



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2014 – 04:39 PM EDT

PDB ID : 4URM  
Title : Crystal Structure of Staph GyraseB 24kDa in complex with Kibdelomycin  
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Deposited on : 2014-06-30  
Resolution : 2.94 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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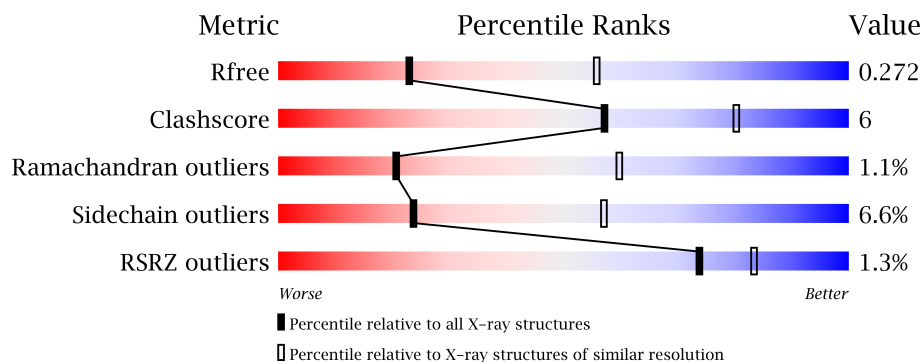
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.94 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))
$R_{free}$	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	231	
1	B	231	
1	C	231	
1	D	231	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6149 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

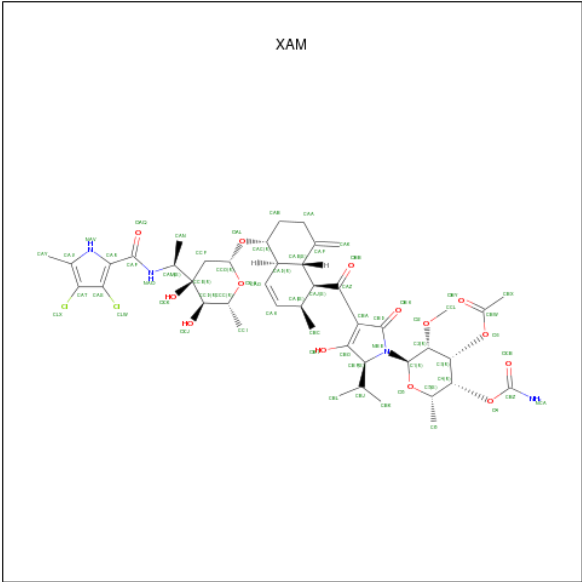
- Molecule 1 is a protein called DNA GYRASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1484	932	261	290	1			
1	B	195	Total	C	N	O		0	0	0
			1486	933	262	291				
1	C	191	Total	C	N	O	S	0	0	0
			1451	911	253	286	1			
1	D	190	Total	C	N	O		0	0	0
			1454	916	252	286				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	VAL	CONFLICT	UNP P0A0K8
B	28	ALA	VAL	CONFLICT	UNP P0A0K8
C	28	ALA	VAL	CONFLICT	UNP P0A0K8
D	28	ALA	VAL	CONFLICT	UNP P0A0K8

- Molecule 2 is (1R,4AS,5S,6S,8AR)-5-[[[(5S)-1-(3-O-ACETYL-4-O-CARBAMOYL-6-DEOXY-2-O-METHYL-ALPHA-L-TALOPYRANOSYL)-4-HYDROXY-2-OXO-5-(PROPAN-2-YL)-2,5-DIHYDRO-1H-PYRROL-3-YL]CARBONYL]-6-METHYL-4-METHYLIDENE-1,2,3,4,4A,5,6,8A-OCTAHYDRONAPHTHALEN-1-YL2,6-DIDEOXY-3-C-[(1S)-1-[(3,4-DICHLORO-5-METHYL-1H-PYRROL-2-YL)CARBONYL]AMINO}ETHYL]-BETA-D-RIBO-H EXOPYRANOSIDE (three-letter code: XAM) (formula: C<sub>44</sub>H<sub>60</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			64	44	2	4	14		
2	B	1	Total	C	Cl	N	O	0	0
			64	44	2	4	14		
2	C	1	Total	C	Cl	N	O	0	0
			64	44	2	4	14		
2	D	1	Total	C	Cl	N	O	0	0
			64	44	2	4	14		

- Molecule 3 is water.

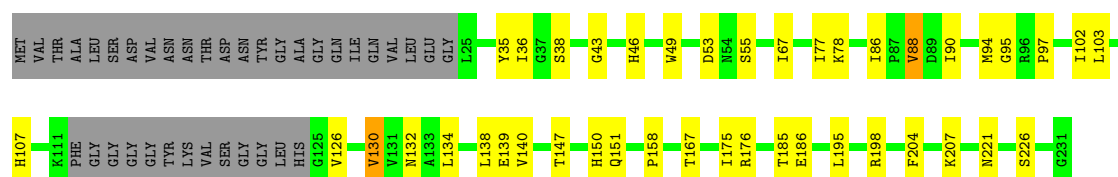
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	5	Total	O	0	0
			5	5		
3	C	3	Total	O	0	0
			3	3		
3	D	5	Total	O	0	0
			5	5		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

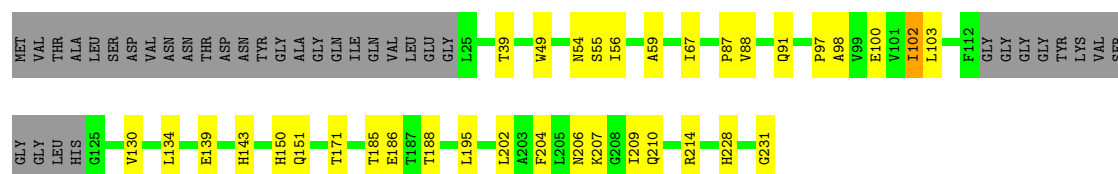
#### • Molecule 1: DNA GYRASE SUBUNIT B

Chain A:



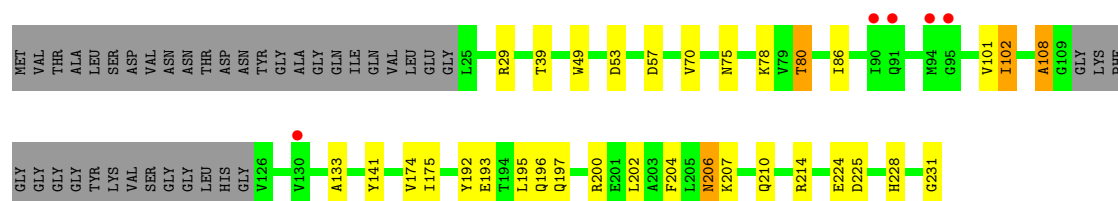
#### • Molecule 1: DNA GYRASE SUBUNIT B

Chain B:



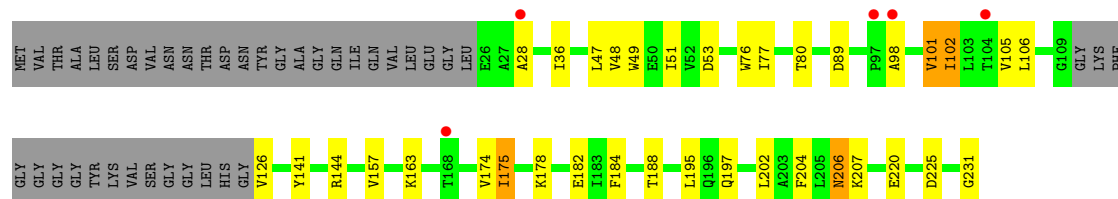
#### • Molecule 1: DNA GYRASE SUBUNIT B

Chain C:



#### • Molecule 1: DNA GYRASE SUBUNIT B

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.28Å 75.55Å 90.45Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	30.44 – 2.94 30.15 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.44-2.94) 99.6 (30.15-2.94)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.195 , 0.256 0.206 , 0.272	Depositor DCC
$R_{free}$ test set	1012 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.3	EDS
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20004 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6149	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAM

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	0/1509	0.78	0/2052
1	B	0.59	0/1511	0.77	0/2056
1	C	0.56	0/1475	0.72	0/2008
1	D	0.55	0/1479	0.74	0/2014
All	All	0.57	0/5974	0.76	0/8130

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1484	0	1402	21	0
1	B	1486	0	1397	18	0
1	C	1451	0	1359	20	0
1	D	1454	0	1368	16	0
2	A	64	0	0	0	0
2	B	64	0	0	2	0
2	C	64	0	0	2	0
2	D	64	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	0	0
All	All	6149	0	5526	74	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (74) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:202:LEU:O	1:C:206:ASN:ND2	1.96	0.99
1:D:202:LEU:O	1:D:206:ASN:ND2	2.03	0.92
1:C:29:ARG:NH1	1:C:133:ALA:O	2.09	0.84
1:D:204:PHE:O	1:D:207:LYS:HE2	1.76	0.83
1:B:49:TRP:HH2	1:B:195:LEU:HA	1.49	0.75
1:C:80:THR:HG23	1:C:174:VAL:HG22	1.75	0.68
1:A:221:ASN:HD21	1:C:200:ARG:HE	1.41	0.68
1:C:204:PHE:O	1:C:207:LYS:HE2	1.96	0.65
1:A:204:PHE:O	1:A:207:LYS:HE2	1.97	0.64
1:B:206:ASN:HB2	1:B:209:ILE:HD11	1.81	0.63
1:D:141:TYR:HB2	1:D:174:VAL:HB	1.81	0.62
1:A:49:TRP:CH2	1:A:198:ARG:HB3	2.36	0.61
1:A:77:ILE:O	1:A:176:ARG:HA	2.03	0.59
1:C:49:TRP:HH2	1:C:195:LEU:HA	1.68	0.58
1:C:210:GLN:HG3	1:C:228:HIS:HB2	1.85	0.57
1:B:102:ILE:HD12	1:B:103:LEU:HG	1.86	0.57
1:C:141:TYR:HB2	1:C:174:VAL:HB	1.86	0.57
1:A:151:GLN:NE2	1:A:158:PRO:HB3	2.20	0.56
1:B:56:ILE:HD13	1:B:202:LEU:HD22	1.86	0.56
1:B:143:HIS:O	1:B:171:THR:HA	2.04	0.56
1:B:49:TRP:CH2	1:B:195:LEU:HA	2.37	0.56
1:A:151:GLN:HE21	1:A:158:PRO:HB3	1.70	0.55
1:B:100:GLU:HG3	1:B:151:GLN:HE22	1.70	0.55
1:C:175:ILE:HD12	2:C:2000:XAM:CLX	2.43	0.54
1:C:207:LYS:HD2	1:C:231:GLY:HA2	1.90	0.52
1:A:35:TYR:HE1	1:A:107:HIS:CE1	2.26	0.52
1:D:28:ALA:HB2	1:D:106:LEU:HD21	1.90	0.52
1:A:88:VAL:O	1:A:97:PRO:HB3	2.09	0.52
1:D:49:TRP:HH2	1:D:195:LEU:HA	1.75	0.52
1:B:55:SER:HB3	1:B:67:ILE:HG12	1.91	0.52
1:D:47:LEU:HD11	1:D:184:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2000:XAM:CAH	1:C:200:ARG:HH12	2.24	0.51
1:B:87:PRO:O	1:B:98:ALA:HB3	2.10	0.51
1:B:139:GLU:HG2	1:B:150:HIS:HE1	1.77	0.50
1:C:49:TRP:CH2	1:C:195:LEU:HD23	2.47	0.50
1:A:90:ILE:HG23	1:A:95:GLY:O	2.12	0.49
1:D:80:THR:HG23	1:D:174:VAL:HG22	1.94	0.49
1:D:175:ILE:HD13	2:D:2000:XAM:CLX	2.49	0.49
1:A:78:LYS:HG3	1:A:176:ARG:HG2	1.95	0.48
1:B:210:GLN:HG3	1:B:228:HIS:HB2	1.96	0.48
1:C:70:VAL:HB	1:C:78:LYS:HB3	1.95	0.48
1:C:192:TYR:HE1	1:C:196:GLN:NE2	2.12	0.48
1:A:102:ILE:HD12	1:A:103:LEU:HG	1.94	0.47
1:C:175:ILE:CD1	2:C:2000:XAM:CLX	3.00	0.46
1:D:49:TRP:CH2	1:D:195:LEU:HA	2.51	0.46
1:A:126:VAL:HG22	1:A:130:VAL:HG11	1.97	0.45
1:A:55:SER:HB3	1:A:67:ILE:HG12	1.99	0.45
1:B:206:ASN:CB	1:B:209:ILE:HD11	2.46	0.45
1:C:102:ILE:HG22	1:C:108:ALA:HB3	1.99	0.45
1:D:206:ASN:N	1:D:206:ASN:ND2	2.63	0.45
1:A:147:THR:HG22	1:A:167:THR:HG22	1.98	0.45
1:B:207:LYS:NZ	1:B:231:GLY:O	2.49	0.45
1:D:102:ILE:HG13	1:D:102:ILE:H	1.62	0.44
1:A:86:ILE:HG21	1:A:102:ILE:HD11	1.99	0.44
1:C:86:ILE:HG23	1:C:102:ILE:HD11	1.99	0.44
1:D:101:VAL:O	1:D:105:VAL:HG12	2.18	0.44
1:D:48:VAL:HG22	1:D:77:ILE:HG21	2.00	0.44
1:A:49:TRP:HH2	1:A:195:LEU:HA	1.84	0.43
1:A:139:GLU:HG2	1:A:150:HIS:HE1	1.83	0.43
1:D:207:LYS:NZ	1:D:231:GLY:O	2.40	0.43
1:A:132:ASN:HA	1:A:138:LEU:HD13	2.00	0.43
1:B:204:PHE:O	1:B:207:LYS:HE2	2.19	0.43
1:C:214:ARG:HG2	1:C:224:GLU:HG3	2.01	0.42
1:A:46:HIS:HA	1:A:49:TRP:CD1	2.54	0.42
1:B:59:ALA:HB1	1:B:209:ILE:HG21	2.02	0.41
1:B:54:ASN:HB3	2:B:2000:XAM:CAS	2.50	0.41
1:A:140:VAL:O	1:A:150:HIS:HA	2.20	0.41
1:A:38:SER:O	1:A:43:GLY:HA3	2.19	0.41
1:B:206:ASN:O	1:B:209:ILE:HG12	2.20	0.41
1:C:192:TYR:HE1	1:C:196:GLN:HE21	1.69	0.41
1:B:88:VAL:O	1:B:97:PRO:HB3	2.21	0.41
1:D:51:ILE:HD12	1:D:175:ILE:HG21	2.03	0.40
1:C:193:GLU:HA	1:C:196:GLN:HG2	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:76:TRP:CE2	1:D:178:LYS:HB2	2.57	0.40

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	190/231 (82%)	178 (94%)	11 (6%)	1 (0%)	38	78
1	B	191/231 (83%)	180 (94%)	10 (5%)	1 (0%)	38	78
1	C	187/231 (81%)	173 (92%)	11 (6%)	3 (2%)	14	47
1	D	186/231 (80%)	171 (92%)	12 (6%)	3 (2%)	14	47
All	All	754/924 (82%)	702 (93%)	44 (6%)	8 (1%)	21	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU
1	B	186	GLU
1	D	89	ASP
1	C	108	ALA
1	C	75	ASN
1	D	98	ALA
1	D	101	VAL
1	C	101	VAL

### 5.3.2 Protein sidechains ⓘ

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	150/192 (78%)	141 (94%)	9 (6%)	27	63
1	B	149/192 (78%)	141 (95%)	8 (5%)	31	68
1	C	146/192 (76%)	138 (94%)	8 (6%)	30	67
1	D	147/192 (77%)	133 (90%)	14 (10%)	12	35
All	All	592/768 (77%)	553 (93%)	39 (7%)	24	57

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	53	ASP
1	A	88	VAL
1	A	94	MET
1	A	130	VAL
1	A	134	LEU
1	A	175	ILE
1	A	185	THR
1	A	226	SER
1	B	39	THR
1	B	91	GLN
1	B	102	ILE
1	B	130	VAL
1	B	134	LEU
1	B	185	THR
1	B	188	THR
1	B	214	ARG
1	C	39	THR
1	C	53	ASP
1	C	57	ASP
1	C	80	THR
1	C	102	ILE
1	C	197	GLN
1	C	206	ASN
1	C	225	ASP
1	D	36	ILE
1	D	53	ASP
1	D	102	ILE
1	D	126	VAL
1	D	144	ARG
1	D	157	VAL
1	D	163	LYS
1	D	175	ILE

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Mol	Chain	Res	Type
1	D	182	GLU
1	D	188	THR
1	D	197	GLN
1	D	206	ASN
1	D	220	GLU
1	D	225	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	143	HIS
1	A	221	ASN
1	B	136	GLN
1	B	143	HIS
1	B	151	GLN
1	C	196	GLN
1	D	159	GLN
1	D	196	GLN
1	D	210	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	XAM	A	2000	-	69,69,69	1.62	10 (14%)	106,106,106	1.74	22 (20%)
2	XAM	B	2000	-	69,69,69	1.62	13 (18%)	106,106,106	1.71	19 (17%)
2	XAM	C	2000	-	69,69,69	1.71	10 (14%)	106,106,106	1.76	22 (20%)
2	XAM	D	2000	-	69,69,69	1.70	11 (15%)	106,106,106	1.72	20 (18%)

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
2	XAM	A	2000	-	-	2/38/133/133	0/6/6/6
2	XAM	B	2000	-	-	2/38/133/133	0/6/6/6
2	XAM	C	2000	-	-	2/38/133/133	0/6/6/6
2	XAM	D	2000	-	-	2/38/133/133	0/6/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2000	XAM	OBB-CAZ	7.73	1.36	1.22
2	B	2000	XAM	OBB-CAZ	7.72	1.36	1.22
2	A	2000	XAM	OBB-CAZ	7.69	1.36	1.22
2	D	2000	XAM	OBB-CAZ	6.93	1.34	1.22
2	D	2000	XAM	CCE-CCD	5.67	1.63	1.54
2	C	2000	XAM	CCE-CCD	5.04	1.62	1.54
2	D	2000	XAM	C1-NBE	4.88	1.55	1.44
2	C	2000	XAM	C1-NBE	4.77	1.55	1.44
2	A	2000	XAM	CBA-CBG	4.24	1.46	1.36
2	C	2000	XAM	CBA-CBG	4.08	1.46	1.36
2	B	2000	XAM	CBA-CAZ	-4.03	1.37	1.46
2	B	2000	XAM	CBA-CBG	3.96	1.46	1.36
2	D	2000	XAM	CBA-CBG	3.92	1.45	1.36
2	A	2000	XAM	CBA-CAZ	-3.90	1.37	1.46
2	A	2000	XAM	CCE-CCD	3.86	1.60	1.54
2	B	2000	XAM	CCE-CCD	3.61	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2000	XAM	CBD-NBE	3.61	1.44	1.36
2	A	2000	XAM	O4-CBZ	3.49	1.41	1.35
2	D	2000	XAM	CBD-NBE	3.45	1.44	1.36
2	B	2000	XAM	CBF-CBG	3.41	1.57	1.51
2	B	2000	XAM	OBI-CBG	-3.40	1.22	1.33
2	D	2000	XAM	OBI-CBG	-3.40	1.22	1.33
2	A	2000	XAM	OBI-CBG	-3.34	1.22	1.33
2	C	2000	XAM	OBI-CBG	-3.33	1.22	1.33
2	C	2000	XAM	CAJ-CAZ	3.25	1.57	1.50
2	A	2000	XAM	CBF-CBG	3.22	1.57	1.51
2	B	2000	XAM	C1-NBE	3.21	1.51	1.44
2	D	2000	XAM	CBA-CAZ	-3.21	1.39	1.46
2	A	2000	XAM	CAJ-CAZ	3.11	1.57	1.50
2	C	2000	XAM	CBF-CBG	2.96	1.56	1.51
2	B	2000	XAM	CAJ-CAZ	2.94	1.57	1.50
2	C	2000	XAM	O4-CBZ	2.90	1.40	1.35
2	B	2000	XAM	CAS-CAT	2.86	1.45	1.36
2	D	2000	XAM	CAS-CAT	2.80	1.44	1.36
2	D	2000	XAM	CAJ-CAZ	2.73	1.56	1.50
2	D	2000	XAM	O4-CBZ	2.69	1.40	1.35
2	A	2000	XAM	C1-NBE	2.66	1.50	1.44
2	B	2000	XAM	CCE-CAM	2.55	1.62	1.55
2	C	2000	XAM	CBA-CAZ	-2.46	1.41	1.46
2	B	2000	XAM	CBD-NBE	2.37	1.41	1.36
2	D	2000	XAM	CBF-CBG	2.29	1.55	1.51
2	B	2000	XAM	O4-CBZ	2.11	1.39	1.35
2	B	2000	XAM	CAM-NAO	2.02	1.51	1.46
2	A	2000	XAM	CBD-NBE	2.00	1.41	1.36

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	XAM	C5-O5-C1	7.31	122.22	112.53
2	D	2000	XAM	CBG-CBF-NBE	7.00	104.44	101.32
2	B	2000	XAM	C5-O5-C1	6.91	121.70	112.53
2	C	2000	XAM	CBG-CBF-NBE	6.44	104.19	101.32
2	D	2000	XAM	C5-O5-C1	6.30	120.89	112.53
2	C	2000	XAM	C5-O5-C1	6.23	120.79	112.53
2	B	2000	XAM	CAS-CAR-CAP	5.41	134.65	124.14
2	C	2000	XAM	O4-CBZ-OCB	-5.12	119.46	124.26
2	A	2000	XAM	CAS-CAR-CAP	4.98	133.82	124.14
2	A	2000	XAM	CAU-CAT-CLX	4.82	131.70	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2000	XAM	C4-O4-CBZ	4.58	123.56	117.03
2	D	2000	XAM	C4-O4-CBZ	4.44	123.36	117.03
2	A	2000	XAM	O4-CBZ-OCB	-4.38	120.15	124.26
2	A	2000	XAM	O2-C2-C1	4.32	117.39	108.60
2	C	2000	XAM	CAS-CAR-CAP	4.32	132.53	124.14
2	A	2000	XAM	C4-O4-CBZ	4.15	122.95	117.03
2	B	2000	XAM	CAT-CAU-NAV	4.10	108.91	106.55
2	D	2000	XAM	CAT-CAU-NAV	3.97	108.83	106.55
2	A	2000	XAM	OCK-CCE-CAM	-3.92	104.03	109.87
2	B	2000	XAM	O4-CBZ-OCB	-3.85	120.65	124.26
2	B	2000	XAM	CAU-CAT-CLX	3.83	130.51	125.90
2	B	2000	XAM	OCK-CCE-CAM	-3.73	104.32	109.87
2	D	2000	XAM	O4-CBZ-OCB	-3.71	120.78	124.26
2	C	2000	XAM	CAU-CAT-CLX	3.68	130.33	125.90
2	B	2000	XAM	C4-O4-CBZ	3.48	121.99	117.03
2	D	2000	XAM	CAS-CAR-CAP	3.41	130.78	124.14
2	B	2000	XAM	O5-C1-NBE	-3.40	105.28	108.23
2	C	2000	XAM	O5-C1-NBE	-3.39	105.28	108.23
2	B	2000	XAM	CAM-NAO-CAP	3.37	127.62	123.47
2	D	2000	XAM	CAU-CAT-CLX	3.33	129.91	125.90
2	D	2000	XAM	OCK-CCE-CAM	-3.27	104.99	109.87
2	B	2000	XAM	C2-C1-NBE	3.10	117.63	113.61
2	D	2000	XAM	CBJ-CBF-NBE	3.03	119.27	113.72
2	B	2000	XAM	OCJ-CCD-CCE	-3.00	101.88	109.51
2	A	2000	XAM	C2-C1-NBE	2.92	117.40	113.61
2	A	2000	XAM	CAT-CAU-NAV	2.83	108.18	106.55
2	D	2000	XAM	CBF-CBG-CBA	-2.82	107.76	113.21
2	C	2000	XAM	OBB-CAZ-CBA	-2.81	116.10	119.96
2	C	2000	XAM	CBF-CBG-CBA	-2.80	107.81	113.21
2	C	2000	XAM	CCE-CAM-NAO	-2.79	109.03	111.35
2	D	2000	XAM	OBB-CAZ-CBA	-2.77	116.16	119.96
2	C	2000	XAM	CCF-CCE-CCD	2.75	113.69	110.27
2	C	2000	XAM	CAJ-CAE-CAF	2.74	122.28	114.74
2	A	2000	XAM	CBD-CBA-CAZ	-2.73	123.34	128.45
2	D	2000	XAM	O5-C1-NBE	-2.65	105.92	108.23
2	A	2000	XAM	CBF-CBG-CBA	-2.61	108.18	113.21
2	B	2000	XAM	CBD-CBA-CAZ	-2.56	123.67	128.45
2	C	2000	XAM	O4-CBZ-NCA	2.53	115.06	110.55
2	B	2000	XAM	CBF-CBG-CBA	-2.49	108.41	113.21
2	A	2000	XAM	O5-C1-NBE	-2.48	106.08	108.23
2	C	2000	XAM	C2-C3-C4	2.46	115.53	110.44
2	C	2000	XAM	CAT-CAU-NAV	2.43	107.95	106.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2000	XAM	OCK-CCE-CAM	-2.41	106.28	109.87
2	B	2000	XAM	CAN-CAM-CCE	2.37	116.13	113.43
2	A	2000	XAM	CBJ-CBF-NBE	-2.37	109.39	113.72
2	B	2000	XAM	CCF-CCE-CAM	2.35	113.73	110.52
2	A	2000	XAM	OAL-CAC-CAD	2.31	110.94	107.73
2	C	2000	XAM	C3-C2-C1	2.31	113.98	109.60
2	D	2000	XAM	CBJ-CBF-CBG	-2.29	108.31	111.52
2	B	2000	XAM	CAB-CAC-CAD	2.29	118.23	112.30
2	A	2000	XAM	OBB-CAZ-CBA	-2.27	116.84	119.96
2	D	2000	XAM	CAM-NAO-CAP	2.28	126.26	123.47
2	A	2000	XAM	O4-CBZ-NCA	2.26	114.59	110.55
2	A	2000	XAM	CAS-CAT-CLX	-2.26	122.48	126.35
2	D	2000	XAM	CCE-CCD-CCC	2.24	116.78	111.75
2	A	2000	XAM	CCE-CAM-NAO	-2.20	109.52	111.35
2	A	2000	XAM	CAJ-CAE-CAF	2.19	120.77	114.74
2	A	2000	XAM	OBH-CBD-NBE	-2.18	122.15	125.95
2	C	2000	XAM	CAS-CAT-CLX	-2.17	122.64	126.35
2	D	2000	XAM	O2-C2-C1	2.17	113.01	108.60
2	D	2000	XAM	CAE-CAJ-CAI	2.16	119.12	111.51
2	C	2000	XAM	OBH-CBD-NBE	-2.15	122.21	125.95
2	D	2000	XAM	OCJ-CCD-CCE	-2.13	104.09	109.51
2	D	2000	XAM	CCF-CCE-CCD	2.13	112.92	110.27
2	D	2000	XAM	OBH-CBD-NBE	-2.12	122.26	125.95
2	A	2000	XAM	OCJ-CCD-CCE	-2.09	104.18	109.51
2	C	2000	XAM	C3-C4-C5	2.09	113.38	110.39
2	C	2000	XAM	CAT-CAS-CLW	-2.08	122.80	126.35
2	C	2000	XAM	CAE-CAD-CAG	2.06	111.20	108.25
2	B	2000	XAM	CAD-CAE-CAF	-2.06	103.75	109.34
2	B	2000	XAM	CAY-CAU-NAV	-2.01	120.28	122.64
2	A	2000	XAM	CAT-CAS-CLW	-2.00	122.92	126.35
2	B	2000	XAM	CCE-CCD-CCC	2.00	116.25	111.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	XAM	C4-O4-CBZ-NCA
2	A	2000	XAM	C4-O4-CBZ-OCB
2	C	2000	XAM	C4-O4-CBZ-NCA
2	C	2000	XAM	C4-O4-CBZ-OCB
2	D	2000	XAM	C4-O4-CBZ-NCA
2	D	2000	XAM	C4-O4-CBZ-OCB

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Mol	Chain	Res	Type	Atoms
2	B	2000	XAM	C4-O4-CBZ-NCA
2	B	2000	XAM	C4-O4-CBZ-OCB

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	194/231 (83%)	-0.16	0	100	100	24, 38, 66, 79	0
1	B	195/231 (84%)	-0.16	0	100	100	20, 38, 67, 73	0
1	C	191/231 (82%)	0.12	5 (2%)	53	64	33, 55, 86, 99	0
1	D	190/231 (82%)	0.17	5 (2%)	53	64	32, 56, 84, 96	0
All	All	770/924 (83%)	-0.01	10 (1%)	74	83	20, 48, 78, 99	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	168	THR	4.7
1	C	94	MET	3.5
1	C	90	ILE	2.9
1	D	98	ALA	2.9
1	C	95	GLY	2.7
1	C	130	VAL	2.6
1	D	97	PRO	2.6
1	D	104	THR	2.3
1	D	28	ALA	2.1
1	C	91	GLN	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 carbohydrates in this entry.

## 6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	XAM	C	2000	64/64	0.23	0.44	52,72,91,93	0
2	XAM	D	2000	64/64	0.22	0.18	56,79,88,92	0
2	XAM	A	2000	64/64	0.18	0.09	19,45,64,73	0
2	XAM	B	2000	64/64	0.20	0.08	19,47,58,63	0

## 6.5 Other polymers

There are no such residues in this entry.