



# Full wwPDB X-ray Structure Validation Report i

Nov 12, 2024 – 06:42 PM EST

PDB ID : 3UQZ  
Title : X-ray structure of DNA processing protein A (DprA) from Streptococcus pneumoniae  
Authors : Quevillon-Cheruel, S.; Brooks, M.A.; Li de la Sierra-Gallay, I.  
Deposited on : 2011-11-21  
Resolution : 2.70 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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

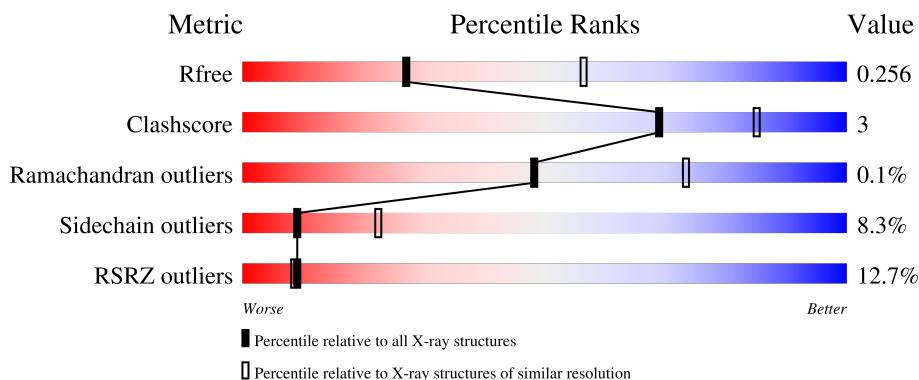
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

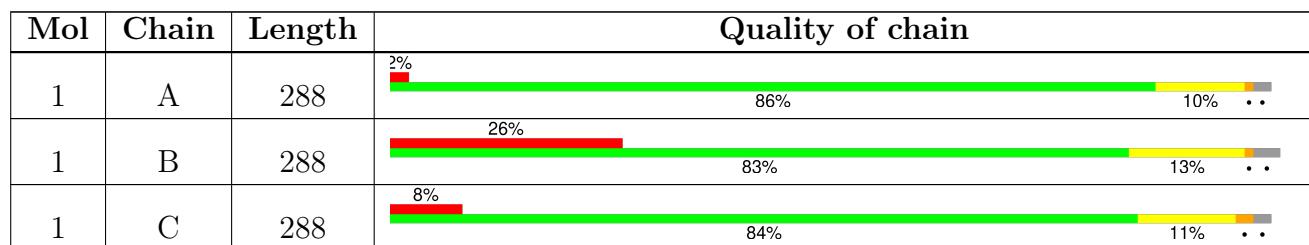
The reported resolution of this entry is 2.70 Å.

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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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 of 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.



## 2 Entry composition [\(i\)](#)

There are 3 unique types of molecules in this entry. The entry contains 6732 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 processing protein DprA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	283	Total	C 2194	N 1401	O 370	S 412	Se 6	0	0	0
1	B	280	Total	C 2164	N 1381	O 365	S 407	Se 6	0	0	0
1	C	282	Total	C 2184	N 1395	O 367	S 411	Se 6	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	HIS	-	expression tag	UNP Q97QF0
A	284	HIS	-	expression tag	UNP Q97QF0
A	285	HIS	-	expression tag	UNP Q97QF0
A	286	HIS	-	expression tag	UNP Q97QF0
A	287	HIS	-	expression tag	UNP Q97QF0
A	288	HIS	-	expression tag	UNP Q97QF0
B	283	HIS	-	expression tag	UNP Q97QF0
B	284	HIS	-	expression tag	UNP Q97QF0
B	285	HIS	-	expression tag	UNP Q97QF0
B	286	HIS	-	expression tag	UNP Q97QF0
B	287	HIS	-	expression tag	UNP Q97QF0
B	288	HIS	-	expression tag	UNP Q97QF0
C	283	HIS	-	expression tag	UNP Q97QF0
C	284	HIS	-	expression tag	UNP Q97QF0
C	285	HIS	-	expression tag	UNP Q97QF0
C	286	HIS	-	expression tag	UNP Q97QF0
C	287	HIS	-	expression tag	UNP Q97QF0
C	288	HIS	-	expression tag	UNP Q97QF0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 10 8 2	0	1
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

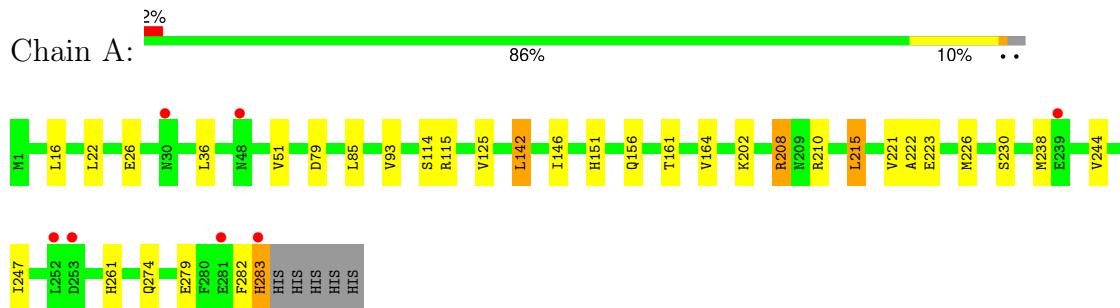
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	44	Total O 44 44	0	0
3	C	22	Total O 22 22	0	0

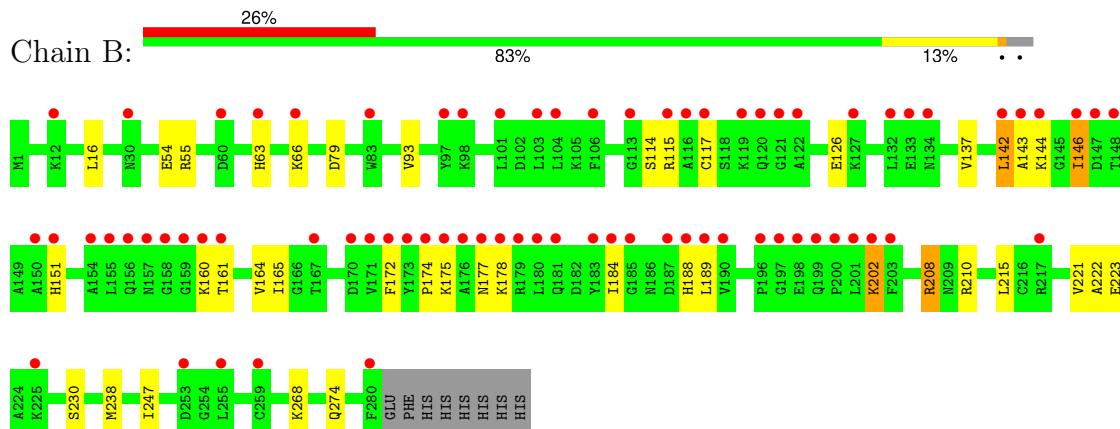
### 3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

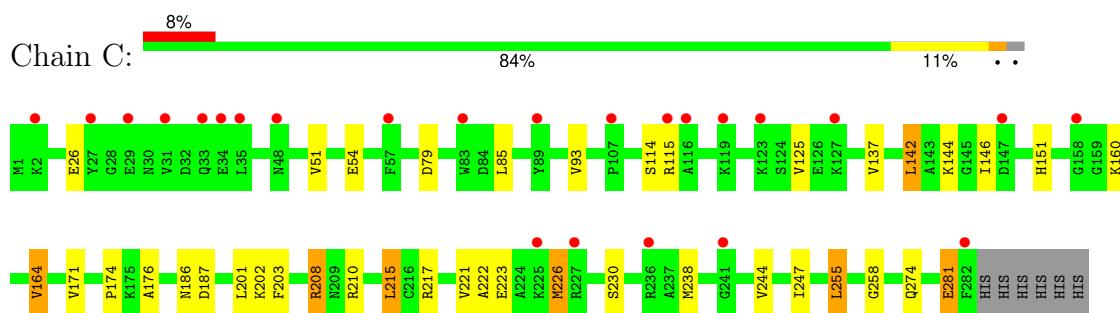
- Molecule 1: DNA processing protein DprA



- Molecule 1: DNA processing protein DprA



- Molecule 1: DNA processing protein DprA



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	300.24Å    300.24Å    78.34Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	41.76 – 2.70 41.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.76-2.70) 96.2 (41.76-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.19 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
$R$ , $R_{free}$	0.219 , 0.245 0.224 , 0.256	Depositor DCC
$R_{free}$ test set	2420 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.3	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.48$ , $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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  $< |L| >$ ,  $< L^2 >$  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:  
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	0.43	0/2231	0.67	0/3003
1	B	0.47	0/2199	0.68	0/2960
1	C	0.44	0/2220	0.67	0/2988
All	All	0.45	0/6650	0.67	0/8951

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [\(i\)](#)

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	2194	0	2205	15	0
1	B	2164	0	2183	17	0
1	C	2184	0	2198	15	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	99	0	0	0	0
3	B	44	0	0	1	0
3	C	22	0	0	0	0
All	All	6732	0	6586	45	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 3.

All (45) 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:C:226:MSE:HE3	1:C:258:GLY:HA2	1.67	0.76
1:A:164:VAL:O	1:A:208:ARG:HD3	2.00	0.61
1:C:142:LEU:H	1:C:151:HIS:HE1	1.50	0.60
1:A:142:LEU:H	1:A:151:HIS:HE1	1.50	0.60
1:B:137:VAL:HG22	1:B:160:LYS:HG3	1.85	0.59
1:B:142:LEU:H	1:B:151:HIS:HE1	1.50	0.58
1:C:137:VAL:HG22	1:C:160:LYS:HG3	1.85	0.57
1:A:151:HIS:HD2	1:A:161:THR:OG1	1.88	0.56
1:B:175:LYS:O	1:B:178:LYS:HG3	2.06	0.56
1:A:282:PHE:O	1:A:283:HIS:HB2	2.06	0.55
1:B:184:ILE:HG23	1:B:188:HIS:HB2	1.89	0.55
1:A:114:SER:HB2	1:A:223:GLU:O	2.08	0.53
1:B:63:HIS:O	1:B:63:HIS:ND1	2.43	0.52
1:A:164:VAL:HG12	1:A:208:ARG:HG2	1.91	0.52
1:A:226:MSE:HE1	1:A:261:HIS:HB2	1.91	0.52
1:C:217:ARG:HD3	1:C:281:GLU:HB3	1.93	0.51
1:C:164:VAL:HG22	1:C:208:ARG:HG2	1.94	0.50
1:B:165:ILE:HG12	3:B:422:HOH:O	2.12	0.49
1:C:114:SER:HB2	1:C:223:GLU:O	2.13	0.49
1:A:22:LEU:O	1:A:26:GLU:HG3	2.12	0.49
1:A:115:ARG:HH22	1:A:208:ARG:HH22	1.60	0.48
1:B:174:PRO:HG2	1:B:177:ASN:HD22	1.78	0.47
1:B:114:SER:HB2	1:B:223:GLU:O	2.15	0.46
1:B:115:ARG:HH22	1:B:208:ARG:HH22	1.64	0.46
1:B:143:ALA:HA	1:B:174:PRO:HD3	1.98	0.45
1:B:114:SER:N	1:B:146:ILE:HD11	2.33	0.44
1:C:115:ARG:HH22	1:C:208:ARG:HH22	1.65	0.44
1:A:36:LEU:HD21	1:C:51:VAL:HG21	1.99	0.44
1:A:115:ARG:HH22	1:A:208:ARG:NH2	2.16	0.43
1:A:222:ALA:HB2	1:A:247:ILE:HD12	2.00	0.42
1:A:283:HIS:CD2	1:C:176:ALA:HB2	2.54	0.42
1:C:255:LEU:H	1:C:255:LEU:HG	1.71	0.42
1:C:125:VAL:HG21	1:C:146:ILE:HG23	2.02	0.42
1:C:222:ALA:HB2	1:C:247:ILE:HD12	2.01	0.42
1:B:115:ARG:HA	1:B:144:LYS:O	2.20	0.42
1:B:151:HIS:HD2	1:B:161:THR:OG1	2.03	0.42
1:B:115:ARG:HH22	1:B:208:ARG:NH2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LYS:HG3	1:C:174:PRO:HG3	2.00	0.41
1:C:85:LEU:HD22	1:C:215:LEU:HD13	2.03	0.41
1:C:201:LEU:HD23	1:C:203:PHE:HE2	1.86	0.41
1:B:172:PHE:CB	1:B:178:LYS:HG2	2.51	0.41
1:A:85:LEU:HD22	1:A:215:LEU:HD13	2.04	0.40
1:B:222:ALA:HB2	1:B:247:ILE:HD12	2.03	0.40
1:A:125:VAL:HG21	1:A:146:ILE:HG23	2.02	0.40
1:B:202:LYS:HD3	1:B:202:LYS:HA	1.76	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	281/288 (98%)	273 (97%)	8 (3%)	0	100 100
1	B	278/288 (96%)	267 (96%)	11 (4%)	0	100 100
1	C	280/288 (97%)	276 (99%)	3 (1%)	1 (0%)	30 55
All	All	839/864 (97%)	816 (97%)	22 (3%)	1 (0%)	48 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	ASP

#### 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	235/235 (100%)	218 (93%)	17 (7%)	12 30
1	B	232/235 (99%)	211 (91%)	21 (9%)	7 19
1	C	234/235 (100%)	214 (92%)	20 (8%)	8 21
All	All	701/705 (99%)	643 (92%)	58 (8%)	9 22

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	51	VAL
1	A	79	ASP
1	A	93	VAL
1	A	142	LEU
1	A	156	GLN
1	A	202	LYS
1	A	208	ARG
1	A	210	ARG
1	A	215	LEU
1	A	221	VAL
1	A	230	SER
1	A	238	MSE
1	A	244	VAL
1	A	274	GLN
1	A	279	GLU
1	A	283	HIS
1	B	16	LEU
1	B	54	GLU
1	B	55	ARG
1	B	66	LYS
1	B	79	ASP
1	B	93	VAL
1	B	117	CYS
1	B	126	GLU
1	B	142	LEU
1	B	146	ILE
1	B	164	VAL
1	B	189	LEU
1	B	202	LYS
1	B	208	ARG
1	B	210	ARG

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Mol	Chain	Res	Type
1	B	215	LEU
1	B	221	VAL
1	B	230	SER
1	B	238	MSE
1	B	268	LYS
1	B	274	GLN
1	C	26	GLU
1	C	54	GLU
1	C	79	ASP
1	C	93	VAL
1	C	142	LEU
1	C	164	VAL
1	C	171	VAL
1	C	186	ASN
1	C	202	LYS
1	C	208	ARG
1	C	210	ARG
1	C	215	LEU
1	C	221	VAL
1	C	226	MSE
1	C	230	SER
1	C	238	MSE
1	C	244	VAL
1	C	255	LEU
1	C	274	GLN
1	C	281	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	186	ASN
1	B	151	HIS
1	B	177	ASN
1	C	151	HIS
1	C	199	GLN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

5 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	SO4	A	302	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	C	300	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	B	300	-	4,4,4	0.30	0	6,6,6	0.19	0
2	SO4	A	301[A]	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	A	301[B]	-	4,4,4	0.35	0	6,6,6	0.18	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 [\(i\)](#)

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	278/288 (96%)	-0.07	7 (2%) 58 57	26, 43, 65, 91	0
1	B	275/288 (95%)	1.23	74 (26%) 2 2	34, 59, 86, 105	0
1	C	277/288 (96%)	0.87	24 (8%) 17 16	46, 67, 89, 109	0
All	All	830/864 (96%)	0.68	105 (12%) 9 8	26, 57, 85, 109	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	LYS	5.8
1	B	174	PRO	5.6
1	C	282	PHE	5.4
1	B	177	ASN	5.2
1	B	155	LEU	5.0
1	B	158	GLY	5.0
1	B	159	GLY	4.9
1	B	183	TYR	4.4
1	B	184	ILE	4.4
1	B	185	GLY	4.2
1	B	106	PHE	4.1
1	B	175	LYS	4.1
1	B	98	LYS	4.1
1	C	119	LYS	3.9
1	B	173	TYR	3.9
1	C	236	ARG	3.9
1	B	280	PHE	3.8
1	B	154	ALA	3.8
1	B	180	LEU	3.8
1	B	202	LYS	3.8
1	B	199	GLN	3.8
1	B	146	ILE	3.7
1	A	283	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	151	HIS	3.7
1	B	143	ALA	3.6
1	B	188	HIS	3.6
1	B	133	GLU	3.6
1	B	156	GLN	3.5
1	B	66	LYS	3.4
1	B	134	ASN	3.4
1	B	117	CYS	3.4
1	B	172	PHE	3.4
1	B	120	GLN	3.3
1	C	29	GLU	3.3
1	C	227	ARG	3.2
1	A	48	ASN	3.2
1	B	176	ALA	3.2
1	C	225	LYS	3.2
1	B	189	LEU	3.1
1	B	217	ARG	3.1
1	B	171	VAL	3.1
1	B	190	VAL	3.0
1	B	132	LEU	3.0
1	C	57	PHE	3.0
1	A	30	ASN	2.9
1	B	83	TRP	2.9
1	C	83	TRP	2.9
1	B	200	PRO	2.9
1	B	187	ASP	2.8
1	B	147	ASP	2.8
1	C	31	VAL	2.8
1	B	142	LEU	2.8
1	B	97	TYR	2.8
1	C	89	TYR	2.8
1	B	196	PRO	2.7
1	B	115	ARG	2.7
1	B	63	HIS	2.7
1	B	148	THR	2.6
1	C	107	PRO	2.6
1	C	2	LYS	2.6
1	C	123	LYS	2.5
1	B	255	LEU	2.5
1	B	179	ARG	2.5
1	B	116	ALA	2.5
1	C	115	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	60	ASP	2.5
1	C	241	GLY	2.5
1	C	35	LEU	2.5
1	B	161	THR	2.4
1	B	104	LEU	2.4
1	C	34	GLU	2.4
1	B	122	ALA	2.4
1	C	116	ALA	2.3
1	B	101	LEU	2.3
1	B	181	GLN	2.3
1	B	121	GLY	2.3
1	B	259	CYS	2.3
1	C	158	GLY	2.3
1	B	198	GLU	2.3
1	A	252	LEU	2.3
1	A	281	GLU	2.2
1	B	150	ALA	2.2
1	B	197	GLY	2.2
1	B	170	ASP	2.2
1	C	33	GLN	2.2
1	B	178	LYS	2.2
1	B	113	GLY	2.2
1	B	225	LYS	2.2
1	A	239	GLU	2.2
1	B	30	ASN	2.2
1	B	103	LEU	2.2
1	B	203	PHE	2.1
1	C	48	ASN	2.1
1	B	127	LYS	2.1
1	C	127	LYS	2.1
1	B	253	ASP	2.1
1	C	147	ASP	2.1
1	B	160	LYS	2.1
1	B	167	THR	2.1
1	B	12	LYS	2.0
1	B	144	LYS	2.0
1	A	253	ASP	2.0
1	C	27	TYR	2.0
1	B	201	LEU	2.0
1	B	157	ASN	2.0

## 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 monosaccharides 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
2	SO4	B	300	5/5	0.77	0.17	116,120,120,122	0
2	SO4	A	301[B]	5/5	0.85	0.30	35,39,40,41	5
2	SO4	A	301[A]	5/5	0.85	0.30	64,68,69,69	5
2	SO4	C	300	5/5	0.85	0.14	98,102,103,103	0
2	SO4	A	302	5/5	0.97	0.07	50,53,55,57	0

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

There are no such residues in this entry.