



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:29 PM UTC

PDB ID : 2QRD / pdb_00002qrd
Title : Crystal Structure of the Adenylate Sensor from AMP-activated Protein Kinase
in complex with ADP and ATP
Authors : Jin, X.; Townley, R.; Shapiro, L.
Deposited on : 2007-07-28
Resolution : 2.41 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

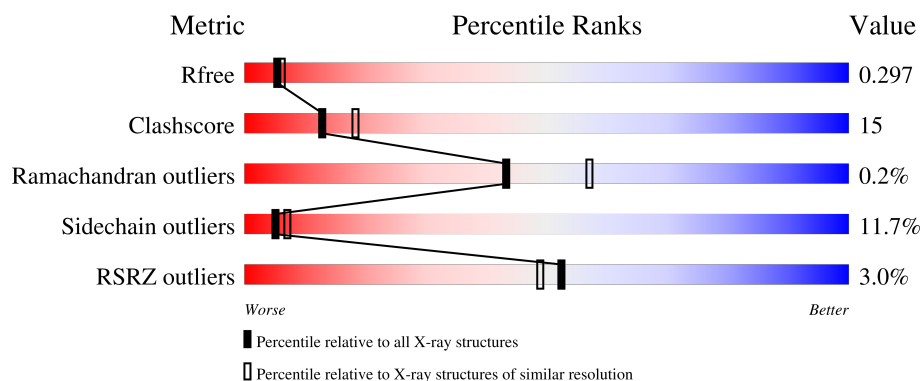
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	137	
1	C	137	
2	B	97	
2	D	97	
3	E	334	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	334	2% 74% 19%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8951 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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			916	593	154	160	9			
1	C	114	Total	C	N	O	S	0	0	0
			914	592	156	157	9			

- Molecule 2 is a protein called SPCC1919.03c protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	S	0	0	0
			699	445	120	132	2			
2	D	92	Total	C	N	O	S	0	0	0
			727	464	124	137	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	MET	-	expression tag	UNP P78789
D	202	MET	-	expression tag	UNP P78789

- Molecule 3 is a protein called Protein C1556.08c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	325	Total	C	N	O	S	0	1	0
			2554	1631	425	483	15			
3	E	324	Total	C	N	O	S	0	1	0
			2551	1629	424	482	16			

There are 4 discrepancies between the modelled and reference sequences:

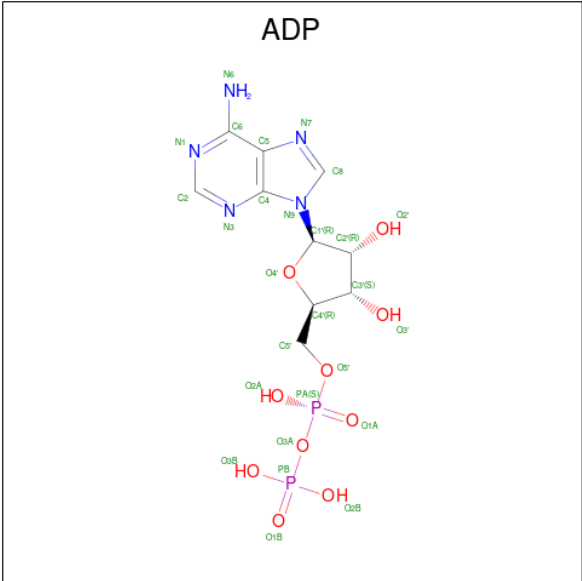
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	expression tag	UNP Q10343
G	2	MET	-	expression tag	UNP Q10343

Continued on next page...

Continued from previous page...

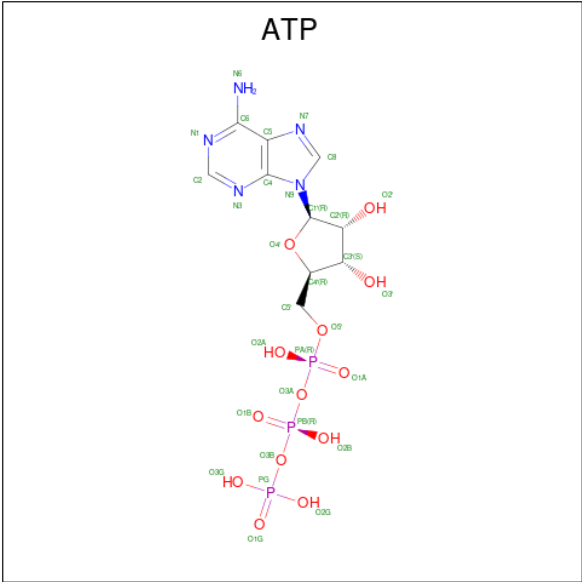
Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ALA	-	expression tag	UNP Q10343
E	2	MET	-	expression tag	UNP Q10343

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
5	G	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
5	E	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
5	E	1	Total	C	N	O	P	0	1
			31	10	5	13	3		

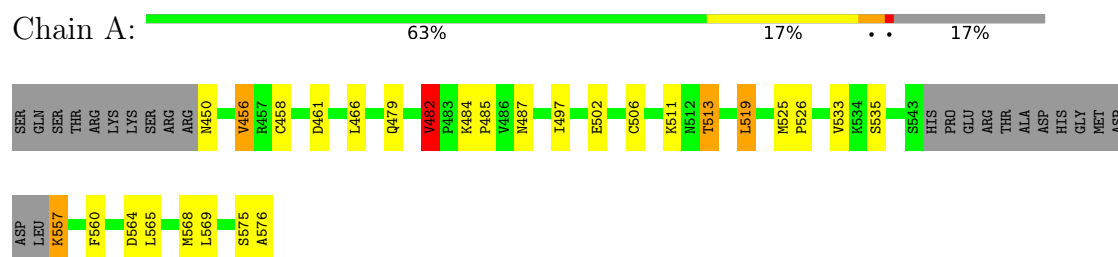
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		
6	B	39	Total	O	0	0
			39	39		
6	G	133	Total	O	0	0
			133	133		
6	C	37	Total	O	0	0
			37	37		
6	D	41	Total	O	0	0
			41	41		
6	E	116	Total	O	0	0
			116	116		

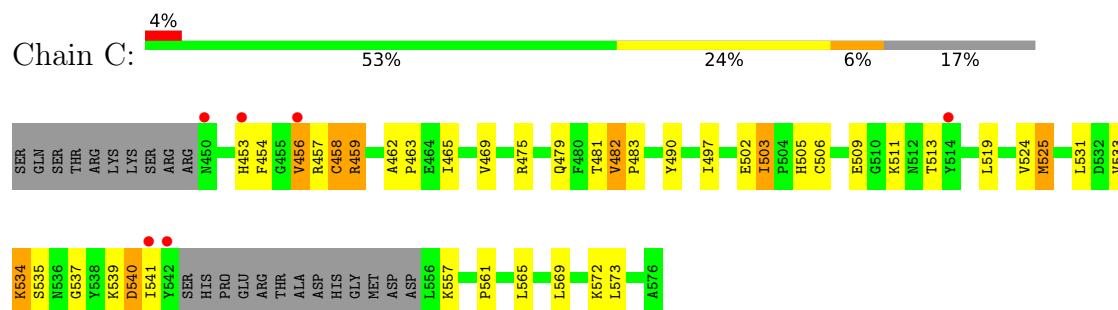
3 Residue-property plots [i](#)

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.

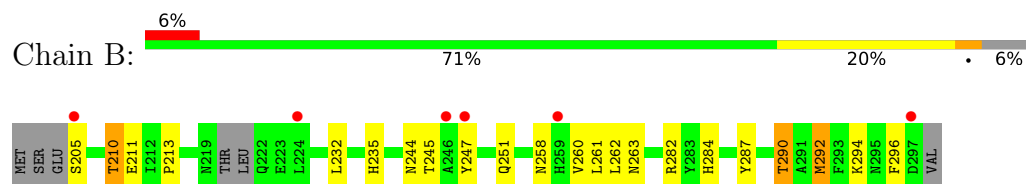
- Molecule 1: SNF1-like protein kinase ssp2



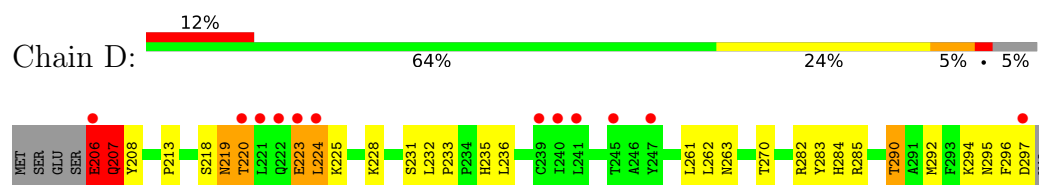
- Molecule 1: SNF1-like protein kinase ssp2



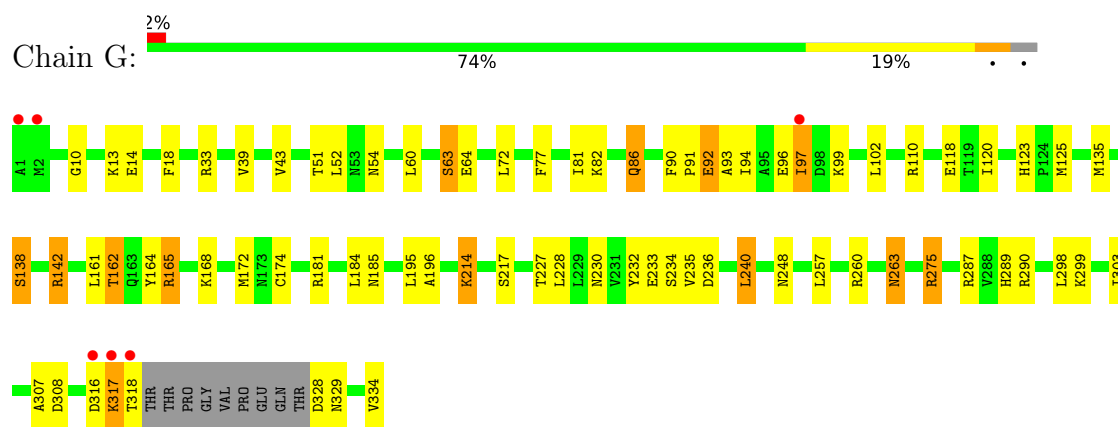
- Molecule 2: SPCC1919.03c protein



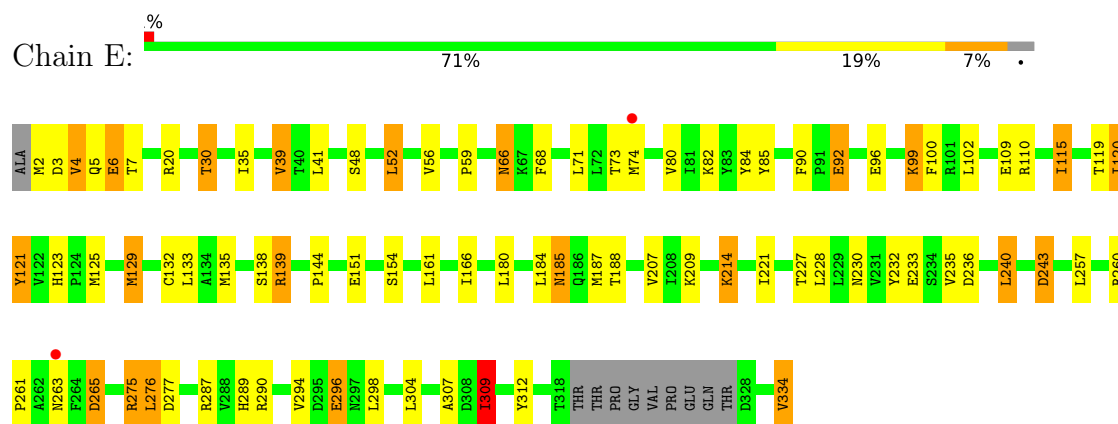
- Molecule 2: SPCC1919.03c protein



- Molecule 3: Protein C1556.08c



• Molecule 3: Protein C1556.08c



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.26Å 78.36Å 109.01Å 90.00° 124.18° 90.00°	Depositor
Resolution (Å)	35.94 – 2.41 35.94 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.94-2.41) 99.1 (35.94-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.262 (Not available) , 0.297	Depositor DCC
R_{free} test set	2279 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8951	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, 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	0.86	1/940 (0.1%)	0.97	3/1266 (0.2%)
1	C	0.77	0/937	0.96	1/1261 (0.1%)
2	B	0.84	0/716	0.99	0/978
2	D	0.87	1/745 (0.1%)	1.13	3/1018 (0.3%)
3	E	0.92	4/2596 (0.2%)	1.02	6/3515 (0.2%)
3	G	0.92	0/2599	1.08	5/3520 (0.1%)
All	All	0.89	6/8533 (0.1%)	1.04	18/11558 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	4
3	G	0	1
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	6	GLU	CA-C	9.22	1.64	1.52
3	E	6	GLU	N-CA	7.35	1.55	1.46
1	A	456	VAL	CA-CB	6.94	1.64	1.54
2	D	297	ASP	CG-OD1	6.71	1.38	1.25
3	E	309	ILE	CA-CB	5.45	1.60	1.54
3	E	6	GLU	CA-CB	-5.37	1.45	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	207	GLN	N-CA-C	11.84	127.07	109.07
3	G	138	SER	N-CA-C	-7.62	101.04	110.41
1	C	525	MET	N-CA-C	-7.55	101.43	108.22
3	G	138	SER	CA-C-N	-6.28	112.53	122.95
3	G	138	SER	C-N-CA	-6.28	112.53	122.95
2	D	297	ASP	N-CA-CB	6.07	120.81	110.50
1	A	482	VAL	CB-CA-C	5.82	115.03	109.33
3	E	39	VAL	CB-CA-C	-5.45	101.38	111.79
3	E	90	PHE	CA-C-N	5.42	125.50	119.32
3	E	90	PHE	C-N-CA	5.42	125.50	119.32
3	G	168	LYS	CA-C-N	5.24	127.30	120.28
3	G	168	LYS	C-N-CA	5.24	127.30	120.28
3	E	115	ILE	CA-C-N	5.16	123.42	119.66
3	E	115	ILE	C-N-CA	5.16	123.42	119.66
1	A	502	GLU	CA-C-N	-5.09	118.93	122.59
1	A	502	GLU	C-N-CA	-5.09	118.93	122.59
2	D	296	PHE	CB-CA-C	-5.02	101.20	113.15
3	E	100	PHE	N-CA-C	5.02	117.18	110.35

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	296	PHE	Peptide
2	D	206	GLU	Peptide
2	D	207	GLN	Peptide
2	D	219	ASN	Peptide
2	D	283	TYR	Peptide
3	G	317	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	916	0	903	24	0
1	C	914	0	909	47	0
2	B	699	0	681	20	0
2	D	727	0	730	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2551	0	2588	83	0
3	G	2554	0	2591	63	0
4	E	27	0	12	0	0
4	G	27	0	12	4	0
5	E	62	0	24	7	0
5	G	62	0	24	11	0
6	A	46	0	0	11	0
6	B	39	0	0	1	0
6	C	37	0	0	3	0
6	D	41	0	0	3	0
6	E	116	0	0	6	0
6	G	133	0	0	9	0
All	All	8951	0	8474	257	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 (257) 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:E:2:MET:CE	3:E:7:THR:HA	1.43	1.48
1:C:482:VAL:CG2	2:D:213:PRO:HG3	1.69	1.22
3:E:2:MET:HE1	3:E:7:THR:HA	1.23	1.18
3:E:307:ALA:HB3	5:E:1002[A]:ATP:O2A	1.42	1.18
3:E:2:MET:HE3	3:E:7:THR:CA	1.72	1.17
2:D:219:ASN:HA	2:D:220:THR:HB	1.28	1.15
3:E:2:MET:CE	3:E:7:THR:CA	2.27	1.13
6:A:339:HOH:O	2:B:292:MET:HG2	1.48	1.10
1:C:482:VAL:HG13	1:C:483:PRO:HD2	1.28	1.09
1:C:482:VAL:HG22	2:D:213:PRO:HG3	1.12	1.07
3:G:289:HIS:O	5:G:1501[B]:ATP:O2G	1.72	1.07
3:G:94:ILE:HG13	6:G:1618:HOH:O	1.54	1.05
3:E:2:MET:HE3	3:E:7:THR:HA	1.17	1.05
3:E:56:VAL:O	3:E:74[B]:MET:HE2	1.59	1.03
1:C:482:VAL:HG22	2:D:213:PRO:CG	1.92	1.00
1:C:513:THR:HG22	1:C:540:ASP:HA	1.45	0.97
1:C:481:THR:HG21	2:D:206:GLU:HG3	1.46	0.97
3:G:92:GLU:HG2	6:C:127:HOH:O	1.65	0.96
1:C:503:ILE:HD12	1:C:561:PRO:HG3	1.49	0.93
3:G:287:ARG:NH1	4:G:1003:ADP:O1B	2.02	0.93
3:E:289:HIS:O	5:E:1502[B]:ATP:O2G	1.87	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:162:THR:HG21	4:G:1003:ADP:O2B	1.68	0.92
2:D:219:ASN:CA	2:D:220:THR:HB	2.00	0.92
3:E:296:GLU:CD	3:E:296:GLU:H	1.81	0.89
1:C:482:VAL:HG13	1:C:483:PRO:CD	2.03	0.88
3:G:162:THR:HG22	3:G:165:ARG:H	1.39	0.88
3:E:123:HIS:HD2	3:E:125:MET:H	1.21	0.86
2:D:207:GLN:HG3	2:D:208:TYR:H	1.38	0.86
3:G:317:LYS:N	3:G:318:THR:CB	2.42	0.83
3:G:165:ARG:HH11	3:G:165:ARG:CG	1.92	0.82
3:G:13:LYS:HG3	6:G:1576:HOH:O	1.79	0.82
1:A:484:LYS:HD2	1:A:485:PRO:HD2	1.62	0.80
6:A:339:HOH:O	2:B:292:MET:CE	2.29	0.79
3:G:275:ARG:HH21	3:G:275:ARG:HG3	1.48	0.79
6:A:339:HOH:O	2:B:292:MET:HE2	1.84	0.78
3:E:2:MET:HE3	3:E:7:THR:N	1.98	0.78
3:E:30:THR:HB	6:E:1614:HOH:O	1.84	0.77
3:G:142:ARG:NH2	4:G:1003:ADP:O2A	2.17	0.77
1:C:503:ILE:HD11	1:C:505:HIS:CE1	2.20	0.77
1:C:482:VAL:HG21	2:D:213:PRO:HG3	1.66	0.75
1:A:506:CYS:HB3	1:A:513:THR:CG2	2.17	0.75
3:E:74[B]:MET:HE3	3:E:74[B]:MET:H	1.52	0.75
1:C:534:LYS:HD2	6:C:401:HOH:O	1.86	0.74
3:E:73:THR:HB	3:E:74[B]:MET:HE3	1.71	0.72
1:C:541:ILE:HG22	1:C:541:ILE:O	1.88	0.71
3:G:217:SER:N	5:G:1001[A]:ATP:O1B	2.22	0.71
1:C:537:GLY:HA2	1:C:557:LYS:HE3	1.72	0.71
3:E:3:ASP:HB3	3:E:6:GLU:H	1.56	0.71
3:E:123:HIS:CD2	3:E:125:MET:H	2.08	0.71
3:E:66:ASN:HB3	3:E:154:SER:HB2	1.73	0.70
2:D:207:GLN:HG3	2:D:208:TYR:N	2.07	0.70
3:G:217:SER:OG	5:G:1001[A]:ATP:O2G	2.10	0.70
5:E:1002[A]:ATP:O2B	5:E:1002[A]:ATP:O5'	2.09	0.69
2:D:235:HIS:HD2	2:D:261:LEU:HD21	1.56	0.69
2:D:219:ASN:CA	2:D:220:THR:CB	2.71	0.69
1:C:513:THR:HG22	1:C:540:ASP:CA	2.22	0.69
1:A:568:MET:HG3	6:A:24:HOH:O	1.92	0.69
3:G:275:ARG:HH21	3:G:275:ARG:CG	2.05	0.68
3:G:123:HIS:HD2	3:G:125:MET:H	1.41	0.68
3:G:195:LEU:HD22	3:G:303:ILE:HD12	1.73	0.67
3:E:309:ILE:HD13	3:E:309:ILE:N	2.09	0.66
6:G:1629:HOH:O	1:C:459:ARG:HB3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:275:ARG:HG3	3:G:275:ARG:NH2	2.10	0.66
3:E:304:LEU:HG	3:E:309:ILE:HD11	1.78	0.66
3:E:138:SER:O	3:E:139:ARG:HB2	1.96	0.65
3:E:4:VAL:CG1	3:E:5:GLN:N	2.60	0.64
2:D:218:SER:O	2:D:220:THR:HB	1.98	0.64
3:E:243:ASP:HB3	6:E:1602:HOH:O	1.97	0.63
2:D:206:GLU:O	2:D:207:GLN:HB2	1.97	0.63
3:E:307:ALA:CB	5:E:1002[A]:ATP:O2A	2.34	0.63
3:G:165:ARG:HH11	3:G:165:ARG:HG3	1.63	0.63
3:E:85:TYR:HB3	3:E:209:LYS:HZ2	1.64	0.62
1:A:557:LYS:HG3	6:A:86:HOH:O	1.99	0.62
2:D:223:GLU:HA	2:D:224:LEU:O	1.99	0.62
3:E:129:MET:CE	3:E:132:CYS:HB2	2.29	0.62
1:C:479:GLN:HB3	2:D:208:TYR:HB3	1.82	0.62
2:B:292:MET:HE3	2:B:294:LYS:HD2	1.81	0.61
1:C:482:VAL:CG2	2:D:213:PRO:CG	2.61	0.61
3:G:307:ALA:HB3	5:G:1001[A]:ATP:O2A	2.01	0.61
1:A:506:CYS:CB	1:A:513:THR:HG23	2.31	0.61
3:E:275:ARG:CG	3:E:275:ARG:HH21	2.14	0.61
3:E:109:GLU:HB3	3:E:115:ILE:HG13	1.82	0.61
1:A:525:MET:HB2	1:A:526:PRO:HD2	1.84	0.60
3:E:139:ARG:NH2	5:E:1002[A]:ATP:O1A	2.34	0.60
3:G:123:HIS:CD2	3:G:125:MET:H	2.19	0.60
1:C:511:LYS:HD3	1:C:513:THR:HG21	1.83	0.60
5:G:1001[A]:ATP:O2B	5:G:1001[A]:ATP:O5'	2.20	0.60
1:A:482:VAL:HG22	2:B:213:PRO:HG3	1.82	0.59
3:E:294:VAL:HG21	3:E:298:LEU:HD23	1.85	0.59
1:A:506:CYS:CB	1:A:513:THR:CG2	2.81	0.59
3:E:4:VAL:HG13	3:E:5:GLN:N	2.16	0.59
3:E:74[B]:MET:SD	3:E:334:VAL:HG12	2.43	0.59
3:G:240:LEU:HG	3:G:248:ASN:HB3	1.84	0.59
3:G:165:ARG:CG	3:G:165:ARG:NH1	2.63	0.58
1:A:557:LYS:CG	6:A:86:HOH:O	2.50	0.58
3:E:263:ASN:CG	3:E:263:ASN:O	2.46	0.58
3:E:187:MET:HE1	3:E:276:LEU:CD2	2.34	0.58
3:E:230:ASN:OD1	3:E:260:ARG:NH2	2.36	0.58
2:D:223:GLU:HA	2:D:224:LEU:C	2.29	0.58
2:B:244:ASN:OD1	2:B:247:TYR:HB3	2.04	0.57
2:D:290:THR:CG2	6:D:321:HOH:O	2.53	0.57
1:C:511:LYS:HB3	1:C:513:THR:HG23	1.86	0.57
3:G:165:ARG:HH11	3:G:165:ARG:HG2	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:90:PHE:CZ	1:C:573:LEU:HD22	2.40	0.56
3:E:133:LEU:HD12	6:E:1515:HOH:O	2.05	0.56
1:A:560:PHE:HD2	1:A:564:ASP:OD1	1.88	0.56
6:A:6:HOH:O	2:B:290:THR:HG23	2.06	0.56
3:E:129:MET:HE2	3:E:132:CYS:HB2	1.87	0.56
1:A:557:LYS:HD2	6:A:86:HOH:O	2.05	0.55
3:G:316:ASP:C	3:G:318:THR:CB	2.79	0.55
3:E:139:ARG:CZ	3:E:139:ARG:HA	2.35	0.55
1:C:503:ILE:HG23	1:C:513:THR:O	2.05	0.55
1:C:503:ILE:HD12	1:C:561:PRO:CG	2.30	0.55
1:C:541:ILE:O	1:C:541:ILE:CG2	2.53	0.54
3:E:2:MET:CE	3:E:7:THR:CB	2.86	0.54
3:G:317:LYS:CA	3:G:318:THR:CB	2.86	0.54
3:G:307:ALA:HB2	5:G:1501[B]:ATP:O1B	2.07	0.54
3:E:71:LEU:HD22	3:E:144:PRO:HD3	1.90	0.54
3:E:187:MET:HE1	3:E:276:LEU:HD21	1.89	0.54
3:G:142:ARG:HD2	3:G:334:VAL:O	2.08	0.54
3:G:195:LEU:HD22	3:G:303:ILE:CD1	2.37	0.53
2:D:292:MET:CE	2:D:294:LYS:HD2	2.37	0.53
2:D:290:THR:HG22	6:D:321:HOH:O	2.08	0.53
3:E:214:LYS:NZ	6:E:1575:HOH:O	2.41	0.53
6:A:6:HOH:O	2:B:290:THR:CG2	2.56	0.53
2:B:251:GLN:HE22	3:G:54:ASN:HD22	1.57	0.53
3:E:129:MET:HE2	3:E:129:MET:HA	1.91	0.53
6:A:302:HOH:O	3:E:92:GLU:HG2	2.09	0.53
2:D:295:ASN:ND2	3:E:41:LEU:HD23	2.23	0.53
3:E:92:GLU:HG3	6:E:1581:HOH:O	2.09	0.53
1:C:503:ILE:CD1	1:C:506:CYS:SG	2.97	0.53
1:C:519:LEU:HD13	1:C:533:VAL:HG22	1.91	0.53
3:G:307:ALA:HB3	5:G:1001[A]:ATP:PA	2.49	0.53
1:C:481:THR:HG21	2:D:206:GLU:CG	2.31	0.53
3:E:307:ALA:HB2	5:E:1502[B]:ATP:O1B	2.08	0.53
3:G:93:ALA:O	3:G:96:GLU:HB3	2.09	0.52
1:C:540:ASP:HB3	3:E:151:GLU:OE2	2.08	0.52
3:E:121:TYR:HD1	3:E:121:TYR:H	1.54	0.52
3:E:304:LEU:CG	3:E:309:ILE:HD11	2.39	0.52
2:D:282:ARG:HG2	2:D:284:HIS:O	2.11	0.51
3:E:233:GLU:O	3:E:236:ASP:HB2	2.11	0.51
3:G:308:ASP:OD2	5:G:1501[B]:ATP:O2'	2.24	0.51
2:D:228:LYS:HB3	6:D:330:HOH:O	2.09	0.51
2:D:235:HIS:CD2	2:D:261:LEU:HD21	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:ARG:HG2	2:B:284:HIS:O	2.11	0.51
2:B:244:ASN:CG	2:B:247:TYR:HB3	2.36	0.51
2:D:206:GLU:O	2:D:207:GLN:OE1	2.30	0.50
3:E:2:MET:HE2	3:E:7:THR:OG1	2.11	0.50
3:E:123:HIS:HD2	3:E:125:MET:N	2.01	0.50
3:E:187:MET:HE3	3:E:312:TYR:CE1	2.46	0.50
3:E:121:TYR:CD1	3:E:121:TYR:N	2.77	0.49
3:E:48:SER:O	3:E:52:LEU:HB2	2.12	0.49
1:C:535:SER:HB3	2:D:263:ASN:HB3	1.94	0.49
3:E:232:TYR:OH	3:E:240:LEU:HD22	2.11	0.49
3:G:162:THR:CG2	3:G:165:ARG:H	2.19	0.49
2:D:223:GLU:OE1	2:D:224:LEU:HA	2.13	0.48
3:E:221:ILE:HD11	3:E:232:TYR:HB2	1.95	0.48
3:G:81:ILE:CD1	3:G:94:ILE:HD11	2.44	0.48
1:C:482:VAL:CG1	1:C:483:PRO:CD	2.85	0.48
3:G:123:HIS:HD2	3:G:125:MET:N	2.10	0.48
3:E:275:ARG:CG	3:E:275:ARG:NH2	2.74	0.48
3:E:135:MET:HE1	3:E:166:ILE:HD12	1.95	0.48
6:G:1629:HOH:O	1:C:459:ARG:CB	2.57	0.48
3:G:328:ASP:OD2	3:G:329:ASN:N	2.47	0.48
1:A:575:SER:O	1:A:576:ALA:C	2.57	0.47
1:A:466:LEU:CD1	1:A:497:ILE:HD11	2.43	0.47
3:G:275:ARG:CG	3:G:275:ARG:NH2	2.72	0.47
3:E:74[B]:MET:SD	3:E:334:VAL:CG1	3.03	0.47
3:G:165:ARG:NH1	4:G:1003:ADP:O2B	2.47	0.47
3:G:290:ARG:HE	5:G:1001[A]:ATP:PG	2.38	0.47
3:G:307:ALA:CB	5:G:1001[A]:ATP:O2A	2.63	0.47
3:G:77:PHE:O	3:G:81:ILE:HG12	2.15	0.47
3:E:139:ARG:HA	3:E:139:ARG:NE	2.30	0.47
3:E:85:TYR:HB3	3:E:209:LYS:NZ	2.27	0.47
3:G:96:GLU:HG2	3:G:99:LYS:HE2	1.97	0.47
3:E:265:ASP:OD2	3:E:265:ASP:N	2.46	0.47
2:B:282:ARG:NH1	2:B:287:TYR:OH	2.48	0.47
3:G:18:PHE:CD1	3:G:174:CYS:SG	3.08	0.47
1:A:519:LEU:HD12	1:A:533:VAL:HG22	1.98	0.46
3:G:135:MET:O	3:G:138:SER:O	2.34	0.46
1:A:506:CYS:HB3	1:A:513:THR:HG23	1.91	0.46
1:C:475:ARG:NH2	1:C:572:LYS:O	2.49	0.46
3:E:74[B]:MET:H	3:E:74[B]:MET:CE	2.24	0.46
1:A:557:LYS:HB3	6:G:1608:HOH:O	2.15	0.46
3:G:240:LEU:HD13	6:G:1572:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LYS:HB3	1:A:511:LYS:HE2	1.82	0.46
3:G:196:ALA:HB2	3:G:214:LYS:HD2	1.99	0.45
3:G:230:ASN:OD1	3:G:260:ARG:NH2	2.45	0.45
3:E:129:MET:HE2	3:E:129:MET:O	2.17	0.45
3:G:91:PRO:HD2	6:C:127:HOH:O	2.16	0.45
3:G:162:THR:HG23	3:G:164:TYR:H	1.80	0.45
3:G:240:LEU:HD12	3:G:240:LEU:HA	1.83	0.45
1:C:483:PRO:HB2	1:C:490:TYR:CE2	2.51	0.45
3:E:275:ARG:NH2	3:E:275:ARG:HG3	2.32	0.45
3:G:60:LEU:HD21	3:G:72:LEU:HB2	1.99	0.45
3:E:185:ASN:C	3:E:185:ASN:HD22	2.24	0.45
2:B:235:HIS:HD2	2:B:261:LEU:HD21	1.82	0.45
3:G:234:SER:OG	3:G:334:VAL:HG11	2.17	0.45
2:D:292:MET:HE2	2:D:294:LYS:HD2	1.99	0.45
1:A:564:ASP:OD2	3:G:63:SER:HB2	2.17	0.45
3:E:2:MET:CE	3:E:7:THR:OG1	2.65	0.44
1:C:458:CYS:HB2	1:C:465:ILE:HD13	1.99	0.44
1:C:497:ILE:HB	1:C:519:LEU:HB2	1.99	0.44
3:E:120:ILE:H	3:E:120:ILE:HG13	1.52	0.44
1:A:557:LYS:CB	6:G:1608:HOH:O	2.65	0.44
1:C:482:VAL:CG1	1:C:483:PRO:N	2.80	0.44
3:E:309:ILE:N	3:E:309:ILE:CD1	2.80	0.44
3:G:97:ILE:HD13	6:G:1618:HOH:O	2.18	0.44
2:B:258:ASN:OD1	2:B:260:VAL:HG22	2.18	0.43
1:C:524:VAL:HG22	2:D:232:LEU:HD13	2.00	0.43
5:G:1001[A]:ATP:H5'2	6:G:1508:HOH:O	2.18	0.43
1:A:506:CYS:SG	1:A:513:THR:HG21	2.58	0.43
3:G:165:ARG:NH1	3:G:165:ARG:HG2	2.32	0.43
1:C:465:ILE:O	1:C:469:VAL:HG23	2.18	0.43
2:D:218:SER:C	2:D:220:THR:HB	2.44	0.43
3:E:129:MET:CE	3:E:129:MET:HA	2.48	0.43
3:E:290:ARG:HE	5:E:1002[A]:ATP:PG	2.39	0.43
3:G:233:GLU:O	3:G:236:ASP:HB2	2.19	0.43
3:E:68:PHE:CZ	3:E:144:PRO:HG3	2.54	0.43
1:A:535:SER:HB3	2:B:263:ASN:HB3	2.00	0.42
2:B:235:HIS:CD2	2:B:261:LEU:HD21	2.54	0.42
1:C:511:LYS:HD3	1:C:513:THR:CG2	2.49	0.42
3:E:96:GLU:HG2	3:E:99:LYS:HD3	2.01	0.42
1:C:503:ILE:HD11	1:C:506:CYS:SG	2.60	0.42
3:E:80:VAL:O	3:E:84:TYR:HD2	2.01	0.42
1:C:503:ILE:O	1:C:503:ILE:HG12	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:THR:HG22	1:C:540:ASP:CB	2.50	0.42
3:E:92:GLU:CG	6:E:1581:HOH:O	2.66	0.42
1:C:454:PHE:CZ	2:D:261:LEU:HD13	2.54	0.42
1:A:525:MET:O	1:A:526:PRO:C	2.61	0.42
1:C:462:ALA:HB3	1:C:463:PRO:HD3	2.01	0.42
2:D:235:HIS:O	2:D:261:LEU:HD11	2.20	0.42
2:D:233:PRO:HG2	2:D:236:LEU:HD12	2.02	0.42
2:B:210:THR:HG23	2:B:211:GLU:HG2	2.02	0.42
3:E:180:LEU:O	3:E:277:ASP:HB3	2.20	0.42
2:D:218:SER:O	2:D:220:THR:CB	2.66	0.42
3:G:10:GLY:O	3:G:14:GLU:HG2	2.20	0.41
3:E:261:PRO:C	3:E:263:ASN:H	2.27	0.41
3:E:4:VAL:CG1	3:E:5:GLN:H	2.31	0.41
3:G:86:GLN:HE21	3:G:86:GLN:HB3	1.61	0.41
2:B:247:TYR:H	2:B:247:TYR:HD1	1.67	0.41
2:B:205:SER:N	6:B:323:HOH:O	2.53	0.41
1:C:456:VAL:HG13	1:C:531:LEU:HB3	2.02	0.41
2:D:223:GLU:CA	2:D:224:LEU:C	2.92	0.41
3:E:121:TYR:HD1	3:E:121:TYR:N	2.18	0.41
1:A:466:LEU:HD11	1:A:497:ILE:HD11	2.03	0.41
3:G:81:ILE:HD12	3:G:94:ILE:HD11	2.03	0.41
1:C:482:VAL:HG13	1:C:483:PRO:N	2.35	0.41
2:B:251:GLN:O	3:G:33:ARG:NH1	2.53	0.40
1:C:503:ILE:CG2	1:C:513:THR:O	2.69	0.40
3:G:90:PHE:HA	3:G:91:PRO:HD3	1.83	0.40
3:E:2:MET:HB2	3:E:7:THR:OG1	2.22	0.40
3:G:232:TYR:OH	3:G:240:LEU:HD22	2.21	0.40
1:C:453:HIS:CE1	1:C:457:ARG:HG3	2.56	0.40
3:E:35:ILE:O	3:E:59:PRO:HD2	2.21	0.40
1:A:557:LYS:HE2	6:A:326:HOH:O	2.21	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	110/137 (80%)	109 (99%)	1 (1%)	0	100	100
1	C	110/137 (80%)	104 (94%)	6 (6%)	0	100	100
2	B	87/97 (90%)	82 (94%)	5 (6%)	0	100	100
2	D	90/97 (93%)	80 (89%)	9 (10%)	1 (1%)	11	16
3	E	321/334 (96%)	313 (98%)	8 (2%)	0	100	100
3	G	322/334 (96%)	311 (97%)	10 (3%)	1 (0%)	36	49
All	All	1040/1136 (92%)	999 (96%)	39 (4%)	2 (0%)	43	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	220	THR
3	G	263	ASN

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	97/120 (81%)	85 (88%)	12 (12%)	4	6
1	C	96/120 (80%)	83 (86%)	13 (14%)	4	4
2	B	77/88 (88%)	71 (92%)	6 (8%)	11	18
2	D	83/88 (94%)	73 (88%)	10 (12%)	5	6
3	E	286/296 (97%)	251 (88%)	35 (12%)	5	6
3	G	285/296 (96%)	253 (89%)	32 (11%)	6	8
All	All	924/1008 (92%)	816 (88%)	108 (12%)	5	7

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	456	VAL
1	A	458	CYS
1	A	461	ASP
1	A	479	GLN
1	A	482	VAL
1	A	487	ASN
1	A	513	THR
1	A	519	LEU
1	A	557	LYS
1	A	565	LEU
1	A	569	LEU
2	B	210	THR
2	B	232	LEU
2	B	245	THR
2	B	262	LEU
2	B	290	THR
2	B	292	MET
3	G	39	VAL
3	G	43	VAL
3	G	51	THR
3	G	52	LEU
3	G	63	SER
3	G	64	GLU
3	G	82	LYS
3	G	86	GLN
3	G	92	GLU
3	G	97	ILE
3	G	102	LEU
3	G	110	ARG
3	G	118	GLU
3	G	120	ILE
3	G	142	ARG
3	G	161	LEU
3	G	162	THR
3	G	165	ARG
3	G	172	MET
3	G	181	ARG
3	G	184	LEU
3	G	185	ASN
3	G	214	LYS
3	G	227	THR
3	G	228	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	235	VAL
3	G	240	LEU
3	G	257	LEU
3	G	263	ASN
3	G	275	ARG
3	G	298	LEU
3	G	299	LYS
1	C	456	VAL
1	C	458	CYS
1	C	459	ARG
1	C	482	VAL
1	C	502	GLU
1	C	503	ILE
1	C	509	GLU
1	C	525	MET
1	C	534	LYS
1	C	539	LYS
1	C	540	ASP
1	C	565	LEU
1	C	569	LEU
2	D	206	GLU
2	D	207	GLN
2	D	223	GLU
2	D	224	LEU
2	D	225	LYS
2	D	231	SER
2	D	262	LEU
2	D	270	THR
2	D	285	ARG
2	D	290	THR
3	E	4	VAL
3	E	20	ARG
3	E	30	THR
3	E	39	VAL
3	E	52	LEU
3	E	66	ASN
3	E	82	LYS
3	E	92	GLU
3	E	99	LYS
3	E	102	LEU
3	E	110	ARG
3	E	119	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	120	ILE
3	E	121	TYR
3	E	129	MET
3	E	139	ARG
3	E	161	LEU
3	E	184	LEU
3	E	185	ASN
3	E	188	THR
3	E	207	VAL
3	E	214	LYS
3	E	227	THR
3	E	228	LEU
3	E	235	VAL
3	E	240	LEU
3	E	243	ASP
3	E	257	LEU
3	E	265	ASP
3	E	275	ARG
3	E	276	LEU
3	E	287	ARG
3	E	296	GLU
3	E	309	ILE
3	E	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	536	ASN
2	B	207	GLN
2	B	251	GLN
2	B	259	HIS
2	B	263	ASN
2	B	269	ASN
3	G	66	ASN
3	G	86	GLN
3	G	123	HIS
3	G	163	GLN
3	G	185	ASN
3	G	242	GLN
3	G	263	ASN
3	G	311	ASN
3	G	329	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	453	HIS
1	C	505	HIS
2	D	207	GLN
2	D	235	HIS
2	D	251	GLN
2	D	263	ASN
2	D	295	ASN
3	E	5	GLN
3	E	53	ASN
3	E	54	ASN
3	E	123	HIS
3	E	163	GLN
3	E	185	ASN
3	E	263	ASN

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](#)

6 ligands are modelled in this entry.

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
5	ATP	E	1002[A]	-	32,33,33	1.34	4 (12%)	48,52,52	1.81	10 (20%)
4	ADP	G	1003	-	28,29,29	1.37	2 (7%)	43,45,45	1.82	9 (20%)
5	ATP	G	1001[A]	-	32,33,33	1.40	3 (9%)	48,52,52	1.89	12 (25%)
5	ATP	E	1502[B]	-	32,33,33	1.37	5 (15%)	48,52,52	1.78	11 (22%)
5	ATP	G	1501[B]	-	32,33,33	1.45	4 (12%)	48,52,52	1.81	12 (25%)
4	ADP	E	1004	-	28,29,29	1.25	3 (10%)	43,45,45	1.84	12 (27%)

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
5	ATP	E	1002[A]	-	-	6/22/38/38	0/3/3/3
4	ADP	G	1003	-	-	0/16/32/32	0/3/3/3
5	ATP	G	1001[A]	-	-	6/22/38/38	0/3/3/3
5	ATP	E	1502[B]	-	-	2/22/38/38	0/3/3/3
5	ATP	G	1501[B]	-	-	6/22/38/38	0/3/3/3
4	ADP	E	1004	-	-	0/16/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1501[B]	ATP	C5-C4	5.18	1.48	1.39
4	G	1003	ADP	C5-C4	5.07	1.48	1.39
5	G	1001[A]	ATP	C5-C4	5.07	1.48	1.39
5	E	1002[A]	ATP	C5-C4	4.70	1.47	1.39
5	E	1502[B]	ATP	C5-C4	4.62	1.47	1.39
4	E	1004	ADP	C5-C4	3.65	1.45	1.39
4	G	1003	ADP	C5-C6	3.04	1.49	1.41
5	G	1501[B]	ATP	PB-O3A	3.00	1.62	1.59
5	G	1501[B]	ATP	C5-C6	2.86	1.49	1.41
5	G	1001[A]	ATP	C5-C6	2.85	1.48	1.41
5	E	1002[A]	ATP	C5-C6	2.64	1.48	1.41
5	E	1502[B]	ATP	C5-C6	2.61	1.48	1.41
4	E	1004	ADP	PA-O3A	2.51	1.62	1.59
5	G	1001[A]	ATP	C8-N7	2.50	1.36	1.31
5	G	1501[B]	ATP	C8-N7	2.46	1.36	1.31
5	E	1002[A]	ATP	C5-N7	-2.30	1.34	1.39
5	E	1002[A]	ATP	C8-N7	2.24	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1502[B]	ATP	C8-N7	2.22	1.35	1.31
4	E	1004	ADP	C5-C6	2.13	1.46	1.41
5	E	1502[B]	ATP	C4-N9	-2.03	1.33	1.37
5	E	1502[B]	ATP	C5-N7	-2.01	1.35	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1501[B]	ATP	C5-C4-N3	-5.58	119.04	126.72
5	G	1001[A]	ATP	C5-C4-N3	-5.49	119.16	126.72
5	E	1002[A]	ATP	C5-C4-N3	-5.44	119.22	126.72
5	E	1502[B]	ATP	C5-C4-N3	-4.95	119.89	126.72
4	G	1003	ADP	C5-C4-N3	-4.83	120.07	126.72
4	E	1004	ADP	C5-C4-N3	-4.69	120.27	126.72
5	G	1501[B]	ATP	N3-C4-N9	4.59	134.97	127.17
5	E	1002[A]	ATP	N3-C4-N9	4.58	134.96	127.17
5	G	1001[A]	ATP	N3-C4-N9	4.52	134.85	127.17
4	E	1004	ADP	N3-C4-N9	4.44	134.72	127.17
4	G	1003	ADP	N3-C4-N9	4.40	134.65	127.17
5	E	1502[B]	ATP	N3-C4-N9	4.33	134.53	127.17
4	E	1004	ADP	N3-C2-N1	-4.31	122.06	128.58
5	E	1502[B]	ATP	N3-C2-N1	-3.94	122.62	128.58
5	E	1002[A]	ATP	C2-N3-C4	3.80	121.11	111.83
5	E	1002[A]	ATP	N3-C2-N1	-3.79	122.84	128.58
5	E	1502[B]	ATP	C2-N3-C4	3.76	121.02	111.83
5	E	1502[B]	ATP	C4-N9-C8	3.65	109.57	105.74
5	G	1001[A]	ATP	C2-N3-C4	3.64	120.72	111.83
4	E	1004	ADP	C2-N3-C4	3.59	120.59	111.83
5	G	1501[B]	ATP	C2-N3-C4	3.56	120.52	111.83
5	G	1001[A]	ATP	N3-C2-N1	-3.53	123.24	128.58
5	G	1001[A]	ATP	C4-C5-N7	-3.42	106.67	110.58
4	G	1003	ADP	C2-N3-C4	3.37	120.05	111.83
5	G	1501[B]	ATP	C4-C5-N7	-3.35	106.75	110.58
4	G	1003	ADP	N3-C2-N1	-3.34	123.52	128.58
5	G	1501[B]	ATP	N3-C2-N1	-3.19	123.75	128.58
5	G	1001[A]	ATP	O4'-C1'-N9	3.19	114.21	108.09
5	E	1002[A]	ATP	C4-C5-N7	-3.16	106.96	110.58
5	E	1002[A]	ATP	C4-N9-C8	3.09	108.98	105.74
5	G	1001[A]	ATP	C4-N9-C8	3.08	108.97	105.74
4	G	1003	ADP	O2B-PB-O3A	-3.06	94.37	104.64
5	E	1502[B]	ATP	C4-C5-N7	-3.02	107.12	110.58
5	G	1501[B]	ATP	C4-N9-C8	3.02	108.90	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1002[A]	ATP	O4'-C1'-N9	2.99	113.84	108.09
4	G	1003	ADP	C4-N9-C8	2.91	108.79	105.74
4	E	1004	ADP	C4-N9-C8	2.87	108.75	105.74
5	E	1502[B]	ATP	N9-C8-N7	-2.75	110.03	113.94
4	G	1003	ADP	C2-N1-C6	2.72	123.20	118.73
5	G	1501[B]	ATP	C5-N7-C8	2.72	107.72	103.45
5	E	1502[B]	ATP	C5-N7-C8	2.70	107.69	103.45
5	G	1001[A]	ATP	C5-N7-C8	2.69	107.67	103.45
5	E	1002[A]	ATP	C5-N7-C8	2.62	107.56	103.45
4	G	1003	ADP	C4-C5-N7	-2.60	107.61	110.58
4	G	1003	ADP	O3B-PB-O1B	2.54	120.74	110.83
5	E	1502[B]	ATP	C6-C5-N7	2.41	136.74	132.09
5	G	1501[B]	ATP	N9-C8-N7	-2.33	110.62	113.94
5	G	1001[A]	ATP	C6-C5-N7	2.32	136.57	132.09
4	E	1004	ADP	C2-N1-C6	2.32	122.54	118.73
5	E	1002[A]	ATP	N9-C8-N7	-2.30	110.67	113.94
5	G	1001[A]	ATP	N9-C8-N7	-2.29	110.69	113.94
5	G	1001[A]	ATP	O3A-PB-O1B	-2.28	103.83	110.70
5	G	1501[B]	ATP	O3A-PA-O1A	-2.27	103.89	110.70
5	G	1001[A]	ATP	C2-N1-C6	2.26	122.44	118.73
5	G	1501[B]	ATP	C6-C5-N7	2.23	136.39	132.09
5	E	1002[A]	ATP	C6-C5-N7	2.20	136.34	132.09
4	E	1004	ADP	O3B-PB-O2B	2.19	116.00	107.80
5	G	1501[B]	ATP	O2A-PA-O3A	2.18	113.17	107.27
4	E	1004	ADP	O4'-C1'-N9	2.15	112.22	108.09
4	E	1004	ADP	O3B-PB-O3A	-2.14	97.45	104.64
4	E	1004	ADP	N6-C6-N1	2.11	123.08	118.38
5	E	1502[B]	ATP	C2-N1-C6	2.07	122.12	118.73
5	G	1501[B]	ATP	C2-N1-C6	2.05	122.09	118.73
5	E	1502[B]	ATP	O4'-C1'-N9	-2.04	104.17	108.09
4	E	1004	ADP	C4-C5-N7	-2.02	108.27	110.58
4	E	1004	ADP	C5-N7-C8	2.01	106.61	103.45

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1001[A]	ATP	C5'-O5'-PA-O1A
5	G	1001[A]	ATP	C5'-O5'-PA-O3A
5	G	1501[B]	ATP	C5'-O5'-PA-O1A
5	G	1501[B]	ATP	C5'-O5'-PA-O2A
5	G	1501[B]	ATP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	E	1002[A]	ATP	C5'-O5'-PA-O1A
5	G	1001[A]	ATP	PB-O3A-PA-O5'
5	E	1002[A]	ATP	PB-O3A-PA-O5'
5	G	1501[B]	ATP	C2'-C1'-N9-C8
5	E	1502[B]	ATP	C2'-C1'-N9-C8
5	G	1001[A]	ATP	C5'-O5'-PA-O2A
5	G	1001[A]	ATP	PB-O3B-PG-O1G
5	G	1001[A]	ATP	PB-O3A-PA-O1A
5	E	1502[B]	ATP	PA-O3A-PB-O2B
5	G	1501[B]	ATP	C2'-C1'-N9-C4
5	E	1002[A]	ATP	PB-O3B-PG-O1G
5	G	1501[B]	ATP	O4'-C1'-N9-C8
5	E	1002[A]	ATP	PA-O3A-PB-O1B
5	E	1002[A]	ATP	PA-O3A-PB-O2B
5	E	1002[A]	ATP	PB-O3A-PA-O2A

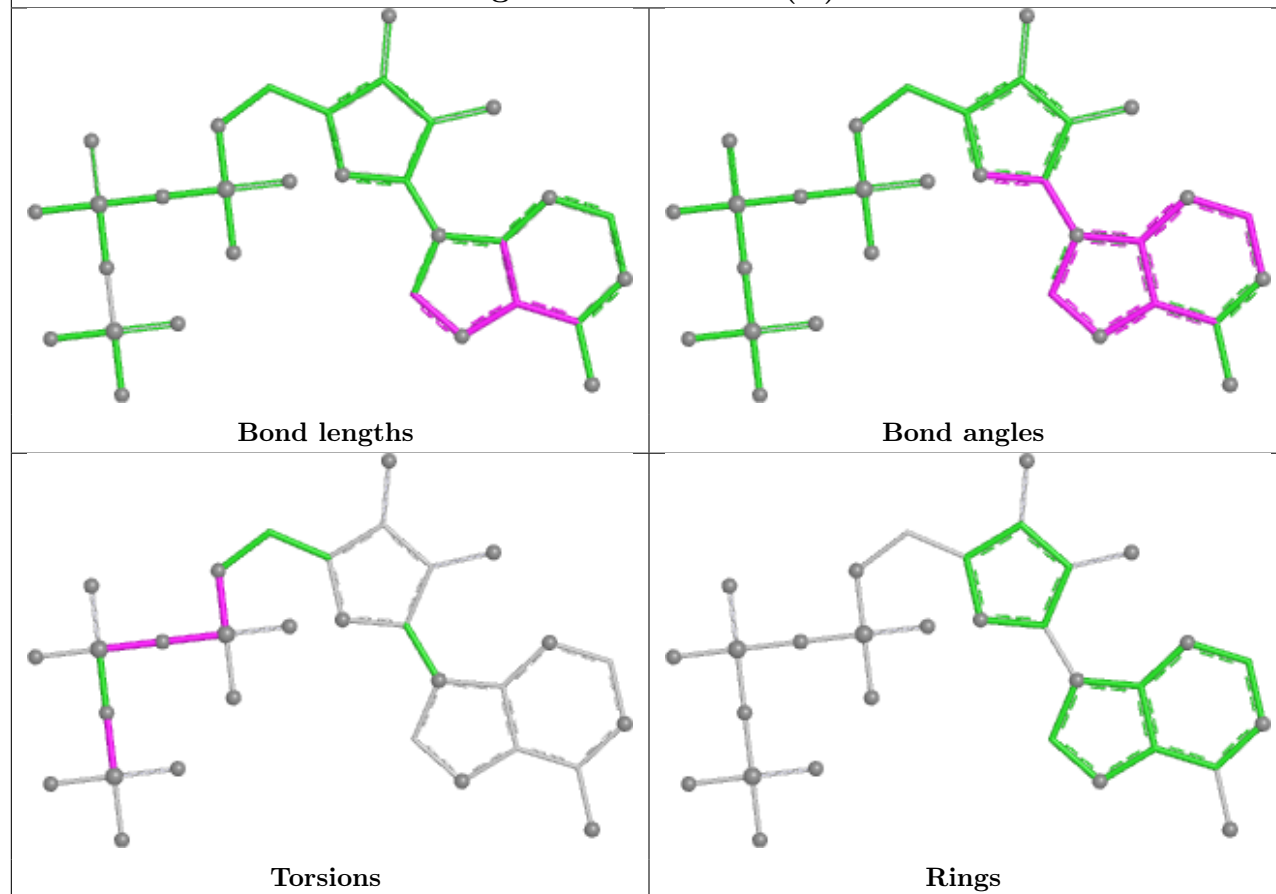
There are no ring outliers.

5 monomers are involved in 22 short contacts:

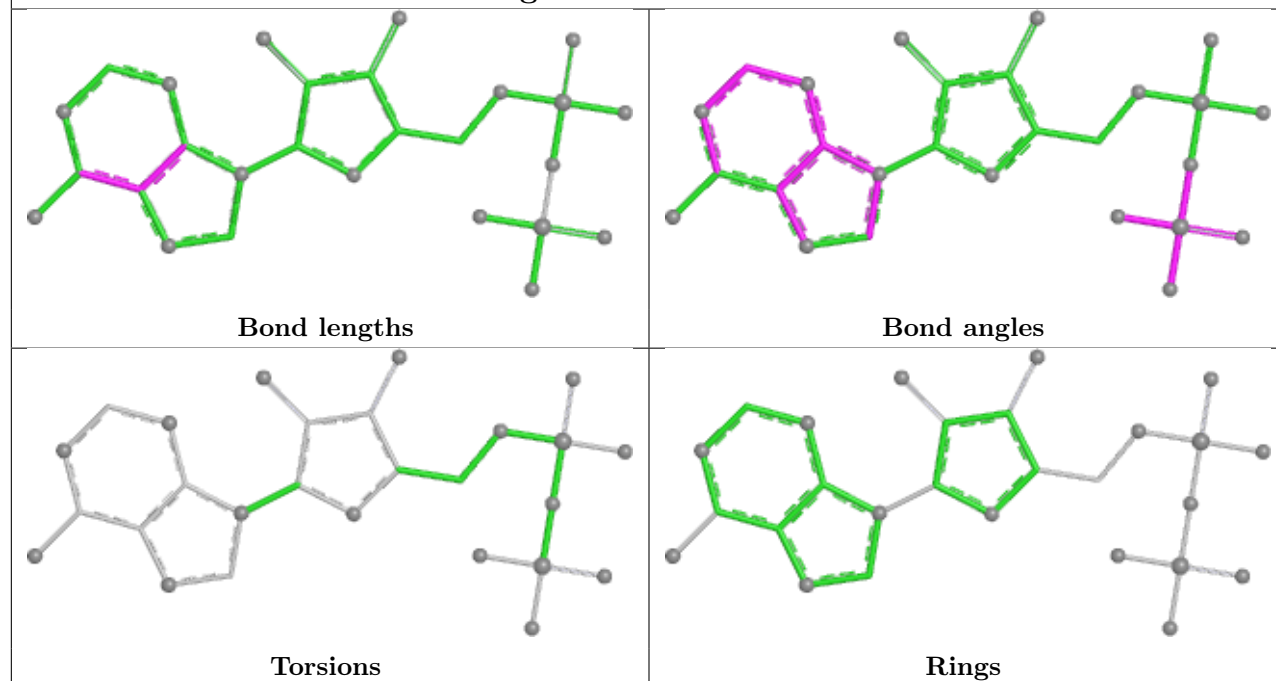
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1002[A]	ATP	5	0
4	G	1003	ADP	4	0
5	G	1001[A]	ATP	8	0
5	E	1502[B]	ATP	2	0
5	G	1501[B]	ATP	3	0

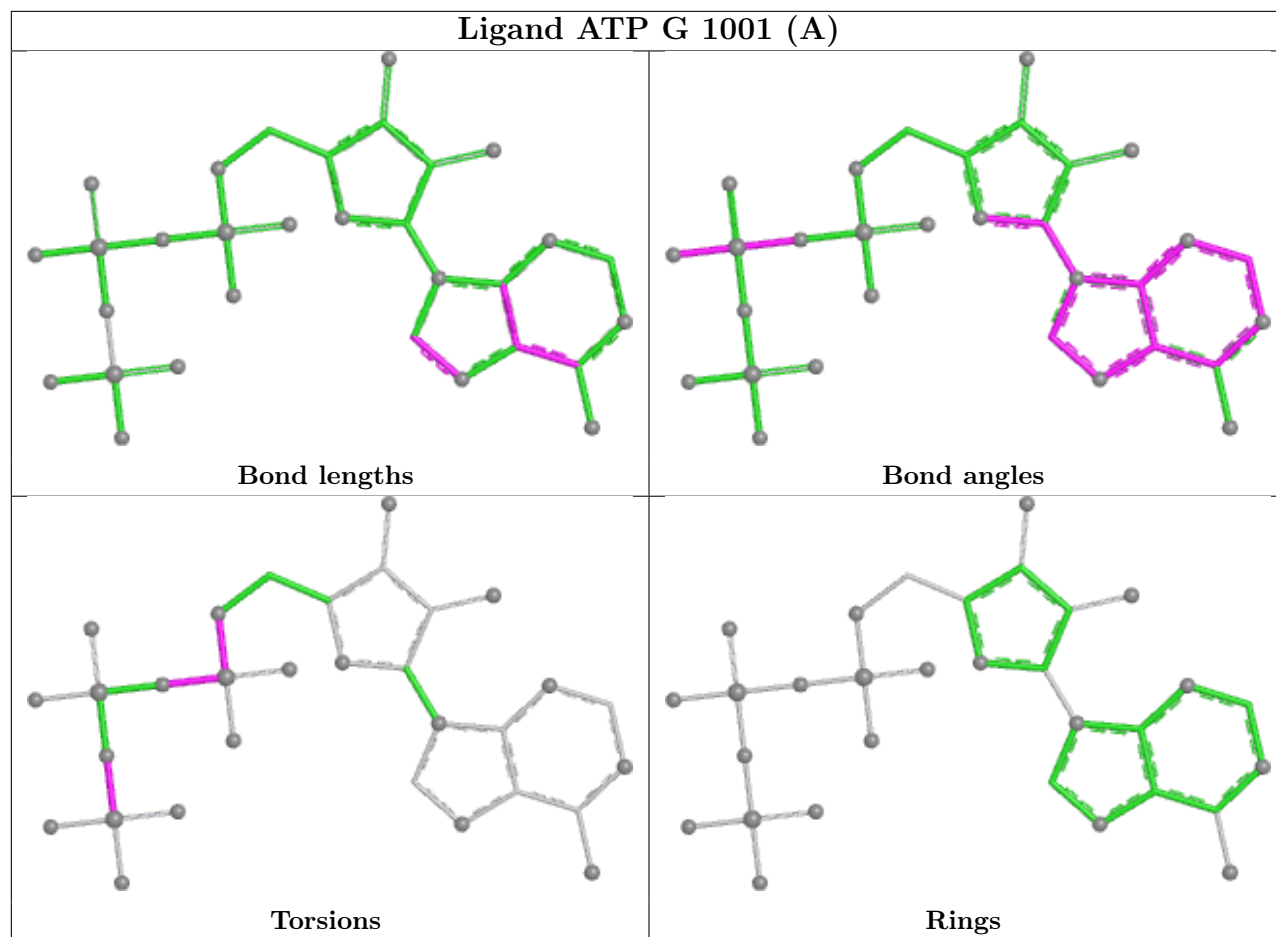
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

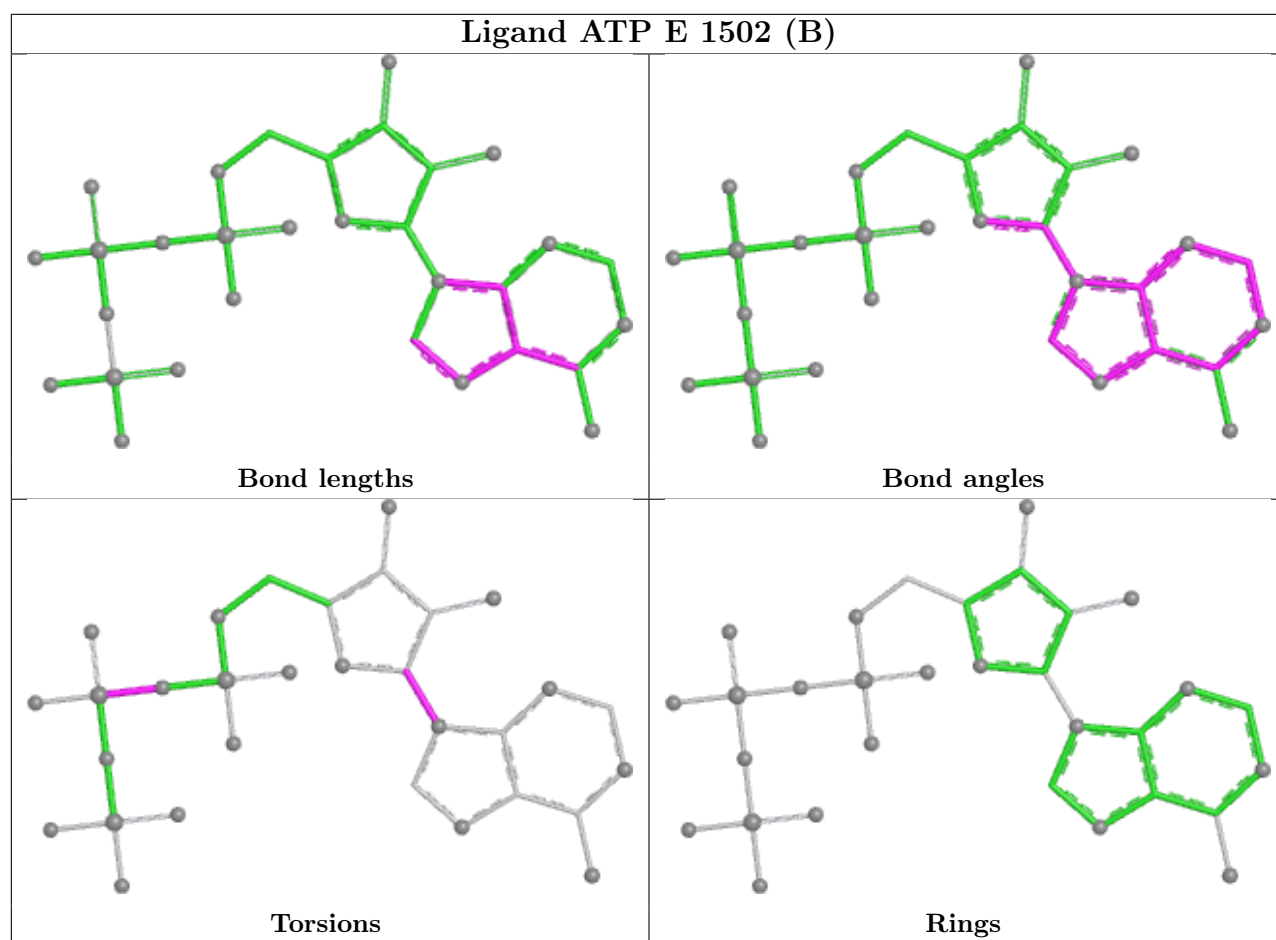
Ligand ATP E 1002 (A)



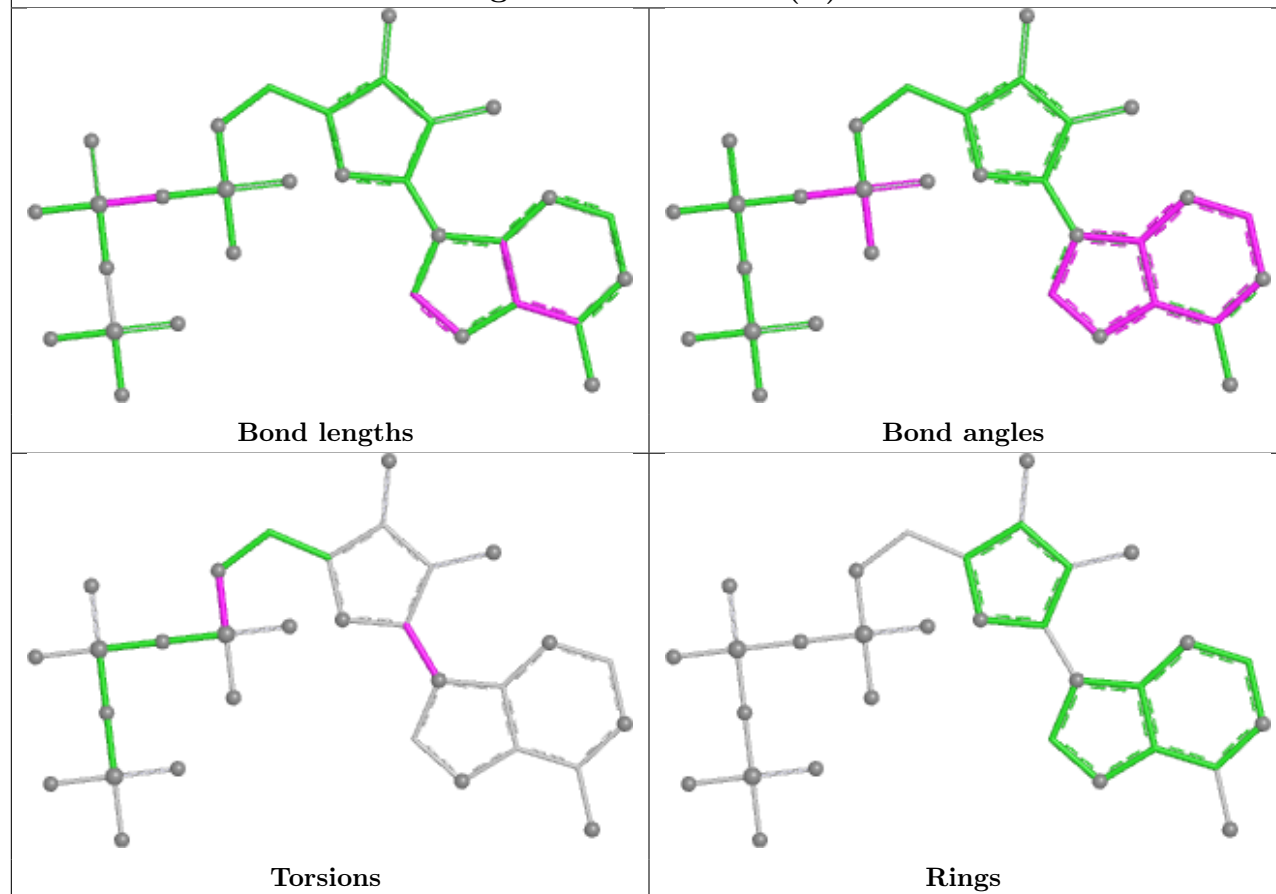
Ligand ADP G 1003



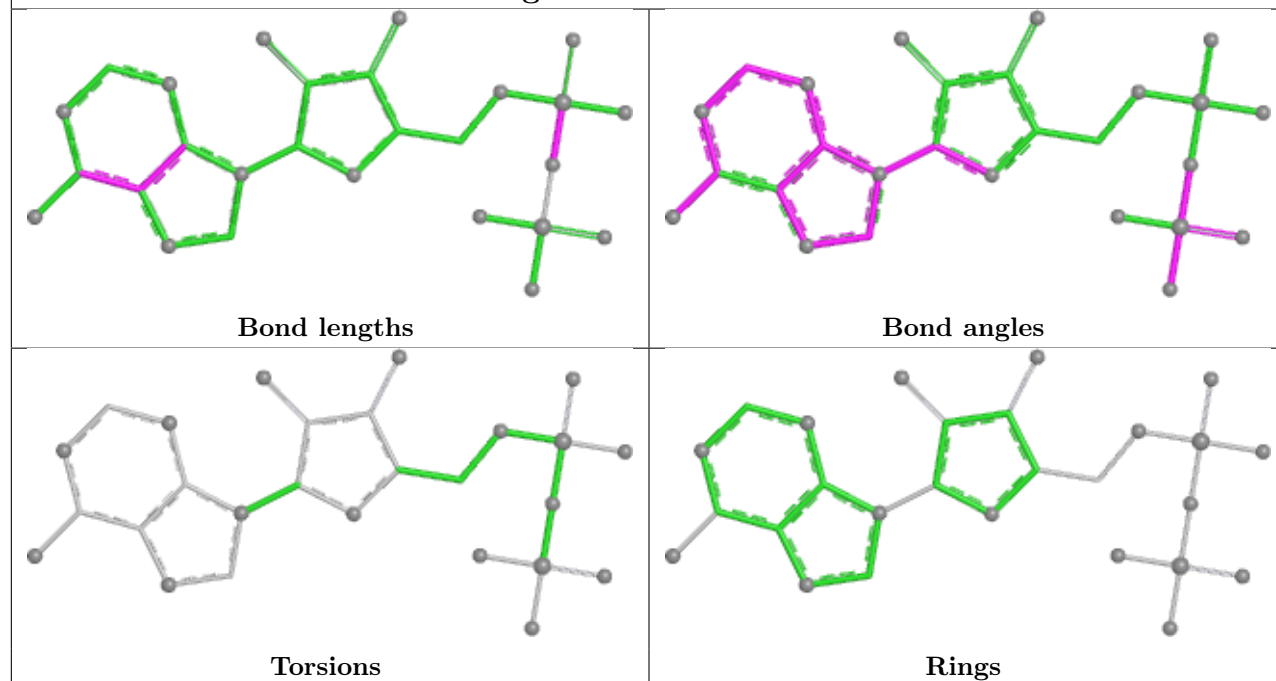




Ligand ATP G 1501 (B)



Ligand ADP E 1004



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	114/137 (83%)	0.19	0 100 100	45, 52, 60, 64	0
1	C	114/137 (83%)	0.71	6 (5%) 32 28	45, 53, 58, 61	0
2	B	91/97 (93%)	0.42	6 (6%) 24 20	46, 52, 59, 66	0
2	D	92/97 (94%)	0.82	12 (13%) 7 5	24, 52, 60, 66	0
3	E	324/334 (97%)	0.22	2 (0%) 85 84	26, 52, 63, 77	1 (0%)
3	G	325/334 (97%)	0.22	6 (1%) 67 64	24, 51, 61, 80	1 (0%)
All	All	1060/1136 (93%)	0.34	32 (3%) 52 49	24, 52, 61, 80	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	TYR	5.1
3	G	1	ALA	4.5
3	G	2	MET	4.4
1	C	542	TYR	3.8
2	D	206	GLU	3.6
3	G	316	ASP	3.5
1	C	450	ASN	3.4
2	D	245	THR	3.4
3	E	263	ASN	3.3
2	D	220	THR	3.2
3	G	318	THR	3.0
1	C	541	ILE	3.0
2	D	224	LEU	2.9
2	D	247	TYR	2.9
2	B	246	ALA	2.8
2	D	221	LEU	2.8
2	B	297	ASP	2.6
2	D	240	ILE	2.6
1	C	456	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	514	TYR	2.6
2	D	297	ASP	2.4
2	D	241	LEU	2.4
3	G	317	LYS	2.3
3	E	74[A]	MET	2.3
2	D	222	GLN	2.3
2	B	224	LEU	2.1
2	B	205	SER	2.1
1	C	453	HIS	2.1
2	D	223	GLU	2.0
2	B	259	HIS	2.0
2	D	239	CYS	2.0
3	G	97	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

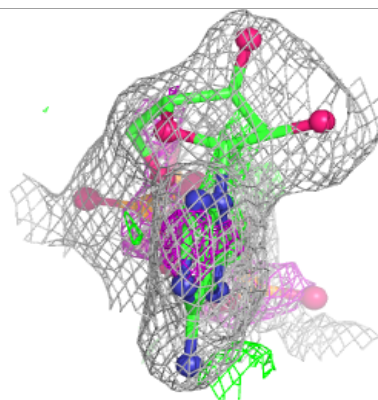
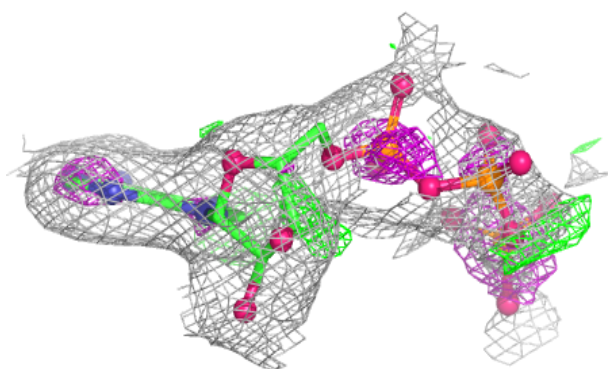
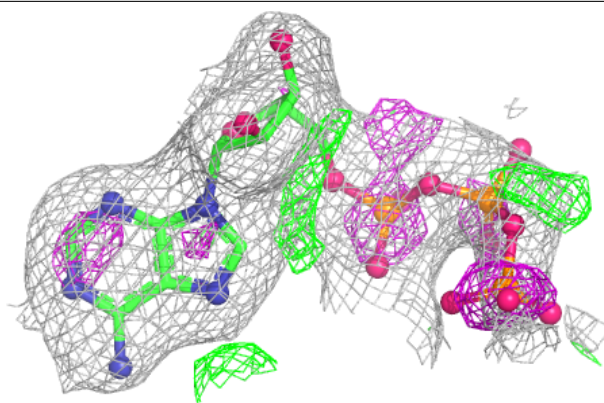
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	ATP	E	1502[B]	31/31	0.84	0.12	31,33,51,52	31
5	ATP	E	1002[A]	31/31	0.88	0.14	48,53,60,61	31
5	ATP	G	1001[A]	31/31	0.89	0.14	36,54,56,57	31
5	ATP	G	1501[B]	31/31	0.89	0.12	27,31,48,49	31
4	ADP	E	1004	27/27	0.94	0.09	33,40,46,49	0
4	ADP	G	1003	27/27	0.95	0.09	36,38,42,45	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.

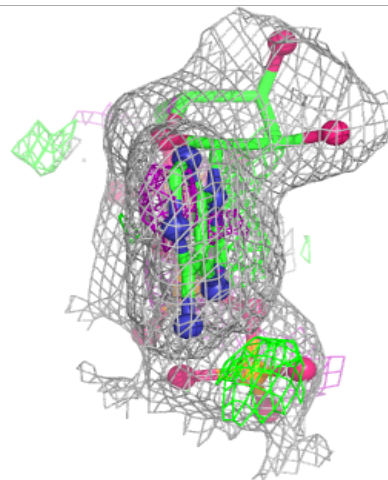
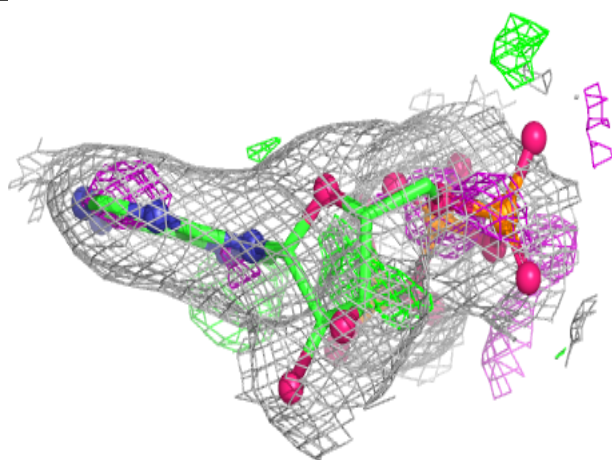
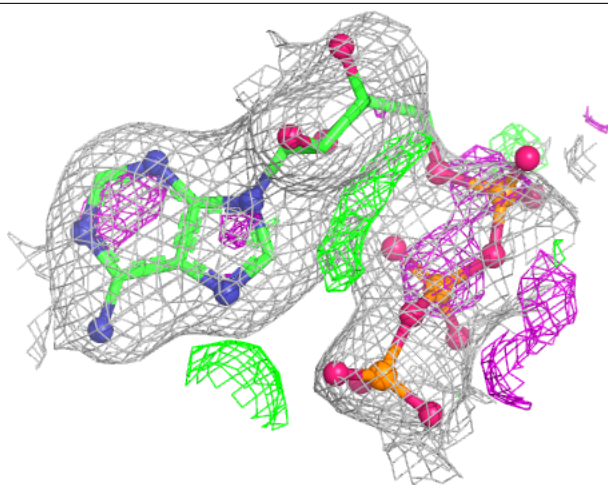
Electron density around ATP E 1502 (B):

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



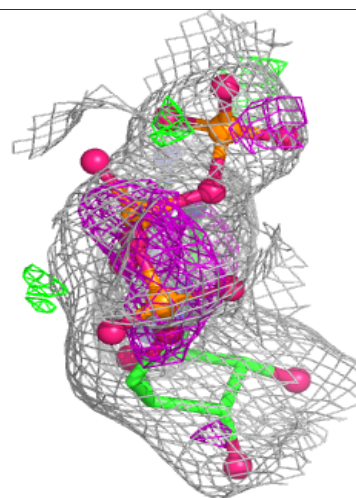
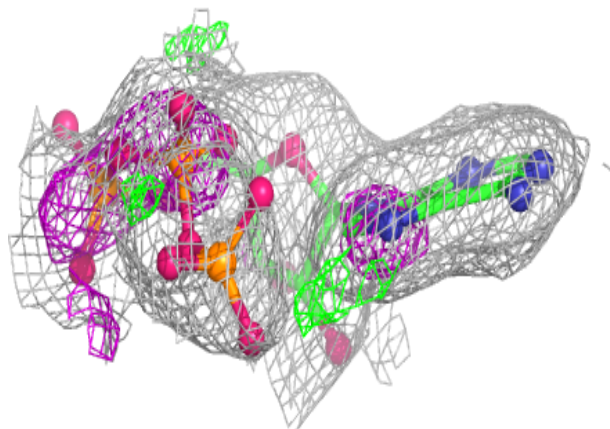
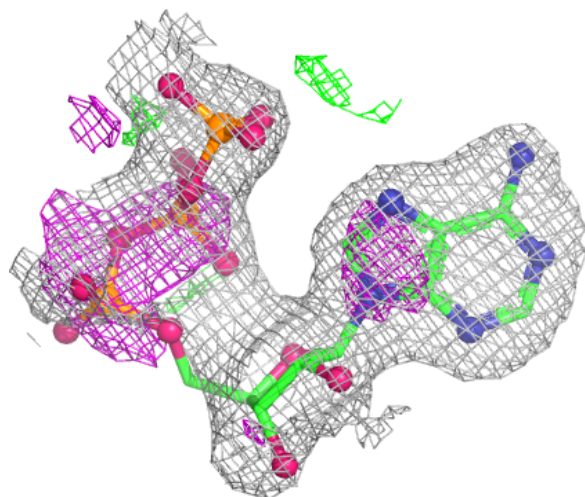
Electron density around ATP E 1002 (A):

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



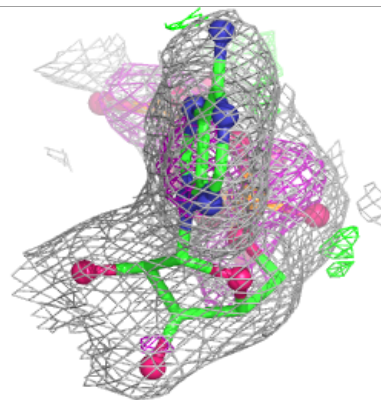
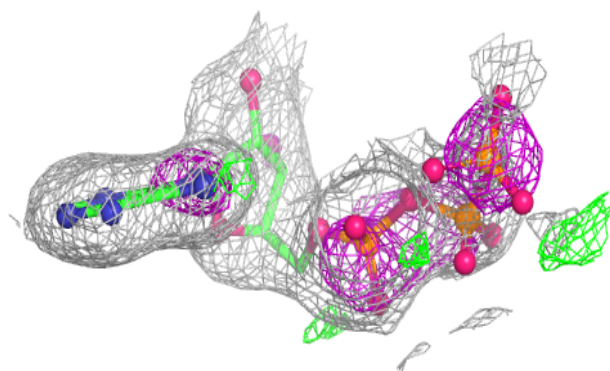
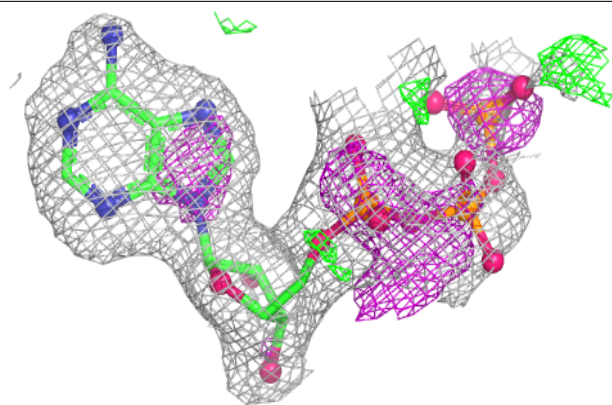
Electron density around ATP G 1001 (A):

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

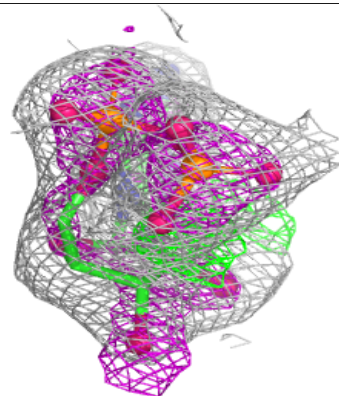
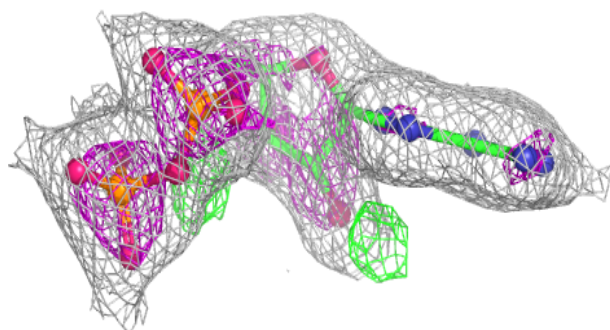
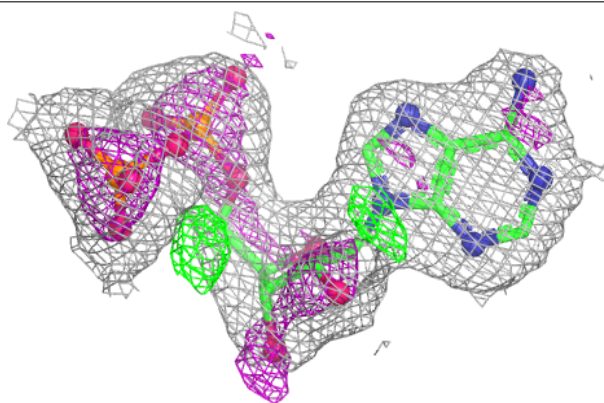


Electron density around ATP G 1501 (B):

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

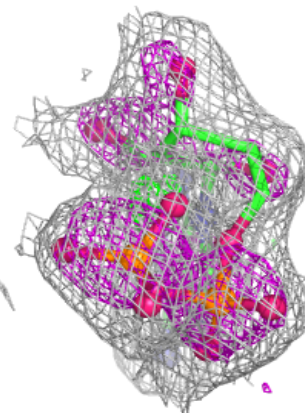
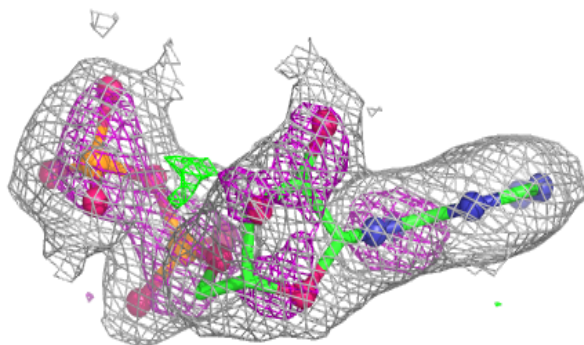
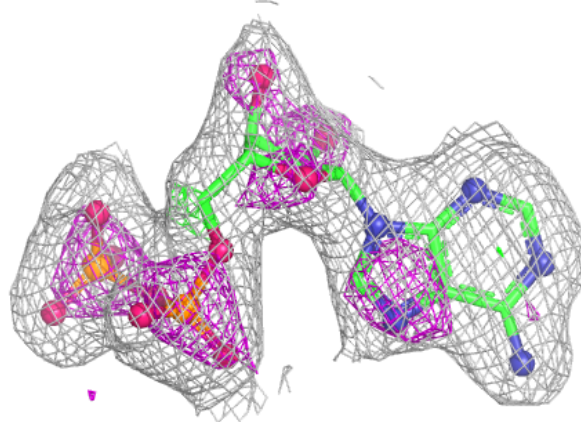
**Electron density around ADP E 1004:**

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



Electron density around ADP G 1003:

$2mF_o-DF_c$ (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.