



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:02 AM UTC

PDB ID : 3GTC / pdb_00003gtc
Title : AmpC beta-lactamase in complex with Fragment-based Inhibitor
Authors : Teotico, D.T.; Shoichet, B.K.
Deposited on : 2009-03-27
Resolution : 1.90 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

<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

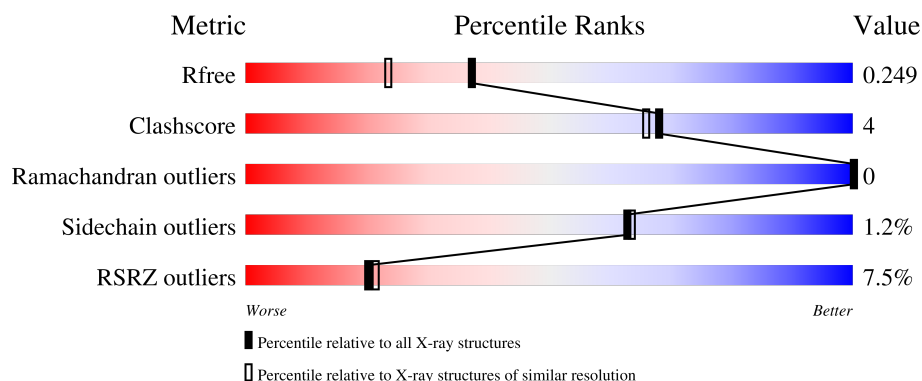
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	92% 7%
1	B	358	14% 91% 9%

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	GTC	B	363	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6395 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.

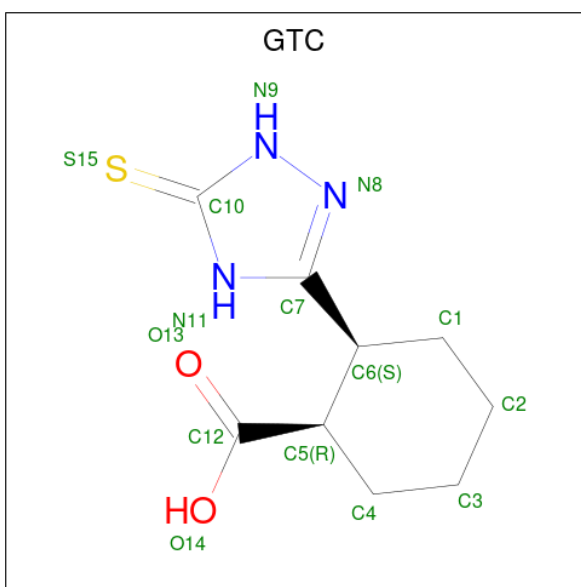
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	2	0
			2815	1812	478	519	6			
1	B	358	Total	C	N	O	S	0	0	0
			2800	1804	476	514	6			

- 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	1
			5	4	1		

- Molecule 3 is (1R,2S)-2-(5-thioxo-4,5-dihydro-1H-1,2,4-triazol-3-yl)cyclohexanecarboxylic acid (CCD ID: GTC) (formula: C₉H₁₃N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 15	C 9	N 3	O 2	S 1	0	0
3	A	1	Total 15	C 9	N 3	O 2	S 1	0	1
3	B	1	Total 15	C 9	N 3	O 2	S 1	0	0
3	B	1	Total 15	C 9	N 3	O 2	S 1	0	0
3	B	1	Total 15	C 9	N 3	O 2	S 1	0	0

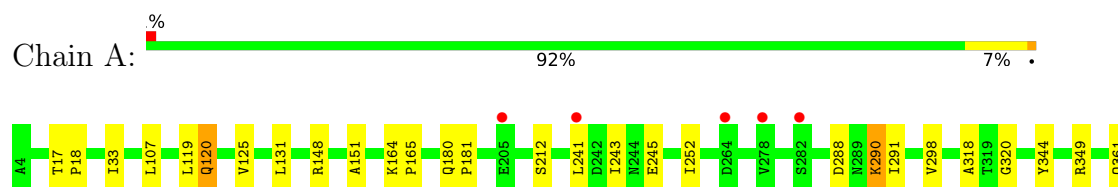
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	386	Total O 386 386	0	0
4	B	309	Total O 309 309	0	0

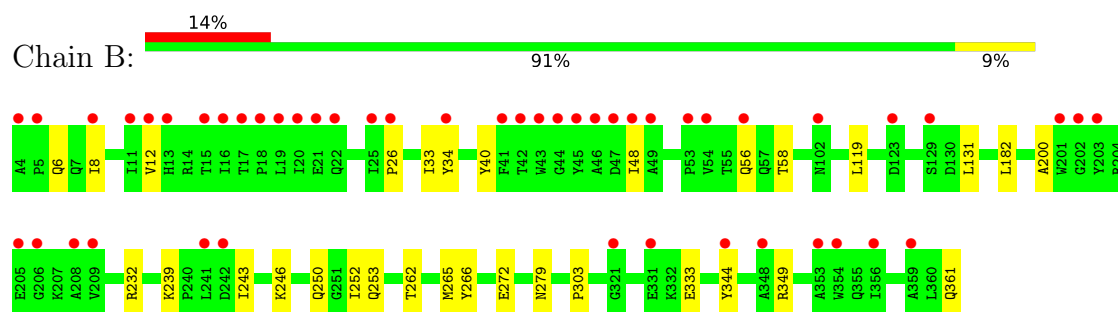
3 Residue-property plots [i](#)

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: 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	118.45Å 77.95Å 97.88Å 90.00° 115.76° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-1.90) 98.7 (30.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.247 0.209 , 0.249	Depositor DCC
R_{free} test set	3184 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.7	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	6395	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 9.50% 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: GTC, 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	0.51	0/2895	0.74	0/3953
1	B	0.49	0/2880	0.73	0/3933
All	All	0.50	0/5775	0.73	0/7886

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	2815	0	2787	22	1
1	B	2800	0	2778	21	0
2	A	10	0	0	0	0
3	A	30	0	24	5	0
3	B	45	0	35	5	1
4	A	386	0	0	1	0
4	B	309	0	0	0	0
All	All	6395	0	5624	41	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 (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:320:GLY:N	3:A:362:GTC:HN11	1.67	0.92
1:A:320:GLY:H	3:A:362:GTC:HN11	0.84	0.71
1:B:279:ASN:ND2	3:B:363:GTC:S15	2.65	0.69
1:B:243:ILE:CD1	1:B:252:ILE:HD12	2.24	0.67
1:A:288:ASP:OD1	1:A:290:LYS:HG3	2.03	0.59
1:B:243:ILE:HD12	1:B:252:ILE:HD12	1.86	0.56
1:A:241:LEU:HD13	1:B:246:LYS:HG2	1.90	0.54
1:B:279:ASN:CG	3:B:363:GTC:S15	2.91	0.54
1:A:120:GLN:NE2	4:A:563:HOH:O	2.26	0.54
1:A:17:THR:HB	1:A:18:PRO:HD3	1.91	0.51
1:A:344:TYR:CZ	1:A:349:ARG:HG2	2.46	0.51
1:B:33:ILE:HD12	1:B:33:ILE:N	2.26	0.51
1:B:344:TYR:CE1	1:B:349:ARG:HG2	2.47	0.50
1:B:131:LEU:HD23	3:B:362:GTC:H3	1.95	0.49
1:B:26:PRO:HB3	1:B:48:ILE:HD11	1.95	0.48
1:A:344:TYR:CE1	1:A:349:ARG:HG2	2.49	0.48
1:A:243:ILE:CD1	1:A:252:ILE:HD12	2.44	0.47
1:B:262:THR:O	1:B:262:THR:HG23	2.15	0.47
1:B:265:MET:HE3	1:B:272:GLU:HG2	1.96	0.47
1:B:131:LEU:HD23	3:B:362:GTC:C3	2.45	0.46
1:A:318:ALA:O	3:A:364[B]:GTC:N8	2.48	0.46
1:A:119:LEU:HD21	3:A:364[B]:GTC:H2	1.99	0.45
1:B:265:MET:HE2	1:B:266:TYR:O	2.16	0.45
1:B:8:ILE:O	1:B:12:VAL:HG23	2.17	0.44
1:A:243:ILE:HD12	1:A:252:ILE:HD12	1.99	0.44
1:A:33:ILE:HD12	1:A:33:ILE:N	2.32	0.44
1:B:182:LEU:O	1:B:232:ARG:HD3	2.17	0.44
1:B:119:LEU:HD21	3:B:1:GTC:H2	1.98	0.43
1:B:250:GLN:HA	1:B:253:GLN:HE21	1.84	0.43
1:A:245:GLU:OE1	1:A:245:GLU:N	2.52	0.42
1:A:212:SER:H	3:A:362:GTC:HN9	1.66	0.42
1:A:125:VAL:HG11	1:A:131:LEU:HD23	2.02	0.42
1:A:290:LYS:HD2	1:A:291:ILE:HG13	2.02	0.42
1:A:164:LYS:HB2	1:A:165:PRO:HD3	2.02	0.41
1:B:40:TYR:HB2	1:B:56:GLN:OE1	2.20	0.41
1:A:107:LEU:HD22	1:B:303:PRO:HD3	2.02	0.41
1:A:180:GLN:HB2	1:A:181:PRO:HD3	2.03	0.41
1:B:8:ILE:HD11	1:B:34:TYR:CG	2.55	0.41
1:B:58:THR:CG2	1:B:200:ALA:HB2	2.50	0.41
1:A:119:LEU:HA	1:A:151:ALA:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:HB2	1:A:298:VAL:HG11	2.03	0.41

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:164:LYS:NZ	3:B:363:GTC:O14[2_655]	1.90	0.30

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	358/358 (100%)	352 (98%)	6 (2%)	0	100	100
1	B	356/358 (99%)	349 (98%)	7 (2%)	0	100	100
All	All	714/716 (100%)	701 (98%)	13 (2%)	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	294/292 (101%)	291 (99%)	3 (1%)	68	70
1	B	292/292 (100%)	288 (99%)	4 (1%)	59	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	586/584 (100%)	579 (99%)	7 (1%)	63	63

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	290	LYS
1	A	361	GLN
1	B	6	GLN
1	B	239	LYS
1	B	333	GLU
1	B	361	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	23	GLN
1	A	35	GLN
1	A	102	ASN
1	A	137	ASN
1	A	175	GLN
1	A	185	ASN
1	B	23	GLN
1	B	102	ASN
1	B	137	ASN
1	B	249	GLN
1	B	253	GLN
1	B	256	GLN
1	B	279	ASN
1	B	361	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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
2	PO4	A	1	-	4,4,4	0.92	0	6,6,6	0.51	0
3	GTC	B	1	-	14,16,16	2.18	3 (21%)	16,22,22	4.27	4 (25%)
3	GTC	B	363	-	14,16,16	2.17	2 (14%)	16,22,22	5.02	7 (43%)
3	GTC	B	362	-	14,16,16	2.07	2 (14%)	16,22,22	4.14	1 (6%)
3	GTC	A	362	-	14,16,16	2.34	4 (28%)	16,22,22	3.52	3 (18%)
2	PO4	A	363[A]	-	4,4,4	0.91	0	6,6,6	0.49	0
3	GTC	A	364[B]	-	14,16,16	1.94	2 (14%)	16,22,22	4.58	2 (12%)

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
3	GTC	B	1	-	-	1/7/19/19	0/2/2/2
3	GTC	B	363	-	1/1/3/3	4/7/19/19	0/2/2/2
3	GTC	B	362	-	-	2/7/19/19	0/2/2/2
3	GTC	A	362	-	-	7/7/19/19	0/2/2/2
3	GTC	A	364[B]	-	-	3/7/19/19	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	362	GTC	C7-N8	6.36	1.37	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	GTC	C7-N8	6.18	1.36	1.30
3	B	363	GTC	C7-N8	6.07	1.36	1.30
3	B	362	GTC	C7-N8	5.68	1.36	1.30
3	A	364[B]	GTC	C7-N8	4.89	1.35	1.30
3	A	362	GTC	C10-S15	4.33	1.77	1.68
3	B	1	GTC	C10-S15	4.12	1.77	1.68
3	A	364[B]	GTC	C10-S15	4.10	1.77	1.68
3	B	362	GTC	C10-S15	4.09	1.77	1.68
3	B	363	GTC	C10-S15	4.09	1.77	1.68
3	A	362	GTC	C10-N11	-2.78	1.33	1.37
3	A	362	GTC	N9-N8	2.26	1.41	1.36
3	B	1	GTC	N9-N8	2.10	1.41	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	364[B]	GTC	C7-N8-N9	17.65	109.97	104.09
3	B	363	GTC	C7-N8-N9	17.25	109.84	104.09
3	B	1	GTC	C7-N8-N9	16.31	109.53	104.09
3	B	362	GTC	C7-N8-N9	16.24	109.50	104.09
3	A	362	GTC	C7-N8-N9	12.71	108.33	104.09
3	B	363	GTC	C4-C5-C12	5.41	122.88	110.71
3	B	363	GTC	C6-C5-C12	4.70	119.38	112.12
3	B	363	GTC	C3-C4-C5	-4.34	104.31	111.76
3	A	362	GTC	S15-C10-N11	-3.50	118.97	125.94
3	B	363	GTC	C2-C1-C6	3.32	117.44	111.76
3	A	362	GTC	C6-C7-N8	3.24	130.00	125.14
3	B	363	GTC	C4-C5-C6	2.77	116.27	110.83
3	B	363	GTC	C2-C3-C4	-2.48	106.32	111.42
3	B	1	GTC	C5-C6-C7	2.26	116.55	112.48
3	A	364[B]	GTC	C3-C4-C5	2.24	115.61	111.76
3	B	1	GTC	C1-C6-C7	-2.10	109.03	111.97
3	B	1	GTC	O14-C12-C5	2.02	119.18	113.93

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	363	GTC	C5

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	362	GTC	C1-C6-C7-N11
3	B	1	GTC	C5-C6-C7-N11
3	B	362	GTC	C5-C6-C7-N11
3	B	362	GTC	C1-C6-C7-N11
3	B	363	GTC	C5-C6-C7-N11
3	B	363	GTC	C1-C6-C7-N11
3	B	363	GTC	O14-C12-C5-C6
3	A	362	GTC	O14-C12-C5-C6
3	A	362	GTC	O14-C12-C5-C4
3	A	362	GTC	O13-C12-C5-C4
3	A	362	GTC	C5-C6-C7-N11
3	A	364[B]	GTC	C5-C6-C7-N11
3	A	362	GTC	O13-C12-C5-C6
3	B	363	GTC	O13-C12-C5-C6
3	A	362	GTC	C1-C6-C7-N8
3	A	364[B]	GTC	C1-C6-C7-N8
3	A	364[B]	GTC	C1-C6-C7-N11

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	GTC	1	0
3	B	363	GTC	2	1
3	B	362	GTC	2	0
3	A	362	GTC	3	0
3	A	364[B]	GTC	2	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	358/358 (100%)	0.07	5 (1%) 73 76	7, 20, 31, 37	4 (1%)
1	B	358/358 (100%)	0.74	49 (13%) 6 7	13, 26, 45, 49	1 (0%)
All	All	716/716 (100%)	0.41	54 (7%) 20 21	7, 22, 43, 49	5 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	TYR	3.9
1	B	19	LEU	3.6
1	B	17	THR	3.6
1	B	48	ILE	3.5
1	B	54	VAL	3.5
1	B	12	VAL	3.3
1	B	44	GLY	3.3
1	B	43	TRP	3.2
1	B	49	ALA	3.2
1	B	241	LEU	3.2
1	B	53	PRO	3.1
1	B	16	ILE	3.1
1	B	359	ALA	3.0
1	B	356	ILE	2.8
1	B	18	PRO	2.8
1	B	20	ILE	2.8
1	B	205	GLU	2.8
1	B	46	ALA	2.8
1	B	206	GLY	2.7
1	B	203	TYR	2.7
1	B	21	GLU	2.7
1	B	26	PRO	2.6
1	B	42	THR	2.6
1	B	331	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	354	TRP	2.5
1	B	8	ILE	2.5
1	A	278	VAL	2.5
1	B	25	ILE	2.5
1	B	201	TRP	2.4
1	B	34	TYR	2.4
1	B	344	TYR	2.4
1	B	13	HIS	2.4
1	B	41	PHE	2.4
1	B	202	GLY	2.4
1	B	47	ASP	2.3
1	B	22	GLN	2.3
1	B	11	ILE	2.3
1	B	56	GLN	2.3
1	B	123	ASP	2.2
1	B	102	ASN	2.2
1	B	321	GLY	2.2
1	A	205	GLU	2.2
1	A	282	SER	2.2
1	B	208	ALA	2.2
1	B	4	ALA	2.1
1	B	348	ALA	2.1
1	B	242	ASP	2.1
1	B	129	SER	2.1
1	B	5	PRO	2.1
1	A	241	LEU	2.1
1	B	209	VAL	2.0
1	B	353	ALA	2.0
1	A	264	ASP	2.0
1	B	15	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
3	GTC	A	364[B]	15/15	0.64	0.26	29,29,30,31	15
3	GTC	A	362	15/15	0.68	0.19	45,47,51,51	0
3	GTC	B	1	15/15	0.68	0.21	71,71,71,72	0
2	PO4	A	363[A]	5/5	0.73	0.23	44,45,45,45	5
3	GTC	B	362	15/15	0.79	0.16	52,52,54,54	0
3	GTC	B	363	15/15	0.80	0.14	39,39,41,41	0
2	PO4	A	1	5/5	0.84	0.11	45,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.