



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2022 – 01:40 AM JST

PDB ID : 7F00  
Title : Crystal structure of SPD\_0310  
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Deposited on : 2021-06-03  
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : ?? (??), CSD ??CSD?? (????)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
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) : 2.29

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

 $R_{free}$ 

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.

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## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7357 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.

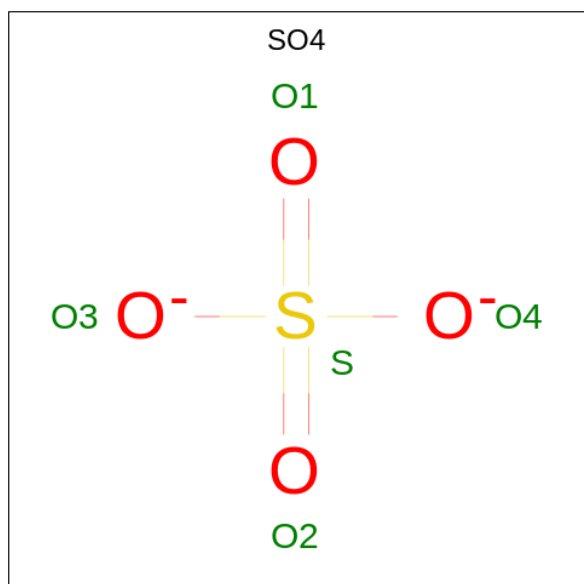
- Molecule 1 is a protein called UPF0371 protein SPRM200\_0309.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3695	2349	627	707	12			
1	B	468	Total	C	N	O	S	0	0	0
			3627	2304	612	699	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A2U3RY31
A	0	SER	-	expression tag	UNP A0A2U3RY31
B	-1	GLY	-	expression tag	UNP A0A2U3RY31
B	0	SER	-	expression tag	UNP A0A2U3RY31

- 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	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	B	1	Total	O	S	0	0
			5	4	1		

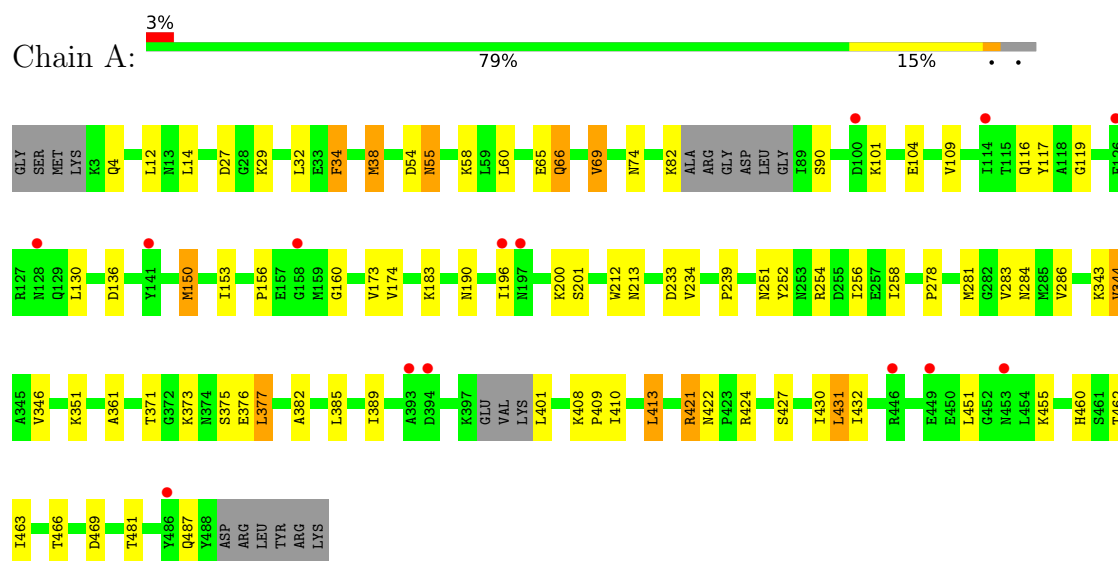
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	9	Total	O	0	0
			9	9		

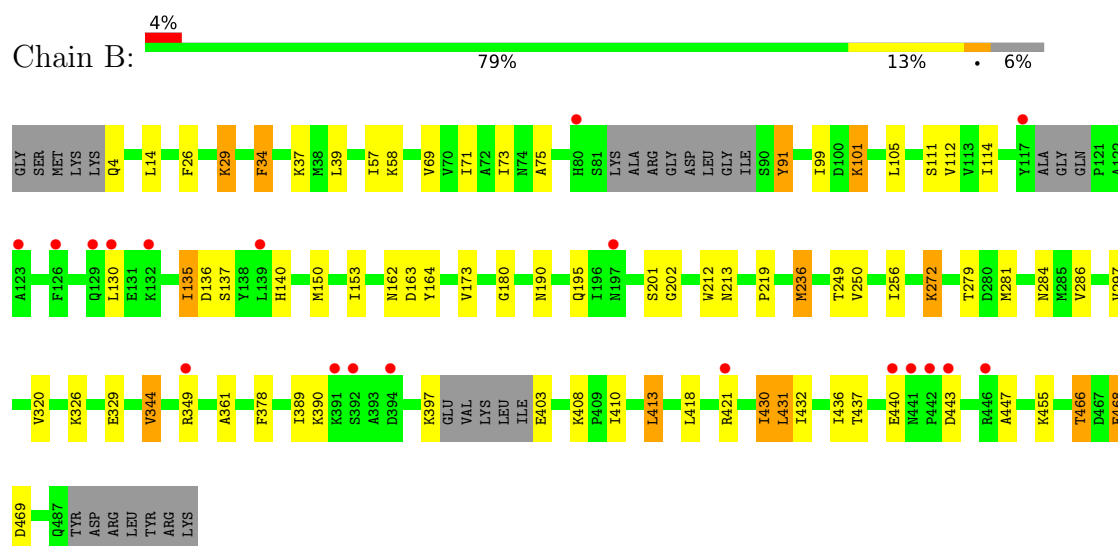
### 3 Residue-property plots [i](#)

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: UPF0371 protein SPRM200\_0309



#### • Molecule 1: UPF0371 protein SPRM200\_0309



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.85Å 87.85Å 326.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.70 43.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.01-2.70) 98.1 (43.53-2.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.97 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, $R_{free}$	0.221 , 0.265 0.221 , 0.265	Depositor DCC
$R_{free}$ test set	1795 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% 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	0.36	0/3765	0.53	0/5104
1	B	0.37	0/3696	0.52	0/5009
All	All	0.37	0/7461	0.53	0/10113

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

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	3695	0	3665	46	0
1	B	3627	0	3573	39	0
2	A	5	0	0	0	0
2	B	15	0	0	1	0
3	A	6	0	0	0	0
3	B	9	0	0	0	0
All	All	7357	0	7238	79	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 5.

All (79) 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:421:ARG:HD2	1:A:422:ASN:H	1.50	0.74
1:A:233:ASP:OD2	1:A:254:ARG:NH1	2.26	0.68
1:B:236:MET:HG3	1:B:256:ILE:HD12	1.77	0.64
1:B:29:LYS:HD3	1:B:201:SER:HB3	1.79	0.63
1:A:278:PRO:HA	1:A:281:MET:HG2	1.81	0.63
1:A:431:LEU:HB3	1:B:413:LEU:HD11	1.83	0.60
1:A:413:LEU:HD11	1:B:431:LEU:HB3	1.84	0.60
1:B:249:THR:HG21	1:B:279:THR:OG1	2.02	0.60
1:A:409:PRO:HG2	1:B:436:ILE:HD13	1.84	0.59
1:A:104:GLU:OE2	1:B:421:ARG:NH2	2.34	0.59
1:A:38:MET:HE1	1:A:60:LEU:HD11	1.86	0.57
1:B:403:GLU:HG2	1:B:437:THR:HG21	1.87	0.55
1:B:73:ILE:HD11	1:B:91:TYR:HB3	1.89	0.53
1:B:75:ALA:HA	1:B:114:ILE:HD11	1.89	0.53
1:B:112:VAL:O	1:B:137:SER:HA	2.08	0.53
1:B:39:LEU:HD21	1:B:101:LYS:HG2	1.90	0.53
1:A:27:ASP:HB2	1:A:200:LYS:HD3	1.92	0.52
1:A:239:PRO:HD2	1:A:256:ILE:HD12	1.92	0.52
1:A:38:MET:CE	1:A:60:LEU:HD11	2.40	0.52
1:B:99:ILE:HD13	1:B:135:ILE:HD12	1.91	0.52
1:A:252:TYR:O	1:A:256:ILE:HG12	2.10	0.52
1:A:65:GLU:HG3	1:A:66:GLN:HG2	1.93	0.51
1:B:284:ASN:OD1	1:B:286:VAL:HG12	2.11	0.51
1:A:150:MET:HE2	1:A:153:ILE:HD11	1.92	0.51
1:A:117:TYR:CZ	1:A:119:GLY:HA2	2.45	0.51
1:A:389:ILE:HD11	1:A:451:LEU:HD23	1.94	0.50
1:A:466:THR:HG23	1:A:469:ASP:H	1.76	0.50
1:B:413:LEU:HD22	1:B:418:LEU:HD13	1.93	0.50
1:A:156:PRO:HA	1:A:160:GLY:HA3	1.93	0.50
1:A:69:VAL:HG22	1:A:109:VAL:HA	1.96	0.48
1:A:74:ASN:ND2	1:A:116:GLN:HG3	2.29	0.47
1:A:54:ASP:OD2	1:A:58:LYS:HE2	2.15	0.47
1:A:212:TRP:CZ3	1:A:213:ASN:HB3	2.49	0.47
1:A:251:ASN:HB3	1:A:256:ILE:HD11	1.97	0.47
1:A:343:LYS:O	1:A:346:VAL:HG22	2.15	0.46
1:A:183:LYS:HE3	1:A:183:LYS:HB2	1.75	0.46
1:B:150:MET:HB3	1:B:150:MET:HE3	1.75	0.46
1:B:326:LYS:HD3	1:B:329:GLU:OE1	2.16	0.46
1:B:29:LYS:HD3	1:B:201:SER:CB	2.44	0.46
1:B:26:PHE:CD1	1:B:202:GLY:HA3	2.51	0.46
1:A:422:ASN:OD1	1:A:424:ARG:NE	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PHE:CD1	1:A:173:VAL:HG13	2.52	0.45
1:B:180:GLY:N	2:B:501:SO4:O2	2.32	0.45
1:B:466:THR:OG1	1:B:468:GLU:HG2	2.16	0.45
1:B:71:ILE:HB	1:B:112:VAL:HG22	1.97	0.45
1:A:12:LEU:HD21	1:A:55:ASN:HB2	1.97	0.45
1:A:233:ASP:OD1	1:A:254:ARG:HD3	2.17	0.45
1:B:389:ILE:HG21	1:B:447:ALA:HB1	1.99	0.45
1:A:410:ILE:HG12	1:B:432:ILE:HG23	1.99	0.45
1:A:375:SER:O	1:A:424:ARG:HD3	2.17	0.45
1:B:140:HIS:ND1	1:B:162:ASN:HB3	2.31	0.45
1:B:466:THR:HG23	1:B:469:ASP:H	1.81	0.45
1:B:219:PRO:HG2	1:B:297:VAL:HG13	1.98	0.45
1:B:212:TRP:HB2	1:B:249:THR:HG23	1.99	0.45
1:A:254:ARG:O	1:A:258:ILE:HG12	2.17	0.44
1:A:29:LYS:HB3	1:A:201:SER:HB3	1.99	0.44
1:A:432:ILE:HG23	1:B:410:ILE:HG12	1.99	0.44
1:A:377:LEU:HD22	1:A:377:LEU:H	1.82	0.44
1:A:375:SER:OG	1:A:376:GLU:N	2.50	0.44
1:B:212:TRP:CZ3	1:B:213:ASN:HB3	2.53	0.44
1:A:430:ILE:HD13	1:A:430:ILE:HA	1.91	0.43
1:A:382:ALA:HB1	1:A:430:ILE:HG13	2.00	0.43
1:A:463:ILE:HG21	1:A:487:GLN:HG2	1.99	0.43
1:A:460:HIS:HA	1:A:481:THR:O	2.19	0.43
1:A:284:ASN:OD1	1:A:286:VAL:HG12	2.18	0.43
1:B:430:ILE:HA	1:B:430:ILE:HD12	1.77	0.43
1:A:351:LYS:HG3	1:A:371:THR:HG21	2.00	0.43
1:B:390:LYS:NZ	1:B:397:LYS:HA	2.34	0.42
1:B:378:PHE:CE2	1:B:430:ILE:HD11	2.54	0.42
1:A:385:LEU:HD12	1:A:427:SER:HB2	2.01	0.42
1:A:344:VAL:O	1:A:361:ALA:HB3	2.19	0.42
1:A:174:VAL:HG12	1:A:183:LYS:HG2	2.02	0.41
1:B:140:HIS:HE1	1:B:163:ASP:O	2.03	0.41
1:B:212:TRP:CE3	1:B:213:ASN:HB3	2.55	0.41
1:B:344:VAL:O	1:B:361:ALA:HB3	2.21	0.41
1:B:34:PHE:CD1	1:B:173:VAL:HG13	2.55	0.41
1:B:57:ILE:HG23	1:B:105:LEU:HD13	2.01	0.41
1:A:212:TRP:CE3	1:A:213:ASN:HB3	2.56	0.40
1:B:272:LYS:HE2	1:B:272:LYS:HB2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	471/496 (95%)	459 (98%)	12 (2%)	0	100	100
1	B	460/496 (93%)	446 (97%)	14 (3%)	0	100	100
All	All	931/992 (94%)	905 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	392/417 (94%)	364 (93%)	28 (7%)	14	34
1	B	384/417 (92%)	351 (91%)	33 (9%)	10	24
All	All	776/834 (93%)	715 (92%)	61 (8%)	12	28

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	14	LEU
1	A	32	LEU
1	A	34	PHE
1	A	38	MET
1	A	55	ASN
1	A	66	GLN
1	A	69	VAL

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Mol	Chain	Res	Type
1	A	82	LYS
1	A	90	SER
1	A	101	LYS
1	A	130	LEU
1	A	136	ASP
1	A	150	MET
1	A	190	ASN
1	A	196	ILE
1	A	234	VAL
1	A	283	VAL
1	A	344	VAL
1	A	373	LYS
1	A	377	LEU
1	A	401	LEU
1	A	408	LYS
1	A	413	LEU
1	A	421	ARG
1	A	431	LEU
1	A	455	LYS
1	A	462	THR
1	B	4	GLN
1	B	14	LEU
1	B	29	LYS
1	B	34	PHE
1	B	37	LYS
1	B	58	LYS
1	B	69	VAL
1	B	91	TYR
1	B	101	LYS
1	B	111	SER
1	B	130	LEU
1	B	135	ILE
1	B	136	ASP
1	B	153	ILE
1	B	164	TYR
1	B	190	ASN
1	B	195	GLN
1	B	236	MET
1	B	250	VAL
1	B	272	LYS
1	B	281	MET
1	B	320	VAL

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Mol	Chain	Res	Type
1	B	344	VAL
1	B	349	ARG
1	B	408	LYS
1	B	413	LEU
1	B	430	ILE
1	B	431	LEU
1	B	440	GLU
1	B	443	ASP
1	B	455	LYS
1	B	466	THR
1	B	468	GLU

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

Mol	Chain	Res	Type
1	A	77	ASN
1	B	487	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	477/496 (96%)	0.14	14 (2%) 51 52	23, 54, 83, 95	0
1	B	468/496 (94%)	0.21	19 (4%) 37 36	26, 53, 82, 99	0
All	All	945/992 (95%)	0.18	33 (3%) 44 44	23, 53, 83, 99	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	4.7
1	B	442	PRO	4.3
1	A	394	ASP	4.0
1	B	394	ASP	3.6
1	A	446	ARG	3.5
1	A	197	ASN	3.4
1	B	117	TYR	2.9
1	B	446	ARG	2.7
1	A	486	TYR	2.7
1	B	126	PHE	2.7
1	B	440	GLU	2.7
1	B	441	ASN	2.6
1	B	139	LEU	2.6
1	A	453	ASN	2.6
1	B	130	LEU	2.6
1	B	123	ALA	2.5
1	A	100	ASP	2.5
1	B	443	ASP	2.5
1	B	391	LYS	2.4
1	B	349	ARG	2.4
1	B	132	LYS	2.4
1	A	128	ASN	2.3
1	A	114	ILE	2.3
1	A	126	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	421	ARG	2.1
1	A	141	TYR	2.1
1	A	393	ALA	2.1
1	B	392	SER	2.1
1	B	129	GLN	2.1
1	B	197	ASN	2.1
1	A	158	GLY	2.0
1	B	80	HIS	2.0
1	A	449	GLU	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( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	501	5/5	0.73	0.20	56,57,62,66	5
2	SO4	B	502	5/5	0.77	0.26	58,61,64,67	5
2	SO4	A	501	5/5	0.89	0.15	61,62,64,73	0
2	SO4	B	503	5/5	0.92	0.22	29,29,29,31	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.