



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:32 AM GMT

PDB ID : 2XCT  
Title : THE TWINNED 3.35Å STRUCTURE OF S. AUREUS GYRASE COMPLEX WITH CIPROFLOXACIN AND DNA  
Authors : Bax, B.D.; Chan, P.; Eggleston, D.S.; Fosberry, A.; Gentry, D.R.; Gorrec, F.; Giordano, I.; Hann, M.M.; Hennessy, A.; Hibbs, M.; Huang, J.; Jones, E.; Jones, J.; Brown, K.K.; Lewis, C.J.; May, E.; Singh, O.; Spitzfaden, C.; Shen, C.; Shillings, A.; Theobald, A.; Wohlkonig, A.; Pearson, N.D.; Gwynn, M.N.  
Deposited on : 2010-04-25  
Resolution : 3.35 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](mailto: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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

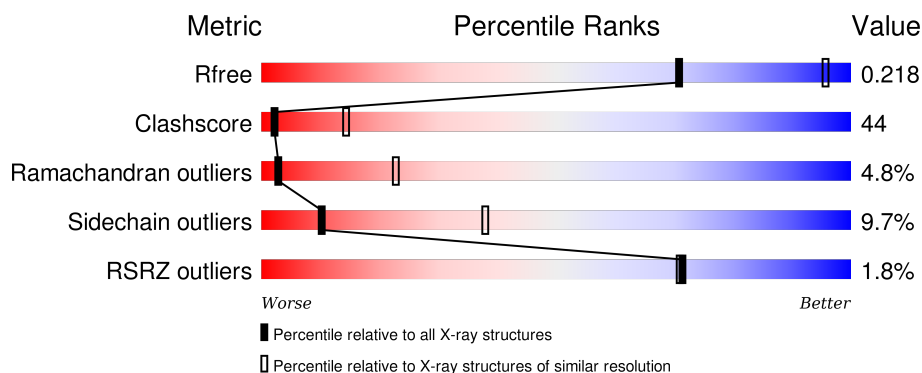
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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.






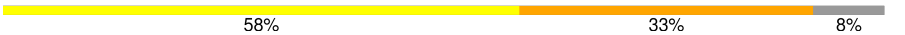



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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. 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	B	692	<div> <div>3%</div> <div>38% 52% 6%</div> </div>
1	D	692	<div> <div>3%</div> <div>39% 50% 8%</div> </div>
1	S	692	<div> <div>3%</div> <div>33% 55% 9%</div> </div>
1	U	692	<div> <div>2%</div> <div>37% 51% 9%</div> </div>
2	E	8	<div> <div>50% 38% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	V	8	
3	F	8	
3	W	8	
4	G	12	
4	X	12	
5	H	12	
5	Y	12	

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
7	CPF	H	1020	-	-	X	-
7	CPF	X	1020	-	-	X	-
7	CPF	Y	1020	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22370 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 DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	669	Total	C	N	O	S	0	2	0
			5262	3277	944	1015	26			
1	D	669	Total	C	N	O	S	0	1	0
			5151	3212	913	1001	25			
1	S	667	Total	C	N	O	S	0	0	1
			5199	3247	920	1007	25			
1	U	665	Total	C	N	O	S	0	0	0
			5193	3239	926	1003	25			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	EXPRESSION TAG	UNP P66937
B	544	THR	-	INSERTION	UNP P66937
B	545	GLY	-	INSERTION	UNP P66937
B	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
D	409	MET	-	EXPRESSION TAG	UNP P66937
D	544	THR	-	INSERTION	UNP P66937
D	545	GLY	-	INSERTION	UNP P66937
D	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
S	409	MET	-	EXPRESSION TAG	UNP P66937
S	544	THR	-	INSERTION	UNP P66937
S	545	GLY	-	INSERTION	UNP P66937
S	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
U	409	MET	-	EXPRESSION TAG	UNP P66937
U	544	THR	-	INSERTION	UNP P66937
U	545	GLY	-	INSERTION	UNP P66937
U	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5

- Molecule 2 is a DNA chain called 5'-D(TP\*GP\*TP\*GP\*CP\*GP\*GP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			147	69	27	44	7			
2	V	7	Total	C	N	O	P	0	0	0
			147	69	27	44	7			

- Molecule 3 is a DNA chain called 5'-D(AP\*GP\*CP\*CP\*GP\*TP\*AP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	P	0	0	0
			145	68	28	42	7			
3	W	6	Total	C	N	O	P	0	0	0
			123	58	23	36	6			

- Molecule 4 is a DNA chain called 5'-D(GP\*TP\*AP\*CP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	11	Total	C	N	O	P	0	0	0
			220	105	42	63	10			
4	X	11	Total	C	N	O	P	0	0	0
			220	105	42	63	10			

- Molecule 5 is a DNA chain called 5'-D(GP\*TP\*AP\*CP\*AP\*CP\*CP\*GP\*CP\*AP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	12	Total	C	N	O	P	0	0	0
			240	115	47	67	11			
5	Y	11	Total	C	N	O	P	0	0	0
			219	105	42	62	10			

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

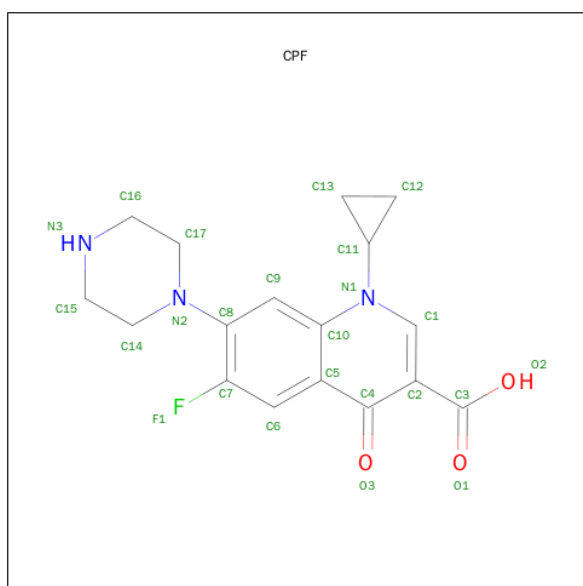
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mn	0	0
			1	1		
6	D	1	Total	Mn	0	0
			1	1		
6	B	1	Total	Mn	0	0
			1	1		
6	W	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	U	1	Total	Mn	0	0
			1	1		
6	S	1	Total	Mn	0	0
			1	1		
6	F	1	Total	Mn	0	0
			1	1		

- Molecule 7 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (three-letter code: CPF) (formula: C<sub>17</sub>H<sub>18</sub>FN<sub>3</sub>O<sub>3</sub>).

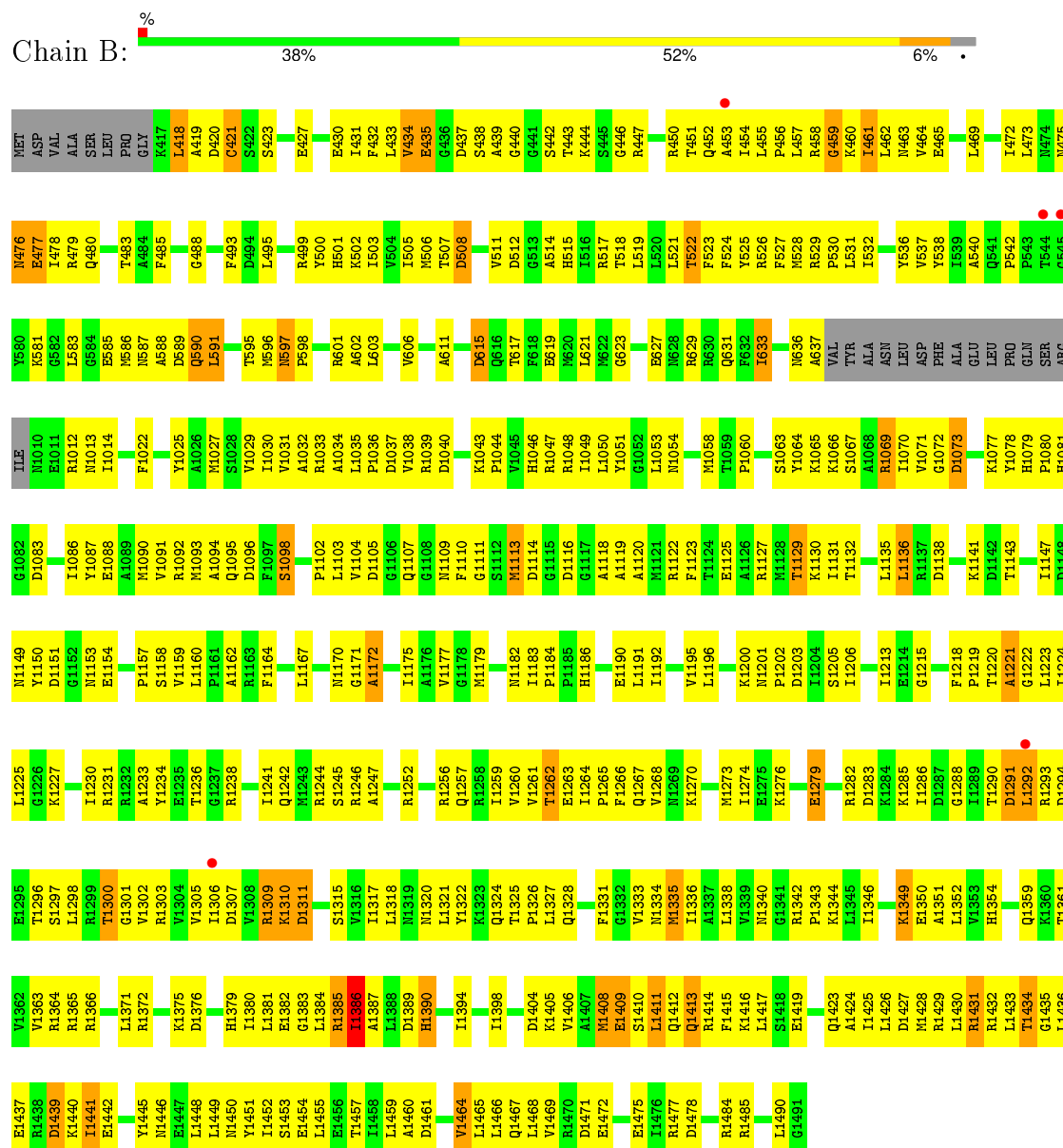


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	G	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
7	H	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
7	X	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
7	Y	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

### 3 Residue-property plots

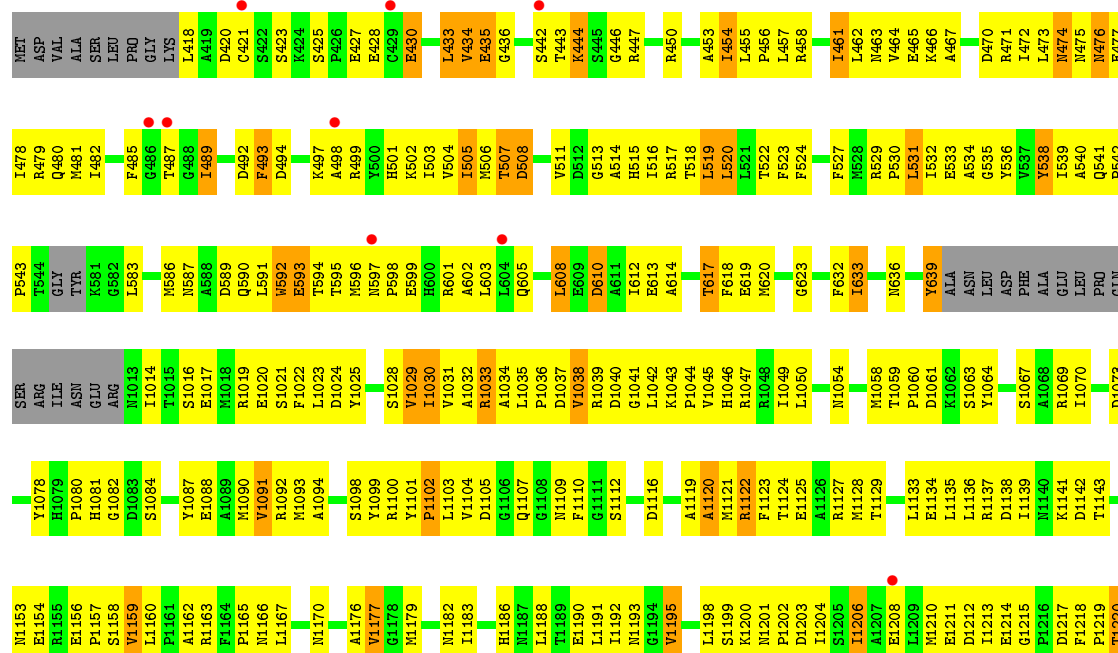
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

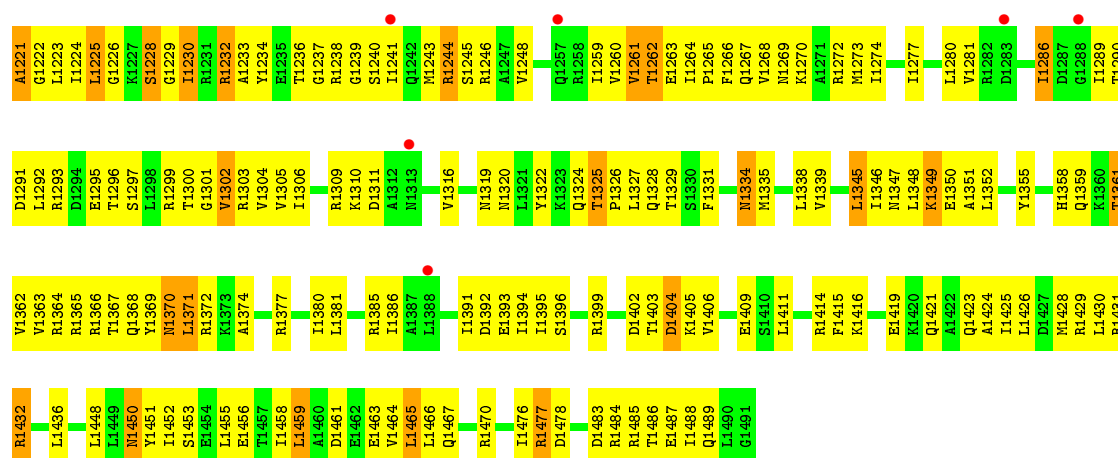
- Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A











- Molecule 2: 5'-D(TP\*GP\*TP\*GP\*CP\*GP\*GP\*T)-3'

Chain E: 50% 38% 13%



- Molecule 2: 5'-D(TP\*GP\*TP\*GP\*CP\*GP\*GP\*T)-3'

Chain V: 13% 50% 25% 13%



- Molecule 3: 5'-D(AP\*GP\*CP\*CP\*GP\*TP\*AP\*G)-3'

Chain F: 13% 50% 25% 13%



- Molecule 3: 5'-D(AP\*GP\*CP\*CP\*GP\*TP\*AP\*G)-3'

Chain W: 13% 38% 25% 25%



- Molecule 4: 5'-D(GP\*TP\*AP\*CP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*T)-3'

Chain G: 58% 33% 8%



- Molecule 4: 5'-D(GP\*TP\*AP\*CP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*T)-3'

Chain X: 8% 25% 58% 8%



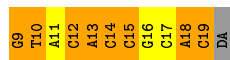
- Molecule 5: 5'-D(GP\*TP\*AP\*CP\*AP\*CP\*CP\*GP\*CP\*AP\*CP\*A)-3'

Chain H:   
25% 75%



- Molecule 5: 5'-D(GP\*TP\*AP\*CP\*AP\*CP\*CP\*GP\*CP\*AP\*CP\*A)-3'

Chain Y:   
25% 67% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.98Å 123.17Å 170.42Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	24.96 – 3.35 24.96 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (24.96-3.35) 97.3 (24.96-3.35)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.166 , 0.236 0.167 , 0.218	Depositor DCC
$R_{free}$ test set	2115 reflections (4.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.1	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.1	EDS
Estimated twinning fraction	0.324 for H,-K,-L 0.277 for h,-k,-l	Xtriage
Reported twinning fraction	0.324 for H,-K,-L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 52173 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MN, CPF

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	B	0.49	0/5332	0.70	0/7190
1	D	0.47	0/5220	0.69	1/7063 (0.0%)
1	S	0.45	0/5269	0.68	1/7112 (0.0%)
1	U	0.49	0/5263	0.71	1/7106 (0.0%)
2	E	1.02	0/164	2.13	7/252 (2.8%)
2	V	0.82	0/164	1.77	3/252 (1.2%)
3	F	0.94	1/162 (0.6%)	2.01	7/248 (2.8%)
3	W	0.80	0/137	1.81	6/209 (2.9%)
4	G	0.98	0/246	1.78	10/377 (2.7%)
4	X	1.00	0/246	2.04	17/377 (4.5%)
5	H	1.33	2/269 (0.7%)	2.72	31/412 (7.5%)
5	Y	1.00	0/245	2.42	18/375 (4.8%)
All	All	0.54	3/22717 (0.0%)	0.90	102/30973 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	17	DC	C3'-O3'	-5.51	1.36	1.44
5	H	16	DG	C3'-O3'	-5.48	1.36	1.44
3	F	6	DT	C1'-N1	5.42	1.56	1.49

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	9	DG	O4'-C1'-N9	17.19	120.03	108.00
5	H	17	DC	O4'-C1'-N1	-13.75	98.38	108.00
5	H	9	DG	O4'-C1'-N9	13.50	117.45	108.00
5	H	10	DT	O4'-C1'-N1	13.39	117.37	108.00
5	Y	9	DG	C1'-O4'-C4'	-11.73	98.36	110.10

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	B	5262	0	5259	446	0
1	D	5151	0	5043	443	0
1	S	5199	0	5178	502	0
1	U	5193	0	5163	464	0
2	E	147	0	80	8	0
2	V	147	0	80	8	0
3	F	145	0	79	14	0
3	W	123	0	68	8	0
4	G	220	0	124	27	0
4	X	220	0	124	35	0
5	H	240	0	135	38	0
5	Y	219	0	124	37	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	S	1	0	0	0	0
6	U	1	0	0	0	0
6	W	2	0	0	0	0
7	G	24	0	17	8	0
7	H	24	0	17	9	0
7	X	24	0	17	20	0
7	Y	24	0	17	10	0
All	All	22370	0	21525	1934	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 44.

The worst 5 of 1934 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)
4:G:12:DC:N3	5:H:9:DG:N2	1.82	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:11:DA:N1	5:Y:10:DT:O4	1.78	1.15
5:H:11:DA:H2"	5:H:12:DC:C5'	1.86	1.06
1:U:1122:ARG:HH22	4:X:9:DG:H5"	1.18	1.06
1:D:1192:ILE:HD12	1:D:1477:ARG:HB2	1.39	1.05

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	B	667/692 (96%)	545 (82%)	100 (15%)	22 (3%)	5	34
1	D	664/692 (96%)	526 (79%)	108 (16%)	30 (4%)	3	24
1	S	661/692 (96%)	493 (75%)	123 (19%)	45 (7%)	1	13
1	U	659/692 (95%)	532 (81%)	97 (15%)	30 (5%)	3	23
All	All	2651/2768 (96%)	2096 (79%)	428 (16%)	127 (5%)	3	23

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1150	TYR
1	B	1291	ASP
1	B	1310	LYS
1	B	1409	GLU
1	B	1431	ARG

### 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	B	563/591 (95%)	518 (92%)	45 (8%)	15	50
1	D	539/591 (91%)	483 (90%)	56 (10%)	9	34
1	S	555/591 (94%)	497 (90%)	58 (10%)	8	33
1	U	553/591 (94%)	499 (90%)	54 (10%)	10	37
All	All	2210/2364 (94%)	1997 (90%)	213 (10%)	10	38

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1432	ARG
1	S	1058	MET
1	U	1262	THR
1	D	1483	ASP
1	S	483	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1334	ASN
1	S	1046	HIS
1	U	1324	GLN
1	D	1421	GLN
1	D	1450	ASN

### 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

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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$
7	CPF	G	1020	6	21,27,27	1.66	2 (9%)	28,40,40	2.20	10 (35%)
7	CPF	H	1020	6	21,27,27	1.77	6 (28%)	28,40,40	2.33	10 (35%)
7	CPF	X	1020	6	21,27,27	1.74	6 (28%)	28,40,40	2.07	7 (25%)
7	CPF	Y	1020	6	21,27,27	2.03	6 (28%)	28,40,40	2.43	9 (32%)

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
7	CPF	G	1020	6	-	0/4/22/22	0/3/4/4
7	CPF	H	1020	6	-	0/4/22/22	0/3/4/4
7	CPF	X	1020	6	-	0/4/22/22	0/3/4/4
7	CPF	Y	1020	6	-	0/4/22/22	0/3/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1020	CPF	C10-N1	-5.07	1.34	1.40
7	Y	1020	CPF	C10-N1	-4.91	1.34	1.40
7	Y	1020	CPF	C5-C10	-4.65	1.38	1.41
7	H	1020	CPF	C10-N1	-4.32	1.35	1.40
7	X	1020	CPF	C10-N1	-4.13	1.35	1.40

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	1020	CPF	C6-C7-C8	-5.65	118.85	123.41
7	Y	1020	CPF	C9-C8-N2	-5.35	115.56	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	1020	CPF	C6-C7-C8	-5.08	119.31	123.41
7	H	1020	CPF	C6-C7-C8	-4.32	119.92	123.41
7	G	1020	CPF	C9-C8-N2	-4.32	116.94	122.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	1020	CPF	8	0
7	H	1020	CPF	9	0
7	X	1020	CPF	20	0
7	Y	1020	CPF	10	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	B	669/692 (96%)	-0.00	5 (0%) 89 89	29, 64, 101, 143	0
1	D	669/692 (96%)	0.00	8 (1%) 81 81	35, 69, 108, 143	0
1	S	667/692 (96%)	0.15	21 (3%) 52 53	43, 78, 119, 218	0
1	U	665/692 (96%)	0.10	15 (2%) 64 64	39, 72, 110, 158	0
2	E	7/8 (87%)	0.02	0 100 100	48, 52, 83, 89	0
2	V	7/8 (87%)	-0.20	0 100 100	51, 62, 76, 86	0
3	F	7/8 (87%)	-0.16	0 100 100	51, 57, 77, 80	0
3	W	6/8 (75%)	-0.22	0 100 100	62, 75, 86, 86	0
4	G	11/12 (91%)	-0.08	0 100 100	60, 67, 90, 120	0
4	X	11/12 (91%)	0.39	0 100 100	68, 88, 102, 125	0
5	H	12/12 (100%)	0.05	0 100 100	48, 77, 111, 123	0
5	Y	11/12 (91%)	-0.00	0 100 100	67, 75, 106, 117	0
All	All	2742/2848 (96%)	0.06	49 (1%) 71 71	29, 71, 112, 218	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1491	GLY	4.8
1	S	619	GLU	4.7
1	U	486	GLY	4.0
1	U	604	LEU	3.9
1	B	545	GLY	3.8

### 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 [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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CPF	H	1020	24/24	0.90	0.24	0.53	86,86,86,86	0
6	MN	S	2492	1/1	0.98	0.16	-0.35	70,70,70,70	0
7	CPF	G	1020	24/24	0.94	0.19	-0.43	70,70,70,70	0
7	CPF	X	1020	24/24	0.92	0.20	-0.47	86,86,86,86	0
7	CPF	Y	1020	24/24	0.93	0.18	-0.56	76,76,76,76	0
6	MN	U	2492	1/1	0.98	0.21	-	64,64,64,64	0
6	MN	D	2492	1/1	0.95	0.21	-	85,85,85,85	0
6	MN	B	2492	1/1	0.96	0.25	-	76,76,76,76	0
6	MN	W	2001	1/1	0.95	0.07	-	76,76,76,76	0
6	MN	W	2000	1/1	0.94	0.12	-	86,86,86,86	0
6	MN	F	2000	1/1	0.86	0.10	-	86,86,86,86	0
6	MN	G	2000	1/1	0.99	0.07	-	70,70,70,70	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.