



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:18 am BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

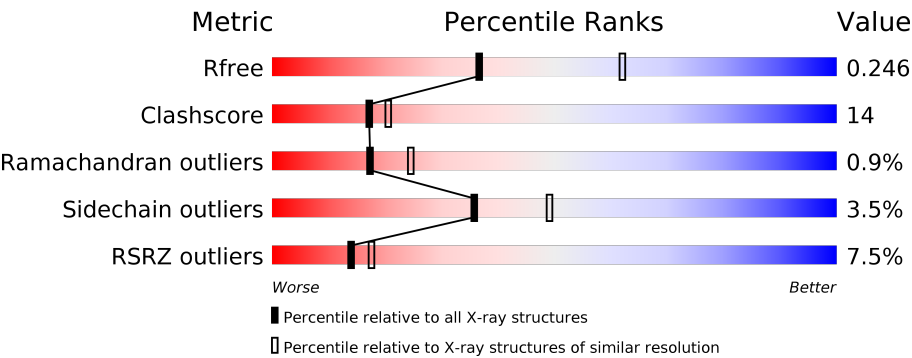
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 respectively. 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><div></div><div>70%</div><div>23%</div><div></div><div></div></div><div></div></div>
2	B	394	<div><div>6%</div><div><div></div><div>34%</div><div>16%</div><div></div><div>48%</div></div><div></div></div>
3	C	372	<div><div>6%</div><div><div></div><div>69%</div><div>24%</div><div></div><div></div></div><div></div></div>
4	D	300	<div><div>2%</div><div><div></div><div>75%</div><div>18%</div><div></div><div>6%</div></div><div></div></div>
5	E	178	<div><div>14%</div><div><div></div><div>54%</div><div>38%</div><div></div><div>6%</div></div><div></div></div>
6	F	168	<div><div>%</div><div><div></div><div>83%</div><div>15%</div><div></div><div></div></div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G	151	<p>11% 69% 17% 3%</p>

## 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			

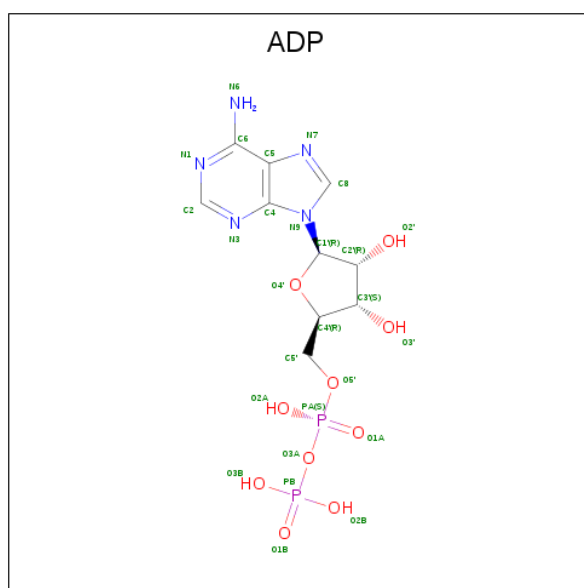
- Molecule 7 is a protein called Arp2/3 Complex 16kDa Subunit.

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	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

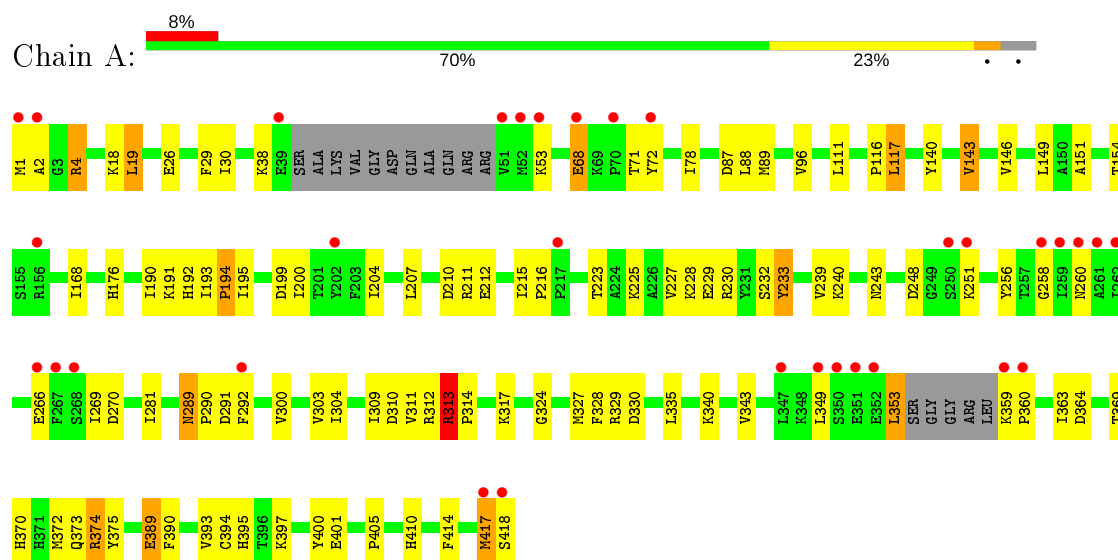
- Molecule 10 is water.

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

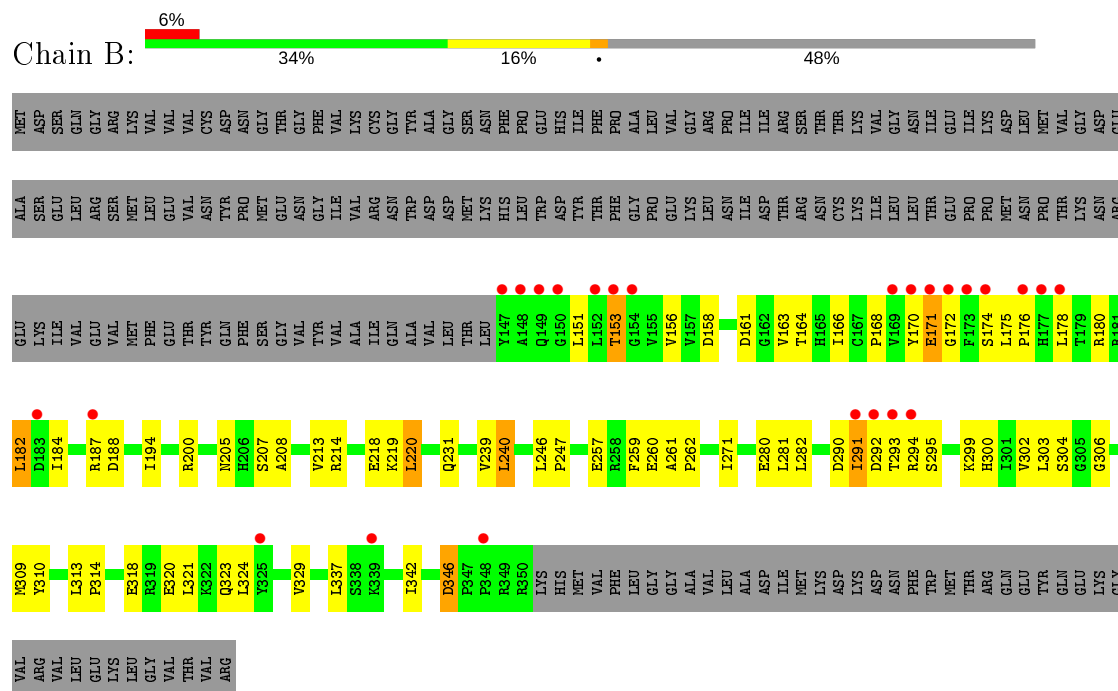
### 3 Residue-property plots

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

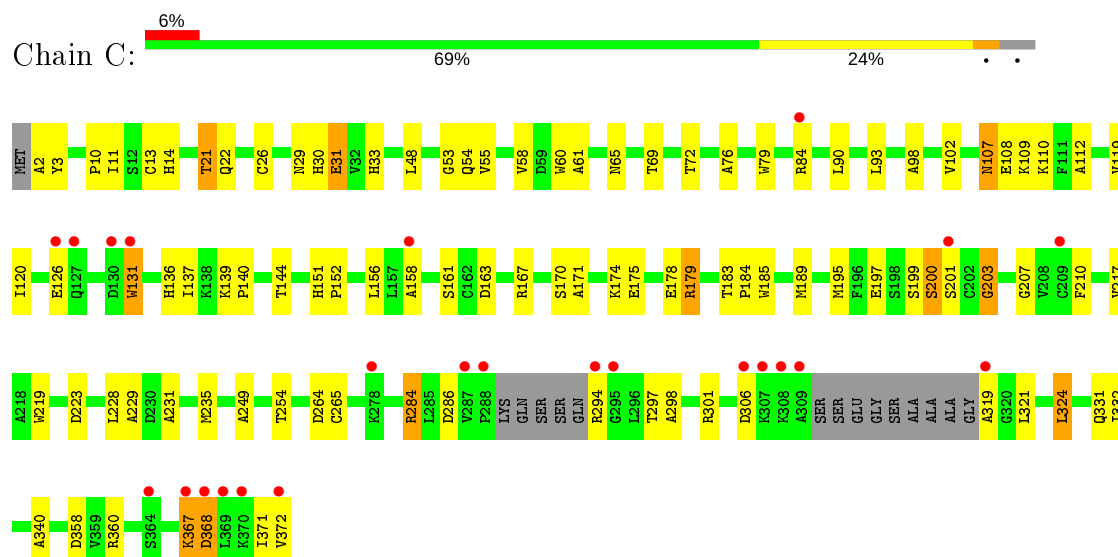
- Molecule 1: Actin-Related Protein 3



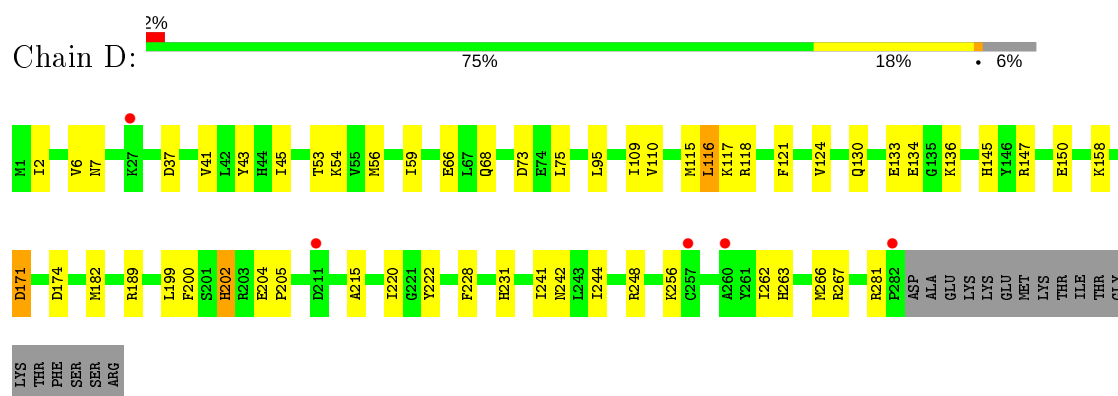
- Molecule 2: Actin-Related Protein 2



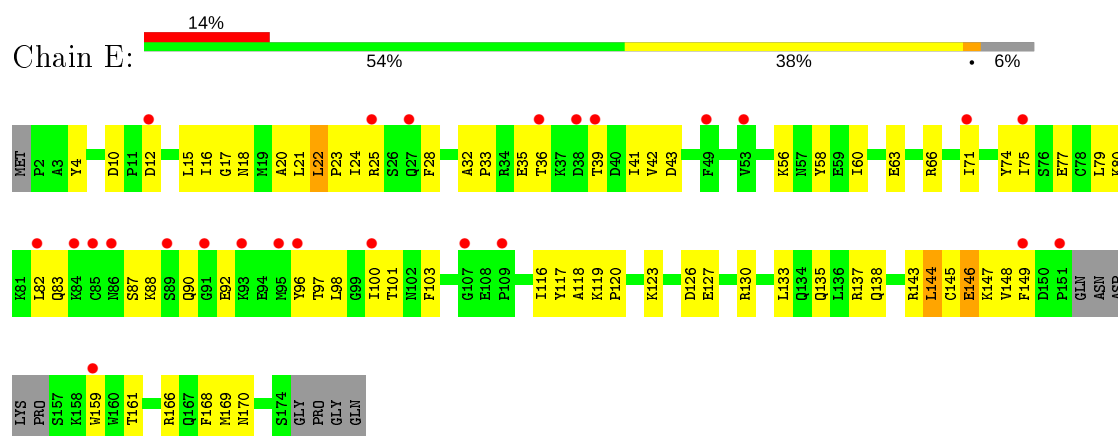
- Molecule 3: Arp2/3 Complex 41Kda Subunit



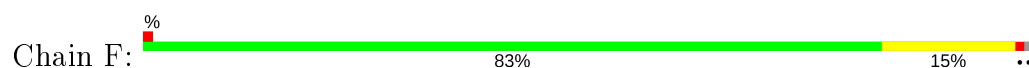
● Molecule 4: Arp2/3 Complex 34Kda Subunit



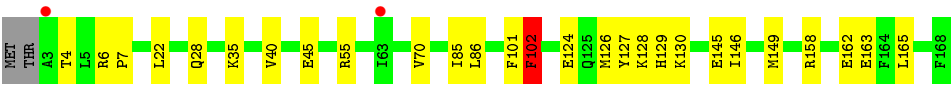
- Molecule 5: Arp2/3 Complex 21Kda Subunit



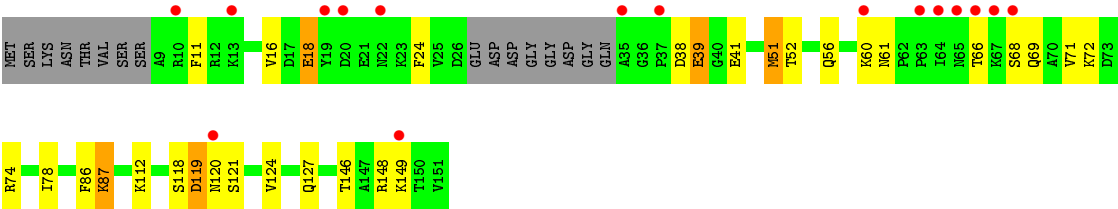
- Molecule 6: Arp2/3 Complex 20Kda Subunit







● 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 0.212 , 0.246	Depositor DCC
$R_{free}$ test set	4565 reflections (5.03%)	wwPDB-VP
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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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

*Continued on next page...*

*Continued from previous page...*

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
3:C:21:THR:HG22	3:C:22:GLN:HG3	1.66	0.77
4:D:281:ARG:HH12	6:F:102:PHE:HZ	1.32	0.77
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.50	0.76
6:F:130:LYS:HE2	6:F:130:LYS:HA	1.68	0.76
3:C:358:ASP:OD1	3:C:360:ARG:HG2	1.85	0.76

*Continued on next page...*

*Continued from previous page...*

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
2:B:291:ILE:HD12	2:B:294:ARG:HH11	1.57	0.69
3:C:107:ASN:HD22	3:C:107:ASN:C	1.96	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
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.76	0.67
7:G:87:LYS:H	7:G:87:LYS:HE3	1.60	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

*Continued on next page...*

*Continued from previous page...*

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
3:C:217:VAL:HG12	3:C:229:ALA:HB3	1.83	0.60
5:E:20:ALA:HB1	5:E:22:LEU:HD13	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
2:B:194:ILE:HG13	2:B:213:VAL:HG11	1.85	0.59
3:C:161:SER:HB2	3:C:163:ASP:OD1	2.02	0.59
7:G:87:LYS:N	7:G:87:LYS:CD	2.65	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
2:B:151:LEU:HD11	2:B:300:HIS:HD2	1.68	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: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

*Continued on next page...*

*Continued from previous page...*

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:111:LEU:HD23	1:A:111:LEU:C	2.27	0.55
1:A:289:ASN:HD22	1:A:289:ASN:C	2.09	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:290:ASP:HB2	2:B:293:THR:OG1	2.08	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
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
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.43	0.53
3:C:30:HIS:HB2	10:C:376:HOH:O	2.07	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
6:F:4:THR:HG23	6:F:55:ARG:NE	2.19	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
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
5:E:88:LYS:O	5:E:92:GLU:HG3	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
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.50	0.52
10:A:1041:HOH:O	4:D:256:LYS:HE2	2.10	0.52
1:A:223:THR:O	1:A:227:VAL:HG23	2.10	0.51
1:A:87:ASP:OD2	4:D:267:ARG:HD2	2.09	0.51
1:A:340:LYS:HA	1:A:343:VAL:HG12	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:GLY:HA2	2:B:309:MET:CE	2.40	0.51
3:C:14:HIS:N	3:C:331:GLN:HE22	1.94	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:102:VAL:HA	3:C:112:ALA:O	2.11	0.51
3:C:297:THR:HG22	3:C:298:ALA:N	2.26	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
1:A:194:PRO:C	1:A:195:ILE:HD12	2.32	0.50
1:A:19:LEU:HD23	1:A:19:LEU:N	2.27	0.50
2:B:205:ASN:ND2	2:B:207:SER:H	2.10	0.50
4:D:281:ARG:NH1	6:F:102:PHE:CZ	2.74	0.50
5:E:168:PHE:CD2	5:E:169:MET:HE2	2.46	0.50
5:E:60:ILE:CD1	5:E:116:ILE:HD13	2.40	0.50
3:C:151:HIS:CG	3:C:152:PRO:HD2	2.47	0.50
6:F:145:GLU:O	6:F:149:MET:HG3	2.11	0.50
4:D:118:ARG:HD3	4:D:118:ARG:C	2.32	0.50
6:F:4:THR:HG23	6:F:55:ARG:NH2	2.27	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
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
3:C:107:ASN:C	3:C:107:ASN:ND2	2.65	0.49
4:D:262:ILE:O	4:D:266:MET:HG3	2.12	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
2:B:346:ASP:OD1	2:B:346:ASP:N	2.45	0.49
5:E:144:LEU:O	5:E:148:VAL:HG23	2.12	0.49
1:A:191:LYS:HB2	1:A:303:VAL:CG2	2.43	0.49
4:D:130:GLN:OE1	4:D:130:GLN:HA	2.13	0.49
5:E:83:GLN:HE21	5:E:161:THR:CG2	2.25	0.48

*Continued on next page...*



*Continued from previous page...*

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
5:E:10:ASP:HB3	5:E:12:ASP:OD1	2.13	0.48
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.95	0.48
3:C:294:ARG:N	3:C:301:ARG:HA	2.29	0.48
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.49	0.48
3:C:144:THR:H	6:F:28:GLN:NE2	2.12	0.48
3:C:185:TRP:CZ3	3:C:235:MET:HG2	2.48	0.48
5:E:82:LEU:HD23	5:E:148:VAL:HG21	1.95	0.48
7:G:87:LYS:H	7:G:87:LYS:CD	2.25	0.48
5:E:98:LEU:HD11	5:E:103:PHE:HZ	1.78	0.48
3:C:10:PRO:HG2	6:F:124:GLU:HG2	1.96	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: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
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.48	0.47
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.43	0.47
3:C:2:ALA:N	10:C:421:HOH:O	2.46	0.47
7:G:149:LYS:HD3	7:G:149:LYS:N	2.29	0.47
3:C:26:CYS:SG	3:C:55:VAL:HB	2.55	0.47
4:D:158:LYS:HD3	4:D:158:LYS:C	2.34	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
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
5:E:20:ALA:CB	5:E:22:LEU:HD13	2.44	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
1:A:53:LYS:HA	10:A:1032:HOH:O	2.13	0.46
2:B:205:ASN:ND2	2:B:208:ALA:H	2.08	0.46
3:C:119:VAL:HG22	3:C:120:ILE:N	2.30	0.46
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.79	0.46
3:C:254:THR:HA	3:C:340:ALA:O	2.15	0.46
1:A:289:ASN:ND2	1:A:289:ASN:C	2.69	0.46
2:B:281:LEU:HD23	2:B:281:LEU:O	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:LEU:O	4:D:75:LEU:HD23	2.15	0.46
1:A:140:TYR:HB2	1:A:394:CYS:SG	2.56	0.46
2:B:151:LEU:HD21	2:B:300:HIS:HD2	1.79	0.46
2:B:214:ARG:NH1	2:B:218:GLU:OE2	2.47	0.46
1:A:395:HIS:HE1	1:A:410:HIS:O	1.98	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:151:ALA:O	1:A:154:THR:HG22	2.16	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:211:ARG:NH1	5:E:159:TRP:CZ3	2.81	0.46
1:A:359:LYS:CD	1:A:359:LYS:O	2.61	0.46
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
2:B:180:ARG:HH11	2:B:180:ARG:HG3	1.81	0.45
6:F:45:GLU:OE2	6:F:45:GLU:N	2.45	0.45
1:A:248:ASP:OD1	1:A:251:LYS:HD3	2.16	0.45
2:B:184:ILE:HD13	2:B:271:ILE:CD1	2.46	0.45
3:C:3:TYR:HB2	3:C:324:LEU:HG	1.99	0.45
5:E:18:ASN:ND2	5:E:118:ALA:H	2.14	0.45
6:F:146:ILE:HA	6:F:149:MET:HE3	1.99	0.45
1:A:232:SER:O	1:A:233:TYR:HB3	2.16	0.45
3:C:31:GLU:OE1	3:C:33:HIS:HE1	1.99	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
2:B:158:ASP:HA	2:B:304:SER:O	2.16	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
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.51	0.45
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.47	0.45
4:D:2:ILE:HG21	6:F:163:GLU:HG2	1.98	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
3:C:72:THR:HA	3:C:98:ALA:HB1	1.99	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
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

*Continued on next page...*

*Continued from previous page...*

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
1:A:313:ARG:N	1:A:314:PRO:CD	2.80	0.45
1:A:329:ARG:O	1:A:330:ASP:HB2	2.17	0.45
2:B:321:LEU:HD12	2:B:342:ILE:HD13	1.99	0.45
5:E:39:THR:HG23	5:E:43:ASP:CB	2.46	0.45
1:A:194:PRO:O	1:A:195:ILE:HD12	2.16	0.44
3:C:158:ALA:HA	3:C:167:ARG:O	2.16	0.44
3:C:61:ALA:HB1	3:C:108:GLU:HG2	1.99	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
4:D:189:ARG:HB2	10:D:317:HOH:O	2.17	0.44
5:E:98:LEU:HD11	5:E:103:PHE:CZ	2.52	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
4:D:7:ASN:OD1	4:D:115:MET:HG2	2.18	0.44
5:E:22:LEU:CD2	5:E:41:ILE:HD13	2.47	0.44
3:C:69:THR:O	3:C:76:ALA:HA	2.17	0.44
1:A:225:LYS:O	1:A:229:GLU:HG2	2.18	0.44
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.99	0.44
5:E:28:PHE:CD2	5:E:138:GLN:HB3	2.53	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
7:G:38:ASP:HB3	7:G:41:GLU:HB2	2.00	0.44
3:C:264:ASP:O	3:C:265:CYS:HB2	2.18	0.44
3:C:228:LEU:HD23	3:C:228:LEU:C	2.38	0.44
7:G:18:GLU:HA	7:G:18:GLU:OE1	2.18	0.44
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.53	0.44
3:C:207:GLY:O	3:C:219:TRP:HA	2.18	0.43
3:C:60:TRP:HE1	3:C:65:ASN:ND2	2.15	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
1:A:71:THR:HG23	1:A:72:TYR:CE1	2.54	0.43
2:B:151:LEU:HD11	2:B:300:HIS:CD2	2.52	0.43
4:D:158:LYS:HE2	4:D:158:LYS:HA	2.00	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

*Continued on next page...*

*Continued from previous page...*

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:59:ILE:HB	4:D:116:LEU:HD13	1.99	0.43
4:D:171:ASP:O	4:D:174:ASP:HB2	2.19	0.43
4:D:95:LEU:HD11	4:D:116:LEU:HG	2.00	0.43
7:G:124:VAL:O	7:G:127:GLN:HB2	2.19	0.43
1:A:200:ILE:CG1	1:A:281:ILE:HD11	2.48	0.42
4:D:228:PHE:H	4:D:231:HIS:CD2	2.25	0.42
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.90	0.42
5:E:15:LEU:HD22	5:E:63:GLU:HG3	2.01	0.42
3:C:201:SER:O	7:G:148:ARG:CG	2.67	0.42
7:G:52:THR:O	7:G:56:GLN:HG3	2.19	0.42
1:A:207:LEU:HD23	5:E:166:ARG:NH2	2.33	0.42
5:E:126:ASP:OD2	5:E:130:ARG:NH1	2.51	0.42
3:C:203:GLY:HA2	10:C:379:HOH:O	2.18	0.42
5:E:88:LYS:NZ	5:E:146:GLU:HG2	2.33	0.42
2:B:170:TYR:O	2:B:172:GLY:N	2.51	0.42
3:C:199:SER:O	3:C:200:SER:HB2	2.18	0.42
4:D:281:ARG:NH1	6:F:102:PHE:HZ	2.09	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
1:A:400:TYR:CE1	1:A:405:PRO:HB3	2.55	0.42
2:B:174:SER:C	2:B:175:LEU:HD23	2.40	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
2:B:151:LEU:CD1	2:B:300:HIS:HD2	2.32	0.41
5:E:145:CYS:C	5:E:147:LYS:N	2.72	0.41
1:A:300:VAL:O	1:A:304:ILE:HG13	2.21	0.41
4:D:41:VAL:HG21	4:D:117:LYS:HE3	2.03	0.41
4:D:68:GLN:NE2	4:D:73:ASP:OD2	2.51	0.41
1:A:312:ARG:O	1:A:312:ARG:HG3	2.19	0.41
3:C:119:VAL:HG21	3:C:136:HIS:HB3	2.03	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
5:E:75:ILE:O	5:E:79:LEU:HG	2.21	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:HD12	1:A:335:LEU:HD11	2.01	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
2:B:178:LEU:O	2:B:180:ARG:HG2	2.21	0.41
2:B:323:GLN:HG2	7:G:16:VAL:HG23	2.02	0.41
3:C:48:LEU:HB3	3:C:79:TRP:CH2	2.56	0.41
7:G:66:THR:OG1	7:G:71:VAL:HG11	2.20	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
1:A:195:ILE:HA	1:A:199:ASP:OD2	2.21	0.41
2:B:231:GLN:HA	2:B:231:GLN:NE2	2.36	0.41
4:D:241:ILE:HA	4:D:244:ILE:HG22	2.02	0.41
1:A:71:THR:HG23	1:A:72:TYR:CD1	2.56	0.41
3:C:29:ASN:O	3:C:54:GLN:HA	2.21	0.41
3:C:48:LEU:HD12	3:C:48:LEU:N	2.35	0.41
4:D:133:GLU:O	4:D:133:GLU:HG2	2.19	0.41
5:E:32:ALA:CB	5:E:135:GLN:OE1	2.68	0.41
1:A:116:PRO:O	1:A:117:LEU:CB	2.62	0.41
5:E:96:TYR:O	5:E:100:ILE:HG12	2.21	0.41
5:E:25:ARG:HD3	5:E:35:GLU:O	2.21	0.41
4:D:109:ILE:HG13	4:D:110:VAL:N	2.36	0.40
4:D:263:HIS:O	4:D:267:ARG:HG3	2.21	0.40
2:B:166:ILE:HD13	2:B:282:LEU:CA	2.51	0.40
5:E:21:LEU:HG	5:E:33:PRO:HD3	2.02	0.40
5:E:22:LEU:HD23	5:E:41:ILE:HD13	2.04	0.40
2:B:259:PHE:CD2	2:B:259:PHE:C	2.94	0.40
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.93	0.40
2:B:302:VAL:HG13	2:B:302:VAL:O	2.22	0.40
5:E:66:ARG:HB3	5:E:117:TYR:CE2	2.56	0.40
6:F:102:PHE:HE1	6:F:126:MET:CE	2.34	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%)	12	16
2	B	202/394 (51%)	183 (91%)	16 (8%)	3 (2%)	10	14
3	C	351/372 (94%)	334 (95%)	14 (4%)	3 (1%)	17	24
4	D	280/300 (93%)	274 (98%)	5 (2%)	1 (0%)	34	46
5	E	164/178 (92%)	154 (94%)	9 (6%)	1 (1%)	25	34
6	F	164/168 (98%)	158 (96%)	5 (3%)	1 (1%)	25	34
7	G	131/151 (87%)	123 (94%)	7 (5%)	1 (1%)	19	27
All	All	1688/1981 (85%)	1593 (94%)	80 (5%)	15 (1%)	17	24

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%)	29	39
2	B	163/345 (47%)	155 (95%)	8 (5%)	25	34
3	C	298/313 (95%)	284 (95%)	14 (5%)	26	35
4	D	248/264 (94%)	244 (98%)	4 (2%)	62	77
5	E	146/159 (92%)	144 (99%)	2 (1%)	67	79
6	F	152/155 (98%)	150 (99%)	2 (1%)	69	80
7	G	108/124 (87%)	102 (94%)	6 (6%)	21	28
All	All	1463/1723 (85%)	1412 (96%)	51 (4%)	36	49

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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	B	1002	-	24,29,29	1.37	3 (12%)	29,45,45	1.47	3 (10%)
9	ADP	A	1001	-	24,29,29	1.36	3 (12%)	29,45,45	1.55	5 (17%)

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	B	1002	-	-	0/12/32/32	0/3/3/3
9	ADP	A	1001	-	-	5/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1001	ADP	C2-N1	3.63	1.40	1.33
9	B	1002	ADP	C2-N1	3.60	1.40	1.33
9	B	1002	ADP	PB-O1B	3.40	1.61	1.50
9	A	1001	ADP	PB-O1B	3.36	1.61	1.50
9	A	1001	ADP	O4'-C1'	2.23	1.44	1.41
9	B	1002	ADP	O4'-C1'	2.21	1.44	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1002	ADP	N3-C2-N1	-5.42	120.21	128.68
9	A	1001	ADP	N3-C2-N1	-5.37	120.29	128.68
9	A	1001	ADP	PA-O3A-PB	-3.17	121.95	132.83
9	B	1002	ADP	PA-O3A-PB	-3.11	122.17	132.83
9	A	1001	ADP	O4'-C1'-C2'	-2.55	103.20	106.93
9	B	1002	ADP	O3B-PB-O3A	2.54	113.15	104.64
9	A	1001	ADP	O3B-PB-O3A	2.39	112.67	104.64
9	A	1001	ADP	C4-C5-N7	-2.03	107.28	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

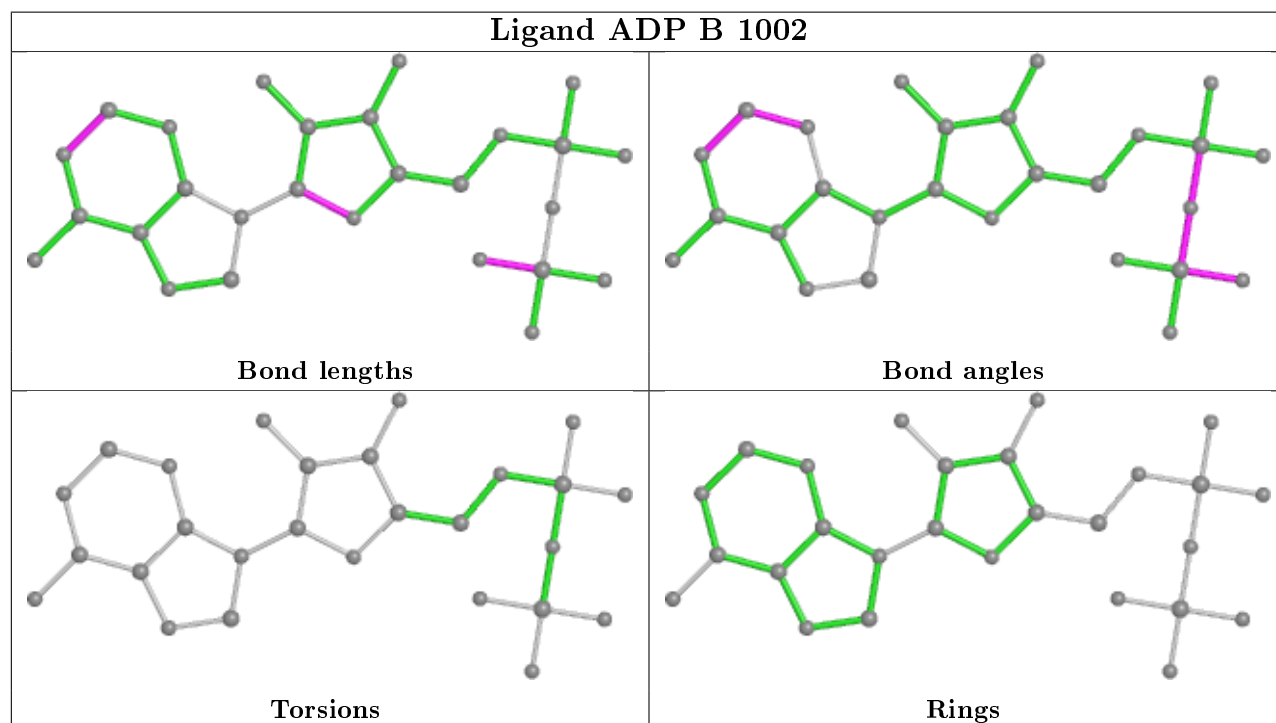
Mol	Chain	Res	Type	Atoms
9	A	1001	ADP	C5'-O5'-PA-O3A
9	A	1001	ADP	C5'-O5'-PA-O1A
9	A	1001	ADP	C5'-O5'-PA-O2A
9	A	1001	ADP	PB-O3A-PA-O2A
9	A	1001	ADP	O4'-C4'-C5'-O5'

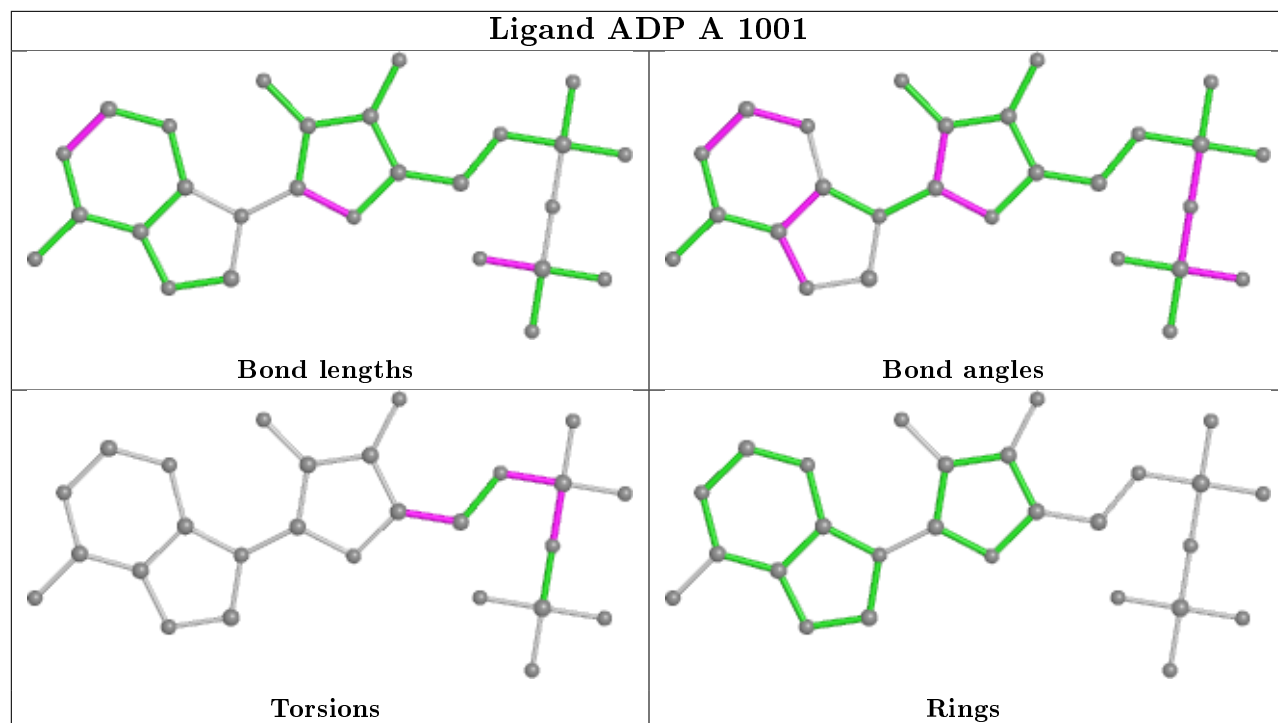
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1002	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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%)	0.38	32 (7%) 12 15	18, 45, 86, 102	0
2	B	204/394 (51%)	0.59	25 (12%) 4 5	26, 53, 93, 100	0
3	C	357/372 (95%)	0.20	24 (6%) 17 21	23, 38, 76, 101	0
4	D	282/300 (94%)	0.04	5 (1%) 68 74	21, 35, 55, 74	0
5	E	168/178 (94%)	0.86	25 (14%) 2 2	42, 59, 93, 97	0
6	F	166/168 (98%)	-0.18	2 (1%) 79 84	21, 30, 43, 62	0
7	G	135/151 (89%)	0.48	16 (11%) 4 5	25, 53, 83, 88	0
All	All	1714/1981 (86%)	0.31	129 (7%) 14 17	18, 42, 85, 102	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	309	ALA	6.5
1	A	1	MET	6.5
5	E	85	CYS	5.7
1	A	51	VAL	5.6
1	A	350	SER	5.3
1	A	359	LYS	5.1
1	A	2	ALA	5.1
5	E	38	ASP	5.0
1	A	418	SER	5.0
7	G	13	LYS	4.9
2	B	292	ASP	4.8
1	A	347	LEU	4.8
5	E	89	SER	4.8
1	A	417	MET	4.8
3	C	306	ASP	4.8
2	B	174	SER	4.7
1	A	351	GLU	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	E	151	PRO	4.6
7	G	64	ILE	4.6
5	E	86	ASN	4.3
1	A	266	GLU	4.2
5	E	36	THR	4.1
3	C	368	ASP	4.0
7	G	68	SER	4.0
6	F	3	ALA	4.0
1	A	250	SER	3.9
3	C	308	LYS	3.9
4	D	211	ASP	3.9
2	B	154	GLY	3.9
5	E	109	PRO	3.9
2	B	171	GLU	3.9
1	A	262	ILE	3.9
3	C	367	LYS	3.7
2	B	187	ARG	3.6
2	B	293	THR	3.6
2	B	153	THR	3.5
2	B	170	TYR	3.5
7	G	66	THR	3.5
3	C	369	LEU	3.5
3	C	201	SER	3.5
1	A	268	SER	3.4
2	B	148	ALA	3.4
2	B	172	GLY	3.4
3	C	294	ARG	3.4
7	G	67	LYS	3.4
1	A	352	GLU	3.3
2	B	178	LEU	3.3
5	E	149	PHE	3.3
3	C	127	GLN	3.3
2	B	173	PHE	3.2
1	A	259	ILE	3.1
5	E	107	GLY	3.1
1	A	260	ASN	3.1
5	E	93	LYS	3.1
3	C	295	GLY	3.1
3	C	131	TRP	3.0
5	E	27	GLN	3.0
1	A	156	ARG	3.0
5	E	75	ILE	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	G	10	ARG	2.9
3	C	370	LYS	2.8
7	G	37	PRO	2.8
5	E	100	ILE	2.8
3	C	278	LYS	2.8
2	B	149	GLN	2.8
3	C	364	SER	2.8
5	E	53	VAL	2.8
1	A	349	LEU	2.8
4	D	282	PRO	2.8
7	G	35	ALA	2.8
2	B	169	VAL	2.7
3	C	307	LYS	2.7
3	C	372	VAL	2.7
7	G	20	ASP	2.7
3	C	319	ALA	2.6
1	A	39	GLU	2.6
2	B	152	LEU	2.6
1	A	267	PHE	2.6
3	C	209	CYS	2.6
3	C	84	ARG	2.6
1	A	261	ALA	2.6
5	E	39	THR	2.6
1	A	217	PRO	2.6
1	A	70	PRO	2.5
7	G	120	ASN	2.5
2	B	294	ARG	2.5
1	A	251	LYS	2.5
5	E	49	PHE	2.5
2	B	150	GLY	2.4
5	E	96	TYR	2.4
4	D	27	LYS	2.4
1	A	202	TYR	2.4
7	G	63	PRO	2.4
1	A	68	GLU	2.4
2	B	177	HIS	2.4
1	A	52	MET	2.4
1	A	292	PHE	2.4
1	A	360	PRO	2.3
3	C	158	ALA	2.3
7	G	60	LYS	2.3
2	B	325	TYR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	E	159	TRP	2.3
3	C	130	ASP	2.3
5	E	12	ASP	2.3
5	E	82	LEU	2.3
5	E	95	MET	2.3
1	A	53	LYS	2.2
2	B	348	PRO	2.2
3	C	288	PRO	2.2
1	A	72	TYR	2.2
3	C	126	GLU	2.2
4	D	260	ALA	2.2
2	B	339	LYS	2.2
2	B	147	TYR	2.2
7	G	65	ASN	2.1
3	C	287	VAL	2.1
7	G	19	TYR	2.1
5	E	71	ILE	2.1
6	F	63	ILE	2.1
5	E	25	ARG	2.1
2	B	176	PRO	2.1
7	G	22	ASN	2.1
5	E	84	LYS	2.1
4	D	257	CYS	2.1
5	E	91	GLY	2.1
1	A	258	GLY	2.0
2	B	183	ASP	2.0
2	B	291	ILE	2.0
7	G	149	LYS	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](#)

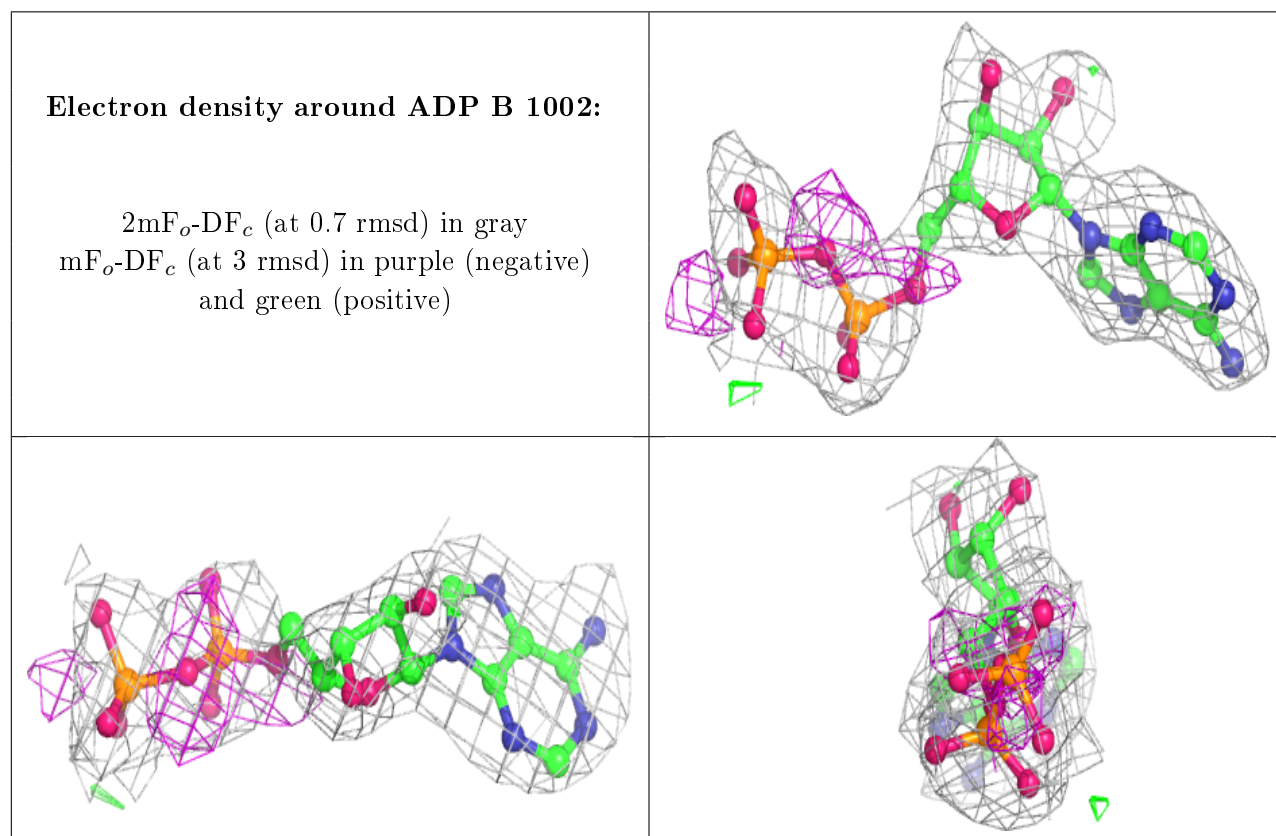
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

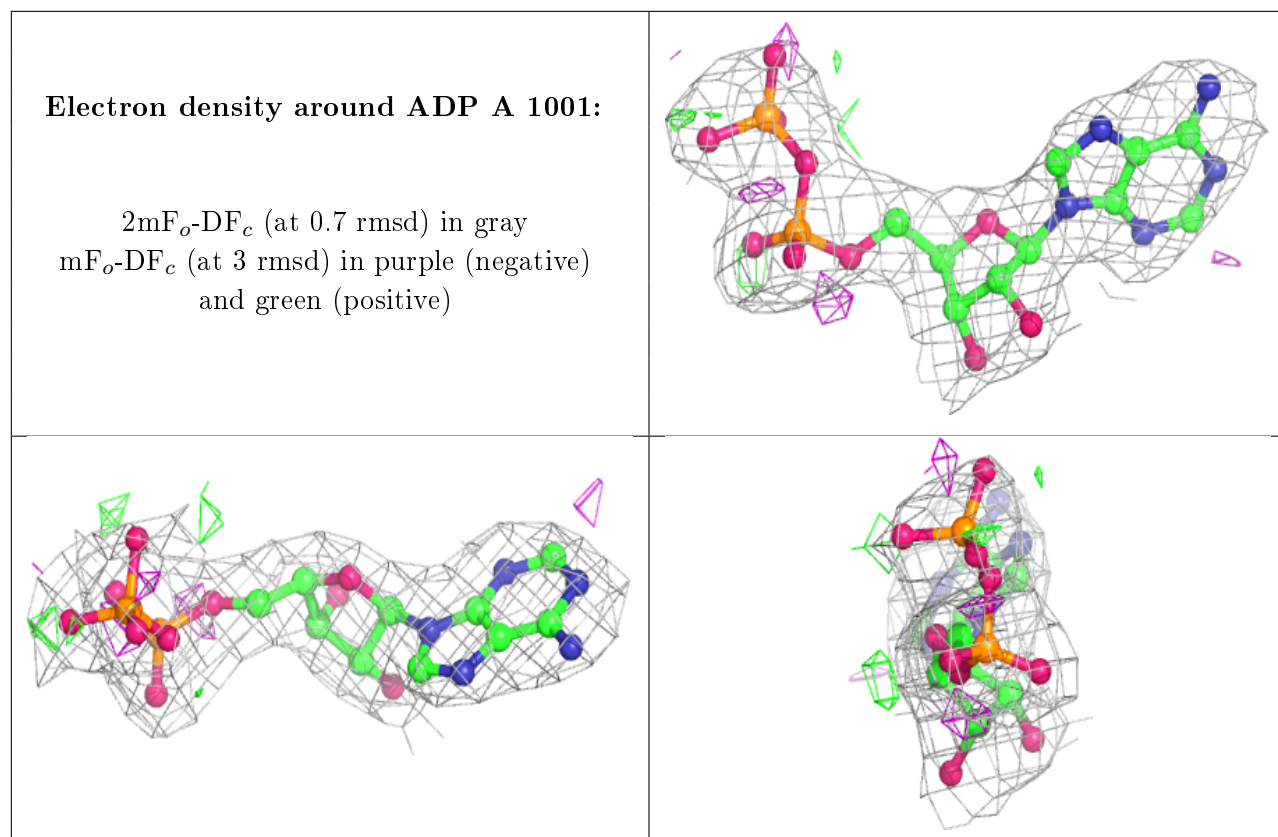


median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	ADP	B	1002	27/27	0.77	0.31	71,80,92,92	0
8	CA	A	500	1/1	0.90	0.40	75,75,75,75	0
9	ADP	A	1001	27/27	0.92	0.16	60,63,70,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.