



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:14 am GMT

PDB ID : 1XOZ
Title : Catalytic Domain Of Human Phosphodiesterase 5A In Complex With Tadalafil
Authors : Card, G.L.; England, B.P.; Suzuki, Y.; Fong, D.; Powell, B.; Lee, B.; Luu, C.;
Tabrizizad, M.; Gillette, S.; Ibrahim, P.N.; Artis, D.R.; Bollag, G.; Milburn,
M.V.; Kim, S.-H.; Schlessinger, J.; Zhang, K.Y.J.
Deposited on : 2004-10-07
Resolution : 1.37 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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

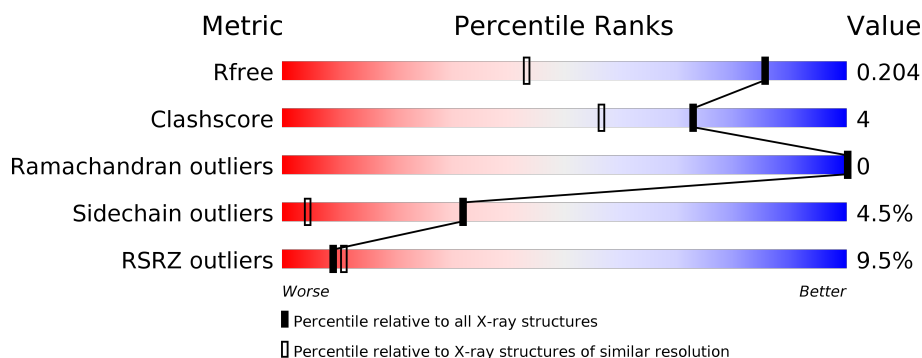
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.37 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	2133 (1.40-1.36)
Clashscore	112137	2266 (1.40-1.36)
Ramachandran outliers	110173	2215 (1.40-1.36)
Sidechain outliers	110143	2214 (1.40-1.36)
RSRZ outliers	101464	2141 (1.40-1.36)

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 ≥ 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	364	<div> <div>9%</div> <div>77%</div> <div>11%</div> <div>10%</div> </div>

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
2	ZN	A	1	-	-	-	X
3	MG	A	2	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3020 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-specific 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2637	1678	451	491	17			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	513	MET	-	INITIATING METHIONINE	UNP O76074
A	514	GLY	-	CLONING ARTIFACT	UNP O76074
A	515	SER	-	CLONING ARTIFACT	UNP O76074
A	516	SER	-	CLONING ARTIFACT	UNP O76074
A	517	HIS	-	EXPRESSION TAG	UNP O76074
A	518	HIS	-	EXPRESSION TAG	UNP O76074
A	519	HIS	-	EXPRESSION TAG	UNP O76074
A	520	HIS	-	EXPRESSION TAG	UNP O76074
A	521	HIS	-	EXPRESSION TAG	UNP O76074
A	522	HIS	-	EXPRESSION TAG	UNP O76074
A	523	SER	-	CLONING ARTIFACT	UNP O76074
A	524	SER	-	CLONING ARTIFACT	UNP O76074
A	525	GLY	-	CLONING ARTIFACT	UNP O76074
A	526	LEU	-	CLONING ARTIFACT	UNP O76074
A	527	VAL	-	CLONING ARTIFACT	UNP O76074
A	528	PRO	-	CLONING ARTIFACT	UNP O76074
A	529	ARG	-	CLONING ARTIFACT	UNP O76074
A	530	GLY	-	CLONING ARTIFACT	UNP O76074
A	531	SER	-	CLONING ARTIFACT	UNP O76074
A	532	HIS	-	CLONING ARTIFACT	UNP O76074
A	533	MET	-	CLONING ARTIFACT	UNP O76074
A	658	PRO	ARG	ENGINEERED	UNP O76074
A	661	SER	ASN	ENGINEERED	UNP O76074
A	663	GLN	SER	ENGINEERED	UNP O76074
A	647	LEU	ILE	ENGINEERED	UNP O76074
A	648	ILE	GLN	ENGINEERED	UNP O76074
A	667	ASN	ARG	ENGINEERED	UNP O76074

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Chain	Residue	Modelled	Actual	Comment	Reference
A	668	THR	SER	ENGINEERED	UNP O76074
A	669	ASN	GLU	ENGINEERED	UNP O76074
A	670	SER	HIS	ENGINEERED	UNP O76074
A	671	GLU	PRO	ENGINEERED	UNP O76074
A	674	LEU	GLN	ENGINEERED	UNP O76074
A	675	MET	LEU	ENGINEERED	UNP O76074
A	676A	ASN	CYS	ENGINEERED	UNP O76074
A	677	ASP	-	ENGINEERED	UNP O76074
A	678	GLU	HIS	ENGINEERED	UNP O76074
A	680	VAL	ILE	ENGINEERED	UNP O76074
A	681	LEU	MET	ENGINEERED	UNP O76074

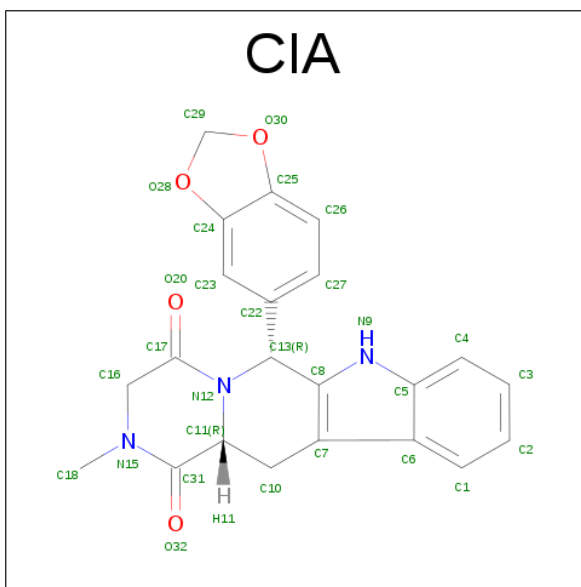
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is 6-BENZO[1,3]DIOXOL-5-YL-2-METHYL-2,3,6,7,12,12A-HEXAHYDRO-PYRAZINO[1',2':1,6]PYRIDO[3,4-B]INDOLE-1,4-DIONE (three-letter code: CIA) (formula: C₂₂H₁₉N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			29	22	3	4		

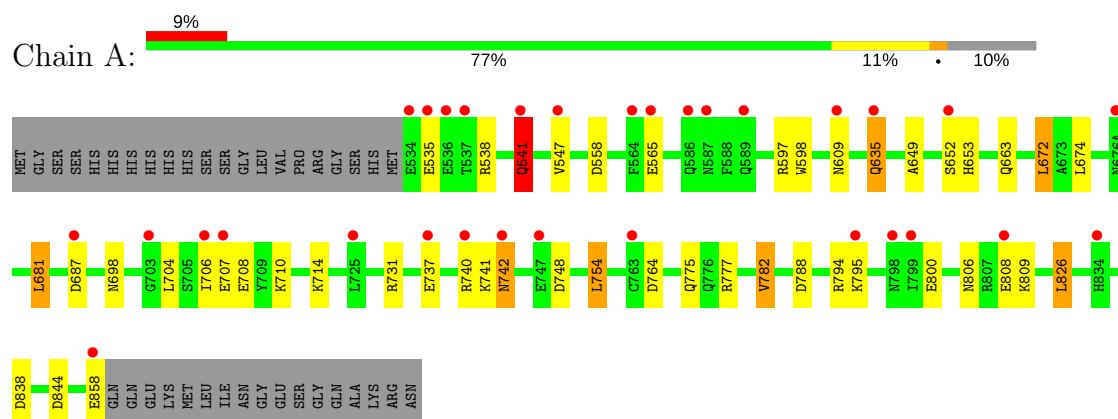
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	352	Total	O	0	0
			352	352		

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-specific 3',5'-cyclic phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	56.10Å 76.40Å 80.70Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	79.06 – 1.37 44.43 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (79.06-1.37) 92.5 (44.43-1.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.152 , 0.193 0.164 , 0.204	Depositor DCC
R_{free} test set	3417 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3020	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, MG, CIA

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	1.05	10/2686 (0.4%)	1.03	19/3629 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	GLN	CD-OE1	9.62	1.45	1.24
1	A	635	GLN	CB-CG	-8.39	1.29	1.52
1	A	635	GLN	CD-NE2	7.85	1.52	1.32
1	A	652	SER	CB-OG	-7.32	1.32	1.42
1	A	794	ARG	NE-CZ	-6.64	1.24	1.33
1	A	708	GLU	CD-OE1	5.80	1.32	1.25
1	A	541	GLN	CG-CD	5.61	1.64	1.51
1	A	782	VAL	CB-CG1	5.47	1.64	1.52
1	A	742	ASN	CG-ND2	5.09	1.45	1.32
1	A	687	ASP	CB-CG	5.07	1.62	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	597	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	597	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	794	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	826	LEU	CB-CG-CD1	6.65	122.31	111.00
1	A	838	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	764	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	681	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	844	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	558	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	748	ASP	CB-CG-OD2	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	740	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	754	LEU	CB-CG-CD2	5.54	120.42	111.00
1	A	788	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	681	LEU	CB-CG-CD2	5.37	120.12	111.00
1	A	777	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	704	LEU	CB-CG-CD2	5.19	119.82	111.00
1	A	687	ASP	OD1-CG-OD2	-5.06	113.69	123.30
1	A	672	LEU	CA-CB-CG	5.01	126.81	115.30

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	2637	0	2643	21	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	29	0	19	1	0
5	A	352	0	0	12	1
All	All	3020	0	2662	21	1

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 (21) 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:809:LYS:HD3	5:A:1060:HOH:O	1.60	0.99
1:A:809:LYS:CD	5:A:1060:HOH:O	2.18	0.90
1:A:635:GLN:HG2	5:A:1019:HOH:O	1.88	0.72
1:A:547:VAL:HG23	5:A:1349:HOH:O	1.98	0.62
1:A:782:VAL:HG21	4:A:501:CIA:C1	2.31	0.61
1:A:808:GLU:HG3	5:A:1098:HOH:O	2.00	0.60
1:A:731:ARG:NH2	5:A:1179:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ASN:OD1	5:A:1202:HOH:O	2.17	0.59
1:A:598:TRP:HA	1:A:698:ASN:HD22	1.68	0.57
1:A:541:GLN:HG3	5:A:1217:HOH:O	2.04	0.56
1:A:706:ILE:HG22	1:A:710:LYS:HE3	1.88	0.55
1:A:806:ASN:ND2	1:A:809:LYS:HE2	2.22	0.55
1:A:737:GLU:HG3	1:A:741:LYS:HE2	1.90	0.53
1:A:547:VAL:HG22	5:A:1082:HOH:O	2.15	0.47
1:A:714:LYS:HG3	5:A:1129:HOH:O	2.15	0.47
1:A:806:ASN:HD22	1:A:809:LYS:HE2	1.80	0.47
1:A:565:GLU:HB2	5:A:1131:HOH:O	2.14	0.47
1:A:535:GLU:OE2	5:A:1188:HOH:O	2.21	0.46
1:A:649:ALA:O	1:A:653:HIS:HB3	2.18	0.44
1:A:706:ILE:CG2	1:A:710:LYS:HE3	2.48	0.42
1:A:737:GLU:CG	1:A:741:LYS:HE2	2.49	0.42

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:GLN:NE2	5:A:1217:HOH:O[3_545]	2.04	0.16

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	324/364 (89%)	323 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	291/323 (90%)	278 (96%)	13 (4%)	32 4

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	ARG
1	A	541	GLN
1	A	672	LEU
1	A	674	LEU
1	A	681	LEU
1	A	707	GLU
1	A	742	ASN
1	A	754	LEU
1	A	775	GLN
1	A	795	LYS
1	A	800	GLU
1	A	826	LEU
1	A	858	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	GLN
1	A	698	ASN
1	A	718	GLN
1	A	776	GLN
1	A	811	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	$\# Z > 2$
4	CIA	A	501	-	33,34,34	1.64	7 (21%)	38,52,52	2.48	12 (31%)

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	CIA	A	501	-	-	0/4/42/42	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	CIA	C8-C13	-3.96	1.48	1.51
4	A	501	CIA	C16-C17	-2.37	1.46	1.51
4	A	501	CIA	C13-N12	-2.10	1.45	1.47
4	A	501	CIA	C3-C4	2.18	1.41	1.36
4	A	501	CIA	C27-C22	2.27	1.42	1.39
4	A	501	CIA	C7-C6	3.03	1.47	1.41
4	A	501	CIA	C22-C13	4.42	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CIA	C22-C13-C8	-5.23	104.04	112.93
4	A	501	CIA	C2-C1-C6	-4.61	114.29	120.88
4	A	501	CIA	C29-O28-C24	-3.67	100.44	105.35
4	A	501	CIA	C3-C4-C5	-2.79	115.87	120.07
4	A	501	CIA	C29-O30-C25	-2.40	102.14	105.35
4	A	501	CIA	C31-C11-N12	2.15	116.85	112.42
4	A	501	CIA	C26-C27-C22	2.20	123.43	121.20
4	A	501	CIA	C1-C6-C5	2.92	122.03	118.17
4	A	501	CIA	C3-C2-C1	3.01	124.73	120.45
4	A	501	CIA	C18-N15-C16	3.25	120.01	116.25
4	A	501	CIA	C8-C13-N12	5.56	115.50	109.96
4	A	501	CIA	C10-C11-C31	7.33	116.75	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	CIA	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, 95th 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 ²)	Q<0.9
1	A	326/364 (89%)	0.85	31 (9%) 9 11	5, 9, 19, 47	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	GLU	6.8
1	A	535	GLU	6.4
1	A	537	THR	6.4
1	A	536	GLU	4.4
1	A	547	VAL	4.3
1	A	586	GLN	4.0
1	A	541	GLN	3.7
1	A	589	GLN	3.7
1	A	706	ILE	3.3
1	A	565	GLU	3.2
1	A	740	ARG	3.1
1	A	858	GLU	3.1
1	A	725	LEU	2.9
1	A	564	PHE	2.8
1	A	676(A)	ASN	2.8
1	A	609	ASN	2.8
1	A	587	ASN	2.7
1	A	707	GLU	2.6
1	A	703	GLY	2.5
1	A	652	SER	2.4
1	A	798	ASN	2.3
1	A	834	HIS	2.2
1	A	742	ASN	2.2
1	A	808	GLU	2.2
1	A	799	ILE	2.2
1	A	747	GLU	2.1
1	A	795	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	737	GLU	2.1
1	A	635	GLN	2.0
1	A	763	CYS	2.0
1	A	687	ASP	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. 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, 95th 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 ²)	Q<0.9
3	MG	A	2	1/1	1.00	0.22	8.48	9,9,9,9	0
2	ZN	A	1	1/1	0.99	0.17	5.05	13,13,13,13	0
4	CIA	A	501	29/29	0.90	0.11	0.21	11,13,16,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.