



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:54 PM UTC

PDB ID : 1U2V / pdb_00001u2v
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

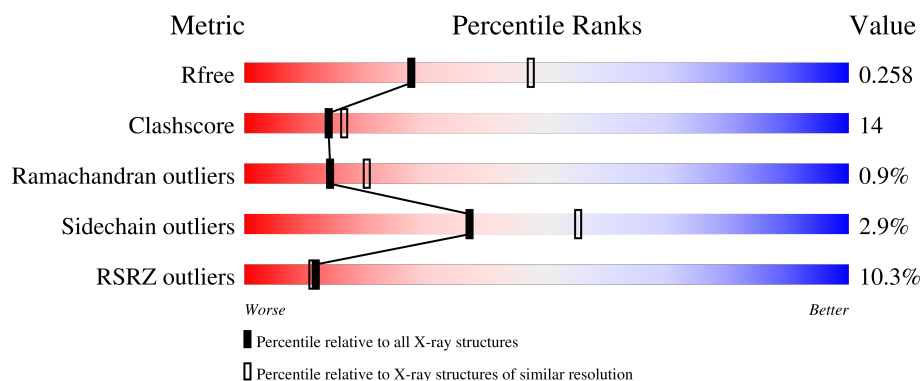
1 Overall quality at a glance

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
2	B	394	
3	C	372	
4	D	300	
5	E	178	

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Mol	Chain	Length	Quality of chain
6	F	168	% 80% 18% ..
7	G	151	10% 69% 17% • 11%

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			

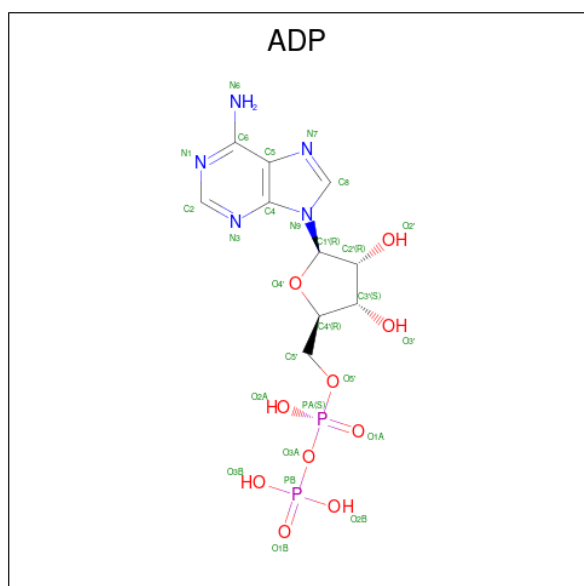
- Molecule 7 is a protein called Arp2/3 Complex 16kDa Subunit.

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

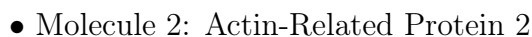


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
9	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

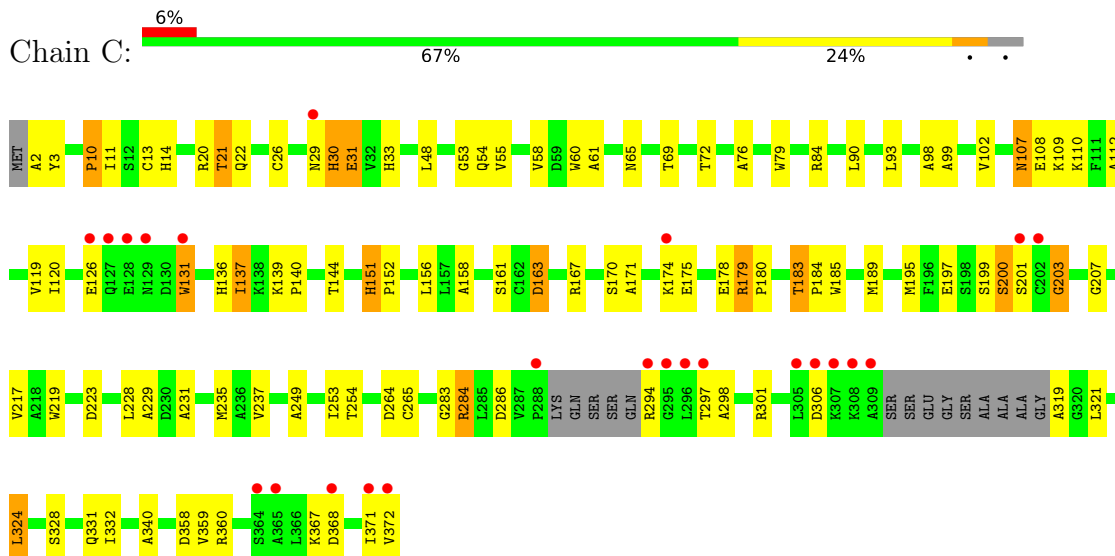
- Molecule 10 is water.

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

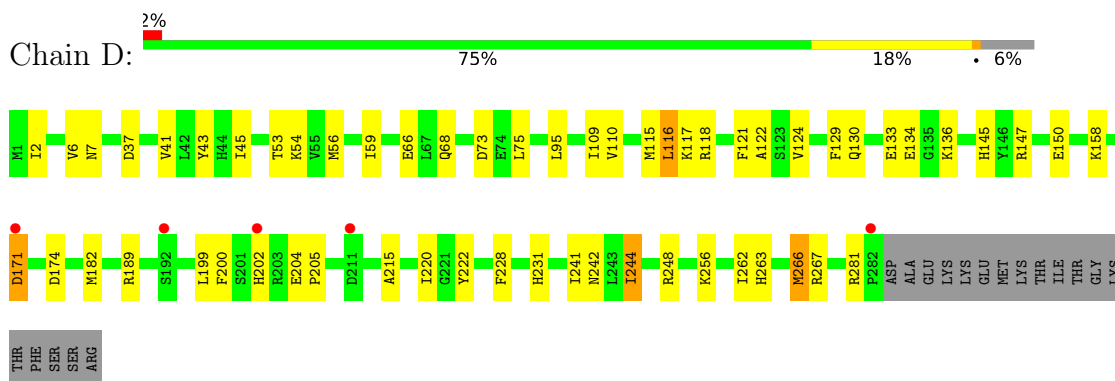
- Molecule 1: Actin-Related Protein 3



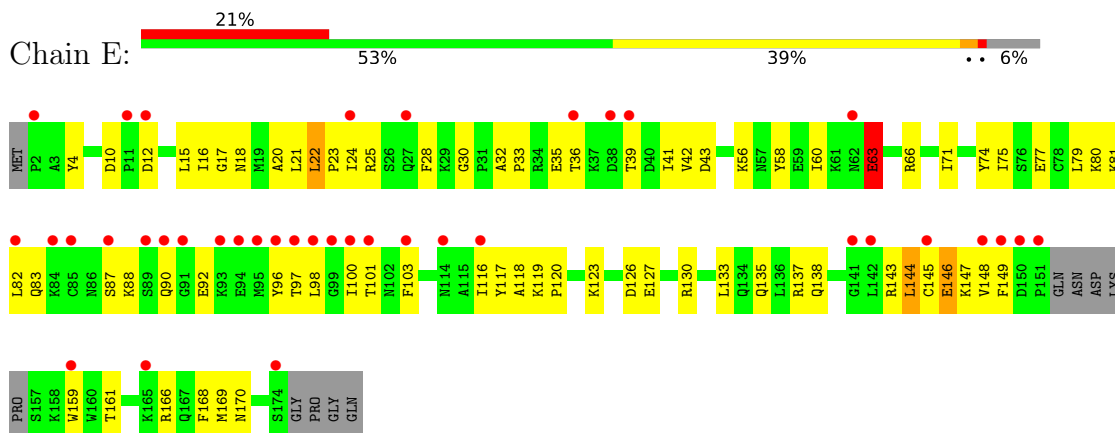
- Molecule 3: Arp2/3 Complex 41Kda Subunit



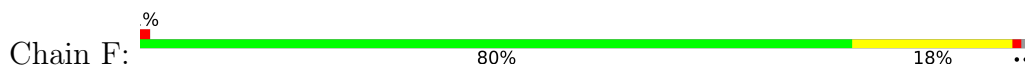
- Molecule 4: Arp2/3 Complex 34Kda Subunit

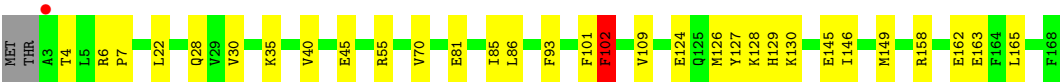


- Molecule 5: Arp2/3 Complex 21Kda Subunit

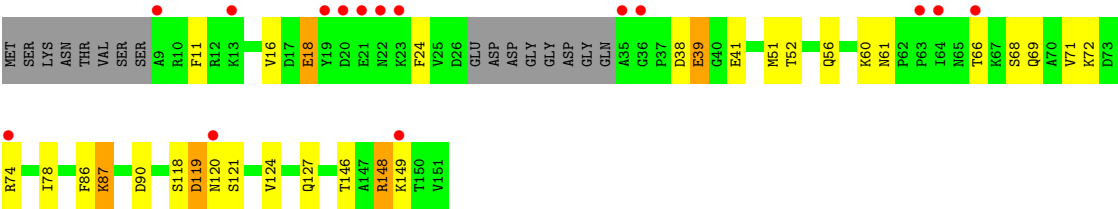


- Molecule 6: Arp2/3 Complex 20Kda Subunit





● 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, α , β , γ	111.30Å 129.30Å 204.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 30.00 – 2.58	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.55) 97.4 (30.00-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.57Å)	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%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.43	0/3290	0.95	12/4464 (0.3%)
2	B	0.39	0/1598	0.88	0/2168
3	C	0.41	0/2830	0.99	13/3837 (0.3%)
4	D	0.43	1/2328 (0.0%)	0.89	3/3143 (0.1%)
5	E	0.35	0/1385	0.86	2/1867 (0.1%)
6	F	0.45	0/1382	0.95	5/1853 (0.3%)
7	G	0.37	0/1033	0.87	1/1390 (0.1%)
All	All	0.41	1/13846 (0.0%)	0.93	36/18722 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	266	MET	SD-CE	-5.10	1.66	1.79

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	283	GLY	N-CA-C	9.24	120.73	111.95
3	C	11	ILE	N-CA-C	-9.22	93.77	107.51
3	C	30	HIS	N-CA-C	-7.67	103.50	113.17
1	A	314	PRO	N-CA-C	-7.33	103.96	113.57
1	A	373	GLN	N-CA-C	7.17	120.13	111.82
6	F	101	PHE	N-CA-C	-7.08	101.72	110.65
1	A	116	PRO	N-CA-C	-6.93	101.02	111.41
5	E	63	GLU	N-CA-C	-6.91	104.11	112.54
4	D	129	PHE	N-CA-C	-6.85	103.74	111.14
1	A	178	ILE	N-CA-C	6.76	114.83	107.60
6	F	102	PHE	N-CA-C	6.46	124.57	110.80
5	E	17	GLY	N-CA-C	-6.44	97.92	113.18
3	C	359	VAL	N-CA-C	6.28	117.03	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	237	VAL	N-CA-C	5.91	116.38	107.75
4	D	122	ALA	N-CA-C	5.87	118.19	111.02
3	C	10	PRO	N-CA-C	5.87	120.54	111.21
3	C	137	ILE	N-CA-C	-5.79	98.89	107.51
6	F	109	VAL	N-CA-C	-5.77	102.13	109.58
3	C	163	ASP	N-CA-C	-5.73	106.51	112.93
3	C	253	ILE	N-CA-C	-5.68	107.58	113.10
1	A	118	ASN	N-CA-C	-5.61	102.09	110.23
1	A	278	GLY	CA-C-N	5.42	125.24	119.28
1	A	278	GLY	C-N-CA	5.42	125.24	119.28
6	F	81	GLU	N-CA-C	5.40	117.16	111.28
6	F	30	VAL	N-CA-C	5.38	115.61	107.75
3	C	151	HIS	N-CA-C	-5.36	102.35	110.39
1	A	109	TYR	N-CA-C	-5.33	102.59	110.48
3	C	99	ALA	N-CA-C	-5.33	102.60	110.48
1	A	78	ILE	N-CA-C	5.29	115.52	108.11
1	A	284	HIS	CA-C-N	5.27	125.58	119.47
1	A	284	HIS	C-N-CA	5.27	125.58	119.47
7	G	148	ARG	N-CA-C	-5.25	105.15	112.45
3	C	20	ARG	N-CA-C	-5.15	105.02	111.92
4	D	244	ILE	N-CA-C	5.13	116.47	110.62
1	A	104	GLU	N-CA-C	-5.13	98.48	109.81
3	C	328	SER	N-CA-C	5.07	117.70	110.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3209	0	3141	97	0
2	B	1569	0	1564	68	0
3	C	2761	0	2707	76	0
4	D	2279	0	2248	47	0
5	E	1354	0	1350	58	0
6	F	1360	0	1399	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1021	0	1038	30	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	390	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 (390) 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:HH11	1:A:4:ARG:HB2	1.20	1.00
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.44	0.99
6:F:146:ILE:HA	6:F:149:MET:HE3	1.45	0.94
3:C:14:HIS:H	3:C:331:GLN:HE22	1.12	0.93
2:B:306:GLY:HA2	2:B:309:MET:HE2	1.50	0.91
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:HH11	1:A:4:ARG:CB	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
6:F:145:GLU:HG3	6:F:149:MET:HE2	1.65	0.76
6:F:130:LYS:HA	6:F:130:LYS:HE2	1.68	0.76
3:C:358:ASP:OD1	3:C:360:ARG:HG2	1.85	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:107:ASN:C	3:C:107:ASN:HD22	1.96	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
3:C:189:MET:HA	3:C:195:MET:HE1	1.73	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
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
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.76	0.67
7:G:87:LYS:HE3	7:G:87:LYS:H	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:HD3	7:G:87:LYS:N	2.12	0.64
5:E:145:CYS:C	5:E:147:LYS:H	2.04	0.64
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
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:PRO:HG2	3:C:189:MET:HE3	1.80	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
3:C:189:MET:HG2	3:C:195:MET:HE3	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
1:A:200:ILE:O	1:A:204:ILE:HG13	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
1:A:417:MET:O	1:A:418:SER:HB2	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
1:A:111:LEU:HD23	1:A:111:LEU:C	2.27	0.60
6:F:6:ARG:HB3	6:F:7:PRO:HD3	1.84	0.60
1:A:289:ASN:C	1:A:289:ASN:HD22	2.09	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
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:24:ILE:O	5:E:24:ILE:HG13	2.02	0.58
5:E:97:THR:O	5:E:101:THR:HG23	2.03	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
1:A:311:VAL:C	1:A:314:PRO:HD2	2.29	0.58
6:F:35:LYS:HD3	6:F:40:VAL:HG11	1.86	0.57
4:D:75:LEU:HD23	4:D:75:LEU:C	2.29	0.57
7:G:118:SER:O	7:G:119:ASP:C	2.47	0.57
1:A:317:LYS:HE2	1:A:364:ASP:OD1	2.05	0.57
3:C:131:TRP:HE3	3:C:131:TRP:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:E:16:ILE:HG23	5:E:16:ILE:O	2.07	0.55
4:D:215:ALA:HB1	4:D:220:ILE:HD13	1.88	0.55
1:A:194:PRO:C	1:A:195:ILE:HD12	2.32	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
4:D:118:ARG:HD3	4:D:118:ARG:C	2.32	0.54
4:D:53:THR:C	4:D:54:LYS:HD2	2.32	0.54
2:B:290:ASP:HB2	2:B:293:THR:OG1	2.08	0.54
2:B:291:ILE:O	2:B:291:ILE:HG22	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
4:D:248:ARG:HD3	4:D:248:ARG:C	2.33	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
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:HA	6:F:130:LYS:CE	2.38	0.53
3:C:254:THR:HG21	3:C:372:VAL:HG22	1.90	0.53
7:G:38:ASP:HB3	7:G:41:GLU:CB	2.39	0.53
4:D:121:PHE:O	4:D:124:VAL:HG12	2.09	0.52
4:D:158:LYS:HD3	4:D:158:LYS:C	2.34	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
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
1:A:340:LYS:HA	1:A:343:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:146:ILE:HA	6:F:149:MET:CE	2.31	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
4:D:266:MET:HE3	6:F:93:PHE:CD1	2.47	0.50
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.92	0.50
1:A:19:LEU:HD23	1:A:19:LEU:N	2.27	0.50
1:A:68:GLU:H	1:A:68:GLU:CD	2.19	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
3:C:178:GLU:O	3:C:179:ARG:C	2.54	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
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
3:C:367:LYS:HD2	3:C:367:LYS:C	2.35	0.49
3:C:107:ASN:HD22	3:C:109:LYS:H	1.57	0.49
6:F:102:PHE:HE1	6:F:126:MET:HE1	1.76	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
4:D:262:ILE:O	4:D:266:MET:HG3	2.12	0.49
1:A:18:LYS:N	1:A:18:LYS:HD3	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
3:C:228:LEU:C	3:C:228:LEU:HD23	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:GLU:H	2:B:257:GLU:CD	2.21	0.48
5:E:83:GLN:HE21	5:E:161:THR:CG2	2.25	0.48
5:E:168:PHE:CD2	5:E:169:MET:HE2	2.48	0.48
1:A:397:LYS:HE2	1:A:401:GLU:OE2	2.13	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
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
2:B:290:ASP:C	2:B:292:ASP:H	2.21	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:2:ALA:N	10:C:421:HOH:O	2.46	0.47
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.43	0.47
7:G:149:LYS:HD3	7:G:149:LYS:N	2.29	0.47
1:A:26:GLU:OE2	1:A:372:MET:HE1	2.14	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
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
3:C:189:MET:HG2	3:C:195:MET:CE	2.44	0.47
5:E:20:ALA:CB	5:E:22:LEU:HD13	2.44	0.47
5:E:145:CYS:C	5:E:147:LYS:N	2.72	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:174:SER:C	2:B:175:LEU:HD23	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:281:LEU:O	2:B:281:LEU:HD23	2.15	0.46
4:D:75:LEU:HD23	4:D:75:LEU:O	2.15	0.46
1:A:140:TYR:HB2	1:A:394:CYS:SG	2.56	0.46
1:A:289:ASN:ND2	1:A:289:ASN:C	2.69	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:170:SER:HB2	3:C:195:MET:CE	2.46	0.46
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.50	0.46
1:A:151:ALA:O	1:A:154:THR:HG22	2.16	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:O	1:A:359:LYS:CD	2.61	0.46
1:A:216:PRO:HG3	1:A:260:ASN:ND2	2.31	0.45
2:B:180:ARG:HG3	2:B:180:ARG:HH11	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
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
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
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.51	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
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.47	0.45
2:B:259:PHE:CD2	2:B:259:PHE:C	2.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:193:ILE:C	1:A:195:ILE:H	2.25	0.44
1:A:194:PRO:O	1:A:195:ILE:HD12	2.16	0.44
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
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:O	1:A:374:ARG:HD3	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
4:D:263:HIS:HA	4:D:266:MET:HE2	1.98	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
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
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.53	0.44
7:G:18:GLU:OE1	7:G:18:GLU:HA	2.18	0.44
1:A:1:MET:O	1:A:2:ALA:C	2.61	0.43
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
4:D:66:GLU:OE2	4:D:145:HIS:ND1	2.37	0.43
2:B:281:LEU:HD23	2:B:281:LEU:C	2.44	0.43
1:A:71:THR:HG23	1:A:72:TYR:CE1	2.54	0.43
1:A:190:ILE:HG22	1:A:191:LYS:N	2.33	0.43
2:B:151:LEU:HD11	2:B:300:HIS:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:LYS:HE2	4:D:158:LYS:HA	2.00	0.43
6:F:85:ILE:HD12	6:F:85:ILE:C	2.44	0.43
7:G:60:LYS:HE2	7:G:61:ASN:ND2	2.33	0.43
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:95:LEU:HD11	4:D:116:LEU:HG	2.00	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
1:A:200:ILE:CG1	1:A:281:ILE:HD11	2.48	0.42
3:C:201:SER:O	7:G:148:ARG:CG	2.67	0.42
4:D:228:PHE:H	4:D:231:HIS:CD2	2.25	0.42
5:E:15:LEU:HD22	5:E:63:GLU:HG3	2.01	0.42
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.90	0.42
6:F:102:PHE:CE1	6:F:126:MET:HE1	2.53	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:30:GLY:HA3	5:E:135:GLN:CD	2.44	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
1:A:78:ILE:HD11	1:A:89:MET:HE1	2.01	0.42
2:B:170:TYR:O	2:B:172:GLY:N	2.51	0.42
5:E:81:LYS:C	5:E:83:GLN:N	2.78	0.42
7:G:87:LYS:NZ	7:G:90:ASP:CG	2.77	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:HD23	2:B:151:LEU:HA	1.86	0.42
4:D:199:LEU:N	4:D:199:LEU:HD12	2.35	0.42
1:A:400:TYR:CE1	1:A:405:PRO:HB3	2.55	0.42
5:E:83:GLN:HE21	5:E:161:THR:HG22	1.85	0.41
5:E:116:ILE:HG22	5:E:117:TYR:CD1	2.55	0.41
2:B:151:LEU:CD1	2:B:300:HIS:HD2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:209:ARG:C	1:A:211:ARG:H	2.27	0.41
2:B:231:GLN:HA	2:B:231:GLN:NE2	2.36	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
4:D:241:ILE:HA	4:D:244:ILE:HG22	2.02	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
3:C:131:TRP:CE3	3:C:131:TRP:C	2.99	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
3:C:107:ASN:C	3:C:107:ASN:ND2	2.65	0.40
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
2:B:290:ASP:C	2:B:292:ASP:N	2.79	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
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.93	0.40
2:B:302:VAL:O	2:B:302:VAL:HG13	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%)	9	12
2	B	202/394 (51%)	183 (91%)	16 (8%)	3 (2%)	8	10
3	C	351/372 (94%)	334 (95%)	14 (4%)	3 (1%)	14	20
4	D	280/300 (93%)	274 (98%)	5 (2%)	1 (0%)	30	39
5	E	164/178 (92%)	154 (94%)	9 (6%)	1 (1%)	21	29
6	F	164/168 (98%)	158 (96%)	5 (3%)	1 (1%)	21	29
7	G	131/151 (87%)	123 (94%)	7 (5%)	1 (1%)	16	22
All	All	1688/1981 (85%)	1593 (94%)	80 (5%)	15 (1%)	14	20

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%)	338 (97%)	10 (3%)	37	55
2	B	163/345 (47%)	154 (94%)	9 (6%)	19	29
3	C	298/313 (95%)	286 (96%)	12 (4%)	28	42
4	D	248/264 (94%)	245 (99%)	3 (1%)	63	78
5	E	146/159 (92%)	143 (98%)	3 (2%)	47	66
6	F	152/155 (98%)	151 (99%)	1 (1%)	76	85
7	G	108/124 (87%)	104 (96%)	4 (4%)	30	45
All	All	1463/1723 (85%)	1421 (97%)	42 (3%)	37	55

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	353	LEU
1	A	366	GLN
1	A	389	GLU
2	B	153	THR
2	B	184	ILE
2	B	200	ARG
2	B	220	LEU
2	B	240	LEU
2	B	303	LEU
2	B	337	LEU
2	B	342	ILE
2	B	346	ASP
3	C	21	THR

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Mol	Chain	Res	Type
3	C	31	GLU
3	C	90	LEU
3	C	107	ASN
3	C	131	TRP
3	C	175	GLU
3	C	179	ARG
3	C	183	THR
3	C	284	ARG
3	C	306	ASP
3	C	321	LEU
3	C	324	LEU
4	D	116	LEU
4	D	171	ASP
4	D	204	GLU
5	E	22	LEU
5	E	63	GLU
5	E	144	LEU
6	F	165	LEU
7	G	18	GLU
7	G	39	GLU
7	G	69	GLN
7	G	87	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	176	HIS
1	A	192	HIS
1	A	219	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
2	B	205	ASN
2	B	231	GLN
2	B	267	GLN
2	B	284	ASN
2	B	300	HIS

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Mol	Chain	Res	Type
2	B	323	GLN
3	C	33	HIS
3	C	46	HIS
3	C	65	ASN
3	C	75	ASN
3	C	107	ASN
3	C	303	GLN
3	C	331	GLN
4	D	49	ASN
4	D	132	GLN
4	D	140	ASN
4	D	202	HIS
4	D	231	HIS
4	D	278	ASN
5	E	62	ASN
5	E	83	GLN
5	E	170	ASN
6	F	28	GLN
6	F	167	ASN
7	G	56	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 oligosaccharides 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	-	28,29,29	1.53	5 (17%)	43,45,45	1.75	9 (20%)
9	ADP	A	1001	-	28,29,29	1.53	5 (17%)	43,45,45	1.78	9 (20%)

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	-	-	0/16/32/32	0/3/3/3
9	ADP	A	1001	-	-	4/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1001	ADP	C2-N1	3.79	1.40	1.33
9	B	1002	ADP	C2-N1	3.76	1.40	1.33
9	B	1002	ADP	PB-O1B	3.55	1.61	1.50
9	A	1001	ADP	PB-O1B	3.51	1.61	1.50
9	B	1002	ADP	C5-N7	-3.14	1.33	1.39
9	A	1001	ADP	C5-N7	-3.11	1.33	1.39
9	B	1002	ADP	C8-N9	-2.31	1.33	1.37
9	A	1001	ADP	C8-N9	-2.23	1.33	1.37
9	A	1001	ADP	C4-N9	-2.21	1.33	1.37
9	B	1002	ADP	C4-N9	-2.03	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1002	ADP	N3-C2-N1	-5.53	120.21	128.58
9	A	1001	ADP	N3-C2-N1	-5.48	120.29	128.58
9	A	1001	ADP	C5-C4-N3	-4.40	120.66	126.72
9	B	1002	ADP	C5-C4-N3	-4.30	120.80	126.72
9	B	1002	ADP	C2-N3-C4	4.14	121.94	111.83
9	A	1001	ADP	C2-N3-C4	4.11	121.87	111.83
9	A	1001	ADP	N9-C8-N7	-3.09	109.55	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1002	ADP	N9-C8-N7	-3.07	109.58	113.94
9	B	1002	ADP	N3-C4-N9	3.01	132.28	127.17
9	A	1001	ADP	N3-C4-N9	2.95	132.18	127.17
9	A	1001	ADP	C4-C5-N7	-2.89	107.28	110.58
9	A	1001	ADP	C5-N7-C8	2.85	107.93	103.45
9	B	1002	ADP	C5-N7-C8	2.81	107.87	103.45
9	B	1002	ADP	C4-C5-N7	-2.71	107.48	110.58
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	B	1002	ADP	C4-N9-C8	2.30	108.15	105.74
9	A	1001	ADP	C4-N9-C8	2.23	108.08	105.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

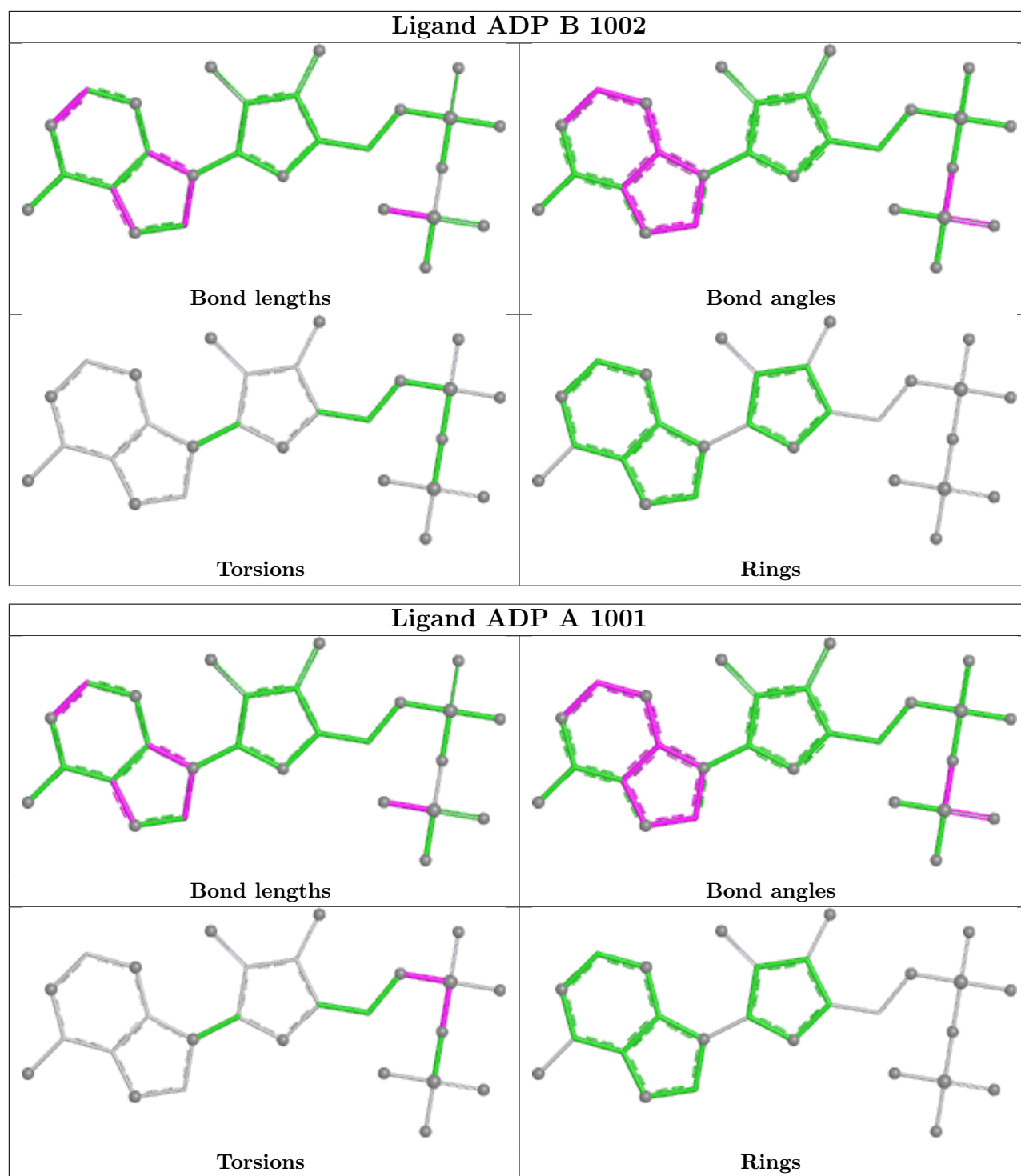
Mol	Chain	Res	Type	Atoms
9	A	1001	ADP	C5'-O5'-PA-O1A
9	A	1001	ADP	C5'-O5'-PA-O2A
9	A	1001	ADP	C5'-O5'-PA-O3A
9	A	1001	ADP	PB-O3A-PA-O2A

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	402/418 (96%)	0.55	54 (13%) 7 5	18, 45, 86, 102	0
2	B	204/394 (51%)	0.96	40 (19%) 3 2	26, 53, 93, 100	0
3	C	357/372 (95%)	0.22	24 (6%) 24 23	23, 38, 76, 101	0
4	D	282/300 (94%)	-0.04	5 (1%) 67 68	21, 35, 55, 74	0
5	E	168/178 (94%)	1.36	38 (22%) 2 2	42, 59, 93, 97	0
6	F	166/168 (98%)	-0.38	1 (0%) 85 88	21, 30, 43, 62	0
7	G	135/151 (89%)	0.80	15 (11%) 10 9	25, 53, 83, 88	0
All	All	1714/1981 (86%)	0.44	177 (10%) 12 11	18, 42, 85, 102	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	85	CYS	7.1
2	B	350	ARG	7.0
2	B	147	TYR	6.7
2	B	291	ILE	6.4
7	G	22	ASN	6.1
1	A	2	ALA	6.0
3	C	309	ALA	5.7
7	G	20	ASP	5.6
5	E	150	ASP	5.1
1	A	262	ILE	5.1
1	A	353	LEU	4.8
3	C	201	SER	4.7
1	A	261	ALA	4.6
7	G	35	ALA	4.6
1	A	52	MET	4.6
1	A	263	SER	4.5
2	B	349	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	350	SER	4.4
1	A	1	MET	4.3
1	A	417	MET	4.3
5	E	95	MET	4.3
5	E	96	TYR	4.2
7	G	21	GLU	4.2
1	A	264	LYS	4.1
1	A	265	LYS	4.0
5	E	151	PRO	4.0
5	E	89	SER	4.0
3	C	127	GLN	3.9
1	A	349	LEU	3.8
5	E	100	ILE	3.8
2	B	161	ASP	3.7
2	B	177	HIS	3.6
2	B	187	ARG	3.6
5	E	2	PRO	3.6
5	E	38	ASP	3.6
5	E	159	TRP	3.6
3	C	294	ARG	3.6
5	E	149	PHE	3.6
5	E	62	ASN	3.6
5	E	36	THR	3.6
5	E	97	THR	3.6
3	C	295	GLY	3.6
7	G	9	ALA	3.5
7	G	63	PRO	3.5
2	B	292	ASP	3.5
3	C	129	ASN	3.5
2	B	149	GLN	3.5
7	G	64	ILE	3.5
2	B	178	LEU	3.4
5	E	84	LYS	3.4
1	A	247	THR	3.4
5	E	82	LEU	3.4
5	E	12	ASP	3.2
1	A	267	PHE	3.2
2	B	333	ASP	3.2
5	E	142	LEU	3.2
5	E	174	SER	3.1
1	A	213	VAL	3.1
1	A	202	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	308	LYS	3.1
3	C	305	LEU	3.0
1	A	260	ASN	3.0
3	C	202	CYS	3.0
3	C	368	ASP	3.0
1	A	418	SER	3.0
2	B	325	TYR	3.0
1	A	343	VAL	3.0
1	A	158	VAL	2.9
3	C	128	GLU	2.9
5	E	39	THR	2.9
7	G	13	LYS	2.9
1	A	209	ARG	2.9
2	B	175	LEU	2.9
2	B	148	ALA	2.9
4	D	282	PRO	2.9
2	B	174	SER	2.8
5	E	98	LEU	2.8
1	A	217	PRO	2.8
1	A	224	ALA	2.7
5	E	27	GLN	2.7
1	A	220	SER	2.7
1	A	250	SER	2.7
1	A	256	TYR	2.7
1	A	268	SER	2.7
1	A	259	ILE	2.7
1	A	53	LYS	2.7
3	C	126	GLU	2.7
4	D	171	ASP	2.6
7	G	23	LYS	2.6
2	B	289	ALA	2.6
1	A	360	PRO	2.6
2	B	342	ILE	2.6
3	C	288	PRO	2.6
1	A	206	GLN	2.6
5	E	93	LYS	2.6
1	A	252	TRP	2.6
2	B	150	GLY	2.6
3	C	364	SER	2.6
2	B	179	THR	2.6
3	C	297	THR	2.6
1	A	257	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	218	GLU	2.5
1	A	51	VAL	2.5
1	A	361	LYS	2.5
3	C	29	ASN	2.5
5	E	165	LYS	2.5
2	B	293	THR	2.5
2	B	290	ASP	2.5
3	C	296	LEU	2.5
5	E	114	ASN	2.5
1	A	68	GLU	2.5
5	E	99	GLY	2.5
7	G	19	TYR	2.5
5	E	116	ILE	2.5
2	B	348	PRO	2.4
5	E	145	CYS	2.4
5	E	91	GLY	2.4
7	G	149	LYS	2.4
5	E	90	GLN	2.4
2	B	296	GLU	2.4
1	A	215	ILE	2.4
1	A	230	ARG	2.4
1	A	347	LEU	2.4
5	E	103	PHE	2.4
2	B	153	THR	2.4
3	C	371	ILE	2.4
2	B	183	ASP	2.4
3	C	306	ASP	2.4
2	B	206	HIS	2.4
3	C	372	VAL	2.4
5	E	101	THR	2.3
1	A	251	LYS	2.3
7	G	120	ASN	2.3
3	C	365	ALA	2.3
5	E	11	PRO	2.3
3	C	131	TRP	2.3
2	B	181	ARG	2.3
5	E	141	GLY	2.3
1	A	266	GLU	2.3
1	A	258	GLY	2.3
4	D	192	SER	2.3
2	B	182	LEU	2.3
5	E	94	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLN	2.3
1	A	348	LYS	2.3
2	B	346	ASP	2.3
5	E	148	VAL	2.3
1	A	359	LYS	2.2
4	D	211	ASP	2.2
3	C	307	LYS	2.2
7	G	74	ARG	2.2
2	B	173	PHE	2.2
2	B	309	MET	2.2
2	B	152	LEU	2.2
2	B	294	ARG	2.2
1	A	289	ASN	2.2
2	B	329	VAL	2.1
1	A	345	ALA	2.1
2	B	284	ASN	2.1
6	F	3	ALA	2.1
2	B	286	ILE	2.1
2	B	343	ARG	2.1
5	E	87	SER	2.1
1	A	392	GLN	2.1
2	B	151	LEU	2.1
1	A	269	ILE	2.1
3	C	174	LYS	2.1
7	G	66	THR	2.1
2	B	184	ILE	2.1
1	A	245	TYR	2.1
4	D	202	HIS	2.1
1	A	288	ALA	2.0
7	G	36	GLY	2.0
2	B	326	LEU	2.0
5	E	24	ILE	2.0
1	A	70	PRO	2.0
1	A	155	SER	2.0

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

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

6.3 Carbohydrates [i](#)

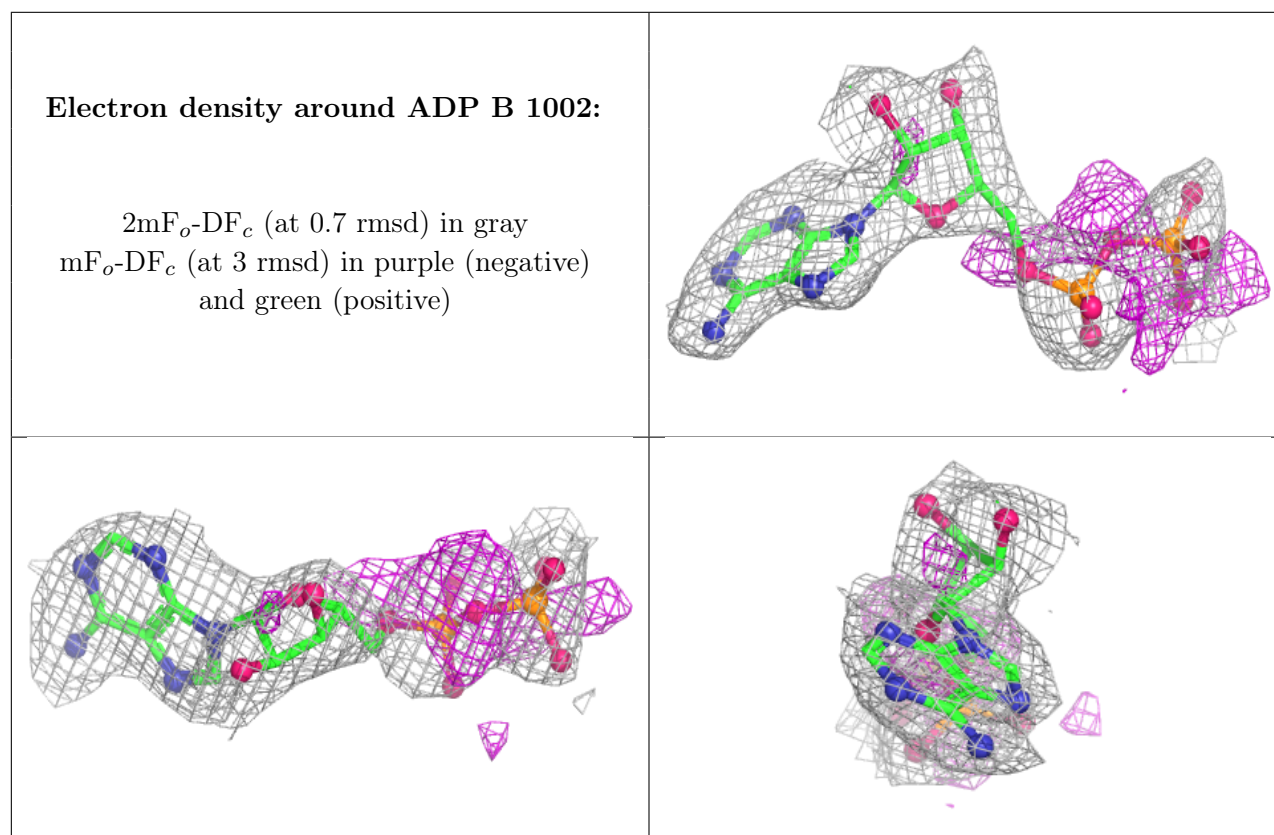
There are no oligosaccharides in this entry.

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, 95th 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.

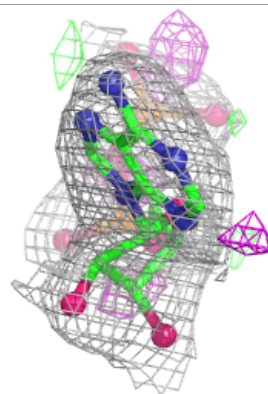
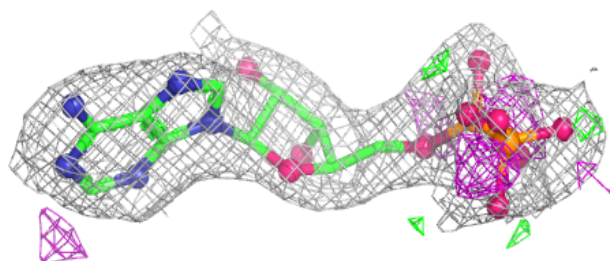
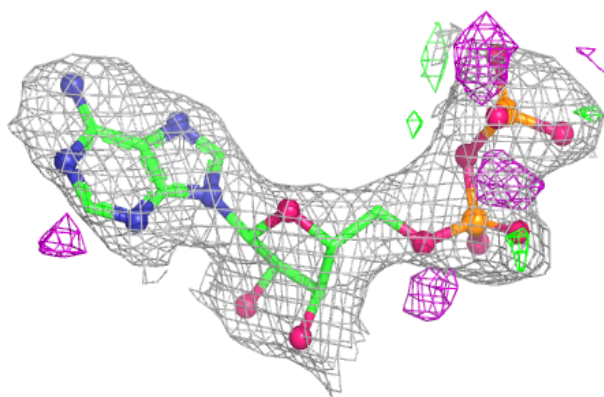
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ADP	B	1002	27/27	0.77	0.17	71,80,92,92	0
8	CA	A	500	1/1	0.86	0.22	75,75,75,75	0
9	ADP	A	1001	27/27	0.88	0.13	60,63,70,71	0

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.



Electron density around ADP A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.