



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:54 pm BST

PDB ID : 2P9K
Title : Crystal structure of bovine Arp2/3 complex co-crystallized with ATP and crosslinked with glutaraldehyde
Authors : Nolen, B.J.; Pollard, T.D.
Deposited on : 2007-03-26
Resolution : 2.59 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 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

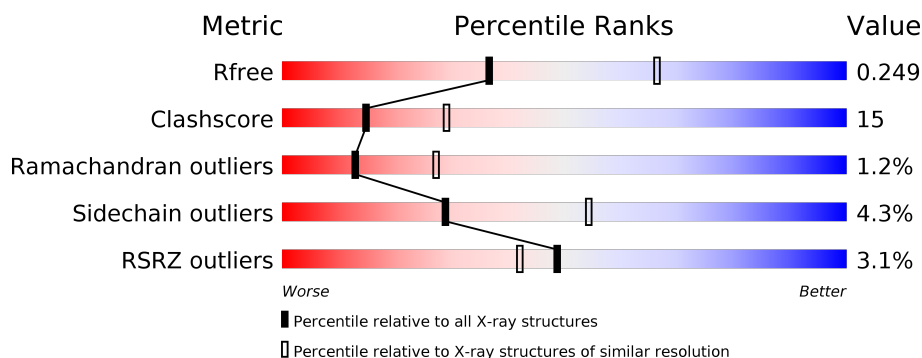
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 ≥ 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>3%</div> <div> <div></div> <div>67%</div> <div>23%</div> <div>• 6%</div> </div> </div>
2	B	394	<div> <div>5%</div> <div> <div></div> <div>47%</div> <div>20%</div> <div>• 30%</div> </div> </div>
3	C	372	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>• 8%</div> </div> </div>
4	D	300	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 8%</div> </div> </div>
5	E	178	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>
6	F	168	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	G	151	<div><div></div><div>6%</div><div>70%</div><div>19%</div><div>• 10%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14360 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
			3150	2023	524	588	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	275	Total	C	N	O	S	0	0	0
			2039	1299	356	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
			2648	1680	464	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	277	Total	C	N	O	S	0	0	0
			2237	1422	389	418	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	136	Total	C	N	O	S	0	0	0
			1040	651	182	204	3			

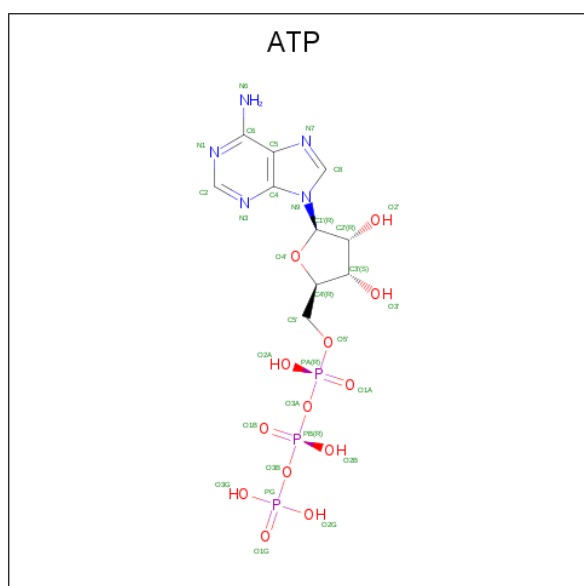
There are 2 discrepancies between the modelled and reference sequences:

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	B	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

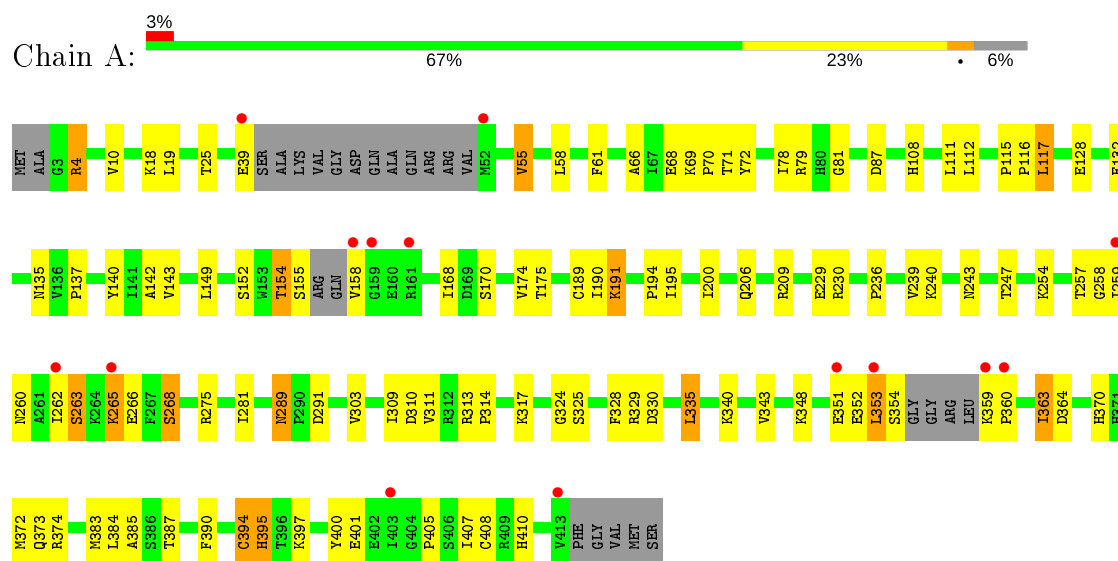
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	75	Total	O	0	0
			75	75		
10	B	38	Total	O	0	0
			38	38		
10	C	88	Total	O	0	0
			88	88		
10	D	87	Total	O	0	0
			87	87		
10	E	30	Total	O	0	0
			30	30		
10	F	59	Total	O	0	0
			59	59		
10	G	19	Total	O	0	0
			19	19		

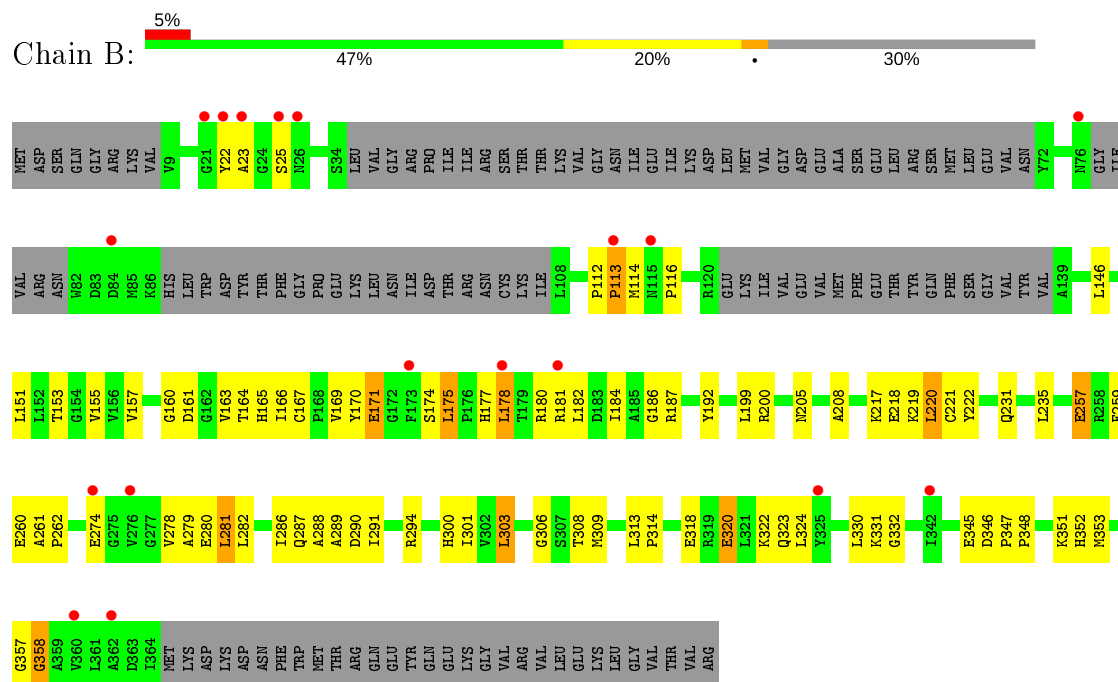
3 Residue-property plots

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.

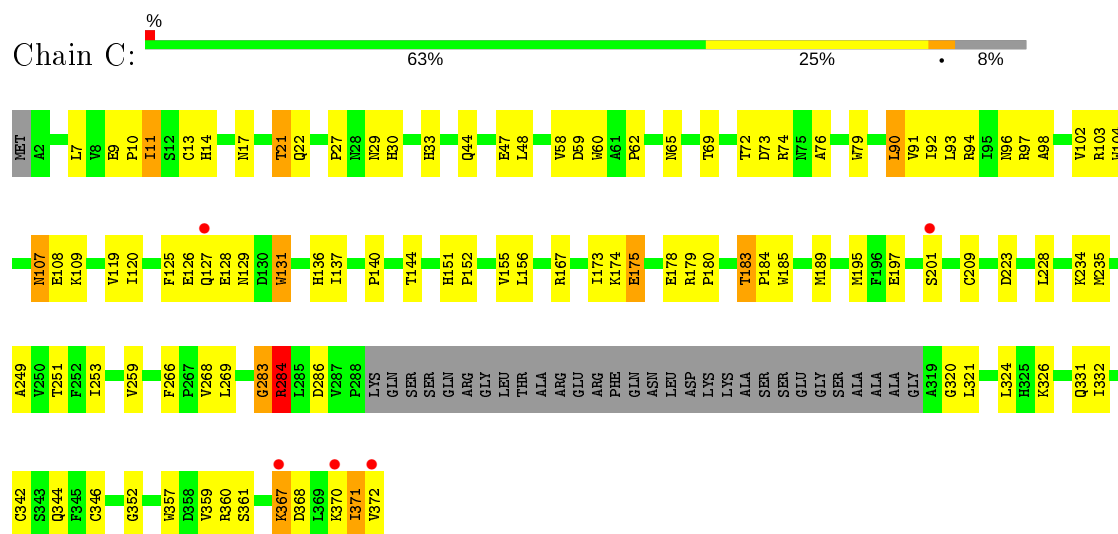
• Molecule 1: Actin-like protein 3



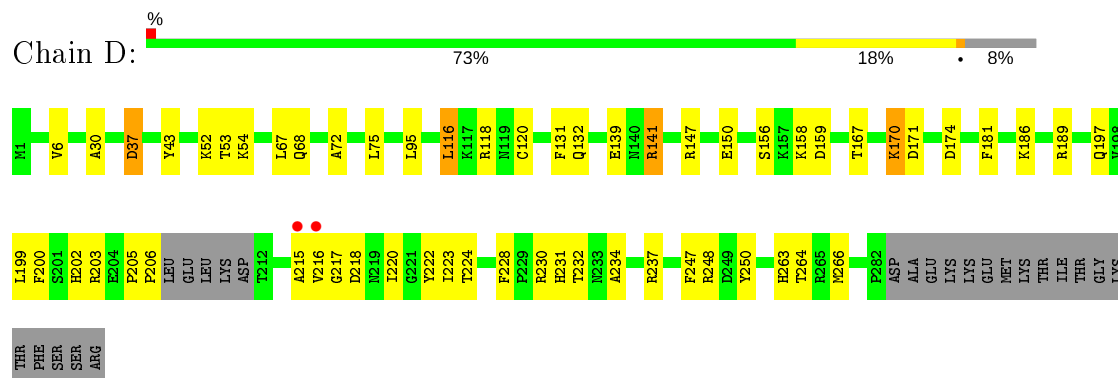
• Molecule 2: Actin-like protein 2



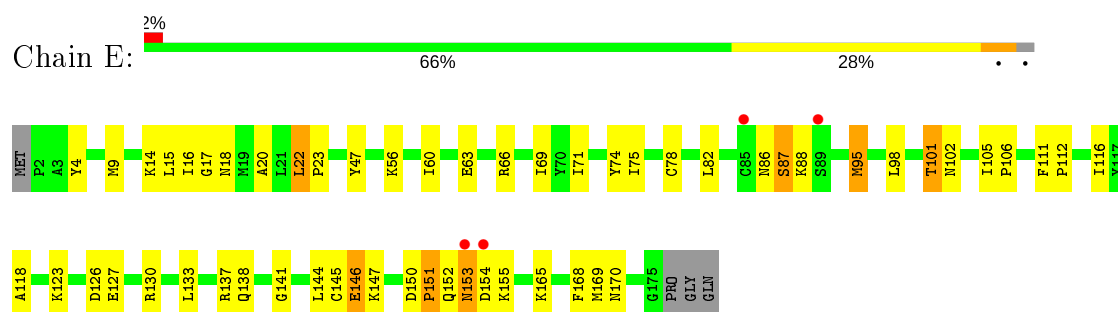
- Molecule 3: Actin-related protein 2/3 complex subunit 1B



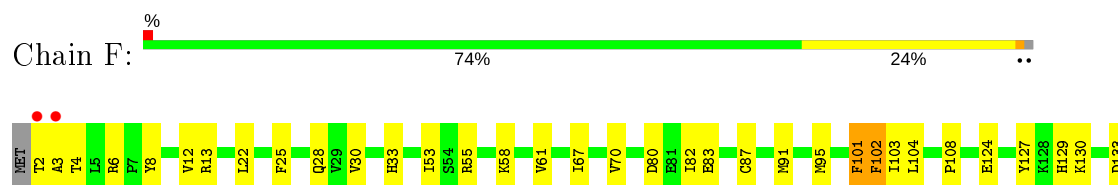
- Molecule 4: Actin-related protein 2/3 complex subunit 2



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

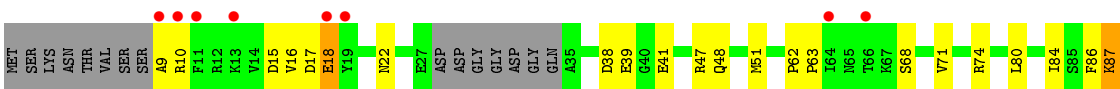


- Molecule 6: Actin-related protein 2/3 complex subunit 4





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.62Å 128.05Å 198.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 45.24 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.59) 96.1 (45.24-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.260 0.211 , 0.249	Depositor DCC
R_{free} test set	4422 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14360	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: CA, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/3229	0.61	0/4380
2	B	0.34	0/2078	0.61	1/2822 (0.0%)
3	C	0.38	0/2717	0.68	2/3688 (0.1%)
4	D	0.37	0/2285	0.60	0/3084
5	E	0.35	0/1449	0.62	1/1954 (0.1%)
6	F	0.40	0/1393	0.61	0/1868
7	G	0.47	1/1052 (0.1%)	0.63	0/1415
All	All	0.38	1/14203 (0.0%)	0.63	4/19211 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	9	ALA	CA-CB	5.27	1.63	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	PRO	N-CA-CB	5.89	110.36	103.30
3	C	283	GLY	N-CA-C	5.73	127.42	113.10
3	C	11	ILE	N-CA-C	-5.46	96.25	111.00
5	E	17	GLY	N-CA-C	-5.02	100.54	113.10

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	3150	0	3097	98	0
2	B	2039	0	1915	79	0
3	C	2648	0	2602	99	0
4	D	2237	0	2202	47	0
5	E	1415	0	1416	61	0
6	F	1371	0	1410	30	0
7	G	1040	0	1054	24	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	31	0	12	3	0
9	B	31	0	12	3	0
10	A	75	0	0	4	0
10	B	38	0	0	1	0
10	C	88	0	0	2	0
10	D	87	0	0	2	0
10	E	30	0	0	1	0
10	F	59	0	0	0	0
10	G	19	0	0	0	0
All	All	14360	0	13720	422	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 15.

All (422) 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)
1:A:257:THR:HG22	1:A:268:SER:HB3	1.18	1.16
3:C:223:ASP:HB3	7:G:146:THR:HG21	1.34	1.08
6:F:4:THR:HG23	6:F:55:ARG:HE	1.25	1.02
2:B:205:ASN:HD22	2:B:208:ALA:H	1.02	0.92
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.49	0.92
1:A:206:GLN:HE22	1:A:209:ARG:NH1	1.67	0.91
4:D:234:ALA:HA	4:D:237:ARG:HD3	1.54	0.89
4:D:186:LYS:HZ3	4:D:200:PHE:H	1.19	0.88
3:C:107:ASN:HD22	3:C:107:ASN:C	1.76	0.87
3:C:183:THR:HG22	3:C:185:TRP:H	1.40	0.86
2:B:205:ASN:ND2	2:B:208:ALA:H	1.72	0.86
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.57	0.86
4:D:186:LYS:NZ	4:D:200:PHE:H	1.73	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:HIS:O	2:B:178:LEU:HB2	1.77	0.83
1:A:259:ILE:HD11	1:A:266:GLU:HG3	1.62	0.81
2:B:165:HIS:CD2	2:B:181:ARG:HG2	2.15	0.81
3:C:107:ASN:ND2	3:C:109:LYS:H	1.79	0.81
3:C:14:HIS:H	3:C:331:GLN:HE22	1.29	0.81
5:E:152:GLN:HB3	5:E:155:LYS:NZ	1.96	0.81
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.62	0.80
4:D:170:LYS:HE2	4:D:170:LYS:HA	1.63	0.80
5:E:126:ASP:O	5:E:130:ARG:HG3	1.83	0.79
2:B:22:TYR:O	2:B:25:SER:HB3	1.82	0.78
2:B:309:MET:HE3	2:B:351:LYS:HB2	1.66	0.77
1:A:343:VAL:HG11	1:A:363:ILE:HG13	1.67	0.77
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.49	0.76
2:B:351:LYS:HE3	2:B:352:HIS:NE2	2.00	0.76
1:A:116:PRO:O	1:A:117:LEU:HB2	1.85	0.76
6:F:130:LYS:HE2	6:F:130:LYS:HA	1.67	0.75
2:B:23:ALA:C	2:B:25:SER:H	1.88	0.75
3:C:179:ARG:HH11	3:C:179:ARG:HG3	1.53	0.74
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.71	0.73
3:C:223:ASP:CB	7:G:146:THR:HG21	2.17	0.73
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.18	0.73
1:A:206:GLN:HE22	1:A:209:ARG:HH11	1.36	0.73
1:A:410:HIS:HB2	2:B:199:LEU:O	1.90	0.72
6:F:4:THR:HG23	6:F:55:ARG:NE	2.03	0.72
1:A:194:PRO:O	1:A:195:ILE:HD12	1.90	0.71
1:A:4:ARG:HB2	1:A:4:ARG:HH11	1.56	0.71
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.73	0.71
3:C:17:ASN:HD21	3:C:21:THR:HG22	1.56	0.70
2:B:205:ASN:HD22	2:B:208:ALA:N	1.85	0.70
7:G:118:SER:O	7:G:120:ASN:N	2.25	0.69
5:E:98:LEU:O	5:E:101:THR:HG23	1.92	0.69
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.28	0.69
3:C:183:THR:CG2	3:C:185:TRP:H	2.05	0.68
5:E:152:GLN:HB3	5:E:155:LYS:HZ1	1.56	0.68
2:B:178:LEU:HD21	2:B:288:ALA:O	1.93	0.68
4:D:150:GLU:HG2	4:D:167:THR:HA	1.76	0.68
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.75	0.68
4:D:228:PHE:H	4:D:231:HIS:HD2	1.42	0.68
3:C:370:LYS:H	3:C:370:LYS:HE2	1.57	0.68
4:D:263:HIS:HD2	4:D:266:MET:CE	2.07	0.68
3:C:321:LEU:HD21	6:F:129:HIS:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:O	1:A:79:ARG:HD2	1.94	0.67
3:C:107:ASN:C	3:C:107:ASN:ND2	2.48	0.67
5:E:86:ASN:HB3	5:E:154:ASP:OD2	1.95	0.67
7:G:15:ASP:O	7:G:18:GLU:HB2	1.95	0.66
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.77	0.66
2:B:314:PRO:O	2:B:318:GLU:HG3	1.95	0.66
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.31	0.66
3:C:107:ASN:HD22	3:C:108:GLU:N	1.93	0.65
1:A:259:ILE:CD1	1:A:266:GLU:HG3	2.28	0.64
1:A:262:ILE:HG22	1:A:262:ILE:O	1.98	0.63
1:A:353:LEU:HD13	1:A:353:LEU:O	1.99	0.63
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.28	0.63
2:B:257:GLU:HA	2:B:260:GLU:HB2	1.80	0.63
2:B:291:ILE:HA	2:B:294:ARG:HD3	1.79	0.63
2:B:309:MET:CE	2:B:351:LYS:HB2	2.28	0.63
5:E:95:MET:HG3	5:E:141:GLY:HA3	1.79	0.63
2:B:309:MET:HE2	2:B:351:LYS:H	1.65	0.62
2:B:180:ARG:HD2	2:B:281:LEU:HD21	1.82	0.62
1:A:263:SER:C	1:A:265:LYS:H	2.03	0.62
7:G:121:SER:O	7:G:124:VAL:HG12	2.01	0.61
2:B:279:ALA:HB3	2:B:320:GLU:HG2	1.81	0.61
3:C:360:ARG:HG3	3:C:361:SER:N	2.15	0.61
4:D:199:LEU:HB2	4:D:224:THR:HB	1.82	0.61
1:A:343:VAL:HG13	1:A:363:ILE:HD11	1.83	0.60
3:C:144:THR:H	6:F:28:GLN:NE2	2.00	0.60
2:B:279:ALA:CB	2:B:320:GLU:HG2	2.31	0.60
1:A:200:ILE:HG12	1:A:281:ILE:HD11	1.83	0.60
3:C:269:LEU:H	3:C:283:GLY:CA	2.15	0.60
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.84	0.60
4:D:217:GLY:HA3	4:D:220:ILE:HD13	1.82	0.60
3:C:179:ARG:NH1	3:C:179:ARG:HG3	2.15	0.60
3:C:155:VAL:HG11	3:C:180:PRO:HG2	1.84	0.59
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.84	0.59
1:A:395:HIS:N	1:A:395:HIS:CD2	2.68	0.59
1:A:259:ILE:HG13	1:A:266:GLU:HA	1.84	0.59
1:A:348:LYS:HE2	1:A:352:GLU:OE2	2.02	0.59
3:C:370:LYS:O	3:C:371:ILE:HB	2.03	0.59
5:E:86:ASN:O	5:E:87:SER:CB	2.51	0.59
6:F:158:ARG:O	6:F:162:GLU:HG3	2.03	0.58
6:F:4:THR:CG2	6:F:55:ARG:HE	2.08	0.58
2:B:291:ILE:CD1	2:B:294:ARG:HH11	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:O	1:A:55:VAL:HG13	2.04	0.58
3:C:201:SER:O	7:G:148:ARG:HG3	2.04	0.58
5:E:56:LYS:HE3	5:E:170:ASN:OD1	2.04	0.58
2:B:345:GLU:C	2:B:347:PRO:HD3	2.24	0.58
1:A:206:GLN:NE2	1:A:209:ARG:HH11	2.00	0.57
2:B:166:ILE:HD13	2:B:282:LEU:HA	1.86	0.57
3:C:284:ARG:NH1	3:C:286:ASP:O	2.35	0.57
4:D:203:ARG:O	4:D:216:VAL:HG13	2.05	0.57
5:E:152:GLN:O	5:E:153:ASN:O	2.23	0.57
5:E:95:MET:HA	5:E:95:MET:CE	2.34	0.57
2:B:291:ILE:HD13	2:B:294:ARG:HD3	1.87	0.57
2:B:146:LEU:CD1	2:B:169:VAL:HB	2.35	0.56
2:B:153:THR:HA	2:B:169:VAL:O	2.05	0.56
4:D:220:ILE:N	4:D:220:ILE:HD12	2.20	0.56
5:E:150:ASP:O	5:E:152:GLN:N	2.37	0.56
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.86	0.56
1:A:374:ARG:HH11	1:A:374:ARG:HG2	1.71	0.56
3:C:269:LEU:H	3:C:283:GLY:HA3	1.71	0.56
6:F:145:GLU:O	6:F:149:MET:HG3	2.06	0.56
2:B:231:GLN:HA	2:B:231:GLN:HE21	1.70	0.56
5:E:15:LEU:HD22	5:E:63:GLU:HG3	1.88	0.56
1:A:374:ARG:HD2	1:A:374:ARG:O	2.06	0.56
1:A:229:GLU:HG2	9:A:601:ATP:C5	2.41	0.55
1:A:395:HIS:CE1	1:A:408:CYS:HA	2.41	0.55
3:C:234:LYS:O	3:C:235:MET:HB2	2.05	0.55
3:C:371:ILE:O	3:C:372:VAL:HB	2.07	0.55
3:C:60:TRP:HE1	3:C:65:ASN:ND2	2.05	0.55
4:D:53:THR:C	4:D:54:LYS:HD2	2.26	0.55
2:B:182:LEU:HD22	2:B:184:ILE:HB	1.89	0.55
1:A:317:LYS:HE3	1:A:364:ASP:OD1	2.07	0.55
3:C:183:THR:HG22	3:C:185:TRP:N	2.15	0.55
7:G:87:LYS:N	7:G:87:LYS:HD3	2.22	0.55
4:D:68:GLN:HA	4:D:72:ALA:HB3	1.90	0.54
6:F:82:ILE:CG2	6:F:150:LYS:HE3	2.37	0.54
2:B:155:VAL:HG21	2:B:286:ILE:HD11	1.89	0.54
3:C:96:ASN:OD1	3:C:97:ARG:HG2	2.07	0.54
7:G:38:ASP:HB3	7:G:41:GLU:CB	2.37	0.54
1:A:135:ASN:HB3	1:A:397:LYS:HZ2	1.72	0.54
1:A:343:VAL:CG1	1:A:363:ILE:HG13	2.35	0.54
3:C:131:TRP:HB2	10:C:488:HOH:O	2.06	0.54
1:A:289:ASN:HD22	1:A:289:ASN:C	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLU:HG2	9:B:602:ATP:C5	2.43	0.54
1:A:257:THR:CG2	1:A:268:SER:HB3	2.13	0.54
1:A:329:ARG:O	1:A:330:ASP:HB2	2.08	0.54
6:F:95:MET:SD	6:F:108:PRO:HD3	2.48	0.54
4:D:158:LYS:O	4:D:158:LYS:HD3	2.08	0.54
3:C:119:VAL:HG22	3:C:120:ILE:N	2.22	0.53
1:A:135:ASN:HB3	1:A:397:LYS:NZ	2.23	0.53
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.90	0.53
6:F:82:ILE:HG21	6:F:150:LYS:HE3	1.90	0.53
2:B:322:LYS:HB3	7:G:16:VAL:HG11	1.91	0.53
5:E:16:ILE:O	5:E:16:ILE:HG23	2.09	0.53
1:A:239:VAL:HG13	5:E:4:TYR:CZ	2.43	0.53
2:B:23:ALA:C	2:B:25:SER:N	2.58	0.53
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.91	0.53
1:A:111:LEU:HD23	1:A:111:LEU:C	2.29	0.52
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.44	0.52
3:C:107:ASN:HD22	3:C:109:LYS:H	1.57	0.52
3:C:268:VAL:HA	3:C:284:ARG:H	1.75	0.52
3:C:332:ILE:HA	3:C:346:CYS:O	2.09	0.52
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.45	0.52
1:A:259:ILE:HG23	1:A:265:LYS:O	2.09	0.52
5:E:71:ILE:O	5:E:75:ILE:HG13	2.08	0.52
3:C:368:ASP:O	3:C:370:LYS:NZ	2.42	0.52
5:E:88:LYS:H	5:E:153:ASN:HD21	1.56	0.52
2:B:161:ASP:O	2:B:187:ARG:HG3	2.10	0.52
1:A:55:VAL:HG22	1:A:58:LEU:HD12	1.92	0.52
1:A:69:LYS:CB	1:A:72:TYR:HB2	2.40	0.51
3:C:367:LYS:HD2	3:C:368:ASP:H	1.75	0.51
4:D:248:ARG:C	4:D:248:ARG:HD3	2.30	0.51
5:E:78:CYS:HA	5:E:95:MET:HE1	1.93	0.51
1:A:236:PRO:HD2	10:A:673:HOH:O	2.10	0.51
5:E:152:GLN:OE1	5:E:152:GLN:HA	2.09	0.51
5:E:95:MET:HA	5:E:95:MET:HE3	1.91	0.51
7:G:80:LEU:O	7:G:84:ILE:HD13	2.10	0.51
1:A:206:GLN:NE2	1:A:209:ARG:NH1	2.48	0.51
3:C:151:HIS:CG	3:C:152:PRO:HD2	2.45	0.51
3:C:90:LEU:HD22	3:C:91:VAL:H	1.76	0.51
4:D:158:LYS:HD3	4:D:158:LYS:C	2.32	0.51
6:F:87:CYS:O	6:F:91:MET:HG2	2.11	0.51
1:A:258:GLY:C	1:A:259:ILE:HD12	2.31	0.51
2:B:330:LEU:C	2:B:332:GLY:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:ASN:O	5:E:87:SER:HB3	2.11	0.51
1:A:155:SER:O	1:A:158:VAL:N	2.44	0.51
1:A:352:GLU:C	1:A:354:SER:H	2.14	0.51
3:C:11:ILE:HG13	3:C:352:GLY:HA2	1.93	0.51
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.26	0.51
7:G:149:LYS:N	7:G:149:LYS:HD3	2.26	0.50
2:B:175:LEU:N	2:B:175:LEU:HD23	2.25	0.50
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.92	0.50
3:C:72:THR:HA	3:C:98:ALA:HB1	1.92	0.50
4:D:171:ASP:O	4:D:174:ASP:HB2	2.12	0.50
6:F:80:ASP:OD1	6:F:83:GLU:HG3	2.11	0.50
2:B:146:LEU:HD12	2:B:169:VAL:HB	1.94	0.50
6:F:130:LYS:CE	6:F:130:LYS:HA	2.41	0.50
2:B:347:PRO:HB2	2:B:353:MET:CE	2.41	0.50
1:A:194:PRO:C	1:A:195:ILE:HD12	2.32	0.50
2:B:320:GLU:HA	2:B:323:GLN:HE21	1.77	0.50
5:E:20:ALA:HB3	5:E:22:LEU:CD2	2.42	0.50
3:C:228:LEU:HD23	3:C:228:LEU:C	2.32	0.50
2:B:157:VAL:HB	2:B:303:LEU:HD12	1.92	0.49
5:E:88:LYS:H	5:E:153:ASN:ND2	2.08	0.49
2:B:177:HIS:O	2:B:178:LEU:CB	2.51	0.49
2:B:231:GLN:HA	2:B:231:GLN:NE2	2.27	0.49
3:C:131:TRP:O	3:C:131:TRP:HE3	1.95	0.49
1:A:190:ILE:O	1:A:191:LYS:HD3	2.12	0.49
1:A:243:ASN:O	1:A:247:THR:HB	2.13	0.49
5:E:152:GLN:O	5:E:155:LYS:HD2	2.12	0.49
3:C:119:VAL:HG23	3:C:137:ILE:O	2.12	0.49
3:C:119:VAL:HG21	3:C:136:HIS:HB3	1.95	0.49
3:C:173:ILE:HG22	3:C:175:GLU:HG2	1.93	0.49
3:C:14:HIS:N	3:C:331:GLN:HE22	2.04	0.49
2:B:330:LEU:O	2:B:332:GLY:N	2.44	0.49
7:G:118:SER:O	7:G:119:ASP:C	2.50	0.49
1:A:395:HIS:HB3	1:A:407:ILE:HD12	1.94	0.49
3:C:33:HIS:HD2	10:C:404:HOH:O	1.96	0.49
3:C:90:LEU:HD22	3:C:91:VAL:N	2.28	0.48
4:D:158:LYS:HG3	4:D:159:ASP:OD2	2.12	0.48
1:A:70:PRO:HD2	10:A:628:HOH:O	2.13	0.48
4:D:232:THR:O	4:D:237:ARG:HG3	2.13	0.48
1:A:400:TYR:CE1	1:A:405:PRO:HA	2.48	0.48
2:B:160:GLY:HA3	9:B:602:ATP:O2G	2.12	0.48
3:C:367:LYS:HD2	3:C:368:ASP:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:GLY:O	2:B:358:GLY:C	2.50	0.48
5:E:87:SER:HA	5:E:153:ASN:OD1	2.14	0.48
2:B:306:GLY:HA2	2:B:351:LYS:HG3	1.95	0.48
4:D:95:LEU:HD11	4:D:116:LEU:HG	1.95	0.48
1:A:243:ASN:HD22	5:E:47:TYR:HE1	1.62	0.48
3:C:27:PRO:HG2	3:C:29:ASN:ND2	2.29	0.48
3:C:73:ASP:O	3:C:74:ARG:HB2	2.14	0.48
2:B:23:ALA:O	2:B:25:SER:N	2.46	0.48
2:B:280:GLU:HA	2:B:324:LEU:HD11	1.95	0.48
3:C:21:THR:HG22	3:C:22:GLN:HG3	1.96	0.48
1:A:260:ASN:HB3	1:A:263:SER:OG	2.13	0.48
1:A:170:SER:OG	1:A:325:SER:HB2	2.14	0.48
5:E:9:MET:CE	5:E:63:GLU:HG2	2.44	0.48
2:B:309:MET:HE2	2:B:351:LYS:N	2.28	0.47
1:A:289:ASN:HD22	1:A:291:ASP:H	1.60	0.47
3:C:344:GLN:HA	3:C:357:TRP:O	2.14	0.47
7:G:68:SER:CB	7:G:71:VAL:HG12	2.44	0.47
3:C:90:LEU:CD2	3:C:91:VAL:H	2.27	0.47
4:D:189:ARG:HH12	4:D:197:GLN:NE2	2.12	0.47
2:B:170:TYR:O	2:B:171:GLU:C	2.52	0.47
3:C:321:LEU:HD22	3:C:321:LEU:N	2.29	0.47
4:D:205:PRO:HA	4:D:206:PRO:HD3	1.75	0.47
1:A:128:GLU:O	1:A:132:GLU:HB2	2.14	0.47
1:A:311:VAL:O	1:A:314:PRO:HG2	2.15	0.47
1:A:87:ASP:OD2	4:D:264:THR:HG22	2.15	0.47
1:A:61:PHE:C	1:A:66:ALA:HB2	2.35	0.47
1:A:324:GLY:HA3	9:A:601:ATP:O4'	2.15	0.47
2:B:308:THR:HA	2:B:313:LEU:CD2	2.45	0.47
3:C:173:ILE:CG2	3:C:175:GLU:HG2	2.45	0.47
1:A:174:VAL:HG12	1:A:175:THR:N	2.29	0.47
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.55	0.47
3:C:48:LEU:HG	3:C:79:TRP:CE3	2.50	0.47
4:D:141:ARG:HH11	4:D:141:ARG:HB2	1.79	0.47
6:F:53:ILE:N	6:F:53:ILE:HD12	2.29	0.47
3:C:92:ILE:HD12	3:C:92:ILE:N	2.30	0.47
1:A:116:PRO:HG3	10:A:640:HOH:O	2.15	0.46
2:B:163:VAL:HG22	2:B:164:THR:N	2.29	0.46
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.98	0.46
4:D:170:LYS:HG2	10:D:457:HOH:O	2.15	0.46
6:F:8:TYR:OH	6:F:61:VAL:HG23	2.15	0.46
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:146:GLU:HG2	5:E:147:LYS:N	2.31	0.46
5:E:150:ASP:C	5:E:152:GLN:H	2.18	0.46
6:F:58:LYS:HA	6:F:58:LYS:HE2	1.97	0.46
2:B:291:ILE:HD12	2:B:294:ARG:NH1	2.31	0.46
5:E:150:ASP:C	5:E:152:GLN:N	2.68	0.46
1:A:254:LYS:HE2	1:A:275:ARG:HH12	1.81	0.46
2:B:174:SER:C	2:B:175:LEU:HD23	2.36	0.46
3:C:14:HIS:H	3:C:331:GLN:NE2	2.07	0.46
3:C:189:MET:HG2	3:C:195:MET:HE3	1.98	0.46
2:B:291:ILE:CD1	2:B:294:ARG:NH1	2.79	0.46
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.78	0.46
5:E:95:MET:HG2	5:E:141:GLY:O	2.16	0.46
2:B:192:TYR:CD2	2:B:261:ALA:HA	2.51	0.46
2:B:186:GLY:HA3	9:B:602:ATP:O3'	2.16	0.46
5:E:18:ASN:ND2	5:E:66:ARG:NE	2.64	0.45
2:B:347:PRO:HB2	2:B:353:MET:HE1	1.97	0.45
4:D:223:ILE:HD12	4:D:223:ILE:N	2.31	0.45
1:A:81:GLY:O	1:A:115:PRO:CG	2.65	0.45
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.97	0.45
3:C:178:GLU:O	3:C:179:ARG:C	2.55	0.45
3:C:269:LEU:H	3:C:283:GLY:HA2	1.80	0.45
4:D:141:ARG:CB	4:D:141:ARG:HH11	2.30	0.45
5:E:165:LYS:HB2	10:E:435:HOH:O	2.15	0.45
1:A:289:ASN:ND2	1:A:291:ASP:H	2.15	0.45
3:C:360:ARG:HG2	3:C:360:ARG:HH11	1.82	0.45
4:D:202:HIS:HE1	4:D:218:ASP:O	1.99	0.45
1:A:313:ARG:CZ	1:A:363:ILE:HG22	2.47	0.45
3:C:253:ILE:HD13	3:C:259:VAL:HG23	1.98	0.45
1:A:263:SER:O	1:A:265:LYS:N	2.48	0.45
1:A:359:LYS:N	1:A:360:PRO:HD3	2.32	0.45
5:E:138:GLN:HA	5:E:138:GLN:OE1	2.17	0.45
6:F:4:THR:CG2	6:F:55:ARG:HH21	2.30	0.45
5:E:153:ASN:O	5:E:154:ASP:HB3	2.17	0.44
1:A:352:GLU:C	1:A:354:SER:N	2.70	0.44
3:C:209:CYS:SG	3:C:251:THR:HA	2.58	0.44
5:E:14:LYS:O	5:E:15:LEU:HD23	2.16	0.44
5:E:60:ILE:CD1	5:E:116:ILE:HG21	2.47	0.44
1:A:140:TYR:HB2	1:A:394:CYS:SG	2.57	0.44
1:A:343:VAL:CG1	1:A:363:ILE:HD11	2.47	0.44
1:A:55:VAL:CG2	1:A:58:LEU:HD12	2.47	0.44
5:E:18:ASN:ND2	5:E:66:ARG:CZ	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG23	1:A:240:LYS:N	2.31	0.44
2:B:200:ARG:HD2	2:B:257:GLU:OE2	2.18	0.44
4:D:75:LEU:C	4:D:75:LEU:HD23	2.38	0.44
3:C:10:PRO:HG2	6:F:124:GLU:HG2	1.99	0.44
3:C:201:SER:O	7:G:148:ARG:CG	2.66	0.44
3:C:59:ASP:OD2	3:C:104:TRP:N	2.37	0.44
3:C:92:ILE:HG22	3:C:94:ARG:HG3	1.99	0.44
7:G:15:ASP:OD1	7:G:17:ASP:HB2	2.18	0.44
1:A:10:VAL:HB	1:A:112:LEU:CD2	2.47	0.44
2:B:200:ARG:HD3	10:B:631:HOH:O	2.17	0.44
4:D:228:PHE:H	4:D:231:HIS:CD2	2.29	0.44
6:F:22:LEU:HD21	6:F:70:VAL:HG23	1.99	0.44
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.47	0.44
3:C:266:PHE:HB2	3:C:286:ASP:HB3	2.00	0.44
1:A:81:GLY:O	1:A:115:PRO:HG3	2.18	0.43
1:A:309:ILE:HG23	1:A:310:ASP:N	2.33	0.43
2:B:280:GLU:HA	2:B:324:LEU:CD1	2.47	0.43
2:B:346:ASP:OD1	2:B:346:ASP:N	2.47	0.43
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.53	0.43
5:E:150:ASP:OD2	5:E:152:GLN:HB2	2.18	0.43
2:B:151:LEU:HD13	2:B:300:HIS:HD2	1.83	0.43
4:D:231:HIS:HE1	10:D:446:HOH:O	2.00	0.43
5:E:74:TYR:OH	5:E:98:LEU:HD12	2.18	0.43
6:F:25:PHE:CD1	6:F:67:ILE:HD13	2.53	0.43
1:A:69:LYS:HB3	1:A:72:TYR:HB2	1.99	0.43
2:B:170:TYR:H	2:B:175:LEU:CD2	2.32	0.43
3:C:144:THR:H	6:F:28:GLN:HE21	1.66	0.43
4:D:118:ARG:HD3	4:D:118:ARG:C	2.39	0.43
3:C:183:THR:HG23	3:C:184:PRO:HD2	2.01	0.43
3:C:107:ASN:HD21	3:C:109:LYS:H	1.62	0.43
6:F:8:TYR:O	6:F:12:VAL:HG23	2.19	0.43
1:A:359:LYS:HG2	1:A:359:LYS:O	2.19	0.43
2:B:345:GLU:O	2:B:347:PRO:HD3	2.19	0.43
3:C:174:LYS:HB3	3:C:174:LYS:HE2	1.83	0.43
3:C:179:ARG:HA	3:C:180:PRO:HD3	1.80	0.43
2:B:231:GLN:CA	2:B:231:GLN:HE21	2.31	0.43
1:A:352:GLU:O	1:A:354:SER:N	2.52	0.43
4:D:203:ARG:HA	4:D:217:GLY:O	2.19	0.43
4:D:203:ARG:NE	4:D:218:ASP:OD1	2.52	0.43
3:C:253:ILE:HD13	3:C:259:VAL:CG2	2.48	0.43
1:A:18:LYS:HD3	1:A:18:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:PHE:CE1	9:A:601:ATP:H2	2.37	0.42
5:E:168:PHE:CE2	5:E:169:MET:HE1	2.54	0.42
4:D:67:LEU:HD13	4:D:120:CYS:O	2.19	0.42
2:B:165:HIS:NE2	2:B:181:ARG:HG2	2.33	0.42
5:E:105:ILE:O	5:E:106:PRO:C	2.58	0.42
6:F:101:PHE:O	6:F:103:ILE:N	2.52	0.42
1:A:108:HIS:O	1:A:137:PRO:HD2	2.19	0.42
1:A:25:THR:HG23	1:A:372:MET:CE	2.49	0.42
1:A:263:SER:C	1:A:265:LYS:N	2.71	0.42
1:A:370:HIS:O	1:A:373:GLN:HG3	2.19	0.42
2:B:222:TYR:O	2:B:259:PHE:HA	2.19	0.42
3:C:126:GLU:CB	3:C:131:TRP:HZ3	2.24	0.42
3:C:7:LEU:N	3:C:7:LEU:HD23	2.34	0.42
4:D:170:LYS:CA	4:D:170:LYS:HE2	2.44	0.42
5:E:126:ASP:OD2	5:E:130:ARG:HD2	2.19	0.42
3:C:125:PHE:CD1	3:C:127:GLN:HG3	2.54	0.42
7:G:74:ARG:HH11	7:G:74:ARG:HG3	1.84	0.42
1:A:140:TYR:HE2	1:A:142:ALA:HB2	1.84	0.42
2:B:347:PRO:HA	2:B:348:PRO:HD3	1.88	0.42
3:C:283:GLY:O	3:C:284:ARG:HB2	2.19	0.42
3:C:326:LYS:HA	3:C:326:LYS:HD3	1.84	0.42
3:C:21:THR:CG2	3:C:22:GLN:HG3	2.50	0.42
3:C:372:VAL:HG12	3:C:372:VAL:OXT	2.19	0.42
4:D:247:PHE:O	4:D:250:TYR:HB3	2.19	0.42
5:E:153:ASN:OD1	5:E:154:ASP:N	2.53	0.42
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.92	0.41
1:A:152:SER:C	1:A:154:THR:H	2.23	0.41
2:B:180:ARG:HD2	2:B:281:LEU:CD2	2.49	0.41
7:G:51:MET:HB3	7:G:86:PHE:CZ	2.55	0.41
2:B:180:ARG:HH11	2:B:180:ARG:HG3	1.85	0.41
6:F:13:ARG:NH1	6:F:133:ASP:OD1	2.45	0.41
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.75	0.41
1:A:189:CYS:O	1:A:303:VAL:HG13	2.20	0.41
5:E:152:GLN:HB3	5:E:155:LYS:HZ2	1.77	0.41
6:F:30:VAL:HG11	6:F:33:HIS:CE1	2.56	0.41
7:G:87:LYS:N	7:G:87:LYS:CD	2.83	0.41
1:A:385:ALA:HA	1:A:390:PHE:CG	2.55	0.41
4:D:132:GLN:HB2	4:D:156:SER:OG	2.20	0.41
5:E:18:ASN:CG	5:E:118:ALA:H	2.23	0.41
1:A:343:VAL:CG1	1:A:363:ILE:CD1	2.99	0.41
1:A:383:MET:O	1:A:387:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:VAL:O	3:C:103:ARG:HG2	2.20	0.41
3:C:127:GLN:C	3:C:128:GLU:HG3	2.40	0.41
4:D:181:PHE:CE2	6:F:157:ALA:HA	2.55	0.41
4:D:215:ALA:O	4:D:222:TYR:OH	2.36	0.41
5:E:123:LYS:O	5:E:127:GLU:HG3	2.20	0.41
7:G:51:MET:HE2	7:G:51:MET:HA	2.02	0.41
2:B:112:PRO:HA	2:B:113:PRO:HD3	1.76	0.41
3:C:342:CYS:O	3:C:359:VAL:HG21	2.20	0.41
7:G:38:ASP:CG	7:G:41:GLU:HB2	2.40	0.41
2:B:217:LYS:O	2:B:221:CYS:HB2	2.21	0.41
5:E:9:MET:HE2	5:E:63:GLU:HG2	2.02	0.41
5:E:152:GLN:O	5:E:155:LYS:CD	2.69	0.41
1:A:39:GLU:HG3	1:A:39:GLU:O	2.21	0.41
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.51	0.41
5:E:111:PHE:CD2	5:E:112:PRO:O	2.74	0.41
5:E:150:ASP:OD1	5:E:151:PRO:HD2	2.20	0.41
6:F:2:THR:OG1	6:F:3:ALA:N	2.54	0.41
1:A:158:VAL:HG11	10:A:674:HOH:O	2.19	0.41
1:A:191:LYS:HB2	1:A:303:VAL:HG22	2.03	0.41
2:B:113:PRO:HG2	2:B:167:CYS:SG	2.61	0.41
4:D:6:VAL:HG11	4:D:118:ARG:HG3	2.03	0.41
4:D:30:ALA:HA	4:D:52:LYS:HG2	2.02	0.41
3:C:144:THR:N	6:F:28:GLN:NE2	2.69	0.41
3:C:44:GLN:HE21	3:C:47:GLU:CG	2.34	0.40
3:C:69:THR:O	3:C:76:ALA:HA	2.21	0.40
3:C:7:LEU:HD12	3:C:9:GLU:HB2	2.03	0.40
5:E:74:TYR:CE2	5:E:78:CYS:SG	3.15	0.40
5:E:98:LEU:HA	5:E:101:THR:CG2	2.51	0.40
1:A:154:THR:HG23	1:A:154:THR:O	2.20	0.40
4:D:131:PHE:CE1	4:D:139:GLU:HG3	2.56	0.40
4:D:54:LYS:HD2	4:D:54:LYS:N	2.37	0.40
7:G:74:ARG:HG3	7:G:74:ARG:NH1	2.36	0.40
1:A:263:SER:OG	1:A:265:LYS:HB2	2.21	0.40
1:A:384:LEU:O	1:A:390:PHE:HB2	2.22	0.40
2:B:287:GLN:C	2:B:289:ALA:H	2.24	0.40
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.88	0.40
5:E:69:ILE:HG23	5:E:169:MET:HE1	2.02	0.40
5:E:87:SER:N	5:E:154:ASP:HA	2.36	0.40
3:C:324:LEU:HA	3:C:324:LEU:HD12	1.95	0.40
5:E:60:ILE:CD1	5:E:116:ILE:CG2	2.99	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	385/418 (92%)	367 (95%)	15 (4%)	3 (1%)	19	39
2	B	265/394 (67%)	239 (90%)	19 (7%)	7 (3%)	5	9
3	C	337/372 (91%)	314 (93%)	19 (6%)	4 (1%)	13	27
4	D	273/300 (91%)	265 (97%)	7 (3%)	1 (0%)	34	57
5	E	172/178 (97%)	163 (95%)	6 (4%)	3 (2%)	9	18
6	F	165/168 (98%)	158 (96%)	6 (4%)	1 (1%)	25	47
7	G	132/151 (87%)	118 (89%)	12 (9%)	2 (2%)	10	21
All	All	1729/1981 (87%)	1624 (94%)	84 (5%)	21 (1%)	13	27

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	114	MET
5	E	87	SER
5	E	153	ASN
6	F	102	PHE
7	G	119	ASP
1	A	263	SER
2	B	171	GLU
3	C	371	ILE
7	G	22	ASN
2	B	178	LEU
3	C	320	GLY
1	A	265	LYS
1	A	353	LEU
2	B	331	LYS
4	D	170	LYS
5	E	151	PRO
2	B	358	GLY
3	C	284	ARG

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Mol	Chain	Res	Type
2	B	113	PRO
3	C	62	PRO
2	B	278	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/363 (95%)	326 (94%)	19 (6%)	21	43
2	B	197/346 (57%)	188 (95%)	9 (5%)	27	51
3	C	290/313 (93%)	280 (97%)	10 (3%)	37	63
4	D	243/264 (92%)	239 (98%)	4 (2%)	62	82
5	E	156/159 (98%)	147 (94%)	9 (6%)	20	40
6	F	154/155 (99%)	148 (96%)	6 (4%)	32	58
7	G	112/124 (90%)	105 (94%)	7 (6%)	18	36
All	All	1497/1724 (87%)	1433 (96%)	64 (4%)	29	54

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	19	LEU
1	A	55	VAL
1	A	68	GLU
1	A	71	THR
1	A	117	LEU
1	A	143	VAL
1	A	154	THR
1	A	191	LYS
1	A	230	ARG
1	A	268	SER
1	A	289	ASN
1	A	335	LEU
1	A	340	LYS

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Mol	Chain	Res	Type
1	A	351	GLU
1	A	363	ILE
1	A	394	CYS
1	A	395	HIS
1	A	401	GLU
2	B	175	LEU
2	B	220	LEU
2	B	235	LEU
2	B	257	GLU
2	B	274	GLU
2	B	281	LEU
2	B	290	ASP
2	B	303	LEU
2	B	320	GLU
3	C	21	THR
3	C	30	HIS
3	C	90	LEU
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	175	GLU
3	C	183	THR
3	C	284	ARG
3	C	367	LYS
4	D	37	ASP
4	D	116	LEU
4	D	141	ARG
4	D	230	ARG
5	E	22	LEU
5	E	82	LEU
5	E	95	MET
5	E	101	THR
5	E	102	ASN
5	E	133	LEU
5	E	144	LEU
5	E	145	CYS
5	E	146	GLU
6	F	6	ARG
6	F	101	PHE
6	F	102	PHE
6	F	104	LEU
6	F	152	SER

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Mol	Chain	Res	Type
6	F	165	LEU
7	G	10	ARG
7	G	18	GLU
7	G	39	GLU
7	G	47	ARG
7	G	48	GLN
7	G	87	LYS
7	G	90	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	205	GLN
1	A	206	GLN
1	A	289	ASN
1	A	306	ASN
1	A	318	ASN
2	B	205	ASN
2	B	231	GLN
2	B	284	ASN
2	B	300	HIS
2	B	323	GLN
3	C	33	HIS
3	C	44	GLN
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
4	D	263	HIS
5	E	102	ASN
6	F	24	ASN
6	F	28	GLN
6	F	125	GLN
6	F	129	HIS
7	G	48	GLN
7	G	96	GLN

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 carbohydrates 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	ATP	A	601	8	26,33,33	1.35	3 (11%)	31,52,52	1.67	5 (16%)
9	ATP	B	602	8	26,33,33	1.35	3 (11%)	31,52,52	1.61	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	A	601	8	-	1/18/38/38	0/3/3/3
9	ATP	B	602	8	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	ATP	C2-N1	3.78	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	602	ATP	C2-N1	3.54	1.40	1.33
9	A	601	ATP	PG-O1G	3.40	1.61	1.50
9	B	602	ATP	PG-O1G	3.38	1.61	1.50
9	B	602	ATP	O4'-C1'	2.23	1.44	1.41
9	A	601	ATP	O4'-C1'	2.03	1.43	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	601	ATP	N3-C2-N1	-5.50	120.08	128.68
9	B	602	ATP	N3-C2-N1	-5.47	120.13	128.68
9	B	602	ATP	PB-O3B-PG	-3.61	120.45	132.83
9	A	601	ATP	O4'-C1'-C2'	-3.17	102.30	106.93
9	B	602	ATP	PA-O3A-PB	-3.16	121.98	132.83
9	A	601	ATP	PA-O3A-PB	-3.12	122.12	132.83
9	A	601	ATP	PB-O3B-PG	-2.96	122.67	132.83
9	A	601	ATP	O3G-PG-O3B	2.60	113.34	104.64
9	B	602	ATP	O3G-PG-O3B	2.51	113.06	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	ATP	PB-O3B-PG-O1G

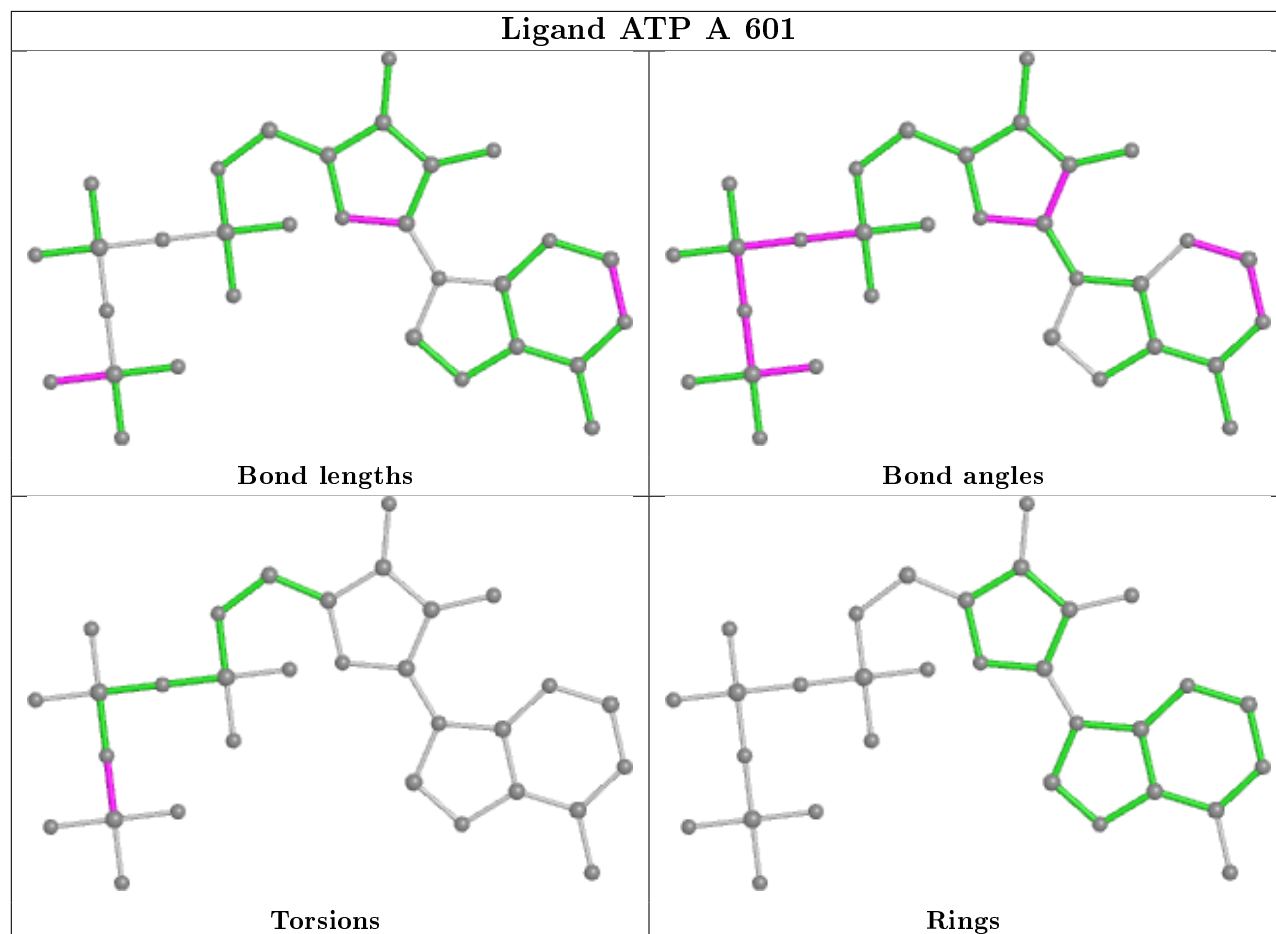
There are no ring outliers.

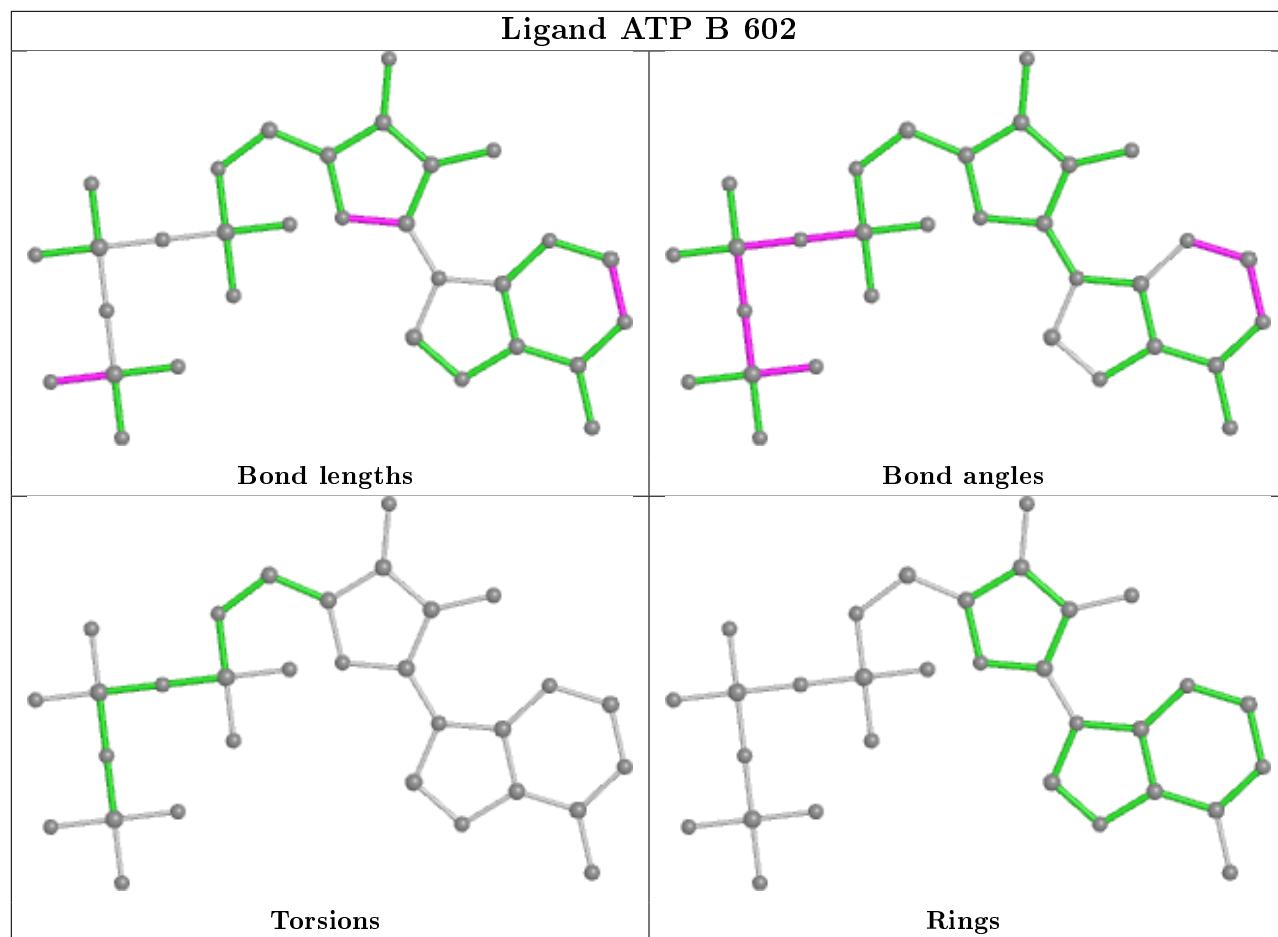
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	601	ATP	3	0
9	B	602	ATP	3	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, 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	393/418 (94%)	-0.02	14 (3%) 42 35	12, 31, 70, 80	0
2	B	275/394 (69%)	0.25	18 (6%) 18 14	16, 48, 76, 83	0
3	C	341/372 (91%)	-0.19	5 (1%) 73 70	15, 26, 58, 78	0
4	D	277/300 (92%)	-0.26	2 (0%) 87 86	15, 28, 52, 86	0
5	E	174/178 (97%)	-0.14	4 (2%) 60 54	21, 36, 60, 79	0
6	F	167/168 (99%)	-0.41	2 (1%) 79 76	14, 22, 38, 72	0
7	G	136/151 (90%)	0.18	9 (6%) 18 13	20, 46, 67, 78	0
All	All	1763/1981 (88%)	-0.08	54 (3%) 49 42	12, 31, 70, 86	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	22	TYR	5.6
1	A	262	ILE	5.2
4	D	215	ALA	4.5
2	B	173	PHE	4.4
1	A	52	MET	4.3
1	A	403	ILE	4.0
6	F	2	THR	3.9
2	B	362	ALA	3.7
7	G	9	ALA	3.7
5	E	154	ASP	3.6
4	D	216	VAL	3.6
2	B	342	ILE	3.5
1	A	259	ILE	3.4
7	G	13	LYS	3.2
2	B	26	ASN	3.2
1	A	353	LEU	3.2
1	A	359	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
7	G	10	ARG	3.1
1	A	159	GLY	3.0
5	E	153	ASN	3.0
2	B	181	ARG	2.9
3	C	370	LYS	2.8
2	B	178	LEU	2.8
2	B	274	GLU	2.7
2	B	113	PRO	2.7
5	E	89	SER	2.7
7	G	64	ILE	2.7
1	A	161	ARG	2.7
2	B	76	ASN	2.6
2	B	360	VAL	2.6
1	A	39	GLU	2.6
3	C	201	SER	2.6
3	C	372	VAL	2.5
3	C	367	LYS	2.5
1	A	158	VAL	2.5
1	A	351	GLU	2.4
6	F	3	ALA	2.4
1	A	360	PRO	2.4
5	E	85	CYS	2.3
7	G	11	PHE	2.3
2	B	23	ALA	2.3
2	B	25	SER	2.3
7	G	19	TYR	2.3
7	G	120	ASN	2.2
7	G	66	THR	2.2
3	C	127	GLN	2.2
2	B	21	GLY	2.1
2	B	115	ASN	2.1
2	B	276	VAL	2.1
2	B	84	ASP	2.1
1	A	265	LYS	2.0
1	A	413	VAL	2.0
2	B	325	TYR	2.0
7	G	18	GLU	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](#)

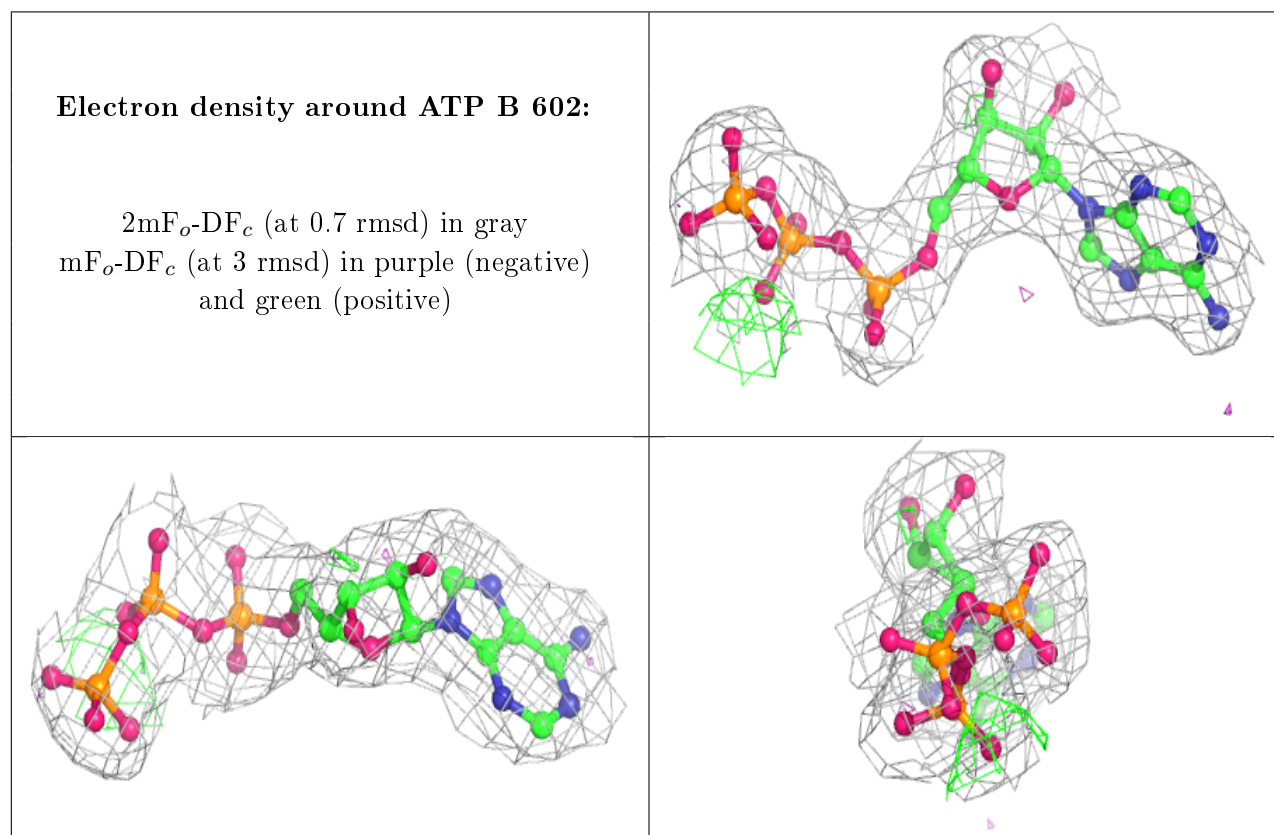
There are no carbohydrates in this entry.

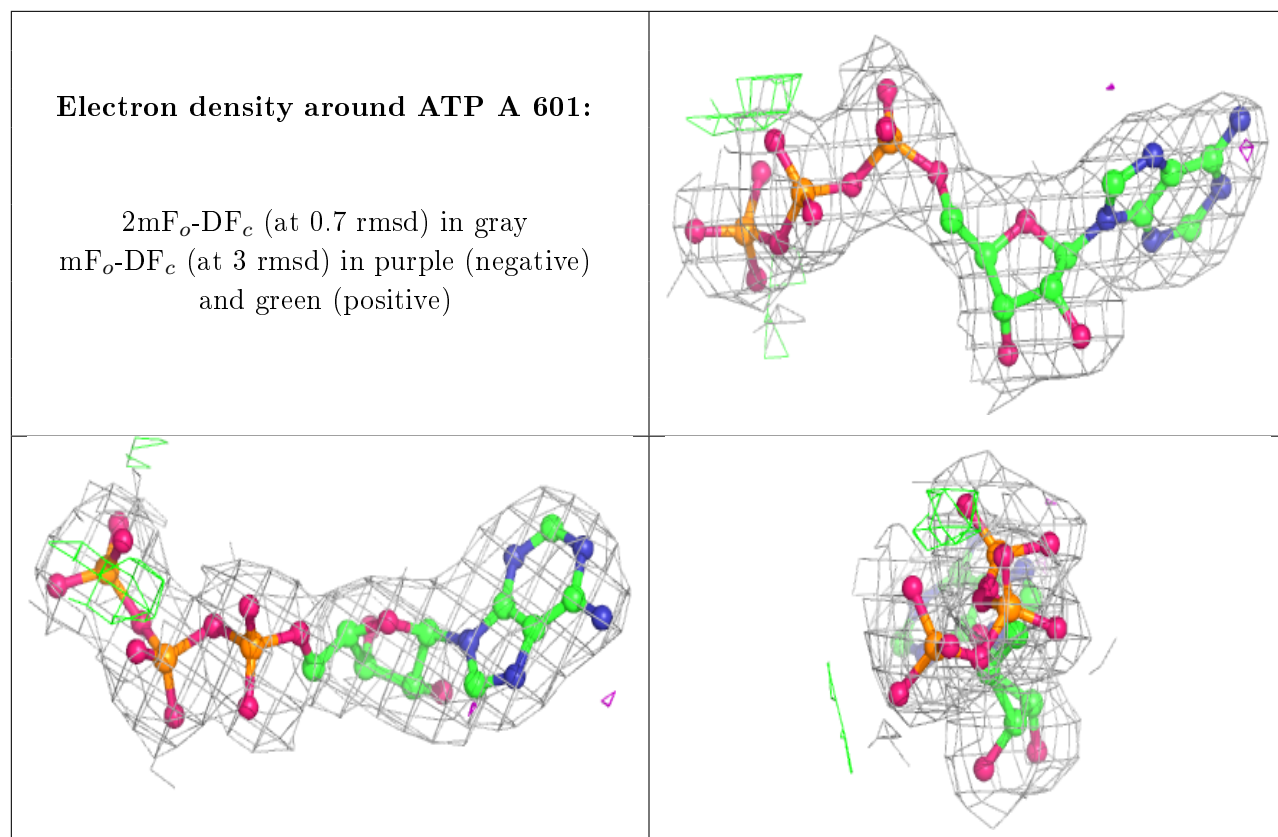
6.4 Ligands [i](#)

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, 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(Å ²)	Q<0.9
8	CA	A	500	1/1	0.94	0.26	41,41,41,41	0
8	CA	B	501	1/1	0.95	0.29	58,58,58,58	0
9	ATP	B	602	31/31	0.97	0.14	22,28,44,47	0
9	ATP	A	601	31/31	0.98	0.13	22,26,31,36	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.