



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:31 PM GMT

PDB ID : 1TYQ  
Title : Crystal structure of Arp2/3 complex with bound ATP and calcium  
Authors : Nolen, B.J.; Littlefield, R.S.; Pollard, T.D.  
Deposited on : 2004-07-08  
Resolution : 2.55 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

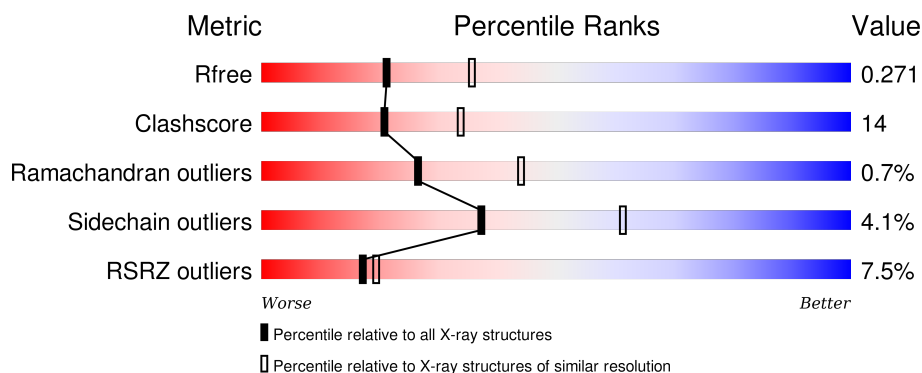
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	418	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• 5%</div> </div> </div>
2	B	394	<div> <div>8%</div> <div> <div></div> <div>32%</div> <div>20%</div> <div>•</div> <div>47%</div> </div> </div>
3	C	372	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>• 8%</div> </div> </div>
4	D	300	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>• 9%</div> </div> </div>
5	E	178	<div> <div>12%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	F	168	<div><div></div><div>2%66%29%. .</div></div>
7	G	151	<div><div></div><div>13%62%26%. 11%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13586 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3166	2031	527	594	14			

- Molecule 2 is a protein called Actin-related Protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1558	998	267	289	4			

- Molecule 3 is a protein called Arp2/3 complex 41kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	342	Total	C	N	O	S	0	0	0
			2641	1674	464	484	19			

- Molecule 4 is a protein called Arp2/3 complex 34kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	274	Total	C	N	O	S	0	0	0
			2219	1411	386	414	8			

- Molecule 5 is a protein called Arp2/3 complex 21kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	169	Total	C	N	O	S	0	0	0
			1379	888	229	253	9			

- Molecule 6 is a protein called Arp2/3 complex 20kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	166	Total	C	N	O	S	0	0	0
			1364	871	238	246	9			

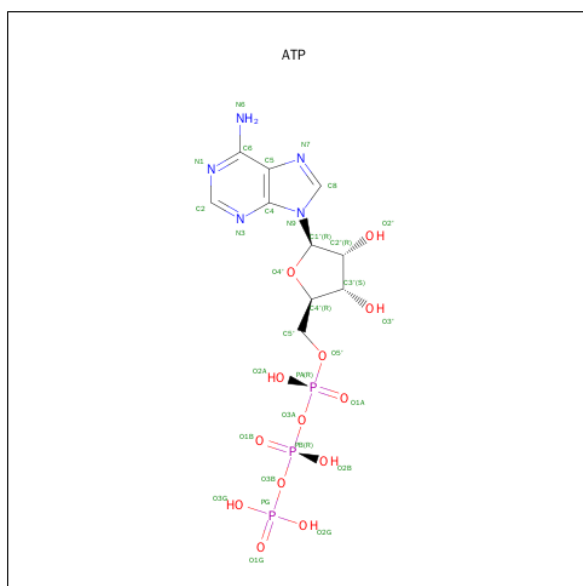
- Molecule 7 is a protein called Arp2/3 Complex 16kDa Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	134	Total	C	N	O	S	0	0	0
			1014	637	174	200	3			

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



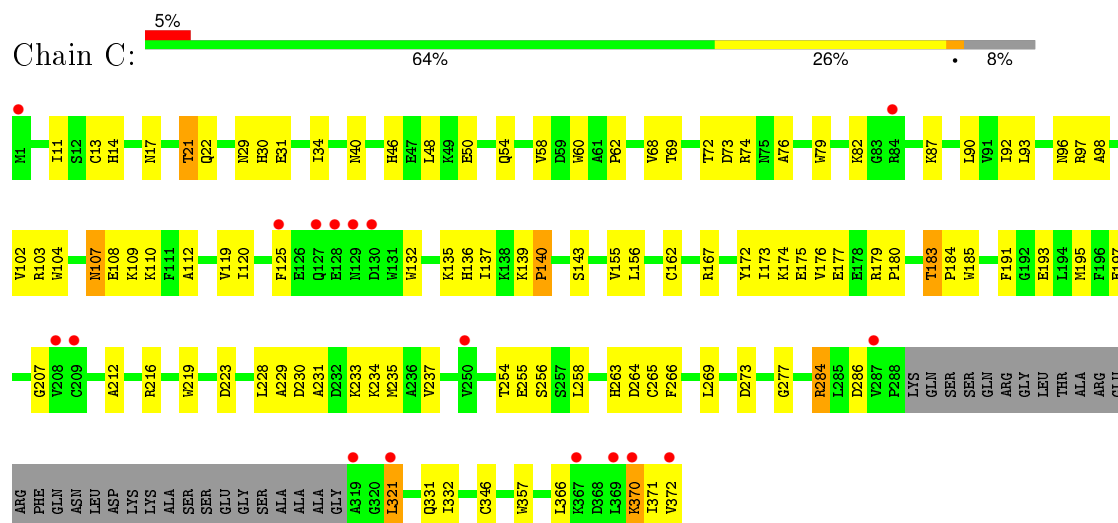
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 10 is water.

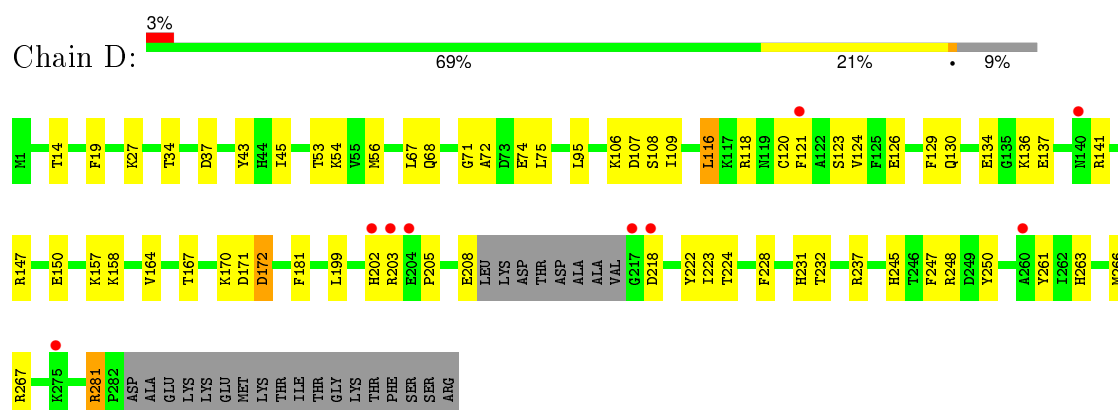
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	22	Total 22	O 22	0	0
10	B	13	Total 13	O 13	0	0
10	C	59	Total 59	O 59	0	0
10	D	41	Total 41	O 41	0	0
10	E	2	Total 2	O 2	0	0
10	F	37	Total 37	O 37	0	0
10	G	7	Total 7	O 7	0	0



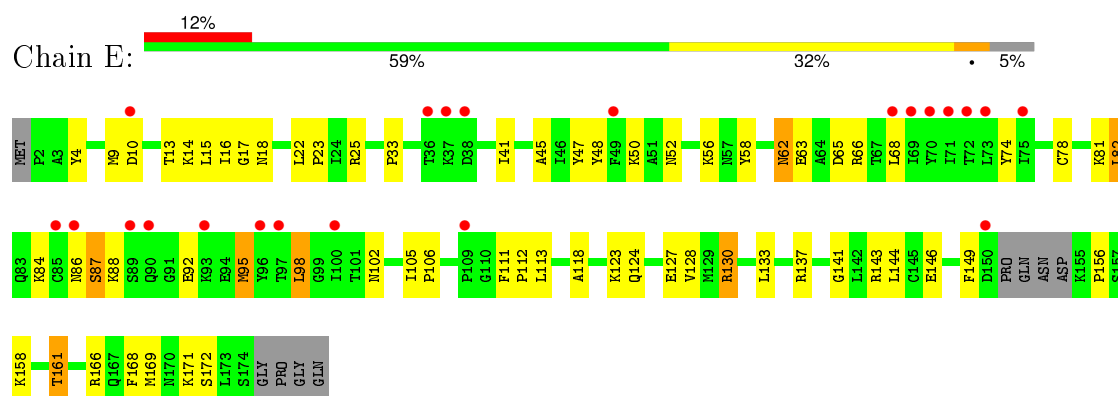
- Molecule 3: Arp2/3 complex 41kDa subunit



- Molecule 4: Arp2/3 complex 34kDa subunit



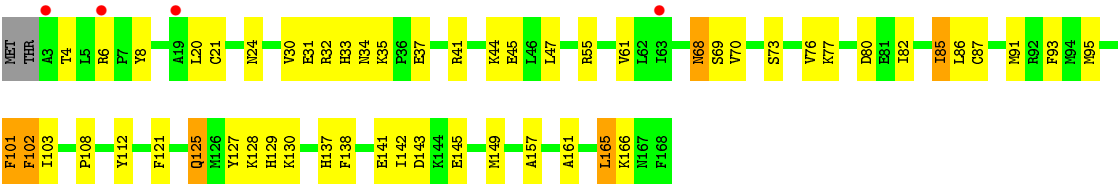
- Molecule 5: Arp2/3 complex 21kDa subunit



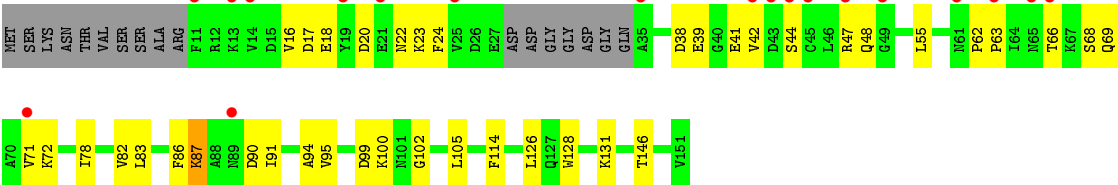
- Molecule 6: Arp2/3 complex 20kDa subunit







● Molecule 7: Arp2/3 Complex 16kDa Subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.37Å 129.39Å 199.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 29.60 – 2.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.55) 78.4 (29.60-2.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.57Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.232 , 0.272 0.232 , 0.271	Depositor DCC
$R_{free}$ test set	3662 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 72816 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CA, 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	0.38	0/3247	0.59	0/4411
2	B	0.35	0/1586	0.59	0/2157
3	C	0.39	0/2708	0.66	1/3675 (0.0%)
4	D	0.38	0/2267	0.59	0/3058
5	E	0.34	0/1411	0.59	1/1900 (0.1%)
6	F	0.41	0/1386	0.62	0/1858
7	G	0.34	0/1026	0.55	0/1382
All	All	0.38	0/13631	0.60	2/18441 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	17	GLY	N-CA-C	-5.88	98.41	113.10
3	C	11	ILE	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	261	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3166	0	3062	79	0
2	B	1558	0	1506	67	0
3	C	2641	0	2597	81	0
4	D	2219	0	2180	56	0
5	E	1379	0	1387	46	0
6	F	1364	0	1403	41	0
7	G	1014	0	1021	29	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	31	0	12	4	0
9	B	31	0	12	4	0
10	A	22	0	0	2	0
10	B	13	0	0	0	0
10	C	59	0	0	1	0
10	D	41	0	0	1	0
10	E	2	0	0	0	0
10	F	37	0	0	3	0
10	G	7	0	0	0	0
All	All	13586	0	13180	384	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 14.

All (384) 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)
6:F:130:LYS:HE2	6:F:130:LYS:HA	1.40	1.00
4:D:170:LYS:HE2	4:D:170:LYS:HA	1.44	0.99
3:C:223:ASP:HB3	7:G:146:THR:HG21	1.43	0.99
3:C:216:ARG:HG2	3:C:230:ASP:HB3	1.47	0.97
2:B:205:ASN:HD22	2:B:208:ALA:H	1.13	0.97
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.45	0.96
6:F:4:THR:HG23	6:F:55:ARG:HE	1.29	0.95
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.50	0.94
1:A:257:THR:HG22	1:A:268:SER:HB3	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:THR:HG22	3:C:185:TRP:H	1.33	0.91
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.53	0.89
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.54	0.87
2:B:326:LEU:HD12	2:B:337:LEU:HD12	1.57	0.87
3:C:370:LYS:HD2	3:C:370:LYS:O	1.79	0.83
2:B:302:VAL:HG22	2:B:350:ARG:HH22	1.45	0.81
1:A:309:ILE:HD13	1:A:312:ARG:CZ	2.11	0.80
6:F:37:GLU:H	6:F:68:ASN:HD21	1.30	0.80
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.63	0.80
3:C:14:HIS:H	3:C:331:GLN:HE22	1.29	0.79
3:C:223:ASP:CB	7:G:146:THR:HG21	2.14	0.77
1:A:248:ASP:O	1:A:250:SER:N	2.18	0.76
2:B:314:PRO:O	2:B:318:GLU:HG3	1.86	0.75
2:B:205:ASN:HD22	2:B:208:ALA:N	1.84	0.74
7:G:62:PRO:CG	7:G:105:LEU:HD21	2.17	0.74
2:B:349:ARG:O	2:B:350:ARG:HB2	1.87	0.72
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.72	0.72
3:C:183:THR:HG22	3:C:185:TRP:N	2.05	0.71
2:B:157:VAL:HB	2:B:303:LEU:HD13	1.71	0.71
6:F:130:LYS:CE	6:F:130:LYS:HA	2.21	0.71
5:E:48:TYR:HB3	5:E:52:ASN:ND2	2.07	0.70
2:B:304:SER:HB3	2:B:350:ARG:NH1	2.07	0.69
7:G:62:PRO:HG2	7:G:105:LEU:HD21	1.73	0.69
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.75	0.68
5:E:9:MET:CE	5:E:13:THR:HB	2.23	0.68
5:E:123:LYS:O	5:E:127:GLU:HG3	1.93	0.68
3:C:321:LEU:N	3:C:321:LEU:HD12	2.09	0.68
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.24	0.68
2:B:166:ILE:O	2:B:168:PRO:HD3	1.94	0.68
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.76	0.68
5:E:88:LYS:O	5:E:92:GLU:HG3	1.94	0.68
3:C:107:ASN:HD22	3:C:107:ASN:C	1.97	0.67
3:C:107:ASN:ND2	3:C:109:LYS:H	1.92	0.67
3:C:21:THR:HG22	3:C:22:GLN:HG3	1.77	0.67
3:C:119:VAL:HG23	3:C:137:ILE:O	1.94	0.67
7:G:87:LYS:HZ3	7:G:87:LYS:HB2	1.59	0.66
1:A:289:ASN:HD22	1:A:289:ASN:C	1.99	0.66
6:F:101:PHE:O	6:F:103:ILE:N	2.28	0.66
4:D:203:ARG:NH1	4:D:218:ASP:HA	2.11	0.66
1:A:194:PRO:O	1:A:195:ILE:HD12	1.96	0.66
5:E:62:ASN:HD22	5:E:62:ASN:C	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:ARG:NH2	4:D:218:ASP:OD1	2.27	0.65
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.77	0.65
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.78	0.65
3:C:229:ALA:HB2	3:C:237:VAL:HG22	1.78	0.65
1:A:91:ARG:O	1:A:94:GLU:HB2	1.97	0.64
6:F:4:THR:CG2	6:F:55:ARG:HE	2.08	0.64
7:G:95:VAL:HG21	7:G:131:LYS:HB3	1.80	0.64
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.81	0.63
1:A:243:ASN:ND2	5:E:47:TYR:HE1	1.96	0.63
4:D:129:PHE:HD2	4:D:237:ARG:HG3	1.65	0.62
2:B:218:GLU:HG2	9:B:1002:ATP:C5	2.34	0.62
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.80	0.62
5:E:62:ASN:ND2	5:E:65:ASP:H	1.98	0.62
3:C:193:GLU:HG3	3:C:195:MET:CE	2.30	0.62
2:B:184:ILE:HD12	2:B:185:ALA:N	2.14	0.61
5:E:130:ARG:HG3	5:E:130:ARG:HH11	1.65	0.61
3:C:14:HIS:H	3:C:331:GLN:NE2	1.98	0.61
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.36	0.61
2:B:345:GLU:C	2:B:347:PRO:HD3	2.21	0.61
4:D:137:GLU:CD	4:D:158:LYS:HE2	2.21	0.61
1:A:230:ARG:CB	1:A:230:ARG:HH11	2.14	0.61
1:A:246:ASP:OD1	5:E:50:LYS:HE3	2.01	0.61
4:D:228:PHE:H	4:D:231:HIS:HD2	1.49	0.61
7:G:86:PHE:C	7:G:87:LYS:HD3	2.22	0.60
6:F:145:GLU:O	6:F:149:MET:HG3	2.01	0.60
2:B:180:ARG:CB	2:B:281:LEU:HD21	2.31	0.60
6:F:20:LEU:HD23	6:F:70:VAL:HG21	1.84	0.60
1:A:120:PRO:HB2	1:A:409:ARG:HG2	1.83	0.60
1:A:229:GLU:HG2	9:A:1001:ATP:C5	2.36	0.60
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.83	0.60
6:F:137:HIS:CE1	6:F:141:GLU:HG3	2.37	0.60
3:C:193:GLU:HG3	3:C:195:MET:HE1	1.83	0.60
2:B:163:VAL:HG22	2:B:164:THR:N	2.17	0.60
6:F:80:ASP:OD1	6:F:82:ILE:HG22	2.02	0.60
6:F:68:ASN:C	6:F:68:ASN:HD22	2.06	0.59
3:C:119:VAL:HG22	3:C:120:ILE:N	2.17	0.59
6:F:121:PHE:O	6:F:125:GLN:HG2	2.02	0.59
1:A:384:LEU:HB3	1:A:414:PHE:CE1	2.36	0.59
2:B:205:ASN:ND2	2:B:208:ALA:H	1.92	0.59
7:G:62:PRO:HG3	7:G:105:LEU:HD21	1.84	0.59
2:B:151:LEU:HD13	2:B:300:HIS:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:VAL:HG21	2:B:286:ILE:HD11	1.84	0.58
7:G:87:LYS:N	7:G:87:LYS:HD3	2.19	0.58
1:A:230:ARG:HB3	1:A:230:ARG:HH11	1.69	0.57
2:B:326:LEU:HD12	2:B:337:LEU:CD1	2.31	0.57
2:B:205:ASN:HB3	2:B:208:ALA:HB3	1.86	0.57
2:B:182:LEU:HD22	2:B:184:ILE:HG23	1.86	0.57
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.40	0.57
3:C:29:ASN:HB3	3:C:31:GLU:H	1.69	0.57
2:B:184:ILE:CD1	2:B:188:ASP:HB2	2.35	0.57
1:A:176:HIS:HD2	1:A:192:HIS:ND1	2.02	0.57
3:C:107:ASN:HD22	3:C:108:GLU:N	2.02	0.56
4:D:95:LEU:HD11	4:D:116:LEU:HG	1.87	0.56
7:G:62:PRO:HG2	7:G:105:LEU:CD2	2.36	0.56
3:C:143:SER:OG	3:C:162:CYS:HB2	2.05	0.56
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.88	0.56
4:D:223:ILE:HD12	4:D:223:ILE:N	2.21	0.56
3:C:184:PRO:HB2	3:C:231:ALA:CB	2.35	0.56
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.40	0.56
1:A:374:ARG:NH1	9:A:1001:ATP:H8	2.02	0.56
1:A:111:LEU:HD23	1:A:111:LEU:C	2.26	0.56
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.41	0.56
2:B:156:VAL:HG22	2:B:302:VAL:HG12	1.88	0.56
1:A:339:LEU:O	1:A:343:VAL:HG12	2.06	0.56
4:D:121:PHE:O	4:D:124:VAL:HG12	2.06	0.55
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.41	0.55
7:G:44:SER:O	7:G:47:ARG:HG2	2.06	0.55
5:E:16:ILE:O	5:E:16:ILE:HG23	2.07	0.55
1:A:36:ALA:HB1	1:A:72:TYR:HB3	1.88	0.54
7:G:47:ARG:HG3	7:G:48:GLN:HG3	1.90	0.54
5:E:56:LYS:HA	5:E:169:MET:HA	1.89	0.54
3:C:183:THR:CG2	3:C:185:TRP:H	2.12	0.54
6:F:95:MET:SD	6:F:108:PRO:HD3	2.48	0.54
3:C:72:THR:HA	3:C:98:ALA:HB1	1.90	0.54
1:A:191:LYS:HB2	1:A:303:VAL:HG22	1.89	0.53
5:E:78:CYS:O	5:E:82:LEU:HB2	2.09	0.53
4:D:106:LYS:O	4:D:109:ILE:HG12	2.08	0.53
2:B:310:TYR:CE1	9:B:1002:ATP:H2	2.26	0.53
5:E:112:PRO:HG3	5:E:172:SER:O	2.08	0.53
1:A:289:ASN:HD22	1:A:290:PRO:N	2.05	0.53
2:B:302:VAL:HG22	2:B:350:ARG:NH2	2.20	0.53
1:A:30:ILE:HG12	1:A:375:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:HIS:HB3	1:A:407:ILE:HD12	1.90	0.53
4:D:137:GLU:OE2	4:D:158:LYS:HE2	2.09	0.53
4:D:171:ASP:OD2	4:D:172:ASP:N	2.42	0.53
1:A:189:CYS:O	1:A:303:VAL:HG13	2.09	0.53
4:D:71:GLY:HA2	4:D:74:GLU:OE1	2.09	0.53
3:C:135:LYS:HB3	3:C:191:PHE:CZ	2.43	0.53
4:D:203:ARG:NH1	4:D:218:ASP:OD1	2.43	0.52
1:A:106:GLU:HG2	1:A:135:ASN:HB3	1.90	0.52
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.44	0.52
1:A:81:GLY:O	1:A:115:PRO:HG2	2.09	0.52
4:D:37:ASP:HB2	4:D:43:TYR:HE1	1.73	0.52
4:D:106:LYS:O	4:D:109:ILE:N	2.41	0.52
1:A:176:HIS:CD2	1:A:192:HIS:ND1	2.78	0.52
4:D:247:PHE:O	4:D:250:TYR:HB3	2.08	0.52
1:A:311:VAL:C	1:A:314:PRO:HD2	2.30	0.52
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.92	0.52
3:C:156:LEU:HD22	3:C:195:MET:HG3	1.92	0.51
2:B:346:ASP:N	2:B:347:PRO:HD3	2.25	0.51
2:B:304:SER:HB3	2:B:350:ARG:CZ	2.40	0.51
2:B:326:LEU:O	2:B:326:LEU:HD23	2.11	0.51
1:A:343:VAL:CG2	1:A:363:ILE:HD12	2.41	0.51
7:G:68:SER:O	7:G:71:VAL:HG12	2.10	0.51
6:F:4:THR:HG23	6:F:55:ARG:NE	2.12	0.51
3:C:173:ILE:HG22	3:C:175:GLU:HG2	1.92	0.51
10:A:1022:HOH:O	4:D:34:THR:HG21	2.10	0.51
2:B:189:ILE:HD11	2:B:265:LEU:HG	1.93	0.51
4:D:202:HIS:O	4:D:203:ARG:HG3	2.10	0.51
4:D:129:PHE:CG	4:D:232:THR:HB	2.45	0.51
2:B:160:GLY:HA3	9:B:1002:ATP:O2G	2.11	0.51
4:D:118:ARG:HD3	4:D:118:ARG:C	2.30	0.51
2:B:319:ARG:NH1	7:G:17:ASP:OD2	2.44	0.51
4:D:281:ARG:NH1	6:F:102:PHE:CZ	2.79	0.51
5:E:149:PHE:CE2	5:E:156:PRO:HG3	2.46	0.51
1:A:349:LEU:O	1:A:353:LEU:HD23	2.10	0.51
4:D:202:HIS:C	4:D:203:ARG:HG3	2.32	0.50
2:B:155:VAL:HG21	2:B:286:ILE:CD1	2.41	0.50
4:D:75:LEU:HD13	4:D:123:SER:N	2.26	0.50
5:E:124:GLN:O	5:E:128:VAL:HG23	2.12	0.50
4:D:53:THR:C	4:D:54:LYS:HD2	2.31	0.50
3:C:48:LEU:HG	3:C:79:TRP:CE3	2.47	0.50
1:A:191:LYS:HB2	1:A:303:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:VAL:CG2	2:B:350:ARG:HH22	2.18	0.50
4:D:150:GLU:HG2	4:D:167:THR:HA	1.92	0.50
1:A:370:HIS:HD2	1:A:372:MET:N	2.10	0.50
1:A:157:GLN:HB2	1:A:368:ILE:HD12	1.93	0.50
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.41	0.50
3:C:193:GLU:CG	3:C:195:MET:CE	2.90	0.50
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.77	0.50
6:F:68:ASN:HD22	6:F:69:SER:N	2.08	0.50
1:A:374:ARG:NH1	9:A:1001:ATP:C8	2.80	0.50
7:G:20:ASP:OD1	7:G:22:ASN:HB2	2.11	0.50
1:A:389:GLU:CD	1:A:414:PHE:HB2	2.31	0.50
1:A:192:HIS:N	1:A:192:HIS:CD2	2.80	0.50
6:F:87:CYS:O	6:F:91:MET:HG2	2.11	0.50
4:D:19:PHE:HB3	4:D:106:LYS:HD3	1.94	0.50
3:C:184:PRO:HB2	3:C:231:ALA:HB1	1.93	0.49
4:D:263:HIS:HD2	4:D:266:MET:CE	2.24	0.49
2:B:231:GLN:O	2:B:235:LEU:HB2	2.11	0.49
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.42	0.49
3:C:107:ASN:C	3:C:107:ASN:ND2	2.66	0.49
3:C:212:ALA:HB3	3:C:255:GLU:OE2	2.13	0.49
3:C:125:PHE:HD2	3:C:132:TRP:CE2	2.30	0.49
3:C:119:VAL:HG21	3:C:136:HIS:HB3	1.95	0.49
4:D:199:LEU:HB2	4:D:224:THR:HB	1.95	0.49
1:A:191:LYS:HZ1	1:A:306:ASN:HD22	1.60	0.49
5:E:9:MET:HE3	5:E:13:THR:HB	1.93	0.49
3:C:254:THR:HG21	3:C:372:VAL:HG22	1.95	0.48
1:A:191:LYS:NZ	1:A:306:ASN:HD22	2.12	0.48
2:B:227:ILE:HD11	2:B:263:GLU:OE2	2.12	0.48
5:E:62:ASN:ND2	5:E:62:ASN:C	2.65	0.48
6:F:76:VAL:HG12	6:F:77:LYS:N	2.28	0.48
3:C:82:LYS:HG3	3:C:87:LYS:HG3	1.95	0.48
6:F:24:ASN:HD21	6:F:34:ASN:HD21	1.60	0.48
3:C:284:ARG:HD3	3:C:286:ASP:O	2.13	0.48
3:C:216:ARG:HH12	3:C:256:SER:HB3	1.79	0.48
1:A:38:LYS:O	1:A:39:GLU:HB3	2.13	0.48
5:E:111:PHE:HA	5:E:112:PRO:HD3	1.70	0.48
3:C:110:LYS:NZ	3:C:177:GLU:OE1	2.45	0.48
1:A:147:LEU:HD12	1:A:377:VAL:HG13	1.94	0.48
1:A:149:LEU:HD23	1:A:320:VAL:HG21	1.96	0.48
2:B:287:GLN:NE2	2:B:298:TYR:OH	2.46	0.48
1:A:260:ASN:O	1:A:264:LYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:58:TYR:CD1	5:E:168:PHE:HZ	2.32	0.48
3:C:102:VAL:HA	3:C:112:ALA:O	2.14	0.47
1:A:191:LYS:HE2	1:A:303:VAL:CG2	2.31	0.47
1:A:243:ASN:ND2	5:E:47:TYR:CE1	2.81	0.47
6:F:86:LEU:HD22	6:F:149:MET:CE	2.45	0.47
5:E:95:MET:HG2	5:E:141:GLY:O	2.15	0.47
2:B:321:LEU:HD12	2:B:342:ILE:HD11	1.95	0.47
2:B:184:ILE:HD12	2:B:185:ALA:H	1.76	0.47
2:B:151:LEU:CD1	2:B:300:HIS:HD2	2.26	0.47
6:F:68:ASN:ND2	6:F:68:ASN:C	2.67	0.47
6:F:31:GLU:OE2	6:F:32:ARG:NE	2.41	0.47
1:A:135:ASN:OD1	1:A:135:ASN:O	2.33	0.47
3:C:321:LEU:HD11	6:F:129:HIS:CE1	2.50	0.47
3:C:119:VAL:CG2	3:C:120:ILE:N	2.78	0.47
4:D:129:PHE:CD2	4:D:237:ARG:HG3	2.49	0.47
1:A:114:GLU:O	1:A:144:GLN:HG3	2.14	0.47
3:C:332:ILE:HA	3:C:346:CYS:O	2.15	0.47
6:F:73:SER:HB3	6:F:112:TYR:CG	2.50	0.47
7:G:91:ILE:O	7:G:95:VAL:HG23	2.15	0.47
2:B:155:VAL:HG21	2:B:286:ILE:CG1	2.45	0.46
1:A:311:VAL:O	1:A:315:LEU:HG	2.15	0.46
4:D:68:GLN:HA	4:D:72:ALA:HB3	1.98	0.46
1:A:289:ASN:ND2	1:A:289:ASN:C	2.69	0.46
3:C:254:THR:HG21	3:C:372:VAL:CG2	2.46	0.46
3:C:228:LEU:HD23	3:C:228:LEU:C	2.36	0.46
2:B:155:VAL:HG21	2:B:286:ILE:HG12	1.97	0.46
2:B:326:LEU:HD23	2:B:326:LEU:C	2.36	0.46
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.72	0.46
2:B:278:VAL:HG13	2:B:279:ALA:N	2.29	0.46
1:A:384:LEU:HB3	1:A:414:PHE:CZ	2.50	0.46
3:C:234:LYS:O	3:C:235:MET:HB2	2.16	0.46
5:E:143:ARG:O	5:E:146:GLU:HG2	2.15	0.45
1:A:21:TYR:OH	1:A:103:ALA:HB2	2.17	0.45
4:D:67:LEU:HD13	4:D:120:CYS:O	2.16	0.45
3:C:109:LYS:HD3	3:C:176:VAL:O	2.16	0.45
5:E:130:ARG:NH1	5:E:130:ARG:HG3	2.31	0.45
1:A:389:GLU:OE2	1:A:414:PHE:HB2	2.17	0.45
2:B:171:GLU:OE2	2:B:171:GLU:HA	2.17	0.45
5:E:23:PRO:HG3	5:E:33:PRO:HB2	1.99	0.45
1:A:193:ILE:O	1:A:195:ILE:N	2.45	0.45
1:A:239:VAL:HG23	1:A:240:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:GLU:O	4:D:130:GLN:HB2	2.16	0.45
7:G:78:ILE:O	7:G:82:VAL:HG23	2.16	0.45
1:A:398:LYS:HD2	10:A:1020:HOH:O	2.17	0.45
3:C:73:ASP:O	3:C:74:ARG:HB2	2.16	0.45
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.47	0.45
6:F:76:VAL:HG13	10:F:188:HOH:O	2.17	0.45
6:F:44:LYS:HG2	10:F:193:HOH:O	2.17	0.45
4:D:27:LYS:HA	4:D:27:LYS:HD3	1.88	0.45
5:E:82:LEU:HD13	5:E:95:MET:SD	2.57	0.44
5:E:166:ARG:HG2	5:E:166:ARG:HH11	1.82	0.44
3:C:107:ASN:HD22	3:C:109:LYS:H	1.65	0.44
3:C:184:PRO:HB2	3:C:231:ALA:HB3	2.00	0.44
2:B:347:PRO:HA	2:B:348:PRO:HD3	1.75	0.44
6:F:125:GLN:H	6:F:125:GLN:HG2	1.59	0.44
3:C:40:ASN:ND2	10:C:405:HOH:O	2.50	0.44
5:E:113:LEU:HD21	5:E:171:LYS:HG3	2.00	0.44
4:D:45:ILE:HA	4:D:56:MET:O	2.17	0.44
2:B:310:TYR:CZ	9:B:1002:ATP:H2	2.36	0.44
3:C:68:VAL:HG12	3:C:104:TRP:NE1	2.32	0.44
2:B:146:LEU:CD1	2:B:169:VAL:HB	2.48	0.44
5:E:41:ILE:O	5:E:41:ILE:HG13	2.18	0.43
3:C:263:HIS:CD2	6:F:21:CYS:HB3	2.53	0.43
4:D:203:ARG:HH12	4:D:218:ASP:HA	1.79	0.43
3:C:174:LYS:HG3	3:C:175:GLU:N	2.33	0.43
5:E:86:ASN:O	5:E:87:SER:HB3	2.18	0.43
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.99	0.43
3:C:96:ASN:OD1	3:C:97:ARG:HG2	2.18	0.43
4:D:170:LYS:CA	4:D:170:LYS:HE2	2.31	0.43
2:B:239:VAL:HG23	2:B:240:LEU:CD1	2.46	0.43
6:F:41:ARG:HB3	6:F:47:LEU:HD11	2.01	0.43
4:D:208:GLU:HB3	10:D:327:HOH:O	2.18	0.43
6:F:86:LEU:HD22	6:F:149:MET:HE3	1.99	0.43
3:C:258:LEU:O	3:C:269:LEU:HD12	2.19	0.43
4:D:137:GLU:OE1	4:D:158:LYS:HB2	2.19	0.43
1:A:229:GLU:HG2	9:A:1001:ATP:C4	2.53	0.43
4:D:164:VAL:HG22	4:D:224:THR:HG23	2.00	0.43
4:D:14:THR:HG21	4:D:45:ILE:HG21	2.01	0.43
3:C:185:TRP:CD2	3:C:231:ALA:HB2	2.54	0.43
5:E:84:LYS:HD3	5:E:84:LYS:HA	1.91	0.43
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.53	0.43
3:C:321:LEU:N	3:C:321:LEU:CD1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:ILE:HG13	6:F:86:LEU:N	2.33	0.43
2:B:163:VAL:CG2	2:B:164:THR:N	2.81	0.43
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.58	0.43
7:G:55:LEU:HD22	7:G:94:ALA:HB1	2.01	0.42
5:E:14:LYS:O	5:E:15:LEU:HD23	2.19	0.42
6:F:8:TYR:OH	6:F:61:VAL:HG23	2.19	0.42
5:E:9:MET:SD	5:E:63:GLU:HG2	2.59	0.42
1:A:289:ASN:ND2	1:A:291:ASP:H	2.16	0.42
3:C:264:ASP:O	3:C:265:CYS:HB2	2.19	0.42
4:D:223:ILE:HG21	4:D:247:PHE:CE2	2.54	0.42
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.55	0.42
7:G:38:ASP:O	7:G:42:VAL:HG23	2.18	0.42
7:G:18:GLU:OE1	7:G:23:LYS:NZ	2.52	0.42
3:C:230:ASP:OD2	3:C:233:LYS:HG3	2.19	0.42
5:E:18:ASN:O	5:E:63:GLU:HB3	2.20	0.42
1:A:117:LEU:HD11	1:A:192:HIS:HE1	1.85	0.42
4:D:106:LYS:O	4:D:108:SER:N	2.52	0.42
4:D:75:LEU:C	4:D:75:LEU:HD23	2.40	0.42
5:E:105:ILE:HB	5:E:106:PRO:HD2	2.02	0.42
1:A:239:VAL:HG13	5:E:4:TYR:CZ	2.55	0.42
4:D:54:LYS:HD2	4:D:54:LYS:N	2.33	0.42
3:C:266:PHE:CE1	3:C:284:ARG:HG3	2.55	0.42
2:B:177:HIS:ND1	2:B:178:LEU:HG	2.35	0.42
2:B:246:LEU:HB3	2:B:247:PRO:HD2	2.01	0.42
3:C:179:ARG:HA	3:C:180:PRO:HD3	1.80	0.42
1:A:2:ALA:HB2	1:A:391:TYR:CE1	2.55	0.42
1:A:19:LEU:HD23	1:A:19:LEU:N	2.34	0.42
4:D:202:HIS:O	4:D:202:HIS:CG	2.73	0.42
4:D:223:ILE:HG21	4:D:247:PHE:CZ	2.54	0.42
7:G:99:ASP:O	7:G:102:GLY:N	2.52	0.42
4:D:205:PRO:HG3	4:D:222:TYR:CZ	2.55	0.42
1:A:234:VAL:HG11	1:A:334:ARG:HG2	2.01	0.42
1:A:237:ASP:OD2	1:A:240:LYS:HG3	2.20	0.41
1:A:61:PHE:C	1:A:66:ALA:HB2	2.41	0.41
1:A:319:ILE:HB	1:A:367:VAL:HG22	2.02	0.41
2:B:295:SER:O	2:B:299:LYS:HG2	2.21	0.41
5:E:66:ARG:HG3	5:E:66:ARG:HH11	1.85	0.41
3:C:366:LEU:N	3:C:366:LEU:HD12	2.35	0.41
1:A:152:SER:HB3	1:A:320:VAL:CG1	2.51	0.41
2:B:161:ASP:OD1	2:B:187:ARG:HG3	2.20	0.41
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:9:MET:HB2	5:E:62:ASN:OD1	2.20	0.41
7:G:55:LEU:CD2	7:G:94:ALA:HB1	2.51	0.41
7:G:100:LYS:HA	7:G:100:LYS:HD3	1.76	0.41
2:B:155:VAL:O	2:B:301:ILE:HA	2.20	0.41
1:A:242:PHE:CE1	5:E:50:LYS:HB3	2.56	0.41
2:B:153:THR:HA	2:B:169:VAL:O	2.21	0.41
1:A:177:VAL:HG11	1:A:300:VAL:HA	2.01	0.41
4:D:134:GLU:HB2	4:D:136:LYS:HG3	2.03	0.41
2:B:306:GLY:HA2	2:B:309:MET:CE	2.51	0.41
1:A:329:ARG:O	1:A:330:ASP:HB2	2.20	0.41
3:C:286:ASP:HB2	3:C:357:TRP:CH2	2.56	0.41
3:C:102:VAL:O	3:C:103:ARG:NH1	2.54	0.41
3:C:183:THR:HG21	3:C:185:TRP:HD1	1.85	0.41
2:B:159:SER:HB2	2:B:164:THR:HG23	2.03	0.41
4:D:263:HIS:O	4:D:267:ARG:HG3	2.20	0.41
5:E:144:LEU:O	5:E:144:LEU:HD13	2.21	0.41
6:F:161:ALA:O	6:F:165:LEU:HB2	2.20	0.41
7:G:114:PHE:CZ	7:G:126:LEU:HD23	2.56	0.41
3:C:139:LYS:HA	3:C:140:PRO:HA	1.85	0.41
3:C:34:ILE:HB	3:C:46:HIS:HB2	2.02	0.41
3:C:92:ILE:N	3:C:92:ILE:HD12	2.36	0.41
3:C:69:THR:O	3:C:76:ALA:HA	2.21	0.41
7:G:66:THR:O	7:G:72:LYS:HE3	2.21	0.41
4:D:181:PHE:CE2	6:F:157:ALA:HA	2.55	0.41
3:C:17:ASN:HB3	3:C:60:TRP:CZ2	2.56	0.41
6:F:33:HIS:ND1	6:F:35:LYS:HE2	2.35	0.41
4:D:267:ARG:HG2	6:F:93:PHE:HZ	1.86	0.40
5:E:81:LYS:HE2	5:E:98:LEU:HD21	2.03	0.40
6:F:35:LYS:NZ	10:F:171:HOH:O	2.54	0.40
1:A:340:LYS:HE3	1:A:340:LYS:HB3	1.95	0.40
3:C:172:TYR:C	3:C:172:TYR:CD2	2.92	0.40
2:B:317:LEU:HB2	2:B:344:ILE:HD12	2.03	0.40
3:C:29:ASN:O	3:C:54:GLN:HA	2.21	0.40
2:B:319:ARG:O	2:B:323:GLN:HG3	2.22	0.40
1:A:157:GLN:HB3	1:A:366:GLN:NE2	2.36	0.40
6:F:30:VAL:HG11	6:F:33:HIS:CE1	2.56	0.40
6:F:138:PHE:O	6:F:142:ILE:HG23	2.22	0.40
3:C:273:ASP:O	3:C:277:GLY:N	2.51	0.40
1:A:247:THR:O	1:A:247:THR:HG22	2.20	0.40
1:A:129:ILE:O	1:A:133:SER:HB2	2.21	0.40
1:A:128:GLU:HG3	1:A:132:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:248:ARG:C	4:D:248:ARG:HD3	2.42	0.40
3:C:207:GLY:O	3:C:219:TRP:HA	2.22	0.40
5:E:18:ASN:ND2	5:E:118:ALA:HB2	2.37	0.40
1:A:311:VAL:HG22	1:A:311:VAL:O	2.21	0.40
5:E:158:LYS:HA	5:E:161:THR:OG1	2.21	0.40
5:E:45:ALA:HA	5:E:68:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	393/418 (94%)	371 (94%)	20 (5%)	2 (0%)	34	54
2	B	206/394 (52%)	184 (89%)	18 (9%)	4 (2%)	10	15
3	C	338/372 (91%)	312 (92%)	24 (7%)	2 (1%)	30	48
4	D	270/300 (90%)	260 (96%)	9 (3%)	1 (0%)	39	60
5	E	165/178 (93%)	152 (92%)	12 (7%)	1 (1%)	30	48
6	F	164/168 (98%)	160 (98%)	3 (2%)	1 (1%)	30	48
7	G	130/151 (86%)	123 (95%)	6 (5%)	1 (1%)	24	40
All	All	1666/1981 (84%)	1562 (94%)	92 (6%)	12 (1%)	26	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	GLY
2	B	329	VAL
2	B	331	LYS
6	F	102	PHE
5	E	87	SER

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Mol	Chain	Res	Type
2	B	179	THR
3	C	50	GLU
4	D	107	ASP
1	A	194	PRO
2	B	342	ILE
3	C	62	PRO
7	G	16	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	339/363 (93%)	326 (96%)	13 (4%)	40	65
2	B	154/345 (45%)	147 (96%)	7 (4%)	34	56
3	C	288/313 (92%)	279 (97%)	9 (3%)	47	73
4	D	241/264 (91%)	235 (98%)	6 (2%)	55	80
5	E	152/159 (96%)	141 (93%)	11 (7%)	18	31
6	F	153/155 (99%)	144 (94%)	9 (6%)	24	42
7	G	109/124 (88%)	105 (96%)	4 (4%)	41	66
All	All	1436/1723 (83%)	1377 (96%)	59 (4%)	37	61

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	68	GLU
1	A	88	LEU
1	A	143	VAL
1	A	191	LYS
1	A	230	ARG
1	A	255	GLN
1	A	268	SER
1	A	289	ASN
1	A	310	ASP

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Mol	Chain	Res	Type
1	A	318	ASN
1	A	335	LEU
1	A	394	CYS
2	B	182	LEU
2	B	183	ASP
2	B	184	ILE
2	B	200	ARG
2	B	220	LEU
2	B	274	GLU
2	B	281	LEU
3	C	21	THR
3	C	30	HIS
3	C	90	LEU
3	C	107	ASN
3	C	140	PRO
3	C	183	THR
3	C	284	ARG
3	C	321	LEU
3	C	370	LYS
4	D	116	LEU
4	D	141	ARG
4	D	157	LYS
4	D	172	ASP
4	D	245	HIS
4	D	281	ARG
5	E	10	ASP
5	E	22	LEU
5	E	25	ARG
5	E	62	ASN
5	E	82	LEU
5	E	95	MET
5	E	98	LEU
5	E	102	ASN
5	E	130	ARG
5	E	133	LEU
5	E	161	THR
6	F	6	ARG
6	F	68	ASN
6	F	85	ILE
6	F	101	PHE
6	F	125	GLN
6	F	128	LYS

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Mol	Chain	Res	Type
6	F	143	ASP
6	F	165	LEU
6	F	166	LYS
7	G	39	GLU
7	G	69	GLN
7	G	87	LYS
7	G	90	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	157	GLN
1	A	176	HIS
1	A	205	GLN
1	A	206	GLN
1	A	255	GLN
1	A	289	ASN
1	A	306	ASN
1	A	318	ASN
1	A	366	GLN
1	A	370	HIS
1	A	395	HIS
2	B	205	ASN
2	B	229	GLN
2	B	231	GLN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	22	GLN
3	C	29	ASN
3	C	33	HIS
3	C	44	GLN
3	C	46	HIS
3	C	54	GLN
3	C	65	ASN
3	C	107	ASN
3	C	331	GLN
4	D	21	ASN
4	D	26	ASN
4	D	49	ASN
4	D	140	ASN

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Mol	Chain	Res	Type
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
5	E	62	ASN
5	E	83	GLN
6	F	24	ASN
6	F	28	GLN
6	F	68	ASN
6	F	125	GLN
6	F	137	HIS
7	G	50	ASN
7	G	56	GLN
7	G	96	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	ATP	A	1001	8	24,33,33	1.37	3 (12%)	31,52,52	2.45	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ATP	B	1002	8	24,33,33	1.38	3 (12%)	31,52,52	2.38	4 (12%)

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
9	ATP	A	1001	8	-	0/18/38/38	0/3/3/3
9	ATP	B	1002	8	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1001	ATP	O4'-C1'	2.17	1.43	1.41
9	B	1002	ATP	O4'-C1'	2.43	1.44	1.41
9	A	1001	ATP	PG-O1G	3.12	1.61	1.51
9	B	1002	ATP	PG-O1G	3.12	1.61	1.51
9	B	1002	ATP	C2-N1	3.47	1.40	1.33
9	A	1001	ATP	C2-N1	3.51	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1001	ATP	N3-C2-N1	-11.43	120.15	128.89
9	B	1002	ATP	N3-C2-N1	-11.08	120.41	128.89
9	A	1001	ATP	PA-O3A-PB	-4.00	121.50	132.73
9	B	1002	ATP	PA-O3A-PB	-3.73	122.26	132.73
9	B	1002	ATP	PB-O3B-PG	-3.24	121.81	132.67
9	A	1001	ATP	PB-O3B-PG	-3.06	122.41	132.67
9	A	1001	ATP	C4'-O4'-C1'	-2.83	106.61	109.72
9	B	1002	ATP	C4-C5-N7	-2.23	107.42	109.48
9	A	1001	ATP	C4-C5-N7	-2.07	107.58	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1001	ATP	4	0
9	B	1002	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	399/418 (95%)	0.38	25 (6%) 23 27	23, 49, 76, 102	0
2	B	208/394 (52%)	0.65	31 (14%) 3 3	31, 60, 92, 100	0
3	C	342/372 (91%)	0.09	17 (4%) 32 38	27, 40, 67, 89	0
4	D	274/300 (91%)	0.22	9 (3%) 50 56	26, 44, 69, 82	0
5	E	169/178 (94%)	0.65	22 (13%) 5 5	40, 57, 81, 92	0
6	F	166/168 (98%)	-0.03	4 (2%) 62 67	28, 41, 55, 73	0
7	G	134/151 (88%)	0.83	19 (14%) 4 4	32, 66, 85, 105	0
All	All	1692/1981 (85%)	0.35	127 (7%) 17 19	23, 47, 83, 105	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	35	ALA	5.5
2	B	350	ARG	5.4
7	G	66	THR	5.3
1	A	72	TYR	5.3
1	A	418	SER	5.3
1	A	351	GLU	5.0
1	A	353	LEU	4.8
3	C	1	MET	4.8
1	A	348	LYS	4.4
5	E	109	PRO	4.3
7	G	25	VAL	4.3
2	B	334	VAL	4.2
1	A	349	LEU	4.2
5	E	71	ILE	4.2
1	A	159	GLY	4.1
2	B	288	ALA	4.0
7	G	49	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
4	D	202	HIS	3.8
1	A	156	ARG	3.8
7	G	44	SER	3.7
1	A	70	PRO	3.7
1	A	347	LEU	3.7
5	E	85	CYS	3.7
1	A	352	GLU	3.6
1	A	417	MET	3.6
5	E	86	ASN	3.6
2	B	292	ASP	3.6
6	F	3	ALA	3.6
2	B	150	GLY	3.6
5	E	38	ASP	3.6
1	A	39	GLU	3.5
5	E	49	PHE	3.5
2	B	293	THR	3.4
3	C	367	LYS	3.4
5	E	37	LYS	3.4
7	G	19	TYR	3.4
7	G	65	ASN	3.3
7	G	63	PRO	3.3
5	E	75	ILE	3.1
7	G	71	VAL	3.1
2	B	333	ASP	3.1
5	E	93	LYS	3.1
1	A	157	GLN	3.0
3	C	130	ASP	3.0
5	E	90	GLN	3.0
5	E	96	TYR	3.0
7	G	13	LYS	3.0
2	B	174	SER	3.0
2	B	173	PHE	2.9
5	E	150	ASP	2.9
7	G	11	PHE	2.9
3	C	370	LYS	2.9
2	B	171	GLU	2.8
4	D	218	ASP	2.8
2	B	274	GLU	2.8
3	C	127	GLN	2.8
2	B	273	VAL	2.8
2	B	178	LEU	2.7
3	C	319	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
7	G	43	ASP	2.7
4	D	275	LYS	2.7
2	B	169	VAL	2.7
4	D	203	ARG	2.7
3	C	321	LEU	2.7
7	G	45	CYS	2.7
1	A	158	VAL	2.6
1	A	168	ILE	2.6
2	B	282	LEU	2.6
2	B	151	LEU	2.6
7	G	47	ARG	2.6
7	G	89	ASN	2.6
1	A	291	ASP	2.6
5	E	70	TYR	2.6
1	A	71	THR	2.5
4	D	121	PHE	2.5
5	E	89	SER	2.5
1	A	202	TYR	2.5
2	B	278	VAL	2.5
7	G	21	GLU	2.5
2	B	143	VAL	2.5
2	B	176	PRO	2.5
3	C	209	CYS	2.4
3	C	208	VAL	2.4
6	F	63	ILE	2.4
3	C	129	ASN	2.4
4	D	217	GLY	2.4
5	E	10	ASP	2.4
6	F	19	ALA	2.4
2	B	154	GLY	2.4
3	C	287	VAL	2.4
1	A	248	ASP	2.4
5	E	97	THR	2.4
4	D	204	GLU	2.4
5	E	100	ILE	2.4
2	B	265	LEU	2.3
1	A	2	ALA	2.3
2	B	152	LEU	2.3
3	C	372	VAL	2.3
7	G	14	VAL	2.3
4	D	260	ALA	2.2
7	G	42	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	347	PRO	2.2
5	E	36	THR	2.2
5	E	73	LEU	2.2
2	B	148	ALA	2.2
1	A	292	PHE	2.2
2	B	317	LEU	2.2
3	C	84	ARG	2.2
2	B	299	LYS	2.2
2	B	147	TYR	2.1
3	C	369	LEU	2.1
2	B	183	ASP	2.1
3	C	125	PHE	2.1
1	A	167	VAL	2.1
2	B	170	TYR	2.1
4	D	140	ASN	2.1
1	A	388	PRO	2.1
2	B	328	ARG	2.1
6	F	6	ARG	2.1
7	G	61	ASN	2.1
2	B	272	ASN	2.1
5	E	69	ILE	2.1
1	A	68	GLU	2.1
5	E	72	THR	2.1
3	C	128	GLU	2.0
5	E	68	LEU	2.0
3	C	250	VAL	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( $\text{\AA}^2$ )	Q<0.9
9	ATP	A	1001	31/31	0.96	0.14	-0.41	46,52,58,60	0
9	ATP	B	1002	31/31	0.95	0.15	-0.77	52,59,74,76	0
8	CA	B	501	1/1	0.89	0.10	-	95,95,95,95	0
8	CA	A	500	1/1	0.96	0.30	-	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.