



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:50 am BST

PDB ID : 6B98  
Title : PDE2 in complex with compound 1  
Authors : Lu, J.  
Deposited on : 2017-10-10  
Resolution : 1.97 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.

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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 : 2.11  
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

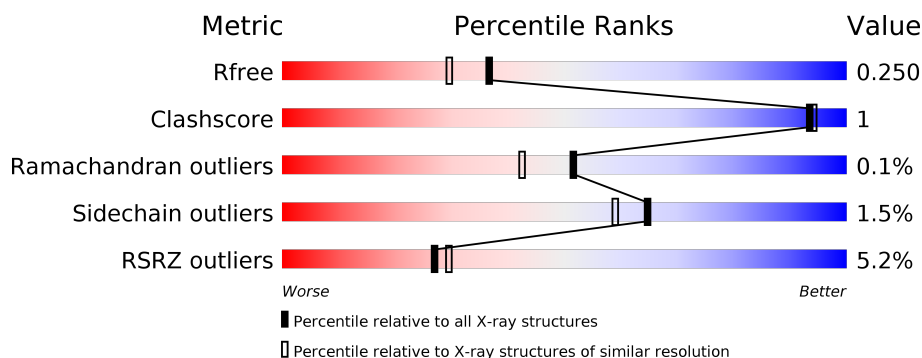
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	373	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
1	B	373	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>•</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5833 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-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	1	0
			2757	1767	462	503	25			
1	B	349	Total	C	N	O	S	0	1	0
			2815	1798	479	513	25			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	547	MET	-	expression tag	UNP O00408
A	548	HIS	-	expression tag	UNP O00408
A	549	HIS	-	expression tag	UNP O00408
A	550	HIS	-	expression tag	UNP O00408
A	551	HIS	-	expression tag	UNP O00408
A	552	HIS	-	expression tag	UNP O00408
A	553	HIS	-	expression tag	UNP O00408
A	554	GLU	-	expression tag	UNP O00408
A	555	ASN	-	expression tag	UNP O00408
A	556	LEU	-	expression tag	UNP O00408
A	557	TYR	-	expression tag	UNP O00408
A	558	PHE	-	expression tag	UNP O00408
A	559	GLN	-	expression tag	UNP O00408
A	560	GLY	-	expression tag	UNP O00408
A	561	GLU	-	expression tag	UNP O00408
A	562	LEU	-	expression tag	UNP O00408
A	563	SER	-	expression tag	UNP O00408
A	564	THR	-	expression tag	UNP O00408
A	565	SER	-	expression tag	UNP O00408
A	566	LEU	-	expression tag	UNP O00408
A	567	TYR	-	expression tag	UNP O00408
A	568	LYS	-	expression tag	UNP O00408
A	569	LYS	-	expression tag	UNP O00408
A	570	ALA	-	expression tag	UNP O00408
A	571	GLY	-	expression tag	UNP O00408

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Chain	Residue	Modelled	Actual	Comment	Reference
A	572	PHE	-	expression tag	UNP O00408
A	573	ASP	-	expression tag	UNP O00408
A	574	ASP	-	expression tag	UNP O00408
A	575	ASP	-	expression tag	UNP O00408
A	576	ASP	-	expression tag	UNP O00408
A	577	LYS	-	expression tag	UNP O00408
B	547	MET	-	expression tag	UNP O00408
B	548	HIS	-	expression tag	UNP O00408
B	549	HIS	-	expression tag	UNP O00408
B	550	HIS	-	expression tag	UNP O00408
B	551	HIS	-	expression tag	UNP O00408
B	552	HIS	-	expression tag	UNP O00408
B	553	HIS	-	expression tag	UNP O00408
B	554	GLU	-	expression tag	UNP O00408
B	555	ASN	-	expression tag	UNP O00408
B	556	LEU	-	expression tag	UNP O00408
B	557	TYR	-	expression tag	UNP O00408
B	558	PHE	-	expression tag	UNP O00408
B	559	GLN	-	expression tag	UNP O00408
B	560	GLY	-	expression tag	UNP O00408
B	561	GLU	-	expression tag	UNP O00408
B	562	LEU	-	expression tag	UNP O00408
B	563	SER	-	expression tag	UNP O00408
B	564	THR	-	expression tag	UNP O00408
B	565	SER	-	expression tag	UNP O00408
B	566	LEU	-	expression tag	UNP O00408
B	567	TYR	-	expression tag	UNP O00408
B	568	LYS	-	expression tag	UNP O00408
B	569	LYS	-	expression tag	UNP O00408
B	570	ALA	-	expression tag	UNP O00408
B	571	GLY	-	expression tag	UNP O00408
B	572	PHE	-	expression tag	UNP O00408
B	573	ASP	-	expression tag	UNP O00408
B	574	ASP	-	expression tag	UNP O00408
B	575	ASP	-	expression tag	UNP O00408
B	576	ASP	-	expression tag	UNP O00408
B	577	LYS	-	expression tag	UNP O00408

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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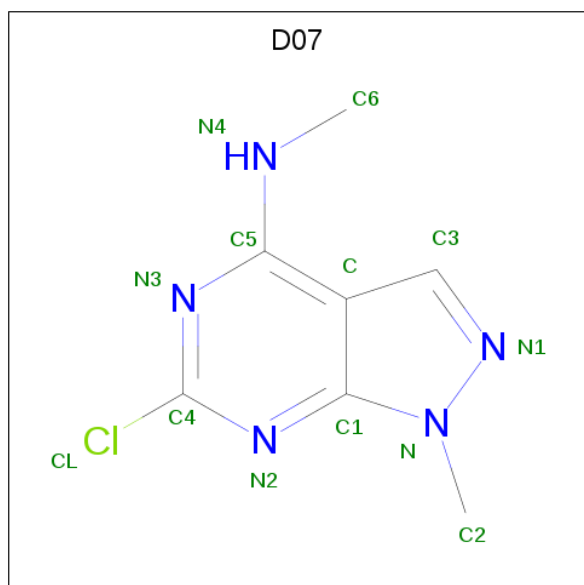
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

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

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

- Molecule 4 is 6-chloro-N,1-dimethyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: D07) (formula: C<sub>7</sub>H<sub>8</sub>ClN<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N 13 7 1 5	0	0
4	B	1	Total C Cl N 13 7 1 5	0	0

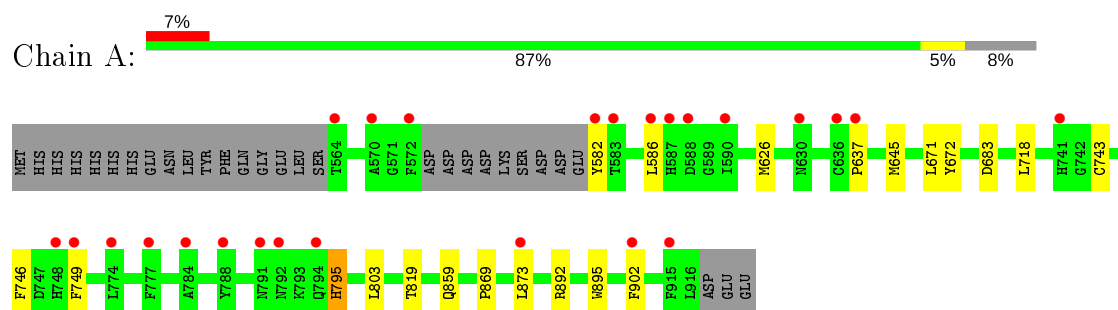
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total 109	O 109	0	0
5	B	122	Total 122	O 122	0	0

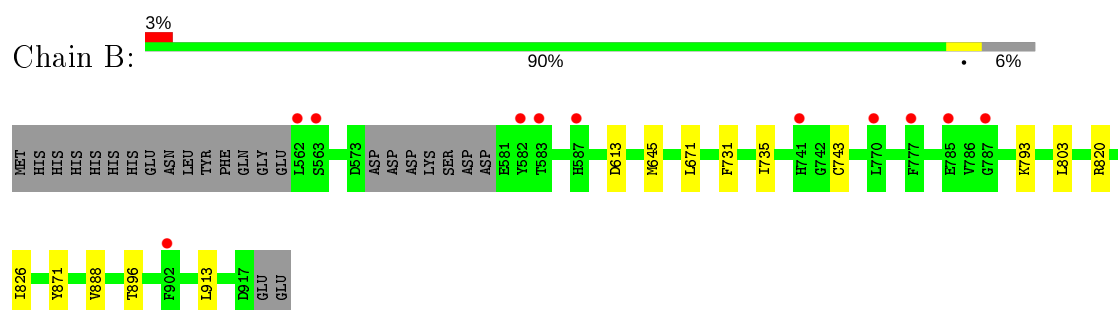
### 3 Residue-property plots [i](#)

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

- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.03 Å 94.19 Å 102.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 1.97 45.03 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.09-1.97) 99.9 (45.03-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 1.97 Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.199 , 0.240 0.208 , 0.250	Depositor DCC
$R_{free}$ test set	2530 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	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	0.95	EDS
Total number of atoms	5833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8271e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: D07, ZN, 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	0/2825	0.64	0/3824
1	B	0.50	0/2883	0.62	0/3895
All	All	0.50	0/5708	0.63	0/7719

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2757	0	2642	9	0
1	B	2815	0	2722	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	0	0	0
4	B	13	0	0	0	0
5	A	109	0	0	0	0
5	B	122	0	0	0	0
All	All	5833	0	5364	15	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 1.

All (15) 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:819:THR:HG22	1:A:895:TRP:HE1	1.58	0.67
1:A:819:THR:CG2	1:A:895:TRP:HE1	2.08	0.65
1:A:859:GLN:HG2	1:A:895:TRP:CE2	2.46	0.51
1:B:671:LEU:HD13	1:B:803:LEU:HD22	1.95	0.49
1:B:871:TYR:CD2	1:B:888:VAL:HG21	2.50	0.46
1:B:820:ARG:HE	1:B:913:LEU:HB3	1.81	0.46
1:B:731:PHE:CE1	1:B:735:ILE:HD11	2.52	0.44
1:A:671:LEU:HD13	1:A:803:LEU:HD22	1.98	0.44
1:A:869:PRO:O	1:A:873:LEU:HG	2.17	0.43
1:B:793:LYS:HD3	1:B:793:LYS:HA	1.82	0.43
1:A:746:PHE:O	1:A:749:PHE:HB2	2.18	0.43
1:A:645:MET:HG3	1:A:743:CYS:SG	2.59	0.42
1:A:586:LEU:HD11	1:A:637:PRO:HA	2.00	0.42
1:B:645:MET:HG3	1:B:743:CYS:SG	2.61	0.41
1:A:626:MET:HG2	1:A:672:TYR:CD1	2.56	0.41

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	341/373 (91%)	335 (98%)	5 (2%)	1 (0%)	41	29
1	B	346/373 (93%)	341 (99%)	5 (1%)	0	100	100
All	All	687/746 (92%)	676 (98%)	10 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	795	HIS

### 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	294/337 (87%)	288 (98%)	6 (2%)	55	48
1	B	304/337 (90%)	301 (99%)	3 (1%)	76	73
All	All	598/674 (89%)	589 (98%)	9 (2%)	65	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	582	TYR
1	A	683	ASP
1	A	718	LEU
1	A	795	HIS
1	A	892	ARG
1	A	902	PHE
1	B	613	ASP
1	B	826	ILE
1	B	896	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	630	ASN

### 5.3.3 RNA [i](#)

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 ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	D07	B	1003	-	12,14,14	2.23	4 (33%)	13,20,20	3.08	7 (53%)
4	D07	A	1003	-	12,14,14	2.19	4 (33%)	13,20,20	2.51	8 (61%)

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	D07	B	1003	-	-	2/2/2/2	0/2/2/2
4	D07	A	1003	-	-	1/2/2/2	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	D07	C4-N2	6.09	1.35	1.30
4	A	1003	D07	C4-N2	5.69	1.34	1.30
4	B	1003	D07	C5-C	-3.00	1.41	1.44
4	A	1003	D07	C5-N3	2.95	1.36	1.32
4	A	1003	D07	C5-C	-2.72	1.41	1.44
4	B	1003	D07	C5-N3	2.52	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	D07	C4-N3	2.16	1.36	1.32
4	B	1003	D07	C4-N3	2.02	1.36	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	D07	C6-N4-C5	6.17	128.18	122.87
4	B	1003	D07	C-C5-N4	5.02	125.36	120.63
4	B	1003	D07	N4-C5-N3	-4.95	112.31	118.50
4	A	1003	D07	N4-C5-N3	-3.86	113.67	118.50
4	A	1003	D07	CL-C4-N2	-3.81	112.45	115.70
4	A	1003	D07	C6-N4-C5	3.76	126.11	122.87
4	B	1003	D07	C3-N1-N	3.67	108.05	104.23
4	A	1003	D07	C-C5-N4	3.34	123.77	120.63
4	B	1003	D07	C4-N2-C1	-2.97	111.75	114.09
4	A	1003	D07	C3-N1-N	2.70	107.05	104.23
4	A	1003	D07	CL-C4-N3	2.32	118.46	115.15
4	A	1003	D07	C4-N2-C1	-2.27	112.30	114.09
4	A	1003	D07	C3-C-C1	-2.08	103.27	105.20
4	B	1003	D07	CL-C4-N2	-2.02	113.98	115.70
4	B	1003	D07	C3-C-C1	-2.00	103.34	105.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1003	D07	N3-C5-N4-C6
4	A	1003	D07	C-C5-N4-C6
4	B	1003	D07	C-C5-N4-C6

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 ⓘ

### 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	344/373 (92%)	0.45	25 (7%) 15 16	20, 37, 65, 83	0
1	B	349/373 (93%)	0.24	11 (3%) 47 50	19, 34, 55, 92	0
All	All	693/746 (92%)	0.34	36 (5%) 27 29	19, 35, 62, 92	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	ASN	5.1
1	A	586	LEU	4.5
1	B	902	PHE	4.2
1	A	777	PHE	3.8
1	A	583	THR	3.8
1	A	587	HIS	3.8
1	A	637	PRO	3.8
1	A	570	ALA	3.5
1	A	784	ALA	3.5
1	A	564	THR	3.4
1	A	582	TYR	3.3
1	B	583	THR	3.3
1	A	636	CYS	3.1
1	A	774	LEU	2.9
1	A	590	ILE	2.9
1	B	582	TYR	2.9
1	A	873	LEU	2.9
1	A	902	PHE	2.8
1	B	770	LEU	2.6
1	B	562	LEU	2.6
1	B	563	SER	2.5
1	B	587	HIS	2.5
1	B	777	PHE	2.5
1	A	588	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	748	HIS	2.3
1	A	915	PHE	2.3
1	A	792	ASN	2.3
1	A	794	GLN	2.3
1	B	787	GLY	2.3
1	B	741	HIS	2.3
1	A	741	HIS	2.2
1	A	788	TYR	2.2
1	A	572	PHE	2.1
1	B	785	GLU	2.1
1	A	630	ASN	2.1
1	A	749	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	D07	B	1003	13/13	0.88	0.17	48,50,55,57	0
4	D07	A	1003	13/13	0.90	0.17	49,51,57,59	0
3	MG	A	1002	1/1	0.95	0.03	36,36,36,36	0
3	MG	B	1002	1/1	0.97	0.07	31,31,31,31	0
2	ZN	B	1001	1/1	0.99	0.07	30,30,30,30	0
2	ZN	A	1001	1/1	1.00	0.04	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.