



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:03 PM UTC

PDB ID : 3GSG / pdb_00003gsg
Title : AmpC beta-lactamase in complex with Fragment-based Inhibitor
Authors : Teotico, D.T.; Shoichet, B.K.
Deposited on : 2009-03-26
Resolution : 2.10 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

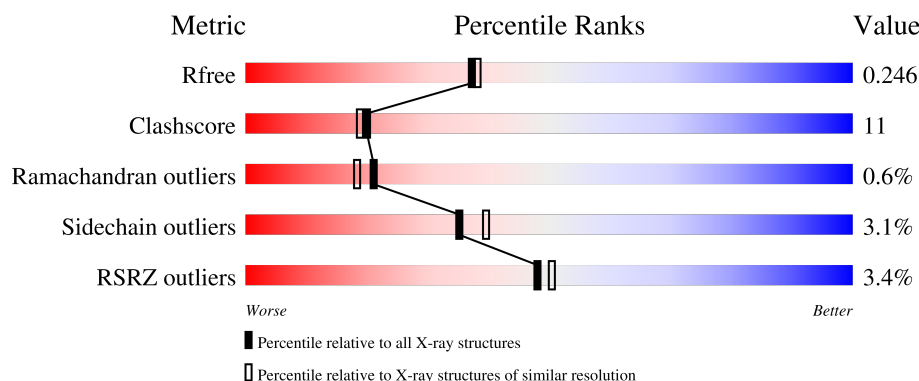
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 ≥ 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	358	5% 83% 13% ..
1	B	358	2% 89% 10% .

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
3	DMS	A	365	-	X	X	-
3	DMS	B	363	-	-	X	-
4	GF1	A	366	X	-	X	-
4	GF1	A	367	X	-	-	-
4	GF1	B	365	X	-	X	-

2 Entry composition [i](#)

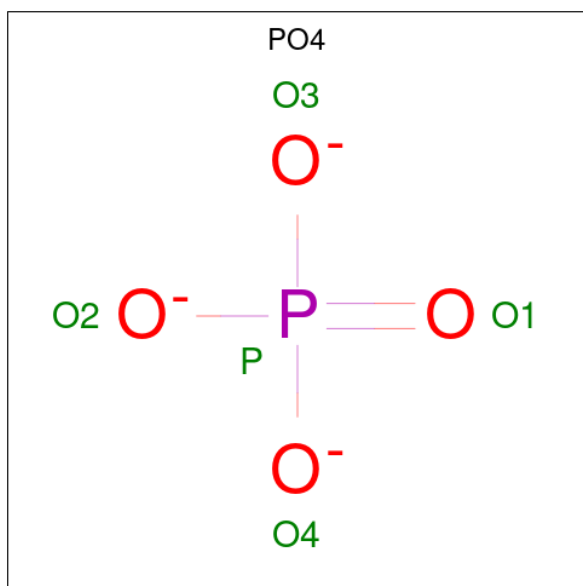
There are 5 unique types of molecules in this entry. The entry contains 6548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	22	27	0
			2886	1849	494	536	7			
1	B	358	Total	C	N	O	S	27	32	0
			2906	1867	499	532	8			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



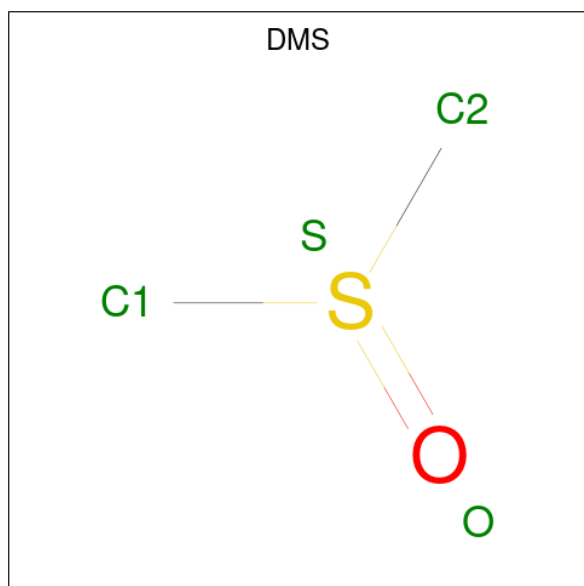
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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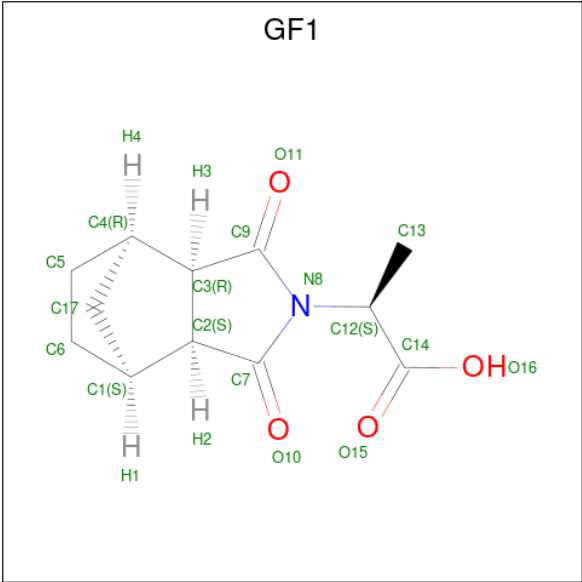
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 4 is (2S)-2-[(3aR,4R,7S,7aS)-1,3-dioxooctahydro-2H-4,7-methanoisoindol-2-yl]propionic acid (CCD ID: GF1) (formula: C₁₂H₁₅NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	12	1	4		
4	A	1	Total	C	N	O	0	0
			17	12	1	4		
4	B	1	Total	C	N	O	0	0
			17	12	1	4		

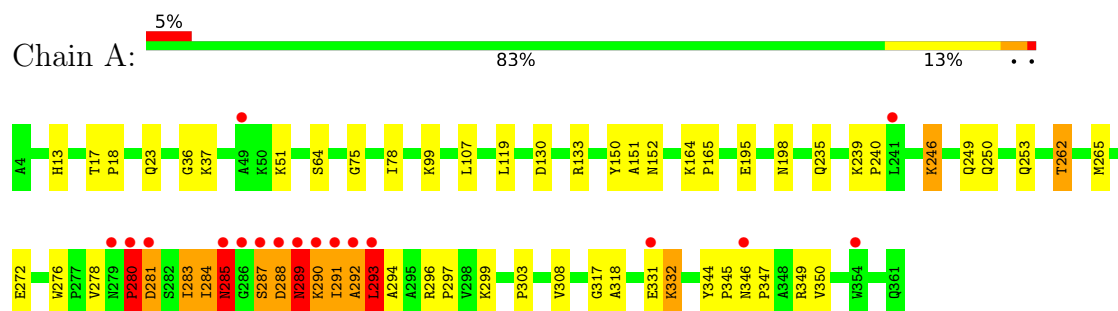
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	344	Total	O	0	0
			344	344		
5	B	308	Total	O	0	0
			308	308		

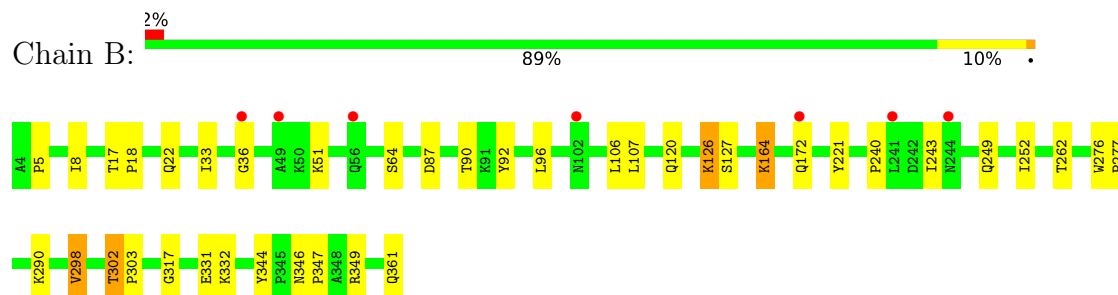
3 Residue-property plots

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: Beta-lactamase



• Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.59Å 75.93Å 97.66Å 90.00° 116.37° 90.00°	Depositor
Resolution (Å)	45.27 – 2.10 45.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.27-2.10) 99.9 (45.27-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.244 0.193 , 0.246	Depositor DCC
R_{free} test set	2263 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6548	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.94% 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: GF1, DMS, PO4

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	0.59	3/3089 (0.1%)	0.80	1/4218 (0.0%)
1	B	0.57	0/3152	0.82	1/4301 (0.0%)
All	All	0.58	3/6241 (0.0%)	0.81	2/8519 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	7
1	B	0	1
All	All	4	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	LYS	CE-NZ	7.58	1.72	1.49
1	A	332	LYS	CD-CE	-6.53	1.32	1.52
1	A	99	LYS	CG-CD	-5.98	1.34	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	LYS	CB-CG-CD	5.31	123.52	111.30
1	A	37	LYS	CG-CD-CE	-5.19	99.37	111.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	285	ASN	CA
1	A	289	ASN	CA
1	A	290	LYS	CA
1	A	292	ALA	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	PRO	Peptide
1	A	284	ILE	Peptide
1	A	285	ASN	Peptide
1	A	287	SER	Peptide
1	A	288	ASP	Peptide

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	2886	0	2850	96	0
1	B	2906	0	2896	36	0
2	A	20	0	0	1	0
2	B	5	0	0	0	0
3	A	8	0	12	14	0
3	B	20	0	30	9	0
4	A	34	0	28	17	0
4	B	17	0	14	7	0
5	A	344	0	0	7	0
5	B	308	0	0	4	0
All	All	6548	0	5830	133	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 11.

The worst 5 of 133 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:291:ILE:CG2	3:A:365:DMS:H12	1.30	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HG22	3:A:365:DMS:C1	1.32	1.53
1:A:291:ILE:HA	1:A:292:ALA:CB	1.41	1.29
3:A:365:DMS:S	3:A:365:DMS:O	1.90	1.28
1:A:291:ILE:CA	1:A:292:ALA:HB2	1.65	1.26

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	383/358 (107%)	369 (96%)	10 (3%)	4 (1%)	12	9
1	B	388/358 (108%)	379 (98%)	9 (2%)	0	100	100
All	All	771/716 (108%)	748 (97%)	19 (2%)	4 (0%)	21	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ASN
1	A	289	ASN
1	A	291	ILE
1	A	280	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	316/292 (108%)	303 (96%)	13 (4%)	27	29
1	B	324/292 (111%)	317 (98%)	7 (2%)	45	53
All	All	640/584 (110%)	620 (97%)	20 (3%)	35	39

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	172	GLN
1	B	302	THR
1	B	361	GLN
1	B	331	GLU
1	A	281	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	285	ASN
1	B	361	GLN
1	A	289	ASN
1	B	6	GLN
1	B	23	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 ligands 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	GF1	A	366	-	19,19,19	1.49	3 (15%)	29,30,30	3.83	19 (65%)
2	PO4	A	363	-	4,4,4	0.86	0	6,6,6	0.43	0
3	DMS	B	363	-	3,3,3	2.75	1 (33%)	3,3,3	0.40	0
2	PO4	B	3	-	4,4,4	0.86	0	6,6,6	0.51	0
3	DMS	B	1	-	3,3,3	2.63	1 (33%)	3,3,3	0.66	0
2	PO4	A	362	-	4,4,4	0.92	0	6,6,6	0.52	0
3	DMS	A	364	-	3,3,3	2.80	1 (33%)	3,3,3	0.58	0
3	DMS	B	362	-	3,3,3	2.66	1 (33%)	3,3,3	0.70	0
4	GF1	A	367	-	19,19,19	2.08	7 (36%)	29,30,30	4.65	14 (48%)
2	PO4	A	1	-	4,4,4	0.98	0	6,6,6	0.62	0
3	DMS	A	365	-	3,3,3	3.94	2 (66%)	3,3,3	1.69	1 (33%)
3	DMS	B	366	-	3,3,3	3.19	1 (33%)	3,3,3	1.01	0
3	DMS	B	364	-	3,3,3	2.75	1 (33%)	3,3,3	0.79	0
2	PO4	A	2	-	4,4,4	0.92	0	6,6,6	0.55	0
4	GF1	B	365	-	19,19,19	2.00	6 (31%)	29,30,30	2.15	12 (41%)

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	GF1	A	367	-	1/1/9/9	3/8/45/45	0/4/3/3
4	GF1	A	366	-	3/3/9/9	2/8/45/45	0/4/3/3
4	GF1	B	365	-	3/3/9/9	2/8/45/45	0/4/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	365	DMS	O-S	6.13	1.90	1.50
3	B	366	DMS	O-S	4.99	1.83	1.50
3	A	364	DMS	O-S	4.68	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	363	DMS	O-S	4.64	1.80	1.50
3	B	364	DMS	O-S	4.59	1.80	1.50

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	367	GF1	C6-C1-C2	16.07	129.70	108.04
4	A	367	GF1	C1-C2-C7	-12.49	92.10	115.49
4	A	366	GF1	C2-C3-C4	8.28	113.14	103.15
4	A	366	GF1	C1-C2-C7	7.87	130.23	115.49
4	A	366	GF1	C5-C4-C3	-7.25	98.26	108.04

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	366	GF1	C1
4	A	366	GF1	C4
4	A	366	GF1	C12
4	A	367	GF1	C12
4	B	365	GF1	C1

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	366	GF1	C14-C12-N8-C9
4	A	367	GF1	C14-C12-N8-C9
4	A	367	GF1	C14-C12-N8-C7
4	B	365	GF1	C13-C12-C14-O16
4	B	365	GF1	C13-C12-C14-O15

There are no ring outliers.

10 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	366	GF1	15	0
3	B	363	DMS	4	0
2	A	362	PO4	1	0
3	A	364	DMS	1	0
3	B	362	DMS	3	0
4	A	367	GF1	2	0
3	A	365	DMS	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	366	DMS	1	0
3	B	364	DMS	1	0
4	B	365	GF1	7	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 [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, 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	358/358 (100%)	0.19	17 (4%) 36 38	9, 21, 36, 46	47 (13%)
1	B	358/358 (100%)	0.06	7 (1%) 65 67	10, 22, 32, 40	47 (13%)
All	All	716/716 (100%)	0.13	24 (3%) 48 50	9, 22, 33, 46	94 (13%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	8.6
1	A	292	ALA	5.3
1	B	36	GLY	5.0
1	B	172	GLN	4.2
1	A	280	PRO	4.1

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
4	GF1	A	367	17/17	0.58	0.18	35,37,38,38	17
3	DMS	A	365	4/4	0.63	0.20	32,32,32,33	1
4	GF1	A	366	17/17	0.65	0.18	31,33,34,34	13
2	PO4	A	363	5/5	0.73	0.20	49,49,50,50	5
2	PO4	A	362	5/5	0.73	0.18	34,34,34,35	5
3	DMS	B	366	4/4	0.76	0.21	36,36,36,37	4
2	PO4	B	3	5/5	0.78	0.15	43,43,44,44	5
4	GF1	B	365	17/17	0.79	0.13	31,32,33,33	2
3	DMS	B	362	4/4	0.80	0.23	38,38,38,39	0
3	DMS	A	364	4/4	0.83	0.20	30,31,31,32	4
3	DMS	B	363	4/4	0.84	0.20	26,27,27,27	4
2	PO4	A	2	5/5	0.85	0.23	49,50,50,50	0
2	PO4	A	1	5/5	0.85	0.17	43,44,44,44	5
3	DMS	B	364	4/4	0.88	0.17	32,32,33,33	4
3	DMS	B	1	4/4	0.95	0.10	32,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.