



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 09:07 am BST

PDB ID : 5WHO  
Title : Kelch domain of human Keap1 bound to small molecule inhibitor fragment: 4-oxo-4H-1-benzopyran-2-carboxylic acid  
Authors : Carolan, J.P.; Lynch, A.J.; Allen, K.N.  
Deposited on : 2017-07-17  
Resolution : 2.23 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

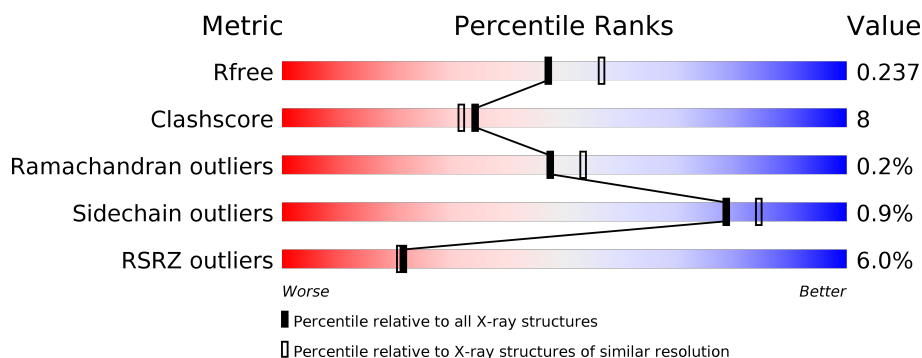
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	336	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>18%</div> <div>17%</div> </div> </div>
1	B	336	<div> <div></div> <div>75%</div> <div>10%</div> <div>14%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4546 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	289	Total	C	N	O	S	0	0	0
			2215	1377	401	421	16			
1	A	280	Total	C	N	O	S	0	0	0
			2142	1330	389	408	15			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	289	MET	-	initiating methionine	UNP Q14145
B	290	GLY	-	expression tag	UNP Q14145
B	291	SER	-	expression tag	UNP Q14145
B	292	SER	-	expression tag	UNP Q14145
B	293	HIS	-	expression tag	UNP Q14145
B	294	HIS	-	expression tag	UNP Q14145
B	295	HIS	-	expression tag	UNP Q14145
B	296	HIS	-	expression tag	UNP Q14145
B	297	HIS	-	expression tag	UNP Q14145
B	298	HIS	-	expression tag	UNP Q14145
B	299	SER	-	expression tag	UNP Q14145
B	300	SER	-	expression tag	UNP Q14145
B	301	GLY	-	expression tag	UNP Q14145
B	302	GLY	-	expression tag	UNP Q14145
B	303	GLU	-	expression tag	UNP Q14145
B	304	ASN	-	expression tag	UNP Q14145
B	305	LEU	-	expression tag	UNP Q14145
B	306	TYR	-	expression tag	UNP Q14145
B	307	PHE	-	expression tag	UNP Q14145
B	308	GLN	-	expression tag	UNP Q14145
B	309	GLY	-	expression tag	UNP Q14145
B	310	HIS	-	expression tag	UNP Q14145
B	311	MET	-	expression tag	UNP Q14145
B	319	SER	CYS	engineered mutation	UNP Q14145
B	540	ALA	GLU	engineered mutation	UNP Q14145

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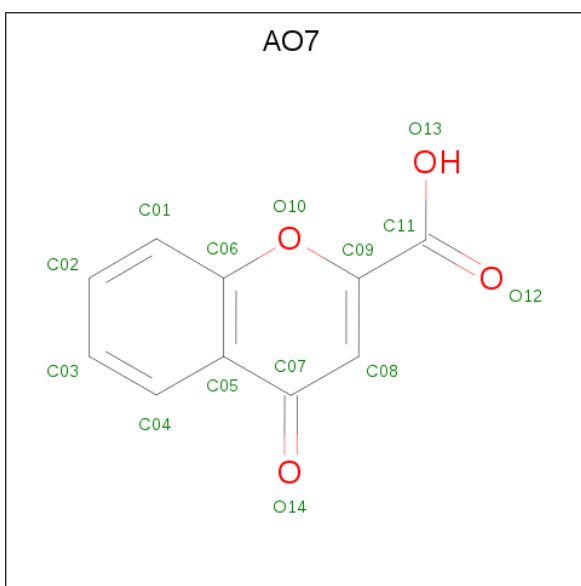
Chain	Residue	Modelled	Actual	Comment	Reference
B	542	ALA	GLU	engineered mutation	UNP Q14145
B	613	SER	CYS	engineered mutation	UNP Q14145
B	622	SER	CYS	engineered mutation	UNP Q14145
B	624	SER	CYS	engineered mutation	UNP Q14145
A	289	MET	-	initiating methionine	UNP Q14145
A	290	GLY	-	expression tag	UNP Q14145
A	291	SER	-	expression tag	UNP Q14145
A	292	SER	-	expression tag	UNP Q14145
A	293	HIS	-	expression tag	UNP Q14145
A	294	HIS	-	expression tag	UNP Q14145
A	295	HIS	-	expression tag	UNP Q14145
A	296	HIS	-	expression tag	UNP Q14145
A	297	HIS	-	expression tag	UNP Q14145
A	298	HIS	-	expression tag	UNP Q14145
A	299	SER	-	expression tag	UNP Q14145
A	300	SER	-	expression tag	UNP Q14145
A	301	GLY	-	expression tag	UNP Q14145
A	302	GLY	-	expression tag	UNP Q14145
A	303	GLU	-	expression tag	UNP Q14145
A	304	ASN	-	expression tag	UNP Q14145
A	305	LEU	-	expression tag	UNP Q14145
A	306	TYR	-	expression tag	UNP Q14145
A	307	PHE	-	expression tag	UNP Q14145
A	308	GLN	-	expression tag	UNP Q14145
A	309	GLY	-	expression tag	UNP Q14145
A	310	HIS	-	expression tag	UNP Q14145
A	311	MET	-	expression tag	UNP Q14145
A	319	SER	CYS	engineered mutation	UNP Q14145
A	540	ALA	GLU	engineered mutation	UNP Q14145
A	542	ALA	GLU	engineered mutation	UNP Q14145
A	613	SER	CYS	engineered mutation	UNP Q14145
A	622	SER	CYS	engineered mutation	UNP Q14145
A	624	SER	CYS	engineered mutation	UNP Q14145

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



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

- Molecule 3 is 4-oxo-4H-1-benzopyran-2-carboxylic acid (three-letter code: AO7) (formula: C<sub>10</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	10	4		

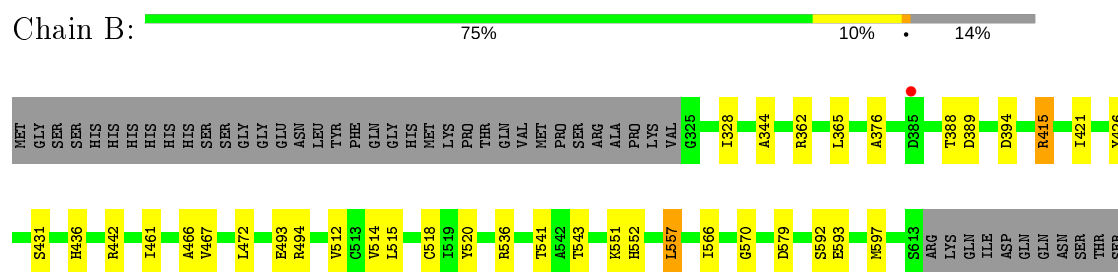
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	130	Total	O	0	0
			130	130		
4	A	25	Total	O	0	0
			25	25		

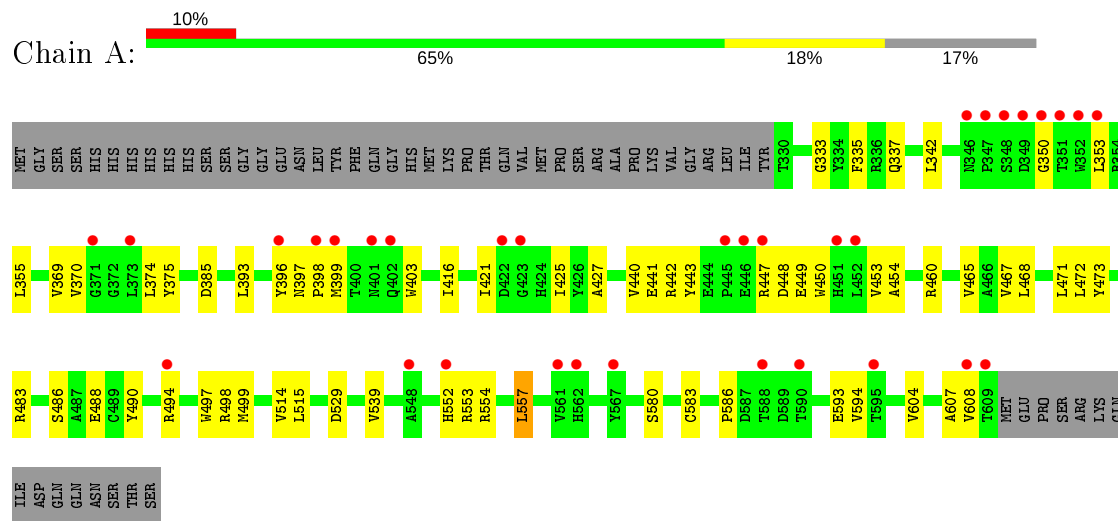
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.46 Å 69.09 Å 143.21 Å 90.00° 91.11° 90.00°	Depositor
Resolution (Å)	51.85 – 2.23 51.85 – 2.23	Depositor EDS
% Data completeness (in resolution range)	96.6 (51.85-2.23) 96.1 (51.85-2.23)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.22 Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.196 , 0.237 0.196 , 0.237	Depositor DCC
$R_{free}$ test set	1999 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: AO7, 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	0.35	0/2194	0.57	0/2989
1	B	0.44	0/2269	0.62	1/3090 (0.0%)
All	All	0.40	0/4463	0.60	1/6079 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	ARG	NE-CZ-NH2	-5.45	117.57	120.30

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	2142	0	2035	47	0
1	B	2215	0	2109	27	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
3	A	14	0	0	1	0
4	A	25	0	0	0	0
4	B	130	0	0	1	0
All	All	4546	0	4144	72	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 8.

The worst 5 of 72 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:466:ALA:HB1	1:B:514:VAL:HG23	1.73	0.71
1:A:554:ARG:HG3	1:A:557:LEU:HD22	1.74	0.70
1:A:515:LEU:HD21	1:A:586:PRO:HG3	1.79	0.65
1:A:583:CYS:HB2	1:A:594:VAL:HG21	1.80	0.63
1:B:436:HIS:HB3	1:B:461:ILE:HD11	1.80	0.63

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	278/336 (83%)	263 (95%)	14 (5%)	1 (0%)	34	35
1	B	287/336 (85%)	278 (97%)	9 (3%)	0	100	100
All	All	565/672 (84%)	541 (96%)	23 (4%)	1 (0%)	47	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	GLY

### 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	225/275 (82%)	222 (99%)	3 (1%)	69	76
1	B	233/275 (85%)	232 (100%)	1 (0%)	91	93
All	All	458/550 (83%)	454 (99%)	4 (1%)	78	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	557	LEU
1	A	557	LEU
1	A	580	SER
1	A	593	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	424	HIS
1	A	469	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](#)

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
3	AO7	A	702	-	9,15,15	4.13	5 (55%)	7,21,21	3.58	3 (42%)
2	SO4	B	701	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	A	701	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	B	703	-	4,4,4	0.22	0	6,6,6	0.61	0
2	SO4	B	702	-	4,4,4	0.29	0	6,6,6	0.38	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
3	AO7	A	702	-	-	0/0/4/4	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	AO7	O14-C07	9.85	1.40	1.23
3	A	702	AO7	O10-C06	5.37	1.46	1.36
3	A	702	AO7	C05-C06	2.81	1.45	1.41
3	A	702	AO7	C08-C09	-2.56	1.31	1.36
3	A	702	AO7	C08-C07	-2.14	1.33	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	AO7	O10-C06-C05	-8.37	113.12	121.20
3	A	702	AO7	C08-C07-C05	-2.53	120.24	123.05
3	A	702	AO7	C04-C05-C06	2.28	119.14	116.50

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	A	702	AO7	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	280/336 (83%)	0.58	33 (11%) 4 3	26, 52, 80, 100	0
1	B	289/336 (86%)	-0.25	1 (0%) 94 94	21, 29, 49, 66	0
All	All	569/672 (84%)	0.16	34 (5%) 21 21	21, 39, 74, 100	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	THR	7.6
1	A	446	GLU	5.4
1	A	608	VAL	5.2
1	A	399	MET	5.0
1	A	402	GLN	4.4

### 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
3	AO7	A	702	14/14	0.73	0.26	48,53,61,65	0
2	SO4	B	703	5/5	0.93	0.22	33,46,54,63	0
2	SO4	B	702	5/5	0.95	0.11	35,41,53,55	0
2	SO4	A	701	5/5	0.96	0.19	56,60,69,71	0
2	SO4	B	701	5/5	0.98	0.11	42,46,48,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.