



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:32 am GMT

PDB ID : 1MAW  
Title : Crystal Structure of Tryptophanyl-tRNA Synthetase Complexed with ATP in an Open Conformation  
Authors : Retailleau, P.; Huang, X.; Yin, Y.; Hu, M.; Weinreb, V.; Vachette, P.; Vonrhein, C.; Bricogne, G.; Roversi, P.; Ilyin, V.; Carter Jr., C.W.  
Deposited on : 2002-08-02  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

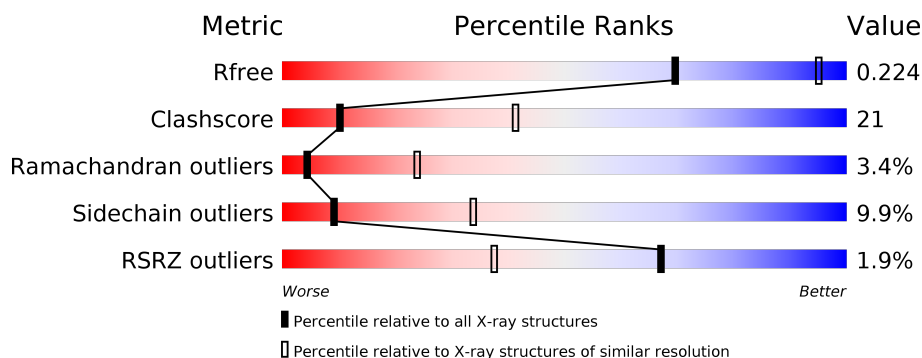
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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> <div></div> <div>56%</div> <div>38%</div> <div>5%</div> </div> </div>
1	B	328	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>37%</div> <div>5%</div> </div> </div>
1	C	328	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>38%</div> <div>5%</div> </div> </div>
1	D	328	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>36%</div> <div>5%</div> </div> </div>
1	E	328	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>35%</div> <div>5%</div> </div> </div>
1	F	328	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>6%</div> </div> </div>

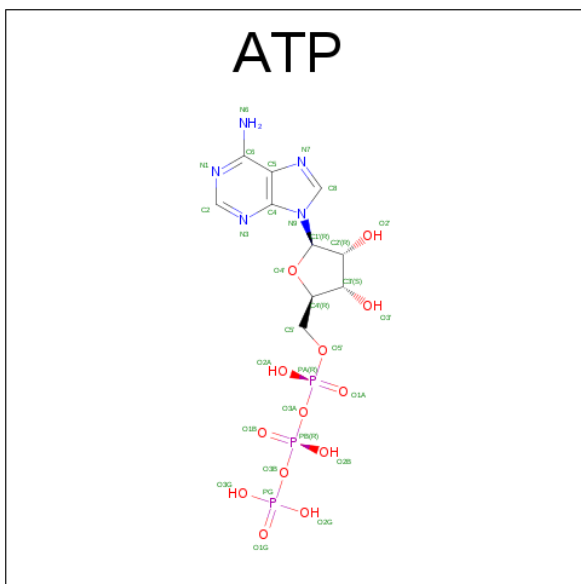


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TRYPTOPHAN-TRNA LIGASE.

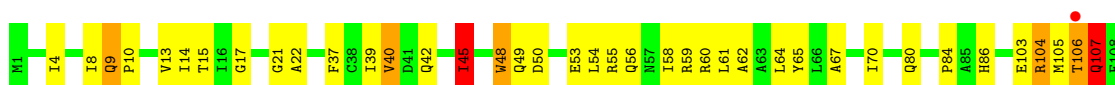
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	B	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	C	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	D	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	E	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0
1	F	326	Total 2563	C 1624	N 442	O 484	S 13	0	0	0

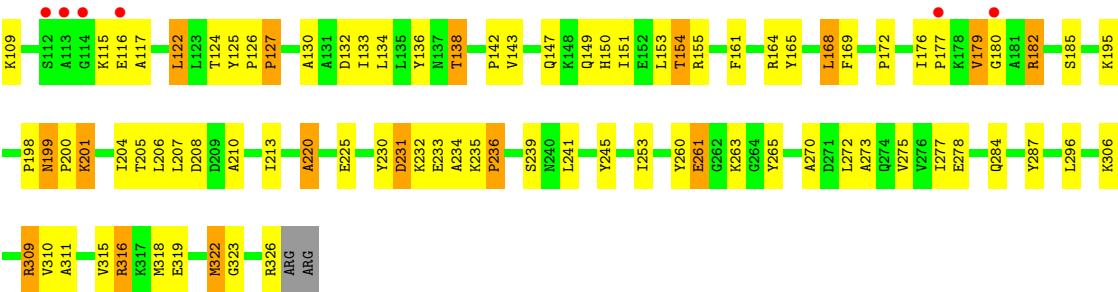
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.55Å 91.98Å 156.89Å 90.00° 132.34° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.05 – 2.99	Depositor EDS
% Data completeness (in resolution range)	88.4 (15.00-3.00) 87.6 (15.05-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.253 0.193 , 0.224	Depositor DCC
$R_{free}$ test set	4285 reflections (11.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 71.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.022 for -h-2*1,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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 27.27 % 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 2.2682e-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, 0.333 respectively for untwinned datasets, and 0.375, 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: ATP

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	0.49	0/2611	0.73	0/3532
1	B	0.47	0/2611	0.73	0/3532
1	C	0.49	0/2611	0.76	0/3532
1	D	0.50	0/2611	0.75	0/3532
1	E	0.50	0/2611	0.75	0/3532
1	F	0.45	0/2611	0.73	1/3532 (0.0%)
All	All	0.48	0/15666	0.74	1/21192 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	180	GLY	N-CA-C	-5.67	98.93	113.10

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	2563	0	2554	104	0
1	B	2563	0	2554	131	0
1	C	2563	0	2554	111	0
1	D	2563	0	2554	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2563	0	2554	102	0
1	F	2563	0	2554	104	0
2	A	31	0	12	2	0
2	B	31	0	12	2	0
2	C	31	0	12	3	0
2	D	31	0	12	3	0
2	E	31	0	12	5	0
2	F	31	0	12	4	0
All	All	15564	0	15396	647	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 21.

All (647) 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:F:205:THR:HG22	1:F:207:LEU:H	1.17	1.05
1:F:8:ILE:HG22	1:F:61:LEU:HD21	1.48	0.93
1:F:309:ARG:HD3	1:F:310:VAL:HG23	1.51	0.92
1:F:106:THR:H	1:F:149:GLN:HE22	1.18	0.92
1:B:205:THR:HG22	1:B:207:LEU:H	1.34	0.89
1:A:205:THR:HG22	1:A:207:LEU:H	1.36	0.89
1:D:106:THR:N	1:D:149:GLN:HE22	1.70	0.87
1:E:14:ILE:HA	1:E:195:LYS:HE2	1.56	0.87
1:A:105:MET:HE3	1:A:105:MET:HA	1.57	0.87
1:A:124:THR:O	1:A:127:PRO:HD2	1.74	0.87
1:A:92:MET:HG2	1:A:322:MET:CE	2.05	0.86
1:C:205:THR:HG22	1:C:207:LEU:H	1.40	0.86
1:D:205:THR:HG22	1:D:207:LEU:H	1.38	0.86
1:B:324:LEU:HD21	1:E:45:ILE:HD13	1.59	0.85
1:D:176:ILE:HG23	1:D:177:PRO:HD2	1.59	0.85
1:A:8:ILE:HG22	1:A:61:LEU:HD21	1.60	0.84
1:F:106:THR:N	1:F:149:GLN:HE22	1.75	0.84
1:E:126:PRO:HB2	1:E:127:PRO:HD3	1.60	0.83
1:D:39:ILE:HG21	1:D:58:ILE:HG23	1.62	0.81
1:F:126:PRO:HB2	1:F:127:PRO:HD3	1.61	0.81
1:C:86:HIS:HD2	1:C:132:ASP:OD1	1.65	0.80
1:D:5:PHE:HB2	1:D:138:THR:HG21	1.63	0.79
1:E:86:HIS:HD2	1:E:132:ASP:OD1	1.64	0.79
1:A:92:MET:HG2	1:A:322:MET:HE2	1.65	0.79
1:A:8:ILE:CG2	1:A:61:LEU:HD21	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ILE:HG21	1:C:174:ALA:HB2	1.65	0.78
1:D:124:THR:O	1:D:127:PRO:HD2	1.82	0.77
1:C:18:ASN:C	1:C:18:ASN:HD22	1.88	0.77
1:B:324:LEU:CD2	1:E:45:ILE:HD13	2.14	0.77
1:B:8:ILE:HG22	1:B:61:LEU:HD21	1.66	0.76
1:E:150:HIS:O	1:E:154:THR:HG22	1.85	0.76
1:E:19:TYR:HE2	1:E:68:VAL:HG13	1.51	0.76
1:C:54:LEU:HD23	1:F:323:GLY:O	1.85	0.76
1:B:176:ILE:HB	1:B:177:PRO:HD2	1.68	0.75
1:A:125:TYR:CD2	1:A:126:PRO:HD3	2.22	0.74
1:B:126:PRO:HB2	1:B:127:PRO:HD3	1.68	0.74
1:B:198:PRO:O	1:B:200:PRO:HD3	1.87	0.74
1:F:8:ILE:CG2	1:F:61:LEU:HD21	2.17	0.74
1:B:13:VAL:O	1:B:195:LYS:HD3	1.89	0.73
1:F:306:LYS:O	1:F:309:ARG:HD2	1.88	0.73
1:E:195:LYS:HD2	2:E:403:ATP:PG	2.29	0.73
1:F:205:THR:HG22	1:F:207:LEU:N	1.99	0.73
1:D:8:ILE:CG2	1:D:61:LEU:HD21	2.19	0.72
1:D:11:SER:O	1:D:13:VAL:HG12	1.90	0.72
1:A:179:VAL:HG12	1:A:181:ALA:H	1.54	0.72
1:C:185:SER:HB3	1:C:188:ASP:O	1.89	0.72
1:D:106:THR:H	1:D:149:GLN:HE22	1.35	0.72
1:B:29:LEU:HD21	1:B:175:ARG:HH22	1.54	0.72
1:D:106:THR:H	1:D:149:GLN:NE2	1.88	0.72
1:D:189:PRO:HD3	1:D:221:VAL:HG21	1.72	0.72
1:D:55:ARG:HG2	1:D:55:ARG:HH11	1.55	0.72
1:C:31:HIS:ND1	1:C:74:GLN:HG2	2.05	0.71
1:D:176:ILE:HG23	1:D:177:PRO:CD	2.19	0.71
1:E:205:THR:HG22	1:E:207:LEU:H	1.54	0.71
1:A:176:ILE:HG13	1:A:177:PRO:HD2	1.71	0.71
1:A:92:MET:HG2	1:A:322:MET:HE1	1.72	0.70
1:D:92:MET:HG2	1:D:322:MET:CE	2.21	0.70
1:C:243:ASN:O	1:C:247:THR:HG23	1.92	0.70
1:D:42:GLN:HB2	1:D:80:GLN:OE1	1.91	0.70
1:C:108:PHE:CZ	1:C:123:LEU:HD13	2.27	0.69
1:F:105:MET:HE1	1:F:153:LEU:HD22	1.73	0.69
1:B:45:ILE:HG22	1:E:95:CYS:SG	2.32	0.69
1:A:189:PRO:HD3	1:A:221:VAL:HG21	1.75	0.69
1:A:245:TYR:CD2	1:A:272:LEU:HD13	2.28	0.69
1:E:176:ILE:HG13	1:E:177:PRO:HD2	1.75	0.69
1:E:86:HIS:CD2	1:E:132:ASP:OD1	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:HB3	1:A:321:ALA:HB1	1.75	0.68
1:D:59:ARG:NH2	1:D:296:LEU:HD23	2.08	0.68
1:C:8:ILE:CG2	1:C:61:LEU:HD21	2.23	0.68
1:D:40:VAL:HA	1:D:80:GLN:HB2	1.76	0.67
1:C:280:LEU:HA	1:C:283:ILE:HD12	1.76	0.67
1:C:225:GLU:OE1	1:C:235:LYS:NZ	2.19	0.67
1:E:32:GLU:HG3	1:E:33:TYR:HD1	1.59	0.67
1:A:106:THR:H	1:A:149:GLN:NE2	1.93	0.67
1:B:5:PHE:HB2	1:B:138:THR:HG21	1.76	0.67
1:C:238:ILE:HD11	1:C:265:TYR:CE1	2.30	0.66
1:A:133:ILE:HD13	1:A:141:VAL:HG21	1.78	0.66
1:A:181:ALA:O	1:A:182:ARG:HB2	1.93	0.66
1:B:9:GLN:NE2	1:B:10:PRO:HD2	2.11	0.66
1:F:106:THR:H	1:F:149:GLN:NE2	1.90	0.66
1:C:211:LYS:HB3	1:C:211:LYS:NZ	2.11	0.66
1:F:133:ILE:O	1:F:138:THR:HG23	1.95	0.66
1:A:106:THR:H	1:A:149:GLN:HE22	1.44	0.65
1:A:151:ILE:HG21	1:A:174:ALA:HB2	1.78	0.65
1:F:8:ILE:HD12	1:F:65:TYR:OH	1.96	0.65
1:A:316:ARG:HA	1:A:316:ARG:NH1	2.11	0.65
1:B:133:ILE:O	1:B:138:THR:HG23	1.96	0.65
1:C:108:PHE:CE2	1:C:123:LEU:HD13	2.31	0.65
1:C:105:MET:HE1	1:C:153:LEU:HD22	1.78	0.65
1:F:179:VAL:HG13	1:F:182:ARG:HG3	1.77	0.65
1:D:254:GLU:H	1:D:254:GLU:CD	1.99	0.65
1:C:165:TYR:HB3	1:C:321:ALA:HB1	1.79	0.65
1:C:226:GLY:HA2	1:C:265:TYR:CE2	2.32	0.65
1:B:235:LYS:N	1:B:236:PRO:HD3	2.13	0.64
1:E:32:GLU:HG3	1:E:33:TYR:CD1	2.32	0.64
1:D:40:VAL:HG23	1:D:40:VAL:O	1.97	0.64
1:A:189:PRO:HD3	1:A:221:VAL:CG2	2.27	0.64
1:C:27:VAL:O	1:C:30:GLN:HG2	1.97	0.64
1:B:23:LEU:HD12	1:B:68:VAL:HG11	1.79	0.64
1:E:195:LYS:HD2	2:E:403:ATP:O3G	1.98	0.64
1:E:176:ILE:HG13	1:E:177:PRO:CD	2.26	0.64
1:A:55:ARG:HG2	1:A:55:ARG:HH11	1.63	0.63
1:C:238:ILE:HD11	1:C:265:TYR:CD1	2.33	0.63
1:A:50:ASP:HB3	1:A:53:GLU:HB2	1.80	0.63
1:C:55:ARG:HE	1:F:323:GLY:HA2	1.63	0.63
1:B:207:LEU:HA	1:B:284:GLN:HE21	1.63	0.63
1:E:25:GLN:O	1:E:28:GLU:OE1	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:ARG:HH11	1:F:310:VAL:HG23	1.63	0.63
1:D:85:ALA:HB1	1:D:315:VAL:HG21	1.81	0.63
1:D:159:GLU:O	1:D:163:LYS:HG3	1.98	0.62
1:E:151:ILE:HG21	1:E:174:ALA:HB2	1.80	0.62
1:B:316:ARG:HH11	1:B:316:ARG:HA	1.64	0.62
1:F:311:ALA:O	1:F:315:VAL:HG23	1.98	0.62
1:C:150:HIS:O	1:C:154:THR:HG23	1.99	0.62
1:A:151:ILE:O	1:A:155:ARG:HG3	1.99	0.62
1:A:295:GLU:O	1:A:299:VAL:HG23	1.99	0.62
1:D:151:ILE:O	1:D:155:ARG:HG3	1.98	0.62
1:C:184:MET:HG3	1:C:189:PRO:O	1.99	0.62
1:A:126:PRO:HB2	1:A:127:PRO:HD3	1.81	0.62
1:C:97:VAL:HB	1:C:157:LEU:HD21	1.81	0.61
1:D:85:ALA:HB1	1:D:315:VAL:CG2	2.29	0.61
1:C:140:ILE:HG12	1:C:175:ARG:HG3	1.83	0.61
1:F:21:GLY:HA3	2:F:405:ATP:N3	2.16	0.61
1:B:176:ILE:HB	1:B:177:PRO:CD	2.31	0.61
1:C:141:VAL:HG12	1:C:143:VAL:HG13	1.82	0.61
1:F:230:TYR:CD2	1:F:253:ILE:HD13	2.35	0.61
1:C:153:LEU:O	1:C:157:LEU:HD12	2.00	0.61
1:C:105:MET:O	1:C:107:GLN:N	2.34	0.61
1:E:13:VAL:O	1:E:195:LYS:HG2	2.01	0.61
1:B:281:ARG:O	1:B:285:GLU:HG3	2.00	0.61
1:B:143:VAL:HG11	1:B:151:ILE:HD11	1.83	0.60
1:B:143:VAL:HG22	1:B:174:ALA:HB1	1.82	0.60
1:C:125:TYR:CD2	1:C:126:PRO:HD3	2.35	0.60
1:D:85:ALA:HB3	1:D:311:ALA:HB1	1.83	0.60
1:D:199:ASN:HD22	1:D:200:PRO:HD2	1.66	0.60
1:E:135:LEU:HD21	1:E:315:VAL:HG23	1.82	0.60
1:B:175:ARG:HG2	1:B:176:ILE:H	1.66	0.60
1:B:200:PRO:O	1:B:216:LYS:HE2	2.01	0.60
1:B:8:ILE:CG2	1:B:61:LEU:HD21	2.29	0.60
1:A:86:HIS:CD2	1:A:132:ASP:HA	2.37	0.60
1:B:316:ARG:HA	1:B:316:ARG:NH1	2.17	0.60
1:C:124:THR:HG21	1:F:124:THR:HG21	1.81	0.60
1:F:198:PRO:O	1:F:200:PRO:HD3	2.01	0.60
1:A:205:THR:N	1:A:208:ASP:OD2	2.27	0.60
1:A:210:ALA:HB1	1:A:277:ILE:HD13	1.84	0.60
1:E:23:LEU:HD21	1:E:65:TYR:CZ	2.37	0.60
1:D:19:TYR:HA	1:D:23:LEU:HB2	1.83	0.59
1:C:8:ILE:HG22	1:C:61:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LEU:HD12	1:D:68:VAL:HG11	1.83	0.59
1:B:205:THR:HG22	1:B:207:LEU:N	2.13	0.59
1:C:14:ILE:HD11	1:C:206:LEU:HD12	1.84	0.59
1:D:133:ILE:O	1:D:138:THR:HG23	2.03	0.59
1:E:185:SER:HB3	1:E:188:ASP:O	2.02	0.59
1:A:230:TYR:CE2	1:A:239:SER:HB3	2.38	0.59
1:C:133:ILE:HD13	1:C:141:VAL:HG21	1.84	0.59
1:C:316:ARG:HA	1:C:316:ARG:NH1	2.17	0.59
1:B:143:VAL:HB	1:B:147:GLN:CB	2.32	0.59
1:C:93:LEU:O	1:C:97:VAL:HG12	2.02	0.59
1:D:316:ARG:NH1	1:D:316:ARG:HA	2.18	0.59
1:C:95:CYS:SG	1:F:45:ILE:HG22	2.43	0.58
1:B:231:ASP:HB3	1:B:235:LYS:HB2	1.85	0.58
1:F:233:GLU:O	1:F:234:ALA:HB3	2.03	0.58
1:A:42:GLN:HB2	1:A:80:GLN:OE1	2.03	0.58
1:C:235:LYS:N	1:C:236:PRO:HD3	2.18	0.58
1:E:272:LEU:O	1:E:276:VAL:HG23	2.03	0.58
1:C:11:SER:O	1:C:13:VAL:HG12	2.04	0.58
1:F:55:ARG:HG2	1:F:55:ARG:HH11	1.69	0.57
1:A:150:HIS:O	1:A:154:THR:HG23	2.03	0.57
1:C:19:TYR:HA	1:C:23:LEU:HB3	1.87	0.57
1:C:226:GLY:HA2	1:C:265:TYR:CZ	2.39	0.57
1:D:189:PRO:HB2	1:D:236:PRO:HB2	1.86	0.57
1:B:46:THR:HG22	1:B:121:GLY:HA3	1.86	0.57
1:C:233:GLU:O	1:C:234:ALA:HB3	2.04	0.57
1:B:21:GLY:HA3	2:B:401:ATP:N3	2.20	0.57
1:E:140:ILE:HG21	1:E:175:ARG:HG3	1.87	0.57
1:D:8:ILE:HG22	1:D:61:LEU:HD21	1.85	0.57
1:E:41:ASP:OD2	1:E:81:SER:OG	2.20	0.57
1:E:64:LEU:O	1:E:68:VAL:HG23	2.04	0.57
1:A:85:ALA:HB3	1:A:311:ALA:HB1	1.86	0.56
1:C:281:ARG:O	1:C:285:GLU:HG3	2.05	0.56
1:D:171:ILE:N	1:D:171:ILE:HD12	2.20	0.56
1:B:106:THR:H	1:B:149:GLN:NE2	2.03	0.56
1:A:175:ARG:HG2	1:A:176:ILE:N	2.20	0.56
1:B:11:SER:O	1:B:13:VAL:HG12	2.04	0.56
1:B:29:LEU:HD21	1:B:175:ARG:NH2	2.20	0.56
1:B:25:GLN:O	1:B:29:LEU:HB2	2.06	0.56
1:A:16:ILE:O	1:A:20:ILE:HG13	2.05	0.56
1:A:74:GLN:HA	1:E:218:LYS:NZ	2.21	0.56
1:C:55:ARG:HG2	1:C:55:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:403:ATP:PA	2:E:403:ATP:O3G	2.64	0.56
1:D:225:GLU:OE1	1:D:235:LYS:HD2	2.06	0.56
1:B:176:ILE:HD12	1:B:176:ILE:H	1.71	0.55
1:B:205:THR:CG2	1:B:207:LEU:H	2.14	0.55
1:C:101:GLU:HA	1:C:104:ARG:HH11	1.70	0.55
1:F:86:HIS:HD2	1:F:132:ASP:OD1	1.88	0.55
1:D:92:MET:HG2	1:D:322:MET:HE1	1.88	0.55
1:D:185:SER:HB3	1:D:188:ASP:O	2.07	0.55
1:F:125:TYR:N	1:F:126:PRO:CD	2.68	0.55
1:C:126:PRO:HB2	1:C:127:PRO:HD3	1.88	0.55
1:F:306:LYS:O	1:F:309:ARG:CD	2.55	0.55
1:B:105:MET:HA	1:B:105:MET:HE2	1.89	0.55
1:B:23:LEU:O	1:B:26:PHE:HB2	2.07	0.55
1:B:318:MET:O	1:B:322:MET:HG2	2.07	0.55
1:F:161:PHE:HE2	1:F:168:LEU:HD12	1.70	0.55
1:E:186:LEU:O	1:E:221:VAL:HG22	2.06	0.55
1:B:126:PRO:O	1:B:129:MET:N	2.37	0.54
1:B:11:SER:O	1:B:13:VAL:N	2.38	0.54
1:E:189:PRO:HB2	1:E:236:PRO:HB2	1.87	0.54
1:B:86:HIS:HD2	1:B:132:ASP:OD1	1.90	0.54
1:B:9:GLN:C	1:B:9:GLN:HE21	2.10	0.54
1:F:149:GLN:O	1:F:149:GLN:HG2	2.07	0.54
1:D:65:TYR:O	1:D:70:ILE:HG12	2.07	0.54
1:E:151:ILE:O	1:E:154:THR:HG23	2.07	0.54
1:D:212:THR:CG2	1:D:216:LYS:HE3	2.37	0.54
1:E:189:PRO:HD3	1:E:221:VAL:HG21	1.89	0.54
1:E:195:LYS:N	2:E:403:ATP:O2G	2.37	0.54
1:A:193:MET:HB3	2:A:400:ATP:N6	2.22	0.54
1:A:231:ASP:HB3	1:A:235:LYS:HB2	1.88	0.54
1:B:176:ILE:CB	1:B:177:PRO:HD2	2.36	0.54
1:C:60:ARG:HG2	1:C:287:TYR:OH	2.08	0.54
1:F:179:VAL:O	1:F:179:VAL:HG12	2.08	0.54
1:E:106:THR:N	1:E:149:GLN:HE22	2.06	0.54
1:B:107:GLN:C	1:B:109:LYS:H	2.12	0.54
1:E:187:VAL:HG22	1:E:202:ALA:HB2	1.90	0.54
1:B:59:ARG:NH2	1:B:296:LEU:HD23	2.23	0.54
1:F:260:TYR:HA	1:F:263:LYS:HG3	1.89	0.54
1:B:175:ARG:HG2	1:B:176:ILE:N	2.22	0.54
1:C:18:ASN:ND2	1:C:18:ASN:C	2.59	0.54
1:B:316:ARG:HH12	1:B:319:GLU:CD	2.11	0.53
1:A:143:VAL:HB	1:A:147:GLN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:MET:HA	1:C:149:GLN:HE22	1.73	0.53
1:D:126:PRO:HB2	1:D:127:PRO:HD3	1.90	0.53
1:A:86:HIS:HD2	1:A:132:ASP:HA	1.73	0.53
1:F:45:ILE:HG23	1:F:45:ILE:O	2.09	0.53
1:D:55:ARG:HG2	1:D:55:ARG:NH1	2.23	0.53
1:A:143:VAL:HG11	1:A:151:ILE:HD11	1.89	0.53
1:C:21:GLY:HA2	1:C:180:GLY:HA3	1.90	0.53
1:E:211:LYS:NZ	1:E:211:LYS:HB3	2.22	0.53
1:A:11:SER:O	1:A:13:VAL:HG12	2.09	0.53
1:A:217:ILE:O	1:A:269:LYS:HD3	2.08	0.53
1:F:143:VAL:HB	1:F:147:GLN:CB	2.39	0.53
1:A:40:VAL:HA	1:A:80:GLN:HB2	1.90	0.52
1:B:27:VAL:O	1:B:30:GLN:HG2	2.09	0.52
1:D:8:ILE:HG21	1:D:61:LEU:HD21	1.89	0.52
1:F:309:ARG:HH11	1:F:310:VAL:CG2	2.21	0.52
1:B:176:ILE:CB	1:B:177:PRO:CD	2.86	0.52
1:F:150:HIS:O	1:F:154:THR:HG23	2.09	0.52
1:F:42:GLN:HB2	1:F:80:GLN:OE1	2.09	0.52
1:A:179:VAL:CG1	1:A:182:ARG:H	2.21	0.52
1:E:31:HIS:HD2	1:E:74:GLN:HE21	1.57	0.52
1:E:10:PRO:HA	1:E:61:LEU:HD22	1.92	0.52
1:F:177:PRO:HG3	2:F:405:ATP:O2'	2.10	0.52
1:B:123:LEU:HD23	1:B:124:THR:HG23	1.92	0.52
1:D:228:ILE:HD11	1:D:265:TYR:HD1	1.75	0.52
1:F:9:GLN:NE2	1:F:10:PRO:HD2	2.25	0.52
1:B:169:PHE:HZ	1:B:318:MET:SD	2.32	0.52
1:D:3:THR:HB	1:D:138:THR:HA	1.92	0.52
1:D:134:LEU:HB3	1:D:169:PHE:CD1	2.43	0.52
1:F:245:TYR:HB2	1:F:272:LEU:HD13	1.92	0.52
1:A:195:LYS:HE3	2:A:400:ATP:O3B	2.10	0.51
1:B:14:ILE:HD11	1:B:206:LEU:HD12	1.93	0.51
1:A:233:GLU:O	1:A:234:ALA:HB3	2.10	0.51
1:E:13:VAL:O	1:E:13:VAL:HG13	2.09	0.51
1:F:39:ILE:HD11	1:F:62:ALA:HB2	1.91	0.51
1:C:86:HIS:CD2	1:C:132:ASP:OD1	2.54	0.51
1:C:140:ILE:HG23	1:C:175:ARG:HB2	1.91	0.51
1:D:147:GLN:O	1:D:149:GLN:N	2.44	0.51
1:C:8:ILE:HD12	1:C:65:TYR:OH	2.10	0.51
1:A:101:GLU:HA	1:A:104:ARG:HH11	1.76	0.51
1:A:66:LEU:CD2	1:A:72:PRO:HD3	2.41	0.51
1:F:14:ILE:HD11	1:F:206:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:VAL:O	1:F:195:LYS:HD3	2.11	0.51
1:F:48:TRP:O	1:F:49:GLN:HG2	2.10	0.51
1:A:68:VAL:O	1:A:68:VAL:HG12	2.11	0.51
1:B:45:ILE:HD13	1:E:324:LEU:HD21	1.92	0.51
1:C:198:PRO:O	1:C:200:PRO:HD3	2.10	0.51
1:E:233:GLU:O	1:E:234:ALA:HB3	2.11	0.51
1:E:79:ILE:HB	1:E:82:GLU:HG3	1.93	0.51
1:B:123:LEU:O	1:B:123:LEU:HG	2.08	0.51
1:B:143:VAL:HB	1:B:147:GLN:HB2	1.93	0.51
1:C:3:THR:HB	1:C:138:THR:HA	1.92	0.51
1:C:206:LEU:HD22	1:C:280:LEU:HD22	1.93	0.51
1:E:126:PRO:HB2	1:E:127:PRO:CD	2.38	0.51
1:B:189:PRO:HD3	1:B:221:VAL:HG21	1.93	0.50
1:B:14:ILE:CD1	1:B:206:LEU:HD12	2.41	0.50
1:F:272:LEU:O	1:F:275:VAL:HG12	2.10	0.50
1:A:233:GLU:H	1:A:233:GLU:CD	2.14	0.50
1:B:252:SER:HB2	1:B:254:GLU:OE1	2.12	0.50
1:C:88:GLN:NE2	1:F:84:PRO:HG3	2.27	0.50
1:B:105:MET:HA	1:B:105:MET:CE	2.41	0.50
1:B:279:THR:HG22	1:B:280:LEU:HD23	1.93	0.50
1:D:105:MET:O	1:D:107:GLN:N	2.44	0.50
1:A:3:THR:HB	1:A:138:THR:HA	1.94	0.50
1:C:125:TYR:CG	1:C:126:PRO:HD3	2.46	0.50
1:D:233:GLU:O	1:D:234:ALA:HB3	2.11	0.50
1:E:43:HIS:HE1	1:E:132:ASP:OD2	1.94	0.50
1:E:11:SER:O	1:E:13:VAL:HG12	2.10	0.50
1:D:316:ARG:HH11	1:D:316:ARG:HA	1.75	0.50
1:A:316:ARG:HA	1:A:316:ARG:HH11	1.75	0.50
1:B:143:VAL:HB	1:B:147:GLN:HB3	1.93	0.50
1:B:282:PRO:HA	1:B:285:GLU:OE1	2.12	0.50
1:D:37:PHE:HB2	1:D:77:LEU:HD12	1.93	0.50
1:E:165:TYR:HB3	1:E:321:ALA:HB1	1.92	0.50
1:A:43:HIS:CE1	1:A:129:MET:HB2	2.47	0.50
1:A:59:ARG:NH2	1:A:296:LEU:HD23	2.26	0.50
1:B:230:TYR:CD2	1:B:253:ILE:HD13	2.47	0.50
1:A:4:ILE:HG12	1:A:140:ILE:HB	1.94	0.49
1:B:171:ILE:N	1:B:171:ILE:HD12	2.27	0.49
1:E:133:ILE:HD13	1:E:141:VAL:HG21	1.93	0.49
1:E:45:ILE:HG23	1:E:45:ILE:O	2.12	0.49
1:F:143:VAL:HB	1:F:147:GLN:HB2	1.93	0.49
1:F:105:MET:CE	1:F:153:LEU:HD22	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:HB2	1:B:135:LEU:HD21	1.93	0.49
1:B:125:TYR:N	1:B:126:PRO:CD	2.74	0.49
1:B:165:TYR:HB3	1:B:321:ALA:HB1	1.93	0.49
1:D:199:ASN:HD22	1:D:200:PRO:CD	2.25	0.49
1:E:188:ASP:OD2	1:E:191:LYS:HB2	2.13	0.49
1:A:74:GLN:HA	1:E:218:LYS:HZ1	1.77	0.49
1:D:165:TYR:HB3	1:D:321:ALA:HB1	1.94	0.49
1:B:233:GLU:O	1:B:234:ALA:HB3	2.12	0.49
1:B:9:GLN:NE2	1:B:10:PRO:CD	2.75	0.49
1:F:39:ILE:HG21	1:F:58:ILE:HG23	1.94	0.49
1:B:207:LEU:CA	1:B:284:GLN:HE21	2.26	0.49
1:D:4:ILE:HG12	1:D:140:ILE:HB	1.95	0.49
1:E:170:THR:O	1:E:172:PRO:HD3	2.12	0.49
1:C:134:LEU:HD13	1:C:169:PHE:CD2	2.48	0.49
1:D:149:GLN:O	1:D:152:GLU:HB2	2.13	0.49
1:A:29:LEU:HD21	1:A:175:ARG:HH12	1.78	0.49
1:A:24:ARG:HH12	1:A:247:THR:HB	1.78	0.49
1:A:10:PRO:HA	1:A:61:LEU:HD22	1.94	0.48
1:D:25:GLN:HE22	1:D:178:LYS:HB2	1.78	0.48
1:F:21:GLY:HA3	2:F:405:ATP:C2	2.47	0.48
1:A:151:ILE:HG13	1:A:174:ALA:HB2	1.96	0.48
1:C:211:LYS:HZ2	1:C:211:LYS:HB3	1.76	0.48
1:F:86:HIS:HE1	1:F:136:TYR:OH	1.97	0.48
1:E:23:LEU:HD21	1:E:65:TYR:CE1	2.48	0.48
1:D:106:THR:N	1:D:149:GLN:NE2	2.45	0.48
1:A:19:TYR:HA	1:A:23:LEU:HB3	1.95	0.48
1:B:106:THR:N	1:B:149:GLN:HE22	2.11	0.48
1:D:231:ASP:HB2	1:D:235:LYS:HB2	1.94	0.48
1:B:181:ALA:O	1:B:182:ARG:C	2.51	0.48
1:C:155:ARG:O	1:C:158:ALA:HB3	2.14	0.48
1:A:267:VAL:HG23	1:A:268:PHE:N	2.29	0.48
1:E:155:ARG:NH1	1:E:172:PRO:O	2.47	0.48
1:F:59:ARG:NH2	1:F:296:LEU:HD23	2.28	0.48
1:C:143:VAL:HB	1:C:147:GLN:HB2	1.96	0.48
1:C:180:GLY:O	1:C:182:ARG:N	2.46	0.48
1:D:92:MET:HG2	1:D:322:MET:HE2	1.95	0.48
1:F:208:ASP:O	1:F:284:GLN:NE2	2.46	0.48
1:F:236:PRO:O	1:F:239:SER:HB2	2.14	0.48
1:A:273:ALA:O	1:A:277:ILE:HG13	2.14	0.48
1:B:11:SER:C	1:B:13:VAL:H	2.17	0.48
1:C:145:GLU:CD	1:C:145:GLU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ARG:O	1:D:261:GLU:HB2	2.14	0.48
1:D:54:LEU:O	1:D:58:ILE:HG13	2.14	0.48
1:F:103:GLU:C	1:F:105:MET:H	2.17	0.48
1:A:245:TYR:HD2	1:A:272:LEU:HD13	1.76	0.48
1:C:288:HIS:O	1:C:292:GLU:HG2	2.14	0.48
1:D:171:ILE:N	1:D:171:ILE:CD1	2.77	0.48
1:A:5:PHE:O	1:A:142:PRO:HD2	2.14	0.47
1:C:140:ILE:CG2	1:C:175:ARG:HB2	2.44	0.47
1:E:25:GLN:O	1:E:29:LEU:HB2	2.14	0.47
1:C:238:ILE:CD1	1:C:265:TYR:CE1	2.96	0.47
1:D:19:TYR:HA	1:D:23:LEU:CB	2.44	0.47
1:D:176:ILE:CG2	1:D:177:PRO:N	2.77	0.47
1:A:68:VAL:CG1	1:A:68:VAL:O	2.63	0.47
1:C:170:THR:O	1:C:172:PRO:HD3	2.15	0.47
1:D:212:THR:HG22	1:D:216:LYS:HE3	1.95	0.47
1:D:25:GLN:OE1	1:D:178:LYS:NZ	2.48	0.47
1:E:106:THR:O	1:E:107:GLN:HB2	2.15	0.47
1:C:8:ILE:O	1:C:40:VAL:HG22	2.14	0.47
1:F:210:ALA:HB1	1:F:277:ILE:HD13	1.96	0.47
1:F:316:ARG:NH1	1:F:319:GLU:OE2	2.47	0.47
1:E:195:LYS:HD2	2:E:403:ATP:O2G	2.15	0.47
1:F:231:ASP:HB3	1:F:235:LYS:HB2	1.97	0.47
1:A:179:VAL:HG12	1:A:181:ALA:N	2.24	0.47
1:C:108:PHE:C	1:C:110:GLU:N	2.65	0.47
1:C:91:TRP:O	1:C:94:GLN:HB2	2.15	0.47
1:A:42:GLN:O	1:A:45:ILE:HG22	2.14	0.47
1:B:205:THR:N	1:B:208:ASP:OD2	2.46	0.47
1:D:15:THR:C	1:D:17:GLY:N	2.68	0.47
1:D:228:ILE:HD13	1:D:265:TYR:CE1	2.50	0.47
1:D:195:LYS:HG3	2:D:402:ATP:O1G	2.15	0.47
1:E:3:THR:HB	1:E:138:THR:HA	1.97	0.47
1:F:45:ILE:O	1:F:45:ILE:CG2	2.63	0.47
1:C:323:GLY:HA2	1:F:55:ARG:HE	1.80	0.47
1:B:177:PRO:O	1:B:178:LYS:HB2	2.15	0.46
1:B:195:LYS:HE3	2:B:401:ATP:O3B	2.14	0.46
1:C:195:LYS:HG3	2:C:404:ATP:O3G	2.15	0.46
1:F:231:ASP:CB	1:F:235:LYS:HB2	2.45	0.46
1:B:74:GLN:HA	1:B:74:GLN:OE1	2.15	0.46
1:F:60:ARG:HG2	1:F:287:TYR:OH	2.15	0.46
1:B:125:TYR:CD2	1:B:126:PRO:HD3	2.50	0.46
1:B:199:ASN:ND2	1:B:201:LYS:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HD11	1:B:62:ALA:HB2	1.97	0.46
1:C:13:VAL:HG23	1:C:205:THR:HG23	1.96	0.46
1:D:209:ASP:O	1:D:213:ILE:HG13	2.15	0.46
1:E:140:ILE:CG2	1:E:175:ARG:HG3	2.45	0.46
1:A:29:LEU:O	1:A:31:HIS:N	2.49	0.46
1:B:109:LYS:C	1:B:111:LYS:H	2.18	0.46
1:F:155:ARG:NH1	1:F:172:PRO:O	2.49	0.46
1:B:280:LEU:O	1:B:281:ARG:C	2.54	0.46
1:D:168:LEU:HD21	1:D:314:MET:SD	2.56	0.46
1:D:78:PHE:CD1	1:D:78:PHE:N	2.82	0.46
1:F:270:ALA:O	1:F:273:ALA:HB3	2.16	0.46
1:D:151:ILE:HG21	1:D:174:ALA:HB2	1.98	0.46
1:F:115:LYS:C	1:F:117:ALA:H	2.18	0.46
1:B:122:LEU:HD12	1:B:122:LEU:HA	1.76	0.46
1:D:153:LEU:O	1:D:156:ASP:N	2.48	0.46
1:D:188:ASP:OD1	1:D:190:THR:OG1	2.30	0.46
1:E:29:LEU:HD21	1:E:175:ARG:HH22	1.80	0.46
1:E:252:SER:OG	1:E:255:GLU:HB2	2.16	0.46
1:D:18:ASN:ND2	2:D:402:ATP:C8	2.83	0.46
1:E:238:ILE:HD13	1:E:238:ILE:HA	1.73	0.46
1:E:31:HIS:HD2	1:E:74:GLN:NE2	2.13	0.46
1:A:238:ILE:HD13	1:A:238:ILE:HA	1.79	0.46
1:C:151:ILE:O	1:C:155:ARG:HG3	2.16	0.46
1:D:43:HIS:CD2	1:D:125:TYR:HB2	2.51	0.46
1:E:15:THR:HG23	1:E:195:LYS:HG3	1.98	0.46
1:B:158:ALA:O	1:B:159:GLU:C	2.55	0.45
1:B:124:THR:HG21	1:E:124:THR:HG21	1.98	0.45
1:F:230:TYR:HD2	1:F:253:ILE:HD13	1.79	0.45
1:A:212:THR:CG2	1:A:216:LYS:HE3	2.46	0.45
1:B:179:VAL:HG12	1:B:180:GLY:H	1.81	0.45
1:C:179:VAL:C	1:C:181:ALA:H	2.18	0.45
1:D:43:HIS:HD2	1:D:125:TYR:HB2	1.81	0.45
1:D:15:THR:C	1:D:17:GLY:H	2.20	0.45
1:E:27:VAL:O	1:E:30:GLN:HG2	2.17	0.45
1:F:15:THR:C	1:F:17:GLY:N	2.69	0.45
1:A:105:MET:HA	1:A:149:GLN:HE22	1.81	0.45
1:B:281:ARG:N	1:B:282:PRO:HD2	2.32	0.45
1:D:176:ILE:HG23	1:D:177:PRO:N	2.31	0.45
1:D:254:GLU:N	1:D:254:GLU:CD	2.69	0.45
1:E:105:MET:CE	1:E:149:GLN:HE21	2.30	0.45
1:C:165:TYR:CE2	1:C:322:MET:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:GLU:CD	1:E:145:GLU:H	2.18	0.45
1:B:79:ILE:CD1	1:E:326:ARG:HD2	2.47	0.45
1:B:126:PRO:HB2	1:B:127:PRO:CD	2.43	0.45
1:D:188:ASP:HA	1:D:189:PRO:HD2	1.79	0.45
1:E:109:LYS:C	1:E:111:LYS:H	2.18	0.45
1:E:129:MET:O	1:E:132:ASP:HB2	2.17	0.45
1:F:318:MET:O	1:F:322:MET:HG2	2.17	0.45
1:B:161:PHE:HE1	1:B:322:MET:SD	2.39	0.45
1:B:82:GLU:OE2	1:E:326:ARG:HD3	2.16	0.45
1:B:99:ILE:HG12	1:E:120:ALA:HA	1.99	0.45
1:F:107:GLN:C	1:F:109:LYS:H	2.20	0.45
1:B:106:THR:N	1:B:149:GLN:NE2	2.65	0.45
1:B:171:ILE:CD1	1:B:171:ILE:N	2.79	0.45
1:B:8:ILE:HD12	1:B:65:TYR:OH	2.16	0.45
1:D:14:ILE:HA	1:D:195:LYS:HE3	1.99	0.45
1:E:240:ASN:O	1:E:244:ILE:HG13	2.17	0.45
1:F:316:ARG:HH12	1:F:319:GLU:CD	2.20	0.45
1:D:185:SER:OG	1:D:202:ALA:HB1	2.17	0.45
1:D:278:GLU:HA	1:D:278:GLU:OE1	2.16	0.45
1:F:14:ILE:CD1	1:F:206:LEU:HD12	2.47	0.45
1:F:204:ILE:HD13	1:F:213:ILE:HG23	1.99	0.45
1:C:153:LEU:HG	1:C:157:LEU:HD12	1.99	0.44
1:C:179:VAL:HB	1:C:180:GLY:H	1.58	0.44
1:C:78:PHE:CE2	1:C:83:VAL:HG21	2.52	0.44
1:F:199:ASN:ND2	1:F:201:LYS:H	2.16	0.44
1:A:29:LEU:C	1:A:31:HIS:H	2.21	0.44
1:A:25:GLN:O	1:A:29:LEU:HD12	2.16	0.44
1:C:193:MET:HB3	2:C:404:ATP:N6	2.32	0.44
1:C:45:ILE:O	1:C:45:ILE:HG23	2.18	0.44
1:D:195:LYS:HG3	2:D:402:ATP:PG	2.57	0.44
1:D:302:GLU:HG2	1:D:302:GLU:O	2.17	0.44
1:F:64:LEU:O	1:F:67:ALA:HB3	2.17	0.44
1:A:105:MET:CE	1:A:149:GLN:NE2	2.81	0.44
1:B:71:ASP:OD2	1:B:74:GLN:HB2	2.18	0.44
1:C:199:ASN:HD22	1:C:199:ASN:C	2.20	0.44
1:D:219:SER:O	1:D:220:ALA:C	2.56	0.44
1:F:164:ARG:HB3	1:F:165:TYR:CD1	2.52	0.44
1:B:159:GLU:HG3	1:B:163:LYS:HE2	2.00	0.44
1:B:263:LYS:HB3	1:B:267:VAL:HG21	1.99	0.44
1:D:168:LEU:HD22	1:D:314:MET:CE	2.47	0.44
1:A:272:LEU:HA	1:A:275:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:HIS:O	1:C:46:THR:HG23	2.18	0.44
1:F:54:LEU:O	1:F:58:ILE:HG13	2.18	0.44
1:E:302:GLU:O	1:E:303:GLY:C	2.55	0.44
1:A:19:TYR:HE2	1:A:68:VAL:HG13	1.83	0.44
1:A:189:PRO:CD	1:A:221:VAL:HG21	2.44	0.44
1:C:169:PHE:HZ	1:C:318:MET:SD	2.40	0.44
1:D:109:LYS:C	1:D:111:LYS:H	2.20	0.44
1:D:59:ARG:CZ	1:D:296:LEU:HD23	2.48	0.44
1:D:5:PHE:HB2	1:D:138:THR:CG2	2.40	0.44
1:F:15:THR:C	1:F:17:GLY:H	2.21	0.44
1:A:105:MET:HE2	1:A:149:GLN:NE2	2.33	0.43
1:D:187:VAL:HG22	1:D:202:ALA:HB2	1.99	0.43
1:E:209:ASP:O	1:E:213:ILE:HG13	2.18	0.43
1:B:47:VAL:O	1:B:49:GLN:HG2	2.18	0.43
1:D:168:LEU:CD2	1:D:314:MET:SD	3.06	0.43
1:E:184:MET:HG3	1:E:189:PRO:O	2.19	0.43
1:B:272:LEU:O	1:B:275:VAL:HG12	2.18	0.43
1:B:19:TYR:HE2	1:B:68:VAL:HG13	1.83	0.43
1:D:143:VAL:HG22	1:D:174:ALA:HB1	2.00	0.43
1:B:322:MET:CE	1:E:45:ILE:HG12	2.48	0.43
1:A:141:VAL:HG12	1:A:143:VAL:HG13	2.00	0.43
1:A:258:ARG:HH22	1:A:261:GLU:CD	2.21	0.43
1:B:282:PRO:HG2	1:B:283:ILE:H	1.83	0.43
1:B:52:HIS:O	1:B:56:GLN:HB2	2.18	0.43
1:C:129:MET:O	1:C:132:ASP:HB2	2.19	0.43
1:C:82:GLU:O	1:C:84:PRO:HD3	2.17	0.43
1:A:118:VAL:O	1:D:99:ILE:HG13	2.19	0.43
1:E:40:VAL:HG23	1:E:40:VAL:O	2.18	0.43
1:F:122:LEU:HD12	1:F:122:LEU:HA	1.89	0.43
1:A:134:LEU:HB3	1:A:169:PHE:CD1	2.53	0.43
1:C:103:GLU:HG2	1:C:123:LEU:HD11	2.01	0.43
1:C:105:MET:SD	1:C:149:GLN:NE2	2.91	0.43
1:D:16:ILE:HG13	1:D:16:ILE:O	2.18	0.43
1:F:4:ILE:HG23	1:F:142:PRO:HD3	2.00	0.43
1:F:143:VAL:HG11	1:F:151:ILE:HD11	2.00	0.43
1:B:43:HIS:HE1	1:B:132:ASP:OD2	2.01	0.43
1:D:147:GLN:O	1:D:148:LYS:C	2.57	0.43
1:D:231:ASP:CB	1:D:235:LYS:HB2	2.49	0.43
1:F:40:VAL:HG23	1:F:40:VAL:O	2.19	0.43
1:A:183:ILE:O	1:A:193:MET:HB3	2.19	0.43
1:A:302:GLU:O	1:A:306:LYS:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:C	1:B:236:PRO:HD3	2.38	0.43
1:C:219:SER:O	1:C:220:ALA:C	2.57	0.43
1:C:316:ARG:HA	1:C:316:ARG:HH11	1.81	0.43
1:D:153:LEU:O	1:D:156:ASP:HB2	2.19	0.43
1:D:189:PRO:HD3	1:D:221:VAL:CG2	2.46	0.43
1:F:210:ALA:HA	1:F:213:ILE:HD12	2.01	0.43
1:F:195:LYS:HB2	2:F:405:ATP:O2G	2.18	0.43
1:C:19:TYR:HE2	1:C:68:VAL:HG13	1.84	0.43
1:F:260:TYR:O	1:F:261:GLU:C	2.57	0.43
1:A:234:ALA:C	1:A:236:PRO:HD3	2.38	0.43
1:A:92:MET:SD	1:A:322:MET:HG3	2.59	0.43
1:D:101:GLU:HA	1:D:104:ARG:HH11	1.84	0.43
1:D:143:VAL:CG2	1:D:174:ALA:HB1	2.48	0.43
1:A:188:ASP:OD1	1:A:190:THR:OG1	2.24	0.43
1:C:95:CYS:SG	1:F:45:ILE:CG2	3.06	0.43
1:E:8:ILE:HG22	1:E:61:LEU:HD21	2.00	0.43
1:A:119:SER:C	1:A:121:GLY:N	2.71	0.42
1:B:220:ALA:O	1:B:269:LYS:NZ	2.46	0.42
1:F:125:TYR:N	1:F:126:PRO:HD3	2.33	0.42
1:F:130:ALA:O	1:F:134:LEU:HG	2.19	0.42
1:F:161:PHE:CD2	1:F:169:PHE:CE2	3.07	0.42
1:F:176:ILE:HA	1:F:177:PRO:HD2	1.85	0.42
1:A:153:LEU:O	1:A:156:ASP:HB2	2.19	0.42
1:B:1:MET:H3	1:B:1:MET:CE	2.32	0.42
1:B:207:LEU:C	1:B:284:GLN:HE21	2.22	0.42
1:C:41:ASP:OD2	1:C:81:SER:OG	2.32	0.42
1:D:40:VAL:HA	1:D:80:GLN:CB	2.46	0.42
1:F:233:GLU:O	1:F:234:ALA:CB	2.67	0.42
1:F:309:ARG:NH1	1:F:310:VAL:HG23	2.33	0.42
1:B:176:ILE:N	1:B:176:ILE:HD12	2.33	0.42
1:C:183:ILE:HD12	1:C:244:ILE:HG12	2.01	0.42
1:E:55:ARG:HH11	1:E:55:ARG:HG2	1.84	0.42
1:A:241:LEU:HA	1:A:241:LEU:HD12	1.76	0.42
1:A:281:ARG:N	1:A:282:PRO:HD2	2.34	0.42
1:A:55:ARG:NH1	1:A:55:ARG:HG2	2.30	0.42
1:E:238:ILE:HG13	1:E:265:TYR:CE1	2.54	0.42
1:B:9:GLN:HE21	1:B:10:PRO:N	2.18	0.42
1:D:217:ILE:HD12	1:D:272:LEU:HD23	1.99	0.42
1:C:208:ASP:O	1:C:284:GLN:NE2	2.52	0.42
1:D:223:ASP:CG	1:D:235:LYS:HZ2	2.22	0.42
1:D:50:ASP:HB3	1:D:53:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ASN:C	1:E:199:ASN:HD22	2.22	0.42
1:E:231:ASP:O	1:E:232:LYS:C	2.57	0.42
1:F:220:ALA:HB1	1:F:241:LEU:HD11	2.00	0.42
1:A:288:HIS:O	1:A:292:GLU:HG2	2.19	0.42
1:C:40:VAL:O	1:C:40:VAL:HG23	2.20	0.42
1:C:77:LEU:O	1:C:303:GLY:HA3	2.20	0.42
1:D:205:THR:N	1:D:208:ASP:OD2	2.38	0.42
1:C:124:THR:O	1:C:127:PRO:HD2	2.20	0.42
1:D:102:LEU:HD13	1:D:123:LEU:O	2.19	0.42
1:E:122:LEU:HD12	1:E:122:LEU:HA	1.77	0.42
1:E:84:PRO:O	1:E:86:HIS:N	2.53	0.42
1:B:76:THR:O	1:B:76:THR:HG22	2.20	0.42
1:B:322:MET:HE2	1:E:45:ILE:HG12	2.02	0.42
1:F:232:LYS:HB2	1:F:233:GLU:OE2	2.19	0.42
1:D:85:ALA:CB	1:D:315:VAL:HG21	2.47	0.42
1:E:60:ARG:HG2	1:E:287:TYR:OH	2.20	0.42
1:E:77:LEU:O	1:E:303:GLY:HA3	2.20	0.42
1:C:8:ILE:HG21	1:C:61:LEU:HD21	1.99	0.41
1:E:141:VAL:HG12	1:E:143:VAL:HG13	2.02	0.41
1:F:115:LYS:O	1:F:117:ALA:N	2.46	0.41
1:B:240:ASN:O	1:B:243:ASN:HB2	2.20	0.41
1:B:43:HIS:O	1:B:46:THR:OG1	2.33	0.41
1:B:47:VAL:O	1:B:48:TRP:C	2.58	0.41
1:D:258:ARG:NH2	1:D:261:GLU:OE1	2.54	0.41
1:E:100:GLY:O	1:E:104:ARG:HG2	2.20	0.41
1:B:45:ILE:CG2	1:E:95:CYS:SG	3.06	0.41
1:B:17:GLY:HA2	1:B:183:ILE:HG13	2.02	0.41
1:D:300:LEU:HA	1:D:300:LEU:HD23	1.88	0.41
1:E:30:GLN:OE1	1:E:71:ASP:HB3	2.20	0.41
1:F:122:LEU:O	1:F:125:TYR:HD2	2.02	0.41
1:A:115:LYS:O	1:A:117:ALA:N	2.52	0.41
1:A:125:TYR:N	1:A:126:PRO:CD	2.84	0.41
1:A:23:LEU:HG	1:A:68:VAL:HG11	2.01	0.41
1:E:84:PRO:O	1:E:85:ALA:C	2.58	0.41
1:A:205:THR:O	1:A:207:LEU:N	2.54	0.41
1:B:177:PRO:C	1:B:179:VAL:H	2.23	0.41
1:C:52:HIS:O	1:C:56:GLN:HB2	2.21	0.41
1:D:189:PRO:HB2	1:D:236:PRO:CB	2.48	0.41
1:D:311:ALA:O	1:D:314:MET:N	2.54	0.41
1:D:30:GLN:NE2	1:D:69:GLY:O	2.54	0.41
1:E:150:HIS:O	1:E:154:THR:CG2	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.82	0.41
1:B:8:ILE:O	1:B:40:VAL:HG22	2.19	0.41
1:E:245:TYR:HD2	1:E:268:PHE:CE1	2.39	0.41
1:C:95:CYS:HB3	1:F:45:ILE:O	2.20	0.41
1:C:108:PHE:CE2	1:C:123:LEU:CD1	3.01	0.41
1:D:123:LEU:HG	1:D:123:LEU:O	2.20	0.41
1:D:25:GLN:HB2	1:D:25:GLN:HE21	1.70	0.41
1:B:14:ILE:HG13	1:B:14:ILE:O	2.20	0.41
1:B:225:GLU:OE1	1:B:235:LYS:HD2	2.21	0.41
1:C:108:PHE:C	1:C:110:GLU:H	2.21	0.41
1:C:14:ILE:HG13	1:C:206:LEU:HG	2.03	0.41
1:C:55:ARG:HG2	1:C:55:ARG:NH1	2.34	0.41
1:D:26:PHE:HZ	1:D:142:PRO:HG3	1.85	0.41
1:F:199:ASN:C	1:F:199:ASN:HD22	2.24	0.41
1:A:98:TYR:HB2	1:A:101:GLU:HG3	2.02	0.41
1:B:134:LEU:HB3	1:B:169:PHE:CD1	2.56	0.41
1:C:212:THR:CG2	1:C:216:LYS:HE3	2.51	0.41
1:C:41:ASP:OD1	1:C:41:ASP:N	2.53	0.41
1:E:25:GLN:NE2	1:E:178:LYS:HE3	2.36	0.41
1:E:24:ARG:NH1	1:E:248:LEU:HD23	2.36	0.41
1:F:103:GLU:O	1:F:105:MET:N	2.54	0.41
1:A:106:THR:N	1:A:149:GLN:HE22	2.15	0.41
1:C:195:LYS:HG3	2:C:404:ATP:O2B	2.21	0.41
1:C:230:TYR:CD2	1:C:253:ILE:HD13	2.56	0.41
1:B:124:THR:HG21	1:E:124:THR:CG2	2.51	0.41
1:E:24:ARG:NH1	1:E:247:THR:O	2.53	0.41
1:F:225:GLU:OE1	1:F:235:LYS:HD2	2.21	0.41
1:F:213:ILE:HD12	1:F:277:ILE:HG12	2.02	0.41
1:F:50:ASP:O	1:F:53:GLU:N	2.52	0.41
1:B:176:ILE:HG22	1:B:177:PRO:HD3	2.03	0.41
1:D:133:ILE:HD13	1:D:141:VAL:HG21	2.02	0.41
1:B:9:GLN:HE21	1:B:9:GLN:CA	2.34	0.40
1:D:209:ASP:OD1	1:D:211:LYS:HB3	2.21	0.40
1:F:37:PHE:CE2	1:F:70:ILE:HD12	2.55	0.40
1:A:171:ILE:N	1:A:171:ILE:HD12	2.35	0.40
1:B:136:TYR:HB2	1:B:138:THR:HG22	2.03	0.40
1:E:133:ILE:O	1:E:138:THR:HG23	2.22	0.40
1:A:115:LYS:C	1:A:117:ALA:H	2.25	0.40
1:A:188:ASP:OD1	1:A:188:ASP:C	2.59	0.40
1:B:235:LYS:N	1:B:236:PRO:CD	2.82	0.40
1:E:110:GLU:C	1:E:112:SER:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:PRO:HB2	1:F:127:PRO:CD	2.42	0.40
1:B:42:GLN:HB2	1:B:80:GLN:OE1	2.21	0.40
1:C:13:VAL:HG13	1:C:13:VAL:O	2.22	0.40
1:F:230:TYR:HE1	1:F:232:LYS:HG2	1.86	0.40
1:C:162:ASN:O	1:C:166:GLY:N	2.51	0.40
1:E:125:TYR:CG	1:E:126:PRO:HD3	2.56	0.40
1:E:231:ASP:O	1:E:233:GLU:O	2.39	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	324/328 (99%)	280 (86%)	33 (10%)	11 (3%)	4	24
1	B	324/328 (99%)	276 (85%)	36 (11%)	12 (4%)	4	22
1	C	324/328 (99%)	275 (85%)	36 (11%)	13 (4%)	3	20
1	D	324/328 (99%)	276 (85%)	41 (13%)	7 (2%)	8	36
1	E	324/328 (99%)	282 (87%)	30 (9%)	12 (4%)	4	22
1	F	324/328 (99%)	285 (88%)	27 (8%)	12 (4%)	4	22
All	All	1944/1968 (99%)	1674 (86%)	203 (10%)	67 (3%)	4	24

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	B	107	GLN
1	B	176	ILE
1	B	179	VAL
1	C	105	MET

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Mol	Chain	Res	Type
1	C	106	THR
1	C	137	ASN
1	C	179	VAL
1	C	181	ALA
1	D	106	THR
1	D	148	LYS
1	E	107	GLN
1	E	261	GLU
1	F	107	GLN
1	A	30	GLN
1	A	116	GLU
1	A	179	VAL
1	A	261	GLU
1	B	12	GLY
1	B	106	THR
1	B	116	GLU
1	C	12	GLY
1	C	107	GLN
1	D	13	VAL
1	D	107	GLN
1	E	13	VAL
1	E	85	ALA
1	E	105	MET
1	E	106	THR
1	E	110	GLU
1	E	175	ARG
1	F	106	THR
1	F	261	GLU
1	C	133	ILE
1	D	116	GLU
1	E	12	GLY
1	F	104	ARG
1	F	220	ALA
1	F	265	TYR
1	A	106	THR
1	B	108	PHE
1	B	181	ALA
1	B	182	ARG
1	C	85	ALA
1	C	116	GLU
1	C	220	ALA
1	C	261	GLU

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Mol	Chain	Res	Type
1	D	40	VAL
1	E	22	ALA
1	F	116	GLU
1	F	236	PRO
1	A	133	ILE
1	A	182	ARG
1	A	206	LEU
1	A	325	GLY
1	B	110	GLU
1	B	178	LYS
1	C	182	ARG
1	F	22	ALA
1	F	179	VAL
1	A	178	LYS
1	B	196	SER
1	D	236	PRO
1	E	116	GLU
1	E	250	GLY
1	F	40	VAL
1	F	45	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	270/280 (96%)	244 (90%)	26 (10%)	10	36
1	B	270/280 (96%)	246 (91%)	24 (9%)	11	40
1	C	270/280 (96%)	239 (88%)	31 (12%)	6	27
1	D	270/280 (96%)	242 (90%)	28 (10%)	8	31
1	E	270/280 (96%)	239 (88%)	31 (12%)	6	27
1	F	270/280 (96%)	249 (92%)	21 (8%)	15	47
All	All	1620/1680 (96%)	1459 (90%)	161 (10%)	9	34

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	GLN
1	A	18	ASN
1	A	29	LEU
1	A	30	GLN
1	A	48	TRP
1	A	56	GLN
1	A	104	ARG
1	A	105	MET
1	A	107	GLN
1	A	122	LEU
1	A	138	THR
1	A	154	THR
1	A	168	LEU
1	A	176	ILE
1	A	201	LYS
1	A	214	GLU
1	A	223	ASP
1	A	241	LEU
1	A	243	ASN
1	A	275	VAL
1	A	278	GLU
1	A	289	HIS
1	A	294	GLU
1	A	314	MET
1	A	316	ARG
1	B	1	MET
1	B	9	GLN
1	B	23	LEU
1	B	25	GLN
1	B	29	LEU
1	B	46	THR
1	B	48	TRP
1	B	51	PRO
1	B	55	ARG
1	B	104	ARG
1	B	105	MET
1	B	107	GLN
1	B	122	LEU
1	B	123	LEU
1	B	138	THR
1	B	176	ILE
1	B	177	PRO

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Mol	Chain	Res	Type
1	B	215	LYS
1	B	241	LEU
1	B	245	TYR
1	B	278	GLU
1	B	289	HIS
1	B	309	ARG
1	B	316	ARG
1	C	9	GLN
1	C	18	ASN
1	C	24	ARG
1	C	29	LEU
1	C	45	ILE
1	C	48	TRP
1	C	55	ARG
1	C	64	LEU
1	C	104	ARG
1	C	106	THR
1	C	107	GLN
1	C	122	LEU
1	C	138	THR
1	C	150	HIS
1	C	154	THR
1	C	157	LEU
1	C	168	LEU
1	C	176	ILE
1	C	178	LYS
1	C	179	VAL
1	C	182	ARG
1	C	194	SER
1	C	195	LYS
1	C	199	ASN
1	C	245	TYR
1	C	261	GLU
1	C	275	VAL
1	C	278	GLU
1	C	289	HIS
1	C	316	ARG
1	C	322	MET
1	D	9	GLN
1	D	23	LEU
1	D	24	ARG
1	D	32	GLU

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Mol	Chain	Res	Type
1	D	48	TRP
1	D	56	GLN
1	D	76	THR
1	D	104	ARG
1	D	106	THR
1	D	107	GLN
1	D	138	THR
1	D	145	GLU
1	D	154	THR
1	D	159	GLU
1	D	168	LEU
1	D	178	LYS
1	D	179	VAL
1	D	182	ARG
1	D	194	SER
1	D	199	ASN
1	D	231	ASP
1	D	241	LEU
1	D	275	VAL
1	D	278	GLU
1	D	289	HIS
1	D	297	ASP
1	D	314	MET
1	D	316	ARG
1	E	9	GLN
1	E	18	ASN
1	E	23	LEU
1	E	28	GLU
1	E	45	ILE
1	E	48	TRP
1	E	55	ARG
1	E	56	GLN
1	E	104	ARG
1	E	105	MET
1	E	106	THR
1	E	107	GLN
1	E	122	LEU
1	E	137	ASN
1	E	138	THR
1	E	154	THR
1	E	168	LEU
1	E	175	ARG

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Mol	Chain	Res	Type
1	E	182	ARG
1	E	199	ASN
1	E	218	LYS
1	E	222	THR
1	E	238	ILE
1	E	241	LEU
1	E	245	TYR
1	E	275	VAL
1	E	278	GLU
1	E	289	HIS
1	E	294	GLU
1	E	316	ARG
1	E	326	ARG
1	F	9	GLN
1	F	45	ILE
1	F	48	TRP
1	F	56	GLN
1	F	104	ARG
1	F	107	GLN
1	F	122	LEU
1	F	127	PRO
1	F	138	THR
1	F	154	THR
1	F	168	LEU
1	F	182	ARG
1	F	185	SER
1	F	199	ASN
1	F	201	LYS
1	F	231	ASP
1	F	278	GLU
1	F	309	ARG
1	F	316	ARG
1	F	322	MET
1	F	326	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	43	HIS

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Mol	Chain	Res	Type
1	A	86	HIS
1	A	149	GLN
1	A	199	ASN
1	A	251	GLN
1	A	259	GLN
1	A	308	ASN
1	B	9	GLN
1	B	18	ASN
1	B	25	GLN
1	B	43	HIS
1	B	86	HIS
1	B	149	GLN
1	B	199	ASN
1	B	284	GLN
1	C	18	ASN
1	C	56	GLN
1	C	86	HIS
1	C	149	GLN
1	C	199	ASN
1	C	251	GLN
1	C	259	GLN
1	D	34	ASN
1	D	43	HIS
1	D	56	GLN
1	D	86	HIS
1	D	149	GLN
1	D	199	ASN
1	D	308	ASN
1	E	9	GLN
1	E	25	GLN
1	E	31	HIS
1	E	34	ASN
1	E	43	HIS
1	E	86	HIS
1	E	137	ASN
1	E	199	ASN
1	E	251	GLN
1	E	259	GLN
1	F	9	GLN
1	F	18	ASN
1	F	25	GLN
1	F	34	ASN

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Mol	Chain	Res	Type
1	F	42	GLN
1	F	43	HIS
1	F	56	GLN
1	F	86	HIS
1	F	149	GLN
1	F	199	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	ATP	A	400	-	27,33,33	2.23	7 (25%)	25,52,52	3.26	8 (32%)
2	ATP	B	401	-	27,33,33	2.03	8 (29%)	25,52,52	3.50	11 (44%)
2	ATP	C	404	-	27,33,33	2.19	7 (25%)	25,52,52	3.47	9 (36%)
2	ATP	D	402	-	27,33,33	2.11	6 (22%)	25,52,52	3.42	7 (28%)
2	ATP	E	403	-	27,33,33	2.25	8 (29%)	25,52,52	3.57	10 (40%)
2	ATP	F	405	-	27,33,33	2.04	8 (29%)	25,52,52	3.34	7 (28%)

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	ATP	A	400	-	-	0/18/38/38	0/3/3/3
2	ATP	B	401	-	-	0/18/38/38	0/3/3/3
2	ATP	C	404	-	-	0/18/38/38	0/3/3/3
2	ATP	D	402	-	-	0/18/38/38	0/3/3/3
2	ATP	E	403	-	-	0/18/38/38	0/3/3/3
2	ATP	F	405	-	-	0/18/38/38	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	402	ATP	O5'-C5'	-4.61	1.26	1.44
2	A	400	ATP	O5'-C5'	-4.55	1.26	1.44
2	F	405	ATP	O5'-C5'	-4.48	1.27	1.44
2	E	403	ATP	O5'-C5'	-4.30	1.27	1.44
2	C	404	ATP	O5'-C5'	-4.19	1.28	1.44
2	B	401	ATP	O5'-C5'	-4.17	1.28	1.44
2	F	405	ATP	PA-O5'	-2.86	1.47	1.59
2	D	402	ATP	PA-O5'	-2.78	1.47	1.59
2	B	401	ATP	C8-N7	-2.76	1.29	1.34
2	E	403	ATP	PA-O5'	-2.68	1.47	1.59
2	E	403	ATP	C8-N7	-2.63	1.29	1.34
2	A	400	ATP	PA-O5'	-2.63	1.48	1.59
2	D	402	ATP	C8-N7	-2.58	1.29	1.34
2	B	401	ATP	PA-O5'	-2.56	1.48	1.59
2	C	404	ATP	PA-O5'	-2.55	1.48	1.59
2	F	405	ATP	C8-N7	-2.33	1.30	1.34
2	A	400	ATP	C8-N7	-2.32	1.30	1.34
2	F	405	ATP	PB-O1B	-2.28	1.42	1.50
2	C	404	ATP	C8-N7	-2.27	1.30	1.34
2	C	404	ATP	PB-O1B	-2.24	1.42	1.50
2	E	403	ATP	PB-O1B	-2.08	1.43	1.50
2	B	401	ATP	PB-O1B	-2.04	1.43	1.50
2	B	401	ATP	C2-N3	2.09	1.35	1.32
2	F	405	ATP	C2-N3	2.90	1.37	1.32
2	F	405	ATP	C2'-C1'	2.94	1.58	1.53
2	D	402	ATP	C2'-C1'	2.96	1.58	1.53
2	E	403	ATP	C2-N3	3.02	1.37	1.32
2	A	400	ATP	C2'-C1'	3.22	1.58	1.53
2	B	401	ATP	C2'-C1'	3.40	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	ATP	PG-O3B	3.61	1.65	1.60
2	F	405	ATP	O4'-C1'	3.79	1.46	1.41
2	E	403	ATP	O4'-C1'	3.88	1.46	1.41
2	D	402	ATP	O4'-C1'	4.08	1.46	1.41
2	A	400	ATP	O4'-C1'	4.09	1.46	1.41
2	C	404	ATP	C2'-C1'	4.28	1.60	1.53
2	C	404	ATP	O4'-C1'	4.44	1.47	1.41
2	B	401	ATP	C4-N3	4.52	1.42	1.35
2	B	401	ATP	O4'-C1'	4.62	1.47	1.41
2	F	405	ATP	C4-N3	4.73	1.42	1.35
2	E	403	ATP	C2'-C1'	4.80	1.61	1.53
2	E	403	ATP	C4-N3	5.25	1.43	1.35
2	D	402	ATP	C4-N3	5.52	1.43	1.35
2	A	400	ATP	C4-N3	5.90	1.44	1.35
2	C	404	ATP	C4-N3	6.01	1.44	1.35

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	ATP	O5'-PA-O1A	-7.70	78.19	109.25
2	B	401	ATP	O5'-PA-O1A	-7.68	78.27	109.25
2	F	405	ATP	O5'-PA-O1A	-7.46	79.15	109.25
2	C	404	ATP	O5'-PA-O1A	-7.38	79.47	109.25
2	E	403	ATP	O5'-PA-O1A	-7.20	80.21	109.25
2	D	402	ATP	O5'-PA-O1A	-6.79	81.84	109.25
2	C	404	ATP	C5'-C4'-C3'	-5.75	93.38	115.29
2	E	403	ATP	C5'-C4'-C3'	-5.68	93.65	115.29
2	B	401	ATP	C5'-C4'-C3'	-5.45	94.52	115.29
2	A	400	ATP	C5'-C4'-C3'	-5.42	94.62	115.29
2	D	402	ATP	C5'-C4'-C3'	-5.36	94.88	115.29
2	F	405	ATP	C5'-C4'-C3'	-5.30	95.09	115.29
2	E	403	ATP	O3B-PG-O1G	-4.31	84.90	111.44
2	B	401	ATP	O3B-PG-O1G	-3.87	87.62	111.44
2	C	404	ATP	O3B-PG-O1G	-3.79	88.14	111.44
2	A	400	ATP	O4'-C4'-C5'	-3.10	98.93	109.40
2	D	402	ATP	N3-C2-N1	-3.05	126.20	128.86
2	B	401	ATP	O4'-C4'-C5'	-3.03	99.15	109.40
2	E	403	ATP	N3-C2-N1	-2.82	126.40	128.86
2	C	404	ATP	O4'-C4'-C5'	-2.58	100.69	109.40
2	B	401	ATP	N3-C2-N1	-2.47	126.71	128.86
2	D	402	ATP	C1'-N9-C4	-2.10	123.01	126.64
2	A	400	ATP	N3-C2-N1	-2.05	127.07	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	405	ATP	O2A-PA-O5'	-2.02	98.59	108.14
2	E	403	ATP	O2A-PA-O1A	2.03	122.78	112.28
2	C	404	ATP	O2A-PA-O1A	2.06	122.94	112.28
2	E	403	ATP	O3G-PG-O2G	2.10	116.10	107.61
2	A	400	ATP	C4-C5-N7	2.11	111.45	109.41
2	B	401	ATP	O2A-PA-O1A	2.13	123.31	112.28
2	F	405	ATP	O2A-PA-O1A	2.13	123.32	112.28
2	B	401	ATP	O3'-C3'-C4'	2.15	117.36	111.09
2	A	400	ATP	O2A-PA-O1A	2.23	123.83	112.28
2	C	404	ATP	O3G-PG-O2G	2.25	116.70	107.61
2	D	402	ATP	C4-C5-N7	2.34	111.67	109.41
2	B	401	ATP	C4-C5-N7	2.56	111.89	109.41
2	E	403	ATP	C4-C5-N7	2.88	112.19	109.41
2	F	405	ATP	C4-C5-N7	2.94	112.25	109.41
2	C	404	ATP	O2G-PG-O1G	3.50	124.20	110.50
2	E	403	ATP	O2G-PG-O1G	3.65	124.80	110.50
2	B	401	ATP	O4'-C4'-C3'	3.76	112.65	105.17
2	A	400	ATP	O4'-C4'-C3'	3.77	112.67	105.17
2	D	402	ATP	O4'-C4'-C3'	4.09	113.29	105.17
2	B	401	ATP	O2G-PG-O1G	4.09	126.51	110.50
2	C	404	ATP	O4'-C4'-C3'	4.22	113.56	105.17
2	F	405	ATP	O4'-C4'-C3'	4.37	113.85	105.17
2	E	403	ATP	O4'-C4'-C3'	4.66	114.44	105.17
2	A	400	ATP	O5'-C5'-C4'	11.01	148.03	109.00
2	B	401	ATP	O5'-C5'-C4'	11.08	148.30	109.00
2	C	404	ATP	O5'-C5'-C4'	11.56	149.99	109.00
2	F	405	ATP	O5'-C5'-C4'	11.73	150.59	109.00
2	E	403	ATP	O5'-C5'-C4'	11.79	150.80	109.00
2	D	402	ATP	O5'-C5'-C4'	12.73	154.13	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	ATP	2	0
2	B	401	ATP	2	0
2	C	404	ATP	3	0
2	D	402	ATP	3	0
2	E	403	ATP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	405	ATP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 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	326/328 (99%)	-0.64	5 (1%) 74 47	17, 37, 80, 102	0
1	B	326/328 (99%)	-0.62	6 (1%) 69 40	11, 38, 78, 99	0
1	C	326/328 (99%)	-0.65	6 (1%) 69 40	13, 35, 77, 96	0
1	D	326/328 (99%)	-0.59	7 (2%) 64 34	14, 37, 79, 102	0
1	E	326/328 (99%)	-0.60	7 (2%) 64 34	13, 34, 79, 103	0
1	F	326/328 (99%)	-0.57	7 (2%) 64 34	12, 41, 79, 100	0
All	All	1956/1968 (99%)	-0.61	38 (1%) 67 37	11, 37, 81, 103	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	VAL	5.3
1	F	114	GLY	5.0
1	F	180	GLY	4.9
1	A	177	PRO	4.8
1	F	113	ALA	4.8
1	D	114	GLY	4.6
1	E	177	PRO	4.5
1	F	177	PRO	4.4
1	E	113	ALA	4.3
1	D	113	ALA	4.2
1	B	177	PRO	4.2
1	A	114	GLY	4.1
1	E	114	GLY	3.9
1	B	114	GLY	3.7
1	D	179	VAL	3.4
1	C	106	THR	3.3
1	B	112	SER	3.3
1	B	113	ALA	3.2
1	E	112	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	112	SER	3.0
1	A	113	ALA	3.0
1	E	106	THR	2.8
1	A	180	GLY	2.8
1	F	116	GLU	2.7
1	C	112	SER	2.6
1	E	178	LYS	2.6
1	F	106	THR	2.6
1	C	113	ALA	2.5
1	C	178	LYS	2.5
1	C	179	VAL	2.5
1	B	179	VAL	2.3
1	D	116	GLU	2.3
1	D	180	GLY	2.2
1	B	106	THR	2.1
1	D	112	SER	2.1
1	D	177	PRO	2.1
1	F	112	SER	2.0
1	C	114	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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
2	ATP	C	404	31/31	0.90	0.23	0.56	53,63,78,78	31
2	ATP	F	405	31/31	0.89	0.25	0.43	57,61,79,80	31

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ATP	B	401	31/31	0.89	0.23	0.35	51,56,74,75	31
2	ATP	D	402	31/31	0.91	0.23	0.32	49,60,75,76	31
2	ATP	E	403	31/31	0.91	0.25	0.32	50,58,78,80	31
2	ATP	A	400	31/31	0.86	0.26	0.26	46,59,81,83	31

## 6.5 Other polymers [i](#)

There are no such residues in this entry.