



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 07:56 pm BST

PDB ID : 1JR3  
Title : Crystal Structure of the Processivity Clamp Loader Gamma Complex of E. coli DNA Polymerase III  
Authors : Jeruzalmi, D.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2001-08-10  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (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

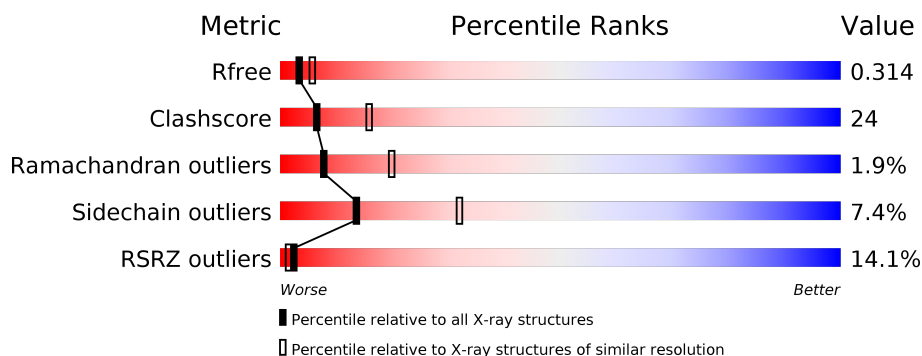
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	373	
1	B	373	
1	C	373	
2	D	343	
3	E	334	

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
5	SO4	A	1500	-	-	X	-
5	SO4	B	2500	-	-	X	-
5	SO4	C	5500	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13845 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 polymerase III subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
1	B	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
1	C	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			

- Molecule 2 is a protein called DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	338	Total	C	N	O	S	0	0	0
			2687	1702	488	487	10			

- Molecule 3 is a protein called DNA polymerase III, delta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

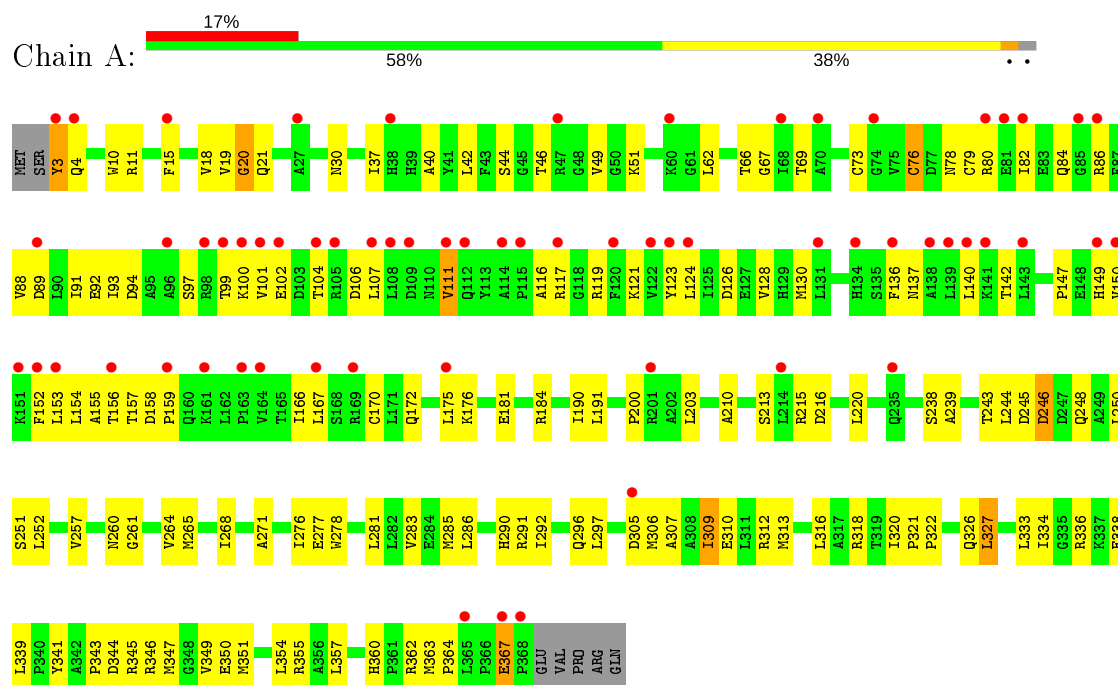


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

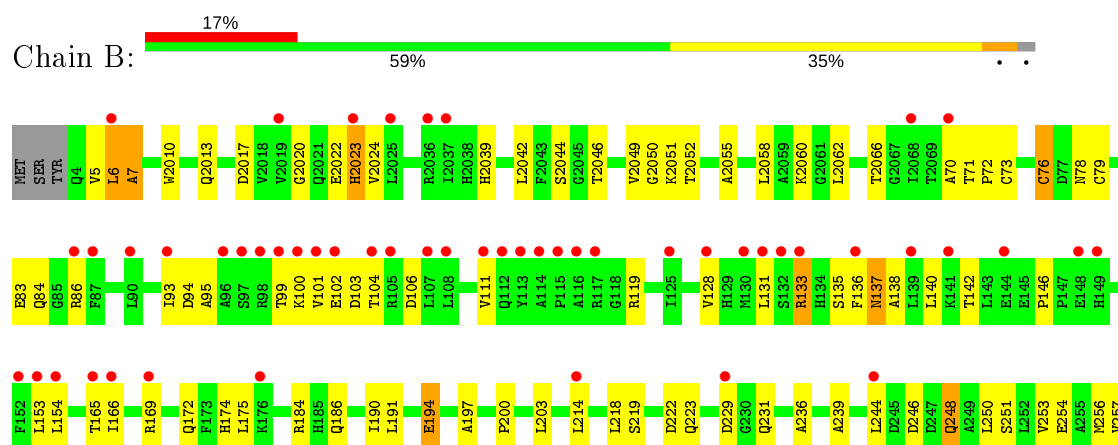
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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 polymerase III subunit gamma

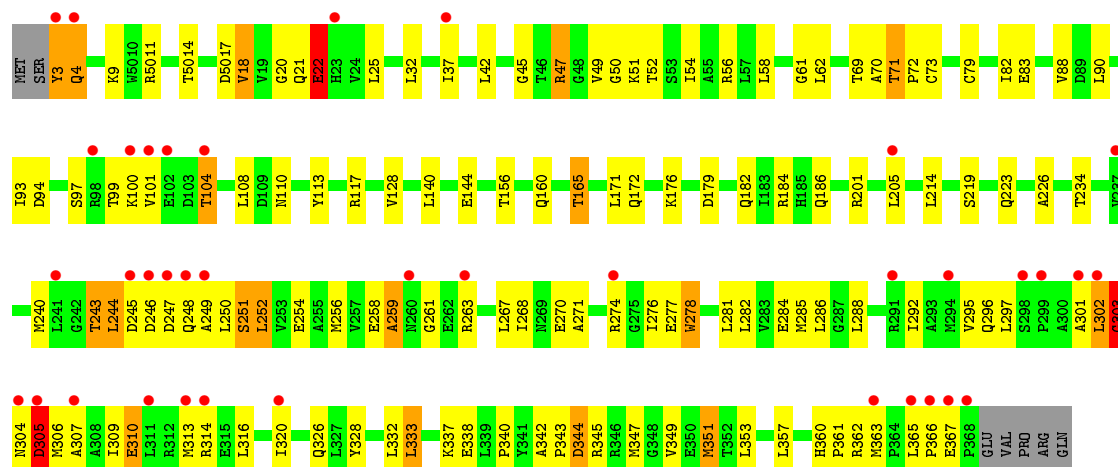


#### • Molecule 1: DNA polymerase III subunit gamma

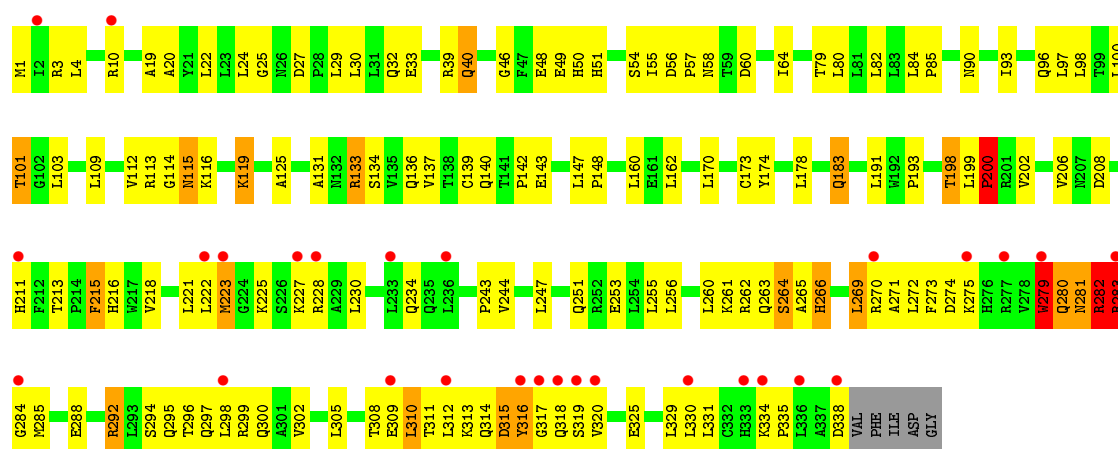




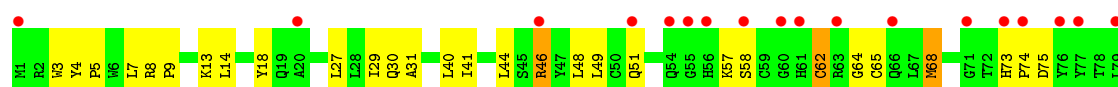
• Molecule 1: DNA polymerase III subunit gamma

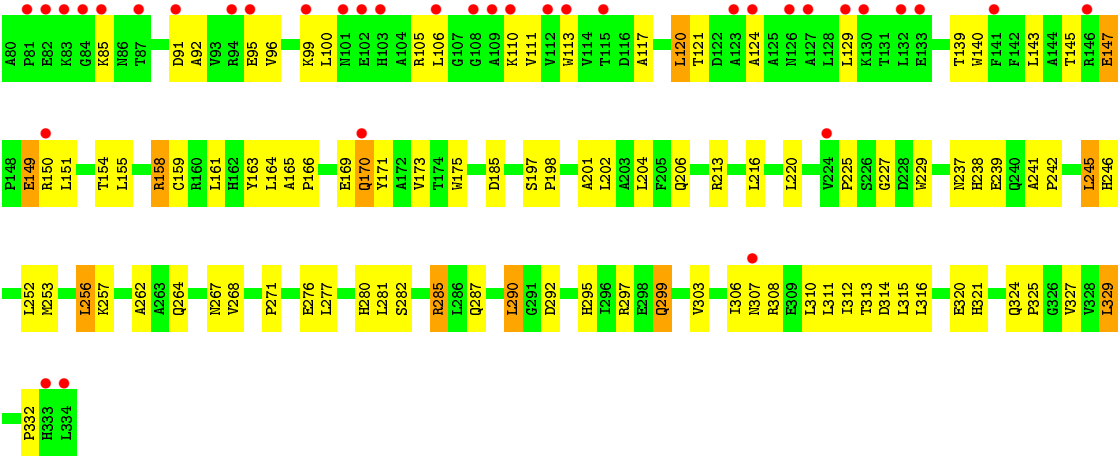


• Molecule 2: DNA polymerase III, delta subunit



• Molecule 3: DNA polymerase III, delta' subunit







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.70 Å 95.86 Å 285.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.70 90.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.70) 76.9 (90.87-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	13.60	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.69 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.268 , 0.304 0.286 , 0.314	Depositor DCC
$R_{free}$ test set	3031 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 71.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13845	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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	0.48	0/2898	0.74	2/3930 (0.1%)
1	B	0.66	7/2885 (0.2%)	0.95	14/3912 (0.4%)
1	C	0.57	0/2898	0.88	10/3930 (0.3%)
2	D	0.85	8/2735 (0.3%)	0.93	10/3716 (0.3%)
3	E	0.49	0/2666	0.70	0/3639
All	All	0.62	15/14082 (0.1%)	0.85	36/19127 (0.2%)

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	B	0	1
2	D	0	4
All	All	0	5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	315	ASP	CB-CG	29.10	2.12	1.51
1	B	133	ARG	CZ-NH2	-10.95	1.18	1.33
2	D	310	LEU	CG-CD2	-9.05	1.18	1.51
1	B	363	MET	CG-SD	8.99	2.04	1.81
1	B	363	MET	SD-CE	8.90	2.27	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	MET	CG-SD-CE	17.06	127.49	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	283	ARG	C-N-CA	12.38	148.31	122.30
1	C	244	LEU	CB-CG-CD2	-11.83	90.88	111.00
2	D	280	GLN	C-N-CA	11.46	150.36	121.70
1	B	133	ARG	NE-CZ-NH1	10.92	125.76	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2023	HIS	Sidechain
2	D	280	GLN	Peptide
2	D	281	ASN	Mainchain
2	D	282	ARG	Mainchain
2	D	319	SER	Mainchain

## 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	2850	0	2896	158	0
1	B	2838	0	2887	195	0
1	C	2850	0	2895	133	1
2	D	2687	0	2741	146	1
3	E	2601	0	2603	100	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	7	0
5	B	5	0	0	2	0
5	C	5	0	0	3	0
All	All	13845	0	14022	664	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 24.

The worst 5 of 664 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:B:363:MET:SD	1:B:363:MET:CG	2.04	1.45
1:C:304:ASN:ND2	2:D:234:GLN:OE1	1.61	1.30
1:B:363:MET:SD	1:B:363:MET:CE	2.27	1.21
1:C:94:ASP:H	1:C:100:LYS:NZ	1.40	1.17
2:D:315:ASP:CB	2:D:315:ASP:CG	2.12	1.16

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:C:117:ARG:NH2	2:D:281:ASN:ND2[4_486]	1.70	0.50

## 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	364/373 (98%)	335 (92%)	23 (6%)	6 (2%)	9	24
1	B	363/373 (97%)	325 (90%)	28 (8%)	10 (3%)	5	11
1	C	364/373 (98%)	334 (92%)	22 (6%)	8 (2%)	6	17
2	D	336/343 (98%)	307 (91%)	22 (6%)	7 (2%)	7	18
3	E	332/334 (99%)	301 (91%)	29 (9%)	2 (1%)	25	50
All	All	1759/1796 (98%)	1602 (91%)	124 (7%)	33 (2%)	8	20

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
1	A	104	THR
1	A	111	VAL
1	A	364	PRO
1	B	2022	GLU

### 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	303/310 (98%)	288 (95%)	15 (5%)	24	51
1	B	302/310 (97%)	289 (96%)	13 (4%)	29	57
1	C	303/310 (98%)	280 (92%)	23 (8%)	13	30
2	D	287/291 (99%)	261 (91%)	26 (9%)	9	21
3	E	270/270 (100%)	239 (88%)	31 (12%)	5	13
All	All	1465/1491 (98%)	1357 (93%)	108 (7%)	13	32

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	344	ASP
2	D	143	GLU
3	E	256	LEU
1	C	357	LEU
2	D	101	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	105	HIS
2	D	204	GLN
3	E	280	HIS
2	D	136	GLN
2	D	211	HIS

### 5.3.3 RNA [i](#)

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z  > 2$
5	SO4	A	1500	-	4,4,4	1.84	2 (50%)	6,6,6	1.06	0
5	SO4	B	2500	-	4,4,4	1.87	2 (50%)	6,6,6	0.91	0
5	SO4	C	5500	-	4,4,4	1.85	2 (50%)	6,6,6	0.94	0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2500	SO4	O1-S	3.07	1.62	1.46
5	C	5500	SO4	O1-S	2.93	1.61	1.46
5	A	1500	SO4	O1-S	2.81	1.61	1.46
5	A	1500	SO4	O3-S	-2.31	1.28	1.47
5	C	5500	SO4	O3-S	-2.25	1.29	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1500	SO4	7	0
5	B	2500	SO4	2	0
5	C	5500	SO4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	366/373 (98%)	1.06	64 (17%)	1 1	32, 76, 152, 173	0
1	B	365/373 (97%)	1.27	65 (17%)	1 1	27, 75, 159, 190	0
1	C	366/373 (98%)	0.85	38 (10%)	6 4	27, 62, 129, 156	0
2	D	338/343 (98%)	0.78	28 (8%)	11 9	38, 69, 121, 142	0
3	E	334/334 (100%)	1.10	54 (16%)	1 1	30, 67, 156, 161	0
All	All	1769/1796 (98%)	1.01	249 (14%)	2 1	27, 69, 151, 190	0

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	PRO	18.7
1	B	365	LEU	15.6
1	B	368	PRO	15.2
1	B	366	PRO	13.3
1	B	359	PHE	11.4

### 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( $\text{\AA}^2$ )	Q<0.9
4	ZN	E	400	1/1	0.57	0.06	156,156,156,156	0
5	SO4	B	2500	5/5	0.95	0.17	68,70,70,70	0
4	ZN	A	400	1/1	0.97	0.18	130,130,130,130	0
5	SO4	A	1500	5/5	0.97	0.14	64,65,66,67	0
4	ZN	B	400	1/1	0.98	0.15	105,105,105,105	0
5	SO4	C	5500	5/5	0.98	0.15	36,36,39,41	0
4	ZN	C	400	1/1	0.99	0.19	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.