



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U2V  
Title : Crystal structure of Arp2/3 complex with bound ADP and calcium  
Authors : Nolen, B.J.; Littlefield, R.S.; Pollard, T.D.  
Deposited on : 2004-07-20  
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

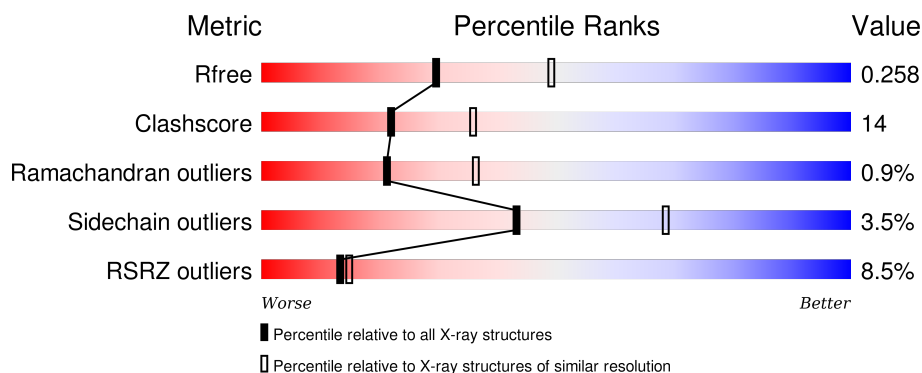
# 1 Overall quality at a glance

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>8%</div> <div>70%</div> <div>23%</div> <div>• •</div> </div>
2	B	394	<div> <div>8%</div> <div>34%</div> <div>16%</div> <div>•</div> <div>48%</div> </div>
3	C	372	<div> <div>7%</div> <div>69%</div> <div>24%</div> <div>• •</div> </div>
4	D	300	<div> <div>2%</div> <div>75%</div> <div>18%</div> <div>• 6%</div> </div>
5	E	178	<div> <div>16%</div> <div>54%</div> <div>38%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	168	<div><div>%</div><div><div></div><div>83%</div><div>15%</div><div>••</div></div></div>
7	G	151	<div><div>12%</div><div><div></div><div>69%</div><div>17%</div><div>•</div><div>11%</div></div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13922 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	402	Total	C	N	O	S	0	0	0
			3209	2059	535	598	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1569	1008	268	289	4			

- Molecule 3 is a protein called Arp2/3 Complex 41Kda Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	357	Total	C	N	O	S	0	0	0
			2761	1750	488	504	19			

- Molecule 4 is a protein called Arp2/3 Complex 34Kda Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	282	Total	C	N	O	S	0	0	0
			2279	1449	395	427	8			

- Molecule 5 is a protein called Arp2/3 Complex 21Kda Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	168	Total	C	N	O	S	0	0	0
			1354	872	227	248	7			

- 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
			1360	869	238	244	9			

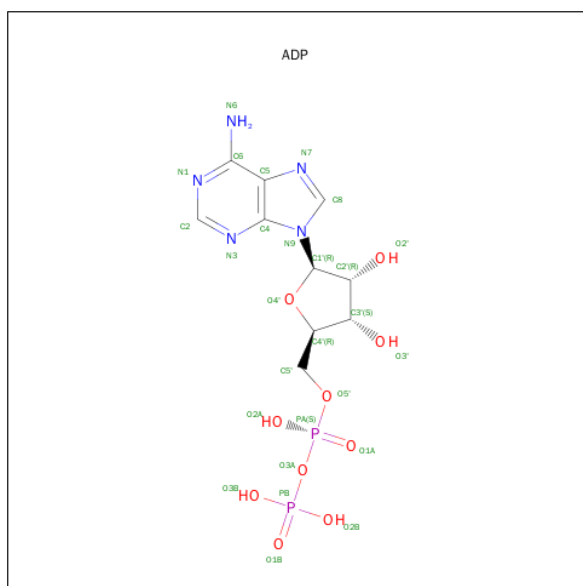
- Molecule 7 is a protein called Arp2/3 Complex 16kDa Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	135	Total	C	N	O	S	0	0	0
			1021	642	180	196	3			

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

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



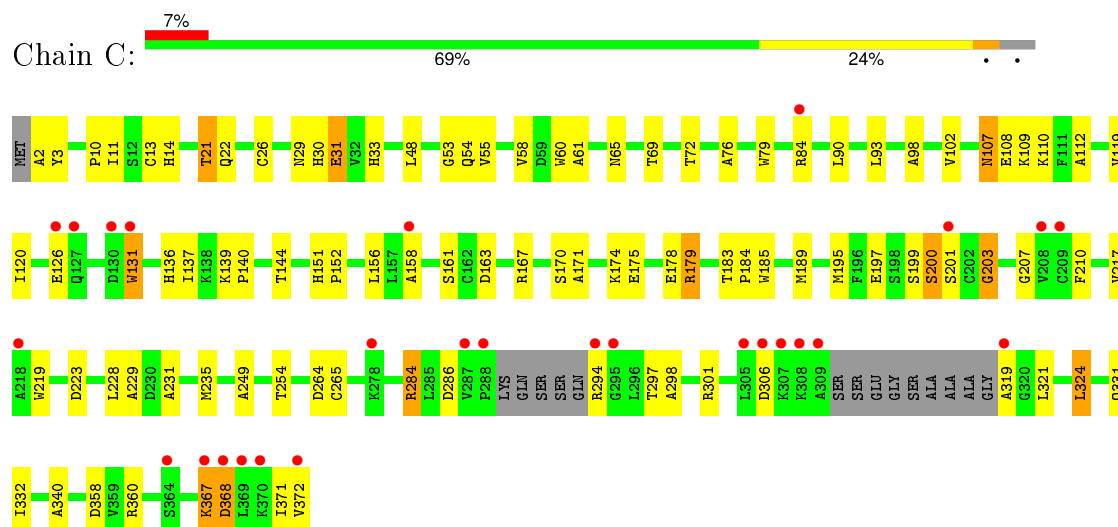
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 10 is water.

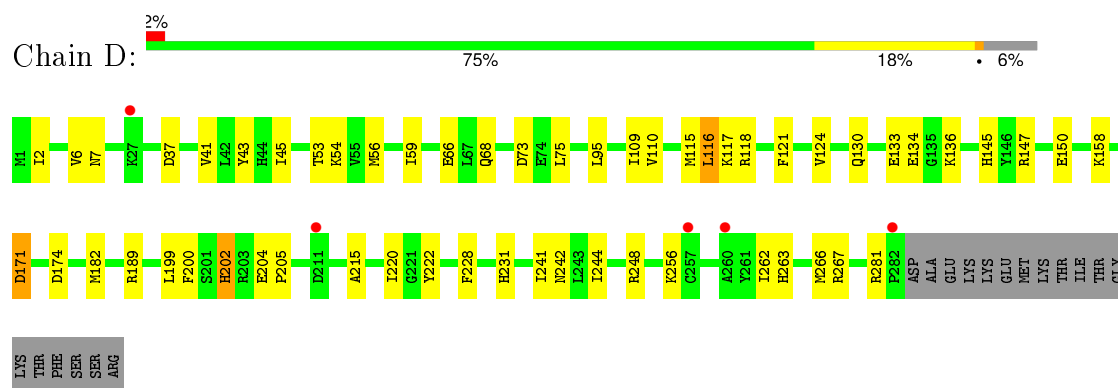
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	68	Total 68	O 68	0	0
10	B	16	Total 16	O 16	0	0
10	C	67	Total 67	O 67	0	0
10	D	66	Total 66	O 66	0	0
10	E	6	Total 6	O 6	0	0
10	F	78	Total 78	O 78	0	0
10	G	13	Total 13	O 13	0	0



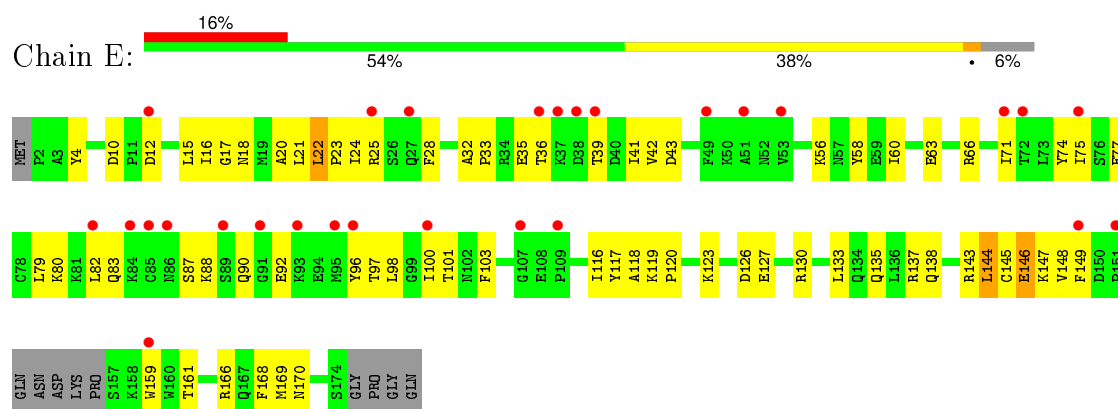
- Molecule 3: Arp2/3 Complex 41Kda Subunit



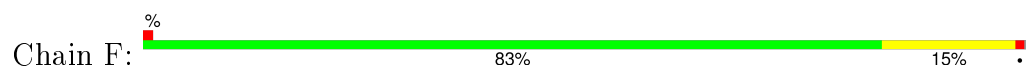
- Molecule 4: Arp2/3 Complex 34Kda Subunit



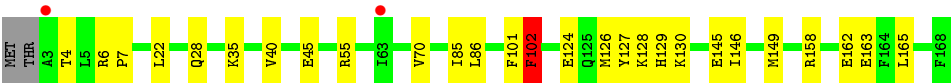
● Molecule 5: Arp2/3 Complex 21Kda Subunit



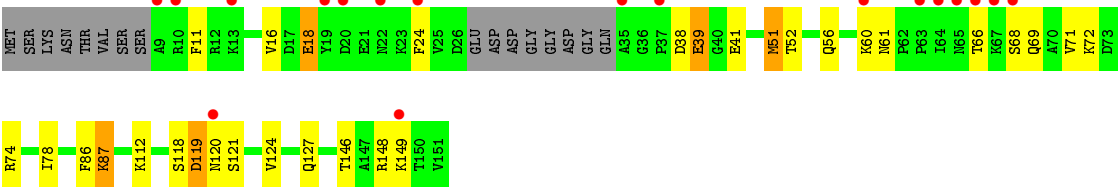
- Molecule 6: Arp2/3 Complex 20Kda Subunit







● 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, $\alpha$ , $\beta$ , $\gamma$	111.30 Å 129.30 Å 204.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 30.17 – 2.58	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.55) 97.5 (30.17-2.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 2.57 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.223 , 0.258 0.223 , 0.258	Depositor DCC
$R_{free}$ test set	4565 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90833 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/3290	0.60	0/4464
2	B	0.32	0/1598	0.57	0/2168
3	C	0.36	0/2830	0.66	1/3837 (0.0%)
4	D	0.38	0/2328	0.59	0/3143
5	E	0.32	0/1385	0.57	1/1867 (0.1%)
6	F	0.39	0/1382	0.64	1/1853 (0.1%)
7	G	0.32	0/1033	0.53	0/1390
All	All	0.36	0/13846	0.60	3/18722 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	11	ILE	N-CA-C	-6.38	93.77	111.00
5	E	17	GLY	N-CA-C	-6.07	97.92	113.10
6	F	102	PHE	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3209	0	3141	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1569	0	1564	67	0
3	C	2761	0	2707	74	0
4	D	2279	0	2248	45	0
5	E	1354	0	1350	56	0
6	F	1360	0	1399	29	0
7	G	1021	0	1038	29	0
8	A	1	0	0	0	0
9	A	27	0	12	0	0
9	B	27	0	12	2	0
10	A	68	0	0	3	0
10	B	16	0	0	1	0
10	C	67	0	0	3	0
10	D	66	0	0	1	0
10	E	6	0	0	0	0
10	F	78	0	0	1	0
10	G	13	0	0	0	0
All	All	13922	0	13471	376	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 (376) 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)
3:C:223:ASP:HB3	7:G:146:THR:HG21	1.36	1.03
3:C:183:THR:HG22	3:C:185:TRP:H	1.23	1.01
1:A:4:ARG:HB2	1:A:4:ARG:HH11	1.20	1.00
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.44	0.99
3:C:14:HIS:H	3:C:331:GLN:HE22	1.12	0.93
3:C:367:LYS:HD2	3:C:368:ASP:N	1.93	0.83
1:A:309:ILE:HD12	1:A:312:ARG:HD2	1.61	0.81
1:A:176:HIS:CD2	1:A:192:HIS:HD2	2.01	0.79
2:B:153:THR:HB	2:B:171:GLU:H	1.47	0.79
1:A:4:ARG:CB	1:A:4:ARG:HH11	1.95	0.79
6:F:4:THR:HG23	6:F:55:ARG:HE	1.48	0.78
5:E:22:LEU:HD23	5:E:41:ILE:HB	1.64	0.78
4:D:281:ARG:HH12	6:F:102:PHE:HZ	1.32	0.77
3:C:21:THR:HG22	3:C:22:GLN:HG3	1.66	0.77
6:F:130:LYS:HE2	6:F:130:LYS:HA	1.68	0.76
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.50	0.76
3:C:358:ASP:OD1	3:C:360:ARG:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLU:OE1	1:A:414:PHE:HB2	1.86	0.75
1:A:349:LEU:O	1:A:353:LEU:HB2	1.87	0.74
1:A:176:HIS:HD2	1:A:192:HIS:CD2	2.05	0.74
1:A:359:LYS:O	1:A:359:LYS:HD3	1.88	0.74
2:B:205:ASN:HD22	2:B:208:ALA:H	1.35	0.74
5:E:60:ILE:HD11	5:E:116:ILE:HD13	1.69	0.74
1:A:116:PRO:O	1:A:117:LEU:HB2	1.87	0.73
1:A:289:ASN:ND2	1:A:291:ASP:H	1.87	0.73
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.71	0.72
1:A:176:HIS:HD2	1:A:192:HIS:HD2	1.35	0.72
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.24	0.71
4:D:228:PHE:H	4:D:231:HIS:HD2	1.36	0.71
7:G:51:MET:HB3	7:G:86:PHE:CZ	2.25	0.71
1:A:324:GLY:O	1:A:327:MET:HG2	1.89	0.71
3:C:107:ASN:ND2	3:C:109:LYS:H	1.89	0.70
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.74	0.69
1:A:258:GLY:O	1:A:266:GLU:HA	1.93	0.69
3:C:107:ASN:HD22	3:C:107:ASN:C	1.96	0.69
2:B:291:ILE:HD12	2:B:294:ARG:HH11	1.57	0.69
3:C:189:MET:HG2	3:C:195:MET:HE3	1.75	0.69
1:A:374:ARG:HD2	1:A:375:TYR:CE2	2.28	0.68
3:C:223:ASP:CB	7:G:146:THR:HG21	2.20	0.68
2:B:174:SER:O	2:B:175:LEU:HD23	1.94	0.67
3:C:14:HIS:H	3:C:331:GLN:NE2	1.90	0.67
3:C:189:MET:HA	3:C:195:MET:HE1	1.75	0.67
7:G:87:LYS:H	7:G:87:LYS:HE3	1.60	0.67
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.76	0.67
6:F:128:LYS:HE2	10:F:189:HOH:O	1.95	0.67
1:A:143:VAL:HG22	1:A:146:VAL:HG23	1.76	0.66
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.76	0.66
5:E:168:PHE:CE2	5:E:169:MET:HE2	2.30	0.66
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.77	0.66
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.78	0.66
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.31	0.66
3:C:29:ASN:HB3	3:C:31:GLU:H	1.62	0.65
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.26	0.65
1:A:211:ARG:NH1	5:E:159:TRP:HZ3	1.95	0.65
5:E:75:ILE:HG23	5:E:144:LEU:HD11	1.78	0.65
4:D:263:HIS:HD2	4:D:266:MET:CE	2.09	0.64
6:F:4:THR:HG23	6:F:55:ARG:HH21	1.62	0.64
7:G:87:LYS:N	7:G:87:LYS:HD3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:HIS:HD2	1:A:372:MET:H	1.43	0.64
2:B:218:GLU:HG2	9:B:1002:ADP:C5	2.32	0.63
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.29	0.62
5:E:39:THR:HG23	5:E:43:ASP:HB2	1.82	0.62
1:A:200:ILE:HG12	1:A:281:ILE:HD11	1.82	0.62
2:B:291:ILE:HA	2:B:294:ARG:HD3	1.83	0.61
3:C:284:ARG:NH1	3:C:286:ASP:O	2.33	0.61
6:F:146:ILE:HA	6:F:149:MET:CE	2.31	0.61
1:A:200:ILE:O	1:A:204:ILE:HG13	2.01	0.61
1:A:417:MET:O	1:A:418:SER:HB2	2.01	0.61
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.83	0.60
4:D:158:LYS:O	4:D:158:LYS:HD3	2.01	0.60
1:A:311:VAL:O	1:A:314:PRO:HD2	2.01	0.60
5:E:20:ALA:HB1	5:E:22:LEU:HD13	1.83	0.60
3:C:217:VAL:HG12	3:C:229:ALA:HB3	1.83	0.60
6:F:6:ARG:HB3	6:F:7:PRO:HD3	1.84	0.60
7:G:39:GLU:HG2	7:G:78:ILE:HD11	1.84	0.60
4:D:134:GLU:OE2	4:D:136:LYS:HE2	2.02	0.59
2:B:166:ILE:O	2:B:168:PRO:HD3	2.02	0.59
5:E:145:CYS:C	5:E:147:LYS:H	2.04	0.59
7:G:87:LYS:N	7:G:87:LYS:CD	2.65	0.59
3:C:161:SER:HB2	3:C:163:ASP:OD1	2.02	0.59
2:B:194:ILE:HG13	2:B:213:VAL:HG11	1.85	0.59
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.85	0.59
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.85	0.59
1:A:343:VAL:CG2	1:A:363:ILE:HD12	2.32	0.58
5:E:97:THR:O	5:E:101:THR:HG23	2.03	0.58
5:E:24:ILE:HG13	5:E:24:ILE:O	2.02	0.58
2:B:151:LEU:HD11	2:B:300:HIS:HD2	1.68	0.58
2:B:151:LEU:HD21	2:B:300:HIS:CD2	2.37	0.58
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.86	0.58
7:G:87:LYS:H	7:G:87:LYS:CE	2.16	0.58
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.34	0.58
6:F:146:ILE:HA	6:F:149:MET:HE2	1.86	0.58
6:F:35:LYS:HD3	6:F:40:VAL:HG11	1.86	0.57
1:A:317:LYS:HE2	1:A:364:ASP:OD1	2.05	0.57
3:C:131:TRP:O	3:C:131:TRP:HE3	1.87	0.57
2:B:163:VAL:HG22	2:B:164:THR:N	2.18	0.57
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.40	0.56
1:A:19:LEU:HD13	1:A:96:VAL:HG13	1.87	0.56
1:A:193:ILE:HG23	1:A:292:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:118:SER:O	7:G:120:ASN:N	2.39	0.56
1:A:30:ILE:HD13	1:A:375:TYR:CZ	2.40	0.56
2:B:161:ASP:O	2:B:187:ARG:HG3	2.06	0.56
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.88	0.55
1:A:289:ASN:HD22	1:A:289:ASN:C	2.09	0.55
1:A:111:LEU:HD23	1:A:111:LEU:C	2.27	0.55
5:E:16:ILE:O	5:E:16:ILE:HG23	2.07	0.55
4:D:215:ALA:HB1	4:D:220:ILE:HD13	1.88	0.55
1:A:289:ASN:HD22	1:A:290:PRO:N	2.05	0.55
5:E:71:ILE:O	5:E:75:ILE:HG13	2.07	0.55
1:A:212:GLU:OE1	1:A:270:ASP:HB2	2.06	0.54
1:A:369:THR:HA	1:A:373:GLN:OE1	2.07	0.54
2:B:291:ILE:HG22	2:B:291:ILE:O	2.07	0.54
5:E:87:SER:OG	5:E:90:GLN:HB2	2.08	0.54
2:B:290:ASP:HB2	2:B:293:THR:OG1	2.08	0.54
1:A:19:LEU:HG	1:A:29:PHE:HB2	1.89	0.54
3:C:119:VAL:HG23	3:C:137:ILE:O	2.08	0.54
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.23	0.53
1:A:311:VAL:C	1:A:314:PRO:HD2	2.29	0.53
6:F:4:THR:CG2	6:F:55:ARG:HE	2.20	0.53
3:C:30:HIS:HB2	10:C:376:HOH:O	2.07	0.53
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.43	0.53
6:F:4:THR:HG23	6:F:55:ARG:NE	2.19	0.53
2:B:184:ILE:HD13	2:B:271:ILE:HD11	1.91	0.53
4:D:75:LEU:C	4:D:75:LEU:HD23	2.29	0.53
2:B:166:ILE:HD13	2:B:282:LEU:HA	1.91	0.53
6:F:130:LYS:CE	6:F:130:LYS:HA	2.38	0.53
3:C:254:THR:HG21	3:C:372:VAL:HG22	1.90	0.53
7:G:118:SER:O	7:G:119:ASP:C	2.47	0.53
7:G:38:ASP:HB3	7:G:41:GLU:CB	2.39	0.53
5:E:88:LYS:O	5:E:92:GLU:HG3	2.09	0.52
2:B:306:GLY:HA2	2:B:309:MET:HE2	1.91	0.52
4:D:121:PHE:O	4:D:124:VAL:HG12	2.09	0.52
3:C:107:ASN:HD22	3:C:108:GLU:N	2.07	0.52
6:F:22:LEU:HD21	6:F:70:VAL:HG23	1.92	0.52
1:A:78:ILE:HD11	1:A:89:MET:HE1	1.92	0.52
10:A:1041:HOH:O	4:D:256:LYS:HE2	2.10	0.52
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.50	0.52
1:A:87:ASP:OD2	4:D:267:ARG:HD2	2.09	0.51
1:A:223:THR:O	1:A:227:VAL:HG23	2.10	0.51
3:C:14:HIS:N	3:C:331:GLN:HE22	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:HA	1:A:343:VAL:HG12	1.92	0.51
2:B:306:GLY:HA2	2:B:309:MET:CE	2.40	0.51
5:E:77:GLU:O	5:E:80:LYS:HB2	2.10	0.51
7:G:118:SER:O	7:G:121:SER:N	2.32	0.51
5:E:123:LYS:O	5:E:127:GLU:HG3	2.11	0.51
1:A:370:HIS:HD2	1:A:372:MET:N	2.06	0.51
3:C:297:THR:HG22	3:C:298:ALA:N	2.26	0.51
3:C:102:VAL:HA	3:C:112:ALA:O	2.11	0.51
1:A:309:ILE:HG23	1:A:310:ASP:N	2.26	0.51
4:D:45:ILE:HA	4:D:56:MET:O	2.11	0.51
5:E:58:TYR:CD1	5:E:168:PHE:HZ	2.29	0.50
2:B:184:ILE:HD12	2:B:188:ASP:CB	2.42	0.50
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.92	0.50
4:D:281:ARG:NH1	6:F:102:PHE:CZ	2.74	0.50
2:B:205:ASN:ND2	2:B:207:SER:H	2.10	0.50
1:A:19:LEU:HD23	1:A:19:LEU:N	2.27	0.50
1:A:194:PRO:C	1:A:195:ILE:HD12	2.32	0.50
5:E:60:ILE:CD1	5:E:116:ILE:HD13	2.40	0.50
5:E:168:PHE:CD2	5:E:169:MET:HE2	2.46	0.50
6:F:145:GLU:O	6:F:149:MET:HG3	2.11	0.50
3:C:151:HIS:CG	3:C:152:PRO:HD2	2.47	0.50
6:F:4:THR:HG23	6:F:55:ARG:NH2	2.27	0.50
4:D:118:ARG:HD3	4:D:118:ARG:C	2.32	0.50
1:A:309:ILE:HD12	1:A:312:ARG:CD	2.37	0.50
1:A:309:ILE:O	1:A:312:ARG:HG2	2.11	0.50
2:B:205:ASN:HB3	2:B:208:ALA:HB3	1.93	0.50
4:D:53:THR:C	4:D:54:LYS:HD2	2.32	0.50
3:C:107:ASN:HD22	3:C:109:LYS:H	1.57	0.49
3:C:183:THR:HG23	3:C:184:PRO:CD	2.43	0.49
4:D:262:ILE:O	4:D:266:MET:HG3	2.12	0.49
3:C:107:ASN:C	3:C:107:ASN:ND2	2.65	0.49
1:A:239:VAL:HG23	1:A:240:LYS:N	2.27	0.49
2:B:240:LEU:HB2	10:B:1007:HOH:O	2.11	0.49
1:A:18:LYS:HD3	1:A:18:LYS:N	2.28	0.49
6:F:158:ARG:O	6:F:162:GLU:HG3	2.13	0.49
2:B:295:SER:O	2:B:299:LYS:HG2	2.12	0.49
5:E:144:LEU:O	5:E:148:VAL:HG23	2.12	0.49
2:B:346:ASP:OD1	2:B:346:ASP:N	2.45	0.49
1:A:191:LYS:HB2	1:A:303:VAL:CG2	2.43	0.49
4:D:130:GLN:HA	4:D:130:GLN:OE1	2.13	0.49
5:E:83:GLN:HE21	5:E:161:THR:CG2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LYS:HE2	1:A:401:GLU:OE2	2.13	0.48
4:D:248:ARG:C	4:D:248:ARG:HD3	2.33	0.48
1:A:30:ILE:HD13	1:A:375:TYR:CE1	2.48	0.48
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.95	0.48
5:E:10:ASP:HB3	5:E:12:ASP:OD1	2.13	0.48
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.49	0.48
3:C:294:ARG:N	3:C:301:ARG:HA	2.29	0.48
3:C:185:TRP:CZ3	3:C:235:MET:HG2	2.48	0.48
7:G:87:LYS:H	7:G:87:LYS:CD	2.25	0.48
5:E:82:LEU:HD23	5:E:148:VAL:HG21	1.95	0.48
3:C:144:THR:H	6:F:28:GLN:NE2	2.12	0.48
3:C:10:PRO:HG2	6:F:124:GLU:HG2	1.96	0.48
5:E:98:LEU:HD11	5:E:103:PHE:HZ	1.78	0.48
6:F:4:THR:CG2	6:F:55:ARG:HH21	2.25	0.48
7:G:66:THR:O	7:G:72:LYS:HE3	2.13	0.48
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.48	0.47
1:A:204:ILE:HD12	1:A:228:LYS:HB2	1.95	0.47
1:A:313:ARG:H	1:A:314:PRO:CD	2.27	0.47
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.43	0.47
7:G:149:LYS:N	7:G:149:LYS:HD3	2.29	0.47
3:C:2:ALA:N	10:C:421:HOH:O	2.46	0.47
4:D:158:LYS:HD3	4:D:158:LYS:C	2.34	0.47
3:C:26:CYS:SG	3:C:55:VAL:HB	2.55	0.47
4:D:53:THR:O	4:D:54:LYS:HD2	2.14	0.47
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.95	0.47
5:E:20:ALA:CB	5:E:22:LEU:HD13	2.44	0.47
1:A:215:ILE:HD11	1:A:269:ILE:HD13	1.96	0.47
2:B:257:GLU:HA	2:B:260:GLU:HB2	1.97	0.47
1:A:228:LYS:O	1:A:232:SER:HB2	2.15	0.47
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.97	0.47
2:B:320:GLU:HG3	7:G:11:PHE:HE1	1.79	0.47
1:A:223:THR:HG23	1:A:256:TYR:HE2	1.76	0.46
1:A:232:SER:HB2	1:A:328:PHE:HE1	1.80	0.46
4:D:182:MET:HG3	4:D:200:PHE:CD1	2.49	0.46
2:B:205:ASN:ND2	2:B:208:ALA:H	2.08	0.46
3:C:254:THR:HA	3:C:340:ALA:O	2.15	0.46
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.79	0.46
3:C:119:VAL:HG22	3:C:120:ILE:N	2.30	0.46
1:A:53:LYS:HA	10:A:1032:HOH:O	2.13	0.46
2:B:281:LEU:HD23	2:B:281:LEU:O	2.15	0.46
1:A:289:ASN:ND2	1:A:289:ASN:C	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:LEU:O	4:D:75:LEU:HD23	2.15	0.46
2:B:214:ARG:NH1	2:B:218:GLU:OE2	2.47	0.46
2:B:151:LEU:HD21	2:B:300:HIS:HD2	1.79	0.46
1:A:140:TYR:HB2	1:A:394:CYS:SG	2.56	0.46
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.50	0.46
3:C:170:SER:HB2	3:C:195:MET:CE	2.46	0.46
1:A:395:HIS:HE1	1:A:410:HIS:O	1.98	0.46
3:C:189:MET:HG2	3:C:195:MET:CE	2.44	0.46
3:C:30:HIS:HA	3:C:53:GLY:O	2.16	0.46
1:A:151:ALA:O	1:A:154:THR:HG22	2.16	0.46
1:A:359:LYS:CD	1:A:359:LYS:O	2.61	0.46
1:A:211:ARG:NH1	5:E:159:TRP:CZ3	2.81	0.46
2:B:180:ARG:HH11	2:B:180:ARG:HG3	1.81	0.45
1:A:216:PRO:HG3	1:A:260:ASN:ND2	2.31	0.45
1:A:68:GLU:CD	1:A:68:GLU:H	2.19	0.45
6:F:45:GLU:OE2	6:F:45:GLU:N	2.45	0.45
2:B:184:ILE:HD13	2:B:271:ILE:CD1	2.46	0.45
6:F:146:ILE:HA	6:F:149:MET:HE3	1.99	0.45
5:E:18:ASN:ND2	5:E:118:ALA:H	2.14	0.45
3:C:3:TYR:HB2	3:C:324:LEU:HG	1.99	0.45
1:A:248:ASP:OD1	1:A:251:LYS:HD3	2.16	0.45
3:C:31:GLU:OE1	3:C:33:HIS:HE1	1.99	0.45
1:A:232:SER:O	1:A:233:TYR:HB3	2.16	0.45
5:E:42:VAL:HB	5:E:143:ARG:NH1	2.32	0.45
3:C:178:GLU:O	3:C:179:ARG:C	2.54	0.45
1:A:309:ILE:CD1	1:A:312:ARG:HD2	2.40	0.45
2:B:299:LYS:HG3	2:B:300:HIS:ND1	2.32	0.45
2:B:153:THR:CB	2:B:171:GLU:H	2.23	0.45
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.51	0.45
3:C:110:LYS:NZ	3:C:171:ALA:O	2.48	0.45
4:D:6:VAL:HG21	4:D:242:ASN:HB3	1.97	0.45
2:B:158:ASP:HA	2:B:304:SER:O	2.16	0.45
4:D:2:ILE:HG21	6:F:163:GLU:HG2	1.98	0.45
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.47	0.45
2:B:180:ARG:CB	2:B:281:LEU:HD21	2.47	0.45
3:C:367:LYS:HD2	3:C:367:LYS:C	2.35	0.45
4:D:205:PRO:HB3	4:D:222:TYR:CE2	2.51	0.45
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.99	0.45
3:C:72:THR:HA	3:C:98:ALA:HB1	1.99	0.45
2:B:153:THR:HB	2:B:170:TYR:HA	1.99	0.45
2:B:163:VAL:CG2	2:B:164:THR:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:GLU:HG2	2:B:342:ILE:HG22	1.99	0.45
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.52	0.45
5:E:39:THR:HG23	5:E:43:ASP:CB	2.46	0.45
1:A:313:ARG:N	1:A:314:PRO:CD	2.80	0.45
2:B:321:LEU:HD12	2:B:342:ILE:HD13	1.99	0.45
1:A:329:ARG:O	1:A:330:ASP:HB2	2.17	0.45
3:C:61:ALA:HB1	3:C:108:GLU:HG2	1.99	0.44
3:C:158:ALA:HA	3:C:167:ARG:O	2.16	0.44
1:A:194:PRO:O	1:A:195:ILE:HD12	2.16	0.44
7:G:71:VAL:O	7:G:74:ARG:HB3	2.16	0.44
2:B:310:TYR:CE1	9:B:1002:ADP:H2	2.36	0.44
5:E:98:LEU:HD11	5:E:103:PHE:CZ	2.52	0.44
4:D:189:ARG:HB2	10:D:317:HOH:O	2.17	0.44
1:A:374:ARG:HD3	1:A:374:ARG:O	2.17	0.44
1:A:176:HIS:CD2	1:A:192:HIS:CD2	2.85	0.44
5:E:22:LEU:CD2	5:E:41:ILE:HD13	2.47	0.44
4:D:7:ASN:OD1	4:D:115:MET:HG2	2.18	0.44
3:C:69:THR:O	3:C:76:ALA:HA	2.17	0.44
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.99	0.44
1:A:225:LYS:O	1:A:229:GLU:HG2	2.18	0.44
5:E:28:PHE:CD2	5:E:138:GLN:HB3	2.53	0.44
7:G:38:ASP:HB3	7:G:41:GLU:HB2	2.00	0.44
1:A:190:ILE:HG22	1:A:191:LYS:N	2.33	0.44
2:B:257:GLU:CD	2:B:257:GLU:H	2.21	0.44
3:C:264:ASP:O	3:C:265:CYS:HB2	2.18	0.44
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.53	0.44
7:G:18:GLU:HA	7:G:18:GLU:OE1	2.18	0.44
3:C:228:LEU:HD23	3:C:228:LEU:C	2.38	0.44
3:C:60:TRP:HE1	3:C:65:ASN:ND2	2.15	0.43
3:C:207:GLY:O	3:C:219:TRP:HA	2.18	0.43
3:C:131:TRP:O	3:C:131:TRP:CE3	2.70	0.43
3:C:297:THR:CG2	3:C:298:ALA:N	2.81	0.43
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.53	0.43
5:E:35:GLU:OE1	5:E:36:THR:N	2.51	0.43
2:B:290:ASP:C	2:B:292:ASP:H	2.21	0.43
4:D:66:GLU:OE2	4:D:145:HIS:ND1	2.37	0.43
4:D:158:LYS:HA	4:D:158:LYS:HE2	2.00	0.43
2:B:151:LEU:HD11	2:B:300:HIS:CD2	2.52	0.43
1:A:71:THR:HG23	1:A:72:TYR:CE1	2.54	0.43
7:G:60:LYS:HE2	7:G:61:ASN:ND2	2.33	0.43
1:A:26:GLU:OE2	1:A:372:MET:HE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:VAL:O	2:B:329:VAL:HG12	2.19	0.43
3:C:84:ARG:O	3:C:84:ARG:HG2	2.18	0.43
3:C:139:LYS:HA	3:C:140:PRO:HA	1.85	0.43
4:D:171:ASP:O	4:D:174:ASP:HB2	2.19	0.43
7:G:124:VAL:O	7:G:127:GLN:HB2	2.19	0.43
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.99	0.43
4:D:95:LEU:HD11	4:D:116:LEU:HG	2.00	0.43
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.90	0.42
4:D:228:PHE:H	4:D:231:HIS:CD2	2.25	0.42
1:A:200:ILE:CG1	1:A:281:ILE:HD11	2.48	0.42
5:E:15:LEU:HD22	5:E:63:GLU:HG3	2.01	0.42
7:G:52:THR:O	7:G:56:GLN:HG3	2.19	0.42
3:C:201:SER:O	7:G:148:ARG:CG	2.67	0.42
5:E:126:ASP:OD2	5:E:130:ARG:NH1	2.51	0.42
1:A:207:LEU:HD23	5:E:166:ARG:NH2	2.33	0.42
5:E:88:LYS:NZ	5:E:146:GLU:HG2	2.33	0.42
3:C:203:GLY:HA2	10:C:379:HOH:O	2.18	0.42
2:B:170:TYR:O	2:B:172:GLY:N	2.51	0.42
4:D:281:ARG:NH1	6:F:102:PHE:HZ	2.09	0.42
3:C:199:SER:O	3:C:200:SER:HB2	2.18	0.42
5:E:82:LEU:HD11	5:E:149:PHE:HE1	1.84	0.42
5:E:119:LYS:HB2	5:E:120:PRO:HD2	2.00	0.42
5:E:133:LEU:HB3	5:E:137:ARG:HH12	1.85	0.42
2:B:151:LEU:HA	2:B:151:LEU:HD23	1.86	0.42
4:D:199:LEU:HD12	4:D:199:LEU:N	2.35	0.42
2:B:174:SER:C	2:B:175:LEU:HD23	2.40	0.42
1:A:400:TYR:CE1	1:A:405:PRO:HB3	2.55	0.42
5:E:116:ILE:HG22	5:E:117:TYR:CD1	2.55	0.41
5:E:83:GLN:HE21	5:E:161:THR:HG22	1.85	0.41
5:E:145:CYS:C	5:E:147:LYS:N	2.72	0.41
2:B:151:LEU:CD1	2:B:300:HIS:HD2	2.32	0.41
4:D:41:VAL:HG21	4:D:117:LYS:HE3	2.03	0.41
1:A:300:VAL:O	1:A:304:ILE:HG13	2.21	0.41
4:D:68:GLN:NE2	4:D:73:ASP:OD2	2.51	0.41
1:A:312:ARG:HG3	1:A:312:ARG:O	2.19	0.41
5:E:75:ILE:O	5:E:79:LEU:HG	2.21	0.41
3:C:319:ALA:HB2	6:F:127:TYR:CZ	2.54	0.41
4:D:215:ALA:HB1	4:D:220:ILE:CD1	2.49	0.41
3:C:119:VAL:HG21	3:C:136:HIS:HB3	2.03	0.41
2:B:280:GLU:HA	2:B:324:LEU:HD11	2.01	0.41
6:F:85:ILE:HD12	6:F:86:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:LEU:O	2:B:180:ARG:HG2	2.21	0.41
1:A:359:LYS:N	1:A:360:PRO:HD3	2.35	0.41
1:A:370:HIS:HE1	10:A:1006:HOH:O	2.04	0.41
1:A:168:ILE:HD12	1:A:335:LEU:HD11	2.01	0.41
7:G:66:THR:OG1	7:G:71:VAL:HG11	2.20	0.41
3:C:48:LEU:HB3	3:C:79:TRP:CH2	2.56	0.41
2:B:323:GLN:HG2	7:G:16:VAL:HG23	2.02	0.41
1:A:335:LEU:HD23	1:A:335:LEU:O	2.20	0.41
1:A:390:PHE:CZ	1:A:394:CYS:SG	3.14	0.41
3:C:29:ASN:O	3:C:54:GLN:HA	2.21	0.41
1:A:71:THR:HG23	1:A:72:TYR:CD1	2.56	0.41
1:A:195:ILE:HA	1:A:199:ASP:OD2	2.21	0.41
3:C:48:LEU:HD12	3:C:48:LEU:N	2.35	0.41
4:D:241:ILE:HA	4:D:244:ILE:HG22	2.02	0.41
2:B:231:GLN:HA	2:B:231:GLN:NE2	2.36	0.41
5:E:32:ALA:CB	5:E:135:GLN:OE1	2.68	0.41
4:D:133:GLU:O	4:D:133:GLU:HG2	2.19	0.41
1:A:116:PRO:O	1:A:117:LEU:CB	2.62	0.41
5:E:25:ARG:HD3	5:E:35:GLU:O	2.21	0.41
5:E:96:TYR:O	5:E:100:ILE:HG12	2.21	0.41
4:D:263:HIS:O	4:D:267:ARG:HG3	2.21	0.40
4:D:109:ILE:HG13	4:D:110:VAL:N	2.36	0.40
2:B:166:ILE:HD13	2:B:282:LEU:CA	2.51	0.40
5:E:22:LEU:HD23	5:E:41:ILE:HD13	2.04	0.40
5:E:21:LEU:HG	5:E:33:PRO:HD3	2.02	0.40
2:B:259:PHE:CD2	2:B:259:PHE:C	2.94	0.40
6:F:102:PHE:HE1	6:F:126:MET:CE	2.34	0.40
5:E:66:ARG:HB3	5:E:117:TYR:CE2	2.56	0.40
2:B:302:VAL:HG13	2:B:302:VAL:O	2.22	0.40
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.93	0.40
7:G:71:VAL:HG13	7:G:72:LYS:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	396/418 (95%)	367 (93%)	24 (6%)	5 (1%)	15	25
2	B	202/394 (51%)	183 (91%)	16 (8%)	3 (2%)	13	22
3	C	351/372 (94%)	334 (95%)	14 (4%)	3 (1%)	21	36
4	D	280/300 (93%)	274 (98%)	5 (2%)	1 (0%)	39	60
5	E	164/178 (92%)	154 (94%)	9 (6%)	1 (1%)	30	48
6	F	164/168 (98%)	158 (96%)	5 (3%)	1 (1%)	30	48
7	G	131/151 (87%)	123 (94%)	7 (5%)	1 (1%)	24	40
All	All	1688/1981 (85%)	1593 (94%)	80 (5%)	15 (1%)	21	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	ARG
2	B	171	GLU
3	C	203	GLY
4	D	202	HIS
7	G	119	ASP
1	A	2	ALA
1	A	210	ASP
3	C	174	LYS
3	C	200	SER
6	F	102	PHE
1	A	233	TYR
5	E	146	GLU
1	A	194	PRO
2	B	176	PRO
2	B	291	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	348/363 (96%)	333 (96%)	15 (4%)	35	59
2	B	163/345 (47%)	155 (95%)	8 (5%)	31	52
3	C	298/313 (95%)	284 (95%)	14 (5%)	32	54
4	D	248/264 (94%)	244 (98%)	4 (2%)	70	89
5	E	146/159 (92%)	144 (99%)	2 (1%)	74	90
6	F	152/155 (98%)	150 (99%)	2 (1%)	76	91
7	G	108/124 (87%)	102 (94%)	6 (6%)	26	45
All	All	1463/1723 (85%)	1412 (96%)	51 (4%)	43	68

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ARG
1	A	19	LEU
1	A	68	GLU
1	A	88	LEU
1	A	117	LEU
1	A	143	VAL
1	A	230	ARG
1	A	243	ASN
1	A	289	ASN
1	A	313	ARG
1	A	353	LEU
1	A	374	ARG
1	A	389	GLU
1	A	417	MET
2	B	153	THR
2	B	182	LEU
2	B	200	ARG
2	B	220	LEU
2	B	240	LEU
2	B	303	LEU
2	B	337	LEU
2	B	346	ASP
3	C	21	THR
3	C	31	GLU
3	C	90	LEU
3	C	107	ASN
3	C	131	TRP
3	C	175	GLU

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Mol	Chain	Res	Type
3	C	179	ARG
3	C	210	PHE
3	C	284	ARG
3	C	306	ASP
3	C	321	LEU
3	C	324	LEU
3	C	367	LYS
3	C	368	ASP
4	D	116	LEU
4	D	171	ASP
4	D	202	HIS
4	D	204	GLU
5	E	22	LEU
5	E	144	LEU
6	F	101	PHE
6	F	165	LEU
7	G	18	GLU
7	G	39	GLU
7	G	51	MET
7	G	69	GLN
7	G	87	LYS
7	G	112	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	176	HIS
1	A	192	HIS
1	A	205	GLN
1	A	243	ASN
1	A	255	GLN
1	A	289	ASN
1	A	305	GLN
1	A	318	ASN
1	A	370	HIS
1	A	395	HIS
1	A	410	HIS
2	B	205	ASN
2	B	231	GLN
2	B	284	ASN
2	B	300	HIS

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Mol	Chain	Res	Type
2	B	323	GLN
3	C	22	GLN
3	C	33	HIS
3	C	46	HIS
3	C	54	GLN
3	C	65	ASN
3	C	107	ASN
3	C	303	GLN
3	C	331	GLN
4	D	49	ASN
4	D	140	ASN
4	D	202	HIS
4	D	231	HIS
5	E	83	GLN
5	E	170	ASN
6	F	28	GLN
7	G	61	ASN
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 3 ligands modelled in this entry, 1 is 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	ADP	A	1001	-	22,29,29	1.39	3 (13%)	27,45,45	2.44	4 (14%)
9	ADP	B	1002	-	22,29,29	1.40	3 (13%)	27,45,45	2.44	3 (11%)

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	ADP	A	1001	-	-	0/12/32/32	0/3/3/3
9	ADP	B	1002	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1002	ADP	O4'-C1'	2.34	1.44	1.41
9	A	1001	ADP	O4'-C1'	2.36	1.44	1.41
9	A	1001	ADP	PB-O1B	3.11	1.61	1.51
9	B	1002	ADP	PB-O1B	3.14	1.61	1.51
9	B	1002	ADP	C2-N1	3.53	1.40	1.33
9	A	1001	ADP	C2-N1	3.56	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1002	ADP	N3-C2-N1	-11.34	120.21	128.89
9	A	1001	ADP	N3-C2-N1	-11.24	120.29	128.89
9	A	1001	ADP	PA-O3A-PB	-3.20	121.95	132.67
9	B	1002	ADP	PA-O3A-PB	-3.13	122.17	132.67
9	A	1001	ADP	C4-C5-N7	-2.39	107.28	109.48
9	A	1001	ADP	C4'-O4'-C1'	-2.32	107.17	109.72
9	B	1002	ADP	C4-C5-N7	-2.17	107.48	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1002	ADP	2	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	402/418 (96%)	0.45	35 (8%) 13 14	18, 45, 86, 102	0
2	B	204/394 (51%)	0.66	30 (14%) 3 3	26, 53, 93, 100	0
3	C	357/372 (95%)	0.26	27 (7%) 17 19	23, 38, 76, 101	0
4	D	282/300 (94%)	0.09	5 (1%) 71 76	21, 35, 55, 74	0
5	E	168/178 (94%)	0.94	28 (16%) 2 2	42, 59, 93, 97	0
6	F	166/168 (98%)	-0.13	2 (1%) 81 84	21, 30, 43, 62	0
7	G	135/151 (89%)	0.55	18 (13%) 4 5	25, 53, 83, 88	0
All	All	1714/1981 (86%)	0.38	145 (8%) 13 15	18, 42, 85, 102	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.8
3	C	309	ALA	6.7
5	E	85	CYS	6.0
1	A	51	VAL	5.8
1	A	350	SER	5.4
1	A	2	ALA	5.4
1	A	359	LYS	5.3
5	E	38	ASP	5.2
1	A	418	SER	5.1
7	G	13	LYS	5.1
1	A	417	MET	5.1
2	B	292	ASP	5.1
1	A	347	LEU	5.0
2	B	174	SER	4.9
5	E	89	SER	4.9
3	C	306	ASP	4.9
1	A	351	GLU	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	E	151	PRO	4.8
7	G	64	ILE	4.7
5	E	86	ASN	4.4
1	A	266	GLU	4.3
5	E	36	THR	4.3
2	B	154	GLY	4.2
3	C	368	ASP	4.2
6	F	3	ALA	4.2
7	G	68	SER	4.1
1	A	250	SER	4.1
4	D	211	ASP	4.1
5	E	109	PRO	4.1
3	C	308	LYS	4.1
1	A	262	ILE	4.0
2	B	171	GLU	4.0
2	B	293	THR	3.9
2	B	187	ARG	3.8
3	C	367	LYS	3.8
2	B	170	TYR	3.7
3	C	369	LEU	3.7
2	B	153	THR	3.7
7	G	66	THR	3.6
3	C	201	SER	3.6
1	A	268	SER	3.5
2	B	148	ALA	3.5
3	C	294	ARG	3.5
2	B	172	GLY	3.5
1	A	352	GLU	3.5
7	G	67	LYS	3.5
3	C	127	GLN	3.4
5	E	149	PHE	3.4
2	B	178	LEU	3.4
5	E	107	GLY	3.4
1	A	259	ILE	3.4
2	B	173	PHE	3.3
5	E	93	LYS	3.3
1	A	260	ASN	3.2
3	C	295	GLY	3.2
3	C	131	TRP	3.2
5	E	27	GLN	3.1
1	A	156	ARG	3.1
5	E	75	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
7	G	10	ARG	3.0
5	E	100	ILE	3.0
5	E	53	VAL	3.0
7	G	37	PRO	3.0
3	C	370	LYS	2.9
2	B	169	VAL	2.9
3	C	278	LYS	2.9
4	D	282	PRO	2.9
2	B	149	GLN	2.9
1	A	349	LEU	2.9
3	C	372	VAL	2.9
7	G	35	ALA	2.8
7	G	20	ASP	2.8
3	C	307	LYS	2.8
3	C	364	SER	2.8
3	C	319	ALA	2.8
2	B	152	LEU	2.8
3	C	209	CYS	2.8
1	A	39	GLU	2.7
1	A	217	PRO	2.7
1	A	267	PHE	2.7
5	E	39	THR	2.7
1	A	70	PRO	2.7
3	C	84	ARG	2.7
2	B	150	GLY	2.7
1	A	261	ALA	2.7
2	B	294	ARG	2.6
7	G	120	ASN	2.6
1	A	251	LYS	2.6
4	D	27	LYS	2.6
7	G	63	PRO	2.6
5	E	96	TYR	2.5
5	E	49	PHE	2.5
2	B	177	HIS	2.5
1	A	202	TYR	2.5
1	A	52	MET	2.5
1	A	68	GLU	2.5
3	C	158	ALA	2.5
1	A	360	PRO	2.5
2	B	325	TYR	2.5
1	A	292	PHE	2.4
5	E	159	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	95	MET	2.4
5	E	82	LEU	2.4
5	E	12	ASP	2.4
2	B	348	PRO	2.4
7	G	60	LYS	2.4
4	D	260	ALA	2.4
3	C	130	ASP	2.4
3	C	288	PRO	2.4
3	C	126	GLU	2.4
1	A	72	TYR	2.3
2	B	339	LYS	2.3
1	A	53	LYS	2.3
7	G	65	ASN	2.3
2	B	176	PRO	2.3
5	E	25	ARG	2.3
5	E	71	ILE	2.2
4	D	257	CYS	2.2
5	E	91	GLY	2.2
3	C	287	VAL	2.2
7	G	19	TYR	2.2
6	F	63	ILE	2.2
2	B	147	TYR	2.2
7	G	22	ASN	2.2
2	B	183	ASP	2.2
3	C	208	VAL	2.2
2	B	151	LEU	2.2
5	E	84	LYS	2.2
1	A	258	GLY	2.1
2	B	291	ILE	2.1
5	E	72	THR	2.1
1	A	218	GLU	2.1
5	E	51	ALA	2.1
3	C	305	LEU	2.1
7	G	9	ALA	2.1
7	G	149	LYS	2.1
3	C	218	ALA	2.0
5	E	37	LYS	2.0
2	B	282	LEU	2.0
1	A	263	SER	2.0
2	B	181	ARG	2.0
7	G	24	PHE	2.0
2	B	350	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	353	LEU	2.0
2	B	321	LEU	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
9	ADP	B	1002	27/27	0.77	0.31	1.41	71,80,92,92	0
9	ADP	A	1001	27/27	0.92	0.16	0.01	60,63,70,71	0
8	CA	A	500	1/1	0.90	0.40	-	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.