



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 10:05 pm BST

PDB ID : 2QRE  
Title : Crystal structure of the adenylate sensor from AMP-activated protein kinase in complex with 5-aminoimidazole-4-carboxamide 1-beta-D-ribofuranotide (ZMP)  
Authors : Jin, X.; Townley, R.; Shapiro, L.  
Deposited on : 2007-07-28  
Resolution : 3.01 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

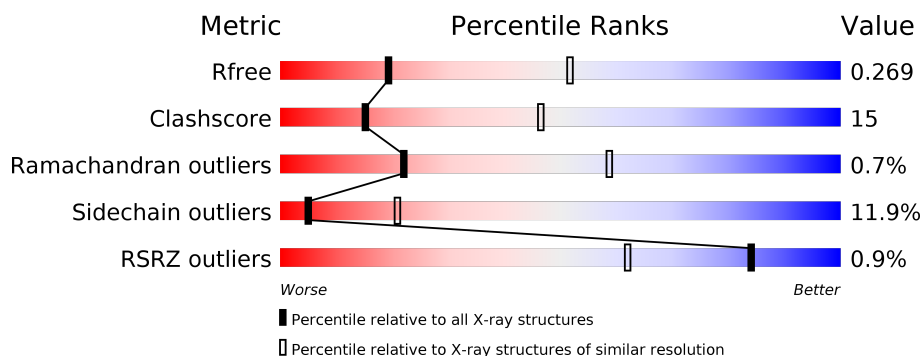
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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>47%</div> <div>28%</div> <div>• •</div> <div>20%</div> </div>
1	C	137	<div> <div>2%</div> <div>55%</div> <div>23%</div> <div>•</div> <div>18%</div> </div>
2	B	97	<div> <div>2%</div> <div>55%</div> <div>27%</div> <div>6%</div> <div>12%</div> </div>
2	D	97	<div> <div>2%</div> <div>57%</div> <div>32%</div> <div>5%</div> <div>6%</div> </div>
3	E	334	<div> <div>•</div> <div>56%</div> <div>34%</div> <div>•</div> <div>6%</div> </div>
3	G	334	<div> <div>63%</div> <div>25%</div> <div>6%</div> <div>6%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8201 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	109	Total	C	N	O	S	0	0	0
			882	572	148	153	9			
1	C	113	Total	C	N	O	S	0	0	0
			903	583	155	156	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	85	Total	C	N	O	S	0	0	0
			668	428	115	123	2			
2	D	91	Total	C	N	O	S	0	0	0
			718	459	123	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	315	Total	C	N	O	S	0	0	0
			2478	1585	414	464	15			
3	E	315	Total	C	N	O	S	0	1	0
			2489	1591	417	466	15			

There are 4 discrepancies between the modelled and reference sequences:

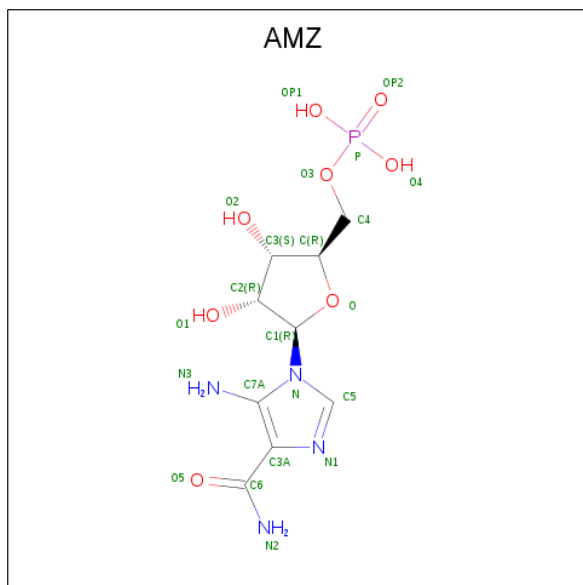
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	EXPRESSION TAG	UNP Q10343
G	2	MET	-	EXPRESSION TAG	UNP Q10343

*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 AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (three-letter code: AMZ) (formula:  $C_9H_{15}N_4O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			22	9	4	8	1		
4	E	1	Total	C	N	O	P	0	0
			22	9	4	8	1		

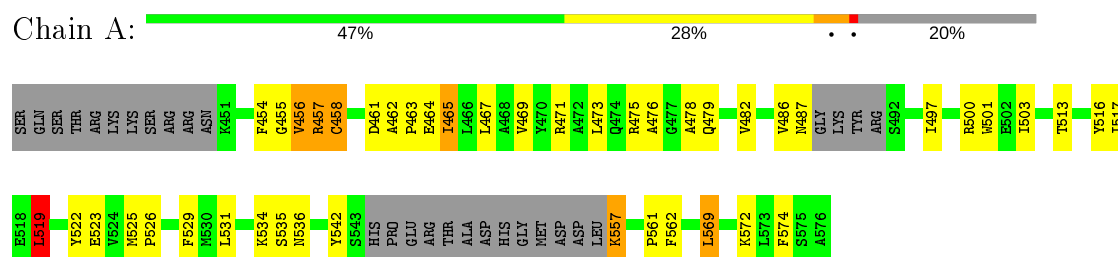
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	G	9	Total	O	0	0
			9	9		
5	C	2	Total	O	0	0
			2	2		
5	D	2	Total	O	0	0
			2	2		
5	E	4	Total	O	0	0
			4	4		

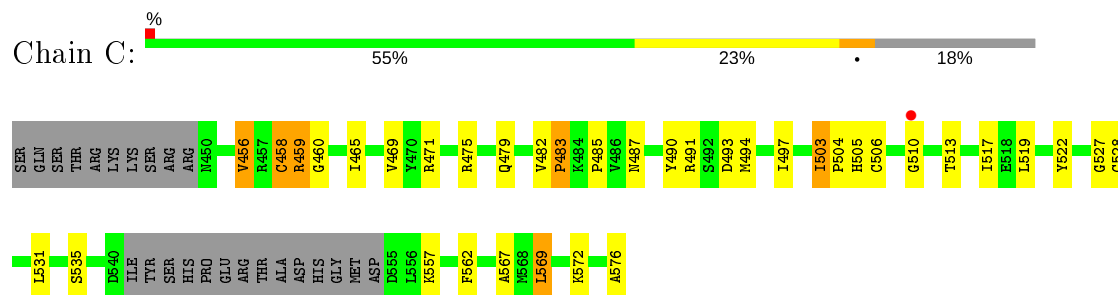
### 3 Residue-property plots

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.

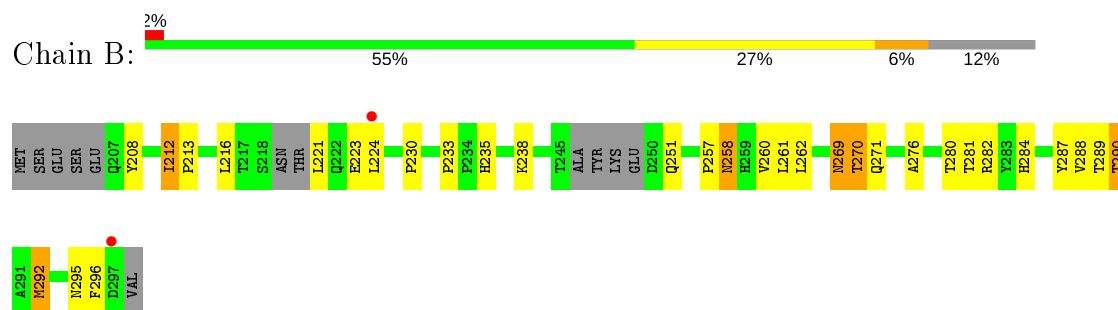
- Molecule 1: SNF1-like protein kinase ssp2



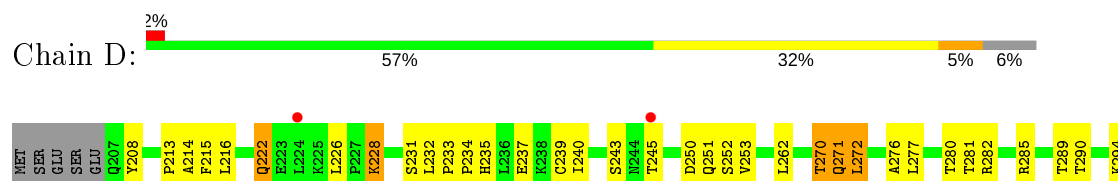
- Molecule 1: SNF1-like protein kinase ssp2



- Molecule 2: SPCC1919.03c protein



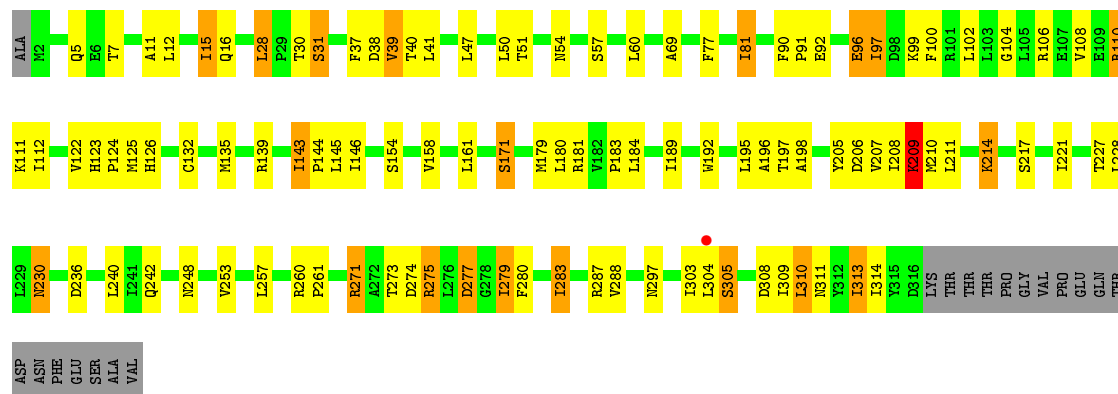
- Molecule 2: SPCC1919.03c protein





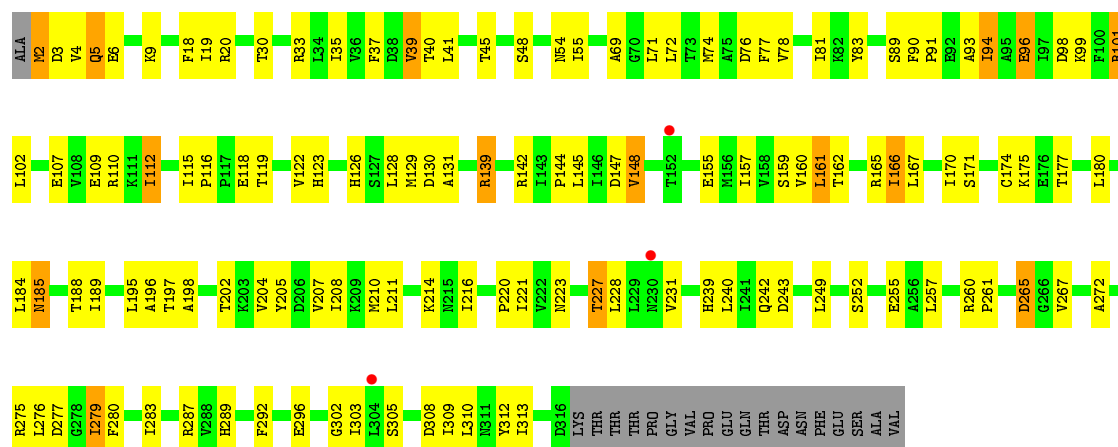
• Molecule 3: Protein C1556.08c

Chain G: 63% 25% 6% 6%



• Molecule 3: Protein C1556.08c

Chain E: 56% 34% 6% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.47Å 78.15Å 108.51Å 90.00° 124.04° 90.00°	Depositor
Resolution (Å)	41.34 – 3.01 41.34 – 3.01	Depositor EDS
% Data completeness (in resolution range)	89.2 (41.34-3.01) 89.2 (41.34-3.01)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.235 , 0.297 0.247 , 0.269	Depositor DCC
$R_{free}$ test set	1074 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 86.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: AMZ

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	0.58	0/904	0.70	2/1215 (0.2%)
1	C	0.55	0/926	0.63	0/1246
2	B	0.49	0/683	0.85	4/931 (0.4%)
2	D	0.49	0/736	0.75	1/1006 (0.1%)
3	E	0.53	0/2534	0.68	0/3433
3	G	0.52	0/2520	0.69	2/3415 (0.1%)
All	All	0.53	0/8303	0.70	9/11246 (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
3	E	0	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	258	ASN	CB-CA-C	6.89	124.17	110.40
2	B	224	LEU	N-CA-C	-6.25	94.13	111.00
2	B	223	GLU	N-CA-C	6.10	127.48	111.00
1	A	519	LEU	CA-CB-CG	5.86	128.79	115.30
2	B	223	GLU	CB-CA-C	-5.77	98.86	110.40
2	D	297	ASP	N-CA-CB	5.60	120.69	110.60
3	G	228	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	569	LEU	CA-CB-CG	5.17	127.18	115.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	96	GLU	CB-CA-C	-5.15	100.10	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	2	MET	Peptide
3	G	209	LYS	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	882	0	880	33	0
1	C	903	0	889	23	0
2	B	668	0	676	23	0
2	D	718	0	724	22	0
3	E	2489	0	2545	90	0
3	G	2478	0	2530	81	0
4	E	22	0	13	1	0
4	G	22	0	13	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	4	0	0	0	0
5	G	9	0	0	0	0
All	All	8201	0	8270	246	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 (246) 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:G:81:ILE:HD11	3:G:208:ILE:CD1	1.41	1.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:81:ILE:CD1	3:G:208:ILE:CD1	2.22	1.18
3:G:81:ILE:CD1	3:G:208:ILE:HD11	1.72	1.16
3:E:3:ASP:O	3:E:4:VAL:HG12	1.57	1.03
3:G:208:ILE:HA	3:G:211:LEU:HD12	1.41	1.02
3:G:81:ILE:HD11	3:G:208:ILE:HD12	1.42	0.98
1:C:456:VAL:HG13	1:C:531:LEU:HB3	1.49	0.94
3:G:81:ILE:HD11	3:G:208:ILE:HD11	0.93	0.91
3:G:81:ILE:CD1	3:G:208:ILE:HD12	1.97	0.89
3:E:239:HIS:HA	3:E:242:GLN:HE21	1.38	0.86
3:E:4:VAL:HG13	3:E:5:GLN:N	1.94	0.83
3:E:4:VAL:CG1	3:E:5:GLN:H	1.93	0.82
3:G:144:PRO:HB2	3:G:146:ILE:CD1	2.09	0.82
3:G:123:HIS:HB3	3:G:126:HIS:CD2	2.15	0.81
3:G:122:VAL:HG22	3:G:143:ILE:HD13	1.63	0.80
3:E:296:GLU:H	3:E:296:GLU:CD	1.86	0.79
3:E:4:VAL:CG1	3:E:5:GLN:N	2.44	0.79
3:G:181:ARG:HA	3:G:275:ARG:HG3	1.64	0.79
3:E:265:ASP:CG	3:E:289:HIS:HE2	1.86	0.78
3:G:207:VAL:O	3:G:210:MET:HB2	1.83	0.78
3:E:123:HIS:HE1	3:E:147:ASP:OD1	1.66	0.77
3:E:83:TYR:CD1	3:E:112:ILE:HD13	2.18	0.77
3:G:81:ILE:CG1	3:G:208:ILE:HD12	2.15	0.77
3:E:123:HIS:CE1	3:E:147:ASP:OD1	2.38	0.76
1:A:462:ALA:HB3	1:A:463:PRO:HD3	1.68	0.74
3:G:283:ILE:HG22	3:G:288:VAL:HB	1.68	0.74
3:E:265:ASP:HB3	3:E:287:ARG:NH2	2.03	0.73
3:G:279:ILE:HD11	3:G:309:ILE:HD13	1.70	0.71
2:D:222:GLN:HA	2:D:222:GLN:HE21	1.56	0.70
1:A:534:LYS:HE3	1:A:536:ASN:HD21	1.58	0.69
3:E:208:ILE:HA	3:E:211:LEU:HD12	1.73	0.69
3:E:37:PHE:HB3	3:E:41:LEU:HD12	1.74	0.68
3:E:205:TYR:HA	3:E:208:ILE:HG12	1.74	0.68
3:G:123:HIS:HD2	3:G:125:MET:H	1.41	0.68
3:G:304:LEU:HD11	3:G:309:ILE:HG22	1.76	0.68
3:G:96:GLU:HG2	3:G:96:GLU:O	1.93	0.67
1:A:465:ILE:HG23	3:E:89:SER:HB3	1.77	0.66
1:A:482:VAL:HG22	2:B:213:PRO:HG3	1.78	0.66
2:D:234:PRO:O	2:D:237:GLU:HB2	1.95	0.66
1:A:557:LYS:O	2:B:281:THR:OG1	2.14	0.66
1:C:485:PRO:HG3	1:C:490:TYR:CE2	2.31	0.65
1:C:503:ILE:HD11	1:C:505:HIS:ND1	2.11	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:VAL:HG12	3:E:5:GLN:H	1.62	0.65
3:G:106:ARG:HH21	3:G:110:ARG:NH1	1.95	0.65
3:E:265:ASP:HB3	3:E:287:ARG:CZ	2.28	0.64
1:C:479:GLN:HB3	2:D:208:TYR:HB3	1.80	0.64
3:G:97:ILE:O	3:G:97:ILE:HG12	1.97	0.64
3:E:122:VAL:HG21	3:E:131:ALA:HB2	1.81	0.63
3:G:81:ILE:HG12	3:G:208:ILE:HD12	1.81	0.62
3:G:221:ILE:HD11	3:G:253:VAL:HG11	1.81	0.62
1:C:503:ILE:HD12	1:C:506:CYS:SG	2.39	0.62
3:G:305:SER:O	3:G:308:ASP:HB2	1.99	0.62
3:G:144:PRO:HB2	3:G:146:ILE:HD13	1.80	0.61
1:C:459:ARG:HD2	1:C:528:CYS:SG	2.40	0.61
3:E:252:SER:OG	3:E:255:GLU:HG3	2.00	0.61
3:G:108:VAL:O	3:G:112:ILE:HG12	2.00	0.61
3:G:196:ALA:HB2	3:G:214:LYS:HD2	1.82	0.60
1:A:475:ARG:HB3	1:A:572:LYS:HE2	1.83	0.60
3:G:210:MET:O	3:G:214:LYS:HB2	2.01	0.60
3:E:167:LEU:HB3	3:E:283:ILE:CD1	2.32	0.60
3:G:16:GLN:HG2	3:G:313:ILE:O	2.03	0.59
2:B:280:THR:HA	2:B:289:THR:HA	1.84	0.59
3:E:77:PHE:O	3:E:81:ILE:HG13	2.03	0.59
1:C:503:ILE:HG22	1:C:513:THR:O	2.03	0.59
1:A:534:LYS:HE3	1:A:536:ASN:ND2	2.18	0.58
3:E:292:PHE:HD2	3:E:303:ILE:HG12	1.68	0.58
3:G:311:ASN:HA	3:G:314:ILE:HG12	1.84	0.58
3:G:77:PHE:O	3:G:81:ILE:HG23	2.04	0.58
2:B:233:PRO:HB2	2:B:235:HIS:CD2	2.39	0.58
3:E:204:VAL:HG11	3:E:240:LEU:HD21	1.85	0.58
2:D:280:THR:OG1	2:D:289:THR:HG23	2.04	0.58
3:G:37:PHE:HB3	3:G:41:LEU:HD12	1.86	0.57
1:C:465:ILE:O	1:C:469:VAL:HG23	2.05	0.57
3:E:305:SER:O	3:E:308:ASP:HB2	2.05	0.56
1:A:458:CYS:HB3	3:E:90:PHE:CD2	2.40	0.56
3:G:38:ASP:OD1	3:G:40:THR:OG1	2.17	0.56
3:G:96:GLU:CG	3:G:96:GLU:O	2.52	0.56
2:B:258:ASN:O	2:B:262:LEU:HD13	2.05	0.56
1:A:503:ILE:HD13	1:A:561:PRO:HG3	1.86	0.56
3:G:39:VAL:HG11	3:G:69:ALA:CB	2.35	0.56
3:G:221:ILE:CD1	3:G:253:VAL:HG11	2.36	0.56
1:C:557:LYS:O	2:D:281:THR:OG1	2.24	0.56
3:E:40:THR:O	3:E:101:ARG:NH1	2.39	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:HB3	1:A:457:ARG:HH11	1.71	0.55
2:D:271:GLN:HG3	2:D:271:GLN:O	2.05	0.55
2:B:296:PHE:CD2	3:E:96:GLU:HG2	2.42	0.55
3:E:3:ASP:O	3:E:4:VAL:CG1	2.44	0.55
3:E:39:VAL:HG11	3:E:69:ALA:CB	2.37	0.55
3:G:205:TYR:HA	3:G:208:ILE:CD1	2.37	0.55
3:E:265:ASP:OD1	3:E:289:HIS:NE2	2.26	0.54
1:C:519:LEU:HD11	1:C:569:LEU:HD11	1.89	0.54
1:A:535:SER:HB2	1:A:562:PHE:CD1	2.42	0.54
3:E:142:ARG:HG2	3:E:162:THR:HG22	1.90	0.54
3:E:214:LYS:O	3:E:216:ILE:HG23	2.06	0.54
3:E:292:PHE:CD2	3:E:303:ILE:HG12	2.43	0.54
1:A:501:TRP:CD1	1:A:517:ILE:HD12	2.43	0.53
3:E:276:LEU:HA	3:E:279:ILE:HG12	1.90	0.53
3:G:139:ARG:O	3:G:139:ARG:HG3	2.08	0.53
1:A:456:VAL:HG13	1:A:531:LEU:HB3	1.91	0.53
3:E:276:LEU:HD13	3:E:279:ILE:HG12	1.91	0.53
3:G:310:LEU:HD23	3:G:313:ILE:HD11	1.92	0.52
1:A:523:GLU:HA	1:A:529:PHE:CD2	2.44	0.52
1:A:486:VAL:O	1:A:486:VAL:HG13	2.08	0.52
2:D:250:ASP:HB3	2:D:252:SER:OG	2.09	0.52
3:E:33[B]:ARG:NH2	3:E:35:ILE:HD11	2.25	0.52
3:G:209:LYS:HG2	3:G:210:MET:N	2.24	0.52
3:E:116:PRO:HG2	3:E:118:GLU:O	2.09	0.52
1:C:471:ARG:O	1:C:475:ARG:HG3	2.08	0.52
1:C:491:ARG:O	1:C:494:MET:HB2	2.10	0.52
3:E:180:LEU:O	3:E:277:ASP:HB3	2.09	0.52
3:E:204:VAL:HG11	3:E:240:LEU:CD2	2.40	0.52
3:E:3:ASP:O	3:E:3:ASP:CG	2.48	0.52
1:C:458:CYS:O	1:C:459:ARG:HD3	2.10	0.52
1:A:465:ILE:CG2	3:E:89:SER:HB3	2.40	0.52
3:E:101:ARG:HH11	3:E:101:ARG:HG2	1.75	0.52
3:G:139:ARG:HD3	4:G:1001:AMZ:H7	1.92	0.52
3:G:236:ASP:OD2	3:G:260:ARG:NH1	2.43	0.52
2:D:272:LEU:HD13	3:E:45:THR:HG23	1.92	0.51
1:A:479:GLN:HB3	2:B:208:TYR:HB3	1.92	0.51
3:E:107:GLU:HG3	3:E:110:ARG:HH21	1.75	0.51
3:G:180:LEU:O	3:G:277:ASP:HB3	2.10	0.51
2:D:251:GLN:OE1	3:E:54:ASN:HB3	2.11	0.51
3:E:231:VAL:HG12	3:E:267:VAL:HG22	1.92	0.51
3:E:195:LEU:HD11	3:E:302:GLY:HA2	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:39:VAL:HG11	3:E:69:ALA:HB1	1.92	0.51
2:B:295:ASN:HD21	3:G:41:LEU:HA	1.76	0.51
3:E:40:THR:O	3:E:101:ARG:HG2	2.11	0.50
1:A:461:ASP:HB3	1:A:464:GLU:HB2	1.93	0.50
3:E:123:HIS:HB3	3:E:126:HIS:ND1	2.26	0.50
3:E:72:LEU:HD22	3:E:102:LEU:HD21	1.93	0.50
3:E:145:LEU:HD11	3:E:161:LEU:HD13	1.92	0.50
3:E:76:ASP:HA	3:E:109:GLU:OE1	2.12	0.50
1:A:497:ILE:HB	1:A:519:LEU:HD23	1.94	0.50
2:B:282:ARG:HG2	2:B:284:HIS:O	2.12	0.49
1:A:478:ALA:HB2	1:A:501:TRP:CD2	2.47	0.49
3:E:223:ASN:OD1	3:E:227:THR:HG23	2.11	0.49
3:G:260:ARG:HG3	3:G:261:PRO:HD2	1.94	0.49
1:A:454:PHE:CZ	2:B:261:LEU:HD13	2.48	0.49
1:A:523:GLU:HG3	1:A:529:PHE:CE2	2.48	0.49
2:D:262:LEU:HD21	2:D:282:ARG:HB2	1.95	0.49
3:E:279:ILE:HG13	3:E:280:PHE:N	2.28	0.49
1:A:500:ARG:HD3	2:B:208:TYR:CE1	2.48	0.48
3:E:205:TYR:O	3:E:208:ILE:HG13	2.13	0.48
3:G:171:SER:HB2	3:G:280:PHE:HD2	1.77	0.48
3:G:39:VAL:CG1	3:G:69:ALA:HB3	2.43	0.48
3:G:7:THR:HG21	3:G:181:ARG:HH21	1.77	0.48
2:B:251:GLN:HE22	3:G:54:ASN:HD22	1.61	0.48
3:E:159:SER:OG	3:E:160:VAL:N	2.46	0.48
1:A:574:PHE:CD1	3:E:93:ALA:HA	2.48	0.48
3:G:240:LEU:HG	3:G:248:ASN:HB3	1.95	0.48
2:B:276:ALA:HA	2:B:292:MET:O	2.14	0.48
3:G:111:LYS:HG2	3:G:112:ILE:HD13	1.96	0.48
3:G:123:HIS:CD2	3:G:125:MET:H	2.28	0.48
3:G:15:ILE:H	3:G:15:ILE:HG12	1.59	0.47
3:E:35:ILE:HD12	3:E:55:ILE:HD13	1.96	0.47
3:G:124:PRO:HG3	3:G:145:LEU:HB3	1.96	0.47
3:E:19:ILE:O	3:E:128:LEU:HB3	2.15	0.47
1:C:517:ILE:HD12	1:C:562:PHE:HD1	1.80	0.47
3:G:39:VAL:HG13	3:G:60:LEU:HB3	1.97	0.46
3:E:166:ILE:H	3:E:166:ILE:HG12	1.59	0.46
3:E:19:ILE:HG22	3:E:128:LEU:HD23	1.96	0.46
3:E:196:ALA:HB2	3:E:214:LYS:HD2	1.97	0.46
3:G:183:PRO:HB3	3:G:273:THR:O	2.16	0.46
3:E:101:ARG:HG2	3:E:101:ARG:NH1	2.30	0.46
3:G:310:LEU:HA	3:G:313:ILE:HD13	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:195:LEU:HD22	3:G:303:ILE:HD12	1.98	0.46
1:A:522:TYR:HA	2:B:230:PRO:O	2.15	0.46
1:A:454:PHE:HZ	2:B:261:LEU:HD13	1.81	0.46
2:B:261:LEU:O	2:B:262:LEU:C	2.53	0.46
2:B:288:VAL:HG12	2:B:290:THR:HG22	1.98	0.46
3:E:4:VAL:HG13	3:E:5:GLN:H	1.63	0.46
3:E:170:ILE:O	3:E:174:CYS:HB2	2.16	0.45
3:G:106:ARG:HH21	3:G:110:ARG:HH12	1.62	0.45
3:E:123:HIS:HB3	3:E:126:HIS:CE1	2.51	0.45
3:G:51:THR:HG21	3:G:242:GLN:OE1	2.16	0.45
1:C:460:GLY:O	1:C:527:GLY:HA2	2.17	0.45
3:G:104:GLY:O	3:G:108:VAL:HG23	2.16	0.45
3:G:171:SER:CB	3:G:280:PHE:HD2	2.28	0.45
2:D:270:THR:HG23	2:D:276:ALA:HB2	1.99	0.45
2:B:270:THR:O	2:B:271:GLN:HB2	2.17	0.44
3:E:171:SER:HA	3:E:177:THR:HG21	1.99	0.44
3:E:210:MET:O	3:E:214:LYS:HB2	2.18	0.44
3:E:198:ALA:HB1	3:E:202:THR:OG1	2.17	0.44
3:E:198:ALA:O	3:E:221:ILE:HG23	2.17	0.44
3:E:6:GLU:O	3:E:9:LYS:HB3	2.18	0.44
3:G:39:VAL:HG11	3:G:69:ALA:HB1	2.00	0.44
1:A:467:LEU:HB2	2:B:216:LEU:HD22	2.00	0.44
1:C:572:LYS:O	1:C:576:ALA:HB2	2.17	0.44
3:G:39:VAL:HG11	3:G:69:ALA:HB3	1.99	0.44
2:B:257:PRO:HG2	2:B:287:TYR:CD2	2.53	0.43
3:G:28:LEU:HD21	3:G:145:LEU:HD12	2.00	0.43
3:G:132:CYS:HB3	3:G:314:ILE:HG21	2.01	0.43
3:G:271:ARG:HB3	3:G:273:THR:OG1	2.18	0.43
2:B:287:TYR:HB2	3:G:31:SER:HB2	2.00	0.43
3:G:16:GLN:CG	3:G:313:ILE:O	2.67	0.43
1:A:458:CYS:HA	3:E:91:PRO:HD3	2.00	0.43
3:G:217:SER:N	4:G:1001:AMZ:OP1	2.51	0.43
3:G:145:LEU:HD11	3:G:161:LEU:HD13	1.99	0.43
1:C:503:ILE:HA	1:C:504:PRO:HD3	1.83	0.43
2:D:276:ALA:O	2:D:277:LEU:HD23	2.19	0.43
3:E:139:ARG:HA	3:E:139:ARG:HD2	1.80	0.43
2:D:250:ASP:HB2	2:D:253:VAL:HG23	1.99	0.43
3:E:71:LEU:HD13	3:E:144:PRO:HG3	1.99	0.43
2:B:212:ILE:HA	2:B:213:PRO:HD3	1.90	0.43
2:B:269:ASN:OD1	2:B:269:ASN:N	2.52	0.43
3:E:189:ILE:HG21	3:E:312:TYR:CD2	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:MET:HB2	1:A:526:PRO:HD2	2.00	0.43
3:G:11:ALA:O	3:G:15:ILE:HG12	2.18	0.43
2:D:214:ALA:C	2:D:216:LEU:H	2.22	0.42
1:C:522:TYR:CD1	2:D:233:PRO:HD3	2.54	0.42
3:E:185:ASN:OD1	3:E:272:ALA:O	2.37	0.42
3:E:72:LEU:HD11	3:E:77:PHE:CE1	2.54	0.42
3:G:97:ILE:HA	3:G:100:PHE:HD1	1.84	0.42
3:E:197:THR:HG22	3:E:220:PRO:HG2	2.00	0.42
2:D:272:LEU:HD22	3:E:48:SER:CB	2.50	0.42
3:G:230:ASN:OD1	3:G:260:ARG:NH2	2.53	0.42
1:C:483:PRO:HB3	1:C:494:MET:HG3	2.02	0.42
3:E:39:VAL:CG1	3:E:69:ALA:CB	2.97	0.42
3:G:205:TYR:O	3:G:208:ILE:HG12	2.19	0.42
3:G:47:LEU:HD23	3:G:50:LEU:HD12	2.02	0.42
3:E:265:ASP:CG	3:E:289:HIS:NE2	2.64	0.42
3:E:189:ILE:CG2	3:E:312:TYR:CD2	3.03	0.42
3:G:198:ALA:O	3:G:221:ILE:HA	2.19	0.42
3:E:74:MET:O	3:E:78:VAL:HG23	2.20	0.41
1:C:483:PRO:O	1:C:485:PRO:HD3	2.20	0.41
2:D:251:GLN:NE2	3:E:54:ASN:OD1	2.47	0.41
3:E:148:VAL:HG12	3:E:155:GLU:HA	2.02	0.41
3:E:260:ARG:HG3	3:E:261:PRO:HD2	2.01	0.41
3:G:184:LEU:HD13	3:G:274:ASP:O	2.20	0.41
1:A:467:LEU:O	1:A:471:ARG:HG3	2.20	0.41
3:E:18:PHE:CE1	3:E:170:ILE:HG22	2.56	0.41
1:C:497:ILE:HB	1:C:519:LEU:HB2	2.03	0.41
3:E:240:LEU:HD23	3:E:249:LEU:HD23	2.02	0.41
3:G:90:PHE:HA	3:G:91:PRO:HD3	1.92	0.41
1:A:500:ARG:HG3	1:A:516:TYR:CE1	2.56	0.41
1:A:476:ALA:HB1	1:A:501:TRP:CZ3	2.56	0.41
3:G:189:ILE:O	3:G:192:TRP:NE1	2.31	0.41
3:G:124:PRO:HG2	3:G:158:VAL:HG21	2.02	0.41
3:G:96:GLU:O	3:G:99:LYS:HG2	2.21	0.41
1:A:469:VAL:O	1:A:473:LEU:HG	2.21	0.40
1:C:482:VAL:HG22	2:D:213:PRO:HG3	2.02	0.40
1:C:567:ALA:HB1	2:D:294:LYS:HE2	2.03	0.40
2:D:228:LYS:HD2	2:D:228:LYS:H	1.85	0.40
2:D:226:LEU:HD12	2:D:226:LEU:H	1.86	0.40
3:E:139:ARG:HH21	4:E:1002:AMZ:P	2.45	0.40
2:D:232:LEU:HA	2:D:233:PRO:HD3	1.90	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	103/137 (75%)	97 (94%)	5 (5%)	1 (1%)	15	50
1	C	109/137 (80%)	102 (94%)	5 (5%)	2 (2%)	8	35
2	B	79/97 (81%)	73 (92%)	6 (8%)	0	100	100
2	D	89/97 (92%)	74 (83%)	13 (15%)	2 (2%)	6	30
3	E	314/334 (94%)	284 (90%)	29 (9%)	1 (0%)	41	75
3	G	313/334 (94%)	291 (93%)	21 (7%)	1 (0%)	41	75
All	All	1007/1136 (89%)	921 (92%)	79 (8%)	7 (1%)	22	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	510	GLY
1	A	455	GLY
3	G	135	MET
2	D	215	PHE
2	D	243	SER
1	C	483	PRO
3	E	94	ILE

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/120 (79%)	85 (90%)	10 (10%)	7	26

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	94/120 (78%)	86 (92%)	8 (8%)	10	36
2	B	77/88 (88%)	69 (90%)	8 (10%)	7	26
2	D	82/88 (93%)	70 (85%)	12 (15%)	3	14
3	E	280/296 (95%)	244 (87%)	36 (13%)	4	18
3	G	278/296 (94%)	244 (88%)	34 (12%)	5	20
All	All	906/1008 (90%)	798 (88%)	108 (12%)	5	21

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

Mol	Chain	Res	Type
1	A	456	VAL
1	A	457	ARG
1	A	458	CYS
1	A	465	ILE
1	A	487	ASN
1	A	513	THR
1	A	519	LEU
1	A	542	TYR
1	A	557	LYS
1	A	569	LEU
2	B	212	ILE
2	B	221	LEU
2	B	238	LYS
2	B	260	VAL
2	B	269	ASN
2	B	270	THR
2	B	290	THR
2	B	292	MET
3	G	5	GLN
3	G	12	LEU
3	G	15	ILE
3	G	28	LEU
3	G	30	THR
3	G	31	SER
3	G	39	VAL
3	G	57	SER
3	G	81	ILE
3	G	92	GLU
3	G	97	ILE
3	G	102	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	110	ARG
3	G	143	ILE
3	G	154	SER
3	G	171	SER
3	G	179	MET
3	G	197	THR
3	G	206	ASP
3	G	209	LYS
3	G	214	LYS
3	G	227	THR
3	G	230	ASN
3	G	257	LEU
3	G	271	ARG
3	G	275	ARG
3	G	277	ASP
3	G	279	ILE
3	G	283	ILE
3	G	287	ARG
3	G	297	ASN
3	G	305	SER
3	G	310	LEU
3	G	313	ILE
1	C	456	VAL
1	C	458	CYS
1	C	459	ARG
1	C	487	ASN
1	C	493	ASP
1	C	503	ILE
1	C	535	SER
1	C	569	LEU
2	D	222	GLN
2	D	228	LYS
2	D	231	SER
2	D	235	HIS
2	D	239	CYS
2	D	240	ILE
2	D	245	THR
2	D	270	THR
2	D	271	GLN
2	D	272	LEU
2	D	285	ARG
2	D	290	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	E	2	MET
3	E	5	GLN
3	E	20	ARG
3	E	30	THR
3	E	39	VAL
3	E	94	ILE
3	E	96	GLU
3	E	98	ASP
3	E	99	LYS
3	E	101	ARG
3	E	112	ILE
3	E	115	ILE
3	E	119	THR
3	E	129	MET
3	E	130	ASP
3	E	139	ARG
3	E	148	VAL
3	E	157	ILE
3	E	161	LEU
3	E	165	ARG
3	E	166	ILE
3	E	175	LYS
3	E	184	LEU
3	E	185	ASN
3	E	188	THR
3	E	207	VAL
3	E	227	THR
3	E	228	LEU
3	E	243	ASP
3	E	257	LEU
3	E	265	ASP
3	E	275	ARG
3	E	279	ILE
3	E	309	ILE
3	E	310	LEU
3	E	313	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	ASN
1	A	536	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	235	HIS
2	B	284	HIS
2	B	295	ASN
3	G	53	ASN
3	G	54	ASN
3	G	86	GLN
3	G	123	HIS
3	G	126	HIS
3	G	173	ASN
3	G	185	ASN
1	C	536	ASN
2	D	219	ASN
2	D	222	GLN
2	D	263	ASN
2	D	284	HIS
3	E	66	ASN
3	E	123	HIS
3	E	163	GLN
3	E	242	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 ⓘ

2 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	AMZ	G	1001	-	18,23,23	0.81	0	22,35,35	1.17	2 (9%)
4	AMZ	E	1002	-	18,23,23	0.77	0	22,35,35	1.36	3 (13%)

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	AMZ	G	1001	-	-	0/6/30/30	0/2/2/2
4	AMZ	E	1002	-	-	5/6/30/30	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1002	AMZ	C5-N1-C3A	2.86	108.44	102.99
4	E	1002	AMZ	C3A-C6-N2	2.65	119.94	115.75
4	G	1001	AMZ	O4-P-OP2	2.14	119.06	110.68
4	G	1001	AMZ	O4-P-O3	-2.04	101.31	106.73
4	E	1002	AMZ	O4-P-OP1	2.03	115.40	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1002	AMZ	C4-O3-P-OP1
4	E	1002	AMZ	C4-O3-P-O4
4	E	1002	AMZ	C4-O3-P-OP2
4	E	1002	AMZ	O-C-C4-O3
4	E	1002	AMZ	C3-C-C4-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

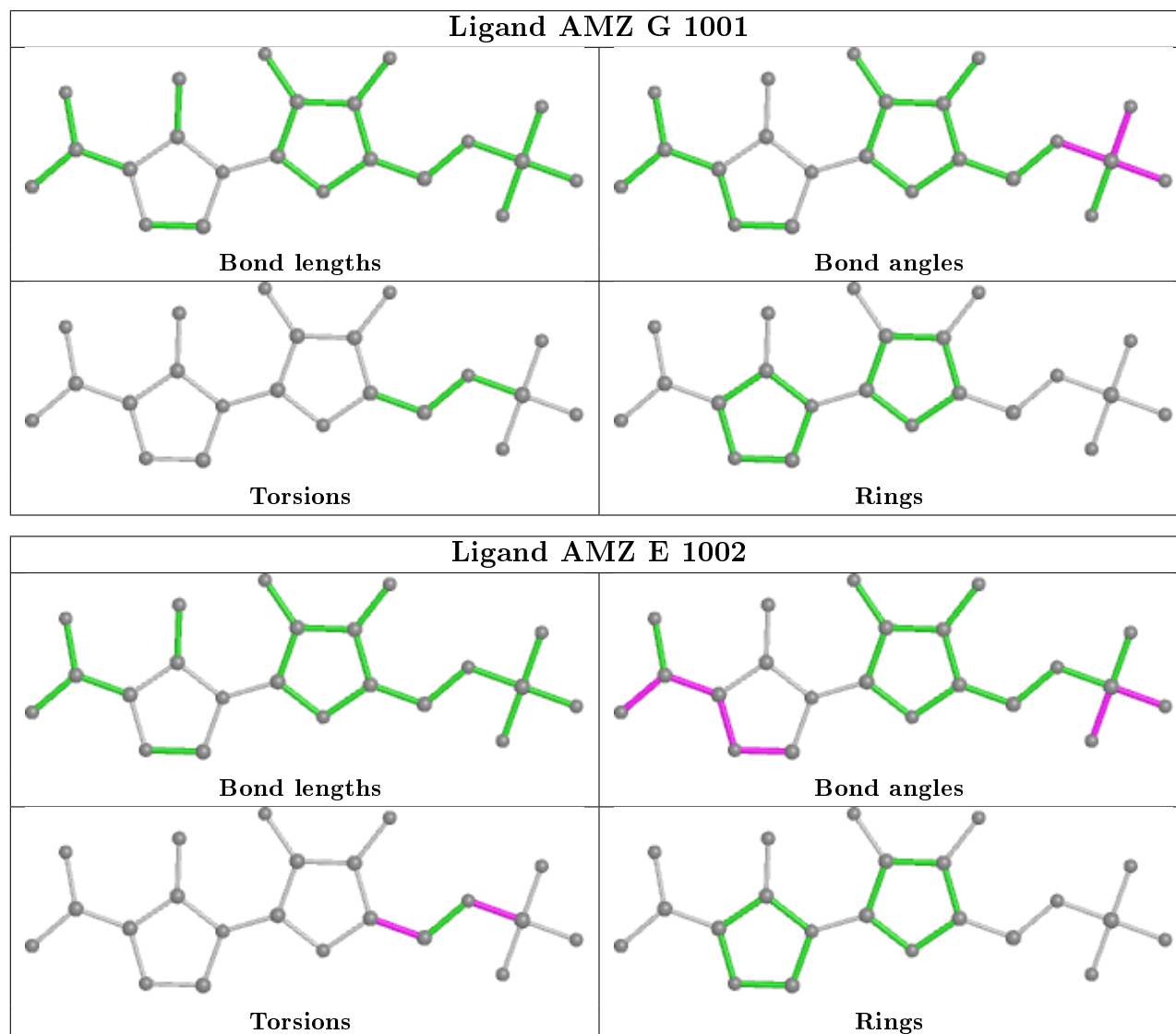
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1001	AMZ	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1002	AMZ	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.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	109/137 (79%)	-0.25	0	100   100	82, 90, 94, 98	1 (0%)
1	C	113/137 (82%)	-0.15	1 (0%)	84   62	84, 90, 95, 98	0
2	B	85/97 (87%)	-0.20	2 (2%)	59   30	28, 89, 95, 99	0
2	D	91/97 (93%)	0.07	2 (2%)	62   32	28, 90, 94, 96	0
3	E	315/334 (94%)	-0.34	3 (0%)	82   58	32, 90, 97, 104	1 (0%)
3	G	315/334 (94%)	-0.39	1 (0%)	94   83	28, 89, 97, 109	1 (0%)
All	All	1028/1136 (90%)	-0.28	9 (0%)	84   62	28, 90, 96, 109	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	224	LEU	3.6
3	E	304	LEU	3.3
2	B	224	LEU	3.3
1	C	510	GLY	3.3
3	E	152	THR	2.6
2	B	297	ASP	2.3
2	D	245	THR	2.3
3	E	230	ASN	2.2
3	G	304	LEU	2.2

### 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](#)

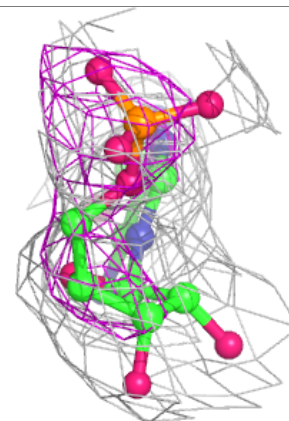
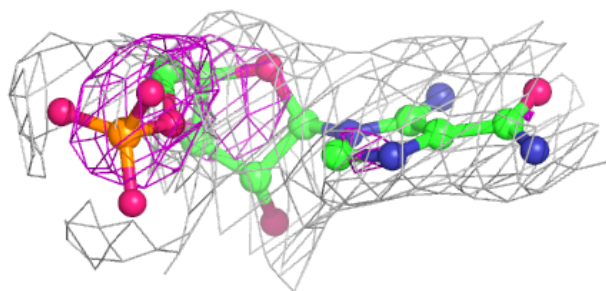
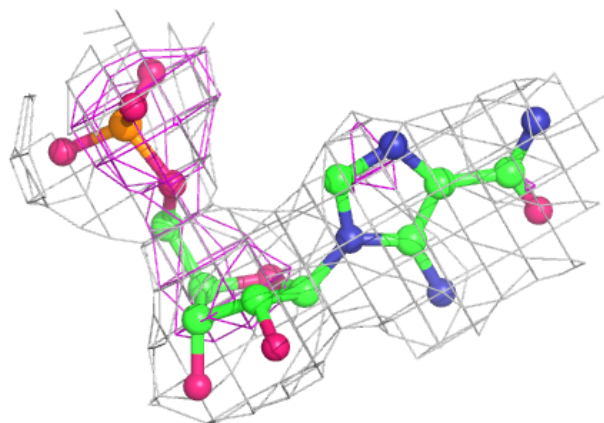
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	AMZ	G	1001	22/22	0.95	0.15	77,79,80,81	0
4	AMZ	E	1002	22/22	0.96	0.14	82,85,90,90	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.

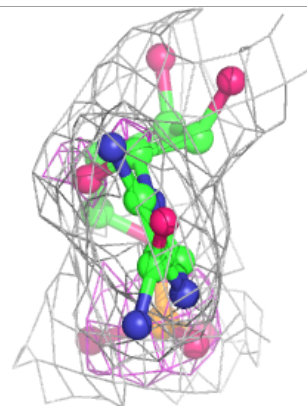
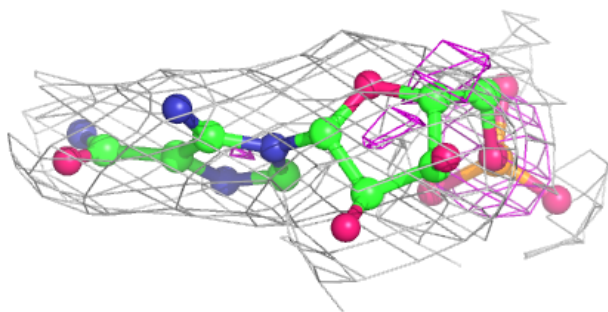
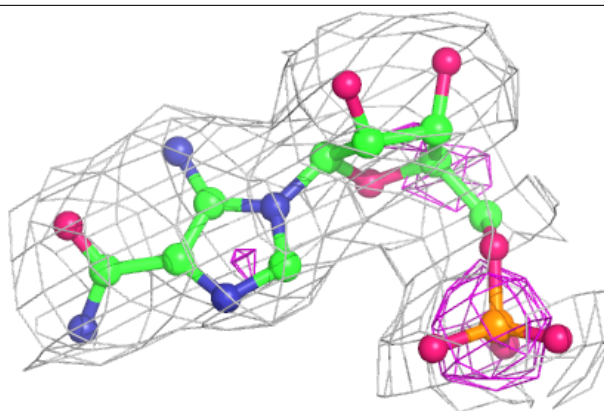
### Electron density around AMZ G 1001:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AMZ 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.