.89	0.54
2:B:1226:ASP:OD1	2:C:122:ASN:ND2	2.35	0.54
2:C:451:GLU:OE2	2:C:452:ASN:ND2	2.41	0.54
3:D:186:LEU:HD22	3:D:233:THR:HG21	1.89	0.54
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.89	0.54
3:E:239:VAL:HG12	3:E:250:ARG:HD2	1.90	0.54
1:A:882:ASP:OD2	1:A:885:THR:OG1	2.24	0.54
2:B:748:GLN:HA	2:C:682:GLN:HE22	1.73	0.54
2:C:504:ASP:OD2	2:C:506:SER:OG	2.26	0.53
3:D:60:ARG:NH2	3:D:87:HIS:O	2.41	0.53
2:C:505:PRO:HG2	2:C:677:ARG:HB2	1.89	0.53
2:B:892:VAL:HG12	2:B:894:VAL:HB	1.91	0.53
2:C:640:GLN:HB2	2:C:646:ASN:HD22	1.71	0.53
1:A:572:LEU:HB3	1:A:584:ILE:HD13	1.89	0.53
2:C:611:GLY:HA3	2:C:635:ILE:O	2.08	0.53
1:A:170:ASN:OD1	1:A:172:PHE:N	2.42	0.53
1:A:44:SER:O	1:A:45:GLN:HB2	2.09	0.53
2:B:674:LYS:HA	2:B:677:ARG:HD3	1.90	0.53
2:C:252:LEU:HD22	2:C:823:ILE:HD13	1.90	0.53
2:B:891:HIS:HA	3:D:242:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:244:VAL:HG13	3:D:247:ARG:HB2	1.90	0.53
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.91	0.53
3:E:176:ARG:HG3	3:E:253:GLU:HB3	1.90	0.53
1:A:943:ILE:HA	1:A:946:VAL:HG12	1.90	0.53
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.90	0.52
1:A:541:LYS:HG2	1:A:975:THR:HG21	1.90	0.52
2:B:217:THR:HB	2:B:219:ILE:HG13	1.91	0.52
2:B:486:VAL:HG21	2:B:709:MET:HB3	1.91	0.52
2:C:865:ILE:HG12	2:C:1041:ARG:HG2	1.91	0.52
1:A:161:TYR:CD2	2:B:1333:ALA:HB1	2.45	0.52
2:B:261:ASP:OD1	2:B:263:ARG:NE	2.41	0.52
2:B:813:LEU:HD11	2:B:1008:LEU:HD13	1.91	0.52
3:E:66:VAL:HG11	3:E:92:ARG:HG3	1.91	0.52
1:A:486:THR:HB	1:A:489:SER:HB3	1.92	0.52
2:C:439:VAL:HG11	2:C:705:VAL:HG21	1.92	0.52
3:D:229:PHE:CE1	3:D:252:LEU:HD11	2.44	0.52
2:C:707:ALA:HB2	2:C:1330:ILE:HG23	1.92	0.52
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.45	0.52
2:B:328:GLY:HA3	2:B:347:ALA:H	1.74	0.52
2:C:495:LEU:HD13	2:C:532:ILE:HG13	1.92	0.52
2:C:156:GLN:HE22	2:C:1309:ILE:H	1.58	0.52
1:A:775:ASP:OD1	1:A:776:SER:N	2.42	0.51
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.91	0.51
1:A:267:THR:OG1	1:A:320:TYR:OH	2.26	0.51
1:A:379:VAL:HG21	1:A:794:LEU:HD13	1.90	0.51
2:C:828:ASP:OD2	2:C:862:ARG:NH2	2.44	0.51
2:C:633:THR:HG21	2:C:710:SER:CB	2.40	0.51
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	1.92	0.51
2:C:1116:ARG:NH1	2:C:1116:ARG:HG2	2.23	0.51
3:D:112:TYR:CZ	3:D:119:ILE:HD13	2.45	0.51
2:B:1134:ARG:NH1	2:B:1158:SER:OG	2.40	0.51
2:B:299:ALA:HB2	2:B:1265:MET:HB3	1.92	0.51
2:C:676:THR:O	2:C:680:THR:HG23	2.11	0.51
3:D:233:THR:HB	3:D:268:THR:HG21	1.93	0.51
1:A:831:ARG:NH1	1:A:832:GLU:OE2	2.44	0.51
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.44	0.50
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	2.26	0.50
2:B:1288:ILE:HG12	3:D:20:ARG:NH2	2.26	0.50
2:B:550:ILE:HG22	2:B:594:LEU:HD21	1.93	0.50
1:A:704:PRO:HG2	1:A:705:PHE:CD2	2.46	0.50
1:A:860:SER:HA	1:A:920:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:VAL:HB	2:C:1242:MET:HB2	1.94	0.50
1:A:887:ILE:HG13	1:A:899:VAL:HG21	1.93	0.50
2:B:1087:ASP:OD2	2:B:1237:SER:OG	2.28	0.50
2:B:357:VAL:HG13	2:B:1054:ARG:HG2	1.92	0.50
2:B:513:GLU:OE2	2:B:760:THR:OG1	2.23	0.50
1:A:539:LEU:HG	1:A:647:LEU:HD12	1.93	0.50
2:B:766:ILE:O	2:B:772:TYR:OH	2.25	0.50
2:B:874:ILE:HD11	2:B:917:VAL:HG13	1.93	0.50
2:C:382:HIS:HE2	2:C:713:MET:H	1.60	0.50
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.94	0.50
2:B:1243:ARG:HD3	2:B:1256:GLY:O	2.12	0.50
3:D:19:ILE:O	3:D:19:ILE:HD12	2.12	0.50
1:A:18:LYS:HA	1:A:112:ARG:HA	1.94	0.50
2:C:748:GLN:HG3	2:C:1000:LEU:HD22	1.92	0.50
2:C:828:ASP:N	2:C:828:ASP:OD1	2.45	0.50
1:A:42:PHE:CE1	1:A:47:ARG:HA	2.47	0.49
1:A:371:GLY:N	1:A:818:PHE:O	2.42	0.49
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	1.93	0.49
3:D:176:ARG:HD3	3:D:253:GLU:HB3	1.94	0.49
3:E:1:MET:HB2	3:E:121:PHE:CE2	2.48	0.49
3:E:221:ARG:O	3:E:225:ARG:HG3	2.11	0.49
3:E:177:ALA:HB3	3:E:252:LEU:HG	1.93	0.49
2:B:990:THR:O	2:B:992:VAL:HG23	2.12	0.49
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	1.94	0.49
2:C:522:PRO:HB3	2:C:609:PRO:HB3	1.93	0.49
1:A:391:ILE:HD11	1:A:757:LEU:HD22	1.95	0.49
1:A:939:GLN:HB2	1:A:998:LEU:HD21	1.95	0.49
2:B:1033:ASP:O	2:B:1034:GLN:HB2	2.12	0.49
1:A:275:ILE:HA	1:A:278:LEU:HD12	1.95	0.49
1:A:557:SER:N	1:A:611:ASP:OD1	2.29	0.49
2:B:704:VAL:HG12	2:B:1330:ILE:HD11	1.93	0.49
2:C:1042:TRP:HD1	2:C:1044:ARG:HG2	1.77	0.49
2:C:865:ILE:HD12	2:C:1042:TRP:HE3	1.77	0.49
2:C:633:THR:HG21	2:C:710:SER:HB2	1.94	0.49
3:D:148:ASP:OD2	3:D:151:ASP:N	2.41	0.49
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.94	0.49
3:E:159:GLU:O	3:E:225:ARG:HG2	2.13	0.49
1:A:1006:MET:HA	1:A:1009:ASP:OD2	2.13	0.49
2:C:225:ILE:HB	2:C:247:TYR:HD1	1.78	0.49
2:C:354:ALA:O	2:C:358:LEU:HG	2.12	0.49
3:E:233:THR:HG22	3:E:252:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1230:ILE:HG12	2:C:119:ASP:HA	1.95	0.49
2:C:164:LEU:HD23	2:C:208:LEU:HA	1.95	0.49
2:B:1150:LEU:HD23	2:C:141:LEU:HD22	1.95	0.49
2:C:503:GLU:O	2:C:666:ARG:NH2	2.39	0.48
1:A:163:ASP:HB3	1:A:180:ASN:ND2	2.28	0.48
1:A:910:ASN:OD1	1:A:910:ASN:N	2.39	0.48
2:B:1214:GLU:HG2	2:B:1215:PRO:HD2	1.95	0.48
2:B:558:TYR:HB3	2:B:568:PHE:CD2	2.47	0.48
3:D:57:PRO:HD3	3:D:139:ASN:ND2	2.28	0.48
2:C:85:ASP:HB2	2:C:161:LYS:HE2	1.96	0.48
2:C:248:VAL:HG11	2:C:971:MET:HG2	1.95	0.48
2:C:525:PHE:CE1	2:C:532:ILE:HD13	2.48	0.48
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.69	0.48
2:C:862:ARG:O	2:C:865:ILE:HG22	2.13	0.48
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.95	0.48
2:B:1189:ASP:HA	2:C:118:THR:HG22	1.96	0.48
2:B:330:THR:OG1	2:B:331:GLU:N	2.47	0.48
2:C:168:VAL:HG11	2:C:196:LEU:HG	1.94	0.48
2:B:419:TYR:HB3	2:B:1005:LEU:HD22	1.95	0.48
1:A:717:THR:HB	1:A:1020:SER:HB2	1.96	0.48
2:C:94:PHE:HB3	2:C:105:MET:HG2	1.95	0.48
2:C:286:LEU:HD11	2:C:290:TYR:HB3	1.96	0.48
2:C:616:ASP:O	2:C:620:ILE:HG13	2.13	0.48
1:A:2:TRP:HD1	1:A:3:HIS:H	1.57	0.48
2:B:1266:ASP:OD1	2:B:1279:SER:OG	2.27	0.48
2:C:1090:PRO:HD3	2:C:1231:TYR:CD2	2.49	0.48
2:C:526:ASN:OD1	2:C:529:LYS:NZ	2.42	0.48
2:B:213:PHE:HB3	2:B:219:ILE:HD12	1.96	0.48
2:B:634:TYR:CE1	2:B:722:GLY:HA3	2.49	0.48
2:B:995:THR:O	2:B:998:GLY:N	2.45	0.48
2:C:422:LEU:HD13	2:C:810:LEU:HD11	1.96	0.48
3:D:26:ALA:HB1	3:D:30:GLN:HG3	1.96	0.48
1:A:377:LEU:HB3	1:A:763:LYS:HB3	1.96	0.48
2:C:704:VAL:HB	2:C:1330:ILE:HD11	1.96	0.48
1:A:43:ASN:HD21	1:A:46:ARG:HD2	1.77	0.47
1:A:724:MET:HG3	1:A:725:PRO:HD2	1.95	0.47
1:A:726:ILE:HG13	1:A:1029:SER:HB2	1.96	0.47
2:B:1159:VAL:HA	2:B:1164:TRP:HB2	1.97	0.47
2:C:1060:ARG:HD3	2:C:1291:LEU:O	2.14	0.47
2:C:626:ARG:HG2	2:C:631:PRO:HB3	1.96	0.47
1:A:426:ARG:HG3	1:A:707:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:THR:HG23	1:A:980:ILE:HG12	1.97	0.47
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.48	0.47
1:A:43:ASN:ND2	1:A:46:ARG:HD2	2.29	0.47
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.96	0.47
1:A:39:LEU:HD11	1:A:52:ARG:HH11	1.79	0.47
2:C:998:GLY:HA3	2:C:1012:LEU:HD21	1.97	0.47
2:C:1073:GLY:HA2	2:C:1168:ILE:O	2.13	0.47
2:C:380:GLN:HB3	2:C:618:LEU:HD22	1.97	0.47
2:C:750:GLU:OE1	2:C:1003:ARG:NH1	2.46	0.47
3:E:229:PHE:O	3:E:233:THR:HG23	2.15	0.47
1:A:275:ILE:HD11	1:A:300:LEU:HD22	1.97	0.47
1:A:531:LYS:HD3	1:A:683:GLN:HG2	1.97	0.47
2:B:992:VAL:O	2:B:993:ASP:HB2	2.15	0.47
2:C:119:ASP:OD1	2:C:119:ASP:N	2.47	0.47
2:C:197:PHE:HB2	2:C:301:LEU:HD21	1.96	0.47
1:A:6:SER:HB2	1:A:251:VAL:O	2.15	0.47
2:B:313:ASP:OD2	2:B:1253:ARG:NH1	2.48	0.47
2:B:886:SER:O	2:B:890:THR:HG23	2.14	0.47
3:D:78:GLY:O	3:D:275:ARG:NH2	2.47	0.47
1:A:488:GLY:HA2	1:A:551:LEU:HD13	1.97	0.47
2:B:1268:GLY:HA3	2:B:1277:LEU:O	2.14	0.47
2:C:629:ARG:HA	2:C:1037:ILE:HG22	1.96	0.47
1:A:289:ASP:OD1	1:A:368:THR:OG1	2.30	0.47
2:B:270:THR:HG22	2:B:291:HIS:HA	1.97	0.47
2:B:512:LEU:HD13	2:B:659:LEU:HD12	1.97	0.47
2:B:522:PRO:HB3	2:B:609:PRO:HB3	1.96	0.47
2:B:612:PHE:CD1	2:B:638:THR:HG22	2.49	0.47
2:C:833:ARG:HG3	2:C:922:TYR:CZ	2.49	0.47
2:C:713:MET:HB2	2:C:713:MET:HE2	1.75	0.47
3:D:93:LEU:HD12	3:D:93:LEU:HA	1.74	0.47
2:B:153:ASP:OD1	2:B:153:ASP:N	2.43	0.46
2:B:720:PHE:CE2	2:B:722:GLY:HA2	2.50	0.46
3:D:17:PHE:HB3	3:D:196:TRP:CE2	2.50	0.46
1:A:302:ASP:O	1:A:306:GLN:HB2	2.16	0.46
1:A:812:VAL:HA	1:A:813:PRO:HA	1.70	0.46
2:B:141:LEU:HD22	2:B:391:GLY:HA3	1.97	0.46
2:B:287:ARG:NH2	2:B:326:GLY:HA3	2.30	0.46
2:C:856:LEU:HD23	2:C:860:ARG:HD3	1.98	0.46
3:D:45:VAL:HG13	3:D:171:VAL:HG12	1.98	0.46
2:B:1180:PRO:HA	2:B:1207:MET:SD	2.55	0.46
2:C:1180:PRO:HD3	2:C:1208:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:281:LYS:O	3:D:285:LEU:HG	2.15	0.46
2:B:347:ALA:HA	2:B:1301:VAL:HA	1.97	0.46
2:B:832:MET:SD	2:B:946:LEU:HG	2.55	0.46
2:C:495:LEU:HD23	2:C:497:LYS:HA	1.98	0.46
2:C:524:GLU:OE1	2:C:758:ILE:HG12	2.15	0.46
1:A:78:TYR:HB3	1:A:79:PRO:HA	1.98	0.46
2:C:332:THR:HG22	2:C:334:LEU:H	1.81	0.46
2:C:362:LEU:HD22	2:C:1303:SER:HB3	1.98	0.46
2:B:446:LYS:HB3	2:B:448:TYR:HD2	1.80	0.46
2:B:833:ARG:HG3	2:B:922:TYR:CZ	2.50	0.46
3:D:35:LEU:HA	3:D:35:LEU:HD12	1.78	0.46
2:B:1106:PHE:CE2	2:B:1119:TYR:HB2	2.51	0.46
2:B:1176:GLU:HB2	2:B:1203:HIS:HE2	1.81	0.46
2:B:873:TYR:HA	2:B:896:LEU:O	2.16	0.46
2:B:949:ALA:HB1	2:B:960:THR:HG22	1.98	0.46
2:C:1031:TYR:CE2	2:C:1041:ARG:HG3	2.51	0.46
2:B:854:GLN:NE2	2:C:647:GLU:OE1	2.48	0.46
1:A:438:LYS:NZ	1:A:626:GLU:OE2	2.47	0.45
2:B:196:LEU:HD22	2:B:296:VAL:HG11	1.98	0.45
2:B:525:PHE:CE1	2:B:532:ILE:HD13	2.51	0.45
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.97	0.45
1:A:129:PRO:CG	2:B:1332:ASN:HB2	2.46	0.45
2:B:489:MET:SD	2:B:527:ARG:HD2	2.56	0.45
2:B:515:ILE:HD12	2:B:659:LEU:HD11	1.97	0.45
2:C:615:THR:HB	2:C:1333:ALA:HB1	1.97	0.45
3:D:29:THR:HG22	3:D:222:ASP:HB2	1.98	0.45
3:E:137:LEU:HD23	3:E:281:LYS:HG3	1.98	0.45
2:B:1075:ARG:HB2	2:B:1233:LEU:HD11	1.98	0.45
2:B:510:VAL:O	2:B:513:GLU:HB3	2.16	0.45
2:B:384:MET:HA	2:B:708:THR:CG2	2.45	0.45
2:C:979:ILE:HD13	2:C:1013:LYS:HB2	1.98	0.45
3:D:53:GLU:CD	3:D:53:GLU:H	2.20	0.45
3:E:62:VAL:HB	3:E:92:ARG:HD3	1.99	0.45
1:A:201:LYS:O	2:B:629:ARG:HG2	2.16	0.45
1:A:613:ILE:HG21	1:A:639:CYS:HB3	1.98	0.45
2:B:309:TRP:CZ2	2:B:1257:ALA:HB1	2.50	0.45
3:E:146:ARG:NH1	3:E:277:GLU:OE2	2.49	0.45
1:A:1020:SER:OG	1:A:1022:PRO:HD2	2.15	0.45
1:A:735:LYS:O	1:A:765:TYR:OH	2.24	0.45
2:B:609:PRO:HD3	2:B:724:HIS:CD2	2.52	0.45
1:A:428:ILE:HG23	1:A:430:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ALA:HB2	1:A:725:PRO:HB3	1.99	0.45
2:B:1176:GLU:HB2	2:B:1203:HIS:NE2	2.32	0.45
2:C:311:ASN:O	2:C:315:THR:HB	2.16	0.45
1:A:474:TYR:HD1	1:A:499:VAL:HG22	1.81	0.45
1:A:722:ASP:N	1:A:722:ASP:OD1	2.44	0.45
2:B:287:ARG:HB2	2:B:329:LEU:O	2.16	0.45
2:C:405:HIS:ND1	2:C:625:PRO:HA	2.31	0.45
2:B:423:GLU:O	2:B:427:VAL:HG23	2.16	0.45
2:B:777:GLN:O	2:B:786:SER:N	2.49	0.45
2:C:1110:LEU:HA	2:C:1110:LEU:HD23	1.76	0.45
1:A:268:TYR:O	1:A:271:ARG:HG2	2.17	0.45
2:B:370:VAL:HG21	2:B:402:ALA:HB2	1.98	0.45
2:B:449:PHE:CE1	2:B:463:VAL:HG22	2.51	0.45
2:C:585:PHE:CE1	2:C:728:LYS:HE2	2.52	0.45
2:C:775:VAL:HA	2:C:776:ARG:HA	1.72	0.45
1:A:1007:LEU:HA	1:A:1007:LEU:HD12	1.86	0.45
1:A:280:PRO:HB3	1:A:304:TYR:CE2	2.52	0.45
1:A:42:PHE:HE1	1:A:47:ARG:HA	1.82	0.45
2:B:813:LEU:HG	2:B:1010:ARG:HH11	1.82	0.45
2:B:502:PHE:CE1	2:B:539:PHE:HB2	2.52	0.45
2:B:619:ALA:HB2	2:B:711:ASN:HA	1.98	0.45
2:C:264:LEU:HD21	2:C:362:LEU:HA	1.99	0.45
1:A:1007:LEU:HD21	1:A:1053:ILE:HG21	1.99	0.44
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.52	0.44
1:A:25:ILE:HD12	1:A:25:ILE:HA	1.82	0.44
1:A:857:GLN:HB3	1:A:877:LYS:HG3	1.98	0.44
2:C:999:LYS:HG2	2:C:1009:THR:HA	1.99	0.44
1:A:315:LEU:O	1:A:319:MET:HG3	2.17	0.44
2:C:1249:ASN:HB3	2:C:1250:GLU:H	1.65	0.44
2:C:332:THR:HG23	2:C:1270:LEU:HD12	2.00	0.44
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.49	0.44
2:C:605:ARG:O	2:C:608:THR:HG23	2.18	0.44
2:C:186:ASP:O	2:C:190:VAL:HB	2.17	0.44
2:C:962:ASP:OD1	2:C:962:ASP:N	2.48	0.44
1:A:7:ILE:HD11	1:A:250:LEU:HD21	1.98	0.44
1:A:417:TYR:CD2	1:A:490:LEU:HD22	2.52	0.44
2:B:347:ALA:HB2	2:B:1301:VAL:HG22	1.98	0.44
2:C:1085:ASP:HA	2:C:1086:PRO:HD3	1.88	0.44
1:A:491:ASP:HA	1:A:494:THR:HG22	1.99	0.44
1:A:50:THR:HA	1:A:170:ASN:ND2	2.33	0.44
2:B:933:ASN:HB3	2:B:935:GLN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.16	0.44
1:A:154:PHE:CD2	1:A:185:HIS:HA	2.52	0.44
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.49	0.44
1:A:470:LEU:HD21	1:A:530:MET:HE2	2.00	0.44
1:A:485:MET:HB2	1:A:491:ASP:OD1	2.18	0.44
1:A:43:ASN:HB3	1:A:48:SER:OG	2.16	0.44
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.52	0.44
2:B:649:ALA:HB1	2:B:692:ASP:OD1	2.17	0.44
2:C:1201:LEU:HD12	2:C:1201:LEU:HA	1.80	0.44
3:E:68:ILE:HA	3:E:68:ILE:HD12	1.89	0.44
1:A:196:LEU:HD13	1:A:349:TYR:CE1	2.52	0.44
2:B:186:ASP:O	2:B:190:VAL:HB	2.17	0.44
1:A:680:THR:HG23	1:A:682:SER:N	2.30	0.44
1:A:400:VAL:HG22	1:A:774:VAL:HG21	1.99	0.44
2:B:169:LYS:O	2:B:202:ALA:N	2.47	0.44
2:B:685:ARG:O	2:B:689:THR:HG23	2.18	0.44
2:B:953:ASP:OD1	2:B:960:THR:OG1	2.34	0.44
2:C:1236:ILE:HD13	2:C:1236:ILE:HA	1.85	0.44
2:C:478:ILE:HG13	2:C:762:ILE:HD11	1.98	0.44
3:E:104:ARG:NH2	3:E:115:GLU:OE2	2.50	0.44
3:E:53:GLU:H	3:E:53:GLU:CD	2.21	0.44
1:A:11:THR:OG1	1:A:254:ASP:OD2	2.36	0.44
1:A:328:MET:HB2	1:A:328:MET:HE2	1.81	0.44
1:A:913:LEU:HD22	1:A:919:TYR:CZ	2.53	0.44
3:E:258:ASN:ND2	3:E:260:MET:SD	2.90	0.44
1:A:154:PHE:HZ	1:A:183:ILE:HB	1.82	0.43
1:A:467:SER:N	1:A:468:PRO:HD2	2.33	0.43
1:A:823:THR:OG1	1:A:825:GLU:OE1	2.36	0.43
3:E:283:LEU:O	3:E:287:PHE:HB2	2.17	0.43
1:A:615:CYS:HB2	1:A:639:CYS:SG	2.58	0.43
2:B:171:GLU:OE2	2:B:174:PHE:N	2.51	0.43
2:C:502:PHE:O	2:C:542:ARG:HG2	2.18	0.43
1:A:844:LEU:HD11	1:A:1017:ILE:HD12	2.00	0.43
2:B:893:ALA:HB1	2:B:915:VAL:HA	2.00	0.43
2:B:826:GLY:HA3	2:B:949:ALA:HB2	2.00	0.43
2:C:1015:GLN:HG2	2:C:1015:GLN:H	1.44	0.43
2:C:1121:HIS:CD2	2:C:1123:PRO:HG2	2.53	0.43
2:C:152:ASP:N	2:C:152:ASP:OD1	2.50	0.43
2:C:439:VAL:HG23	2:C:440:ILE:HG22	2.01	0.43
2:C:865:ILE:CG1	2:C:1041:ARG:HG2	2.49	0.43
1:A:1043:LEU:O	1:A:1047:ASN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.70	0.43
3:D:60:ARG:O	3:D:62:VAL:HG23	2.18	0.43
1:A:532:MET:HG3	1:A:565:ARG:HD2	2.01	0.43
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.99	0.43
3:D:178:LYS:HA	3:D:250:ARG:O	2.19	0.43
3:D:253:GLU:HA	3:D:254:TYR:HA	1.58	0.43
3:D:283:LEU:HA	3:D:286:THR:HG22	2.00	0.43
1:A:485:MET:HG2	1:A:511:ILE:HD11	1.99	0.43
2:B:1059:LEU:HD23	2:B:1059:LEU:HA	1.81	0.43
2:B:617:ASP:OD1	2:B:618:LEU:N	2.51	0.43
2:C:865:ILE:HD12	2:C:1042:TRP:CE3	2.52	0.43
1:A:734:ILE:HD13	1:A:762:LEU:HD13	2.00	0.43
1:A:882:ASP:N	1:A:882:ASP:OD1	2.52	0.43
1:A:95:TRP:O	1:A:98:SER:HB3	2.18	0.43
2:B:409:ILE:HD13	2:B:625:PRO:HB2	2.01	0.43
2:C:265:VAL:HB	2:C:1304:MET:HB3	2.00	0.43
2:C:340:VAL:HG23	2:C:341:LYS:HG2	2.00	0.43
2:C:685:ARG:O	2:C:689:THR:HG23	2.18	0.43
2:C:811:SER:O	2:C:815:LEU:HB2	2.19	0.43
1:A:199:MET:HG3	1:A:205:VAL:HG21	2.00	0.43
1:A:312:LEU:HD11	1:A:361:SER:HB3	2.00	0.43
1:A:767:SER:N	1:A:788:ASP:OD1	2.52	0.43
2:C:1116:ARG:HH22	2:C:1131:PRO:HD2	1.84	0.43
2:C:736:SER:HB2	2:C:738:GLU:OE1	2.19	0.43
3:E:176:ARG:NH1	3:E:253:GLU:OE2	2.45	0.43
1:A:289:ASP:H	1:A:368:THR:HG23	1.84	0.43
1:A:34:LEU:HG	1:A:38:TYR:CZ	2.54	0.43
1:A:377:LEU:HD22	1:A:768:GLU:HA	2.01	0.43
2:B:1148:SER:HB3	2:B:1151:VAL:HG23	2.01	0.43
2:C:442:PRO:HD2	2:C:475:ILE:HG23	2.00	0.43
3:D:68:ILE:HG12	3:D:93:LEU:HD13	2.00	0.43
1:A:261:ILE:HD11	1:A:326:LEU:HD13	2.01	0.42
1:A:586:GLY:HA3	1:A:595:ASN:OD1	2.19	0.42
2:B:286:LEU:HD11	2:B:290:TYR:CD1	2.54	0.42
2:B:484:ARG:HE	2:B:524:GLU:CD	2.13	0.42
2:B:892:VAL:HG13	2:B:951:ILE:HG22	2.01	0.42
2:B:145:THR:HB	2:B:1317:VAL:HG23	2.00	0.42
2:C:1085:ASP:HA	2:C:1243:ARG:HH22	1.85	0.42
2:C:154:PHE:HB3	2:C:264:LEU:HB2	2.02	0.42
2:C:504:ASP:OD1	2:C:504:ASP:N	2.48	0.42
3:E:261:ARG:NH1	3:E:263:ALA:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LYS:HE2	1:A:690:THR:HG22	2.01	0.42
2:B:439:VAL:HG11	2:B:702:LEU:HD13	2.01	0.42
2:B:484:ARG:O	2:B:527:ARG:NH2	2.53	0.42
2:C:391:GLY:HA3	2:C:392:PRO:HD3	1.84	0.42
2:C:1180:PRO:HA	2:C:1207:MET:SD	2.59	0.42
2:C:334:LEU:HA	2:C:334:LEU:HD23	1.77	0.42
3:D:283:LEU:O	3:D:287:PHE:HB2	2.20	0.42
3:D:77:PHE:HB2	3:D:194:VAL:HG23	2.02	0.42
1:A:556:THR:HB	1:A:611:ASP:OD2	2.20	0.42
2:B:171:GLU:HG2	2:B:1181:SER:OG	2.19	0.42
2:B:1242:MET:HG2	2:B:1260:PRO:HD3	2.01	0.42
2:B:515:ILE:HG21	2:B:655:ILE:HG21	2.02	0.42
2:C:1066:ARG:HD2	2:C:1296:ILE:HG13	2.02	0.42
2:C:1267:THR:HB	2:C:1299:SER:HB3	2.01	0.42
3:D:189:LEU:HA	3:D:189:LEU:HD12	1.77	0.42
1:A:628:MET:O	1:A:632:THR:HG22	2.20	0.42
2:B:814:THR:HA	2:B:1010:ARG:HH12	1.84	0.42
2:B:859:ILE:HG13	2:B:859:ILE:H	1.68	0.42
1:A:565:ARG:HA	1:A:565:ARG:HD3	1.73	0.42
2:B:732:TYR:CE1	2:B:1021:ARG:HG3	2.55	0.42
2:B:1043:SER:HB2	2:B:1046:PHE:CE2	2.55	0.42
2:B:1128:TYR:HB3	2:B:1134:ARG:HG2	2.01	0.42
2:B:331:GLU:O	2:B:344:VAL:HA	2.20	0.42
2:B:838:GLU:C	2:B:935:GLN:HG2	2.40	0.42
2:B:954:GLN:NE2	3:D:240:VAL:HG12	2.34	0.42
2:C:1190:ALA:O	2:C:1193:ILE:HG22	2.20	0.42
1:A:251:VAL:HG12	1:A:253:ALA:H	1.84	0.42
1:A:373:ILE:HG12	1:A:817:GLY:N	2.35	0.42
1:A:595:ASN:HD22	1:A:595:ASN:H	1.66	0.42
1:A:936:ALA:HB1	1:A:998:LEU:HD23	2.02	0.42
2:B:664:ASN:O	2:B:668:VAL:HG13	2.20	0.42
2:B:887:VAL:O	2:B:891:HIS:N	2.51	0.42
2:B:924:ASP:O	2:B:927:SER:OG	2.33	0.42
3:D:188:SER:O	3:D:191:ARG:HG3	2.19	0.42
3:E:118:ASN:ND2	3:E:118:ASN:H	2.17	0.42
1:A:259:ARG:NH1	1:A:277:ALA:HB2	2.35	0.42
2:B:382:HIS:HD1	2:B:799:THR:HG23	1.84	0.42
2:B:491:ASN:ND2	2:B:750:GLU:O	2.53	0.42
2:C:385:ILE:HA	2:C:385:ILE:HD13	1.75	0.42
2:B:1129:PRO:HD3	3:E:273:LEU:HD23	2.01	0.41
2:B:533:GLN:HB2	2:B:588:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:379:LEU:HA	2:C:379:LEU:HD23	1.86	0.41
2:B:336:TYR:HA	3:D:64:GLY:HA3	2.01	0.41
1:A:20:ASN:N	1:A:20:ASN:OD1	2.53	0.41
1:A:834:THR:O	1:A:838:LYS:HG2	2.20	0.41
2:B:1305:MET:H	2:B:1305:MET:HG2	1.65	0.41
2:C:609:PRO:HB2	2:C:634:TYR:CE2	2.55	0.41
2:C:612:PHE:HZ	2:C:1330:ILE:HG22	1.84	0.41
2:C:405:HIS:CE1	2:C:625:PRO:HA	2.55	0.41
2:C:828:ASP:OD1	2:C:960:THR:OG1	2.32	0.41
3:D:160:LEU:HB3	3:D:161:ALA:H	1.77	0.41
3:D:1:MET:HB2	3:D:121:PHE:CZ	2.55	0.41
3:D:87:HIS:CE1	3:D:89:TYR:H	2.38	0.41
1:A:384:GLU:HA	1:A:802:THR:HG22	2.01	0.41
1:A:595:ASN:HD22	1:A:595:ASN:N	2.18	0.41
1:A:538:ALA:HB1	1:A:678:LEU:HD11	2.02	0.41
2:B:1224:GLY:HA2	2:C:124:GLN:HG2	2.02	0.41
2:B:147:VAL:HG13	2:B:379:LEU:HD21	2.01	0.41
2:B:233:VAL:HA	2:B:234:PRO:HD2	1.80	0.41
2:B:814:THR:HA	2:B:1010:ARG:NH1	2.36	0.41
2:C:451:GLU:O	2:C:452:ASN:HB2	2.20	0.41
2:C:256:PHE:CE2	2:C:815:LEU:HD22	2.55	0.41
2:C:823:ILE:O	2:C:968:ARG:HD3	2.20	0.41
3:E:182:TRP:CE3	3:E:182:TRP:N	2.88	0.41
3:E:224:PHE:O	3:E:228:LEU:HG	2.20	0.41
1:A:178:PRO:HB2	1:A:179:TYR:CD1	2.55	0.41
1:A:335:LEU:HA	1:A:335:LEU:HD23	1.90	0.41
2:B:208:LEU:HD22	2:B:213:PHE:CE2	2.55	0.41
2:B:376:ILE:HD13	2:B:379:LEU:HD12	2.01	0.41
2:B:537:LEU:HA	2:B:537:LEU:HD22	1.93	0.41
2:C:264:LEU:HA	2:C:264:LEU:HD22	1.87	0.41
2:C:659:LEU:O	2:C:663:VAL:HG23	2.20	0.41
1:A:132:GLN:H	1:A:132:GLN:HG2	1.70	0.41
1:A:309:ASN:OD1	1:A:311:GLN:HG3	2.20	0.41
1:A:461:ARG:HH21	1:A:684:ASN:CG	2.23	0.41
1:A:882:ASP:HA	1:A:883:PRO:HD3	1.95	0.41
2:B:397:LEU:HA	2:B:1309:ILE:HD13	2.02	0.41
2:B:640:GLN:HE22	2:B:647:GLU:HB3	1.86	0.41
2:C:1233:LEU:HD13	2:C:1233:LEU:HA	1.77	0.41
2:C:382:HIS:ND1	2:C:799:THR:HG23	2.35	0.41
3:E:281:LYS:O	3:E:285:LEU:HG	2.21	0.41
1:A:684:ASN:HA	1:A:685:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:LYS:O	2:B:1267:THR:HG22	2.21	0.41
2:C:412:LEU:HA	2:C:412:LEU:HD23	1.80	0.41
2:C:419:TYR:HA	2:C:420:PRO:HD2	1.92	0.41
2:C:635:ILE:HA	2:C:636:PRO:HD3	1.89	0.41
2:C:836:GLN:N	2:C:836:GLN:OE1	2.54	0.41
3:E:182:TRP:NE1	3:E:185:SER:HA	2.35	0.41
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.69	0.41
3:E:9:TYR:H	3:E:204:ASP:CG	2.24	0.41
1:A:557:SER:HB3	1:A:583:ARG:HB2	2.01	0.41
1:A:73:ARG:O	1:A:76:LEU:HB3	2.21	0.41
2:B:1050:LEU:HA	2:B:1050:LEU:HD23	1.83	0.41
2:B:1219:ASP:HA	2:B:1220:PRO:HD3	1.86	0.41
2:C:648:PHE:HB2	2:C:699:THR:HG21	2.03	0.41
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.83	0.41
1:A:177:THR:HA	1:A:178:PRO:HD3	1.93	0.41
1:A:271:ARG:HB3	1:A:271:ARG:HE	1.66	0.41
1:A:647:LEU:HD22	1:A:691:TYR:HB3	2.03	0.41
2:B:1074:VAL:HG22	2:B:1171:ILE:HD12	2.03	0.41
2:B:612:PHE:HZ	2:B:1330:ILE:HG22	1.86	0.41
2:B:635:ILE:HA	2:B:636:PRO:HD3	1.83	0.41
2:C:1280:PRO:HB3	2:C:1285:GLN:O	2.21	0.41
2:C:583:GLU:CD	2:C:583:GLU:H	2.24	0.41
2:C:612:PHE:CZ	2:C:1330:ILE:HG22	2.56	0.41
1:A:583:ARG:HH11	1:A:583:ARG:H	1.68	0.41
2:B:353:PHE:CD2	2:B:1061:LEU:HD23	2.56	0.41
2:B:415:ALA:O	2:B:419:TYR:N	2.45	0.41
2:C:1220:PRO:HA	2:C:1221:PRO:HD3	1.95	0.41
3:D:9:TYR:H	3:D:204:ASP:CG	2.23	0.41
1:A:616:ASP:OD1	1:A:691:TYR:OH	2.31	0.41
1:A:633:ILE:HA	1:A:633:ILE:HD13	1.87	0.41
2:B:1002:LEU:HA	2:B:1002:LEU:HD23	1.87	0.41
2:B:802:GLN:HB2	2:B:997:TYR:CE2	2.56	0.41
2:C:403:PHE:CE2	2:C:625:PRO:HD3	2.56	0.41
2:C:876:GLY:O	2:C:903:ASN:ND2	2.51	0.41
3:D:19:ILE:HG13	3:D:19:ILE:H	1.66	0.41
2:B:1044:ARG:HH22	2:B:1049:GLU:CD	2.24	0.40
2:B:401:LEU:HA	2:B:401:LEU:HD23	1.87	0.40
2:B:817:ASP:OD1	2:B:821:ASN:ND2	2.55	0.40
3:E:273:LEU:O	3:E:277:GLU:HG3	2.21	0.40
1:A:951:LEU:HA	1:A:951:LEU:HD12	1.94	0.40
2:C:1134:ARG:HB3	2:C:1135:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:475:ILE:H	2:C:475:ILE:HG13	1.55	0.40
2:C:833:ARG:HG3	2:C:922:TYR:CE1	2.56	0.40
3:E:109:GLY:HA2	3:E:199:LEU:HD12	2.02	0.40
1:A:431:ALA:O	1:A:435:ILE:HG12	2.22	0.40
2:B:177:LYS:O	2:B:177:LYS:HD3	2.22	0.40
2:C:1271:SER:HB3	2:C:1277:LEU:HD21	2.03	0.40
2:C:166:TYR:HA	2:C:205:ASN:O	2.22	0.40
2:C:331:GLU:HA	2:C:335:ASP:OD2	2.22	0.40
2:C:956:ASP:O	2:C:1044:ARG:NH1	2.55	0.40
3:E:124:PRO:HA	3:E:127:VAL:HG22	2.03	0.40
3:E:189:LEU:HA	3:E:189:LEU:HD12	1.85	0.40
1:A:293:LEU:HD22	1:A:297:LEU:HG	2.02	0.40
1:A:858:VAL:HG22	1:A:918:ILE:HB	2.03	0.40
2:B:1228:ARG:HG2	2:B:1231:TYR:CE1	2.55	0.40
2:B:605:ARG:O	2:B:608:THR:HG23	2.21	0.40
2:C:509:VAL:HG22	2:C:683:TRP:CH2	2.55	0.40
2:C:820:ILE:HA	2:C:820:ILE:HD13	1.97	0.40
1:A:13:VAL:HG23	1:A:213:TRP:HD1	1.85	0.40
1:A:764:SER:HA	1:A:795:GLU:HG3	2.04	0.40
1:A:859:VAL:HB	1:A:919:TYR:CD1	2.56	0.40
1:A:977:HIS:HB2	1:A:981:ARG:HB3	2.03	0.40
2:B:832:MET:SD	2:B:848:ARG:HB3	2.61	0.40
3:D:44:LEU:HG	3:D:174:VAL:HG22	2.04	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%)	1011 (96%)	41 (4%)	3 (0%)	46	80
2	B	1187/1333 (89%)	1133 (96%)	49 (4%)	5 (0%)	39	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1246/1333 (94%)	1180 (95%)	63 (5%)	3 (0%)	52	84
3	D	290/448 (65%)	283 (98%)	5 (2%)	2 (1%)	26	65
3	E	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	46	80
All	All	4068/4620 (88%)	3889 (96%)	165 (4%)	14 (0%)	50	80

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	B	1035	ILE
2	B	1123	PRO
2	C	1267	THR
3	D	61	ASN
3	E	80	SER
2	C	1123	PRO
1	A	483	MET
2	B	503	GLU
2	B	738	GLU
1	A	350	PRO
2	C	340	VAL
2	B	1034	GLN
3	D	244	VAL

### 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%)	852 (90%)	90 (10%)	10	37
2	B	1038/1153 (90%)	967 (93%)	71 (7%)	20	55
2	C	1089/1153 (94%)	1011 (93%)	78 (7%)	18	53
3	D	240/379 (63%)	218 (91%)	22 (9%)	11	40
3	E	240/379 (63%)	214 (89%)	26 (11%)	8	30
All	All	3549/4007 (89%)	3262 (92%)	287 (8%)	19	47

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	13	VAL
1	A	36	THR
1	A	50	THR
1	A	76	LEU
1	A	77	LYS
1	A	88	LEU
1	A	104	VAL
1	A	105	ARG
1	A	108	ASP
1	A	112	ARG
1	A	132	GLN
1	A	133	LEU
1	A	142	ASN
1	A	157	LEU
1	A	166	ILE
1	A	183	ILE
1	A	188	THR
1	A	199	MET
1	A	202	SER
1	A	207	THR
1	A	210	SER
1	A	216	LEU
1	A	242	LYS
1	A	260	LEU
1	A	275	ILE
1	A	293	LEU
1	A	312	LEU
1	A	313	ARG
1	A	314	ARG
1	A	337	LEU
1	A	339	GLN
1	A	357	THR
1	A	360	THR
1	A	377	LEU
1	A	396	THR
1	A	401	ILE
1	A	402	THR
1	A	444	LEU
1	A	451	ARG
1	A	466	LEU
1	A	493	LEU

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Mol	Chain	Res	Type
1	A	506	VAL
1	A	514	LEU
1	A	523	MET
1	A	583	ARG
1	A	598	VAL
1	A	599	ARG
1	A	611	ASP
1	A	613	ILE
1	A	622	ASP
1	A	628	MET
1	A	648	VAL
1	A	680	THR
1	A	697	ILE
1	A	714	ARG
1	A	719	VAL
1	A	721	ASP
1	A	742	SER
1	A	757	LEU
1	A	762	LEU
1	A	763	LYS
1	A	770	THR
1	A	774	VAL
1	A	794	LEU
1	A	823	THR
1	A	832	GLU
1	A	844	LEU
1	A	855	MET
1	A	868	ASP
1	A	872	VAL
1	A	877	LYS
1	A	886	ARG
1	A	890	LEU
1	A	905	GLN
1	A	910	ASN
1	A	914	GLU
1	A	926	MET
1	A	941	ASP
1	A	970	ARG
1	A	977	HIS
1	A	981	ARG
1	A	987	LEU
1	A	1007	LEU

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Mol	Chain	Res	Type
1	A	1013	THR
1	A	1018	ARG
1	A	1024	LEU
1	A	1034	ARG
1	A	1035	LEU
1	A	1047	ASN
2	B	147	VAL
2	B	168	VAL
2	B	217	THR
2	B	223	LYS
2	B	233	VAL
2	B	238	THR
2	B	264	LEU
2	B	265	VAL
2	B	271	THR
2	B	274	MET
2	B	287	ARG
2	B	294	VAL
2	B	323	THR
2	B	330	THR
2	B	334	LEU
2	B	335	ASP
2	B	383	SER
2	B	384	MET
2	B	397	LEU
2	B	439	VAL
2	B	451	GLU
2	B	452	ASN
2	B	457	GLN
2	B	495	LEU
2	B	533	GLN
2	B	537	LEU
2	B	546	VAL
2	B	552	VAL
2	B	567	GLU
2	B	579	LEU
2	B	633	THR
2	B	637	TYR
2	B	643	THR
2	B	654	THR
2	B	661	ASN
2	B	704	VAL

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Mol	Chain	Res	Type
2	B	708	THR
2	B	735	THR
2	B	751	THR
2	B	755	LEU
2	B	774	LEU
2	B	798	THR
2	B	809	VAL
2	B	812	LYS
2	B	815	LEU
2	B	864	HIS
2	B	890	THR
2	B	899	SER
2	B	912	GLU
2	B	945	VAL
2	B	946	LEU
2	B	1032	ASP
2	B	1052	LEU
2	B	1082	ASP
2	B	1110	LEU
2	B	1138	HIS
2	B	1159	VAL
2	B	1179	THR
2	B	1193	ILE
2	B	1212	ARG
2	B	1228	ARG
2	B	1233	LEU
2	B	1234	GLN
2	B	1237	SER
2	B	1270	LEU
2	B	1293	VAL
2	B	1294	ASP
2	B	1311	THR
2	B	1319	ARG
2	B	1320	VAL
2	B	1331	ARG
2	C	79	SER
2	C	97	GLU
2	C	98	ASN
2	C	112	THR
2	C	116	SER
2	C	120	VAL
2	C	134	THR

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Mol	Chain	Res	Type
2	C	175	THR
2	C	180	LEU
2	C	207	ASP
2	C	217	THR
2	C	243	GLN
2	C	263	ARG
2	C	264	LEU
2	C	280	THR
2	C	282	VAL
2	C	294	VAL
2	C	315	THR
2	C	323	THR
2	C	327	LEU
2	C	330	THR
2	C	340	VAL
2	C	362	LEU
2	C	373	ASP
2	C	384	MET
2	C	439	VAL
2	C	451	GLU
2	C	462	LEU
2	C	475	ILE
2	C	495	LEU
2	C	508	ILE
2	C	512	LEU
2	C	527	ARG
2	C	546	VAL
2	C	557	THR
2	C	626	ARG
2	C	630	ASN
2	C	637	TYR
2	C	638	THR
2	C	648	PHE
2	C	654	THR
2	C	656	VAL
2	C	661	ASN
2	C	704	VAL
2	C	767	LEU
2	C	769	GLN
2	C	774	LEU
2	C	776	ARG
2	C	790	GLU

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Mol	Chain	Res	Type
2	C	798	THR
2	C	828	ASP
2	C	833	ARG
2	C	851	THR
2	C	856	LEU
2	C	865	ILE
2	C	892	VAL
2	C	946	LEU
2	C	948	ILE
2	C	951	ILE
2	C	962	ASP
2	C	964	VAL
2	C	980	ARG
2	C	1014	MET
2	C	1015	GLN
2	C	1052	LEU
2	C	1055	LEU
2	C	1110	LEU
2	C	1119	TYR
2	C	1136	HIS
2	C	1148	SER
2	C	1200	LYS
2	C	1201	LEU
2	C	1202	PHE
2	C	1233	LEU
2	C	1250	GLU
2	C	1269	THR
2	C	1291	LEU
2	C	1320	VAL
3	D	2	LEU
3	D	21	ASN
3	D	29	THR
3	D	35	LEU
3	D	47	LYS
3	D	54	THR
3	D	92	ARG
3	D	93	LEU
3	D	100	ASN
3	D	107	LEU
3	D	116	THR
3	D	130	PHE
3	D	133	THR

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Mol	Chain	Res	Type
3	D	189	LEU
3	D	191	ARG
3	D	193	VAL
3	D	194	VAL
3	D	214	ARG
3	D	226	MET
3	D	239	VAL
3	D	252	LEU
3	D	253	GLU
3	E	2	LEU
3	E	24	THR
3	E	29	THR
3	E	35	LEU
3	E	48	THR
3	E	66	VAL
3	E	93	LEU
3	E	94	SER
3	E	98	LEU
3	E	118	ASN
3	E	133	THR
3	E	139	ASN
3	E	142	THR
3	E	158	LEU
3	E	160	LEU
3	E	189	LEU
3	E	194	VAL
3	E	226	MET
3	E	240	VAL
3	E	244	VAL
3	E	247	ARG
3	E	252	LEU
3	E	262	THR
3	E	272	ASP
3	E	287	PHE
3	E	288	THR

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	49	HIS
1	A	114	ASN
1	A	595	ASN

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Mol	Chain	Res	Type
1	A	667	GLN
1	A	1030	ASN
2	B	491	ASN
2	B	1332	ASN
2	C	430	ASN
2	C	981	HIS
2	C	1051	GLN
2	C	1138	HIS

### 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](#)

There are no ligands in this entry.

### 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.