



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:08 pm BST

PDB ID : 3GSG  
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 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.

---

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

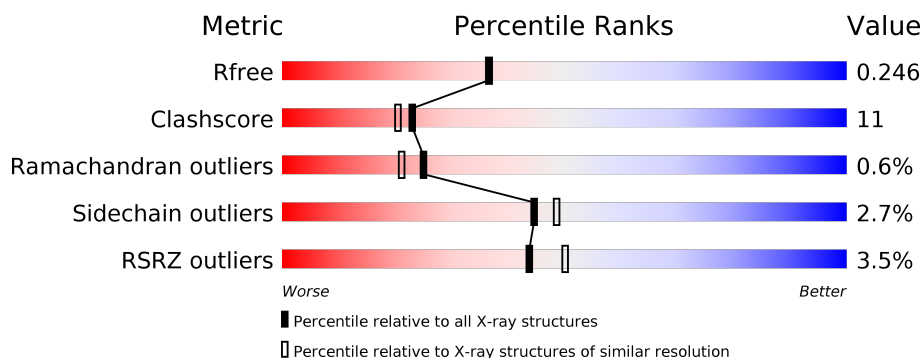
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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	358	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	358	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </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
3	DMS	A	365	-	-	X	-
3	DMS	B	362	-	-	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 (three-letter code: PO4) (formula: O<sub>4</sub>P).



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		

*Continued on next page...*

Continued from previous page...

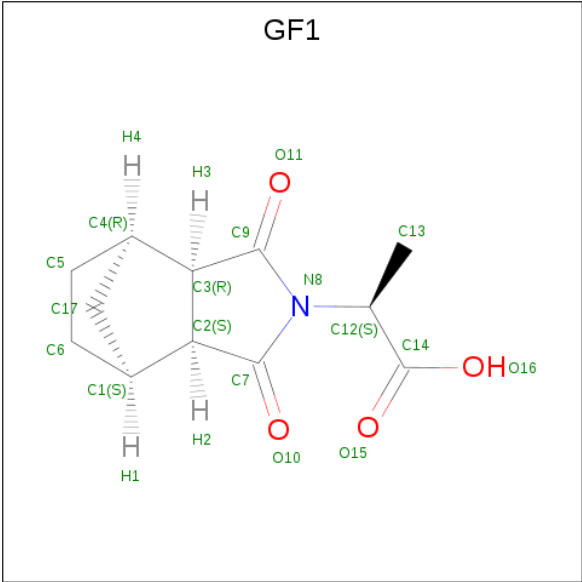
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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]propanoic acid (three-letter code: GF1) (formula:  $C_{12}H_{15}NO_4$ ).



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		

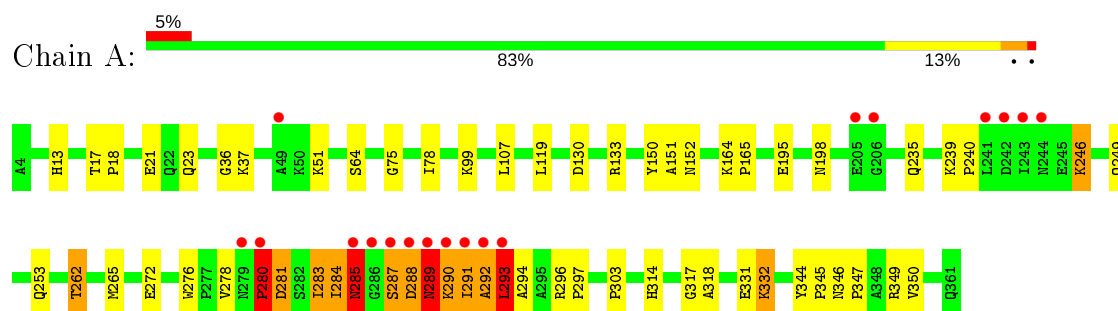
- Molecule 5 is water.

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

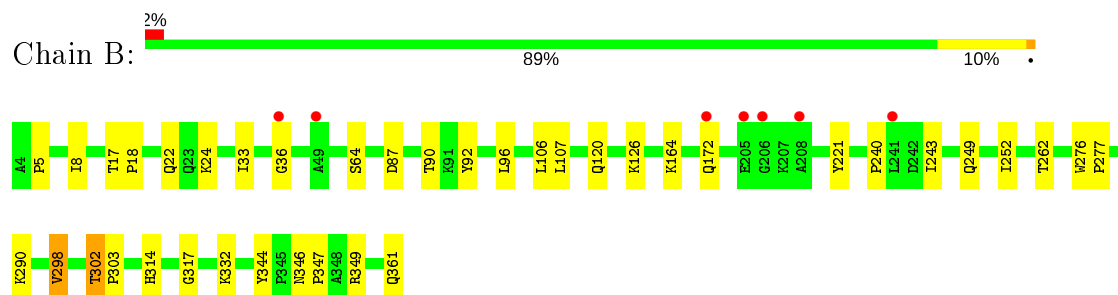
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	118.59Å 75.93Å 97.66Å 90.00° 116.37° 90.00°	Depositor
Resolution (Å)	45.27 – 2.10 45.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.27-2.10) 99.9 (45.26-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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: PO4, GF1, DMS

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	4/3089 (0.1%)	0.57	1/4218 (0.0%)
1	B	0.46	1/3152 (0.0%)	0.57	0/4301
All	All	0.48	5/6241 (0.1%)	0.57	1/8519 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	LYS	CE-NZ	9.21	1.72	1.49
1	A	332	LYS	CD-CE	-7.36	1.32	1.51
1	A	21	GLU	CG-CD	6.42	1.61	1.51
1	A	99	LYS	CG-CD	-5.28	1.34	1.52
1	B	24	LYS	CD-CE	-5.26	1.38	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	LYS	CD-CE-NZ	-6.19	97.46	111.70

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

All (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
1	A	292	ALA	Peptide
1	A	293	LEU	Peptide
1	B	36	GLY	Peptide

## 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	2886	0	2850	97	0
1	B	2906	0	2896	35	0
2	A	20	0	0	1	0
2	B	5	0	0	0	0
3	A	8	0	12	13	0
3	B	20	0	30	8	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.

All (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: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:O	3:A:365:DMS:S	1.90	1.28
1:A:291:ILE:CA	1:A:292:ALA:HB2	1.65	1.26
1:A:291:ILE:CG2	3:A:365:DMS:C1	2.20	1.20
1:A:291:ILE:CG2	3:A:365:DMS:H11	1.70	1.19
1:A:293:LEU:HD23	1:A:293:LEU:O	1.52	1.08
1:A:291:ILE:HG22	3:A:365:DMS:H12	1.10	1.07
1:A:318:ALA:H	4:A:366:GF1:H13B	1.23	1.04
1:A:291:ILE:HG22	3:A:365:DMS:H11	1.20	1.03
1:A:318:ALA:H	4:A:366:GF1:C13	1.73	1.02
1:B:120:GLN:HE22	4:B:365:GF1:H4	1.26	0.99
1:A:291:ILE:CA	1:A:292:ALA:CB	2.30	0.96
1:A:280:PRO:O	1:A:283:ILE:HG13	1.71	0.90
1:B:120:GLN:HE22	4:B:365:GF1:C4	1.86	0.88
1:A:291:ILE:HG23	3:A:365:DMS:H11	1.57	0.84
4:A:367:GF1:O10	4:A:367:GF1:H6	1.76	0.84
1:A:262[B]:THR:HG21	1:A:296:ARG:HB3	1.61	0.82
1:A:284:ILE:HD13	1:A:350:VAL:HG12	1.61	0.82
1:A:291:ILE:HA	1:A:292:ALA:HB2	0.81	0.80
1:A:318:ALA:N	4:A:366:GF1:H13B	1.97	0.80
1:A:291:ILE:HA	1:A:292:ALA:HB3	1.58	0.77
1:B:346:ASN:HD21	3:B:363:DMS:H23	1.53	0.73
1:A:246:LYS:HG2	5:A:373:HOH:O	1.88	0.72
1:A:281:ASP:H	1:A:284:ILE:HG12	1.53	0.72
1:A:291:ILE:HG23	1:A:291:ILE:O	1.89	0.72
1:A:281:ASP:N	1:A:284:ILE:HG12	2.05	0.72
1:A:291:ILE:O	3:A:365:DMS:H11	1.89	0.72
1:A:290:LYS:HE2	1:A:296:ARG:HH21	1.55	0.71
1:A:280:PRO:N	1:A:281:ASP:HB2	2.05	0.70
1:B:332:LYS:HD2	5:B:561:HOH:O	1.90	0.70
1:A:290:LYS:HB2	3:A:365:DMS:H13	1.74	0.69
1:A:291:ILE:CG2	3:A:365:DMS:H12	2.04	0.69
1:A:289:ASN:O	1:A:294:ALA:HB3	1.96	0.66
1:A:293:LEU:C	1:A:293:LEU:HD23	2.15	0.66
1:A:290:LYS:O	1:A:291:ILE:C	2.33	0.65
1:A:64:SER:OG	4:A:366:GF1:C13	2.43	0.65
1:A:318:ALA:O	4:A:366:GF1:H13B	1.96	0.65
1:A:272:GLU:OE1	1:A:288:ASP:CB	2.45	0.64
1:A:278:VAL:HG11	1:A:283:ILE:HG12	1.80	0.64
1:B:164:LYS:HE2	3:B:362:DMS:C2	2.29	0.62
1:A:280:PRO:C	1:A:284:ILE:HG12	2.20	0.61

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:H	4:A:366:GF1:H13	1.61	0.61
1:B:120:GLN:NE2	4:B:365:GF1:H4	2.08	0.61
1:A:13:HIS:HE1	5:A:572:HOH:O	1.83	0.60
1:A:164[B]:LYS:HE2	5:A:452:HOH:O	2.01	0.60
1:A:240:PRO:O	1:A:249:GLN:HG3	2.02	0.60
1:B:64:SER:HB2	1:B:317:GLY:HA2	1.84	0.60
1:A:331:GLU:HG3	1:A:332:LYS:HG3	1.84	0.59
1:A:281:ASP:H	1:A:284:ILE:CG1	2.14	0.59
1:A:291:ILE:CG2	1:A:291:ILE:O	2.51	0.58
1:B:120:GLN:HE22	4:B:365:GF1:C17	2.16	0.58
1:A:290:LYS:HE2	1:A:296:ARG:NH2	2.18	0.57
1:A:150:TYR:CB	1:A:289:ASN:HB3	2.34	0.57
1:A:150:TYR:HB3	1:A:289:ASN:HB3	1.86	0.57
1:A:36:GLY:HA2	1:A:235[B]:GLN:HE22	1.71	0.56
1:A:291:ILE:HG13	1:A:292:ALA:HB3	1.86	0.56
1:B:344:TYR:CZ	1:B:349:ARG:HG2	2.40	0.56
1:A:280:PRO:CA	1:A:281:ASP:HB2	2.37	0.55
1:A:291:ILE:N	1:A:292:ALA:HB2	2.20	0.55
1:B:87:ASP:OD2	1:B:92:TYR:OH	2.17	0.53
1:A:195:GLU:CD	5:A:826:HOH:O	2.48	0.52
1:A:290:LYS:CE	1:A:296:ARG:HH21	2.21	0.51
1:A:303:PRO:HD3	1:B:107:LEU:HD22	1.91	0.51
1:B:346:ASN:ND2	3:B:363:DMS:H23	2.24	0.51
1:A:64:SER:HB2	4:A:366:GF1:H13	1.93	0.51
1:A:284:ILE:HD13	1:A:350:VAL:CG1	2.36	0.51
1:B:221:TYR:CD2	4:B:365:GF1:H5A	2.46	0.50
1:A:17:THR:HB	1:A:18:PRO:HD3	1.93	0.50
1:A:291:ILE:HG22	3:A:365:DMS:S	2.44	0.50
1:B:120:GLN:NE2	4:B:365:GF1:C17	2.74	0.50
1:B:164:LYS:HE2	3:B:362:DMS:H23	1.93	0.49
1:B:346:ASN:ND2	3:B:363:DMS:C2	2.75	0.49
1:B:5:PRO:HD2	1:B:8:ILE:HD12	1.93	0.49
1:A:13:HIS:CE1	5:A:572:HOH:O	2.61	0.49
1:A:262[B]:THR:HG21	1:A:296:ARG:CB	2.37	0.49
1:A:198:ASN:HB2	5:A:826:HOH:O	2.11	0.49
1:B:17:THR:HB	1:B:18:PRO:HD3	1.95	0.49
1:A:130:ASP:OD1	1:A:133[B]:ARG:NH2	2.46	0.49
1:A:164[B]:LYS:HB2	1:A:165:PRO:HD3	1.95	0.49
1:A:64:SER:CB	4:A:366:GF1:H13	2.42	0.49
1:A:107:LEU:HD22	1:B:303:PRO:HD3	1.95	0.49
1:A:290:LYS:O	1:A:291:ILE:O	2.30	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243[A]:ILE:CD1	1:B:252:ILE:HD12	2.43	0.49
1:B:164:LYS:HE2	3:B:362:DMS:H21	1.95	0.48
1:B:346:ASN:HD21	3:B:363:DMS:C2	2.24	0.48
4:A:367:GF1:O10	4:A:367:GF1:O16	2.31	0.48
1:A:347:PRO:HG3	3:A:365:DMS:C2	2.43	0.48
1:A:64:SER:OG	4:A:366:GF1:C12	2.61	0.48
1:B:126:LYS:HG3	5:B:554:HOH:O	2.14	0.48
1:A:280:PRO:HB2	1:A:281:ASP:OD1	2.12	0.48
1:A:344:TYR:CE1	1:A:349:ARG:HG2	2.48	0.48
1:B:240:PRO:O	1:B:249:GLN:HG3	2.14	0.47
1:A:280:PRO:CD	1:A:281:ASP:HB2	2.44	0.47
1:B:262[B]:THR:CG2	1:B:298:VAL:HG12	2.45	0.47
1:A:262[B]:THR:HG23	1:A:297:PRO:O	2.14	0.47
1:A:262[A]:THR:HG23	1:A:265[A]:MET:HG3	1.97	0.46
1:A:64:SER:OG	4:A:366:GF1:H13A	2.15	0.46
1:A:290:LYS:CG	1:A:296:ARG:HH21	2.29	0.46
1:A:290:LYS:HE3	5:A:794:HOH:O	2.15	0.46
1:B:92:TYR:CE1	1:B:106:LEU:HD11	2.49	0.46
1:A:289:ASN:O	1:A:294:ALA:CB	2.63	0.45
1:B:22:GLN:HG3	5:B:700:HOH:O	2.17	0.45
1:A:262[A]:THR:CG2	1:A:265[A]:MET:SD	3.05	0.45
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.52	0.45
1:A:344:TYR:CZ	1:A:349:ARG:HG2	2.52	0.44
1:B:221:TYR:CG	4:B:365:GF1:H5A	2.52	0.44
1:A:290:LYS:HG2	1:A:296:ARG:NH2	2.32	0.44
1:A:152[B]:ASN:ND2	4:A:366:GF1:H4	2.33	0.44
1:A:23:GLN:NE2	1:A:345:PRO:HD2	2.33	0.44
1:B:90[B]:THR:HG22	1:B:96:LEU:O	2.18	0.43
1:A:165:PRO:HB3	2:A:362:PO4:O2	2.18	0.43
1:A:317:GLY:HA2	4:A:366:GF1:H13	2.01	0.42
1:A:75:GLY:HA2	1:A:78:ILE:HD12	2.01	0.42
1:A:318:ALA:CA	4:A:366:GF1:H13B	2.49	0.42
1:A:318:ALA:O	4:A:366:GF1:C13	2.66	0.42
1:A:276:TRP:HE3	1:A:278:VAL:HG23	1.85	0.42
1:A:284:ILE:O	1:A:285:ASN:C	2.58	0.42
1:A:262[A]:THR:HG23	1:A:265[A]:MET:SD	2.60	0.41
1:A:346[A]:ASN:ND2	3:A:365:DMS:O	2.49	0.41
1:A:119:LEU:HA	1:A:151:ALA:HA	2.02	0.41
1:A:64:SER:H	4:A:366:GF1:C13	2.33	0.41
1:B:262[B]:THR:HG22	1:B:298:VAL:HG12	2.03	0.41
1:A:280:PRO:CB	1:A:281:ASP:HB2	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:THR:HG22	5:B:603:HOH:O	2.21	0.41
1:B:346:ASN:HB2	1:B:347:PRO:HD3	2.03	0.41
1:B:164:LYS:CE	3:B:362:DMS:H21	2.50	0.41
1:A:284:ILE:CD1	1:A:350:VAL:HG12	2.39	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	383/358 (107%)	369 (96%)	10 (3%)	4 (1%)	15	11
1	B	388/358 (108%)	379 (98%)	9 (2%)	0	100	100
All	All	771/716 (108%)	748 (97%)	19 (2%)	4 (0%)	25	26

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%)	305 (96%)	11 (4%)	36	38
1	B	324/292 (111%)	318 (98%)	6 (2%)	57	63
All	All	640/584 (110%)	623 (97%)	17 (3%)	44	48

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	LYS
1	A	246	LYS
1	A	262[A]	THR
1	A	262[B]	THR
1	A	281	ASP
1	A	283	ILE
1	A	287	SER
1	A	289	ASN
1	A	290	LYS
1	A	293	LEU
1	A	314	HIS
1	B	172	GLN
1	B	290[B]	LYS
1	B	298	VAL
1	B	302	THR
1	B	314	HIS
1	B	361	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	23	GLN
1	A	35	GLN
1	A	190	ASN
1	A	253	GLN
1	A	289	ASN
1	B	6	GLN
1	B	23	GLN
1	B	120	GLN
1	B	137	ASN
1	B	244	ASN
1	B	285	ASN
1	B	346	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 ⓘ

There are no carbohydrates 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
3	DMS	B	364	-	3,3,3	2.68	1 (33%)	3,3,3	0.77	0
3	DMS	B	363	-	3,3,3	2.68	1 (33%)	3,3,3	0.38	0
2	PO4	A	362	-	4,4,4	0.87	0	6,6,6	0.49	0
3	DMS	A	365	-	3,3,3	3.85	2 (66%)	3,3,3	1.66	0
2	PO4	A	1	-	4,4,4	0.93	0	6,6,6	0.59	0
4	GF1	A	366	-	16,19,19	1.54	3 (18%)	27,30,30	4.83	19 (70%)
2	PO4	A	363	-	4,4,4	0.81	0	6,6,6	0.40	0
3	DMS	B	366	-	3,3,3	3.12	1 (33%)	3,3,3	0.99	0
4	GF1	A	367	-	16,19,19	2.23	9 (56%)	27,30,30	4.67	14 (51%)
3	DMS	B	362	-	3,3,3	2.60	1 (33%)	3,3,3	0.67	0
3	DMS	A	364	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMS	B	1	-	3,3,3	2.57	1 (33%)	3,3,3	0.64	0
2	PO4	B	3	-	4,4,4	0.82	0	6,6,6	0.48	0
4	GF1	B	365	-	16,19,19	2.27	6 (37%)	27,30,30	2.22	14 (51%)
2	PO4	A	2	-	4,4,4	0.87	0	6,6,6	0.52	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
4	GF1	A	367	-	1/1/9/9	4/4/45/45	0/4/3/3
4	GF1	A	366	-	3/3/9/9	0/4/45/45	0/4/3/3
4	GF1	B	365	-	3/3/9/9	0/4/45/45	0/4/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	365	DMS	O-S	5.98	1.90	1.50
3	B	366	DMS	O-S	4.87	1.83	1.50
4	B	365	GF1	C13-C12	4.73	1.63	1.52
3	A	364	DMS	O-S	4.57	1.81	1.50
3	B	363	DMS	O-S	4.53	1.80	1.50
3	B	364	DMS	O-S	4.48	1.80	1.50
3	B	362	DMS	O-S	4.35	1.79	1.50
3	B	1	DMS	O-S	4.29	1.79	1.50
4	A	367	GF1	C7-N8	-4.16	1.31	1.39
4	A	366	GF1	C9-N8	-4.13	1.32	1.39
4	A	367	GF1	C2-C1	-3.89	1.47	1.54
4	B	365	GF1	C7-N8	-3.61	1.32	1.39
4	B	365	GF1	C9-N8	-3.50	1.33	1.39
4	B	365	GF1	C3-C2	-3.15	1.47	1.55
4	B	365	GF1	C12-N8	-3.06	1.44	1.49
4	A	367	GF1	C9-N8	-2.98	1.34	1.39
3	A	365	DMS	C2-S	2.86	1.97	1.75
4	B	365	GF1	C3-C4	-2.57	1.50	1.54
4	A	367	GF1	O10-C7	2.55	1.26	1.22
4	A	367	GF1	C6-C1	-2.37	1.47	1.53
4	A	366	GF1	C3-C2	-2.35	1.49	1.55
4	A	366	GF1	C3-C4	-2.17	1.50	1.54
4	A	367	GF1	C12-N8	-2.13	1.46	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	367	GF1	C5-C6	2.10	1.59	1.54
4	A	367	GF1	C3-C4	2.06	1.58	1.54
4	A	367	GF1	C2-C7	2.05	1.54	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	367	GF1	C6-C1-C2	15.01	129.70	108.13
4	A	366	GF1	C14-C12-N8	14.47	127.78	111.05
4	A	367	GF1	C1-C2-C7	-13.20	92.10	115.64
4	A	366	GF1	C3-C2-C7	-8.20	97.69	104.87
4	A	366	GF1	C1-C2-C7	8.19	130.23	115.64
4	A	366	GF1	C2-C3-C4	7.80	113.14	103.19
4	A	366	GF1	C5-C4-C3	-6.86	98.26	108.13
4	A	367	GF1	C3-C2-C7	-6.57	99.11	104.87
4	A	366	GF1	C12-N8-C7	5.71	134.29	123.07
4	A	367	GF1	C5-C6-C1	-5.46	94.10	103.49
4	A	367	GF1	C14-C12-N8	4.83	116.64	111.05
4	A	366	GF1	C3-C2-C1	-4.75	97.13	103.19
4	B	365	GF1	C3-C2-C7	-4.35	101.06	104.87
4	B	365	GF1	C1-C2-C7	3.81	122.43	115.64
4	A	366	GF1	C9-N8-C7	-3.79	107.73	112.66
4	A	367	GF1	C6-C5-C4	3.66	109.80	103.49
4	A	366	GF1	C2-C3-C9	3.64	108.06	104.87
4	B	365	GF1	C14-C12-N8	3.58	115.19	111.05
4	A	367	GF1	C5-C4-C3	3.57	113.27	108.13
4	B	365	GF1	C2-C3-C9	3.35	107.80	104.87
4	A	367	GF1	C2-C3-C9	-3.33	101.95	104.87
4	A	367	GF1	C17-C4-C5	-3.32	94.40	101.30
4	A	367	GF1	C17-C1-C2	-3.28	96.06	101.94
4	A	366	GF1	C12-N8-C9	-3.25	116.69	123.07
4	A	366	GF1	C13-C12-N8	-3.22	106.48	111.00
4	A	366	GF1	C6-C5-C4	-3.16	98.05	103.49
4	A	366	GF1	C13-C12-C14	-3.15	104.38	113.54
4	A	366	GF1	O10-C7-C2	-3.13	123.96	127.52
4	B	365	GF1	C12-N8-C9	2.93	128.84	123.07
4	A	366	GF1	C3-C9-N8	-2.91	104.44	108.50
4	B	365	GF1	C2-C3-C4	2.78	106.73	103.19
4	A	366	GF1	C17-C1-C6	-2.76	95.57	101.30
4	B	365	GF1	C13-C12-N8	2.72	114.82	111.00
4	B	365	GF1	C12-N8-C7	-2.70	117.77	123.07
4	B	365	GF1	O11-C9-C3	-2.67	124.49	127.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	365	GF1	O11-C9-N8	2.66	129.28	124.83
4	B	365	GF1	C5-C4-C3	-2.54	104.47	108.13
4	A	367	GF1	C9-N8-C7	-2.46	109.46	112.66
4	A	366	GF1	O11-C9-N8	2.46	128.93	124.83
4	A	366	GF1	C5-C6-C1	2.44	107.69	103.49
4	A	367	GF1	C17-C4-C3	-2.24	97.92	101.94
4	A	367	GF1	C13-C12-N8	-2.21	107.90	111.00
4	B	365	GF1	C6-C5-C4	-2.18	99.73	103.49
4	A	366	GF1	C17-C1-C2	2.18	105.85	101.94
4	B	365	GF1	C4-C3-C9	-2.11	111.87	115.64
4	A	367	GF1	C13-C12-C14	-2.03	107.64	113.54
4	B	365	GF1	O10-C7-C2	-2.00	125.24	127.52

All (7) chirality outliers are listed below:

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

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	367	GF1	C14-C12-N8-C7
4	A	367	GF1	C14-C12-N8-C9
4	A	367	GF1	C13-C12-N8-C9
4	A	367	GF1	C13-C12-N8-C7

There are no ring outliers.

7 monomers are involved in 46 short contacts:

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	362	DMS	4	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 ⓘ

### 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	358/358 (100%)	0.06	18 (5%) 28 34	15, 22, 36, 46	20 (5%)
1	B	358/358 (100%)	-0.02	7 (1%) 65 69	15, 23, 34, 40	17 (4%)
All	All	716/716 (100%)	0.02	25 (3%) 44 50	15, 23, 35, 46	37 (5%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	6.6
1	A	287	SER	4.9
1	A	290	LYS	4.9
1	A	241	LEU	4.7
1	A	49	ALA	4.5
1	B	241	LEU	4.3
1	A	292	ALA	4.2
1	B	206	GLY	3.8
1	A	289	ASN	3.7
1	B	49	ALA	3.7
1	B	205	GLU	3.5
1	A	293	LEU	3.3
1	B	36	GLY	3.3
1	A	291	ILE	3.3
1	B	172	GLN	3.1
1	A	206	GLY	3.0
1	A	285	ASN	2.8
1	B	208	ALA	2.8
1	A	286	GLY	2.7
1	A	280	PRO	2.6
1	A	243	ILE	2.6
1	A	205	GLU	2.4
1	A	242	ASP	2.4
1	A	244	ASN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	279	ASN	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. 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(Å <sup>2</sup> )	Q<0.9
4	GF1	A	367	17/17	0.62	0.31	35,37,38,38	17
3	DMS	A	365	4/4	0.65	0.33	32,32,32,33	1
4	GF1	A	366	17/17	0.69	0.30	31,33,34,34	13
2	PO4	A	362	5/5	0.77	0.29	34,34,34,35	5
2	PO4	B	3	5/5	0.80	0.27	43,43,44,44	5
3	DMS	B	362	4/4	0.81	0.28	38,38,38,39	0
4	GF1	B	365	17/17	0.82	0.21	31,32,33,33	2
3	DMS	B	366	4/4	0.83	0.22	36,36,36,37	4
3	DMS	B	363	4/4	0.84	0.27	26,27,27,27	4
3	DMS	A	364	4/4	0.85	0.23	30,31,31,32	4
2	PO4	A	363	5/5	0.88	0.43	49,49,50,50	5
2	PO4	A	1	5/5	0.90	0.20	43,44,44,44	5
2	PO4	A	2	5/5	0.90	0.41	49,50,50,50	0
3	DMS	B	364	4/4	0.91	0.16	32,32,33,33	4
3	DMS	B	1	4/4	0.96	0.13	32,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.