



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2017 – 07:13 PM EDT

PDB ID : 5T45  
Title : Chicken smooth muscle myosin motor domain co-crystallized with the specific CK-571 inhibitor, MgADP.BeFx form  
Authors : Sirigu, S.; Planelles-Herrero, V.J.; Hartman, J.; Houdusse, A.  
Deposited on : unknown  
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

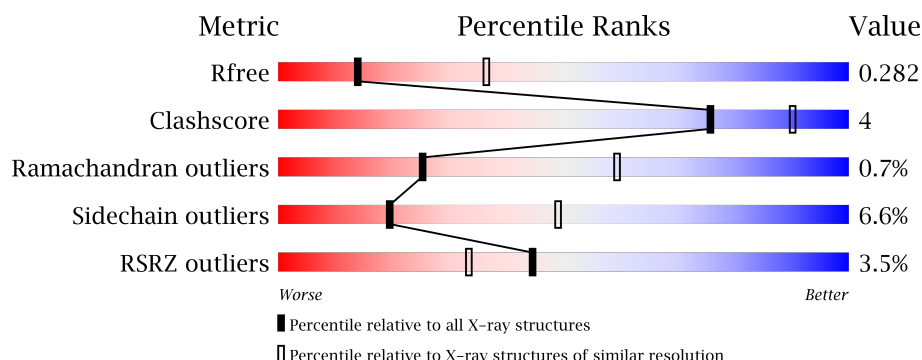
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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. 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	800	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	907	-	-	-	X
7	BCN	A	908	-	-	-	X

## 2 Entry composition [i](#)

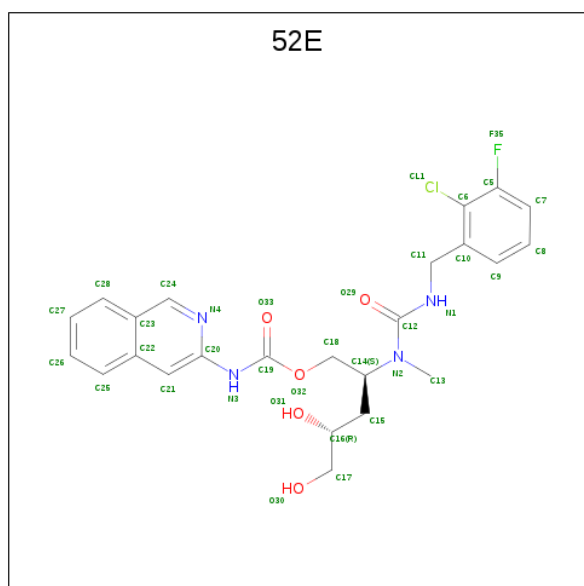
There are 8 unique types of molecules in this entry. The entry contains 5800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myosin-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	2	0
			5621	3578	954	1060	29			

- Molecule 2 is 4-{{[(2-chloro-3-fluorobenzyl)carbamoyl](methyl)amino}-3,4-dideoxy-5-O-(isoquinolin-3-ylcarbamoyl)-D-erythro-pentitol (three-letter code: 52E) (formula: C<sub>24</sub>H<sub>26</sub>ClFN<sub>4</sub>O<sub>5</sub>).

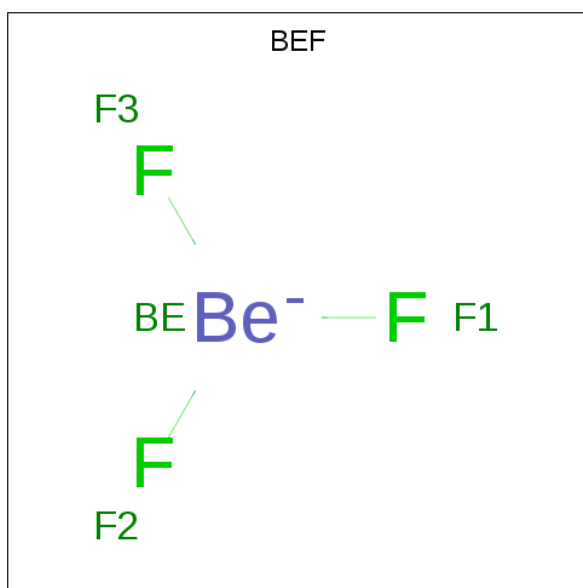


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	
			35	24	1	1	4	5	0

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

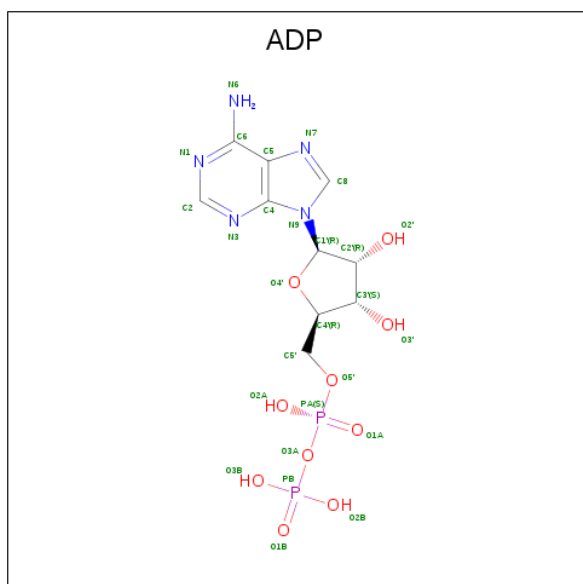
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $\text{BeF}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Be	F	0	0
			4	1	3		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



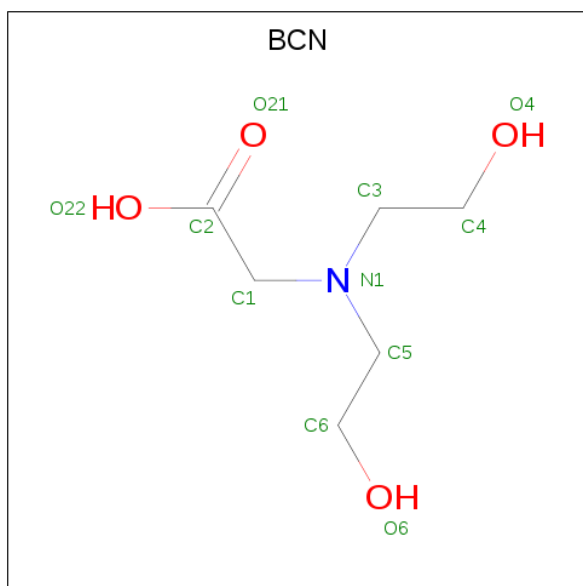
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	83	Total	O	0	0
			83	83		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.94 Å   202.17 Å   67.02 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	44.35 – 2.80 44.35 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.35-2.80) 99.9 (44.35-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.81 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.219   ,   0.271 0.226   ,   0.282	Depositor DCC
$R_{free}$ test set	1260 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.884	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: GOL, BCN, ADP, 52E, BEF, MG

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	0.50	0/5727	0.71	1/7743 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	533	ASN	N-CA-C	-5.58	95.92	111.00

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	5621	0	5490	41	0
2	A	35	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	0	0	0
5	A	27	0	12	0	0
6	A	18	0	24	0	0
7	A	11	0	12	1	0
8	A	83	0	0	0	0
All	All	5800	0	5538	41	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 4.

All (41) 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:A:530:ARG:HE	1:A:534:PRO:HD2	1.52	0.73
1:A:234:PHE:CE1	1:A:289:ILE:HG12	2.30	0.67
1:A:249:GLY:HA3	1:A:466:ILE:CD1	2.29	0.62
1:A:249:GLY:HA3	1:A:466:ILE:HD13	1.83	0.60
1:A:184:THR:HG22	1:A:188:LYS:HE2	1.86	0.57
1:A:51:GLU:HG3	1:A:58:THR:HB	1.86	0.56
1:A:288:HIS:HB3	1:A:292:TYR:CZ	2.42	0.55
1:A:97:GLU:HG2	1:A:711:LEU:HD22	1.87	0.55
1:A:85:LYS:HG2	1:A:106:GLU:HB3	1.90	0.53
1:A:367:PHE:O	1:A:420:LYS:HE2	2.10	0.52
1:A:729:GLU:O	1:A:733:ARG:HB2	2.12	0.50
1:A:293:LEU:HD13	1:A:353:LEU:HD22	1.93	0.50
1:A:242:ASN:HB3	1:A:245:SER:HB2	1.93	0.50
1:A:547:PHE:HB2	1:A:550:ALA:HB2	1.95	0.49
1:A:551:THR:H	1:A:554:SER:HB3	1.78	0.48
1:A:391:MET:HE3	1:A:393:ILE:HD11	1.94	0.48
1:A:239:THR:HG22	1:A:241:LYS:H	1.79	0.48
1:A:173:ILE:HD12	1:A:461:LEU:HD21	1.96	0.48
1:A:184:THR:HA	1:A:465:ASP:OD2	2.14	0.48
1:A:530:ARG:NE	1:A:534:PRO:HD2	2.24	0.46
1:A:471:ILE:HG12	1:A:590:VAL:HG22	1.98	0.45
1:A:308:GLU:O	1:A:312:ASN:HB2	2.16	0.45
1:A:529:GLU:HG3	1:A:530:ARG:H	1.81	0.45
1:A:613:LEU:HB3	1:A:625:TRP:CD1	2.52	0.44
1:A:594:ALA:HA	1:A:597:TRP:CE2	2.53	0.44
1:A:544:GLU:HG3	1:A:555:PHE:HA	1.99	0.44
1:A:252:ILE:HG12	1:A:267:ILE:HG12	1.99	0.44
1:A:107:ARG:NH1	1:A:112:LEU:HB3	2.33	0.43
1:A:766:LEU:HA	1:A:777:ARG:HG3	2.00	0.43
1:A:168:ARG:HH12	1:A:258:VAL:HG12	1.84	0.42
1:A:410:GLY:HA2	1:A:411:ARG:HA	1.89	0.42
1:A:533:ASN:CB	1:A:534:PRO:CD	2.97	0.42
1:A:249:GLY:HA3	1:A:466:ILE:HD12	1.99	0.42
1:A:606:ASN:OD1	1:A:608:ASN:HB2	2.20	0.41
1:A:160:ALA:O	1:A:171:GLN:HG3	2.21	0.41
1:A:192:GLN:HB2	1:A:192:GLN:HE21	1.58	0.41
1:A:90:ALA:HB2	1:A:118:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:THR:O	1:A:554:SER:HB3	2.21	0.41
1:A:594:ALA:HA	1:A:597:TRP:NE1	2.35	0.41
1:A:102:HIS:CE1	1:A:106:GLU:HG3	2.57	0.40
1:A:268:GLU:HG3	7:A:908:BCN:H51	2.03	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	702/800 (88%)	666 (95%)	31 (4%)	5 (1%)	25	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	ARG
1	A	533	ASN
1	A	529	GLU
1	A	309	GLY
1	A	548	PRO

### 5.3.2 Protein sidechains [i](#)

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	596/704 (85%)	556 (93%)	40 (7%)	19	48

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	50	LYS
1	A	59	VAL
1	A	124	ILE
1	A	128	LYS
1	A	168	ARG
1	A	192	GLN
1	A	239	THR
1	A	241	LYS
1	A	258	VAL
1	A	263	VAL
1	A	268	GLU
1	A	286	THR
1	A	300	GLN
1	A	304	ASP
1	A	321	VAL
1	A	371	ARG
1	A	396	THR
1	A	402	ILE
1	A	412	ASP
1	A	434	LYS
1	A	445[A]	ARG
1	A	445[B]	ARG
1	A	451	ASP
1	A	470	GLU
1	A	506	GLN
1	A	515	ILE
1	A	519	LEU
1	A	541	LEU
1	A	609	VAL
1	A	627	ASP
1	A	662	LEU
1	A	718	ARG
1	A	729	GLU
1	A	733	ARG
1	A	737	LEU
1	A	762	LEU
1	A	771	GLN

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Mol	Chain	Res	Type
1	A	784	LEU
1	A	785	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	102	HIS
1	A	192	GLN

### 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](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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$
2	52E	A	901	-	36,37,37	1.60	7 (19%)	40,50,50	1.28	4 (10%)
4	BEF	A	903	-	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	A	904	3	25,29,29	0.63	0	24,45,45	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	905	-	5,5,5	0.18	0	5,5,5	0.49	0
6	GOL	A	906	-	5,5,5	0.12	0	5,5,5	0.52	0
6	GOL	A	907	-	5,5,5	0.18	0	5,5,5	0.14	0
7	BCN	A	908	-	7,10,10	0.60	0	8,11,11	0.94	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
2	52E	A	901	-	-	2/28/28/28	0/3/3/3
4	BEF	A	903	-	-	0/0/0/0	0/0/0/0
5	ADP	A	904	3	-	0/12/32/32	0/3/3/3
6	GOL	A	905	-	-	0/4/4/4	0/0/0/0
6	GOL	A	906	-	-	0/4/4/4	0/0/0/0
6	GOL	A	907	-	-	0/4/4/4	0/0/0/0
7	BCN	A	908	-	-	0/8/10/10	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	52E	C26-C27	2.11	1.43	1.38
2	A	901	52E	C14-N2	2.17	1.51	1.48
2	A	901	52E	C7-C5	2.29	1.42	1.37
2	A	901	52E	C19-N3	2.48	1.41	1.36
2	A	901	52E	C6-C10	2.68	1.42	1.39
2	A	901	52E	C24-C23	2.94	1.47	1.41
2	A	901	52E	C20-N4	4.63	1.43	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	52E	C11-C10-C6	-3.22	116.98	121.09
2	A	901	52E	C18-O32-C19	2.24	120.56	116.07
2	A	901	52E	C13-N2-C14	2.67	120.86	117.84
2	A	901	52E	C10-C6-CL1	3.04	122.46	119.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	52E	N4-C20-N3-C19
2	A	901	52E	C21-C20-N3-C19

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	908	BCN	1	0

## 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	708/800 (88%)	0.16	25 (3%) 44 33	37, 60, 102, 138	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	770	GLY	3.5
1	A	766	LEU	3.4
1	A	725	ILE	3.4
1	A	741	ALA	3.2
1	A	747	MET	3.1
1	A	767	TYR	3.1
1	A	776	PHE	2.8
1	A	217	TYR	2.6
1	A	730	PHE	2.6
1	A	726	VAL	2.6
1	A	546	TRP	2.6
1	A	757	ILE	2.5
1	A	755	LEU	2.5
1	A	547	PHE	2.5
1	A	772	SER	2.4
1	A	746	PHE	2.3
1	A	778	THR	2.2
1	A	780	VAL	2.2
1	A	64	ASN	2.2
1	A	762	LEU	2.2
1	A	65	GLY	2.1
1	A	572	SER	2.1
1	A	784	LEU	2.1
1	A	751	GLN	2.1
1	A	781	LEU	2.1



## 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	907	6/6	0.89	0.34	6.59	53,56,59,62	0
7	BCN	A	908	11/11	0.81	0.32	5.43	58,69,74,77	0
6	GOL	A	905	6/6	0.96	0.29	1.53	48,51,52,55	0
6	GOL	A	906	6/6	0.84	0.23	0.99	80,82,83,84	0
5	ADP	A	904	27/27	0.96	0.23	0.45	40,47,54,55	0
4	BEF	A	903	4/4	0.95	0.24	0.32	48,51,52,52	0
2	52E	A	901	35/35	0.95	0.21	0.13	43,54,69,74	0
3	MG	A	902	1/1	0.97	0.23	-	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.