



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:57 am BST

PDB ID : 2QR1  
Title : Crystal structure of the adenylate sensor from AMP-activated protein kinase  
in complex with ADP  
Authors : Jin, X.; Townley, R.; Shapiro, L.  
Deposited on : 2007-07-27  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

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

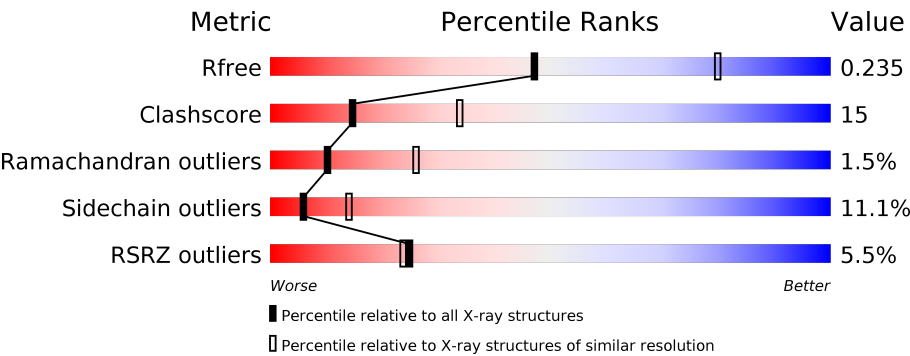
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	137	<div><div>7%</div><div><div></div><div>58%</div><div>22%</div><div>•</div><div>15%</div></div></div>
1	C	137	<div><div>8%</div><div><div></div><div>53%</div><div>26%</div><div>•</div><div>18%</div></div></div>
2	B	97	<div><div>11%</div><div><div></div><div>58%</div><div>24%</div><div>12%</div><div>6%</div></div></div>
2	D	97	<div><div>9%</div><div><div></div><div>66%</div><div>19%</div><div>7%</div><div>•</div><div>6%</div></div></div>
3	E	334	<div><div>2%</div><div><div></div><div>68%</div><div>24%</div><div>•</div><div>•</div></div></div>
3	G	334	<div><div>3%</div><div><div></div><div>62%</div><div>29%</div><div>5%</div><div>•</div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8544 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	116	Total	C	N	O	S	0	0	0
			939	608	159	163	9			
1	C	112	Total	C	N	O	S	0	1	0
			907	587	158	153	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
			711	453	123	133	2			
2	D	91	Total	C	N	O	S	0	0	0
			714	456	122	134	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	324	Total	C	N	O	S	0	0	0
			2543	1624	424	480	15			
3	E	324	Total	C	N	O	S	0	0	0
			2543	1623	424	482	14			

There are 4 discrepancies between the modelled and reference sequences:

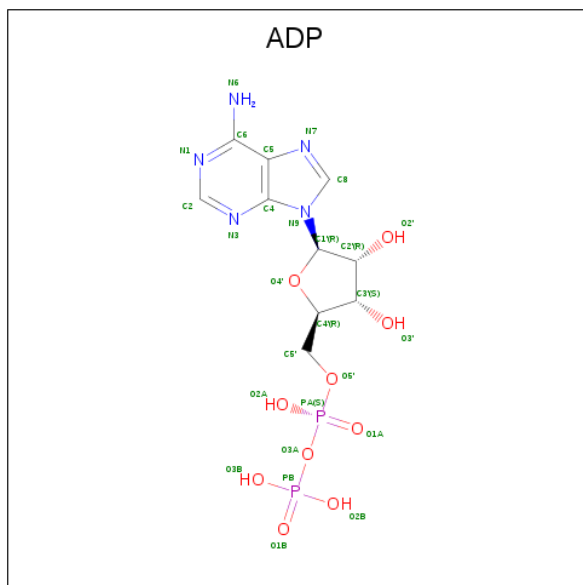
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	EXPRESSION TAG	UNP Q10343
G	2	MET	-	EXPRESSION TAG	UNP Q10343

*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 (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	10	Total	O	0	0
			10	10		
5	G	19	Total	O	0	0
			19	19		
5	C	11	Total	O	0	0
			11	11		

*Continued on next page...*

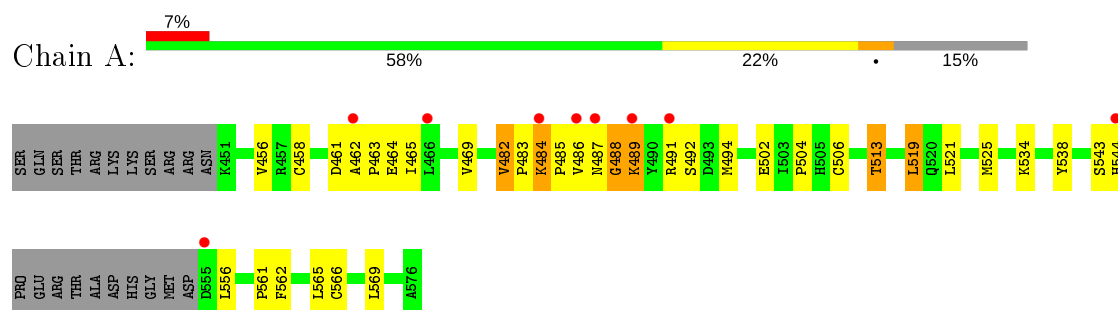
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	11	Total	O	0	0
			11	11		
5	E	20	Total	O	0	0
			20	20		

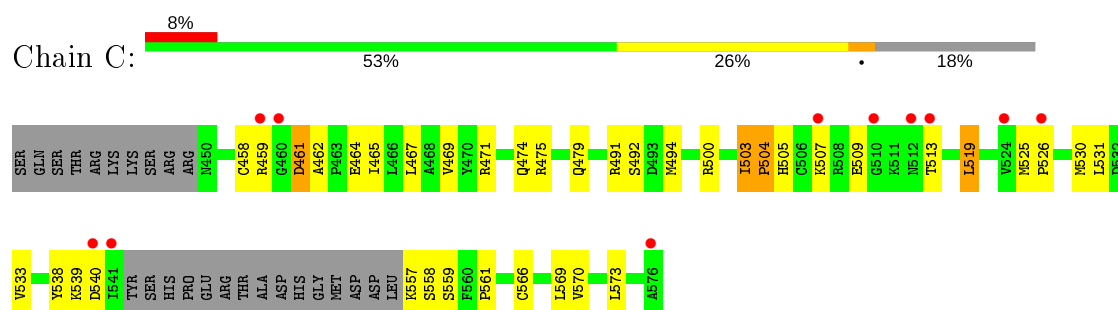
### 3 Residue-property plots [i](#)

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.

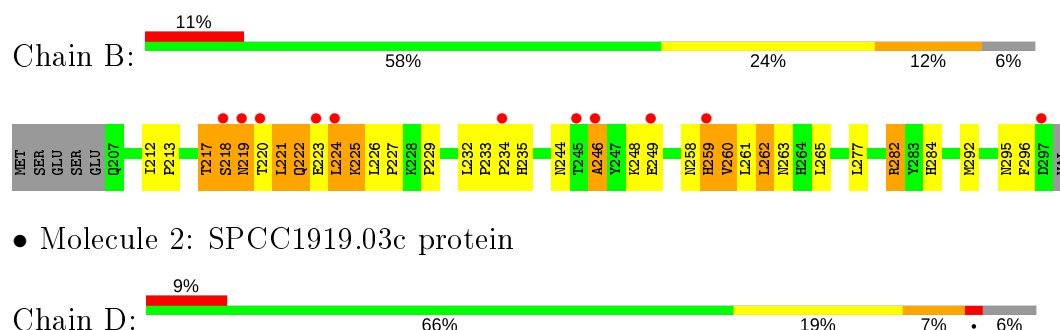
- Molecule 1: SNF1-like protein kinase ssp2



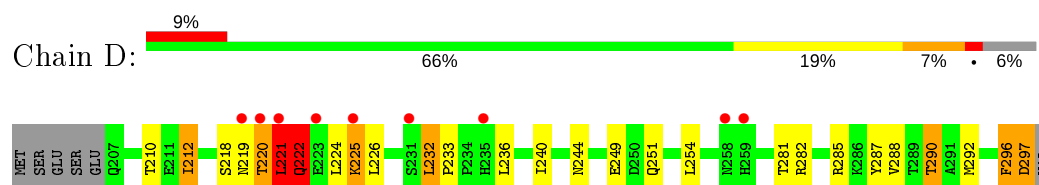
- Molecule 1: SNF1-like protein kinase ssp2



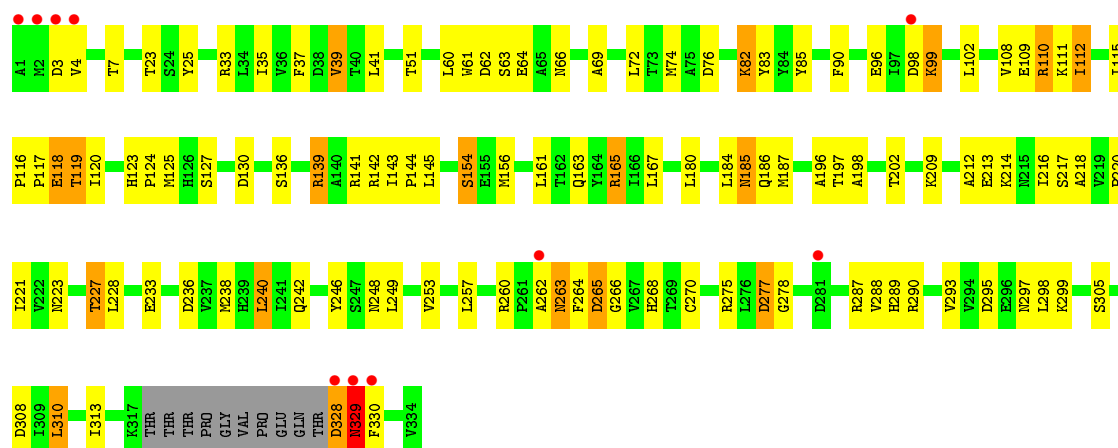
- Molecule 2: SPCC1919.03c protein



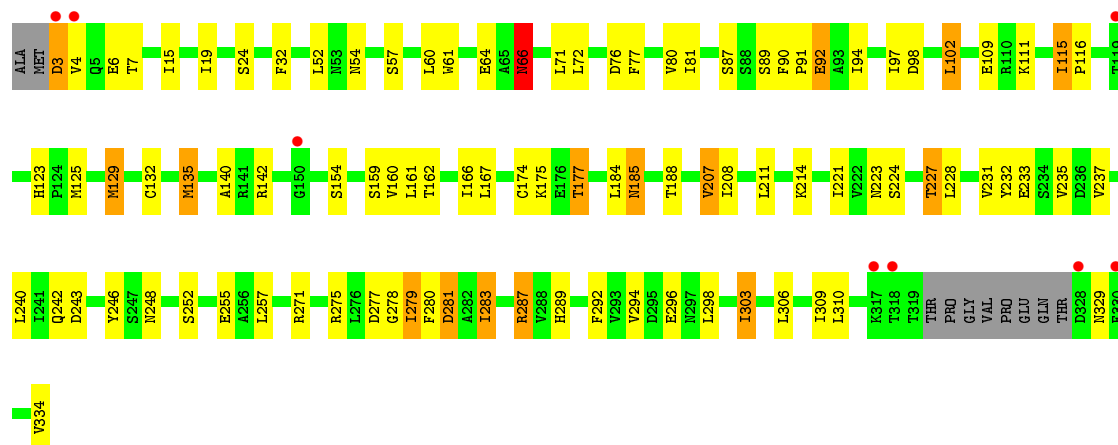
- Molecule 2: SPCC1919.03c protein



- 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, $\alpha$ , $\beta$ , $\gamma$	168.29Å 78.09Å 108.55Å 90.00° 124.13° 90.00°	Depositor
Resolution (Å)	48.28 – 2.70 48.28 – 2.69	Depositor EDS
% Data completeness (in resolution range)	96.3 (48.28-2.70) 89.0 (48.28-2.69)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.206 , 0.289 0.229 , 0.235	Depositor DCC
$R_{free}$ test set	1484 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.65	0/963	0.75	1/1295 (0.1%)
1	C	0.62	0/933	0.73	0/1253
2	B	0.54	0/728	0.96	4/995 (0.4%)
2	D	0.56	0/732	0.79	2/1002 (0.2%)
3	E	0.60	0/2585	0.71	0/3502
3	G	0.62	0/2585	0.76	2/3501 (0.1%)
All	All	0.61	0/8526	0.76	9/11548 (0.1%)

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	4
3	E	0	3
3	G	0	5
All	All	0	12

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	224	LEU	CB-CA-C	14.08	136.95	110.20
2	B	225	LYS	N-CA-CB	11.11	130.60	110.60
3	G	330	PHE	N-CA-CB	9.93	128.48	110.60
2	B	232	LEU	CA-CB-CG	5.68	128.37	115.30
2	D	296	PHE	CB-CA-C	-5.57	99.26	110.40
3	G	120	ILE	CB-CA-C	-5.52	100.57	111.60
2	B	246	ALA	CB-CA-C	-5.35	102.08	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	LEU	CA-CB-CG	5.24	127.35	115.30
2	D	297	ASP	N-CA-CB	5.12	119.82	110.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	218	SER	Peptide
2	B	221	LEU	Peptide
2	B	222	GLN	Peptide
2	B	296	PHE	Peptide
3	E	287	ARG	Sidechain
3	E	3	ASP	Peptide
3	E	66	ASN	Peptide
3	G	118	GLU	Peptide
3	G	262	ALA	Peptide
3	G	263	ASN	Peptide
3	G	328	ASP	Peptide
3	G	329	ASN	Peptide

## 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	939	0	936	27	0
1	C	907	0	909	24	0
2	B	711	0	717	48	0
2	D	714	0	713	37	0
3	E	2543	0	2572	55	0
3	G	2543	0	2583	80	0
4	E	54	0	24	1	0
4	G	54	0	24	8	0
5	A	8	0	0	0	0
5	B	10	0	0	0	0
5	C	11	0	0	1	0
5	D	11	0	0	0	0
5	E	20	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	19	0	0	3	0
All	All	8544	0	8478	259	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 (259) 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)
2:D:219:ASN:CA	2:D:220:THR:HG22	1.17	1.56
2:D:219:ASN:HA	2:D:220:THR:CG2	1.18	1.55
1:A:543:SER:CB	1:A:544:HIS:HA	1.51	1.31
1:A:543:SER:HB3	1:A:544:HIS:CA	1.64	1.26
3:G:217:SER:OG	4:G:1001:ADP:O1B	1.63	1.12
2:D:221:LEU:O	2:D:222:GLN:HB2	1.46	1.08
2:D:219:ASN:N	2:D:220:THR:HG22	1.69	1.05
1:A:488:GLY:HA3	1:A:489:LYS:HB2	1.37	1.02
3:E:61:TRP:HZ2	3:E:66:ASN:ND2	1.60	1.00
1:C:503:ILE:HD11	1:C:505:HIS:CD2	2.01	0.95
2:B:217:THR:C	2:B:219:ASN:HB3	1.87	0.95
2:B:226:LEU:HB3	2:B:227:PRO:HD2	1.49	0.94
2:D:219:ASN:HA	2:D:220:THR:HG23	1.49	0.94
1:A:488:GLY:CA	1:A:489:LYS:HB2	1.97	0.93
2:B:222:GLN:N	2:B:223:GLU:CB	2.32	0.91
2:D:220:THR:O	2:D:221:LEU:HB2	1.70	0.89
2:B:222:GLN:H	2:B:223:GLU:HB2	1.37	0.89
2:B:248:LYS:N	2:B:249:GLU:HA	1.87	0.86
3:E:123:HIS:HD2	3:E:125:MET:H	1.22	0.86
3:E:61:TRP:CZ2	3:E:66:ASN:ND2	2.44	0.86
3:E:142:ARG:HD2	3:E:334:VAL:O	1.76	0.86
2:B:217:THR:O	2:B:219:ASN:HB3	1.75	0.85
3:E:129:MET:HA	3:E:129:MET:HE2	1.59	0.85
2:D:232:LEU:HD22	2:D:233:PRO:HD2	1.59	0.84
3:G:37:PHE:HB3	3:G:41:LEU:HD12	1.60	0.83
2:D:232:LEU:CD2	2:D:233:PRO:HD2	2.07	0.83
3:G:264:PHE:O	3:G:266:GLY:N	2.11	0.83
2:B:235:HIS:HD2	2:B:261:LEU:HD21	1.43	0.83
1:A:488:GLY:HA3	1:A:489:LYS:CB	2.08	0.83
3:G:287:ARG:NH1	4:G:1003:ADP:O1B	2.15	0.80
3:G:217:SER:OG	4:G:1001:ADP:PB	2.41	0.79
2:B:222:GLN:N	2:B:223:GLU:HB2	1.93	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:139:ARG:NH2	3:G:163:GLN:HE22	1.80	0.77
1:A:484:LYS:HD3	1:A:485:PRO:HD2	1.66	0.77
3:E:167:LEU:HB3	3:E:283:ILE:HD11	1.66	0.76
3:G:119:THR:CG2	3:G:119:THR:O	2.33	0.76
2:D:220:THR:O	2:D:220:THR:HG23	1.84	0.76
3:G:119:THR:O	3:G:119:THR:HG23	1.86	0.76
3:G:33:ARG:HD2	5:G:1018:HOH:O	1.85	0.76
2:B:248:LYS:O	2:B:248:LYS:HG3	1.87	0.75
2:D:232:LEU:HD22	2:D:233:PRO:CD	2.16	0.74
3:G:33:ARG:HE	3:G:35:ILE:HD11	1.52	0.74
2:B:222:GLN:N	2:B:223:GLU:HB3	2.01	0.74
2:D:219:ASN:CA	2:D:220:THR:CG2	2.06	0.73
3:E:76:ASP:HA	3:E:109:GLU:OE1	1.89	0.72
2:B:258:ASN:OD1	2:B:260:VAL:HG22	1.89	0.72
3:G:139:ARG:NH2	3:G:163:GLN:NE2	2.37	0.71
1:A:566:CYS:HB3	2:B:265:LEU:HD22	1.72	0.71
3:G:110:ARG:HG2	5:G:1016:HOH:O	1.90	0.70
2:B:259:HIS:CD2	2:B:259:HIS:H	2.10	0.70
3:E:167:LEU:HB3	3:E:283:ILE:CD1	2.21	0.69
1:C:471:ARG:O	1:C:475:ARG:HG3	1.92	0.69
1:A:556:LEU:HD23	3:G:156:MET:SD	2.32	0.69
3:G:51:THR:HG21	3:G:242:GLN:HE22	1.58	0.69
1:C:503:ILE:HD11	1:C:505:HIS:HD2	1.56	0.69
3:G:83:TYR:CZ	3:G:112:ILE:HD11	2.27	0.69
2:B:259:HIS:N	2:B:259:HIS:CD2	2.62	0.68
1:A:465:ILE:O	1:A:469:VAL:HG23	1.93	0.67
3:G:82:LYS:HG3	3:G:212:ALA:HB3	1.74	0.67
3:G:123:HIS:HD2	3:G:125:MET:H	1.40	0.67
3:E:3:ASP:N	3:E:6:GLU:H	1.92	0.67
3:G:198:ALA:O	3:G:221:ILE:HA	1.95	0.66
3:G:236:ASP:OD2	3:G:260:ARG:NH1	2.28	0.66
2:B:222:GLN:H	2:B:223:GLU:CB	1.99	0.66
2:D:288:VAL:HG22	3:E:32:PHE:CZ	2.31	0.66
1:C:503:ILE:HD12	1:C:504:PRO:HD2	1.78	0.66
2:D:218:SER:C	2:D:220:THR:HG22	2.16	0.66
1:A:506:CYS:HB3	1:A:513:THR:HG23	1.78	0.65
2:B:223:GLU:O	2:B:225:LYS:N	2.27	0.65
2:D:282:ARG:HG3	2:D:287:TYR:CE2	2.31	0.65
2:D:221:LEU:O	2:D:222:GLN:CB	2.33	0.65
3:E:296:GLU:CD	3:E:296:GLU:H	2.00	0.65
3:G:139:ARG:HG3	3:G:139:ARG:O	1.96	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:91:PRO:HB2	3:E:92:GLU:OE2	1.98	0.64
3:G:66:ASN:HD22	3:G:154:SER:HB2	1.62	0.64
2:B:295:ASN:HD21	3:G:41:LEU:HA	1.61	0.63
2:D:240:ILE:H	2:D:240:ILE:HD12	1.64	0.63
2:D:220:THR:O	2:D:220:THR:CG2	2.46	0.63
2:D:220:THR:O	2:D:221:LEU:CB	2.45	0.63
1:A:543:SER:HB3	1:A:544:HIS:HA	0.71	0.62
3:E:275:ARG:O	3:E:279:ILE:HG23	1.99	0.62
1:A:543:SER:CB	1:A:544:HIS:CA	2.39	0.62
2:D:232:LEU:HD22	2:D:233:PRO:N	2.15	0.62
3:G:185:ASN:HD22	3:G:186:GLN:N	1.98	0.62
2:B:223:GLU:C	2:B:225:LYS:H	2.03	0.62
3:E:115:ILE:HD13	3:E:116:PRO:O	2.00	0.61
3:G:139:ARG:HH21	3:G:163:GLN:NE2	1.98	0.61
2:B:235:HIS:CD2	2:B:261:LEU:HD21	2.31	0.61
2:B:258:ASN:ND2	2:B:260:VAL:CG2	2.64	0.61
2:D:219:ASN:HB3	2:D:220:THR:O	2.01	0.60
3:G:295:ASP:OD2	3:G:299:LYS:HB3	2.01	0.60
3:G:96:GLU:O	3:G:99:LYS:HG3	2.02	0.59
2:D:219:ASN:CA	2:D:220:THR:CB	2.76	0.59
3:E:223:ASN:OD1	3:E:227:THR:HG23	2.03	0.58
3:G:268:HIS:CD2	3:G:288:VAL:HG22	2.39	0.58
3:G:305:SER:O	3:G:308:ASP:HB2	2.04	0.58
1:A:521:LEU:HD23	2:B:229:PRO:HG3	1.86	0.58
1:C:474:GLN:OE1	2:D:212:ILE:HD11	2.03	0.57
3:G:202:THR:O	3:G:253:VAL:HG23	2.04	0.57
3:G:123:HIS:CD2	3:G:125:MET:H	2.21	0.57
1:A:562:PHE:CE1	1:A:566:CYS:SG	2.98	0.57
2:D:219:ASN:HA	2:D:220:THR:O	2.05	0.56
3:E:185:ASN:C	3:E:185:ASN:HD22	2.08	0.56
3:G:66:ASN:HB3	3:G:154:SER:HB2	1.87	0.56
2:B:221:LEU:C	2:B:223:GLU:HB3	2.25	0.56
2:D:232:LEU:HD23	2:D:233:PRO:HD2	1.85	0.56
2:D:218:SER:O	2:D:219:ASN:OD1	2.24	0.56
1:A:502:GLU:O	1:A:504:PRO:HD3	2.05	0.55
3:G:142:ARG:NH2	4:G:1003:ADP:O2A	2.40	0.55
3:E:289:HIS:O	3:E:306:LEU:HG	2.05	0.55
3:E:294:VAL:HG21	3:E:298:LEU:HD23	1.89	0.55
1:A:484:LYS:HB3	1:A:491:ARG:HH21	1.72	0.55
3:G:246:TYR:O	3:G:249:LEU:HD12	2.06	0.55
2:B:226:LEU:HB3	2:B:227:PRO:CD	2.30	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:ASN:O	2:B:260:VAL:N	2.40	0.54
3:G:51:THR:HG21	3:G:242:GLN:NE2	2.21	0.54
3:E:61:TRP:HZ2	3:E:66:ASN:HD21	1.48	0.54
3:E:174:CYS:O	3:E:177:THR:HG23	2.08	0.54
2:B:259:HIS:N	2:B:259:HIS:HD2	2.06	0.53
2:D:218:SER:C	2:D:220:THR:CG2	2.77	0.53
3:E:72:LEU:HD11	3:E:77:PHE:HE1	1.73	0.53
3:G:185:ASN:HD22	3:G:185:ASN:C	2.13	0.53
1:C:465:ILE:O	1:C:469:VAL:HG23	2.09	0.52
3:E:60:LEU:HD22	3:E:102:LEU:HD23	1.89	0.52
3:G:240:LEU:HG	3:G:248:ASN:HB3	1.91	0.52
3:E:207:VAL:O	3:E:211:LEU:HG	2.10	0.52
2:B:223:GLU:C	2:B:225:LYS:N	2.62	0.52
1:C:491:ARG:O	1:C:494:MET:HB2	2.10	0.52
3:G:196:ALA:O	3:G:220:PRO:HD2	2.09	0.52
1:C:513:THR:HG22	1:C:540:ASP:HA	1.92	0.52
3:E:129:MET:HA	3:E:129:MET:CE	2.37	0.52
3:E:271:ARG:HH12	3:E:296:GLU:HA	1.75	0.52
3:E:279:ILE:O	3:E:283:ILE:HG23	2.10	0.52
3:G:60:LEU:HD21	3:G:72:LEU:HB2	1.91	0.52
3:E:221:ILE:HD11	3:E:232:TYR:HB2	1.92	0.51
3:G:216:ILE:HG22	4:G:1001:ADP:H5'1	1.93	0.51
3:G:76:ASP:HA	3:G:109:GLU:OE1	2.10	0.51
1:A:482:VAL:HG22	2:B:213:PRO:HG3	1.92	0.51
2:B:217:THR:O	2:B:219:ASN:CB	2.54	0.51
3:E:279:ILE:HD11	3:E:309:ILE:HD13	1.93	0.51
3:G:145:LEU:HD21	3:G:161:LEU:HD22	1.92	0.51
1:A:538:TYR:CE1	1:A:561:PRO:HD2	2.46	0.51
2:D:251:GLN:OE1	3:E:54:ASN:HB3	2.11	0.51
1:A:506:CYS:CB	1:A:513:THR:HG23	2.40	0.50
1:A:484:LYS:HD3	1:A:485:PRO:CD	2.39	0.50
3:G:3:ASP:O	3:G:7:THR:N	2.38	0.50
2:D:233:PRO:HG2	2:D:236:LEU:HD12	1.92	0.50
3:G:265:ASP:OD2	3:G:289:HIS:CE1	2.65	0.50
1:A:461:ASP:HB3	1:A:464:GLU:HB2	1.92	0.50
3:G:264:PHE:C	3:G:266:GLY:N	2.64	0.50
2:B:258:ASN:HD21	2:B:260:VAL:CG2	2.25	0.49
1:A:566:CYS:CB	2:B:265:LEU:HD22	2.42	0.49
3:E:98:ASP:OD1	3:E:246:TYR:OH	2.20	0.49
2:B:258:ASN:CG	2:B:260:VAL:CG2	2.81	0.49
2:B:282:ARG:HG2	2:B:284:HIS:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:219:ASN:N	2:D:220:THR:CG2	2.56	0.49
1:C:525:MET:HB2	1:C:526:PRO:HD2	1.95	0.49
3:G:289:HIS:O	3:G:290:ARG:HB3	2.12	0.49
1:A:486:VAL:O	1:A:487:ASN:HB2	2.12	0.49
1:C:464:GLU:O	1:C:467:LEU:HB3	2.13	0.49
3:E:162:THR:HG21	4:E:1004:ADP:O3B	2.11	0.49
3:E:292:PHE:HD2	3:E:303:ILE:HG13	1.78	0.49
3:E:252:SER:OG	3:E:255:GLU:HG3	2.13	0.48
3:G:264:PHE:C	3:G:266:GLY:H	2.16	0.48
3:G:82:LYS:HG3	3:G:212:ALA:CB	2.40	0.48
2:D:219:ASN:CA	2:D:220:THR:O	2.62	0.48
2:B:258:ASN:OD1	2:B:260:VAL:CG2	2.59	0.48
5:C:4:HOH:O	2:D:290:THR:HG22	2.13	0.48
3:E:81:ILE:HG12	3:E:94:ILE:HD11	1.94	0.48
2:B:258:ASN:ND2	2:B:260:VAL:HG23	2.29	0.48
3:G:180:LEU:O	3:G:277:ASP:HB3	2.13	0.48
3:G:214:LYS:HB2	3:G:216:ILE:HG12	1.96	0.48
2:B:244:ASN:C	2:B:246:ALA:H	2.17	0.47
3:E:208:ILE:HD11	3:E:237:VAL:CG2	2.45	0.47
3:E:240:LEU:HG	3:E:248:ASN:HB3	1.96	0.47
2:D:240:ILE:HG22	2:D:254:LEU:HD13	1.97	0.47
3:G:85:TYR:HA	1:C:459[B]:ARG:HH22	1.80	0.47
3:E:240:LEU:HA	3:E:240:LEU:HD12	1.80	0.47
3:G:108:VAL:O	3:G:112:ILE:HB	2.15	0.47
3:E:292:PHE:CD2	3:E:303:ILE:HG13	2.50	0.47
1:C:503:ILE:HD13	1:C:561:PRO:HG3	1.97	0.47
2:D:296:PHE:HB3	2:D:297:ASP:H	1.61	0.46
3:G:165:ARG:HH12	4:G:1003:ADP:H3'	1.80	0.46
3:G:233:GLU:O	3:G:236:ASP:HB2	2.15	0.46
3:G:124:PRO:HG3	3:G:145:LEU:HB3	1.97	0.46
1:C:561:PRO:HB3	3:E:66:ASN:OD1	2.15	0.46
1:C:461:ASP:HB2	1:C:464:GLU:HG3	1.97	0.46
1:A:483:PRO:HG3	1:A:494:MET:HB2	1.97	0.46
3:E:15:ILE:O	3:E:19:ILE:HG23	2.16	0.46
3:G:33:ARG:NE	3:G:35:ILE:HD11	2.26	0.46
3:G:277:ASP:OD2	3:G:278:GLY:N	2.49	0.46
3:G:62:ASP:HB2	3:G:69:ALA:HB2	1.98	0.46
3:G:329:ASN:HD22	3:G:329:ASN:HA	1.56	0.45
3:G:82:LYS:HE2	3:G:329:ASN:O	2.15	0.45
2:B:222:GLN:HB3	2:B:223:GLU:HB2	1.98	0.45
3:E:90:PHE:HA	3:E:91:PRO:HD2	1.87	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:216:ILE:HD12	3:G:218:ALA:O	2.17	0.45
3:E:123:HIS:CD2	3:E:125:MET:H	2.15	0.45
3:G:127:SER:O	3:G:130:ASP:HB2	2.17	0.45
2:B:259:HIS:HD2	2:B:259:HIS:H	1.58	0.44
3:G:165:ARG:NH1	4:G:1003:ADP:H3'	2.33	0.44
2:D:219:ASN:CB	2:D:220:THR:O	2.65	0.44
3:G:33:ARG:HE	3:G:35:ILE:CD1	2.28	0.44
1:A:484:LYS:HB3	1:A:491:ARG:NH2	2.32	0.44
3:E:60:LEU:CD2	3:E:102:LEU:HD23	2.47	0.44
3:E:159:SER:OG	3:E:160:VAL:N	2.51	0.44
1:C:503:ILE:HD12	1:C:504:PRO:CD	2.45	0.44
3:G:116:PRO:HA	3:G:117:PRO:HD3	1.74	0.44
3:E:129:MET:CE	3:E:132:CYS:HB2	2.48	0.44
2:B:248:LYS:CG	2:B:248:LYS:O	2.60	0.43
3:E:233:GLU:HG3	3:E:235:VAL:HG22	2.00	0.43
2:B:258:ASN:HD21	2:B:260:VAL:HG21	1.82	0.43
3:G:223:ASN:ND2	3:G:227:THR:HG23	2.34	0.43
2:B:258:ASN:C	2:B:260:VAL:H	2.21	0.43
1:C:462:ALA:HA	1:C:465:ILE:HD12	2.01	0.43
3:E:135:MET:HG2	3:E:140:ALA:O	2.18	0.43
3:G:264:PHE:O	3:G:265:ASP:C	2.54	0.43
1:A:488:GLY:N	1:A:489:LYS:HB2	2.32	0.43
3:E:161:LEU:HD23	3:E:166:ILE:HD11	2.00	0.43
2:B:219:ASN:N	2:B:219:ASN:OD1	2.52	0.43
3:E:279:ILE:HG13	3:E:280:PHE:N	2.34	0.43
3:G:141:ARG:O	3:G:163:GLN:HG3	2.19	0.43
1:C:479:GLN:OE1	1:C:500:ARG:NH2	2.45	0.43
1:A:462:ALA:HB3	1:A:463:PRO:HD3	2.00	0.42
2:B:233:PRO:HA	2:B:234:PRO:HD3	1.92	0.42
3:G:37:PHE:HB3	3:G:41:LEU:CD1	2.41	0.42
1:C:492:SER:C	1:C:494:MET:N	2.72	0.42
1:C:519:LEU:HD13	1:C:533:VAL:HG13	2.01	0.42
3:G:297:ASN:O	3:G:298:LEU:HB2	2.20	0.42
3:G:90:PHE:CZ	1:C:573:LEU:HD22	2.55	0.42
2:B:212:ILE:H	2:B:212:ILE:HG13	1.60	0.42
3:G:74:MET:SD	3:G:238:MET:HG3	2.59	0.42
1:C:557:LYS:HB3	1:C:558:SER:H	1.57	0.42
3:E:281:ASP:OD1	3:E:281:ASP:C	2.58	0.42
3:G:167:LEU:HG	3:G:310:LEU:HD22	2.01	0.42
1:C:530:MET:HG2	1:C:531:LEU:N	2.34	0.41
2:B:265:LEU:HD11	2:B:277:LEU:HD22	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:61:TRP:CZ2	3:G:66:ASN:HA	2.55	0.41
2:B:262:LEU:O	2:B:263:ASN:HB2	2.19	0.41
3:G:23:THR:OG1	3:G:25:TYR:HB3	2.20	0.41
3:G:270:CYS:O	3:G:293:VAL:HA	2.21	0.41
3:E:111:LYS:HE2	3:E:111:LYS:HB3	1.81	0.41
3:E:214:LYS:HB3	3:E:214:LYS:NZ	2.35	0.41
2:D:220:THR:O	2:D:221:LEU:HD22	2.21	0.41
3:G:143:ILE:HG12	3:G:144:PRO:HD2	2.03	0.41
3:G:213:GLU:HG2	3:G:328:ASP:HA	2.03	0.41
3:G:39:VAL:HG22	3:G:61:TRP:O	2.21	0.41
1:C:538:TYR:CZ	1:C:561:PRO:HD2	2.56	0.41
3:E:231:VAL:O	3:E:231:VAL:HG13	2.20	0.41
3:G:290:ARG:HE	4:G:1001:ADP:PB	2.44	0.41
1:C:566:CYS:O	1:C:570:VAL:HG23	2.21	0.41
3:E:277:ASP:OD2	3:E:278:GLY:N	2.54	0.41
2:B:248:LYS:N	2:B:249:GLU:CA	2.71	0.40
2:D:224:LEU:O	2:D:225:LYS:C	2.59	0.40
2:B:259:HIS:HA	2:B:262:LEU:HD22	2.03	0.40
2:B:212:ILE:HD12	2:B:212:ILE:O	2.21	0.40
2:D:224:LEU:O	2:D:226:LEU:N	2.54	0.40
3:E:76:ASP:O	3:E:80:VAL:HG23	2.21	0.40
3:G:139:ARG:HG2	5:G:1022:HOH:O	2.21	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	112/137 (82%)	104 (93%)	5 (4%)	3 (3%)	5	12
1	C	109/137 (80%)	104 (95%)	4 (4%)	1 (1%)	17	40
2	B	89/97 (92%)	72 (81%)	15 (17%)	2 (2%)	6	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	89/97 (92%)	70 (79%)	15 (17%)	4 (4%)	2	5
3	E	320/334 (96%)	302 (94%)	16 (5%)	2 (1%)	25	50
3	G	320/334 (96%)	302 (94%)	14 (4%)	4 (1%)	12	30
All	All	1039/1136 (92%)	954 (92%)	69 (7%)	16 (2%)	10	26

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	LYS
3	G	263	ASN
3	G	265	ASP
2	D	221	LEU
2	D	222	GLN
3	G	98	ASP
2	D	225	LYS
1	A	488	GLY
1	A	492	SER
2	B	218	SER
3	G	329	ASN
2	D	220	THR
3	E	242	GLN
2	B	219	ASN
3	E	64	GLU
1	C	504	PRO

### 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	100/120 (83%)	90 (90%)	10 (10%)	7	18
1	C	95/120 (79%)	86 (90%)	9 (10%)	8	20
2	B	81/88 (92%)	73 (90%)	8 (10%)	8	18
2	D	81/88 (92%)	70 (86%)	11 (14%)	3	8

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	284/296 (96%)	250 (88%)	34 (12%)	5	11
3	G	284/296 (96%)	253 (89%)	31 (11%)	6	14
All	All	925/1008 (92%)	822 (89%)	103 (11%)	6	14

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	VAL
1	A	458	CYS
1	A	482	VAL
1	A	484	LYS
1	A	513	THR
1	A	519	LEU
1	A	525	MET
1	A	534	LYS
1	A	565	LEU
1	A	569	LEU
2	B	217	THR
2	B	220	THR
2	B	224	LEU
2	B	259	HIS
2	B	260	VAL
2	B	262	LEU
2	B	282	ARG
2	B	292	MET
3	G	4	VAL
3	G	39	VAL
3	G	63	SER
3	G	64	GLU
3	G	82	LYS
3	G	99	LYS
3	G	102	LEU
3	G	110	ARG
3	G	111	LYS
3	G	112	ILE
3	G	115	ILE
3	G	118	GLU
3	G	119	THR
3	G	136	SER
3	G	139	ARG
3	G	154	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	165	ARG
3	G	184	LEU
3	G	185	ASN
3	G	187	MET
3	G	197	THR
3	G	209	LYS
3	G	227	THR
3	G	228	LEU
3	G	240	LEU
3	G	257	LEU
3	G	275	ARG
3	G	277	ASP
3	G	310	LEU
3	G	313	ILE
3	G	329	ASN
1	C	458	CYS
1	C	461	ASP
1	C	503	ILE
1	C	507	LYS
1	C	509	GLU
1	C	519	LEU
1	C	539	LYS
1	C	559	SER
1	C	569	LEU
2	D	210	THR
2	D	212	ILE
2	D	221	LEU
2	D	222	GLN
2	D	232	LEU
2	D	244	ASN
2	D	249	GLU
2	D	281	THR
2	D	285	ARG
2	D	290	THR
2	D	292	MET
3	E	4	VAL
3	E	7	THR
3	E	24	SER
3	E	52	LEU
3	E	57	SER
3	E	66	ASN
3	E	71	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	E	87	SER
3	E	89	SER
3	E	92	GLU
3	E	97	ILE
3	E	102	LEU
3	E	115	ILE
3	E	129	MET
3	E	135	MET
3	E	154	SER
3	E	175	LYS
3	E	177	THR
3	E	184	LEU
3	E	185	ASN
3	E	188	THR
3	E	207	VAL
3	E	224	SER
3	E	227	THR
3	E	228	LEU
3	E	243	ASP
3	E	257	LEU
3	E	279	ILE
3	E	281	ASP
3	E	283	ILE
3	E	287	ARG
3	E	303	ILE
3	E	310	LEU
3	E	329	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	235	HIS
2	B	259	HIS
2	B	284	HIS
2	B	295	ASN
3	G	66	ASN
3	G	123	HIS
3	G	163	GLN
3	G	173	ASN
3	G	185	ASN
3	G	194	ASN
3	G	242	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	268	HIS
3	G	289	HIS
3	G	329	ASN
1	C	505	HIS
1	C	512	ASN
1	C	536	ASN
2	D	235	HIS
2	D	244	ASN
2	D	263	ASN
2	D	284	HIS
3	E	123	HIS
3	E	126	HIS
3	E	185	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
4	ADP	G	1003	-	24,29,29	1.00	1 (4%)	29,45,45	1.37	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ADP	G	1001	-	24,29,29	0.96	2 (8%)	29,45,45	1.41	5 (17%)
4	ADP	E	1002	-	24,29,29	1.00	2 (8%)	29,45,45	1.34	4 (13%)
4	ADP	E	1004	-	24,29,29	1.03	2 (8%)	29,45,45	1.42	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	G	1003	-	-	5/12/32/32	0/3/3/3
4	ADP	G	1001	-	-	6/12/32/32	0/3/3/3
4	ADP	E	1002	-	-	5/12/32/32	0/3/3/3
4	ADP	E	1004	-	-	2/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1003	ADP	C5-C4	3.09	1.49	1.40
4	G	1001	ADP	O4'-C1'	2.66	1.44	1.41
4	E	1004	ADP	C5-C4	2.56	1.47	1.40
4	E	1002	ADP	C5-C4	2.40	1.47	1.40
4	E	1002	ADP	C2-N3	2.33	1.35	1.32
4	G	1001	ADP	C5-C4	2.32	1.47	1.40
4	E	1004	ADP	C2-N3	2.01	1.35	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1001	ADP	N3-C2-N1	-3.56	123.12	128.68
4	G	1003	ADP	N3-C2-N1	-3.46	123.27	128.68
4	E	1004	ADP	PA-O3A-PB	-3.41	121.13	132.83
4	E	1004	ADP	N3-C2-N1	-3.30	123.53	128.68
4	E	1002	ADP	PA-O3A-PB	-3.13	122.08	132.83
4	G	1003	ADP	C2-N1-C6	3.08	124.02	118.75
4	E	1002	ADP	N6-C6-N1	2.62	124.02	118.57
4	G	1001	ADP	PA-O3A-PB	-2.58	123.97	132.83
4	G	1001	ADP	C1'-N9-C4	-2.53	122.20	126.64
4	E	1002	ADP	N3-C2-N1	-2.48	124.80	128.68
4	E	1004	ADP	C3'-C2'-C1'	2.45	104.67	100.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1001	ADP	C2-N1-C6	2.44	122.92	118.75
4	G	1003	ADP	O3B-PB-O2B	2.29	116.38	107.64
4	E	1002	ADP	C5-C6-N6	-2.18	117.03	120.35
4	G	1003	ADP	PA-O3A-PB	-2.12	125.54	132.83
4	G	1003	ADP	C1'-N9-C4	-2.10	122.95	126.64
4	E	1004	ADP	N6-C6-N1	2.06	122.85	118.57
4	G	1003	ADP	C4-C5-N7	-2.01	107.30	109.40
4	G	1001	ADP	C4-C5-N7	-2.01	107.31	109.40
4	E	1004	ADP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (18) torsion outliers are listed below:

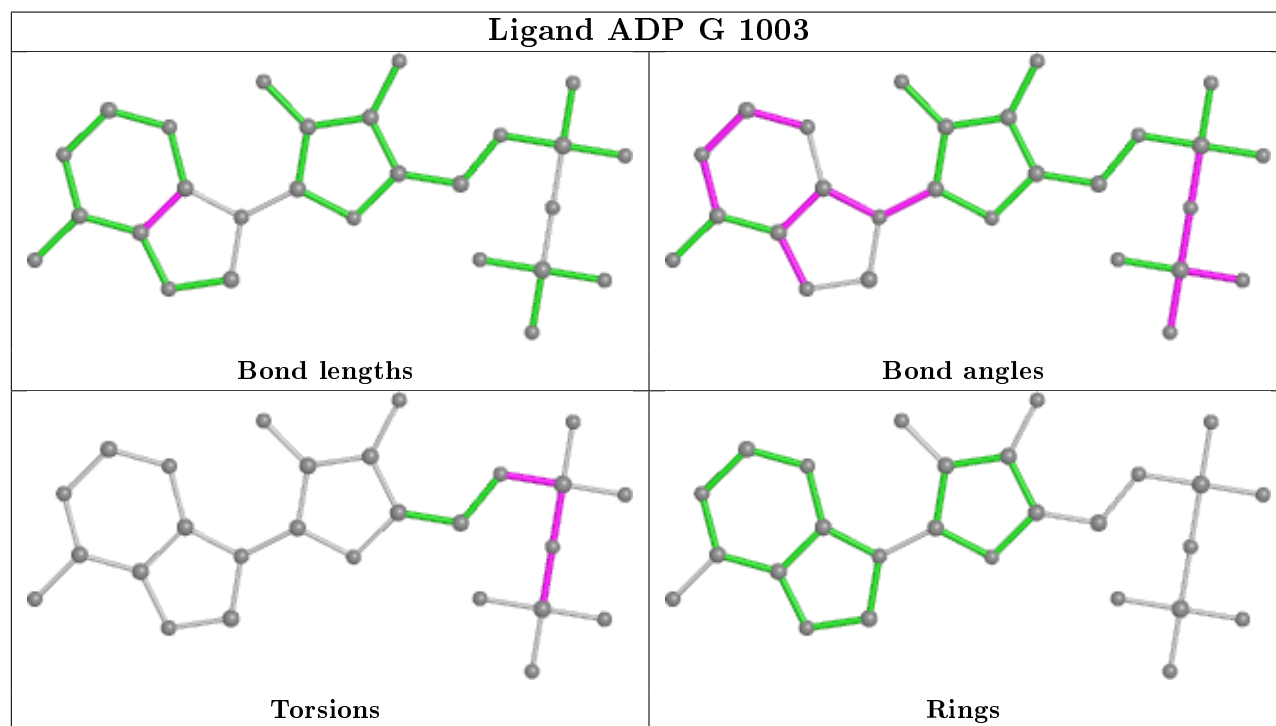
Mol	Chain	Res	Type	Atoms
4	G	1003	ADP	PA-O3A-PB-O3B
4	G	1003	ADP	C5'-O5'-PA-O1A
4	G	1003	ADP	C5'-O5'-PA-O2A
4	G	1001	ADP	PA-O3A-PB-O3B
4	G	1001	ADP	C5'-O5'-PA-O1A
4	E	1002	ADP	C5'-O5'-PA-O1A
4	E	1002	ADP	C5'-O5'-PA-O2A
4	E	1002	ADP	O4'-C4'-C5'-O5'
4	E	1002	ADP	C3'-C4'-C5'-O5'
4	E	1004	ADP	O4'-C4'-C5'-O5'
4	G	1001	ADP	O4'-C4'-C5'-O5'
4	G	1001	ADP	C3'-C4'-C5'-O5'
4	E	1004	ADP	C3'-C4'-C5'-O5'
4	G	1003	ADP	PB-O3A-PA-O5'
4	G	1003	ADP	C5'-O5'-PA-O3A
4	G	1001	ADP	C5'-O5'-PA-O3A
4	G	1001	ADP	C5'-O5'-PA-O2A
4	E	1002	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

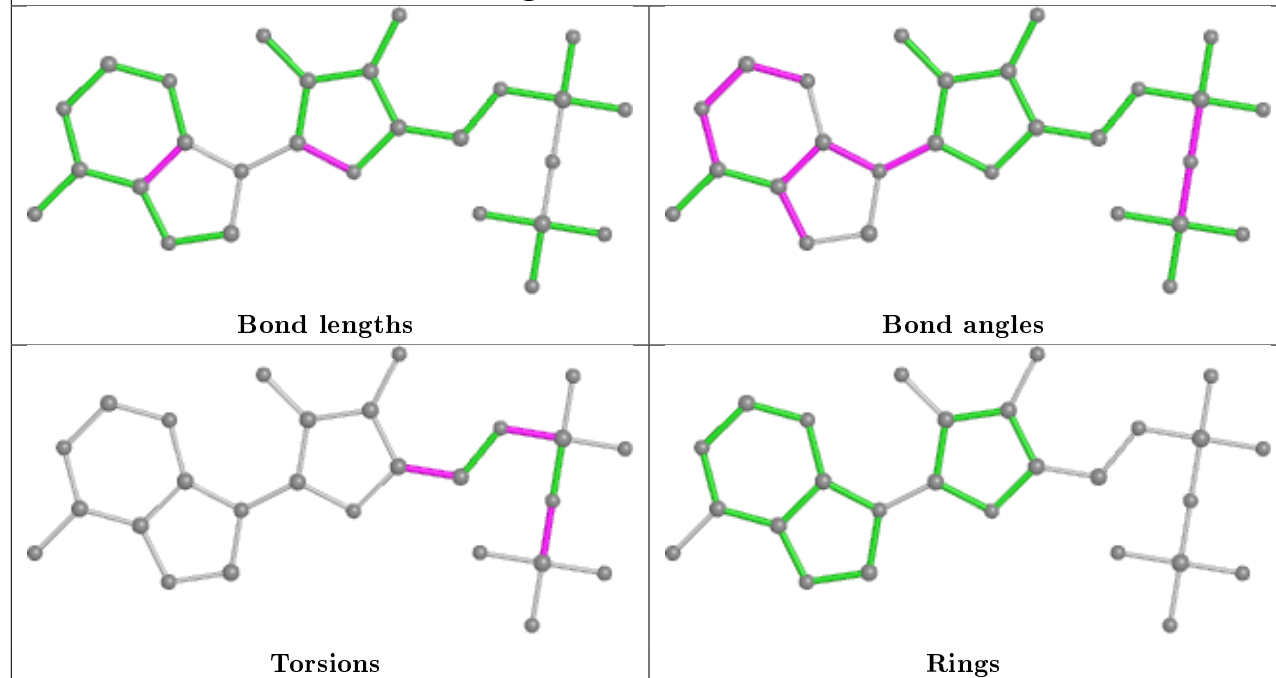
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1003	ADP	4	0
4	G	1001	ADP	4	0
4	E	1004	ADP	1	0

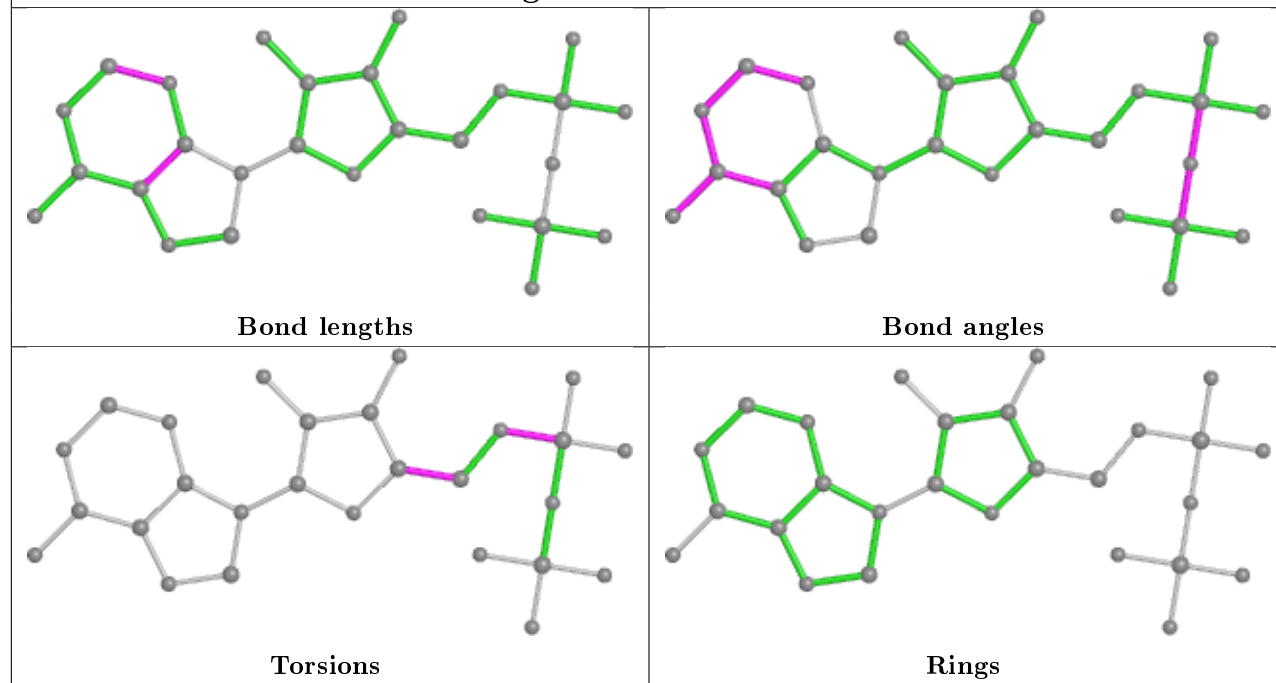
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

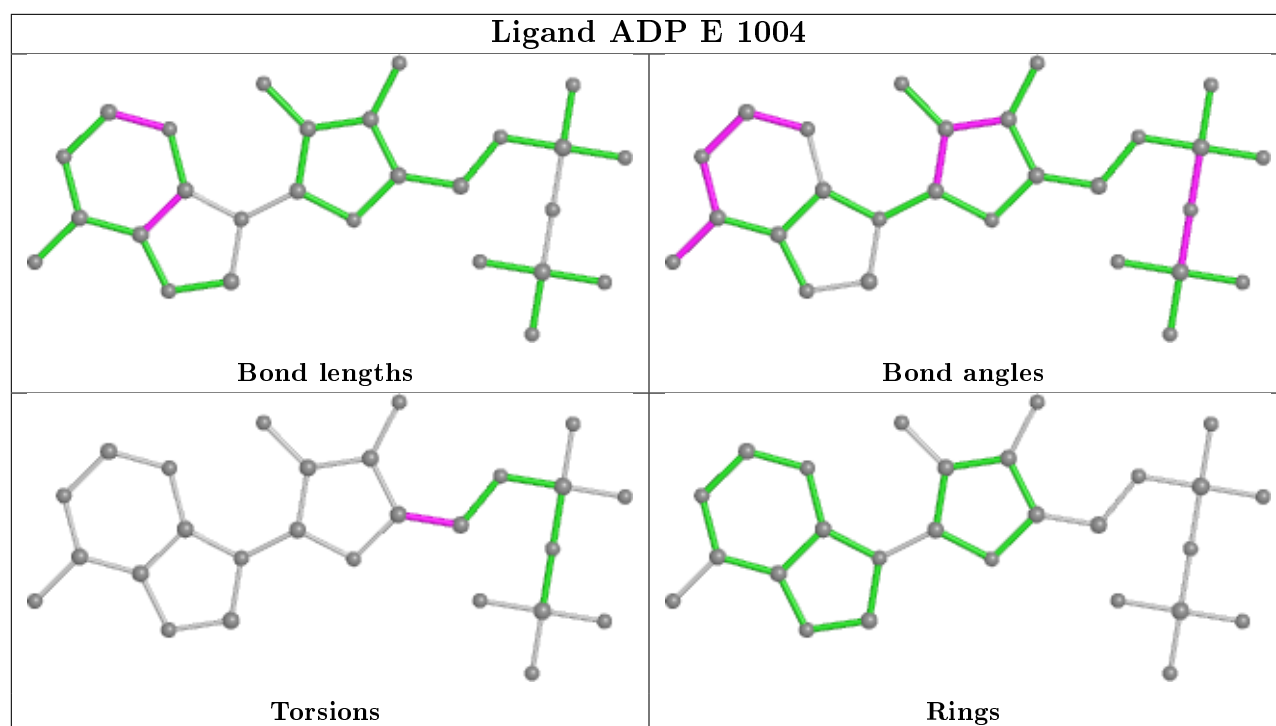


## Ligand ADP G 1001



## Ligand ADP E 1002





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	116/137 (84%)	0.62	9 (7%) 13 11	40, 52, 59, 63	0
1	C	112/137 (81%)	0.61	11 (9%) 7 5	45, 52, 57, 62	0
2	B	91/97 (93%)	1.01	11 (12%) 4 3	47, 52, 61, 65	0
2	D	91/97 (93%)	0.88	9 (9%) 7 5	45, 52, 60, 63	0
3	E	324/334 (97%)	0.50	8 (2%) 57 59	41, 52, 64, 76	0
3	G	324/334 (97%)	0.39	10 (3%) 49 49	42, 52, 61, 74	1 (0%)
All	All	1058/1136 (93%)	0.57	58 (5%) 25 24	40, 52, 61, 76	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	220	THR	9.6
2	B	224	LEU	8.3
3	G	328	ASP	5.6
1	A	544	HIS	5.5
3	E	318	THR	4.7
3	G	4	VAL	4.4
2	B	223	GLU	4.4
2	D	225	LYS	4.4
3	G	2	MET	4.0
2	B	220	THR	3.9
3	E	330	PHE	3.8
3	G	329	ASN	3.7
1	C	576	ALA	3.7
2	B	259	HIS	3.7
1	C	510	GLY	3.6
1	C	512	ASN	3.6
2	B	218	SER	3.6
1	A	487	ASN	3.6
2	B	249	GLU	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	246	ALA	3.2
1	A	491	ARG	3.1
3	E	119	THR	3.0
1	A	489	LYS	3.0
2	D	258	ASN	3.0
1	A	484	LYS	2.9
3	G	1	ALA	2.9
1	C	541	ILE	2.8
3	E	328	ASP	2.8
2	D	223	GLU	2.8
2	B	219	ASN	2.8
3	E	4	VAL	2.7
3	E	317	LYS	2.7
3	G	3	ASP	2.6
1	C	526	PRO	2.6
3	G	281	ASP	2.5
2	D	219	ASN	2.5
3	E	150	GLY	2.5
1	A	486	VAL	2.5
2	D	235	HIS	2.4
3	G	262	ALA	2.4
1	A	555	ASP	2.4
1	C	540	ASP	2.4
1	C	507	LYS	2.3
1	C	459[A]	ARG	2.3
1	A	466	LEU	2.3
2	B	245	THR	2.3
2	B	297	ASP	2.3
2	B	234	PRO	2.3
2	D	221	LEU	2.3
3	G	330	PHE	2.2
2	D	259	HIS	2.2
1	C	524	VAL	2.2
3	E	3	ASP	2.2
1	A	462	ALA	2.1
1	C	460	GLY	2.1
3	G	98	ASP	2.0
1	C	513	THR	2.0
2	D	231	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

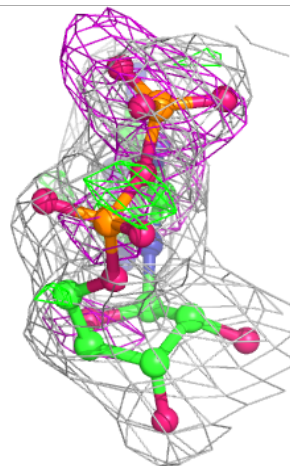
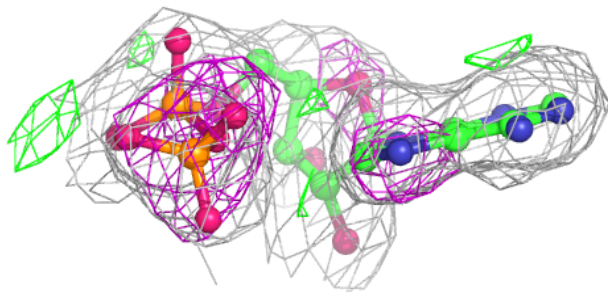
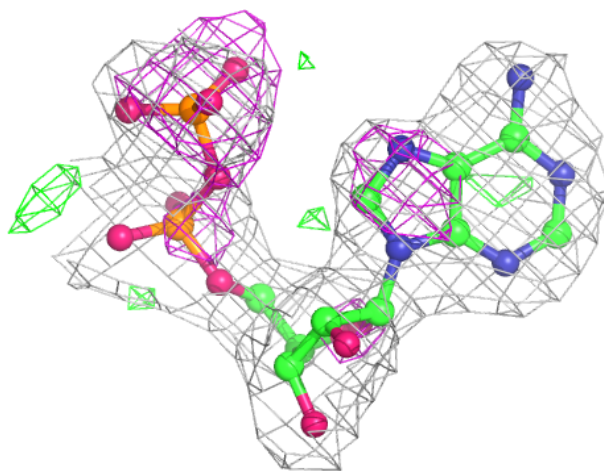
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ADP	G	1001	27/27	0.92	0.22	35,37,54,56	0
4	ADP	G	1003	27/27	0.93	0.19	61,65,74,75	0
4	ADP	E	1002	27/27	0.93	0.16	43,45,63,64	0
4	ADP	E	1004	27/27	0.94	0.20	70,72,80,81	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.

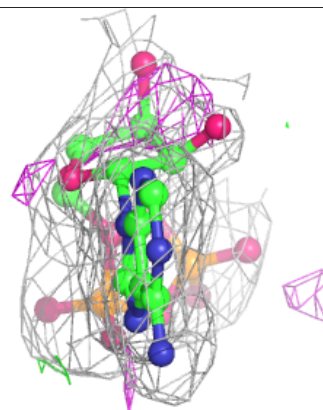
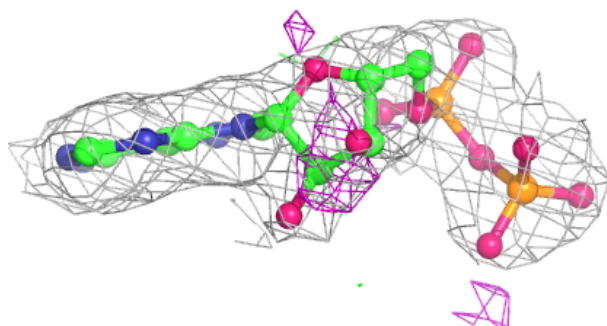
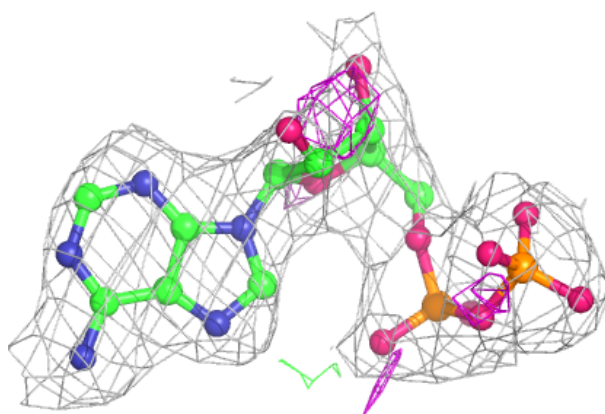
**Electron density around ADP G 1001:**

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



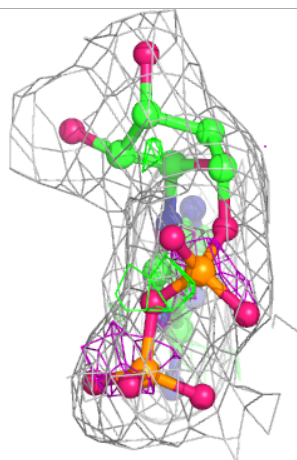
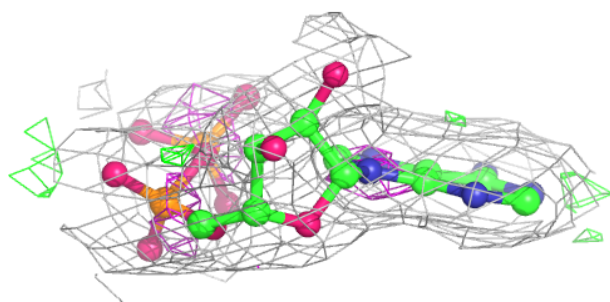
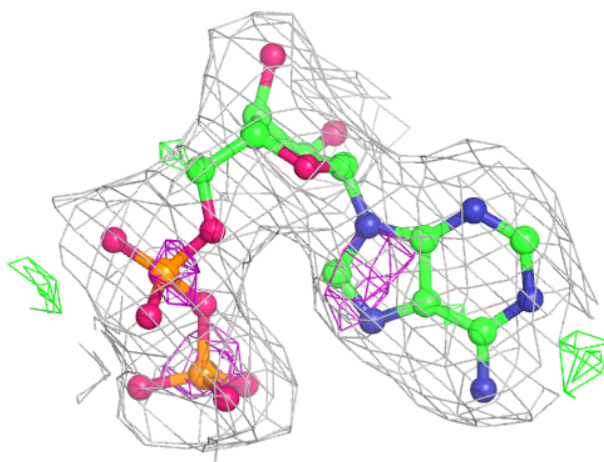
**Electron density around ADP G 1003:**

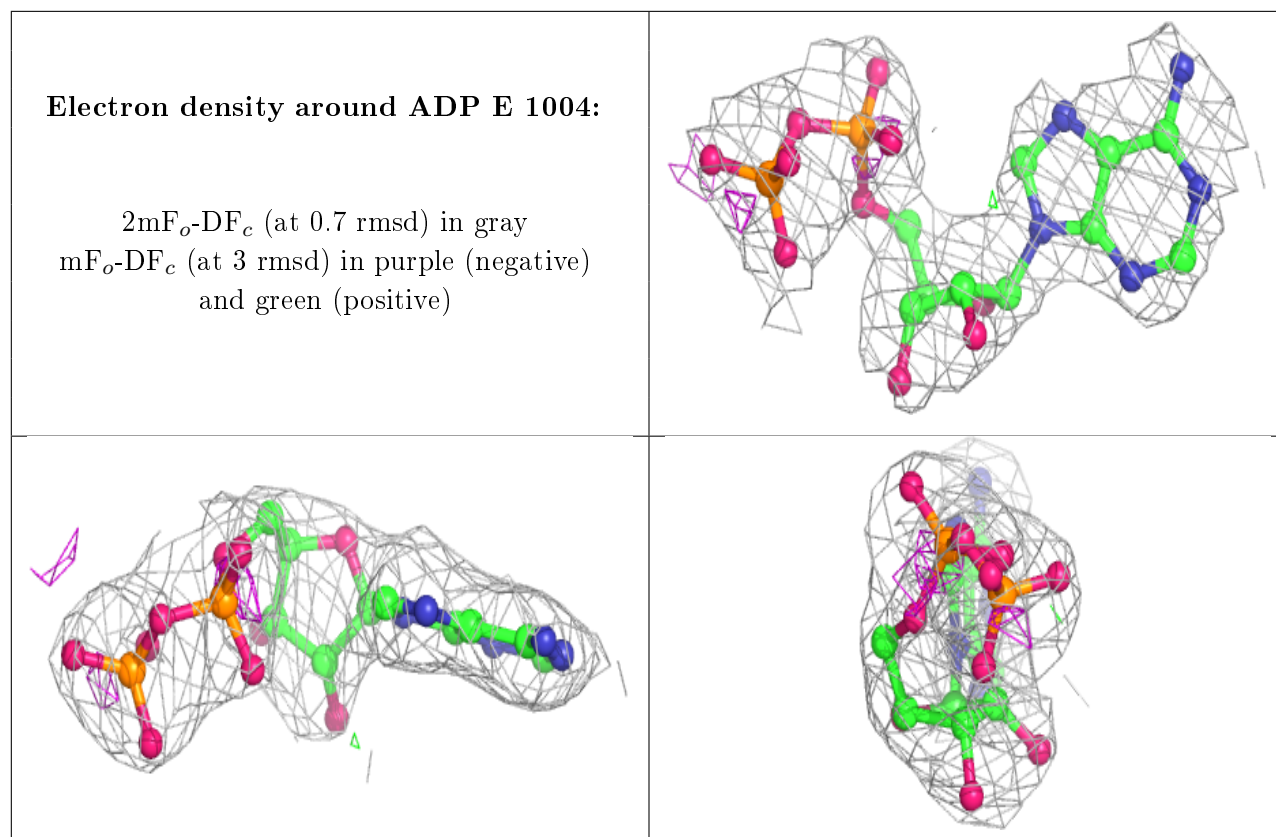
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ADP E 1002:**

$2mF_o-DF_c$  (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.