



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2021 – 10:09 AM EDT

PDB ID : 7L27  
Title : Crystal structure of the catalytic domain of human PDE3A  
Authors : Horner, S.W.; Garvie, C.  
Deposited on : 2020-12-16  
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 : 2.20  
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) : 2.20

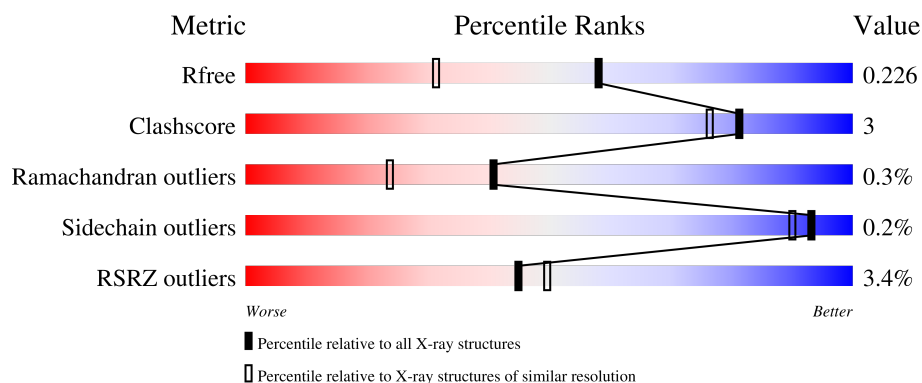
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 of 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	380	<div> <div>3%</div> <div>90%</div> <div>5%</div> <div>.</div> </div>
1	B	380	<div> <div>4%</div> <div>90%</div> <div>.</div> <div>5%</div> </div>
1	C	380	<div> <div>3%</div> <div>92%</div> <div>.</div> <div>.</div> </div>
1	D	380	<div> <div>3%</div> <div>93%</div> <div>.</div> <div>.</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12424 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	1	0
			2935	1893	492	531	19			
1	B	362	Total	C	N	O	S	0	1	0
			2931	1892	491	529	19			
1	C	366	Total	C	N	O	S	0	0	0
			2949	1899	494	538	18			
1	D	370	Total	C	N	O	S	0	2	0
			2982	1920	500	543	19			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	GLY	-	expression tag	UNP Q14432
A	795	GLY	-	linker	UNP Q14432
A	796	GLY	-	linker	UNP Q14432
A	797	SER	-	linker	UNP Q14432
A	798	GLY	-	linker	UNP Q14432
A	799	GLY	-	linker	UNP Q14432
A	800	SER	-	linker	UNP Q14432
A	1062	GLY	-	linker	UNP Q14432
A	1063	GLY	-	linker	UNP Q14432
A	1064	SER	-	linker	UNP Q14432
A	1065	GLY	-	linker	UNP Q14432
A	1066	GLY	-	linker	UNP Q14432
A	1067	SER	-	linker	UNP Q14432
B	668	GLY	-	expression tag	UNP Q14432
B	795	GLY	-	linker	UNP Q14432
B	796	GLY	-	linker	UNP Q14432
B	797	SER	-	linker	UNP Q14432
B	798	GLY	-	linker	UNP Q14432
B	799	GLY	-	linker	UNP Q14432
B	800	SER	-	linker	UNP Q14432
B	1062	GLY	-	linker	UNP Q14432

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1063	GLY	-	linker	UNP Q14432
B	1064	SER	-	linker	UNP Q14432
B	1065	GLY	-	linker	UNP Q14432
B	1066	GLY	-	linker	UNP Q14432
B	1067	SER	-	linker	UNP Q14432
C	668	GLY	-	expression tag	UNP Q14432
C	795	GLY	-	linker	UNP Q14432
C	796	GLY	-	linker	UNP Q14432
C	797	SER	-	linker	UNP Q14432
C	798	GLY	-	linker	UNP Q14432
C	799	GLY	-	linker	UNP Q14432
C	800	SER	-	linker	UNP Q14432
C	1029	GLY	-	linker	UNP Q14432
C	1063	GLY	-	linker	UNP Q14432
C	1064	SER	-	linker	UNP Q14432
C	1065	GLY	-	linker	UNP Q14432
C	1066	GLY	-	linker	UNP Q14432
C	1067	SER	-	linker	UNP Q14432
D	668	GLY	-	expression tag	UNP Q14432
D	795	GLY	-	linker	UNP Q14432
D	796	GLY	-	linker	UNP Q14432
D	797	SER	-	linker	UNP Q14432
D	798	GLY	-	linker	UNP Q14432
D	799	GLY	-	linker	UNP Q14432
D	800	SER	-	linker	UNP Q14432
D	1062	GLY	-	linker	UNP Q14432
D	1063	GLY	-	linker	UNP Q14432
D	1064	SER	-	linker	UNP Q14432
D	1065	GLY	-	linker	UNP Q14432
D	1066	GLY	-	linker	UNP Q14432
D	1067	SER	-	linker	UNP Q14432

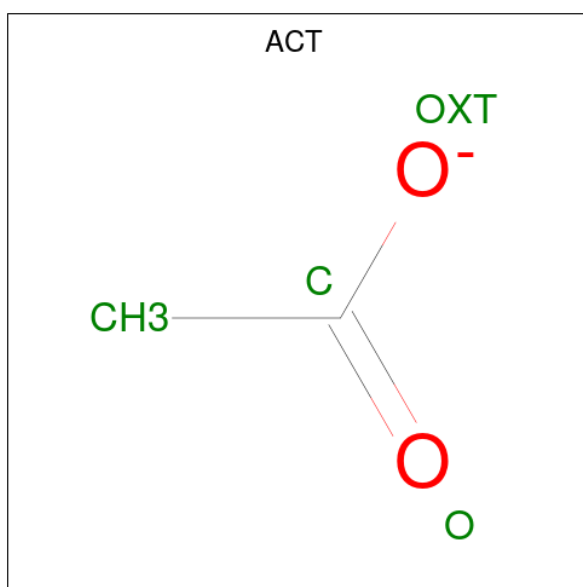
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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

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

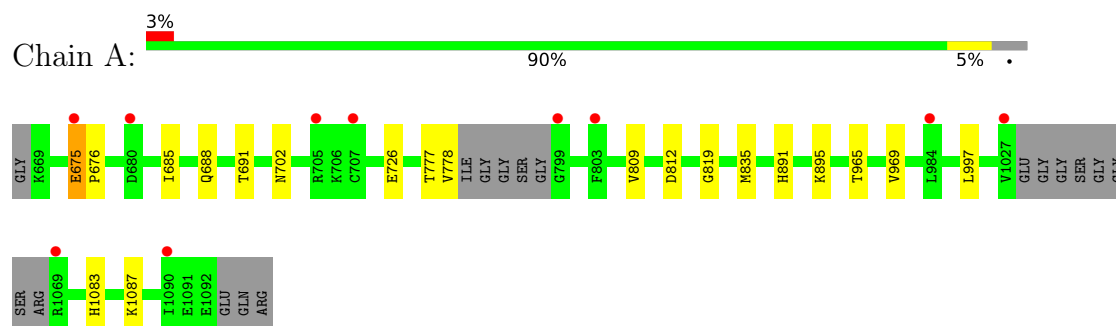
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	139	Total 139	O 139	0	0
6	B	101	Total 101	O 101	0	0
6	C	173	Total 173	O 173	0	0
6	D	189	Total 189	O 189	0	0

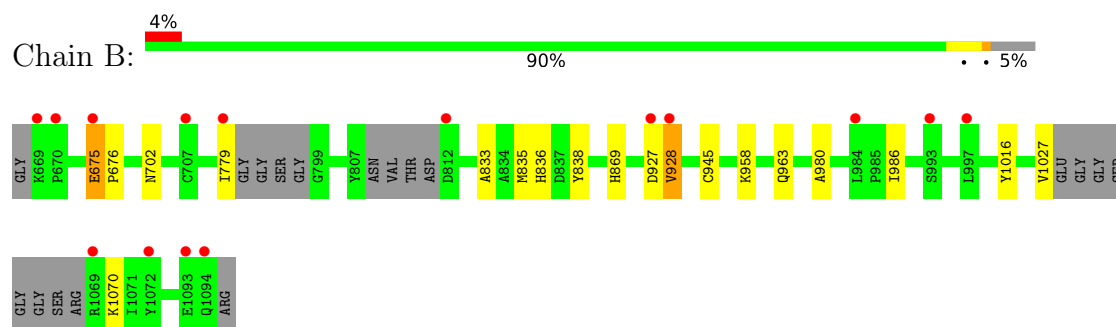
### 3 Residue-property plots [i](#)

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

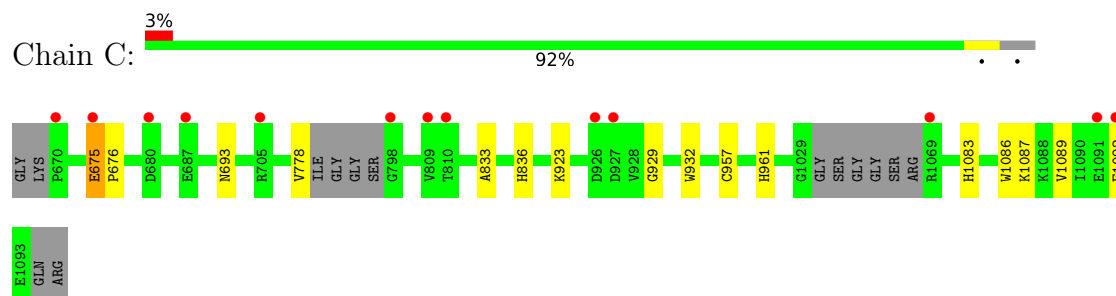
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A

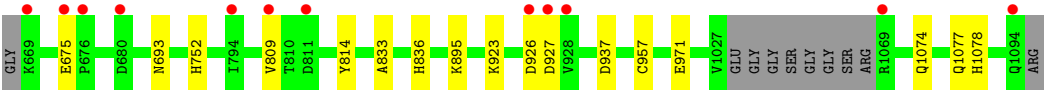


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.37Å 58.79Å 157.66Å 90.00° 90.69° 90.00°	Depositor
Resolution (Å)	47.85 – 1.70 47.85 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.85-1.70) 99.2 (47.85-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.194 , 0.220 0.204 , 0.226	Depositor DCC
$R_{free}$ test set	8214 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, MG, ACT, CA

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	0.51	0/3017	0.66	1/4097 (0.0%)
1	B	0.51	0/3012	0.65	1/4087 (0.0%)
1	C	0.54	0/3028	0.68	0/4111
1	D	0.55	0/3068	0.68	0/4166
All	All	0.53	0/12125	0.67	2/16461 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	MET	CB-CA-C	-5.33	99.73	110.40
1	A	835	MET	CB-CA-C	-5.07	100.27	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2935	0	2863	15	0
1	B	2931	0	2861	18	0
1	C	2949	0	2864	17	0
1	D	2982	0	2908	11	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
5	C	1	0	0	0	0
6	A	139	0	0	0	0
6	B	101	0	0	3	0
6	C	173	0	0	1	0
6	D	189	0	0	2	0
All	All	12424	0	11508	61	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 3.

The worst 5 of 61 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:HIS:HE1	1:C:1086:TRP:HE1	1.12	0.96
1:B:675:GLU:HB3	1:B:676:PRO:CD	1.97	0.95
1:B:675:GLU:HB3	1:B:676:PRO:HD2	1.51	0.93
1:A:675:GLU:HB3	1:A:676:PRO:CD	2.01	0.91
1:A:675:GLU:HB3	1:A:676:PRO:HD2	1.52	0.88

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	358/380 (94%)	351 (98%)	5 (1%)	2 (1%)	25	11
1	B	355/380 (93%)	347 (98%)	6 (2%)	2 (1%)	25	11
1	C	360/380 (95%)	353 (98%)	6 (2%)	1 (0%)	41	24
1	D	368/380 (97%)	359 (98%)	9 (2%)	0	100	100
All	All	1441/1520 (95%)	1410 (98%)	26 (2%)	5 (0%)	41	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	675	GLU
1	B	675	GLU
1	B	928	VAL
1	C	675	GLU
1	A	812	ASP

### 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	319/327 (98%)	318 (100%)	1 (0%)	92	89
1	B	318/327 (97%)	317 (100%)	1 (0%)	92	89
1	C	319/327 (98%)	319 (100%)	0	100	100
1	D	324/327 (99%)	323 (100%)	1 (0%)	92	89
All	All	1280/1308 (98%)	1277 (100%)	3 (0%)	93	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	809	VAL
1	B	702	ASN
1	D	675	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	860	ASN
1	D	963	GLN
1	C	961	HIS
1	D	860	ASN
1	C	888	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	$\# Z  > 2$
4	ACT	B	1103	-	1,3,3	3.97	1 (100%)	0,3,3	0.00	-
4	ACT	C	1104	-	1,3,3	3.71	1 (100%)	0,3,3	0.00	-
4	ACT	D	1103	-	1,3,3	4.27	1 (100%)	0,3,3	0.00	-
4	ACT	A	1103	-	1,3,3	3.69	1 (100%)	0,3,3	0.00	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1103	ACT	CH3-C	4.27	1.54	1.48
4	B	1103	ACT	CH3-C	3.97	1.53	1.48
4	C	1104	ACT	CH3-C	3.71	1.53	1.48
4	A	1103	ACT	CH3-C	3.69	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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	363/380 (95%)	0.03	10 (2%) 53 57	21, 38, 65, 97	0
1	B	362/380 (95%)	0.18	15 (4%) 37 41	21, 41, 73, 109	0
1	C	366/380 (96%)	0.01	13 (3%) 42 47	19, 34, 64, 88	0
1	D	370/380 (97%)	0.10	12 (3%) 47 52	18, 32, 63, 122	0
All	All	1461/1520 (96%)	0.08	50 (3%) 45 50	18, 36, 68, 122	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	675	GLU	7.8
1	D	927	ASP	7.5
1	B	669	LYS	7.1
1	A	705	ARG	6.9
1	B	927	ASP	6.4

### 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 monosaccharides 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	ACT	B	1103	4/4	0.84	0.20	46,59,69,70	0
4	ACT	C	1104	4/4	0.93	0.12	36,38,42,44	0
5	CA	C	1103	1/1	0.94	0.05	46,46,46,46	0
4	ACT	A	1103	4/4	0.95	0.11	38,39,42,43	0
4	ACT	D	1103	4/4	0.96	0.09	23,25,26,30	0
3	MG	B	1102	1/1	0.97	0.12	20,20,20,20	0
2	MN	B	1101	1/1	0.97	0.08	27,27,27,27	0
3	MG	D	1102	1/1	0.98	0.12	15,15,15,15	0
3	MG	C	1102	1/1	0.98	0.10	19,19,19,19	0
2	MN	A	1101	1/1	0.99	0.06	24,24,24,24	0
2	MN	C	1101	1/1	0.99	0.06	26,26,26,26	0
2	MN	D	1101	1/1	0.99	0.09	21,21,21,21	0
3	MG	A	1102	1/1	0.99	0.13	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.