



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:56 AM GMT

PDB ID : 2D1K  
Title : Ternary complex of the WH2 domain of mim with actin-dnase I  
Authors : Chereau, D.; Kerff, F.; Dominguez, R.  
Deposited on : 2005-08-26  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

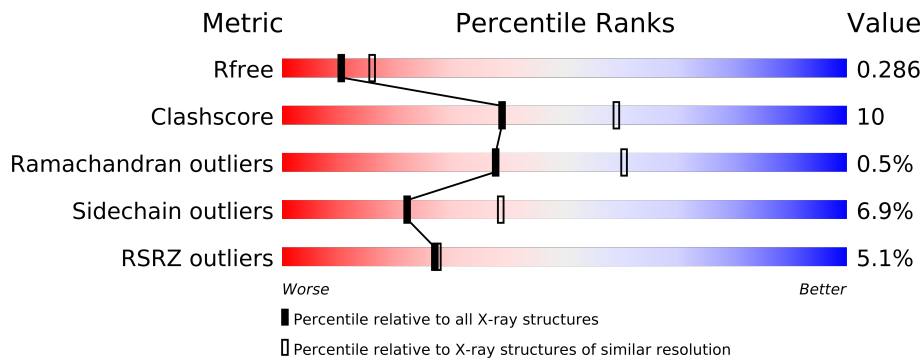
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	375	
2	B	260	
3	C	32	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CA	B	1273	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5355 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2897	1833	489	554	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	MODIFIED RESIDUE	UNP P68135

- Molecule 2 is a protein called Deoxyribonuclease-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	1	0
			2056	1303	344	401	8			

- Molecule 3 is a protein called Metastasis suppressor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	29	Total	C	N	O	S	0	0	0
			226	135	47	43	1			

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

*Continued on next page...*

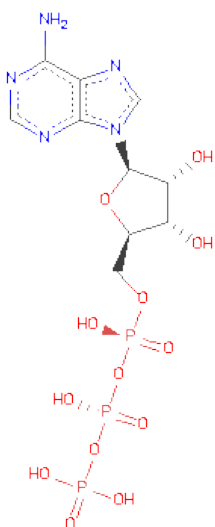
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	34	Total	O	0	0
			34	34		
8	B	68	Total	O	0	0
			68	68		
8	C	1	Total	O	0	0
			1	1		

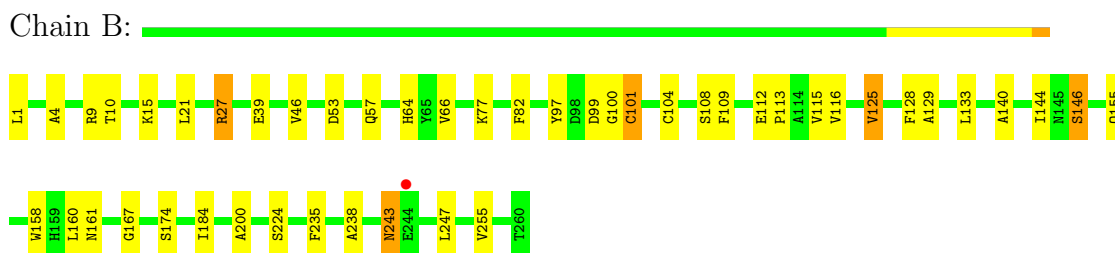
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

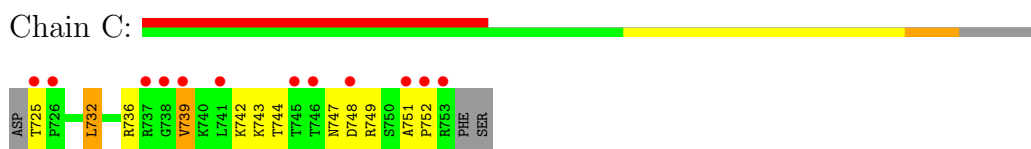
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Deoxyribonuclease-1



- Molecule 3: Metastasis suppressor protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.09Å 75.49Å 228.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.40 – 2.50 41.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.6 (41.40-2.50) 89.6 (41.40-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.217 , 0.284 0.218 , 0.286	Depositor DCC
$R_{free}$ test set	1165 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 71.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 23504 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, CA, HIC, 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	0.47	0/2946	0.64	0/3990
2	B	0.70	0/2105	0.73	0/2867
3	C	0.60	1/227 (0.4%)	0.72	0/303
All	All	0.58	1/5278 (0.0%)	0.68	0/7160

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	749	ARG	CZ-NH2	5.25	1.39	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2897	0	2869	74	0
2	B	2056	0	1993	27	0
3	C	226	0	238	8	0
4	B	39	0	34	1	0
5	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	B	1	0	0	0	0
7	A	31	0	12	3	0
8	A	34	0	0	2	0
8	B	68	0	0	2	0
8	C	1	0	0	0	0
All	All	5355	0	5146	101	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (101) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:25:ASP:N	1:A:26:ALA:HB3	1.77	1.00
1:A:25:ASP:H	1:A:26:ALA:HB3	1.38	0.85
1:A:242:LEU:HB3	1:A:243:PRO:HD2	1.70	0.73
1:A:120:THR:HA	1:A:132:MET:CE	2.20	0.72
1:A:345:ILE:HG23	3:C:739:VAL:HG21	1.71	0.71
1:A:26:ALA:HB1	3:C:744:THR:HB	1.72	0.70
1:A:207:GLU:O	3:C:752:PRO:HB2	1.93	0.68
1:A:59:GLN:O	1:A:62:ARG:HG3	1.94	0.67
1:A:216:LEU:HD13	1:A:250:ILE:HG21	1.74	0.67
1:A:202:THR:OG1	1:A:205:GLU:HB2	1.93	0.67
1:A:25:ASP:N	1:A:26:ALA:CB	2.56	0.65
2:B:9:ARG:HA	2:B:39:GLU:OE1	1.98	0.63
1:A:120:THR:HA	1:A:132:MET:HE3	1.82	0.62
1:A:185:LEU:HD23	1:A:306:TYR:OH	2.00	0.62
1:A:120:THR:HA	1:A:132:MET:HE1	1.82	0.61
1:A:121:GLN:O	1:A:125:GLU:HB2	1.99	0.61
1:A:335:ARG:HA	1:A:338:SER:HB2	1.82	0.61
2:B:125:VAL:HG22	2:B:224:SER:OG	2.01	0.60
1:A:25:ASP:H	1:A:26:ALA:CB	2.10	0.59
1:A:288:ASP:HB3	8:A:1407:HOH:O	2.02	0.58
1:A:136:ILE:HD12	1:A:136:ILE:H	1.69	0.57
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.86	0.56
1:A:18:LYS:HD3	1:A:18:LYS:N	2.20	0.56
3:C:742:LYS:HD3	3:C:743:LYS:H	1.71	0.56
1:A:30:VAL:HB	3:C:748:ASP:HA	1.88	0.56
2:B:99:ASP:HB3	2:B:104:CYS:HB3	1.89	0.55
1:A:37:ARG:HH11	1:A:68:LYS:HD2	1.72	0.55
1:A:177:ARG:NH1	1:A:179:ASP:CG	2.61	0.54
1:A:34:ILE:HG21	1:A:67:LEU:HD22	1.90	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:302:GLY:HA3	7:A:1380:ATP:O4'	2.07	0.54
1:A:297:ASN:HB3	1:A:329:ILE:HG13	1.90	0.54
2:B:100:GLY:O	2:B:101:CYS:HB3	2.08	0.53
1:A:9:VAL:HG21	1:A:344:SER:HA	1.91	0.53
1:A:262:PHE:CE1	1:A:274:ILE:HD11	2.43	0.53
1:A:123:MET:HG3	1:A:132:MET:HE2	1.89	0.53
1:A:242:LEU:HB3	1:A:243:PRO:CD	2.37	0.53
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.90	0.52
1:A:176:MET:HG3	1:A:281:SER:HB2	1.92	0.52
1:A:26:ALA:H	1:A:27:PRO:HD3	1.75	0.52
1:A:34:ILE:CG2	1:A:67:LEU:HD22	2.40	0.51
2:B:155:GLN:NE2	2:B:161:ASN:OD1	2.43	0.51
1:A:124:PHE:O	1:A:128:ASN:HA	2.10	0.50
2:B:128:PHE:HA	2:B:160:LEU:HD21	1.93	0.50
1:A:79:TRP:CZ3	1:A:118:LYS:HB3	2.46	0.50
1:A:177:ARG:HH12	1:A:179:ASP:CG	2.15	0.49
1:A:40:HIS:NE2	2:B:53:ASP:OD1	2.38	0.49
3:C:732:LEU:HB3	3:C:736:ARG:HH21	1.77	0.49
1:A:202:THR:HG1	1:A:205:GLU:HB2	1.77	0.48
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.96	0.48
1:A:97:ALA:O	1:A:101:HIS:HD2	1.97	0.48
2:B:200:ALA:O	8:B:1276:HOH:O	2.20	0.48
2:B:144:ILE:HG22	2:B:184:ILE:CG2	2.44	0.47
1:A:25:ASP:OD1	1:A:26:ALA:HB2	2.15	0.47
2:B:109:PHE:CZ	2:B:146:SER:HB3	2.49	0.47
1:A:55:GLY:O	1:A:58:ALA:HB3	2.15	0.47
1:A:24:ASP:OD1	1:A:24:ASP:N	2.48	0.46
1:A:161:HIS:CE1	1:A:177:ARG:HG3	2.51	0.46
2:B:115:VAL:HG12	2:B:158:TRP:CZ3	2.51	0.45
2:B:133:LEU:O	2:B:167:GLY:HA3	2.17	0.45
2:B:116:VAL:O	2:B:129:ALA:HA	2.16	0.45
1:A:29:ALA:CB	1:A:93:GLU:HG3	2.47	0.45
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.99	0.45
1:A:345:ILE:HG23	3:C:739:VAL:CG2	2.44	0.45
1:A:216:LEU:HD11	1:A:240:TYR:HB2	1.99	0.45
2:B:9:ARG:O	2:B:10:THR:C	2.55	0.45
1:A:214:GLU:HG2	7:A:1380:ATP:C5	2.52	0.45
1:A:102:PRO:HA	1:A:131:ALA:O	2.17	0.45
2:B:97:TYR:HB3	2:B:113:PRO:HD2	1.99	0.45
1:A:190:MET:HG2	1:A:209:VAL:HG11	2.00	0.44
3:C:751:ALA:HA	3:C:752:PRO:HD3	1.85	0.44
2:B:243:ASN:O	2:B:247:LEU:HB2	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:66:VAL:HB	2:B:82:PHE:HB2	2.00	0.43
1:A:104:LEU:HD22	1:A:347:ALA:HB2	2.00	0.43
2:B:144:ILE:HG22	2:B:184:ILE:HG21	2.01	0.43
1:A:104:LEU:HD12	1:A:133:TYR:HB3	2.00	0.43
1:A:41:GLN:HB3	2:B:64:HIS:CD2	2.53	0.43
2:B:4:ALA:HA	2:B:255:VAL:O	2.18	0.43
1:A:318:THR:HA	1:A:327:ILE:HD11	2.00	0.43
1:A:203:THR:OG1	2:B:46:VAL:HG21	2.18	0.43
1:A:336:LYS:HE2	7:A:1380:ATP:C8	2.54	0.43
1:A:189:LEU:HA	1:A:192:ILE:HG12	2.01	0.42
1:A:317:ILE:HG13	1:A:317:ILE:H	1.58	0.42
1:A:297:ASN:HB3	1:A:329:ILE:CG1	2.49	0.42
1:A:139:VAL:HG12	1:A:143:TYR:CZ	2.54	0.42
1:A:252:ASN:O	1:A:256:ARG:HG3	2.19	0.42
2:B:27:ARG:HG2	8:B:1293:HOH:O	2.18	0.42
1:A:208:ILE:HD13	1:A:243:PRO:HD3	2.02	0.41
2:B:140:ALA:O	2:B:144:ILE:HG13	2.20	0.41
1:A:201:VAL:HB	8:A:1403:HOH:O	2.19	0.41
1:A:332:PRO:HB2	1:A:334:GLU:OE2	2.19	0.41
1:A:264:PRO:HG2	1:A:271:SER:O	2.21	0.41
1:A:115:ASN:O	1:A:119:MET:HG3	2.20	0.41
2:B:235:PHE:HA	2:B:238:ALA:HB3	2.03	0.41
1:A:312:ARG:HD2	1:A:316:GLU:HG2	2.03	0.41
2:B:112:GLU:HA	2:B:113:PRO:HD3	1.91	0.41
1:A:287:ILE:HA	1:A:290:ARG:HD2	2.03	0.41
2:B:53:ASP:O	2:B:57:GLN:HB3	2.21	0.40
1:A:340:TRP:O	1:A:343:GLY:N	2.54	0.40
2:B:21:LEU:HD21	4:B:270:NAG:H62	2.03	0.40
1:A:135:ALA:HB3	1:A:140:LEU:HD11	2.04	0.40
1:A:17:VAL:HG23	1:A:33:SER:HB3	2.03	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	368/375 (98%)	339 (92%)	26 (7%)	3 (1%)	27	46
2	B	259/260 (100%)	239 (92%)	20 (8%)	0	100	100
3	C	27/32 (84%)	22 (82%)	5 (18%)	0	100	100
All	All	654/667 (98%)	600 (92%)	51 (8%)	3 (0%)	38	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ALA
1	A	353	GLN
1	A	350	SER

### 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	313/317 (99%)	288 (92%)	25 (8%)	17	31
2	B	230/229 (100%)	220 (96%)	10 (4%)	40	65
3	C	25/28 (89%)	21 (84%)	4 (16%)	3	6
All	All	568/574 (99%)	529 (93%)	39 (7%)	22	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	12	ASN
1	A	18	LYS
1	A	24	ASP
1	A	66	THR
1	A	82	MET
1	A	121	GLN
1	A	132	MET
1	A	183	ARG
1	A	184	ASP
1	A	205	GLU
1	A	206	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	207	GLU
1	A	212	ILE
1	A	224	GLU
1	A	237	GLU
1	A	284	LYS
1	A	303	THR
1	A	334	GLU
1	A	336	LYS
1	A	349	LEU
1	A	355	MET
1	A	358	THR
1	A	359	LYS
1	A	364	GLU
2	B	1	LEU
2	B	15	LYS
2	B	27	ARG
2	B	77	LYS
2	B	101	CYS
2	B	108	SER
2	B	125	VAL
2	B	146	SER
2	B	174	SER
2	B	243	ASN
3	C	725	THR
3	C	732	LEU
3	C	739	VAL
3	C	747	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	121	GLN
1	A	128	ASN
1	A	280	ASN
2	B	44	HIS
3	C	727	GLN
3	C	747	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	HIC	A	73	1	11,11,12	5.45	3 (27%)	12,14,16	1.88	2 (16%)

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
1	HIC	A	73	1	-	0/4/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	O-C	17.48	1.23	1.11
1	A	73	HIC	CD2-CG	3.39	1.39	1.36
1	A	73	HIC	CD2-NE2	-2.05	1.34	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	CG-CB-CA	-4.01	108.36	113.85
1	A	73	HIC	C-CA-N	-3.99	109.84	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

3 carbohydrates 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	NAG	B	270	2,4	12,14,15	0.71	0	15,19,21	1.66	3 (20%)
4	NAG	B	271	4	12,14,15	0.40	0	15,19,21	2.00	5 (33%)
4	BMA	B	272	4	10,11,12	0.73	0	11,15,17	0.74	0

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	NAG	B	270	2,4	-	2/6/23/26	0/1/1/1
4	NAG	B	271	4	-	0/6/23/26	0/1/1/1
4	BMA	B	272	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	271	NAG	O5-C5-C6	4.65	111.86	106.98
4	B	270	NAG	C2-N2-C7	3.71	129.31	123.09
4	B	271	NAG	C2-N2-C7	3.37	128.74	123.09
4	B	271	NAG	C8-C7-N2	2.64	121.27	116.11
4	B	271	NAG	O5-C5-C4	2.36	113.65	110.65
4	B	270	NAG	O4-C4-C3	-2.23	105.36	110.35
4	B	270	NAG	C3-C2-N2	-2.19	108.43	111.76
4	B	271	NAG	C3-C2-N2	2.10	114.96	111.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	270	NAG	O7-C7-N2-C2
4	B	270	NAG	C8-C7-N2-C2

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	ATP	A	1380	5	33,33,33	1.06	2 (6%)	52,52,52	2.08	11 (21%)

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
7	ATP	A	1380	5	-	0/22/38/38	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1380	ATP	C4-N9	-3.25	1.33	1.37
7	A	1380	ATP	C5-C4	3.18	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1380	ATP	N3-C2-N1	-6.51	123.26	128.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1380	ATP	PA-O3A-PB	-5.90	114.37	131.68
7	A	1380	ATP	N3-C4-N9	4.80	134.10	125.43
7	A	1380	ATP	O4'-C1'-N9	4.76	112.87	108.44
7	A	1380	ATP	C8-N9-C4	3.87	109.85	106.90
7	A	1380	ATP	PB-O3B-PG	-3.83	120.44	131.68
7	A	1380	ATP	C4-C5-N7	-3.26	106.73	109.52
7	A	1380	ATP	C5-C4-N3	-2.53	120.19	125.70
7	A	1380	ATP	C2'-C1'-N9	-2.29	107.39	113.27
7	A	1380	ATP	C2-N3-C4	2.26	120.45	114.01
7	A	1380	ATP	C1'-N9-C4	-2.12	122.98	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	371/375 (98%)	0.17	21 (5%) 23 23	44, 71, 86, 99	2 (0%)
2	B	260/260 (100%)	-0.44	1 (0%) 90 92	26, 40, 53, 77	2 (0%)
3	C	29/32 (90%)	2.13	12 (41%) 1 0	75, 88, 108, 112	0
All	All	660/667 (98%)	0.02	34 (5%) 27 27	26, 57, 87, 112	4 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	726	PRO	4.8
3	C	751	ALA	4.6
3	C	752	PRO	4.5
1	A	367	PRO	3.9
1	A	250	ILE	3.9
1	A	374	CYS	3.8
3	C	753	ARG	3.8
3	C	725	THR	3.6
1	A	247	VAL	3.6
1	A	245	GLY	3.5
1	A	242	LEU	3.4
1	A	240	TYR	3.4
1	A	372	ARG	3.4
3	C	748	ASP	3.3
3	C	737	ARG	3.3
1	A	198	TYR	3.1
1	A	244	ASP	3.1
3	C	746	THR	3.0
1	A	370	VAL	2.9
3	C	739	VAL	2.8
1	A	216	LEU	2.8
1	A	243	PRO	2.4
1	A	110	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	2.4
1	A	193	LEU	2.3
1	A	261	LEU	2.3
1	A	131	ALA	2.3
3	C	745	THR	2.3
2	B	244	GLU	2.3
1	A	200	PHE	2.3
1	A	212	ILE	2.3
3	C	738	GLY	2.1
3	C	741	LEU	2.1
1	A	297	ASN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	HIC	A	73	11/12	0.13	-0.38	48,49,53,58	0

## 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	270	14/15	0.14	2.04	54,58,61,66	0
4	NAG	B	271	14/15	0.22	0.20	70,72,76,78	0
4	BMA	B	272	11/12	0.29	-	79,80,82,82	0

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CA	B	1273	1/1	0.14	3.36	36,36,36,36	0
5	CA	A	1381	1/1	0.19	1.39	64,64,64,64	0
7	ATP	A	1380	31/31	0.16	0.74	59,65,67,68	0
6	MG	B	1274	1/1	0.10	-1.22	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.