



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:51 pm GMT

PDB ID : 4B6E  
Title : Discovery of an allosteric mechanism for the regulation of HCV NS3 protein function  
Authors : Saalau-Bethell, S.M.; Woodhead, A.J.; Chessari, G.; Carr, M.G.; Coyle, J.; Graham, B.; Hiscock, S.D.; Murray, C.W.; Pathuri, P.; Rich, S.J.; Richardson, C.J.; Williams, P.A.; Jhoti, H.  
Deposited on : 2012-08-09  
Resolution : 2.46 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

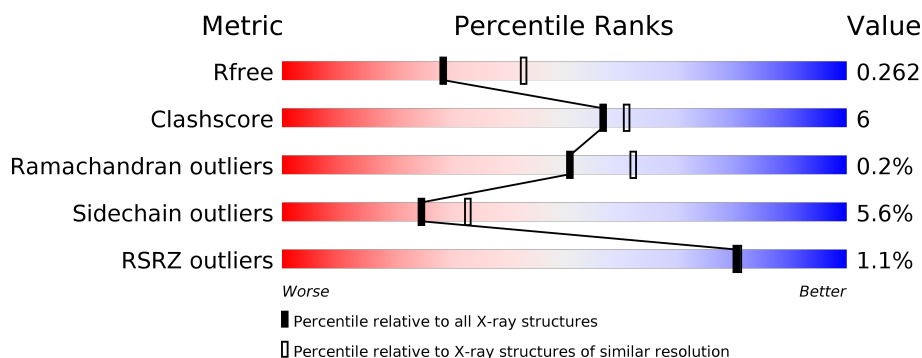
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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))
$R_{free}$	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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	A	683	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>5%</div> </div> </div>
1	B	683	<div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div>

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
2	SO4	B	1721	-	-	-	X
3	10L	B	1722	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9975 atoms, of which 7 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 NON-STRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	646	Total	C	N	O	S	0	0	1
			4808	3026	835	917	30			
1	B	643	Total	C	N	O	S	0	0	1
			4794	3019	832	913	30			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	EXPRESSION TAG	UNP P26663
A	-33	GLY	-	EXPRESSION TAG	UNP P26663
A	-32	SER	-	EXPRESSION TAG	UNP P26663
A	-31	SER	-	EXPRESSION TAG	UNP P26663
A	-30	HIS	-	EXPRESSION TAG	UNP P26663
A	-29	HIS	-	EXPRESSION TAG	UNP P26663
A	-28	HIS	-	EXPRESSION TAG	UNP P26663
A	-27	HIS	-	EXPRESSION TAG	UNP P26663
A	-26	HIS	-	EXPRESSION TAG	UNP P26663
A	-25	HIS	-	EXPRESSION TAG	UNP P26663
A	-24	SER	-	EXPRESSION TAG	UNP P26663
A	-23	SER	-	EXPRESSION TAG	UNP P26663
A	-22	GLY	-	EXPRESSION TAG	UNP P26663
A	-21	LEU	-	EXPRESSION TAG	UNP P26663
A	-20	VAL	-	EXPRESSION TAG	UNP P26663
A	-19	PRO	-	EXPRESSION TAG	UNP P26663
A	-18	ARG	-	EXPRESSION TAG	UNP P26663
A	-17	GLY	-	EXPRESSION TAG	UNP P26663
A	-16	SER	-	EXPRESSION TAG	UNP P26663
A	-15	HIS	-	EXPRESSION TAG	UNP P26663
A	-14	MET	-	EXPRESSION TAG	UNP P26663
A	-1	GLY	-	LINKER	UNP P26663
A	0	SER	-	LINKER	UNP P26663
A	1	GLY	-	LINKER	UNP P26663

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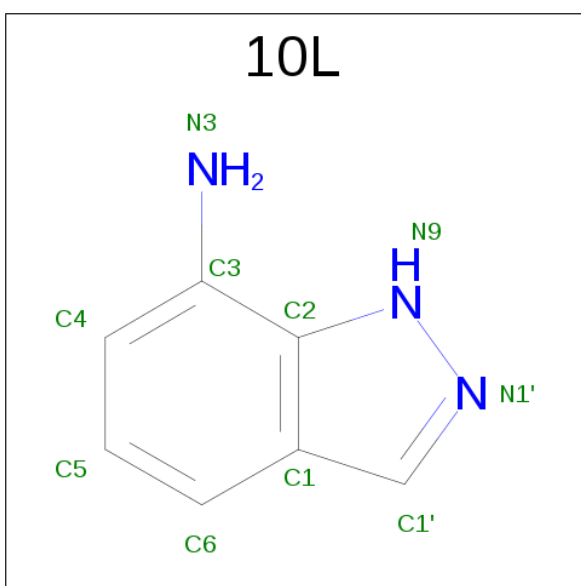
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	LINKER	UNP P26663
B	-34	MET	-	EXPRESSION TAG	UNP P26663
B	-33	GLY	-	EXPRESSION TAG	UNP P26663
B	-32	SER	-	EXPRESSION TAG	UNP P26663
B	-31	SER	-	EXPRESSION TAG	UNP P26663
B	-30	HIS	-	EXPRESSION TAG	UNP P26663
B	-29	HIS	-	EXPRESSION TAG	UNP P26663
B	-28	HIS	-	EXPRESSION TAG	UNP P26663
B	-27	HIS	-	EXPRESSION TAG	UNP P26663
B	-26	HIS	-	EXPRESSION TAG	UNP P26663
B	-25	HIS	-	EXPRESSION TAG	UNP P26663
B	-24	SER	-	EXPRESSION TAG	UNP P26663
B	-23	SER	-	EXPRESSION TAG	UNP P26663
B	-22	GLY	-	EXPRESSION TAG	UNP P26663
B	-21	LEU	-	EXPRESSION TAG	UNP P26663
B	-20	VAL	-	EXPRESSION TAG	UNP P26663
B	-19	PRO	-	EXPRESSION TAG	UNP P26663
B	-18	ARG	-	EXPRESSION TAG	UNP P26663
B	-17	GLY	-	EXPRESSION TAG	UNP P26663
B	-16	SER	-	EXPRESSION TAG	UNP P26663
B	-15	HIS	-	EXPRESSION TAG	UNP P26663
B	-14	MET	-	EXPRESSION TAG	UNP P26663
B	-1	GLY	-	LINKER	UNP P26663
B	0	SER	-	LINKER	UNP P26663
B	1	GLY	-	LINKER	UNP P26663
B	2	SER	-	LINKER	UNP P26663

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



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

- Molecule 3 is 1H-INDAZOL-7-AMINE (three-letter code: 10L) (formula:  $C_7H_7N_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	N	0	0
			17	7	7	3		

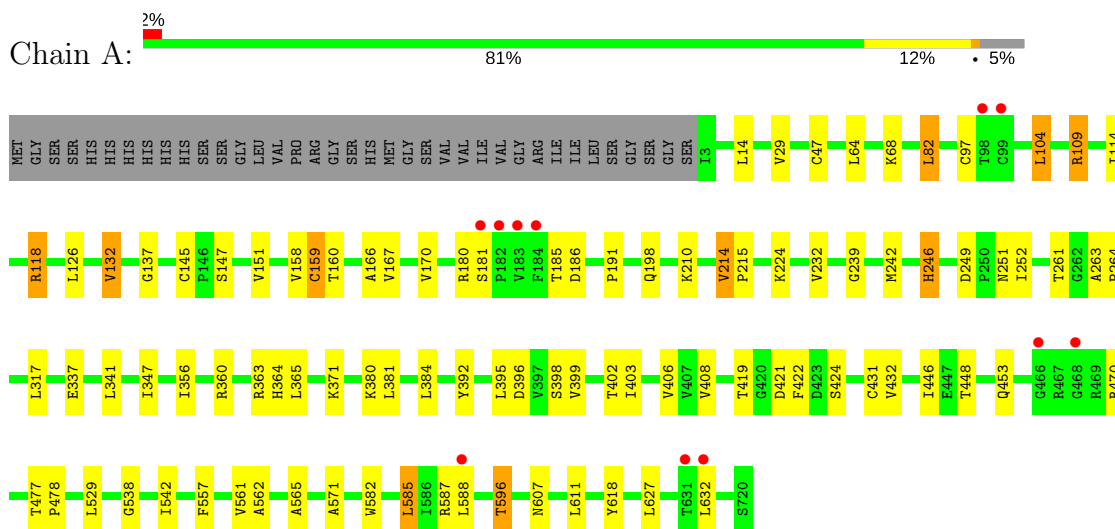
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total 186	O 186	0	0
4	B	160	Total 160	O 160	0	0

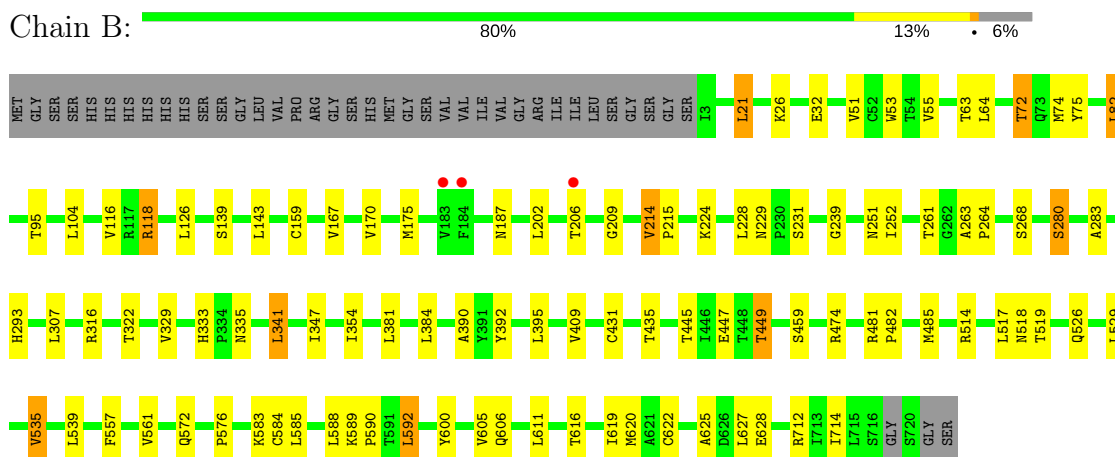
### 3 Residue-property plots [i](#)

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: NON-STRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3



- Molecule 1: NON-STRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.40Å 111.31Å 141.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.57 – 2.46 87.57 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.0 (87.57-2.46) 98.0 (87.57-2.47)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019I	Depositor
R, $R_{free}$	0.187 , 0.257 0.193 , 0.262	Depositor DCC
$R_{free}$ test set	2645 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: SO4, 10L

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	0.58	2/4916 (0.0%)	0.70	2/6713 (0.0%)
1	B	0.59	1/4901 (0.0%)	0.69	0/6692
All	All	0.59	3/9817 (0.0%)	0.69	2/13405 (0.0%)

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	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	CYS	CB-SG	-6.15	1.71	1.82
1	A	47	CYS	CB-SG	-5.98	1.72	1.81
1	A	159	CYS	CB-SG	-5.70	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	109	ARG	NE-CZ-NH2	-5.19	117.70	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	403	ILE	CA

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	4808	0	4783	52	0
1	B	4794	0	4771	59	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	B	10	7	7	1	0
4	A	186	0	0	3	0
4	B	160	0	0	2	0
All	All	9968	7	9561	110	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 6.

The worst 5 of 110 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:A:97:CYS:SG	1:A:151:VAL:HG23	2.02	0.99
1:A:365:LEU:HD13	1:A:408:VAL:HG23	1.54	0.87
1:A:365:LEU:CD1	1:A:408:VAL:HG23	2.08	0.84
1:A:596:THR:HG22	1:A:607:ASN:HD22	1.44	0.83
1:A:365:LEU:HD13	1:A:408:VAL:CG2	2.10	0.80

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	642/683 (94%)	614 (96%)	26 (4%)	2 (0%)	44	55
1	B	638/683 (93%)	616 (97%)	21 (3%)	1 (0%)	51	62
All	All	1280/1366 (94%)	1230 (96%)	47 (4%)	3 (0%)	51	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	A	403	ILE
1	B	572	GLN

### 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	526/557 (94%)	496 (94%)	30 (6%)	24	32
1	B	525/557 (94%)	496 (94%)	29 (6%)	25	33
All	All	1051/1114 (94%)	992 (94%)	59 (6%)	25	33

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	LEU
1	B	64	LEU
1	B	584	CYS
1	A	596	THR
1	A	627	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	ASN

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Mol	Chain	Res	Type
1	B	221	GLN
1	B	293	HIS
1	A	607	ASN
1	B	251	ASN

### 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 carbohydrates in this entry.

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

3 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	1721	-	4,4,4	0.11	0	6,6,6	0.37	0
2	SO4	B	1721	-	4,4,4	0.16	0	6,6,6	0.13	0
3	10L	B	1722	-	10,11,11	0.63	0	6,15,15	0.68	0

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	SO4	A	1721	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1721	-	-	0/0/0/0	0/0/0/0
3	10L	B	1722	-	-	0/0/0/0	0/2/2/2

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1722	10L	1	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	646/683 (94%)	-0.02	11 (1%) 70 67	14, 38, 71, 82	0
1	B	643/683 (94%)	-0.12	3 (0%) 90 92	19, 38, 67, 96	0
All	All	1289/1366 (94%)	-0.07	14 (1%) 80 81	14, 38, 68, 96	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	VAL	5.9
1	A	182	PRO	4.6
1	A	468	GLY	4.1
1	A	99	CYS	4.0
1	B	184	PHE	4.0

### 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 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
3	10L	B	1722	10/10	0.78	0.32	7.53	66,70,71,71	0
2	SO4	B	1721	5/5	0.43	0.30	2.53	142,142,143,143	0
2	SO4	A	1721	5/5	0.98	0.14	0.02	43,43,44,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.