



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 01:46 am BST

PDB ID : 1UNN  
Title : Complex of beta-clamp processivity factor and little finger domain of PolIV  
Authors : Bunting, K.A.; Roe, S.M.; Pearl, L.H.  
Deposited on : 2003-09-11  
Resolution : 1.90 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.

---

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

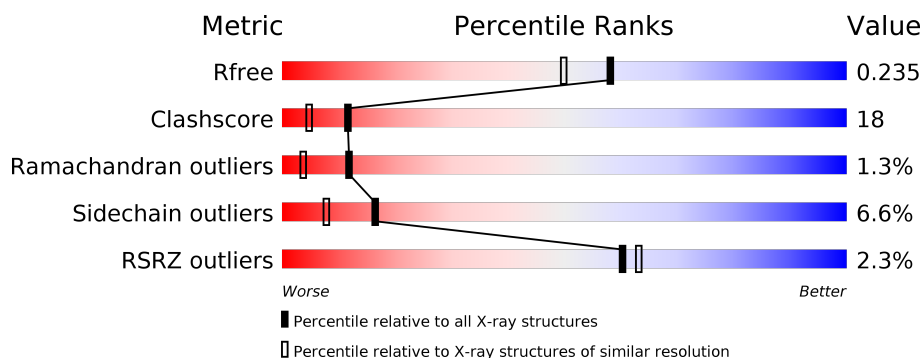
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	366	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	366	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>5%</div> <div>.</div> </div> </div>
2	C	115	<div> <div></div> <div> <div>77%</div> <div>17%</div> <div>.</div> <div>.</div> </div> </div>
2	D	115	<div> <div>%</div> <div> <div>66%</div> <div>23%</div> <div>.</div> <div>.</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8485 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.

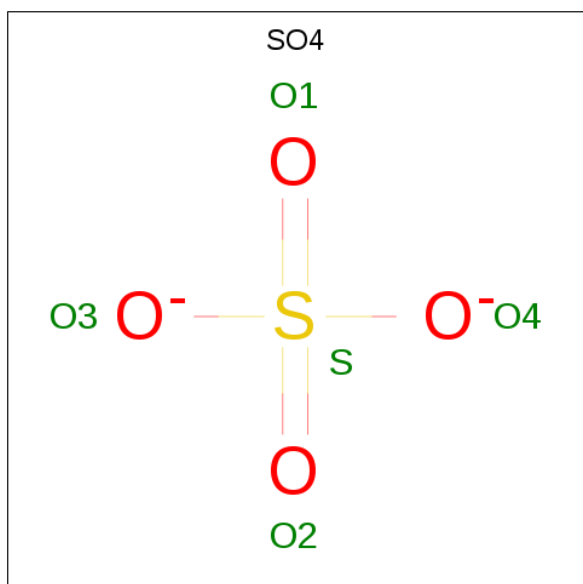
- Molecule 1 is a protein called DNA POLYMERASE III BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2844	1786	498	541	19			
1	B	366	Total	C	N	O	S	0	0	0
			2844	1786	498	541	19			

- Molecule 2 is a protein called DNA POLYMERASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	111	Total	C	N	O	S	0	0	0
			915	576	175	161	3			
2	D	112	Total	C	N	O	S	0	0	0
			925	582	178	162	3			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

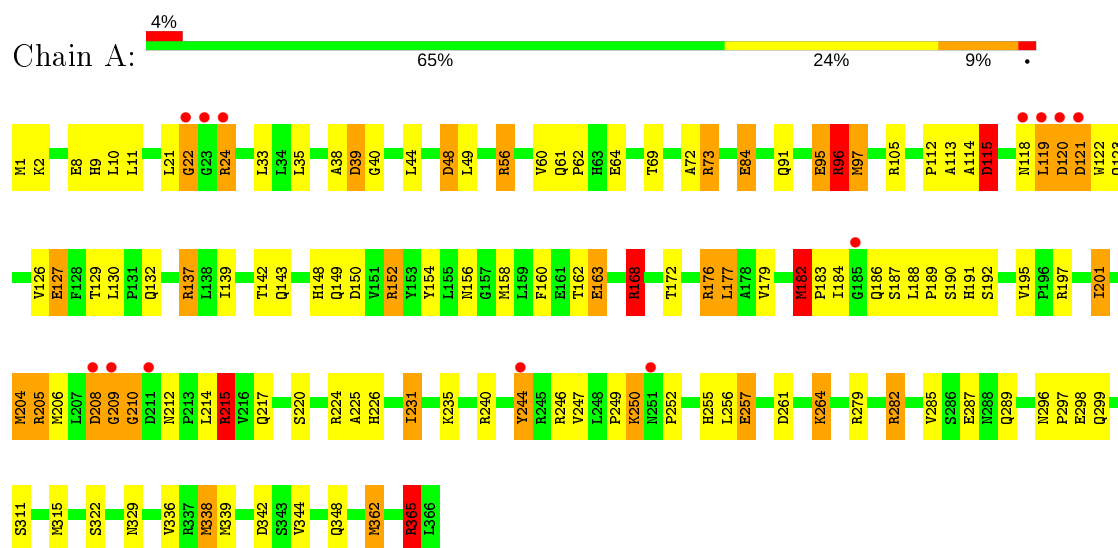
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	304	Total	O	0	0
			304	304		
4	B	375	Total	O	0	0
			375	375		
4	C	116	Total	O	0	0
			116	116		
4	D	152	Total	O	0	0
			152	152		

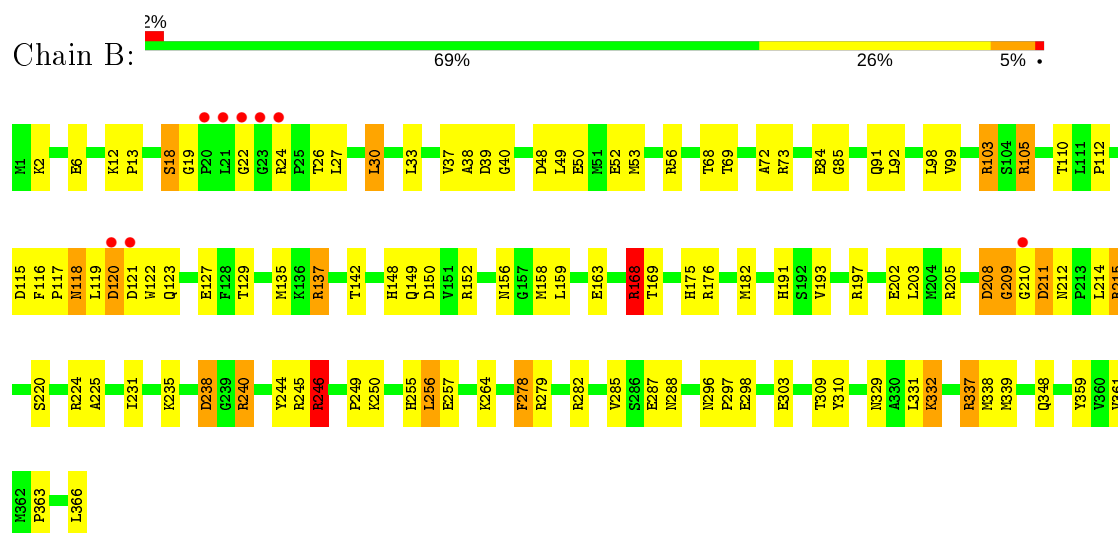
### 3 Residue-property plots [i](#)

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 BETA SUBUNIT



#### • Molecule 1: DNA POLYMERASE III BETA SUBUNIT

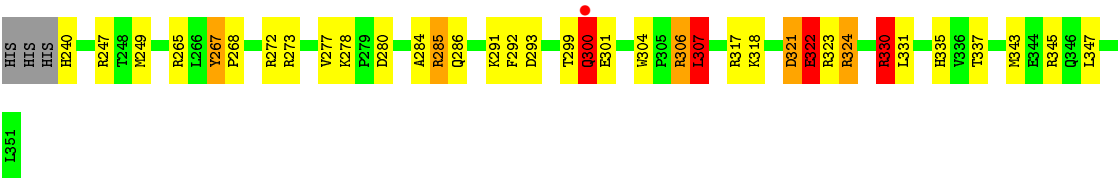


#### • Molecule 2: DNA POLYMERASE IV





● Molecule 2: DNA POLYMERASE IV



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.45Å 70.12Å 110.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.10 – 1.90 61.11 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (62.10-1.90) 96.6 (61.11-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.179 , 0.240 0.178 , 0.235	Depositor DCC
$R_{free}$ test set	4388 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.6	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	0.95	EDS
Total number of atoms	8485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: 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	1.37	21/2893 (0.7%)	1.47	32/3915 (0.8%)
1	B	1.45	17/2893 (0.6%)	1.53	27/3915 (0.7%)
2	C	1.18	2/933 (0.2%)	1.28	5/1258 (0.4%)
2	D	1.64	10/944 (1.1%)	1.83	25/1273 (2.0%)
All	All	1.41	50/7663 (0.7%)	1.52	89/10361 (0.9%)

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	1	1
1	B	2	2
All	All	3	3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	307	LEU	N-CA	19.82	1.85	1.46
2	D	322	GLU	N-CA	12.18	1.70	1.46
1	A	96	ARG	N-CA	10.47	1.67	1.46
1	A	182	MET	CG-SD	-10.05	1.55	1.81
1	B	182	MET	CG-SD	-9.11	1.57	1.81

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ARG	NE-CZ-NH2	-23.66	108.47	120.30
1	A	152	ARG	NE-CZ-NH2	-22.66	108.97	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ARG	NE-CZ-NH1	21.37	130.99	120.30
1	A	152	ARG	NE-CZ-NH1	18.71	129.66	120.30
1	B	215	ARG	NE-CZ-NH2	-15.88	112.36	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	142	THR	CB
1	B	129	THR	CB
1	B	142	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	GLY	Peptide
1	B	18	SER	Peptide
1	B	209	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	2844	0	2861	121	0
1	B	2844	0	2861	80	1
2	C	915	0	929	17	0
2	D	925	0	936	53	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	304	0	0	24	0
4	B	375	0	0	31	2
4	C	116	0	0	6	0
4	D	152	0	0	15	1
All	All	8485	0	7587	265	3

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 18.

The worst 5 of 265 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:168:ARG:CG	1:B:168:ARG:CD	1.74	1.63
2:D:322:GLU:N	2:D:322:GLU:CA	1.70	1.52
2:D:307:LEU:N	2:D:307:LEU:CA	1.86	1.38
2:D:321:ASP:O	2:D:322:GLU:CA	1.72	1.37
1:A:338:MET:SD	1:A:338:MET:CE	2.14	1.35

All (3) 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:B:209:GLY:CA	1:B:209:GLY:CA[2_665]	2.14	0.06
4:B:2018:HOH:O	4:D:2028:HOH:O[2_655]	2.19	0.01
4:B:2114:HOH:O	4:B:2168:HOH:O[2_665]	2.19	0.01

## 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	364/366 (100%)	349 (96%)	8 (2%)	7 (2%)	8	1
1	B	364/366 (100%)	355 (98%)	7 (2%)	2 (0%)	29	18
2	C	109/115 (95%)	108 (99%)	1 (1%)	0	100	100
2	D	110/115 (96%)	103 (94%)	4 (4%)	3 (3%)	5	1
All	All	947/962 (98%)	915 (97%)	20 (2%)	12 (1%)	12	4

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ALA
1	A	115	ASP
2	D	322	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	22	GLY
1	A	119	LEU

### 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	313/313 (100%)	288 (92%)	25 (8%)	12	5
1	B	313/313 (100%)	291 (93%)	22 (7%)	15	7
2	C	97/101 (96%)	92 (95%)	5 (5%)	23	14
2	D	98/101 (97%)	96 (98%)	2 (2%)	55	51
All	All	821/828 (99%)	767 (93%)	54 (7%)	16	8

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ARG
1	B	105	ARG
2	C	299	THR
1	B	24	ARG
1	B	30	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
1	B	132	GLN
2	D	335	HIS
1	A	348	GLN
1	B	9	HIS

### 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 ⓘ

2 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	SO4	C	1352	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	D	1352	-	4,4,4	0.18	0	6,6,6	0.37	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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	366/366 (100%)	0.14	13 (3%) 42 45	5, 20, 40, 69	0
1	B	366/366 (100%)	-0.06	8 (2%) 62 64	5, 15, 36, 70	0
2	C	111/115 (96%)	-0.10	0 100 100	8, 21, 34, 40	0
2	D	112/115 (97%)	-0.28	1 (0%) 84 85	7, 14, 26, 36	0
All	All	955/962 (99%)	-0.01	22 (2%) 60 63	5, 17, 37, 70	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	GLY	10.8
1	A	22	GLY	5.3
1	A	23	GLY	4.6
1	A	119	LEU	4.1
1	A	211	ASP	4.1

### 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( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	1352	5/5	0.85	0.18	91,93,93,94	0
3	SO4	D	1352	5/5	0.90	0.18	79,80,82,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.