Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 01:28 PM EST

PDB ID	:	2P9I
Title	:	Crystal Structure of bovine Arp2/3 Complex co-crystallized with ADP and crosslinked with gluteraldehyde
Authors	:	Nolen, B.J.; Pollard, T.D.
Deposited on	:	2007-03-26
Resolution	:	2.46 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:

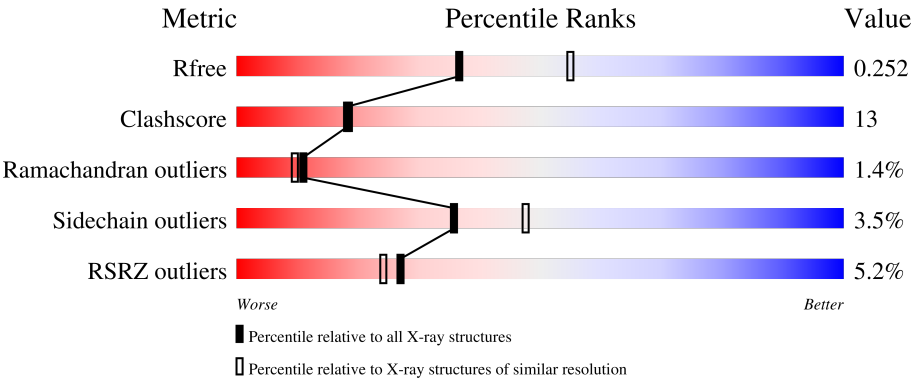
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	6% 73% 19% • 6%
2	B	394	7% 42% 24% • 31%
3	C	372	4% 66% 24% • 8%
4	D	300	2% 75% 17% • 7%
5	E	178	4% 69% 25% • •

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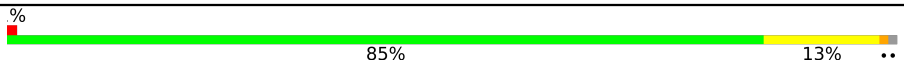
Mol	Chain	Length	Quality of chain
6	F	168	
7	G	151	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14311 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-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3151	2022	528	587	14			

- Molecule 2 is a protein called Actin-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	272	Total	C	N	O	S	0	0	0
			2030	1296	350	376	8			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	341	Total	C	N	O	S	0	0	0
			2642	1677	461	485	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	VAL	ILE	conflict	UNP Q58CQ2

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	280	Total	C	N	O	S	0	0	0
			2263	1439	392	424	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1415	908	236	262	9			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	137	Total	C	N	O	S	0	0	0
			1048	655	183	207	3			

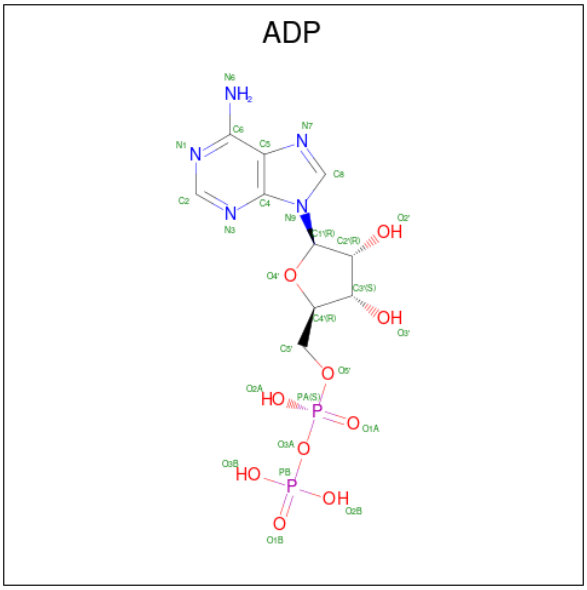
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ASP	GLY	conflict	UNP Q3SYX9
G	28	ASP	GLU	conflict	UNP Q3SYX9

- 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		
8	B	1	Total	Ca	0	0
			1	1		

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



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		

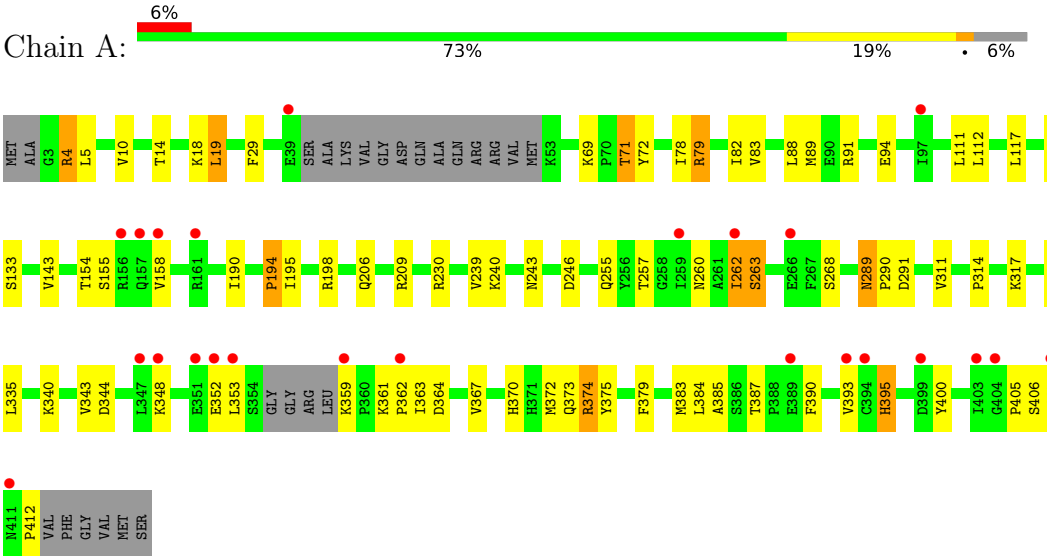
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	75	Total	O	0	0
			75	75		
10	B	32	Total	O	0	0
			32	32		
10	C	64	Total	O	0	0
			64	64		
10	D	72	Total	O	0	0
			72	72		
10	E	17	Total	O	0	0
			17	17		
10	F	66	Total	O	0	0
			66	66		
10	G	9	Total	O	0	0
			9	9		

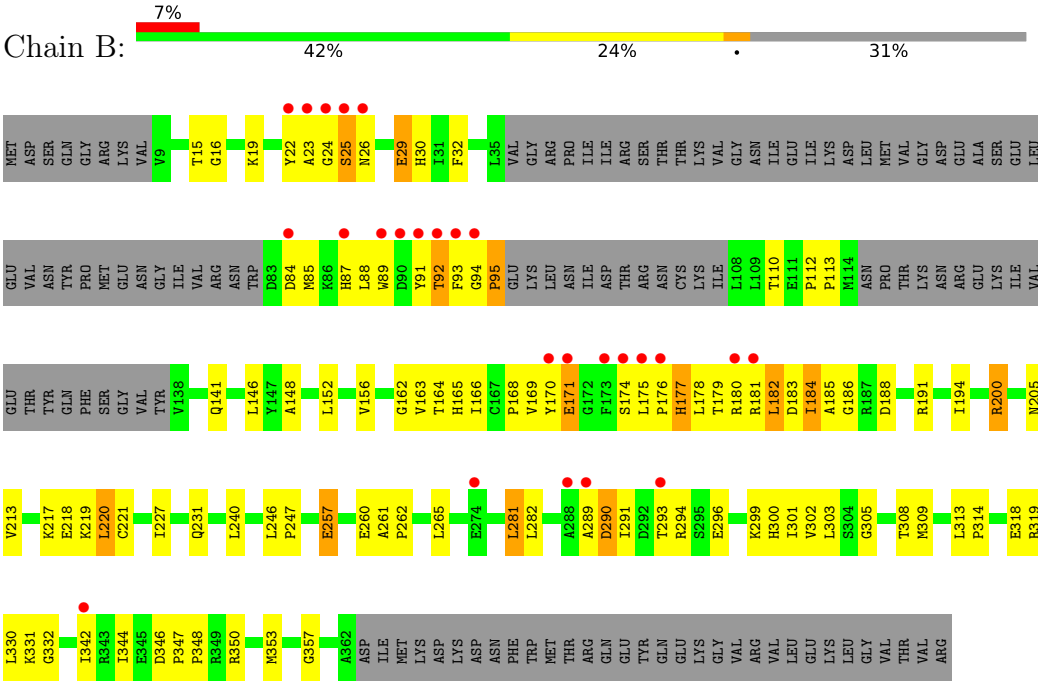
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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-like protein 3

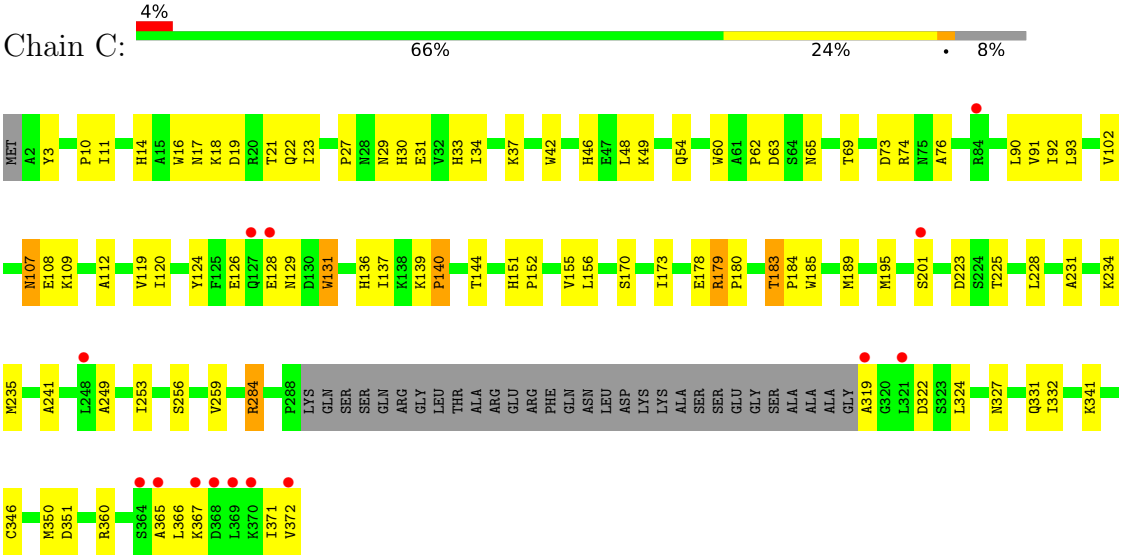


• Molecule 2: Actin-like protein 2



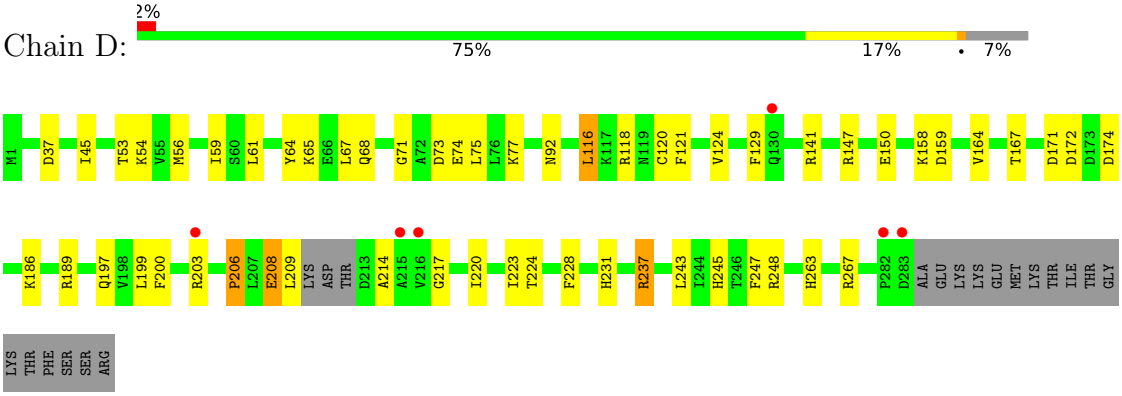
• Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C:



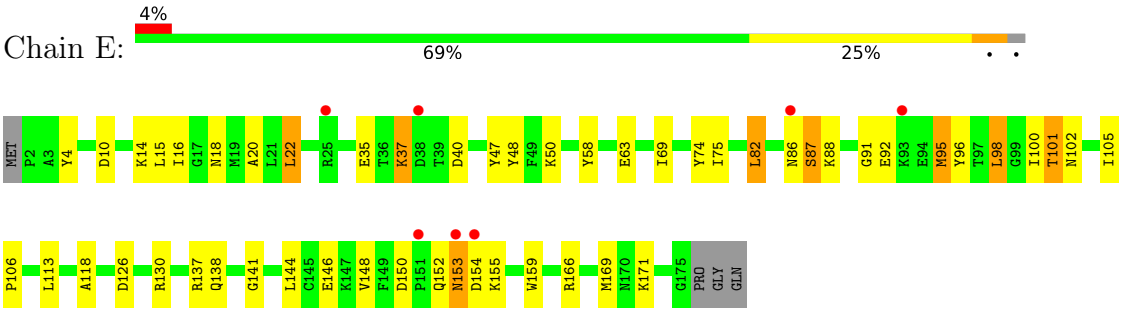
• Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:



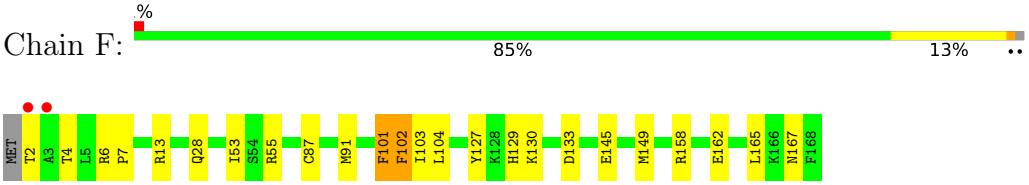
• Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:



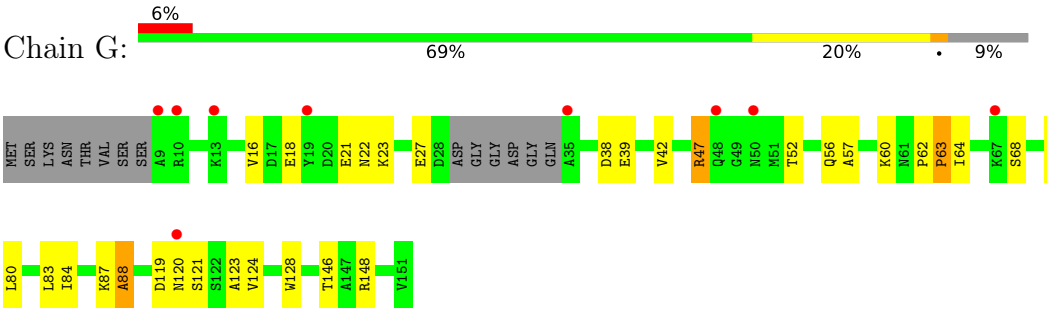
• Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:



• Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.61Å 128.18Å 198.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.46 45.24 – 2.43	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.46) 94.2 (45.24-2.43)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.261 0.207 , 0.252	Depositor DCC
R_{free} test set	5292 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14311	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.36	0/3231	0.58	0/4384
2	B	0.33	0/2071	0.56	1/2813 (0.0%)
3	C	0.37	0/2711	0.64	1/3681 (0.0%)
4	D	0.37	0/2311	0.56	0/3119
5	E	0.34	0/1449	0.58	0/1954
6	F	0.40	0/1393	0.61	0/1868
7	G	0.32	0/1060	0.53	0/1426
All	All	0.36	0/14226	0.59	2/19245 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	112	PRO	N-CA-CB	5.55	109.96	103.30
3	C	11	ILE	N-CA-C	-5.53	96.08	111.00

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	3151	0	3097	75	0
2	B	2030	0	1915	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2642	0	2591	81	0
4	D	2263	0	2227	48	0
5	E	1415	0	1416	51	0
6	F	1371	0	1410	18	0
7	G	1048	0	1058	25	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	27	0	12	1	0
9	B	27	0	12	2	0
10	A	75	0	0	1	0
10	B	32	0	0	0	0
10	C	64	0	0	2	0
10	D	72	0	0	1	0
10	E	17	0	0	0	0
10	F	66	0	0	0	0
10	G	9	0	0	0	0
All	All	14311	0	13738	370	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 13.

All (370) 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	1.31	1.11
6:F:4:THR:HG23	6:F:55:ARG:HH21	1.20	1.04
3:C:183:THR:HG22	3:C:185:TRP:H	1.28	0.97
2:B:309:MET:HE1	2:B:350:ARG:HG3	1.43	0.97
3:C:319:ALA:HB2	6:F:130:LYS:HD2	1.50	0.92
3:C:14:HIS:H	3:C:331:GLN:HE22	1.19	0.86
2:B:205:ASN:HD22	2:B:208:ALA:H	1.30	0.80
5:E:126:ASP:O	5:E:130:ARG:HG3	1.82	0.80
3:C:189:MET:HG2	3:C:195:MET:HE3	1.65	0.79
1:A:393:VAL:HB	1:A:412:PRO:HB2	1.64	0.78
1:A:206:GLN:HE22	1:A:209:ARG:NH1	1.81	0.78
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.66	0.77
3:C:223:ASP:CB	7:G:146:THR:HG21	2.15	0.76
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.01	0.75
5:E:98:LEU:O	5:E:101:THR:HG23	1.87	0.75
5:E:152:GLN:HB3	5:E:155:LYS:HZ1	1.52	0.74
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:HIS:CD2	2:B:181:ARG:HG2	2.23	0.73
5:E:35:GLU:OE1	5:E:37:LYS:HE3	1.88	0.73
4:D:228:PHE:H	4:D:231:HIS:HD2	1.37	0.71
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.72	0.71
4:D:150:GLU:HG2	4:D:167:THR:HA	1.73	0.71
2:B:182:LEU:HD22	2:B:184:ILE:HG23	1.73	0.70
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.72	0.70
4:D:186:LYS:NZ	4:D:200:PHE:H	1.90	0.70
1:A:257:THR:HG22	1:A:268:SER:OG	1.92	0.69
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.27	0.69
2:B:309:MET:CE	2:B:350:ARG:HG3	2.20	0.69
3:C:107:ASN:C	3:C:107:ASN:HD22	1.96	0.69
3:C:126:GLU:HB3	3:C:131:TRP:HZ3	1.57	0.69
4:D:217:GLY:HA3	4:D:220:ILE:HD13	1.75	0.69
3:C:90:LEU:HD23	3:C:91:VAL:N	2.08	0.69
1:A:14:THR:HG23	1:A:79:ARG:HA	1.73	0.68
1:A:409:ARG:HB3	2:B:200:ARG:O	1.94	0.68
1:A:348:LYS:HE2	1:A:352:GLU:OE2	1.94	0.67
2:B:257:GLU:HA	2:B:260:GLU:HB2	1.75	0.67
7:G:120:ASN:HD21	7:G:123:ALA:HB2	1.60	0.66
1:A:343:VAL:HG13	1:A:363:ILE:HD12	1.77	0.66
4:D:186:LYS:HZ2	4:D:200:PHE:H	1.43	0.66
5:E:95:MET:HE3	5:E:95:MET:HA	1.79	0.65
1:A:155:SER:HB2	1:A:370:HIS:HB3	1.79	0.65
2:B:184:ILE:HG13	2:B:265:LEU:HD23	1.80	0.64
6:F:130:LYS:HA	6:F:130:LYS:HE2	1.79	0.64
3:C:14:HIS:H	3:C:331:GLN:NE2	1.94	0.64
7:G:47:ARG:HG3	7:G:47:ARG:HH11	1.62	0.64
3:C:126:GLU:HB3	3:C:131:TRP:CZ3	2.32	0.64
5:E:95:MET:HG3	5:E:141:GLY:HA3	1.80	0.63
1:A:206:GLN:HE22	1:A:209:ARG:HH11	1.45	0.63
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.81	0.63
3:C:256:SER:HB2	3:C:372:VAL:HG13	1.81	0.63
3:C:319:ALA:HB2	6:F:130:LYS:CD	2.27	0.63
3:C:31:GLU:OE2	3:C:49:LYS:HE3	1.99	0.63
6:F:2:THR:HB	6:F:4:THR:HG22	1.81	0.63
1:A:260:ASN:CG	1:A:263:SER:HB3	2.19	0.62
4:D:208:GLU:HG3	4:D:209:LEU:N	2.15	0.62
6:F:158:ARG:O	6:F:162:GLU:HG3	1.99	0.62
3:C:144:THR:H	6:F:28:GLN:NE2	1.98	0.62
4:D:199:LEU:HB2	4:D:224:THR:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ILE:HD12	2:B:185:ALA:N	2.14	0.62
2:B:163:VAL:HG22	2:B:164:THR:N	2.15	0.61
4:D:189:ARG:HH22	4:D:197:GLN:HE21	1.47	0.61
3:C:189:MET:HA	3:C:195:MET:HE1	1.81	0.61
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.81	0.61
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.81	0.61
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.80	0.61
4:D:53:THR:C	4:D:54:LYS:HD2	2.20	0.61
5:E:87:SER:HA	5:E:154:ASP:H	1.65	0.61
4:D:208:GLU:OE2	4:D:209:LEU:HD23	2.00	0.61
1:A:246:ASP:OD1	5:E:50:LYS:HE3	2.00	0.61
2:B:290:ASP:O	2:B:291:ILE:HD13	2.01	0.61
2:B:350:ARG:HA	2:B:353:MET:HE2	1.81	0.60
2:B:290:ASP:O	2:B:294:ARG:HD3	2.02	0.60
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.83	0.60
1:A:353:LEU:HD13	1:A:353:LEU:O	2.01	0.60
3:C:107:ASN:ND2	3:C:109:LYS:H	2.00	0.59
2:B:32:PHE:HZ	2:B:92:THR:HG23	1.67	0.59
1:A:18:LYS:HD2	1:A:18:LYS:N	2.18	0.59
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.85	0.59
7:G:52:THR:HG22	7:G:56:GLN:HE21	1.68	0.59
2:B:146:LEU:CD1	2:B:169:VAL:HB	2.33	0.58
3:C:92:ILE:HD12	3:C:92:ILE:H	1.68	0.58
5:E:113:LEU:HD11	5:E:169:MET:HE3	1.85	0.58
1:A:206:GLN:NE2	1:A:209:ARG:HH11	2.00	0.58
4:D:189:ARG:NH2	4:D:197:GLN:HE21	2.00	0.58
6:F:101:PHE:O	6:F:103:ILE:N	2.37	0.58
5:E:74:TYR:OH	5:E:98:LEU:HD12	2.04	0.58
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.39	0.58
5:E:75:ILE:HG23	5:E:144:LEU:HD11	1.86	0.58
1:A:343:VAL:CG1	1:A:363:ILE:HD12	2.33	0.58
2:B:23:ALA:C	2:B:25:SER:H	2.05	0.58
3:C:107:ASN:HD22	3:C:108:GLU:N	2.01	0.57
3:C:119:VAL:HG23	3:C:137:ILE:O	2.04	0.57
4:D:158:LYS:HG3	4:D:159:ASP:OD2	2.04	0.57
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.86	0.57
1:A:14:THR:HG23	1:A:79:ARG:C	2.24	0.57
4:D:223:ILE:HD12	4:D:223:ILE:N	2.20	0.57
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.35	0.57
1:A:206:GLN:NE2	1:A:209:ARG:NH1	2.52	0.56
1:A:262:ILE:HG22	1:A:262:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:220:ILE:N	4:D:220:ILE:HD12	2.20	0.56
7:G:120:ASN:ND2	7:G:123:ALA:HB2	2.20	0.56
6:F:145:GLU:O	6:F:149:MET:HG3	2.06	0.56
2:B:299:LYS:HG3	2:B:300:HIS:ND1	2.20	0.55
4:D:129:PHE:HD2	4:D:237:ARG:HG3	1.72	0.55
5:E:69:ILE:HG23	5:E:169:MET:HE1	1.88	0.55
1:A:335:LEU:HD12	1:A:367:VAL:HG21	1.87	0.55
2:B:227:ILE:O	2:B:231:GLN:HG3	2.07	0.55
1:A:117:LEU:HD21	1:A:190:ILE:HD12	1.88	0.55
6:F:4:THR:HG23	6:F:55:ARG:NH2	2.05	0.55
2:B:218:GLU:HG2	9:B:402:ADP:C5	2.42	0.55
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.87	0.55
5:E:95:MET:HA	5:E:95:MET:CE	2.36	0.55
4:D:141:ARG:HG2	4:D:141:ARG:HH11	1.71	0.55
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.89	0.55
1:A:78:ILE:HG22	1:A:78:ILE:O	2.06	0.55
3:C:284:ARG:NH2	3:C:322:ASP:OD2	2.40	0.55
4:D:189:ARG:HH12	4:D:197:GLN:NE2	2.05	0.55
5:E:88:LYS:O	5:E:92:GLU:HG3	2.06	0.55
1:A:14:THR:HG22	1:A:198:ARG:NH2	2.23	0.54
2:B:322:LYS:HB3	7:G:16:VAL:HG11	1.90	0.54
2:B:23:ALA:C	2:B:25:SER:N	2.60	0.54
3:C:14:HIS:N	3:C:331:GLN:HE22	1.97	0.54
5:E:86:ASN:C	5:E:154:ASP:HA	2.28	0.54
1:A:154:THR:HG21	1:A:372:MET:HG2	1.89	0.54
1:A:194:PRO:C	1:A:195:ILE:HD12	2.28	0.54
1:A:409:ARG:NH1	2:B:200:ARG:HD2	2.23	0.54
1:A:243:ASN:HD22	5:E:47:TYR:HE1	1.56	0.53
1:A:409:ARG:HH11	2:B:200:ARG:HD2	1.73	0.53
2:B:148:ALA:HB2	2:B:357:GLY:HA2	1.91	0.53
2:B:110:THR:HB	2:B:141:GLN:HG2	1.90	0.53
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.38	0.53
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.91	0.53
2:B:89:TRP:HB3	2:B:93:PHE:CE2	2.44	0.53
3:C:18:LYS:HE2	3:C:63:ASP:OD1	2.09	0.53
4:D:208:GLU:HG3	4:D:209:LEU:H	1.74	0.53
1:A:78:ILE:HD11	1:A:89:MET:SD	2.49	0.53
4:D:121:PHE:O	4:D:124:VAL:HG12	2.09	0.52
1:A:14:THR:HG23	1:A:79:ARG:CA	2.39	0.52
3:C:92:ILE:HD12	3:C:92:ILE:N	2.24	0.52
2:B:146:LEU:HD23	2:B:302:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:ASN:C	3:C:107:ASN:ND2	2.62	0.52
5:E:95:MET:HG2	5:E:141:GLY:O	2.10	0.52
2:B:146:LEU:HD11	2:B:169:VAL:HB	1.92	0.51
2:B:15:THR:HG21	2:B:162:GLY:HA3	1.91	0.51
7:G:56:GLN:O	7:G:60:LYS:HG3	2.11	0.51
2:B:22:TYR:O	2:B:25:SER:HB2	2.11	0.51
2:B:91:TYR:O	2:B:94:GLY:O	2.27	0.51
3:C:360:ARG:NH1	3:C:360:ARG:HB3	2.26	0.51
3:C:17:ASN:ND2	3:C:22:GLN:HB2	2.25	0.51
7:G:80:LEU:O	7:G:84:ILE:HD13	2.10	0.51
3:C:119:VAL:HG22	3:C:120:ILE:N	2.26	0.51
2:B:330:LEU:C	2:B:332:GLY:H	2.14	0.51
3:C:126:GLU:HG2	3:C:128:GLU:HG3	1.92	0.51
1:A:383:MET:O	1:A:387:THR:HG23	2.10	0.51
2:B:350:ARG:HA	2:B:353:MET:CE	2.41	0.51
4:D:171:ASP:HB3	4:D:174:ASP:HB2	1.92	0.51
1:A:71:THR:HG23	1:A:72:TYR:CE1	2.46	0.50
1:A:343:VAL:HG11	1:A:363:ILE:HB	1.92	0.50
2:B:200:ARG:HG3	2:B:200:ARG:HH11	1.76	0.50
4:D:71:GLY:HA2	4:D:74:GLU:OE1	2.11	0.50
1:A:370:HIS:O	1:A:373:GLN:HB2	2.12	0.50
2:B:165:HIS:HD2	2:B:181:ARG:HG2	1.70	0.50
1:A:82:ILE:HG13	1:A:83:VAL:N	2.27	0.50
2:B:194:ILE:HG13	2:B:213:VAL:HG11	1.93	0.50
2:B:318:GLU:HG3	2:B:344:ILE:HD12	1.93	0.50
2:B:170:TYR:OH	2:B:293:THR:HG21	2.12	0.50
5:E:16:ILE:HG23	5:E:16:ILE:O	2.12	0.50
7:G:38:ASP:O	7:G:42:VAL:HG23	2.11	0.50
1:A:82:ILE:HD12	1:A:83:VAL:H	1.77	0.49
2:B:319:ARG:O	2:B:323:GLN:HG3	2.12	0.49
4:D:228:PHE:H	4:D:231:HIS:CD2	2.23	0.49
1:A:410:HIS:O	1:A:412:PRO:HD3	2.12	0.49
7:G:68:SER:O	7:G:71:VAL:HG12	2.12	0.49
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.42	0.49
7:G:121:SER:O	7:G:124:VAL:HG12	2.12	0.49
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.94	0.49
1:A:69:LYS:HB3	1:A:72:TYR:HB2	1.95	0.49
5:E:69:ILE:CG2	5:E:169:MET:HE1	2.42	0.49
4:D:45:ILE:HA	4:D:56:MET:O	2.13	0.49
5:E:82:LEU:HD23	5:E:148:VAL:HG21	1.95	0.49
2:B:177:HIS:CD2	2:B:177:HIS:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASN:C	1:A:289:ASN:HD22	2.15	0.48
4:D:53:THR:O	4:D:54:LYS:HD2	2.13	0.48
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.48	0.48
3:C:371:ILE:O	3:C:372:VAL:HB	2.13	0.48
1:A:400:TYR:CE1	1:A:405:PRO:HB3	2.48	0.48
2:B:85:MET:HA	2:B:88:LEU:CB	2.43	0.48
2:B:289:ALA:O	2:B:290:ASP:O	2.30	0.48
5:E:153:ASN:O	5:E:155:LYS:HG3	2.14	0.48
7:G:62:PRO:C	7:G:64:ILE:H	2.17	0.48
1:A:385:ALA:HA	1:A:390:PHE:CG	2.49	0.48
6:F:13:ARG:NH1	6:F:133:ASP:OD1	2.36	0.48
3:C:131:TRP:N	3:C:131:TRP:HE3	2.12	0.48
4:D:263:HIS:O	4:D:267:ARG:HG3	2.14	0.48
1:A:400:TYR:HE1	1:A:405:PRO:HB3	1.79	0.48
2:B:191:ARG:HG3	2:B:191:ARG:HH11	1.79	0.48
5:E:126:ASP:OD2	5:E:130:ARG:HD2	2.13	0.48
1:A:14:THR:HG22	1:A:198:ARG:HH22	1.79	0.48
1:A:111:LEU:HD23	1:A:111:LEU:C	2.34	0.48
5:E:18:ASN:CG	5:E:118:ALA:H	2.18	0.47
2:B:89:TRP:HA	2:B:92:THR:OG1	2.14	0.47
3:C:10:PRO:HB3	3:C:350:MET:HA	1.96	0.47
4:D:68:GLN:HG3	4:D:73:ASP:OD2	2.14	0.47
2:B:182:LEU:HG	2:B:281:LEU:HD12	1.97	0.47
2:B:186:GLY:HA3	9:B:402:ADP:O3'	2.15	0.47
3:C:69:THR:O	3:C:76:ALA:HA	2.15	0.47
3:C:124:TYR:CD2	3:C:173:ILE:HG21	2.49	0.47
1:A:311:VAL:C	1:A:314:PRO:HD2	2.35	0.47
2:B:170:TYR:CB	2:B:175:LEU:HD21	2.45	0.47
4:D:231:HIS:HE1	10:D:350:HOH:O	1.96	0.47
1:A:239:VAL:HG11	5:E:48:TYR:HD1	1.80	0.47
3:C:60:TRP:HE1	3:C:65:ASN:ND2	2.13	0.47
3:C:225:THR:HG22	3:C:241:ALA:HA	1.97	0.47
4:D:208:GLU:CG	4:D:209:LEU:N	2.78	0.47
5:E:18:ASN:ND2	5:E:118:ALA:H	2.13	0.47
5:E:152:GLN:HA	5:E:152:GLN:OE1	2.15	0.47
1:A:4:ARG:HG3	1:A:5:LEU:HG	1.97	0.47
2:B:170:TYR:HB2	2:B:175:LEU:HD21	1.97	0.47
2:B:205:ASN:ND2	2:B:208:ALA:H	2.06	0.47
4:D:67:LEU:HD13	4:D:120:CYS:O	2.15	0.47
5:E:35:GLU:HG2	5:E:40:ASP:HB3	1.97	0.47
4:D:209:LEU:HD13	4:D:214:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:O	1:A:390:PHE:HB2	2.14	0.46
2:B:163:VAL:CG2	2:B:164:THR:N	2.79	0.46
2:B:170:TYR:O	2:B:171:GLU:C	2.54	0.46
1:A:71:THR:HG23	1:A:72:TYR:CD1	2.50	0.46
3:C:183:THR:HB	10:C:385:HOH:O	2.16	0.46
2:B:184:ILE:CD1	2:B:188:ASP:HB2	2.45	0.46
4:D:189:ARG:NH1	4:D:197:GLN:NE2	2.63	0.46
3:C:144:THR:H	6:F:28:GLN:HE21	1.62	0.46
4:D:223:ILE:HG21	4:D:247:PHE:CE2	2.51	0.46
2:B:169:VAL:HA	2:B:174:SER:HA	1.97	0.46
2:B:175:LEU:O	2:B:177:HIS:N	2.49	0.46
2:B:205:ASN:ND2	2:B:207:SER:H	2.14	0.46
3:C:178:GLU:O	3:C:179:ARG:C	2.53	0.46
5:E:50:LYS:NZ	5:E:159:TRP:O	2.49	0.46
1:A:406:SER:O	1:A:409:ARG:HG3	2.15	0.46
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.51	0.46
2:B:184:ILE:CG1	2:B:265:LEU:HD23	2.45	0.45
2:B:299:LYS:HG3	2:B:300:HIS:CE1	2.52	0.45
1:A:335:LEU:HD12	1:A:367:VAL:CG2	2.46	0.45
6:F:87:CYS:O	6:F:91:MET:HG2	2.16	0.45
2:B:200:ARG:NH1	2:B:257:GLU:OE1	2.49	0.45
2:B:322:LYS:HG2	2:B:342:ILE:HD12	1.98	0.45
3:C:234:LYS:O	3:C:235:MET:HB2	2.16	0.45
7:G:57:ALA:HA	7:G:60:LYS:CD	2.47	0.45
1:A:69:LYS:HD2	1:A:72:TYR:CD1	2.51	0.45
3:C:183:THR:CG2	3:C:185:TRP:H	2.15	0.45
3:C:201:SER:O	7:G:148:ARG:HG3	2.16	0.45
5:E:150:ASP:C	5:E:152:GLN:N	2.69	0.45
1:A:361:LYS:HG3	1:A:362:PRO:HD2	1.98	0.45
2:B:305:GLY:O	2:B:309:MET:HE3	2.15	0.45
2:B:347:PRO:O	2:B:350:ARG:HG2	2.17	0.45
4:D:75:LEU:HD23	4:D:75:LEU:C	2.37	0.45
1:A:340:LYS:HE3	1:A:344:ASP:OD2	2.17	0.45
3:C:319:ALA:N	6:F:129:HIS:HE2	2.15	0.45
1:A:328:PHE:CZ	9:A:501:ADP:H2	2.35	0.45
1:A:359:LYS:O	1:A:359:LYS:HG2	2.17	0.45
4:D:118:ARG:HD3	4:D:118:ARG:C	2.38	0.45
1:A:128:GLU:O	1:A:132:GLU:HB2	2.18	0.44
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.52	0.44
2:B:347:PRO:HB2	2:B:353:MET:HE1	1.98	0.44
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:ALA:C	3:C:366:LEU:HD12	2.37	0.44
5:E:18:ASN:ND2	5:E:118:ALA:N	2.65	0.44
6:F:53:ILE:N	6:F:53:ILE:HD12	2.32	0.44
2:B:152:LEU:HB3	2:B:171:GLU:HA	1.99	0.44
7:G:68:SER:CB	7:G:71:VAL:HG12	2.47	0.44
7:G:52:THR:HG22	7:G:56:GLN:NE2	2.32	0.44
1:A:289:ASN:ND2	1:A:291:ASP:H	2.15	0.44
1:A:329:ARG:O	1:A:330:ASP:HB2	2.17	0.44
2:B:24:GLY:O	2:B:25:SER:O	2.35	0.44
4:D:248:ARG:HD3	4:D:248:ARG:C	2.37	0.44
5:E:113:LEU:HD21	5:E:171:LYS:HG3	1.99	0.44
3:C:16:TRP:CZ2	3:C:23:ILE:HD12	2.53	0.44
3:C:34:ILE:HB	3:C:46:HIS:HB2	2.00	0.44
4:D:61:LEU:N	4:D:61:LEU:HD12	2.32	0.44
3:C:33:HIS:HD2	10:C:374:HOH:O	2.00	0.44
4:D:203:ARG:HG3	4:D:217:GLY:C	2.38	0.44
5:E:18:ASN:ND2	5:E:118:ALA:HB2	2.33	0.44
7:G:87:LYS:O	7:G:88:ALA:C	2.55	0.44
5:E:20:ALA:HB3	5:E:22:LEU:CD2	2.48	0.44
1:A:395:HIS:ND1	1:A:395:HIS:N	2.62	0.43
2:B:166:ILE:HD12	2:B:281:LEU:HD13	2.00	0.43
2:B:347:PRO:HA	2:B:348:PRO:HD3	1.91	0.43
3:C:3:TYR:HB2	3:C:324:LEU:HG	1.99	0.43
3:C:19:ASP:OD1	3:C:21:THR:HG23	2.19	0.43
3:C:131:TRP:HE3	3:C:131:TRP:H	1.65	0.43
1:A:409:ARG:HH11	2:B:200:ARG:CD	2.31	0.43
3:C:183:THR:HG23	3:C:184:PRO:CD	2.45	0.43
4:D:171:ASP:O	4:D:174:ASP:HB2	2.17	0.43
5:E:74:TYR:CE1	5:E:98:LEU:HD12	2.54	0.43
5:E:96:TYR:O	5:E:100:ILE:HG12	2.18	0.43
1:A:239:VAL:HG23	1:A:240:LYS:N	2.33	0.43
2:B:88:LEU:O	2:B:92:THR:OG1	2.36	0.43
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.49	0.43
7:G:57:ALA:HA	7:G:60:LYS:HD3	1.99	0.43
2:B:166:ILE:O	2:B:168:PRO:HD3	2.18	0.43
1:A:19:LEU:HG	1:A:29:PHE:HB2	2.00	0.43
2:B:175:LEU:HB3	2:B:177:HIS:CD2	2.53	0.43
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.53	0.43
2:B:217:LYS:O	2:B:221:CYS:HB2	2.19	0.43
1:A:317:LYS:HE3	1:A:364:ASP:OD1	2.18	0.43
3:C:332:ILE:HA	3:C:346:CYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:119:ASP:O	7:G:120:ASN:HB3	2.18	0.43
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.75	0.43
2:B:29:GLU:OE1	2:B:30:HIS:CE1	2.72	0.42
3:C:183:THR:HG22	3:C:185:TRP:N	2.12	0.42
5:E:74:TYR:CZ	5:E:98:LEU:HD12	2.54	0.42
7:G:68:SER:HB3	7:G:71:VAL:CG1	2.50	0.42
2:B:180:ARG:HD3	2:B:281:LEU:HD21	2.02	0.42
4:D:59:ILE:HB	4:D:116:LEU:HD13	2.00	0.42
5:E:86:ASN:O	5:E:87:SER:HB3	2.19	0.42
1:A:374:ARG:HG3	1:A:375:TYR:CE2	2.54	0.42
3:C:253:ILE:HD13	3:C:259:VAL:CG2	2.50	0.42
2:B:308:THR:HA	2:B:313:LEU:HD23	2.01	0.42
2:B:346:ASP:OD2	3:C:74:ARG:NH1	2.45	0.42
2:B:347:PRO:HB2	2:B:353:MET:CE	2.49	0.42
1:A:129:ILE:O	1:A:133:SER:HB2	2.20	0.42
1:A:289:ASN:HD22	1:A:290:PRO:N	2.17	0.42
4:D:158:LYS:O	4:D:158:LYS:HD3	2.19	0.42
5:E:166:ARG:HG2	5:E:166:ARG:HH11	1.84	0.42
1:A:372:MET:HE2	1:A:379:PHE:CD1	2.54	0.42
3:C:102:VAL:HA	3:C:112:ALA:O	2.20	0.42
3:C:201:SER:OG	7:G:27:GLU:HB2	2.20	0.42
3:C:366:LEU:HD12	3:C:366:LEU:N	2.34	0.42
3:C:151:HIS:CG	3:C:152:PRO:HD2	2.55	0.42
3:C:327:ASN:HB2	3:C:351:ASP:HB3	2.02	0.42
3:C:170:SER:HB2	3:C:195:MET:CE	2.50	0.41
3:C:341:LYS:HG3	3:C:341:LYS:O	2.19	0.41
2:B:19:LYS:HD3	2:B:19:LYS:N	2.36	0.41
2:B:84:ASP:O	2:B:87:HIS:HB2	2.20	0.41
3:C:179:ARG:HA	3:C:180:PRO:HD3	1.90	0.41
3:C:228:LEU:C	3:C:228:LEU:HD23	2.41	0.41
5:E:91:GLY:O	5:E:95:MET:HB2	2.21	0.41
1:A:158:VAL:HG21	10:A:551:HOH:O	2.20	0.41
3:C:27:PRO:HG2	3:C:29:ASN:OD1	2.21	0.41
3:C:139:LYS:HA	3:C:140:PRO:HA	1.87	0.41
2:B:94:GLY:O	2:B:95:PRO:C	2.59	0.41
3:C:253:ILE:HD13	3:C:259:VAL:HG23	2.02	0.41
5:E:18:ASN:HD21	5:E:118:ALA:N	2.19	0.41
1:A:82:ILE:CG1	1:A:83:VAL:N	2.83	0.41
2:B:156:VAL:HG22	2:B:302:VAL:HG13	2.02	0.41
3:C:119:VAL:HG21	3:C:136:HIS:HB3	2.03	0.41
5:E:150:ASP:O	5:E:152:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:LEU:C	2:B:177:HIS:H	2.24	0.41
2:B:330:LEU:O	2:B:332:GLY:N	2.53	0.41
3:C:29:ASN:O	3:C:54:GLN:HA	2.20	0.41
5:E:58:TYR:CD2	5:E:69:ILE:HD11	2.56	0.41
1:A:91:ARG:O	1:A:94:GLU:HB2	2.20	0.41
2:B:246:LEU:HB3	2:B:247:PRO:HD2	2.03	0.41
3:C:37:LYS:HD3	3:C:42:TRP:CZ2	2.56	0.41
3:C:48:LEU:HD12	3:C:48:LEU:N	2.35	0.41
3:C:73:ASP:O	3:C:74:ARG:HB2	2.21	0.41
4:D:150:GLU:CG	4:D:167:THR:HA	2.48	0.41
4:D:243:LEU:HD11	6:F:167:ASN:HB3	2.03	0.41
5:E:14:LYS:O	5:E:15:LEU:HD23	2.21	0.41
5:E:138:GLN:OE1	5:E:138:GLN:HA	2.20	0.41
4:D:77:LYS:HD2	4:D:77:LYS:HA	1.86	0.41
5:E:105:ILE:HB	5:E:106:PRO:HD2	2.03	0.41
1:A:10:VAL:HB	1:A:112:LEU:CD2	2.50	0.40
1:A:407:ILE:HG13	1:A:408:CYS:N	2.35	0.40
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.48	0.40
4:D:64:TYR:CD2	4:D:92:ASN:HB3	2.55	0.40
4:D:203:ARG:O	4:D:203:ARG:HG2	2.20	0.40
2:B:293:THR:O	2:B:296:GLU:HB3	2.21	0.40
6:F:6:ARG:HB3	6:F:7:PRO:HD3	2.03	0.40
4:D:164:VAL:HG11	4:D:206:PRO:HG3	2.02	0.40
1:A:72:TYR:CD1	1:A:72:TYR:N	2.90	0.40
4:D:65:LYS:HD3	4:D:65:LYS:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	387/418 (93%)	367 (95%)	17 (4%)	3 (1%)	19 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	264/394 (67%)	237 (90%)	18 (7%)	9 (3%)	3 1
3	C	337/372 (91%)	321 (95%)	14 (4%)	2 (1%)	25 29
4	D	276/300 (92%)	265 (96%)	9 (3%)	2 (1%)	22 25
5	E	172/178 (97%)	166 (96%)	3 (2%)	3 (2%)	9 7
6	F	165/168 (98%)	157 (95%)	7 (4%)	1 (1%)	25 29
7	G	133/151 (88%)	122 (92%)	7 (5%)	4 (3%)	4 1
All	All	1734/1981 (88%)	1635 (94%)	75 (4%)	24 (1%)	11 9

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	SER
2	B	25	SER
2	B	290	ASP
5	E	153	ASN
6	F	102	PHE
2	B	171	GLU
5	E	37	LYS
7	G	23	LYS
7	G	88	ALA
2	B	176	PRO
2	B	179	THR
4	D	237	ARG
5	E	87	SER
2	B	26	ASN
2	B	113	PRO
4	D	206	PRO
7	G	22	ASN
2	B	331	LYS
3	C	179	ARG
1	A	262	ILE
3	C	62	PRO
7	G	63	PRO
1	A	194	PRO
2	B	16	GLY

5.3.2 Protein sidechains (i)

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	344/363 (95%)	333 (97%)	11 (3%)	39	50
2	B	198/345 (57%)	185 (93%)	13 (7%)	16	20
3	C	289/313 (92%)	282 (98%)	7 (2%)	49	61
4	D	246/264 (93%)	241 (98%)	5 (2%)	55	67
5	E	156/159 (98%)	148 (95%)	8 (5%)	24	31
6	F	154/155 (99%)	150 (97%)	4 (3%)	46	58
7	G	113/124 (91%)	108 (96%)	5 (4%)	28	37
All	All	1500/1723 (87%)	1447 (96%)	53 (4%)	36	47

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	19	LEU
1	A	71	THR
1	A	79	ARG
1	A	88	LEU
1	A	143	VAL
1	A	230	ARG
1	A	255	GLN
1	A	289	ASN
1	A	374	ARG
1	A	395	HIS
2	B	29	GLU
2	B	92	THR
2	B	95	PRO
2	B	177	HIS
2	B	182	LEU
2	B	183	ASP
2	B	184	ILE
2	B	200	ARG
2	B	220	LEU
2	B	240	LEU
2	B	257	GLU
2	B	281	LEU
2	B	303	LEU

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Mol	Chain	Res	Type
3	C	30	HIS
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	183	THR
3	C	284	ARG
3	C	367	LYS
4	D	37	ASP
4	D	116	LEU
4	D	172	ASP
4	D	208	GLU
4	D	245	HIS
5	E	10	ASP
5	E	22	LEU
5	E	82	LEU
5	E	95	MET
5	E	98	LEU
5	E	101	THR
5	E	102	ASN
5	E	146	GLU
6	F	101	PHE
6	F	102	PHE
6	F	104	LEU
6	F	165	LEU
7	G	18	GLU
7	G	21	GLU
7	G	39	GLU
7	G	47	ARG
7	G	73	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	206	GLN
1	A	255	GLN
1	A	289	ASN
1	A	305	GLN
1	A	318	ASN
2	B	30	HIS
2	B	87	HIS
2	B	177	HIS

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Mol	Chain	Res	Type
2	B	205	ASN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	33	HIS
3	C	44	GLN
3	C	46	HIS
3	C	65	ASN
3	C	107	ASN
3	C	331	GLN
4	D	140	ASN
4	D	197	GLN
4	D	202	HIS
4	D	231	HIS
5	E	83	GLN
5	E	102	ASN
5	E	134	GLN
6	F	28	GLN
6	F	125	GLN
6	F	154	ASN
7	G	56	GLN
7	G	69	GLN
7	G	96	GLN
7	G	120	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	ADP	A	501	8	24,29,29	1.35	3 (12%)	29,45,45	1.56	4 (13%)
9	ADP	B	402	8	24,29,29	1.37	3 (12%)	29,45,45	1.47	3 (10%)

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	501	8	-	0/12/32/32	0/3/3/3
9	ADP	B	402	8	-	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	402	ADP	C2-N1	3.58	1.40	1.33
9	A	501	ADP	C2-N1	3.55	1.40	1.33
9	B	402	ADP	PB-O1B	3.40	1.61	1.50
9	A	501	ADP	PB-O1B	3.36	1.61	1.50
9	B	402	ADP	O4'-C1'	2.17	1.44	1.41
9	A	501	ADP	O4'-C1'	2.05	1.43	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	501	ADP	N3-C2-N1	-5.45	120.17	128.68
9	B	402	ADP	N3-C2-N1	-5.44	120.17	128.68
9	B	402	ADP	PA-O3A-PB	-2.98	122.59	132.83
9	A	501	ADP	PA-O3A-PB	-2.97	122.64	132.83
9	A	501	ADP	O4'-C1'-C2'	-2.93	102.65	106.93
9	A	501	ADP	O3B-PB-O3A	2.38	112.61	104.64
9	B	402	ADP	O3B-PB-O3A	2.30	112.36	104.64

There are no chirality outliers.

There are no torsion outliers.

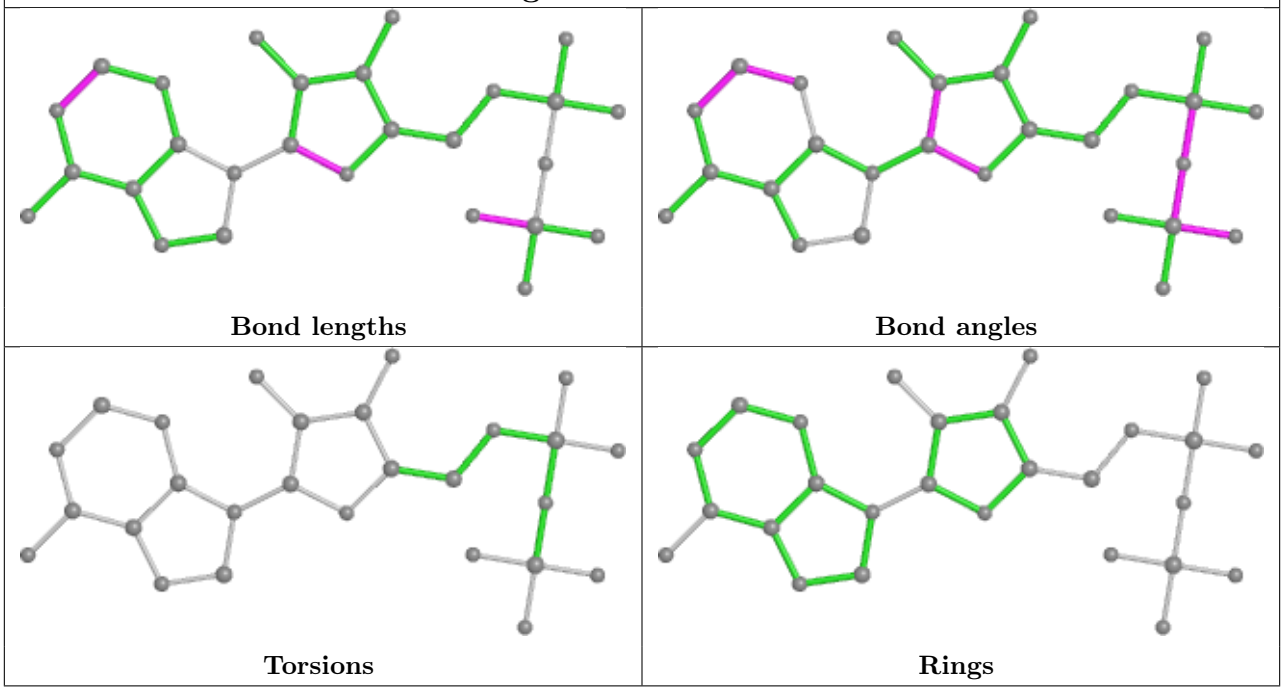
There are no ring outliers.

2 monomers are involved in 3 short contacts:

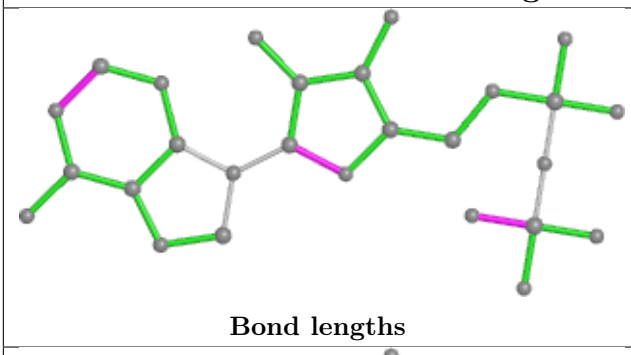
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	501	ADP	1	0
9	B	402	ADP	2	0

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 then 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.

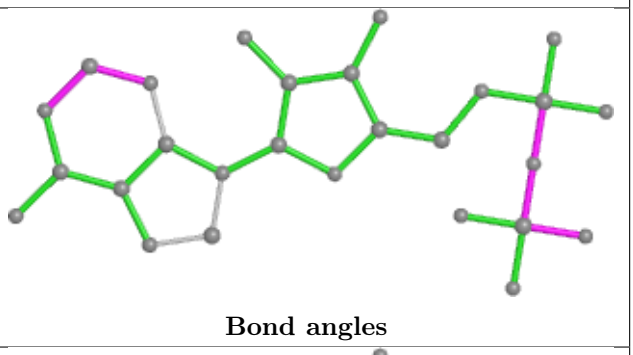
Ligand ADP A 501



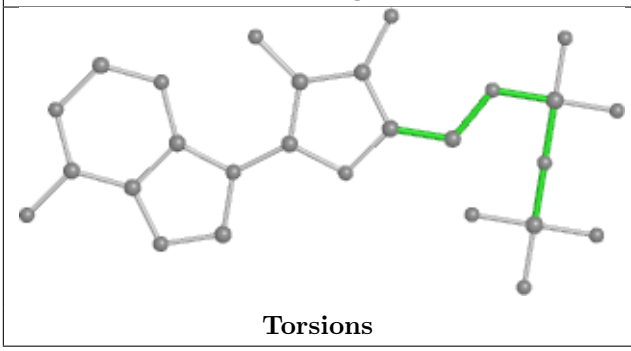
Ligand ADP B 402



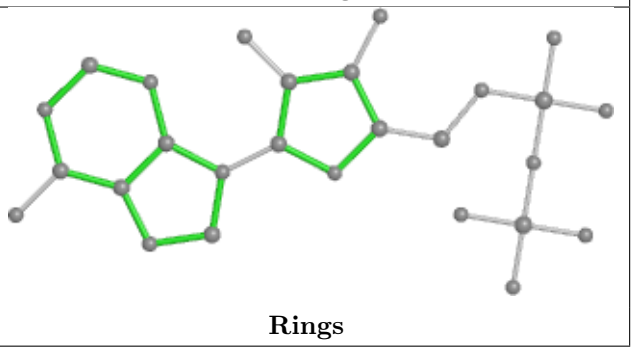
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	393/418 (94%)	0.12	27 (6%)	16	13	20, 42, 93, 118	0
2	B	272/394 (69%)	0.28	26 (9%)	8	5	24, 61, 95, 104	0
3	C	341/372 (91%)	-0.08	14 (4%)	37	34	25, 39, 82, 104	0
4	D	280/300 (93%)	-0.11	6 (2%)	63	60	22, 40, 73, 95	0
5	E	174/178 (97%)	-0.20	7 (4%)	38	35	32, 48, 73, 94	0
6	F	167/168 (99%)	-0.29	2 (1%)	79	77	22, 32, 50, 88	0
7	G	137/151 (90%)	0.22	9 (6%)	18	14	27, 62, 88, 96	0
All	All	1764/1981 (89%)	0.01	91 (5%)	27	24	20, 43, 89, 118	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ARG	7.8
1	A	157	GLN	6.7
4	D	215	ALA	6.3
1	A	408	CYS	6.2
1	A	403	ILE	5.4
2	B	91	TYR	5.4
3	C	368	ASP	4.7
6	F	3	ALA	4.5
4	D	283	ASP	4.5
2	B	93	PHE	4.5
1	A	407	ILE	4.3
7	G	9	ALA	4.2
1	A	353	LEU	4.2
3	C	367	LYS	4.2
2	B	174	SER	4.2
2	B	288	ALA	4.1
2	B	173	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
3	C	369	LEU	3.8
2	B	22	TYR	3.8
7	G	13	LYS	3.7
1	A	352	GLU	3.7
1	A	348	LYS	3.7
2	B	87	HIS	3.7
1	A	409	ARG	3.6
5	E	154	ASP	3.6
7	G	48	GLN	3.6
1	A	161	ARG	3.5
6	F	2	THR	3.4
2	B	23	ALA	3.4
1	A	262	ILE	3.3
2	B	89	TRP	3.3
1	A	359	LYS	3.3
2	B	26	ASN	3.2
3	C	201	SER	3.2
2	B	342	ILE	3.2
3	C	319	ALA	3.2
2	B	94	GLY	3.1
1	A	399	ASP	3.1
3	C	321	LEU	3.0
7	G	67	LYS	3.0
4	D	282	PRO	2.9
4	D	216	VAL	2.9
2	B	24	GLY	2.9
3	C	84	ARG	2.9
1	A	158	VAL	2.9
5	E	93	LYS	2.9
3	C	364	SER	2.8
1	A	393	VAL	2.8
7	G	50	ASN	2.8
3	C	365	ALA	2.7
2	B	274	GLU	2.7
2	B	25	SER	2.7
2	B	92	THR	2.7
1	A	347	LEU	2.6
1	A	404	GLY	2.6
2	B	293	THR	2.6
2	B	84	ASP	2.6
1	A	394	CYS	2.6
1	A	259	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	39	GLU	2.5
2	B	170	TYR	2.5
1	A	362	PRO	2.5
1	A	411	ASN	2.4
7	G	10	ARG	2.4
3	C	248	LEU	2.3
3	C	127	GLN	2.3
1	A	97	ILE	2.3
1	A	351	GLU	2.3
2	B	175	LEU	2.3
1	A	410	HIS	2.3
4	D	203	ARG	2.3
5	E	153	ASN	2.2
1	A	389	GLU	2.2
2	B	180	ARG	2.2
3	C	128	GLU	2.2
5	E	25	ARG	2.2
2	B	171	GLU	2.2
5	E	151	PRO	2.2
7	G	19	TYR	2.2
5	E	38	ASP	2.2
2	B	90	ASP	2.1
5	E	86	ASN	2.1
2	B	176	PRO	2.1
2	B	181	ARG	2.1
7	G	120	ASN	2.1
2	B	289	ALA	2.1
3	C	370	LYS	2.1
1	A	266	GLU	2.1
7	G	35	ALA	2.0
3	C	372	VAL	2.0
4	D	130	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

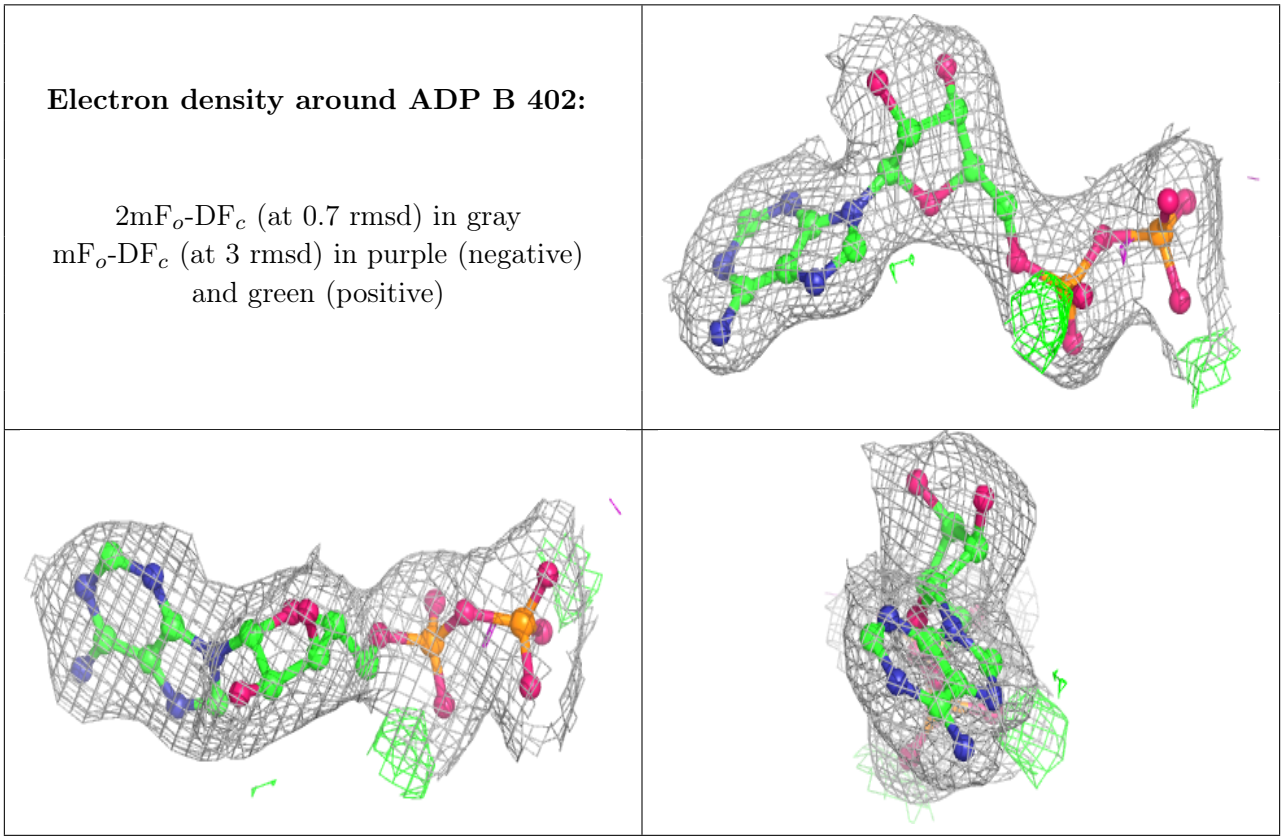
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	CA	B	501	1/1	0.90	0.30	78,78,78,78	0
9	ADP	B	402	27/27	0.97	0.12	29,41,46,48	0
9	ADP	A	501	27/27	0.98	0.14	33,36,40,40	0
8	CA	A	500	1/1	0.98	0.23	43,43,43,43	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.

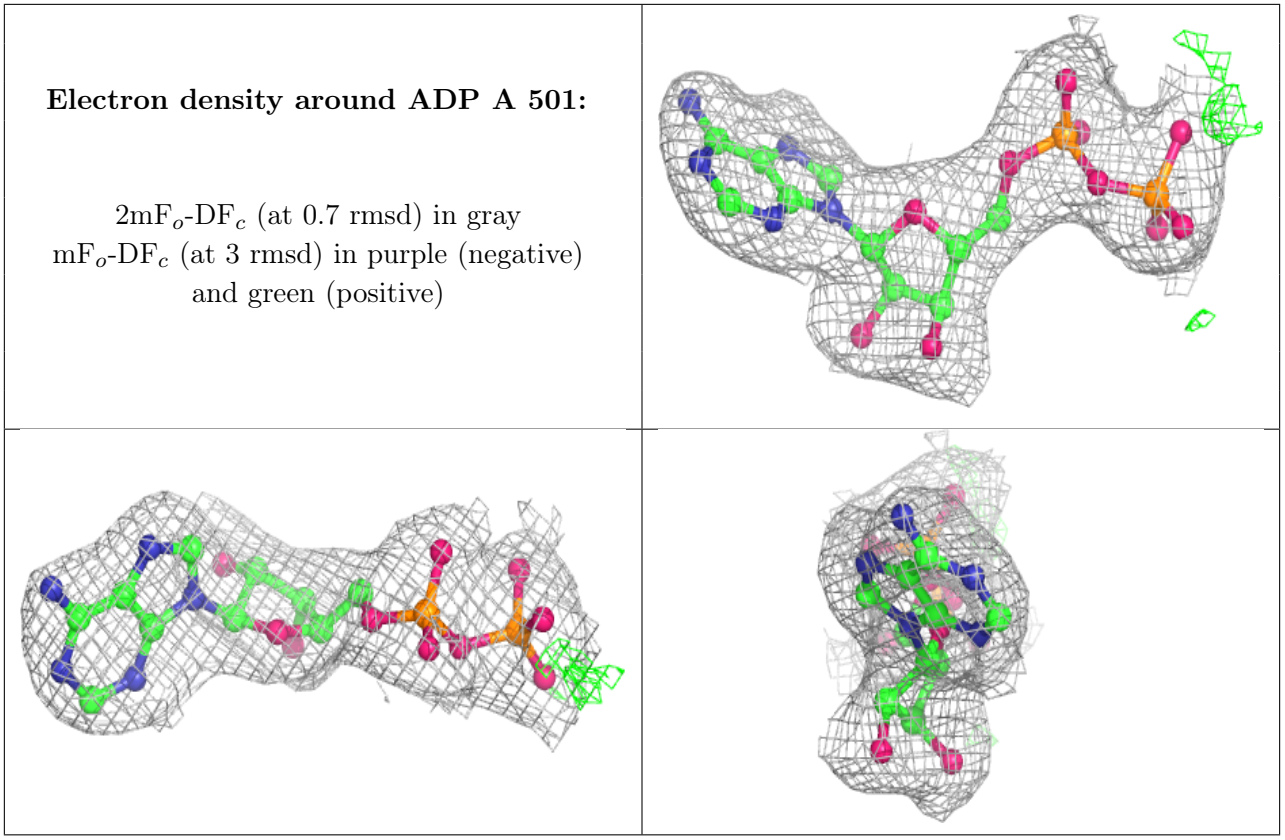
Electron density around ADP B 402:

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



Electron density around ADP A 501:

$2mF_o$-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.