



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:39 AM GMT

PDB ID : 3FHJ  
Title : Independent saturation of three TrpRS subsites generates a partially-assembled state similar to those observed in molecular simulations  
Authors : Laowanapiban, P.; Kapustina, M.; Vonnrhein, C.; Delarue, M.; Koehl, P.; Carter Jr., C.W.  
Deposited on : 2008-12-09  
Resolution : 2.65 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

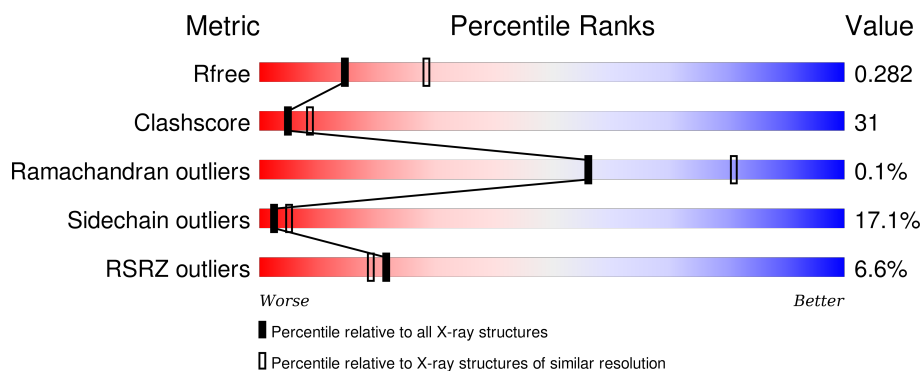
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	328	<div> <div>2%</div> <div>55%</div> <div>29%</div> <div>7%</div> <div>9%</div> </div>
1	B	328	<div> <div>4%</div> <div>45%</div> <div>35%</div> <div>9%</div> <div>11%</div> </div>
1	C	328	<div> <div>9%</div> <div>43%</div> <div>34%</div> <div>9%</div> <div>15%</div> </div>
1	D	328	<div> <div>5%</div> <div>48%</div> <div>30%</div> <div>9%</div> <div>13%</div> </div>
1	E	328	<div> <div>12%</div> <div>43%</div> <div>37%</div> <div>9%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	328	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRP	D	1001	-	-	-	X
3	PO4	A	1002	-	-	X	-
3	PO4	B	1002	-	-	X	-
3	PO4	D	1002	-	-	X	-
4	AMP	A	1003	-	-	-	X
4	AMP	B	1003	-	-	X	X
4	AMP	C	1003	-	-	-	X
4	AMP	D	1003	-	-	-	X
4	AMP	E	1003	-	-	X	X
4	AMP	F	1003	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14203 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

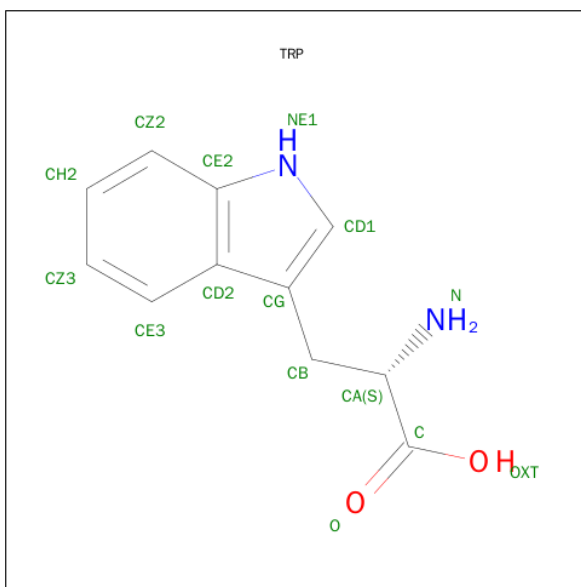
- Molecule 1 is a protein called Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2394	1520	413	448	13			
1	D	286	Total	C	N	O	S	0	0	0
			2281	1451	391	426	13			
1	B	291	Total	C	N	O	S	0	0	0
			2338	1484	401	440	13			
1	C	279	Total	C	N	O	S	0	0	0
			2225	1415	384	413	13			
1	E	292	Total	C	N	O	S	0	0	0
			2337	1485	403	436	13			
1	F	296	Total	C	N	O	S	0	0	0
			2370	1505	408	444	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	LYS	CONFLICT	UNP P00953
D	64	LEU	LYS	CONFLICT	UNP P00953
B	64	LEU	LYS	CONFLICT	UNP P00953
C	64	LEU	LYS	CONFLICT	UNP P00953
E	64	LEU	LYS	CONFLICT	UNP P00953
F	64	LEU	LYS	CONFLICT	UNP P00953

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



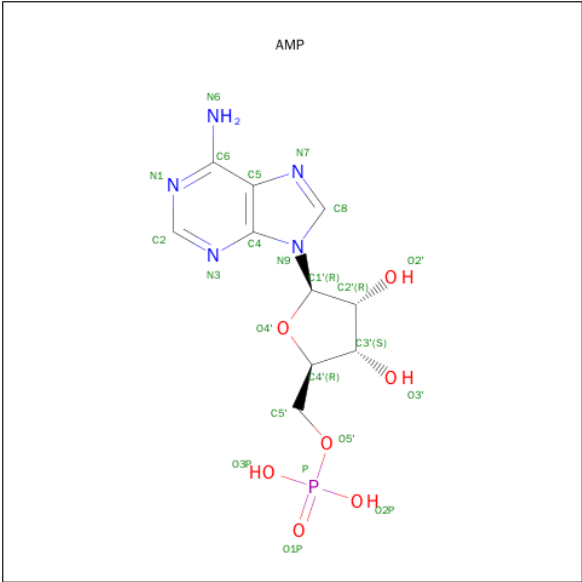
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		
2	F	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

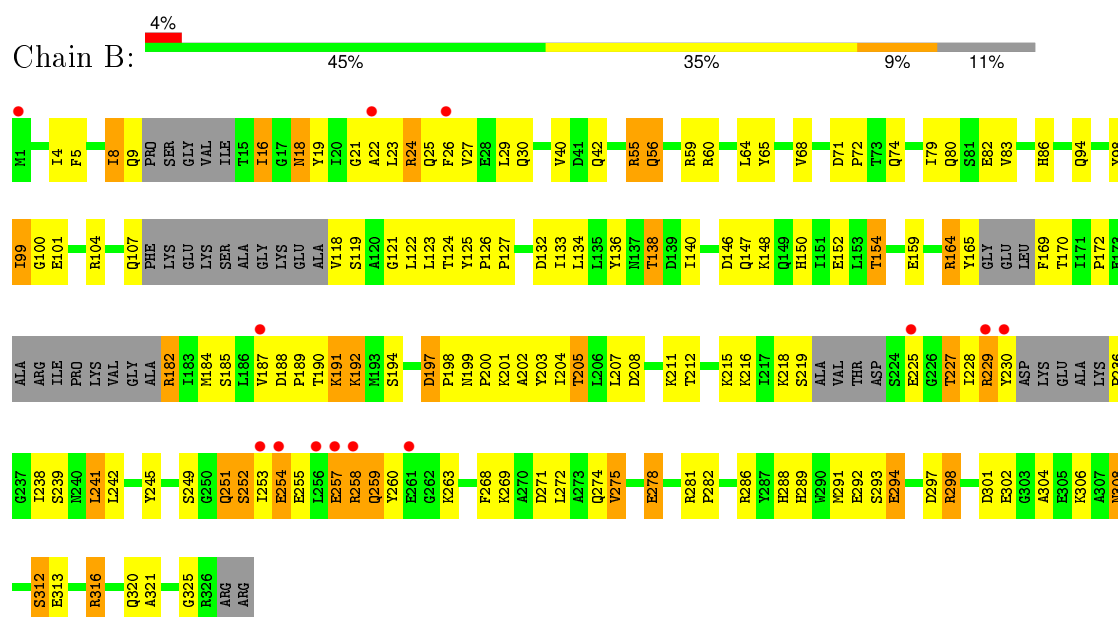
- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



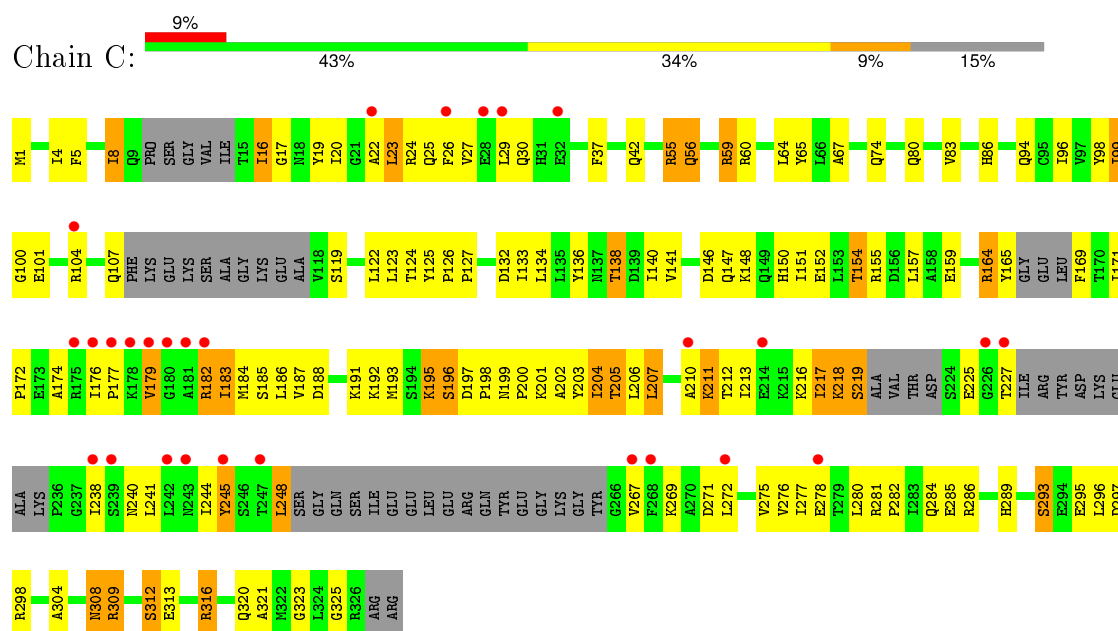
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		



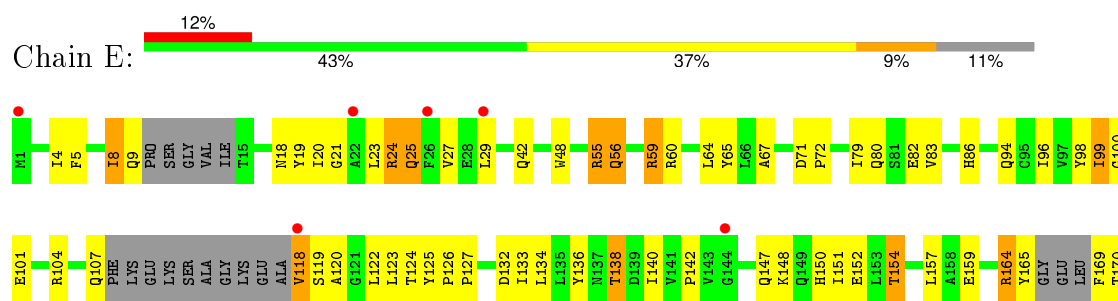




• Molecule 1: Tryptophanyl-tRNA synthetase



• Molecule 1: Tryptophanyl-tRNA synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.61Å 91.99Å 158.32Å 90.00° 134.01° 90.00°	Depositor
Resolution (Å)	25.00 – 2.65 49.86 – 2.31	Depositor EDS
% Data completeness (in resolution range)	92.5 (25.00-2.65) 79.0 (49.86-2.31)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.200 , 0.270 0.271 , 0.282	Depositor DCC
$R_{free}$ test set	3310 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.7	EDS
Estimated twinning fraction	0.000 for h+2*l,k,-h-l 0.000 for h,-k,-h-l 0.005 for -h-2*l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 79981 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.5371e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.40	0/2435	0.42	0/3285
1	B	0.27	0/2377	0.42	0/3205
1	C	0.29	0/2262	0.39	0/3053
1	D	0.24	0/2320	0.39	0/3137
1	E	0.24	0/2378	0.38	0/3210
1	F	0.23	0/2411	0.38	0/3253
All	All	0.28	0/14183	0.40	0/19143

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2394	0	2408	111	0
1	B	2338	0	2341	178	0
1	C	2225	0	2249	174	0
1	D	2281	0	2306	135	0
1	E	2337	0	2355	191	0
1	F	2370	0	2380	145	0
2	A	15	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	0	0
2	E	15	0	9	0	0
2	F	15	0	9	0	0
3	A	5	0	0	3	0
3	B	5	0	0	2	0
3	C	5	0	0	0	0
3	D	5	0	0	4	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
4	A	23	0	12	4	0
4	B	23	0	12	7	0
4	C	23	0	12	5	0
4	D	23	0	12	5	0
4	E	23	0	12	7	0
4	F	23	0	12	7	0
All	All	14203	0	14165	891	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 31.

All (891) 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:118:VAL:CG1	1:B:99:ILE:HG13	1.58	1.32
1:C:206:LEU:CD1	1:C:280:LEU:HD22	1.70	1.20
1:F:13:VAL:HG21	1:F:205:THR:HG23	1.22	1.20
1:E:215:LYS:O	1:E:218:LYS:HG2	1.40	1.19
1:B:23:LEU:HA	1:B:26:PHE:CD2	1.77	1.19
1:C:213:ILE:HG21	1:C:276:VAL:HG12	1.23	1.18
1:B:230:TYR:CE1	1:B:239:SER:HB3	1.78	1.17
1:D:140:ILE:HD11	1:D:175:ARG:CG	1.77	1.15
1:C:206:LEU:CD1	1:C:280:LEU:CD2	2.26	1.14
1:B:16:ILE:HD13	1:B:204:ILE:HB	1.21	1.12
1:B:230:TYR:CD1	1:B:239:SER:HB3	1.84	1.12
1:C:64:LEU:HD21	1:C:207:LEU:HD21	1.22	1.12
1:C:176:ILE:CG2	1:C:179:VAL:HG13	1.79	1.11
1:A:118:VAL:HG12	1:B:99:ILE:CG1	1.80	1.09
1:D:200:PRO:O	1:D:216:LYS:HE2	1.51	1.09
1:E:187:VAL:HG11	1:E:199:ASN:ND2	1.67	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:HG22	1:A:207:LEU:H	1.11	1.08
1:C:206:LEU:HD11	1:C:280:LEU:HD22	1.33	1.07
1:D:140:ILE:HD11	1:D:175:ARG:HG2	1.13	1.07
1:C:272:LEU:HA	1:C:275:VAL:HG13	1.37	1.06
1:F:15:THR:HG22	1:F:18:ASN:H	1.14	1.06
1:E:215:LYS:HG2	1:E:218:LYS:HE2	1.07	1.06
1:C:213:ILE:HG21	1:C:276:VAL:CG1	1.84	1.06
1:C:187:VAL:HG21	1:C:199:ASN:OD1	1.56	1.04
1:D:140:ILE:CD1	1:D:175:ARG:HG2	1.88	1.04
1:E:19:TYR:O	1:E:24:ARG:HB3	1.57	1.04
1:F:104:ARG:HH11	1:F:104:ARG:HG3	1.20	1.03
1:C:182:ARG:HG2	1:C:184:MET:CE	1.88	1.03
1:F:205:THR:HG22	1:F:207:LEU:H	1.20	1.02
1:E:215:LYS:HG2	1:E:218:LYS:CE	1.87	1.02
1:C:206:LEU:HD11	1:C:280:LEU:CD2	1.85	1.01
1:C:176:ILE:HG22	1:C:179:VAL:HG13	1.39	1.01
1:E:215:LYS:CG	1:E:218:LYS:HE2	1.92	1.00
1:C:295:GLU:HG2	1:C:298:ARG:HH21	1.25	1.00
1:E:197:ASP:OD1	1:E:198:PRO:HD2	1.62	0.99
1:F:140:ILE:HD11	1:F:175:ARG:HB3	1.42	0.99
1:D:215:LYS:NZ	1:D:215:LYS:HB3	1.74	0.99
1:B:23:LEU:HA	1:B:26:PHE:HD2	0.85	0.99
1:C:206:LEU:HD12	1:C:280:LEU:HD22	1.45	0.98
4:F:1003:AMP:H5'1	4:F:1003:AMP:H8	1.26	0.98
1:B:187:VAL:HG11	1:B:199:ASN:ND2	1.79	0.97
1:A:140:ILE:HD11	1:A:175:ARG:HD3	1.47	0.95
1:C:210:ALA:HB1	1:C:277:ILE:HD13	1.46	0.94
1:D:19:TYR:O	1:D:24:ARG:HB2	1.65	0.94
1:B:23:LEU:CA	1:B:26:PHE:HD2	1.78	0.94
1:C:64:LEU:HD21	1:C:207:LEU:CD2	1.98	0.93
1:D:140:ILE:HD11	1:D:175:ARG:CD	1.99	0.93
1:C:176:ILE:O	1:C:179:VAL:HG22	1.70	0.92
1:E:305:GLU:O	1:E:309:ARG:HG2	1.68	0.92
1:B:282:PRO:HB2	1:B:286:ARG:NH2	1.84	0.92
1:D:205:THR:HG22	1:D:207:LEU:H	1.34	0.91
1:E:107:GLN:H	1:E:107:GLN:NE2	1.69	0.91
1:E:213:ILE:O	1:E:217:ILE:HG13	1.68	0.91
1:C:213:ILE:CG2	1:C:276:VAL:CG1	2.48	0.91
1:B:205:THR:HG23	1:B:207:LEU:H	1.34	0.91
1:C:206:LEU:HD12	1:C:280:LEU:CD2	1.97	0.90
1:A:118:VAL:HG12	1:B:99:ILE:HG13	0.91	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:TYR:CE2	1:C:24:ARG:HD3	2.07	0.89
1:C:23:LEU:O	1:C:23:LEU:HD12	1.72	0.89
1:D:215:LYS:HB3	1:D:215:LYS:HZ3	1.29	0.89
1:F:15:THR:HG23	1:F:17:GLY:H	1.38	0.89
1:C:218:LYS:CB	1:C:218:LYS:NZ	2.35	0.88
1:E:283:ILE:HG13	1:E:286:ARG:NH2	1.88	0.88
1:C:134:LEU:HB3	1:C:169:PHE:CD1	2.08	0.88
1:A:18:ASN:HD22	1:A:18:ASN:C	1.77	0.88
1:C:213:ILE:CG2	1:C:276:VAL:HG11	2.03	0.88
1:A:99:ILE:HG13	1:B:118:VAL:HG23	1.56	0.88
1:D:215:LYS:CB	1:D:215:LYS:NZ	2.36	0.88
1:C:218:LYS:HZ3	1:C:218:LYS:HB3	1.39	0.86
1:C:26:PHE:O	1:C:30:GLN:HB3	1.75	0.86
1:F:13:VAL:CG2	1:F:14:ILE:N	2.38	0.86
1:E:261:GLU:C	1:E:263:LYS:HE2	1.96	0.86
1:C:16:ILE:O	1:C:20:ILE:HD12	1.75	0.86
1:C:213:ILE:HG23	1:C:276:VAL:HG11	1.56	0.85
1:C:126:PRO:HB2	1:C:127:PRO:HD3	1.58	0.85
1:B:304:ALA:O	1:B:308:ASN:HB2	1.76	0.85
1:F:126:PRO:HB2	1:F:127:PRO:HD3	1.59	0.85
1:E:29:LEU:HD11	1:E:177:PRO:HB2	1.57	0.84
1:B:126:PRO:HB2	1:B:127:PRO:HD3	1.58	0.84
1:E:140:ILE:HD11	1:E:175:ARG:CG	2.08	0.84
1:B:281:ARG:HH11	1:B:281:ARG:HG3	1.43	0.84
1:D:4:ILE:HG12	1:D:140:ILE:HG22	1.59	0.84
1:E:126:PRO:HB2	1:E:127:PRO:HD3	1.58	0.84
1:C:200:PRO:HA	1:C:203:TYR:CE1	2.12	0.83
1:C:206:LEU:CD1	1:C:280:LEU:HD21	2.05	0.83
1:D:217:ILE:O	1:D:220:ALA:HB3	1.78	0.83
1:B:184:MET:HG3	1:B:191:LYS:O	1.78	0.83
1:C:4:ILE:HG12	1:C:140:ILE:HG22	1.60	0.83
1:D:176:ILE:HB	1:D:179:VAL:HG12	1.58	0.83
1:F:205:THR:HG22	1:F:207:LEU:N	1.94	0.82
1:D:126:PRO:HB2	1:D:127:PRO:HD3	1.60	0.82
1:B:205:THR:HG22	1:B:208:ASP:N	1.95	0.82
1:C:64:LEU:CD2	1:C:207:LEU:HD21	2.07	0.82
1:C:281:ARG:N	1:C:282:PRO:HD2	1.94	0.82
1:B:134:LEU:HB3	1:B:169:PHE:CD1	2.15	0.82
1:C:22:ALA:O	1:C:26:PHE:CE2	2.33	0.82
1:E:261:GLU:HG3	1:E:261:GLU:O	1.80	0.82
1:C:16:ILE:HG23	1:C:204:ILE:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PRO:HB2	1:A:127:PRO:HD3	1.59	0.81
1:E:134:LEU:HB3	1:E:169:PHE:CD1	2.14	0.81
1:B:22:ALA:O	1:B:26:PHE:CD2	2.34	0.81
1:B:4:ILE:HG12	1:B:140:ILE:HG22	1.62	0.81
1:F:164:ARG:HD2	1:F:165:TYR:CE2	2.16	0.81
1:C:22:ALA:O	1:C:26:PHE:CD2	2.33	0.81
1:C:281:ARG:H	1:C:282:PRO:HD2	1.46	0.81
1:F:15:THR:CG2	1:F:18:ASN:H	1.92	0.81
1:B:230:TYR:CD1	1:B:239:SER:CB	2.63	0.80
1:F:175:ARG:HG2	1:F:175:ARG:HH11	1.46	0.80
1:C:182:ARG:HG2	1:C:184:MET:HE1	1.61	0.80
1:A:205:THR:HG22	1:A:207:LEU:N	1.93	0.80
1:B:205:THR:HG22	1:B:208:ASP:H	1.46	0.80
1:E:4:ILE:HG12	1:E:140:ILE:HG22	1.61	0.80
1:F:188:ASP:HB3	1:F:191:LYS:HB3	1.63	0.80
1:A:4:ILE:HG12	1:A:140:ILE:HG22	1.64	0.80
1:D:140:ILE:HD11	1:D:175:ARG:HD2	1.64	0.80
1:D:205:THR:CG2	1:D:207:LEU:H	1.95	0.79
1:F:13:VAL:HG21	1:F:205:THR:CG2	2.10	0.79
1:F:140:ILE:CD1	1:F:175:ARG:HB3	2.13	0.79
1:F:175:ARG:HG2	1:F:175:ARG:NH1	1.98	0.79
1:B:60:ARG:HG2	1:B:291:MET:CE	2.13	0.79
1:E:197:ASP:OD1	1:E:198:PRO:CD	2.30	0.79
1:D:320:GLN:HA	1:C:55:ARG:NH2	1.98	0.79
1:F:4:ILE:HG12	1:F:140:ILE:HG22	1.63	0.78
1:B:16:ILE:CD1	1:B:204:ILE:HB	2.10	0.78
1:B:187:VAL:HG22	1:B:202:ALA:HB2	1.65	0.78
1:D:13:VAL:HG21	1:D:205:THR:HG23	1.63	0.78
1:E:55:ARG:HH22	1:F:320:GLN:HA	1.48	0.78
1:D:193:MET:HB3	4:D:1003:AMP:N6	1.98	0.77
1:E:281:ARG:HA	1:E:281:ARG:NE	2.00	0.77
1:B:200:PRO:HA	1:B:203:TYR:CZ	2.18	0.77
1:F:13:VAL:HG22	1:F:14:ILE:N	1.98	0.77
1:E:205:THR:HG22	1:E:207:LEU:H	1.50	0.77
1:E:205:THR:CG2	1:E:207:LEU:H	1.98	0.77
1:A:205:THR:CG2	1:A:207:LEU:H	1.94	0.77
1:A:189:PRO:HB2	1:A:236:PRO:HB2	1.67	0.77
1:E:185:SER:OG	1:E:202:ALA:HB1	1.85	0.77
1:D:22:ALA:O	1:D:26:PHE:CD2	2.39	0.76
1:F:104:ARG:NH1	1:F:104:ARG:HG3	1.91	0.76
1:B:282:PRO:HB2	1:B:286:ARG:HH21	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LEU:CD1	1:C:177:PRO:HB2	2.15	0.76
1:E:29:LEU:CD1	1:E:177:PRO:HB2	2.16	0.76
1:A:124:THR:HG21	1:B:124:THR:HG21	1.68	0.76
1:A:24:ARG:HH11	1:A:24:ARG:HB3	1.50	0.76
1:C:176:ILE:HG21	1:C:179:VAL:HG13	1.67	0.75
1:E:218:LYS:HG3	1:E:219:SER:N	1.99	0.75
1:B:189:PRO:HB2	1:B:236:PRO:HB2	1.68	0.75
1:E:288:HIS:O	1:E:292:GLU:HG2	1.85	0.75
1:E:55:ARG:HD2	1:F:325:GLY:O	1.85	0.75
1:E:320:GLN:HA	1:F:55:ARG:HH22	1.51	0.75
1:F:105:MET:HE2	1:F:150:HIS:CE1	2.21	0.75
1:F:13:VAL:HG23	1:F:14:ILE:H	1.52	0.75
1:E:273:ALA:O	1:E:277:ILE:HD12	1.85	0.75
1:D:198:PRO:HA	1:E:198:PRO:HA	1.69	0.75
1:F:205:THR:CG2	1:F:207:LEU:H	1.97	0.75
1:E:140:ILE:HD11	1:E:175:ARG:HH11	1.51	0.75
1:B:170:THR:O	1:B:172:PRO:HD3	1.86	0.74
1:F:121:GLY:O	1:F:125:TYR:HB3	1.87	0.74
1:E:140:ILE:CD1	1:E:175:ARG:HH11	1.99	0.74
1:E:19:TYR:CE2	1:E:24:ARG:HD2	2.22	0.74
4:F:1003:AMP:H5'1	4:F:1003:AMP:C8	2.20	0.74
1:E:263:LYS:N	1:E:263:LYS:HD3	2.03	0.74
1:F:15:THR:HG23	1:F:17:GLY:N	2.03	0.73
1:F:13:VAL:CG2	1:F:205:THR:HG23	2.13	0.73
1:B:187:VAL:HG22	1:B:202:ALA:CB	2.18	0.73
1:B:252:SER:OG	1:B:254:GLU:HG2	1.88	0.73
1:C:272:LEU:HA	1:C:275:VAL:CG1	2.16	0.73
1:F:140:ILE:HD11	1:F:175:ARG:CB	2.18	0.73
1:C:218:LYS:HZ2	1:C:218:LYS:HB2	1.54	0.73
1:D:16:ILE:HD13	1:D:204:ILE:HB	1.69	0.73
1:E:253:ILE:O	1:E:257:GLU:HG2	1.88	0.73
1:D:187:VAL:HG13	1:D:202:ALA:HA	1.70	0.73
1:B:200:PRO:O	1:B:216:LYS:HE2	1.88	0.73
1:D:185:SER:OG	1:D:202:ALA:HB1	1.89	0.73
1:D:320:GLN:HA	1:C:55:ARG:HH22	1.53	0.72
1:E:265:TYR:O	1:E:269:LYS:HG3	1.88	0.72
1:C:192:LYS:HG2	1:C:193:MET:N	2.05	0.72
1:D:22:ALA:HB1	1:D:26:PHE:CE2	2.25	0.72
1:A:164:ARG:HD2	1:A:165:TYR:CE2	2.23	0.72
1:D:22:ALA:HB1	1:D:26:PHE:HE2	1.53	0.72
1:E:187:VAL:HG11	1:E:199:ASN:HD21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LYS:HB2	1:C:218:LYS:NZ	2.05	0.72
1:F:13:VAL:CG2	1:F:14:ILE:H	2.01	0.71
1:E:295:GLU:HG2	1:E:298:ARG:NH2	2.06	0.71
1:A:134:LEU:HB3	1:A:169:PHE:CD1	2.26	0.71
1:C:23:LEU:HD12	1:C:23:LEU:C	2.11	0.70
1:F:125:TYR:N	1:F:126:PRO:HD2	2.06	0.70
1:E:189:PRO:HB2	1:E:236:PRO:HB2	1.74	0.70
1:E:215:LYS:HG3	1:E:218:LYS:HZ3	1.55	0.70
1:C:210:ALA:CB	1:C:277:ILE:HD13	2.21	0.70
1:B:249:SER:OG	1:B:251:GLN:HG3	1.92	0.70
1:F:134:LEU:HB3	1:F:169:PHE:CD1	2.26	0.70
1:F:184:MET:HG3	1:F:189:PRO:O	1.92	0.70
1:A:320:GLN:HA	1:B:55:ARG:HH22	1.55	0.70
1:C:16:ILE:HD13	1:C:204:ILE:HB	1.72	0.70
1:F:8:ILE:HD12	1:F:65:TYR:OH	1.92	0.70
1:A:304:ALA:O	1:A:308:ASN:HB2	1.92	0.70
1:A:140:ILE:CD1	1:A:175:ARG:HD3	2.19	0.69
1:A:140:ILE:HD11	1:A:175:ARG:CD	2.21	0.69
1:C:16:ILE:CG2	1:C:204:ILE:HG22	2.21	0.69
1:F:212:THR:HG22	1:F:216:LYS:HD2	1.73	0.69
1:D:205:THR:HG22	1:D:207:LEU:N	2.04	0.69
1:C:304:ALA:O	1:C:308:ASN:HB2	1.93	0.69
1:F:14:ILE:HG22	1:F:15:THR:N	2.05	0.69
1:B:60:ARG:HG2	1:B:291:MET:HE2	1.74	0.69
1:A:107:GLN:NE2	1:A:107:GLN:H	1.90	0.69
1:C:100:GLY:O	1:C:104:ARG:HG3	1.93	0.69
1:F:18:ASN:HD21	4:F:1003:AMP:H5'1	1.57	0.68
1:C:29:LEU:HD13	1:C:177:PRO:HB2	1.75	0.68
1:E:100:GLY:O	1:E:104:ARG:HG3	1.93	0.68
1:F:105:MET:CE	1:F:150:HIS:CE1	2.76	0.68
1:A:320:GLN:HA	1:B:55:ARG:NH2	2.07	0.68
1:D:304:ALA:O	1:D:308:ASN:HB2	1.93	0.68
1:E:304:ALA:O	1:E:308:ASN:HB2	1.91	0.68
1:A:288:HIS:O	1:A:292:GLU:HG2	1.93	0.68
1:E:213:ILE:O	1:E:217:ILE:CG1	2.42	0.68
1:F:150:HIS:O	1:F:154:THR:HG22	1.93	0.68
1:A:150:HIS:O	1:A:154:THR:HG22	1.93	0.68
1:B:24:ARG:CB	1:B:24:ARG:HH11	2.07	0.68
1:D:23:LEU:HA	1:D:26:PHE:HD2	1.59	0.68
1:B:150:HIS:O	1:B:154:THR:HG22	1.94	0.68
1:C:150:HIS:O	1:C:154:THR:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:HIS:O	1:E:154:THR:HG22	1.94	0.67
1:B:189:PRO:HB2	1:B:236:PRO:CB	2.23	0.67
1:E:189:PRO:HB3	1:E:237:GLY:HA2	1.76	0.67
1:F:304:ALA:O	1:F:308:ASN:HB2	1.94	0.67
1:D:100:GLY:O	1:D:104:ARG:HG3	1.93	0.67
1:B:187:VAL:HG11	1:B:199:ASN:HD21	1.57	0.67
1:E:283:ILE:HG13	1:E:286:ARG:HH21	1.60	0.67
1:F:282:PRO:HB2	1:F:286:ARG:HH21	1.58	0.67
1:C:16:ILE:CD1	1:C:204:ILE:HB	2.25	0.67
1:F:15:THR:HG22	1:F:18:ASN:N	1.99	0.67
1:E:19:TYR:CZ	1:E:24:ARG:HB2	2.30	0.67
1:B:259:GLN:HG2	1:B:260:TYR:CD2	2.30	0.67
1:D:150:HIS:O	1:D:154:THR:HG22	1.95	0.66
1:A:281:ARG:NH2	1:A:285:GLU:OE2	2.28	0.66
1:C:218:LYS:HB3	1:C:218:LYS:NZ	1.98	0.66
1:A:55:ARG:HH22	1:B:320:GLN:HA	1.59	0.66
1:A:140:ILE:HD11	1:A:175:ARG:HB3	1.76	0.66
1:D:13:VAL:HG21	1:D:205:THR:CG2	2.25	0.66
1:D:13:VAL:CG2	1:D:205:THR:HG23	2.24	0.66
1:C:4:ILE:HG12	1:C:140:ILE:CG2	2.25	0.66
1:F:189:PRO:HB2	1:F:236:PRO:HB2	1.77	0.66
1:E:297:ASP:HA	1:F:326:ARG:NH1	2.10	0.66
1:F:175:ARG:CG	1:F:175:ARG:HH11	2.09	0.66
1:D:193:MET:HB3	4:D:1003:AMP:HN62	1.57	0.66
1:F:67:ALA:O	1:F:286:ARG:NH1	2.29	0.66
1:C:164:ARG:HD2	1:C:165:TYR:CE2	2.31	0.66
1:B:100:GLY:O	1:B:104:ARG:HG3	1.96	0.66
1:C:295:GLU:HG2	1:C:298:ARG:NH2	2.04	0.66
1:D:19:TYR:HA	1:D:23:LEU:HB3	1.78	0.66
1:F:142:PRO:HA	1:F:175:ARG:O	1.95	0.65
1:A:192:LYS:HE2	4:A:1003:AMP:C5	2.31	0.65
1:D:55:ARG:NH2	1:C:320:GLN:HA	2.12	0.65
1:B:182:ARG:CZ	1:B:192:LYS:HD3	2.26	0.65
1:E:182:ARG:HB3	1:E:184:MET:CE	2.26	0.65
1:B:16:ILE:HD13	1:B:204:ILE:CB	2.14	0.65
1:F:125:TYR:N	1:F:126:PRO:CD	2.60	0.65
3:B:1002:PO4:O2	4:B:1003:AMP:H5'1	1.97	0.65
1:D:282:PRO:HB2	1:D:286:ARG:NH2	2.12	0.65
1:D:140:ILE:HD13	1:D:177:PRO:HG3	1.78	0.65
1:D:4:ILE:HG12	1:D:140:ILE:CG2	2.26	0.65
1:C:182:ARG:HG2	1:C:184:MET:HE3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:PRO:O	1:D:200:PRO:HD3	1.97	0.64
1:E:198:PRO:O	1:E:200:PRO:HD3	1.98	0.64
1:B:187:VAL:CG2	1:B:202:ALA:HB2	2.26	0.64
3:D:1002:PO4:O4	4:D:1003:AMP:H5'2	1.98	0.64
1:C:25:GLN:O	1:C:29:LEU:HG	1.97	0.64
1:E:320:GLN:HA	1:F:55:ARG:NH2	2.13	0.64
1:C:83:VAL:HG13	1:C:308:ASN:ND2	2.12	0.64
1:D:30:GLN:O	1:D:74:GLN:HG3	1.97	0.64
1:C:244:ILE:O	1:C:248:LEU:HB2	1.97	0.64
1:F:19:TYR:HA	1:F:23:LEU:HB3	1.78	0.64
1:F:13:VAL:C	1:F:14:ILE:HD13	2.17	0.64
1:B:24:ARG:HB3	1:B:24:ARG:HH11	1.63	0.64
1:B:278:GLU:OE1	1:B:281:ARG:NH2	2.29	0.64
1:E:297:ASP:HA	1:F:326:ARG:HH12	1.61	0.64
1:E:215:LYS:CG	1:E:218:LYS:CE	2.65	0.64
1:F:185:SER:HB3	1:F:188:ASP:O	1.96	0.64
1:A:280:LEU:O	1:A:284:GLN:HG3	1.96	0.64
1:C:185:SER:OG	1:C:202:ALA:HB1	1.98	0.64
1:C:281:ARG:N	1:C:282:PRO:CD	2.61	0.64
1:C:16:ILE:CG2	1:C:204:ILE:O	2.47	0.64
1:C:205:THR:HG23	1:C:206:LEU:H	1.63	0.63
1:F:14:ILE:CG2	1:F:15:THR:N	2.61	0.63
1:E:215:LYS:O	1:E:218:LYS:CG	2.32	0.63
1:F:188:ASP:HB3	1:F:191:LYS:CB	2.27	0.63
1:E:164:ARG:HD2	1:E:165:TYR:CE2	2.32	0.63
1:F:83:VAL:HG13	1:F:308:ASN:ND2	2.13	0.63
1:D:142:PRO:HA	1:D:175:ARG:O	1.99	0.63
1:D:215:LYS:HZ2	1:D:215:LYS:CB	2.11	0.63
1:A:18:ASN:ND2	1:A:18:ASN:C	2.49	0.63
1:E:171:ILE:N	1:E:171:ILE:HD12	2.14	0.63
1:E:215:LYS:CG	1:E:218:LYS:HZ3	2.10	0.63
1:E:142:PRO:HA	1:E:175:ARG:O	1.99	0.63
1:F:281:ARG:HB3	1:F:282:PRO:CD	2.29	0.63
1:A:55:ARG:NH2	1:B:320:GLN:HA	2.12	0.63
1:D:192:LYS:HE3	1:D:193:MET:O	2.00	0.62
1:B:164:ARG:HD2	1:B:165:TYR:CE2	2.34	0.62
1:A:133:ILE:O	1:A:138:THR:HG23	1.99	0.62
1:B:313:GLU:OE2	1:B:316:ARG:NH2	2.32	0.62
1:F:288:HIS:O	1:F:292:GLU:HG3	2.00	0.62
1:C:182:ARG:NH1	1:C:192:LYS:HD2	2.14	0.62
1:B:8:ILE:HD12	1:B:65:TYR:OH	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LYS:CG	1:E:219:SER:H	2.13	0.62
1:D:22:ALA:O	1:D:26:PHE:CE2	2.52	0.62
1:C:24:ARG:O	1:C:27:VAL:HB	2.00	0.62
1:A:281:ARG:HG3	1:A:282:PRO:HD3	1.81	0.62
1:A:100:GLY:O	1:A:104:ARG:HG3	1.98	0.62
1:F:281:ARG:HH11	1:F:281:ARG:HG3	1.64	0.62
1:A:86:HIS:HD2	1:A:132:ASP:OD1	1.83	0.62
1:E:187:VAL:HG11	1:E:199:ASN:HD22	1.57	0.61
1:D:19:TYR:O	1:D:24:ARG:CB	2.45	0.61
1:C:204:ILE:HG22	1:C:204:ILE:O	1.98	0.61
1:A:212:THR:HG22	1:A:216:LYS:HD2	1.80	0.61
1:E:83:VAL:HG13	1:E:308:ASN:ND2	2.15	0.61
1:A:199:ASN:ND2	1:A:201:LYS:H	1.99	0.61
1:B:281:ARG:HB3	1:B:282:PRO:CD	2.31	0.61
1:C:29:LEU:HD13	1:C:177:PRO:CB	2.30	0.61
1:F:200:PRO:O	1:F:216:LYS:HE2	2.01	0.61
1:C:192:LYS:HE2	4:C:1003:AMP:C5	2.35	0.61
1:E:205:THR:HG22	1:E:207:LEU:N	2.15	0.61
1:E:55:ARG:NH2	1:F:320:GLN:HA	2.14	0.61
1:D:124:THR:HG21	1:C:124:THR:HG21	1.82	0.61
1:E:218:LYS:CG	1:E:219:SER:N	2.62	0.61
1:D:200:PRO:O	1:D:216:LYS:CE	2.40	0.61
1:F:16:ILE:HG23	1:F:204:ILE:O	2.01	0.61
1:D:199:ASN:ND2	1:D:201:LYS:HG3	2.16	0.61
1:F:133:ILE:O	1:F:138:THR:HG23	2.01	0.61
1:B:16:ILE:CG2	1:B:204:ILE:HG22	2.31	0.60
1:C:205:THR:HG23	1:C:206:LEU:N	2.16	0.60
1:D:83:VAL:HG13	1:D:308:ASN:ND2	2.15	0.60
1:D:10:PRO:HA	1:D:61:LEU:HD22	1.82	0.60
1:E:218:LYS:HG3	1:E:219:SER:H	1.64	0.60
1:B:189:PRO:CB	1:B:236:PRO:HB2	2.30	0.60
1:F:4:ILE:HG12	1:F:140:ILE:CG2	2.29	0.60
1:D:173:GLU:CD	1:D:175:ARG:NH1	2.54	0.60
1:A:199:ASN:HD22	1:A:201:LYS:H	1.48	0.60
1:C:86:HIS:HD2	1:C:132:ASP:OD1	1.84	0.60
1:D:133:ILE:O	1:D:138:THR:HG23	2.01	0.60
1:B:200:PRO:HA	1:B:203:TYR:CE2	2.36	0.60
1:D:55:ARG:HH22	1:C:320:GLN:HA	1.65	0.60
1:E:182:ARG:HB3	1:E:184:MET:HE1	1.83	0.60
1:E:86:HIS:HD2	1:E:132:ASP:OD1	1.84	0.60
1:E:200:PRO:HA	1:E:203:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:GLU:HG3	1:D:29:LEU:N	2.17	0.60
1:C:16:ILE:HG21	1:C:204:ILE:CG2	2.31	0.60
1:E:4:ILE:HG12	1:E:140:ILE:CG2	2.31	0.60
1:C:197:ASP:OD1	1:C:198:PRO:HD2	2.00	0.60
1:D:313:GLU:OE2	1:D:316:ARG:NH2	2.35	0.60
1:B:133:ILE:O	1:B:138:THR:HG23	2.02	0.60
1:A:182:ARG:HG2	1:A:184:MET:HE2	1.83	0.59
1:E:245:TYR:CB	1:E:272:LEU:HD13	2.32	0.59
1:B:125:TYR:CG	1:B:126:PRO:HD3	2.37	0.59
1:C:267:VAL:O	1:C:271:ASP:CG	2.41	0.59
1:A:24:ARG:HH11	1:A:24:ARG:CB	2.14	0.59
1:A:29:LEU:CD1	1:A:177:PRO:HG2	2.32	0.59
1:E:212:THR:CG2	1:E:216:LYS:HE3	2.32	0.59
1:E:133:ILE:O	1:E:138:THR:HG23	2.02	0.59
1:B:24:ARG:NH1	1:B:25:GLN:HE22	2.00	0.59
1:B:16:ILE:HG23	1:B:204:ILE:HG22	1.82	0.59
1:A:325:GLY:O	1:B:55:ARG:HD2	2.03	0.59
1:E:254:GLU:O	1:E:258:ARG:HG3	2.02	0.59
1:D:238:ILE:O	1:D:242:LEU:HD12	2.02	0.59
1:F:14:ILE:CG2	1:F:15:THR:H	2.16	0.59
1:E:24:ARG:HG2	1:E:25:GLN:NE2	2.17	0.59
1:B:18:ASN:HD21	4:B:1003:AMP:C1'	2.15	0.59
1:E:125:TYR:CG	1:E:126:PRO:HD3	2.38	0.59
1:F:282:PRO:HB2	1:F:286:ARG:NH2	2.17	0.59
1:F:14:ILE:N	1:F:14:ILE:HD13	2.18	0.59
1:D:19:TYR:O	1:D:24:ARG:N	2.36	0.59
1:B:212:THR:HG22	1:B:216:LYS:HD2	1.84	0.59
1:D:199:ASN:HD21	1:D:201:LYS:HG3	1.67	0.59
1:E:313:GLU:OE2	1:E:316:ARG:NH2	2.35	0.59
1:E:124:THR:HG21	1:F:124:THR:CG2	2.33	0.59
1:F:124:THR:O	1:F:127:PRO:HD2	2.02	0.59
1:F:313:GLU:OE2	1:F:316:ARG:NH2	2.36	0.59
1:C:205:THR:CG2	1:C:206:LEU:N	2.66	0.59
1:C:206:LEU:HD12	1:C:280:LEU:CD1	2.32	0.59
1:D:183:ILE:HD13	1:D:183:ILE:N	2.18	0.58
1:B:18:ASN:ND2	4:B:1003:AMP:C1'	2.65	0.58
1:D:86:HIS:HD2	1:D:132:ASP:OD1	1.86	0.58
1:A:313:GLU:OE2	1:A:316:ARG:NH2	2.35	0.58
1:D:13:VAL:O	1:D:195:LYS:HE2	2.02	0.58
1:A:83:VAL:HG13	1:A:308:ASN:ND2	2.18	0.58
1:C:133:ILE:O	1:C:138:THR:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ASP:OD1	1:F:326:ARG:NH2	2.37	0.58
1:F:193:MET:HB3	4:F:1003:AMP:N6	2.19	0.58
1:A:4:ILE:HG12	1:A:140:ILE:CG2	2.32	0.58
1:D:23:LEU:HD21	1:D:68:VAL:HG21	1.84	0.58
1:A:281:ARG:HG3	1:A:282:PRO:CD	2.34	0.58
1:C:280:LEU:O	1:C:284:GLN:HB2	2.03	0.58
1:B:187:VAL:HG11	1:B:199:ASN:HD22	1.62	0.58
1:A:19:TYR:HA	1:A:23:LEU:HB3	1.86	0.58
1:C:313:GLU:OE2	1:C:316:ARG:NH2	2.34	0.58
1:C:125:TYR:CG	1:C:126:PRO:HD3	2.39	0.58
1:A:29:LEU:HD11	1:A:177:PRO:HG2	1.86	0.58
1:B:281:ARG:NH1	1:B:281:ARG:HG3	2.11	0.58
1:C:134:LEU:HB3	1:C:169:PHE:HD1	1.63	0.58
1:E:262:GLY:N	1:E:263:LYS:HE2	2.19	0.58
1:A:125:TYR:CG	1:A:126:PRO:HD3	2.37	0.58
1:B:86:HIS:HD2	1:B:132:ASP:OD1	1.85	0.58
1:B:271:ASP:O	1:B:275:VAL:HG13	2.04	0.57
1:F:86:HIS:HD2	1:F:132:ASP:OD1	1.85	0.57
1:C:19:TYR:CZ	1:C:24:ARG:HD3	2.39	0.57
1:B:118:VAL:O	1:B:118:VAL:HG23	2.03	0.57
1:B:83:VAL:HG13	1:B:308:ASN:ND2	2.19	0.57
1:B:4:ILE:HG12	1:B:140:ILE:CG2	2.31	0.57
1:D:193:MET:O	4:D:1003:AMP:N6	2.36	0.57
1:E:280:LEU:HB3	1:E:284:GLN:OE1	2.04	0.57
1:F:16:ILE:CG2	1:F:204:ILE:HG22	2.34	0.57
1:F:308:ASN:O	1:F:312:SER:HB2	2.05	0.57
1:E:18:ASN:ND2	4:E:1003:AMP:H8	2.02	0.57
1:B:218:LYS:HA	1:B:269:LYS:HD3	1.85	0.57
1:F:18:ASN:ND2	4:F:1003:AMP:H5'1	2.19	0.57
1:B:24:ARG:HH12	1:B:25:GLN:HE22	1.52	0.57
1:C:217:ILE:O	1:C:269:LYS:HG2	2.04	0.57
1:B:230:TYR:HD2	1:B:253:ILE:HG21	1.70	0.57
1:E:140:ILE:HD11	1:E:175:ARG:HG3	1.86	0.57
1:C:308:ASN:O	1:C:312:SER:HB2	2.05	0.57
1:E:67:ALA:HB2	1:E:287:TYR:HA	1.86	0.57
1:C:155:ARG:NH1	1:C:171:ILE:HG22	2.19	0.57
1:B:184:MET:HG2	1:B:189:PRO:O	2.04	0.57
1:C:210:ALA:HA	1:C:277:ILE:HG12	1.87	0.56
1:C:67:ALA:O	1:C:286:ARG:NH1	2.39	0.56
1:D:22:ALA:C	1:D:26:PHE:CE2	2.78	0.56
1:C:218:LYS:HZ3	1:C:218:LYS:CB	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LYS:CG	1:C:219:SER:N	2.69	0.56
1:D:125:TYR:CG	1:D:126:PRO:HD3	2.40	0.56
1:E:245:TYR:HB2	1:E:272:LEU:HD13	1.85	0.56
1:C:282:PRO:HB2	1:C:286:ARG:HH21	1.69	0.56
1:E:213:ILE:HD13	1:E:276:VAL:HG12	1.87	0.56
1:F:125:TYR:CG	1:F:126:PRO:HD3	2.41	0.56
1:B:205:THR:CG2	1:B:207:LEU:H	2.13	0.56
1:C:19:TYR:O	1:C:24:ARG:HB2	2.05	0.56
1:D:187:VAL:HG13	1:D:202:ALA:CA	2.34	0.56
1:B:254:GLU:O	1:B:258:ARG:HG2	2.05	0.56
1:A:281:ARG:CG	1:A:282:PRO:HD3	2.35	0.56
1:B:23:LEU:O	1:B:26:PHE:HB2	2.06	0.56
1:D:176:ILE:O	1:D:179:VAL:HG13	2.05	0.56
1:D:252:SER:OG	1:D:254:GLU:HG2	2.06	0.56
1:A:308:ASN:O	1:A:312:SER:HB2	2.05	0.56
1:B:229:ARG:HB2	1:B:257:GLU:OE2	2.05	0.55
1:E:297:ASP:CA	1:F:326:ARG:HH12	2.19	0.55
1:C:212:THR:CG2	1:C:216:LYS:HE3	2.36	0.55
1:F:125:TYR:H	1:F:126:PRO:HD2	1.69	0.55
1:A:107:GLN:H	1:A:107:GLN:CD	2.07	0.55
1:E:189:PRO:CG	1:E:236:PRO:HB2	2.37	0.55
1:B:24:ARG:NH1	1:B:25:GLN:NE2	2.54	0.55
1:A:171:ILE:HD13	1:A:171:ILE:N	2.21	0.55
1:F:14:ILE:HG23	1:F:18:ASN:CB	2.37	0.55
1:E:215:LYS:C	1:E:218:LYS:HG2	2.23	0.55
1:C:240:ASN:O	1:C:244:ILE:HG13	2.06	0.55
1:B:22:ALA:HB1	1:B:26:PHE:CE2	2.41	0.55
1:D:187:VAL:HG22	1:D:202:ALA:HB2	1.87	0.55
1:F:278:GLU:OE2	1:F:281:ARG:NE	2.35	0.55
1:D:147:GLN:OE1	1:D:150:HIS:HD2	1.90	0.55
1:E:252:SER:O	1:E:256:LEU:HD12	2.07	0.55
1:B:22:ALA:O	1:B:26:PHE:CE2	2.59	0.55
1:C:192:LYS:CG	1:C:193:MET:N	2.70	0.54
1:E:281:ARG:N	1:E:282:PRO:HD2	2.22	0.54
1:E:189:PRO:CB	1:E:236:PRO:HB2	2.36	0.54
1:E:147:GLN:OE1	1:E:150:HIS:HD2	1.90	0.54
1:A:30:GLN:O	1:A:74:GLN:HG3	2.07	0.54
1:F:13:VAL:HG22	1:F:14:ILE:O	2.08	0.54
1:E:107:GLN:H	1:E:107:GLN:HE21	1.50	0.54
1:D:308:ASN:O	1:D:312:SER:HB2	2.06	0.54
1:A:147:GLN:OE1	1:A:150:HIS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:GLN:OE1	1:B:150:HIS:HD2	1.89	0.54
1:C:245:TYR:CD2	1:C:272:LEU:HD13	2.43	0.54
1:E:189:PRO:HB2	1:E:236:PRO:CB	2.37	0.54
1:C:165:TYR:HB3	1:C:321:ALA:HB1	1.90	0.54
1:E:252:SER:O	1:E:255:GLU:HB2	2.08	0.54
1:C:16:ILE:CG2	1:C:204:ILE:CG2	2.85	0.54
1:B:200:PRO:O	1:B:216:LYS:CE	2.54	0.54
1:F:147:GLN:OE1	1:F:150:HIS:HD2	1.90	0.54
1:E:215:LYS:CG	1:E:218:LYS:NZ	2.71	0.54
1:B:255:GLU:O	1:B:259:GLN:HB3	2.08	0.54
1:C:8:ILE:HD12	1:C:65:TYR:OH	2.08	0.54
1:D:23:LEU:HA	1:D:26:PHE:CD2	2.42	0.53
1:B:60:ARG:HG2	1:B:291:MET:HE1	1.86	0.53
1:D:192:LYS:HG2	1:D:193:MET:N	2.23	0.53
1:E:308:ASN:O	1:E:312:SER:HB2	2.08	0.53
1:C:238:ILE:O	1:C:238:ILE:HG22	2.08	0.53
1:E:42:GLN:HB2	1:E:80:GLN:OE1	2.08	0.53
1:F:18:ASN:HD21	4:F:1003:AMP:C5'	2.20	0.53
1:E:192:LYS:HE2	4:E:1003:AMP:C5	2.42	0.53
1:B:8:ILE:HD12	1:B:65:TYR:CZ	2.43	0.53
1:D:326:ARG:NH1	1:C:297:ASP:HA	2.23	0.53
1:C:245:TYR:CG	1:C:272:LEU:HD13	2.43	0.53
1:D:19:TYR:HD1	1:D:23:LEU:HD23	1.73	0.53
1:F:165:TYR:HB3	1:F:321:ALA:HB1	1.91	0.53
1:F:200:PRO:HA	1:F:203:TYR:CE2	2.44	0.53
1:C:147:GLN:OE1	1:C:150:HIS:HD2	1.91	0.53
1:A:281:ARG:HG3	1:A:282:PRO:N	2.23	0.53
1:D:8:ILE:HD12	1:D:65:TYR:OH	2.08	0.53
1:E:19:TYR:CE2	1:E:24:ARG:HB2	2.44	0.53
1:E:19:TYR:HA	1:E:23:LEU:HB3	1.90	0.53
1:A:126:PRO:CB	1:A:127:PRO:HD3	2.36	0.53
1:E:18:ASN:ND2	4:E:1003:AMP:H5'2	2.22	0.53
1:E:118:VAL:HB	1:F:99:ILE:HG13	1.90	0.53
1:C:185:SER:HB3	1:C:188:ASP:O	2.09	0.53
1:A:199:ASN:C	1:A:199:ASN:HD22	2.11	0.53
1:E:59:ARG:NH2	1:E:296:LEU:HD23	2.23	0.53
1:B:254:GLU:HA	1:B:257:GLU:HB2	1.89	0.53
1:F:281:ARG:HB3	1:F:282:PRO:HD3	1.89	0.53
1:E:187:VAL:HG13	1:E:202:ALA:HA	1.90	0.53
1:E:18:ASN:ND2	4:E:1003:AMP:C8	2.77	0.53
1:A:260:TYR:O	1:A:263:LYS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:VAL:O	1:F:195:LYS:CE	2.57	0.53
1:D:19:TYR:HE1	1:D:68:VAL:HG13	1.74	0.53
1:B:165:TYR:HB3	1:B:321:ALA:HB1	1.91	0.53
1:D:151:ILE:HG13	1:D:174:ALA:HB2	1.90	0.53
1:E:140:ILE:HD11	1:E:175:ARG:HG2	1.87	0.52
1:A:24:ARG:CG	1:A:24:ARG:HH11	2.22	0.52
1:F:187:VAL:CG2	1:F:202:ALA:HB2	2.39	0.52
1:A:326:ARG:NH2	1:B:301:ASP:OD1	2.37	0.52
1:E:140:ILE:HD11	1:E:175:ARG:CD	2.39	0.52
1:E:237:GLY:O	1:E:241:LEU:HD22	2.10	0.52
1:B:281:ARG:HB3	1:B:282:PRO:HD3	1.90	0.52
1:F:105:MET:HE2	1:F:150:HIS:HE1	1.69	0.52
1:E:263:LYS:N	1:E:263:LYS:CD	2.67	0.52
1:A:125:TYR:CD2	1:A:126:PRO:HD3	2.45	0.52
1:B:23:LEU:CA	1:B:26:PHE:CD2	2.68	0.52
1:B:229:ARG:CG	1:B:230:TYR:N	2.71	0.52
1:B:27:VAL:CG2	1:B:68:VAL:HG12	2.40	0.52
1:C:281:ARG:HB3	1:C:282:PRO:CD	2.39	0.52
1:B:125:TYR:CD2	1:B:126:PRO:HD3	2.45	0.52
1:C:42:GLN:HB2	1:C:80:GLN:OE1	2.09	0.52
1:B:288:HIS:O	1:B:292:GLU:HG2	2.09	0.52
1:B:42:GLN:HB2	1:B:80:GLN:OE1	2.09	0.52
1:C:192:LYS:NZ	4:C:1003:AMP:H2'	2.25	0.52
1:E:281:ARG:N	1:E:281:ARG:HD2	2.24	0.52
1:C:134:LEU:HB3	1:C:169:PHE:CE1	2.45	0.52
1:F:249:SER:OG	1:F:251:GLN:HG3	2.09	0.52
1:B:24:ARG:HH12	1:B:25:GLN:NE2	2.08	0.52
1:C:192:LYS:HE2	4:C:1003:AMP:C6	2.44	0.51
1:C:23:LEU:HA	1:C:26:PHE:HD2	1.74	0.51
1:A:165:TYR:HB3	1:A:321:ALA:HB1	1.92	0.51
1:E:183:ILE:HB	4:E:1003:AMP:HN62	1.74	0.51
1:B:22:ALA:C	1:B:26:PHE:CD2	2.83	0.51
1:A:106:THR:HB	1:A:107:GLN:NE2	2.25	0.51
1:B:254:GLU:HA	1:B:257:GLU:OE1	2.10	0.51
1:E:8:ILE:HD12	1:E:65:TYR:OH	2.10	0.51
1:B:188:ASP:OD1	1:B:190:THR:OG1	2.28	0.51
1:D:13:VAL:HG22	1:D:14:ILE:N	2.24	0.51
1:E:125:TYR:CD2	1:E:126:PRO:HD3	2.45	0.51
1:E:289:HIS:HA	1:E:292:GLU:OE2	2.10	0.51
1:D:293:SER:OG	1:D:295:GLU:HB2	2.10	0.51
1:A:249:SER:OG	1:A:251:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:TYR:CE1	1:E:24:ARG:HB2	2.46	0.51
1:C:277:ILE:O	1:C:281:ARG:HB2	2.10	0.51
1:C:281:ARG:HB3	1:C:282:PRO:HD3	1.91	0.51
1:C:125:TYR:CD2	1:C:126:PRO:HD3	2.45	0.51
1:E:293:SER:OG	1:E:295:GLU:HB2	2.11	0.51
1:E:165:TYR:HB3	1:E:321:ALA:HB1	1.92	0.51
1:B:197:ASP:OD1	1:B:198:PRO:HD2	2.11	0.51
1:B:272:LEU:O	1:B:275:VAL:HG22	2.10	0.51
1:D:245:TYR:CD2	1:D:272:LEU:HD13	2.45	0.51
1:B:201:LYS:HA	1:B:216:LYS:HE2	1.91	0.51
1:C:96:ILE:HG13	1:C:157:LEU:HD22	1.93	0.51
1:C:206:LEU:HD12	1:C:280:LEU:HD13	1.93	0.51
1:C:16:ILE:O	1:C:20:ILE:CD1	2.55	0.51
1:D:125:TYR:CD2	1:D:126:PRO:HD3	2.45	0.51
1:B:126:PRO:CB	1:B:127:PRO:HD3	2.36	0.50
1:D:183:ILE:HG22	1:D:193:MET:HE3	1.93	0.50
1:E:124:THR:HG21	1:F:124:THR:HG21	1.93	0.50
1:B:22:ALA:C	1:B:26:PHE:CE2	2.85	0.50
1:C:182:ARG:NH1	1:C:192:LYS:HB2	2.25	0.50
1:D:13:VAL:CG2	1:D:14:ILE:N	2.74	0.50
1:C:125:TYR:N	1:C:126:PRO:CD	2.75	0.50
1:E:182:ARG:HG2	1:E:192:LYS:HG3	1.93	0.50
1:D:249:SER:OG	1:D:251:GLN:HG3	2.12	0.50
3:F:1002:PO4:O3	4:F:1003:AMP:O1P	2.30	0.50
1:E:107:GLN:N	1:E:107:GLN:NE2	2.50	0.50
1:D:197:ASP:OD1	1:D:198:PRO:HD2	2.11	0.50
1:C:126:PRO:HB2	1:C:127:PRO:CD	2.38	0.50
1:E:295:GLU:HG2	1:E:298:ARG:CZ	2.42	0.50
1:A:326:ARG:NH1	1:B:297:ASP:HA	2.26	0.50
1:F:42:GLN:HB2	1:F:80:GLN:OE1	2.12	0.50
1:C:271:ASP:O	1:C:275:VAL:HG12	2.12	0.50
1:E:261:GLU:O	1:E:263:LYS:HE2	2.11	0.50
1:F:187:VAL:HG22	1:F:202:ALA:CB	2.41	0.50
1:E:18:ASN:HD22	4:E:1003:AMP:H5'2	1.78	0.49
1:C:182:ARG:HH12	1:C:192:LYS:HD2	1.75	0.49
1:D:22:ALA:CB	1:D:26:PHE:HE2	2.21	0.49
1:F:187:VAL:HG22	1:F:202:ALA:HB2	1.94	0.49
1:D:42:GLN:HB2	1:D:80:GLN:OE1	2.12	0.49
1:D:125:TYR:N	1:D:126:PRO:CD	2.74	0.49
1:A:140:ILE:CG1	1:A:175:ARG:HB3	2.42	0.49
1:E:125:TYR:N	1:E:126:PRO:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:LEU:HB3	1:E:169:PHE:HD1	1.72	0.49
1:D:60:ARG:HG2	1:D:291:MET:HE2	1.93	0.49
1:D:173:GLU:OE2	1:D:175:ARG:NH1	2.46	0.49
1:E:217:ILE:HD12	1:E:273:ALA:HA	1.95	0.49
1:B:304:ALA:O	1:B:308:ASN:N	2.45	0.49
1:E:126:PRO:CB	1:E:127:PRO:HD3	2.36	0.49
3:D:1002:PO4:O4	4:D:1003:AMP:H8	1.96	0.49
1:B:125:TYR:N	1:B:126:PRO:CD	2.76	0.48
1:D:9:GLN:HE21	1:D:10:PRO:HD2	1.77	0.48
1:B:30:GLN:O	1:B:74:GLN:HG3	2.13	0.48
1:A:97:VAL:O	1:B:119:SER:HA	2.13	0.48
1:E:125:TYR:N	1:E:126:PRO:CD	2.75	0.48
1:C:148:LYS:O	1:C:152:GLU:HG3	2.14	0.48
1:B:98:TYR:HB2	1:B:101:GLU:HG3	1.96	0.48
1:D:256:LEU:HG	1:D:256:LEU:H	1.47	0.48
1:E:124:THR:HG21	1:F:124:THR:HG22	1.94	0.48
1:F:126:PRO:CB	1:F:127:PRO:HD3	2.37	0.48
1:C:188:ASP:HB3	1:C:191:LYS:HB2	1.95	0.48
1:D:217:ILE:HA	1:D:220:ALA:HB2	1.95	0.48
1:D:192:LYS:NZ	3:D:1002:PO4:O3	2.42	0.48
1:D:60:ARG:HG2	1:D:291:MET:CE	2.43	0.48
1:F:140:ILE:CG1	1:F:175:ARG:HB3	2.43	0.48
1:A:99:ILE:HG13	1:B:118:VAL:CG2	2.38	0.48
1:C:16:ILE:HG21	1:C:204:ILE:HG22	1.90	0.48
1:A:125:TYR:N	1:A:126:PRO:CD	2.76	0.48
1:A:126:PRO:HB2	1:A:127:PRO:CD	2.39	0.48
1:E:148:LYS:O	1:E:152:GLU:HG3	2.14	0.48
1:F:309:ARG:HB3	1:F:309:ARG:HE	1.50	0.48
1:B:125:TYR:N	1:B:126:PRO:HD2	2.29	0.48
1:A:148:LYS:O	1:A:152:GLU:HG3	2.12	0.48
1:E:261:GLU:CG	1:E:261:GLU:O	2.56	0.48
1:B:184:MET:CG	1:B:191:LYS:O	2.57	0.48
1:D:16:ILE:CD1	1:D:204:ILE:HB	2.43	0.48
1:F:148:LYS:O	1:F:152:GLU:HG3	2.14	0.48
1:D:215:LYS:O	1:D:219:SER:OG	2.31	0.48
1:C:125:TYR:N	1:C:126:PRO:HD2	2.28	0.48
1:C:186:LEU:HB2	1:C:201:LYS:O	2.14	0.48
1:F:98:TYR:HB2	1:F:101:GLU:HG3	1.96	0.48
1:A:18:ASN:ND2	1:A:18:ASN:O	2.42	0.47
1:B:198:PRO:HA	1:C:198:PRO:HA	1.95	0.47
1:F:218:LYS:HA	1:F:269:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:TYR:N	1:D:126:PRO:HD2	2.29	0.47
1:D:281:ARG:N	1:D:282:PRO:HD2	2.30	0.47
1:E:86:HIS:HE1	1:E:136:TYR:OH	1.97	0.47
1:B:148:LYS:O	1:B:152:GLU:HG3	2.14	0.47
1:A:42:GLN:HB2	1:A:80:GLN:OE1	2.14	0.47
1:A:118:VAL:O	1:B:98:TYR:HA	2.14	0.47
1:B:254:GLU:O	1:B:257:GLU:N	2.44	0.47
1:F:126:PRO:HB2	1:F:127:PRO:CD	2.39	0.47
1:C:86:HIS:HE1	1:C:136:TYR:OH	1.98	0.47
1:D:251:GLN:HG3	1:D:256:LEU:CD2	2.45	0.47
1:B:9:GLN:OE1	1:B:40:VAL:HG23	2.14	0.47
1:E:98:TYR:HB2	1:E:101:GLU:HG3	1.96	0.47
1:E:197:ASP:OD1	1:E:198:PRO:N	2.47	0.47
1:C:192:LYS:HZ3	4:C:1003:AMP:H2'	1.79	0.47
1:C:210:ALA:HB1	1:C:277:ILE:CD1	2.32	0.47
1:A:125:TYR:N	1:A:126:PRO:HD2	2.29	0.47
1:D:55:ARG:HD2	1:C:325:GLY:O	2.13	0.47
1:A:140:ILE:HD11	1:A:175:ARG:CB	2.43	0.47
1:C:126:PRO:CB	1:C:127:PRO:HD3	2.36	0.47
1:B:21:GLY:HA3	4:B:1003:AMP:C2	2.48	0.47
1:F:5:PHE:HB2	1:F:138:THR:HG21	1.97	0.47
1:B:5:PHE:HB2	1:B:138:THR:HG21	1.95	0.47
1:A:140:ILE:CD1	1:A:175:ARG:HB3	2.42	0.47
1:B:134:LEU:HB3	1:B:169:PHE:CE1	2.48	0.47
1:A:281:ARG:N	1:A:282:PRO:HD2	2.29	0.47
1:E:212:THR:HG22	1:E:216:LYS:HE3	1.97	0.47
1:C:213:ILE:O	1:C:217:ILE:HG13	2.14	0.47
1:F:188:ASP:CB	1:F:191:LYS:HB3	2.39	0.47
1:C:59:ARG:NH2	1:C:296:LEU:HD23	2.29	0.47
1:A:98:TYR:HB2	1:A:101:GLU:HG3	1.97	0.47
1:F:199:ASN:HD22	1:F:200:PRO:CD	2.28	0.47
1:B:27:VAL:CG2	1:B:68:VAL:CG1	2.93	0.47
1:B:228:ILE:CD1	1:B:268:PHE:HB2	2.45	0.47
1:B:189:PRO:CG	1:B:236:PRO:HB2	2.45	0.47
1:A:86:HIS:HE1	1:A:136:TYR:OH	1.97	0.47
1:E:245:TYR:CD2	1:E:272:LEU:HB2	2.50	0.47
1:D:86:HIS:HE1	1:D:136:TYR:OH	1.98	0.47
1:B:86:HIS:HE1	1:B:136:TYR:OH	1.97	0.47
1:B:19:TYR:CE2	1:B:24:ARG:CD	2.98	0.47
1:D:118:VAL:HB	1:C:99:ILE:HG13	1.97	0.47
1:C:272:LEU:HD12	1:C:275:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ILE:HA	1:E:241:LEU:HD22	1.96	0.46
1:A:5:PHE:HB2	1:A:138:THR:HG21	1.97	0.46
1:D:148:LYS:O	1:D:152:GLU:HG3	2.15	0.46
1:A:118:VAL:HG12	1:A:118:VAL:O	2.15	0.46
1:C:23:LEU:CD1	1:C:23:LEU:C	2.83	0.46
1:C:26:PHE:HB3	1:C:37:PHE:HZ	1.80	0.46
1:F:123:LEU:O	1:F:126:PRO:HD2	2.15	0.46
1:F:14:ILE:CG2	1:F:18:ASN:CB	2.94	0.46
1:D:140:ILE:CD1	1:D:175:ARG:HD2	2.37	0.46
1:D:19:TYR:CZ	1:D:24:ARG:HG3	2.49	0.46
1:E:281:ARG:HA	1:E:281:ARG:HE	1.75	0.46
1:F:124:THR:C	1:F:127:PRO:HD2	2.35	0.46
1:B:182:ARG:NE	1:B:192:LYS:HD3	2.30	0.46
1:A:187:VAL:HG13	1:A:202:ALA:HA	1.98	0.46
1:E:27:VAL:HG12	1:E:27:VAL:O	2.14	0.46
1:A:118:VAL:HG11	1:B:99:ILE:HG13	1.78	0.46
1:C:277:ILE:O	1:C:277:ILE:HG22	2.15	0.46
1:B:126:PRO:HB2	1:B:127:PRO:CD	2.38	0.46
1:D:126:PRO:CB	1:D:127:PRO:HD3	2.37	0.46
1:B:230:TYR:HB2	1:B:242:LEU:HD13	1.98	0.46
1:F:125:TYR:CD2	1:F:126:PRO:HD3	2.50	0.46
1:F:281:ARG:NH1	1:F:281:ARG:HG3	2.29	0.46
1:F:19:TYR:CE2	1:F:24:ARG:HB2	2.51	0.46
1:E:5:PHE:HB2	1:E:138:THR:HG21	1.98	0.46
1:D:239:SER:HA	1:D:242:LEU:HB2	1.98	0.46
1:D:123:LEU:HG	1:D:123:LEU:O	2.16	0.46
1:B:18:ASN:ND2	4:B:1003:AMP:O4'	2.33	0.46
1:F:295:GLU:HG2	1:F:298:ARG:HE	1.81	0.46
1:C:271:ASP:O	1:C:275:VAL:CG1	2.64	0.46
1:E:258:ARG:CB	1:E:258:ARG:CZ	2.94	0.46
1:F:9:GLN:HG2	1:F:40:VAL:CG2	2.46	0.46
1:E:277:ILE:HG23	1:E:281:ARG:HD3	1.96	0.46
1:C:176:ILE:HG21	1:C:179:VAL:CG1	2.43	0.46
1:A:55:ARG:HD2	1:B:325:GLY:O	2.16	0.46
1:A:192:LYS:HE2	4:A:1003:AMP:C6	2.51	0.46
1:D:5:PHE:HB2	1:D:138:THR:HG21	1.98	0.46
1:D:215:LYS:HB2	1:D:215:LYS:HZ2	1.81	0.45
3:B:1002:PO4:P	4:B:1003:AMP:H5'1	2.56	0.45
1:C:98:TYR:HB2	1:C:101:GLU:HG3	1.97	0.45
1:C:141:VAL:O	1:C:174:ALA:HA	2.15	0.45
1:D:98:TYR:HB2	1:D:101:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ILE:H	1:E:171:ILE:HD12	1.81	0.45
1:D:10:PRO:O	1:D:57:ASN:HB3	2.17	0.45
1:C:195:LYS:HB3	1:C:195:LYS:HE3	1.76	0.45
1:F:164:ARG:HD2	1:F:165:TYR:CZ	2.50	0.45
1:A:29:LEU:HD13	1:A:177:PRO:CG	2.46	0.45
1:F:16:ILE:HG21	1:F:204:ILE:CG2	2.47	0.45
1:B:24:ARG:CG	1:B:24:ARG:HH11	2.30	0.45
1:D:19:TYR:CE2	1:D:24:ARG:HG3	2.52	0.45
1:D:56:GLN:O	1:D:60:ARG:HG3	2.16	0.45
1:E:242:LEU:O	1:E:246:SER:HB3	2.16	0.45
1:F:86:HIS:HE1	1:F:136:TYR:OH	1.99	0.45
1:A:120:ALA:HA	1:B:99:ILE:CD1	2.47	0.45
1:C:206:LEU:HD11	1:C:280:LEU:HD21	1.79	0.45
1:B:198:PRO:HB3	1:C:196:SER:O	2.16	0.45
1:E:254:GLU:H	1:E:254:GLU:HG2	1.45	0.45
1:B:27:VAL:HG21	1:B:68:VAL:CG1	2.47	0.45
1:E:219:SER:OG	1:E:219:SER:O	2.32	0.45
1:D:173:GLU:OE1	1:D:175:ARG:NH1	2.44	0.45
1:A:24:ARG:NH1	1:A:24:ARG:CG	2.79	0.45
1:D:209:ASP:O	1:D:213:ILE:HG13	2.16	0.45
1:A:198:PRO:O	1:A:200:PRO:HD3	2.17	0.45
1:D:126:PRO:HB2	1:D:127:PRO:CD	2.40	0.45
1:E:56:GLN:O	1:E:60:ARG:HG3	2.17	0.44
1:B:229:ARG:HG3	1:B:230:TYR:H	1.82	0.44
1:C:272:LEU:HD12	1:C:275:VAL:HG22	1.99	0.44
1:F:125:TYR:C	1:F:125:TYR:CD1	2.89	0.44
1:D:23:LEU:HG	1:D:68:VAL:HG11	2.00	0.44
1:C:5:PHE:HB2	1:C:138:THR:HG21	1.98	0.44
1:C:56:GLN:O	1:C:60:ARG:HG3	2.17	0.44
1:E:305:GLU:O	1:E:309:ARG:CG	2.54	0.44
1:F:199:ASN:HD22	1:F:200:PRO:HD2	1.82	0.44
1:F:56:GLN:O	1:F:60:ARG:HG3	2.18	0.44
1:F:13:VAL:O	1:F:195:LYS:HE3	2.17	0.44
1:C:182:ARG:NH1	1:C:192:LYS:CB	2.81	0.44
1:A:192:LYS:CE	4:A:1003:AMP:C5	2.99	0.44
1:E:20:ILE:O	1:E:20:ILE:HG22	2.16	0.44
1:C:210:ALA:HB2	1:C:277:ILE:HG21	1.99	0.44
1:F:19:TYR:HA	1:F:23:LEU:CB	2.46	0.44
1:E:171:ILE:N	1:E:171:ILE:CD1	2.80	0.44
1:A:56:GLN:O	1:A:60:ARG:HG3	2.17	0.44
1:B:281:ARG:CG	1:B:281:ARG:NH1	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLN:O	1:B:60:ARG:HG3	2.18	0.44
1:E:241:LEU:HD13	1:E:241:LEU:N	2.33	0.44
1:C:309:ARG:HB3	1:C:309:ARG:HE	1.27	0.44
1:E:215:LYS:HG2	1:E:218:LYS:NZ	2.31	0.43
1:B:19:TYR:HA	1:B:23:LEU:HB3	2.00	0.43
1:E:185:SER:HB3	1:E:188:ASP:O	2.18	0.43
1:E:277:ILE:O	1:E:281:ARG:HD2	2.18	0.43
1:B:18:ASN:CG	4:B:1003:AMP:C8	2.92	0.43
1:E:120:ALA:HA	1:F:99:ILE:CD1	2.48	0.43
1:E:98:TYR:HA	1:F:118:VAL:O	2.18	0.43
1:F:14:ILE:HG22	1:F:15:THR:H	1.76	0.43
1:E:213:ILE:HD12	1:E:277:ILE:HG13	2.00	0.43
1:B:64:LEU:HD21	1:B:207:LEU:HD21	1.99	0.43
1:B:294:GLU:HB2	1:B:298:ARG:NH2	2.33	0.43
1:B:230:TYR:C	1:B:230:TYR:CD1	2.90	0.43
1:A:29:LEU:CD1	1:A:177:PRO:CG	2.95	0.43
1:E:260:TYR:CE2	1:E:268:PHE:HA	2.54	0.43
1:F:170:THR:O	1:F:172:PRO:HD3	2.18	0.43
1:C:155:ARG:HG2	1:C:172:PRO:HD2	2.00	0.43
1:B:241:LEU:HB3	1:B:268:PHE:HE2	1.83	0.43
1:F:9:GLN:OE1	1:F:43:HIS:HB3	2.18	0.43
1:B:22:ALA:HB1	1:B:26:PHE:HE2	1.82	0.43
1:A:124:THR:HG21	1:B:124:THR:CG2	2.45	0.43
1:B:60:ARG:HA	1:B:291:MET:HE2	2.01	0.43
1:B:258:ARG:HG3	1:B:258:ARG:HH11	1.84	0.43
1:E:295:GLU:HG2	1:E:298:ARG:HH21	1.83	0.43
1:A:124:THR:CG2	1:B:124:THR:HG21	2.45	0.43
1:D:187:VAL:CG2	1:D:202:ALA:HB2	2.49	0.43
1:E:189:PRO:HG2	1:E:236:PRO:HB2	2.01	0.43
1:E:170:THR:O	1:E:172:PRO:HD3	2.18	0.43
1:E:134:LEU:HB3	1:E:169:PHE:CE1	2.54	0.43
1:A:195:LYS:N	3:A:1002:PO4:O1	2.32	0.43
1:C:188:ASP:HB3	1:C:191:LYS:CB	2.49	0.43
1:A:309:ARG:HB3	1:A:309:ARG:HE	1.27	0.43
1:D:309:ARG:HE	1:D:309:ARG:HB3	1.27	0.43
1:B:215:LYS:O	1:B:219:SER:OG	2.29	0.43
1:D:215:LYS:HZ2	1:D:215:LYS:HB3	1.66	0.42
1:A:140:ILE:HD11	1:A:175:ARG:CG	2.48	0.42
1:F:273:ALA:O	1:F:277:ILE:HD12	2.19	0.42
1:E:123:LEU:HG	1:E:123:LEU:O	2.19	0.42
1:D:194:SER:HA	3:D:1002:PO4:O1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1002:PO4:O4	4:A:1003:AMP:O1P	2.37	0.42
1:D:79:ILE:HB	1:D:82:GLU:HG3	2.01	0.42
1:D:189:PRO:HG2	1:E:48:TRP:CE2	2.54	0.42
1:B:302:GLU:O	1:B:306:LYS:HG3	2.18	0.42
1:C:218:LYS:HG2	1:C:219:SER:H	1.84	0.42
1:E:99:ILE:CD1	1:F:120:ALA:HA	2.50	0.42
1:F:16:ILE:HG13	1:F:17:GLY:N	2.34	0.42
1:B:19:TYR:CE2	1:B:24:ARG:HD2	2.55	0.42
1:E:55:ARG:NH1	1:F:324:LEU:O	2.52	0.42
1:E:265:TYR:O	1:E:269:LYS:CG	2.64	0.42
1:F:24:ARG:NH1	1:F:247:THR:O	2.53	0.42
1:B:119:SER:C	1:B:121:GLY:N	2.72	0.42
1:F:11:SER:HB2	1:F:195:LYS:HD2	2.01	0.42
1:C:293:SER:OG	1:C:295:GLU:HB2	2.19	0.42
1:C:23:LEU:HA	1:C:26:PHE:CD2	2.53	0.42
1:C:30:GLN:O	1:C:74:GLN:HG3	2.20	0.42
1:E:245:TYR:CG	1:E:272:LEU:HD13	2.55	0.42
1:B:205:THR:HG23	1:B:207:LEU:N	2.16	0.42
1:E:126:PRO:HB2	1:E:127:PRO:CD	2.38	0.42
1:E:183:ILE:HB	4:E:1003:AMP:N6	2.34	0.42
1:D:10:PRO:HA	1:D:61:LEU:CD2	2.49	0.42
1:D:151:ILE:HG21	1:D:174:ALA:HB2	2.02	0.42
1:D:51:PRO:HA	1:C:323:GLY:HA3	2.02	0.42
1:A:4:ILE:HG23	1:A:140:ILE:CG2	2.50	0.42
1:F:14:ILE:CG2	1:F:18:ASN:HB3	2.49	0.41
1:B:25:GLN:O	1:B:29:LEU:HG	2.19	0.41
1:E:210:ALA:HA	1:E:277:ILE:HG12	2.01	0.41
1:A:123:LEU:O	1:A:123:LEU:HG	2.20	0.41
1:A:281:ARG:CG	1:A:282:PRO:CD	2.97	0.41
1:B:192:LYS:HB3	1:B:192:LYS:HE2	1.48	0.41
1:C:211:LYS:HE3	1:C:211:LYS:HB3	1.82	0.41
1:A:96:ILE:HG13	1:A:157:LEU:HD22	2.02	0.41
1:C:17:GLY:HA3	4:C:1003:AMP:N6	2.35	0.41
1:B:278:GLU:HA	1:B:278:GLU:OE1	2.18	0.41
1:B:308:ASN:HA	1:B:308:ASN:HD22	1.66	0.41
1:F:151:ILE:O	1:F:154:THR:HG23	2.20	0.41
1:E:189:PRO:HB3	1:E:237:GLY:CA	2.46	0.41
1:E:64:LEU:HG	1:E:287:TYR:CE1	2.55	0.41
1:A:146:ASP:N	1:A:146:ASP:OD1	2.50	0.41
1:B:238:ILE:HA	1:B:238:ILE:HD13	1.79	0.41
1:C:267:VAL:O	1:C:271:ASP:OD2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:THR:O	1:D:215:LYS:HG2	2.20	0.41
1:C:26:PHE:HB3	1:C:37:PHE:CZ	2.55	0.41
1:E:258:ARG:HB2	1:E:258:ARG:NH2	2.35	0.41
1:A:67:ALA:O	1:A:286:ARG:NH1	2.51	0.41
1:F:4:ILE:HG23	1:F:140:ILE:HG23	2.02	0.41
1:D:176:ILE:HB	1:D:179:VAL:CG1	2.40	0.41
1:C:29:LEU:HD11	1:C:177:PRO:HB2	1.96	0.41
1:A:107:GLN:CD	1:A:107:GLN:N	2.74	0.41
1:E:308:ASN:HD22	1:E:308:ASN:HA	1.62	0.41
1:A:151:ILE:HG21	1:A:174:ALA:HB2	2.03	0.41
1:F:14:ILE:N	1:F:14:ILE:CD1	2.83	0.41
1:E:289:HIS:O	1:E:292:GLU:HG3	2.20	0.41
1:F:105:MET:HE1	1:F:150:HIS:CE1	2.55	0.41
1:B:118:VAL:O	1:B:118:VAL:CG2	2.68	0.41
1:A:79:ILE:HB	1:A:82:GLU:HG3	2.02	0.41
1:B:71:ASP:HA	1:B:72:PRO:HD2	1.91	0.41
1:F:205:THR:CG2	1:F:206:LEU:N	2.83	0.41
1:F:104:ARG:CG	1:F:104:ARG:NH1	2.65	0.41
1:B:187:VAL:HG21	1:B:199:ASN:HD22	1.85	0.41
1:E:140:ILE:HD11	1:E:175:ARG:HD3	2.03	0.41
1:A:260:TYR:HH	1:A:271:ASP:CG	2.23	0.41
1:E:71:ASP:HA	1:E:72:PRO:HD2	1.91	0.41
1:E:21:GLY:O	1:E:179:VAL:HG23	2.20	0.41
1:E:187:VAL:HG13	1:E:202:ALA:CA	2.51	0.41
1:C:187:VAL:CG2	1:C:199:ASN:OD1	2.46	0.41
1:E:205:THR:HG23	1:E:207:LEU:H	1.79	0.41
1:F:184:MET:CG	1:F:189:PRO:O	2.66	0.41
1:A:195:LYS:HG2	3:A:1002:PO4:O1	2.21	0.41
1:E:79:ILE:HB	1:E:82:GLU:HG3	2.02	0.41
1:B:79:ILE:HB	1:B:82:GLU:HG3	2.01	0.41
1:B:19:TYR:CE2	1:B:24:ARG:HD3	2.56	0.41
1:B:25:GLN:H	1:B:25:GLN:CD	2.25	0.41
1:B:229:ARG:CG	1:B:230:TYR:H	2.33	0.41
1:B:200:PRO:O	1:B:216:LYS:NZ	2.54	0.41
1:E:151:ILE:O	1:E:154:THR:HG23	2.20	0.41
1:F:79:ILE:HB	1:F:82:GLU:HG3	2.03	0.41
1:B:123:LEU:HG	1:B:123:LEU:O	2.20	0.41
1:B:19:TYR:O	1:B:24:ARG:HB2	2.21	0.40
1:B:258:ARG:H	1:B:258:ARG:HG2	1.37	0.40
1:C:183:ILE:HD13	1:C:183:ILE:N	2.37	0.40
1:D:182:ARG:HE	1:D:184:MET:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASN:O	1:B:312:SER:HB2	2.21	0.40
1:E:118:VAL:O	1:F:99:ILE:CG1	2.69	0.40
1:A:1:MET:SD	1:A:32:GLU:O	2.79	0.40
1:C:123:LEU:O	1:C:123:LEU:HG	2.21	0.40
1:E:24:ARG:CG	1:E:24:ARG:O	2.69	0.40
1:E:213:ILE:CD1	1:E:277:ILE:HG13	2.51	0.40
1:B:134:LEU:HB3	1:B:169:PHE:HD1	1.72	0.40
1:F:161:PHE:CD2	1:F:169:PHE:HE2	2.39	0.40
1:D:14:ILE:HG22	1:D:18:ASN:HB3	2.04	0.40
1:E:283:ILE:N	1:E:286:ARG:HH21	2.19	0.40
1:C:151:ILE:O	1:C:154:THR:HG23	2.21	0.40
1:E:272:LEU:HA	1:E:275:VAL:HG13	2.04	0.40
1:E:96:ILE:HG13	1:E:157:LEU:HD22	2.03	0.40
1:B:225:GLU:OE1	1:B:227:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/328 (88%)	279 (97%)	7 (2%)	1 (0%)	46	72
1	B	277/328 (84%)	269 (97%)	8 (3%)	0	100	100
1	C	265/328 (81%)	250 (94%)	15 (6%)	0	100	100
1	D	276/328 (84%)	263 (95%)	13 (5%)	0	100	100
1	E	282/328 (86%)	263 (93%)	19 (7%)	0	100	100
1	F	284/328 (87%)	273 (96%)	11 (4%)	0	100	100
All	All	1671/1968 (85%)	1597 (96%)	73 (4%)	1 (0%)	56	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	PRO

### 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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/280 (92%)	216 (84%)	42 (16%)	3	6
1	B	253/280 (90%)	208 (82%)	45 (18%)	2	4
1	C	241/280 (86%)	199 (83%)	42 (17%)	2	5
1	D	248/280 (89%)	203 (82%)	45 (18%)	2	4
1	E	252/280 (90%)	209 (83%)	43 (17%)	2	5
1	F	256/280 (91%)	214 (84%)	42 (16%)	3	6
All	All	1508/1680 (90%)	1249 (83%)	259 (17%)	2	5

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	ILE
1	A	9	GLN
1	A	18	ASN
1	A	24	ARG
1	A	25	GLN
1	A	28	GLU
1	A	55	ARG
1	A	56	GLN
1	A	59	ARG
1	A	94	GLN
1	A	99	ILE
1	A	107	GLN
1	A	122	LEU
1	A	138	THR
1	A	146	ASP
1	A	154	THR
1	A	159	GLU

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Mol	Chain	Res	Type
1	A	164	ARG
1	A	171	ILE
1	A	182	ARG
1	A	185	SER
1	A	187	VAL
1	A	191	LYS
1	A	196	SER
1	A	199	ASN
1	A	211	LYS
1	A	224	SER
1	A	225	GLU
1	A	227	THR
1	A	228	ILE
1	A	238	ILE
1	A	241	LEU
1	A	245	TYR
1	A	255	GLU
1	A	271	ASP
1	A	275	VAL
1	A	281	ARG
1	A	308	ASN
1	A	309	ARG
1	A	312	SER
1	A	316	ARG
1	D	1	MET
1	D	8	ILE
1	D	14	ILE
1	D	16	ILE
1	D	28	GLU
1	D	32	GLU
1	D	55	ARG
1	D	56	GLN
1	D	59	ARG
1	D	94	GLN
1	D	99	ILE
1	D	118	VAL
1	D	119	SER
1	D	122	LEU
1	D	138	THR
1	D	146	ASP
1	D	154	THR
1	D	159	GLU

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Mol	Chain	Res	Type
1	D	173	GLU
1	D	175	ARG
1	D	182	ARG
1	D	192	LYS
1	D	195	LYS
1	D	199	ASN
1	D	205	THR
1	D	211	LYS
1	D	215	LYS
1	D	217	ILE
1	D	219	SER
1	D	239	SER
1	D	241	LEU
1	D	242	LEU
1	D	243	ASN
1	D	251	GLN
1	D	256	LEU
1	D	271	ASP
1	D	274	GLN
1	D	278	GLU
1	D	281	ARG
1	D	285	GLU
1	D	294	GLU
1	D	308	ASN
1	D	309	ARG
1	D	312	SER
1	D	316	ARG
1	B	8	ILE
1	B	16	ILE
1	B	18	ASN
1	B	24	ARG
1	B	55	ARG
1	B	56	GLN
1	B	59	ARG
1	B	94	GLN
1	B	99	ILE
1	B	107	GLN
1	B	122	LEU
1	B	138	THR
1	B	146	ASP
1	B	154	THR
1	B	159	GLU

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Mol	Chain	Res	Type
1	B	164	ARG
1	B	182	ARG
1	B	185	SER
1	B	191	LYS
1	B	192	LYS
1	B	194	SER
1	B	197	ASP
1	B	205	THR
1	B	211	LYS
1	B	227	THR
1	B	229	ARG
1	B	241	LEU
1	B	245	TYR
1	B	251	GLN
1	B	252	SER
1	B	254	GLU
1	B	257	GLU
1	B	258	ARG
1	B	259	GLN
1	B	263	LYS
1	B	274	GLN
1	B	275	VAL
1	B	278	GLU
1	B	289	HIS
1	B	293	SER
1	B	294	GLU
1	B	298	ARG
1	B	308	ASN
1	B	312	SER
1	B	316	ARG
1	C	1	MET
1	C	8	ILE
1	C	16	ILE
1	C	23	LEU
1	C	55	ARG
1	C	56	GLN
1	C	59	ARG
1	C	94	GLN
1	C	99	ILE
1	C	107	GLN
1	C	119	SER
1	C	122	LEU

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Mol	Chain	Res	Type
1	C	138	THR
1	C	146	ASP
1	C	154	THR
1	C	159	GLU
1	C	164	ARG
1	C	179	VAL
1	C	182	ARG
1	C	183	ILE
1	C	195	LYS
1	C	196	SER
1	C	204	ILE
1	C	205	THR
1	C	207	LEU
1	C	211	LYS
1	C	217	ILE
1	C	218	LYS
1	C	219	SER
1	C	225	GLU
1	C	227	THR
1	C	241	LEU
1	C	245	TYR
1	C	248	LEU
1	C	278	GLU
1	C	285	GLU
1	C	289	HIS
1	C	293	SER
1	C	308	ASN
1	C	309	ARG
1	C	312	SER
1	C	316	ARG
1	E	8	ILE
1	E	9	GLN
1	E	24	ARG
1	E	25	GLN
1	E	55	ARG
1	E	56	GLN
1	E	59	ARG
1	E	94	GLN
1	E	99	ILE
1	E	118	VAL
1	E	119	SER
1	E	122	LEU

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Mol	Chain	Res	Type
1	E	138	THR
1	E	154	THR
1	E	159	GLU
1	E	164	ARG
1	E	178	LYS
1	E	182	ARG
1	E	205	THR
1	E	211	LYS
1	E	217	ILE
1	E	219	SER
1	E	241	LEU
1	E	245	TYR
1	E	246	SER
1	E	251	GLN
1	E	252	SER
1	E	253	ILE
1	E	254	GLU
1	E	256	LEU
1	E	258	ARG
1	E	259	GLN
1	E	263	LYS
1	E	267	VAL
1	E	281	ARG
1	E	284	GLN
1	E	285	GLU
1	E	293	SER
1	E	294	GLU
1	E	295	GLU
1	E	308	ASN
1	E	312	SER
1	E	316	ARG
1	F	1	MET
1	F	8	ILE
1	F	9	GLN
1	F	13	VAL
1	F	14	ILE
1	F	15	THR
1	F	23	LEU
1	F	55	ARG
1	F	56	GLN
1	F	94	GLN
1	F	99	ILE

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Mol	Chain	Res	Type
1	F	104	ARG
1	F	118	VAL
1	F	119	SER
1	F	122	LEU
1	F	125	TYR
1	F	138	THR
1	F	146	ASP
1	F	154	THR
1	F	159	GLU
1	F	164	ARG
1	F	175	ARG
1	F	188	ASP
1	F	194	SER
1	F	196	SER
1	F	199	ASN
1	F	211	LYS
1	F	225	GLU
1	F	227	THR
1	F	228	ILE
1	F	241	LEU
1	F	245	TYR
1	F	254	GLU
1	F	263	LYS
1	F	274	GLN
1	F	275	VAL
1	F	292	GLU
1	F	295	GLU
1	F	308	ASN
1	F	309	ARG
1	F	312	SER
1	F	316	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	18	ASN
1	A	34	ASN
1	A	86	HIS
1	A	107	GLN
1	A	150	HIS
1	A	199	ASN

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Mol	Chain	Res	Type
1	A	259	GLN
1	A	284	GLN
1	A	308	ASN
1	A	320	GLN
1	D	9	GLN
1	D	34	ASN
1	D	86	HIS
1	D	150	HIS
1	D	199	ASN
1	D	284	GLN
1	D	308	ASN
1	D	320	GLN
1	B	25	GLN
1	B	34	ASN
1	B	86	HIS
1	B	107	GLN
1	B	150	HIS
1	B	308	ASN
1	B	320	GLN
1	C	9	GLN
1	C	34	ASN
1	C	86	HIS
1	C	150	HIS
1	C	308	ASN
1	C	320	GLN
1	E	9	GLN
1	E	18	ASN
1	E	25	GLN
1	E	34	ASN
1	E	86	HIS
1	E	107	GLN
1	E	150	HIS
1	E	199	ASN
1	E	308	ASN
1	E	320	GLN
1	F	9	GLN
1	F	18	ASN
1	F	34	ASN
1	F	86	HIS
1	F	150	HIS
1	F	199	ASN
1	F	259	GLN

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Mol	Chain	Res	Type
1	F	289	HIS
1	F	308	ASN
1	F	320	GLN

### 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](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	TRP	A	1001	-	12,16,16	0.74	0	7,22,22	1.00	0
3	PO4	A	1002	-	4,4,4	1.47	0	6,6,6	0.27	0
4	AMP	A	1003	-	20,25,25	1.20	2 (10%)	22,38,38	1.09	2 (9%)
2	TRP	B	1001	-	12,16,16	0.72	0	7,22,22	1.02	0
3	PO4	B	1002	-	4,4,4	1.47	0	6,6,6	0.26	0
4	AMP	B	1003	-	20,25,25	1.10	1 (5%)	22,38,38	0.80	0
2	TRP	C	1001	-	12,16,16	0.73	0	7,22,22	1.02	0
3	PO4	C	1002	-	4,4,4	1.38	0	6,6,6	0.27	0
4	AMP	C	1003	-	20,25,25	1.13	1 (5%)	22,38,38	0.83	0
2	TRP	D	1001	-	12,16,16	0.71	0	7,22,22	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	D	1002	-	4,4,4	1.36	0	6,6,6	0.27	0
4	AMP	D	1003	-	20,25,25	1.12	1 (5%)	22,38,38	1.07	1 (4%)
2	TRP	E	1001	-	12,16,16	0.72	0	7,22,22	1.02	0
3	PO4	E	1002	-	4,4,4	1.36	0	6,6,6	0.27	0
4	AMP	E	1003	-	20,25,25	1.13	1 (5%)	22,38,38	0.96	1 (4%)
2	TRP	F	1001	-	12,16,16	0.70	0	7,22,22	1.00	0
3	PO4	F	1002	-	4,4,4	1.42	0	6,6,6	0.27	0
4	AMP	F	1003	-	20,25,25	1.08	1 (5%)	22,38,38	0.96	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	A	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	A	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	A	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	B	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	B	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	B	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	C	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	C	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	C	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	D	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	D	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	D	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	E	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	E	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	E	1003	-	-	0/6/26/26	0/3/3/3
2	TRP	F	1001	-	-	0/3/8/8	0/2/2/2
3	PO4	F	1002	-	-	0/0/0/0	0/0/0/0
4	AMP	F	1003	-	-	0/6/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	AMP	C2-N3	2.13	1.36	1.32
4	F	1003	AMP	O4'-C1'	3.68	1.45	1.41
4	D	1003	AMP	O4'-C1'	3.84	1.46	1.41
4	B	1003	AMP	O4'-C1'	3.90	1.46	1.41
4	C	1003	AMP	O4'-C1'	3.90	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1003	AMP	O4'-C1'	3.96	1.46	1.41
4	A	1003	AMP	O4'-C1'	4.22	1.46	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	AMP	C4'-O4'-C1'	-3.17	106.23	109.72
4	D	1003	AMP	C4'-O4'-C1'	-3.07	106.34	109.72
4	E	1003	AMP	C4'-O4'-C1'	-2.64	106.81	109.72
4	F	1003	AMP	C4'-O4'-C1'	-2.14	107.37	109.72
4	A	1003	AMP	C2'-C3'-C4'	-2.08	98.33	102.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	PO4	3	0
4	A	1003	AMP	4	0
3	B	1002	PO4	2	0
4	B	1003	AMP	7	0
4	C	1003	AMP	5	0
3	D	1002	PO4	4	0
4	D	1003	AMP	5	0
4	E	1003	AMP	7	0
3	F	1002	PO4	1	0
4	F	1003	AMP	7	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	299/328 (91%)	0.05	7 (2%) 64 62	36, 53, 75, 101	0
1	B	291/328 (88%)	0.32	13 (4%) 37 35	38, 66, 91, 103	0
1	C	279/328 (85%)	0.63	28 (10%) 9 6	41, 66, 99, 116	0
1	D	286/328 (87%)	0.45	17 (5%) 26 23	39, 64, 96, 109	0
1	E	292/328 (89%)	0.67	39 (13%) 4 3	54, 85, 114, 124	0
1	F	296/328 (90%)	0.13	11 (3%) 45 44	27, 62, 81, 98	0
All	All	1743/1968 (88%)	0.37	115 (6%) 22 19	27, 64, 101, 124	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	GLY	7.8
1	A	179	VAL	7.4
1	D	258	ARG	7.1
1	C	26	PHE	6.7
1	C	242	LEU	6.7
1	E	180	GLY	6.6
1	E	253	ILE	6.5
1	C	181	ALA	6.4
1	D	181	ALA	6.4
1	C	22	ALA	5.9
1	D	180	GLY	5.9
1	C	268	PHE	5.3
1	E	177	PRO	5.2
1	C	227	THR	5.1
1	A	178	LYS	5.1
1	D	238	ILE	5.1
1	E	22	ALA	4.9
1	E	218	LYS	4.8
1	D	254	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	198	PRO	4.6
1	A	181	ALA	4.6
1	D	253	ILE	4.5
1	C	179	VAL	4.3
1	E	179	VAL	4.3
1	B	26	PHE	4.3
1	F	104	ARG	4.1
1	C	178	LYS	4.0
1	C	267	VAL	3.9
1	D	256	LEU	3.8
1	E	176	ILE	3.8
1	E	178	LYS	3.8
1	F	182	ARG	3.8
1	C	210	ALA	3.7
1	B	230	TYR	3.6
1	C	180	GLY	3.5
1	B	22	ALA	3.5
1	B	261	GLU	3.3
1	F	11	SER	3.3
1	C	214	GLU	3.2
1	E	144	GLY	3.2
1	E	29	LEU	3.2
1	E	260	TYR	3.2
1	C	272	LEU	3.1
1	F	28	GLU	3.1
1	D	178	LYS	3.1
1	C	238	ILE	3.1
1	C	243	ASN	3.1
1	B	187	VAL	3.1
1	E	1	MET	3.1
1	C	182	ARG	3.1
1	E	254	GLU	3.1
1	E	245	TYR	3.1
1	B	253	ILE	3.0
1	B	254	GLU	3.0
1	E	196	SER	3.0
1	A	176	ILE	3.0
1	E	257	GLU	3.0
1	D	12	GLY	2.9
1	C	239	SER	2.9
1	C	176	ILE	2.9
1	E	215	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	179	VAL	2.9
1	E	214	GLU	2.8
1	B	1	MET	2.8
1	D	1	MET	2.7
1	C	32	GLU	2.6
1	E	182	ARG	2.6
1	E	247	THR	2.6
1	A	177	PRO	2.6
1	B	225	GLU	2.6
1	D	242	LEU	2.5
1	F	8	ILE	2.5
1	C	177	PRO	2.5
1	B	257	GLU	2.5
1	D	260	TYR	2.5
1	C	104	ARG	2.4
1	C	245	TYR	2.4
1	E	199	ASN	2.4
1	B	229	ARG	2.4
1	E	242	LEU	2.4
1	D	144	GLY	2.4
1	B	258	ARG	2.4
1	A	106	THR	2.4
1	C	247	THR	2.4
1	F	175	ARG	2.4
1	B	256	LEU	2.3
1	E	255	GLU	2.3
1	D	177	PRO	2.3
1	E	256	LEU	2.3
1	C	28	GLU	2.3
1	E	262	GLY	2.3
1	C	226	GLY	2.3
1	F	12	GLY	2.3
1	E	118	VAL	2.3
1	E	211	LYS	2.3
1	D	249	SER	2.3
1	C	278	GLU	2.2
1	E	252	SER	2.2
1	E	207	LEU	2.2
1	E	268	PHE	2.2
1	C	175	ARG	2.2
1	C	29	LEU	2.2
1	E	269	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	211	LYS	2.2
1	E	197	ASP	2.2
1	E	175	ARG	2.1
1	E	238	ILE	2.1
1	E	26	PHE	2.1
1	F	261	GLU	2.1
1	E	274	GLN	2.0
1	F	20	ILE	2.0
1	F	174	ALA	2.0
1	E	241	LEU	2.0
1	D	182	ARG	2.0
1	E	261	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	AMP	D	1003	23/23	0.19	0.91	5.83	62,66,70,71	23
4	AMP	C	1003	23/23	0.02	0.86	5.10	64,67,72,73	23
4	AMP	A	1003	23/23	0.58	0.50	2.94	41,47,54,56	23
4	AMP	F	1003	23/23	0.56	0.47	2.78	55,61,66,67	23
4	AMP	E	1003	23/23	0.38	0.54	2.74	72,76,81,82	23
4	AMP	B	1003	23/23	0.62	0.39	2.52	42,50,57,59	23
2	TRP	D	1001	15/15	0.90	0.22	2.01	44,50,74,75	15
2	TRP	E	1001	15/15	0.86	0.25	1.49	63,70,94,94	15
3	PO4	B	1002	5/5	0.86	0.21	1.06	74,77,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TRP	C	1001	15/15	0.93	0.19	0.73	34,40,65,65	15
2	TRP	B	1001	15/15	0.84	0.20	0.70	36,42,67,67	15
2	TRP	A	1001	15/15	0.91	0.19	0.64	30,36,61,61	15
2	TRP	F	1001	15/15	0.91	0.19	0.55	36,42,67,67	15
3	PO4	D	1002	5/5	0.93	0.21	0.18	73,76,79,80	5
3	PO4	E	1002	5/5	0.84	0.26	-0.16	73,76,79,80	5
3	PO4	F	1002	5/5	0.86	0.17	-0.40	89,92,95,95	0
3	PO4	A	1002	5/5	0.94	0.16	-0.44	55,58,61,62	5
3	PO4	C	1002	5/5	0.92	0.15	-0.99	83,86,89,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.