



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:34 PM BST

PDB ID : 6PRM  
Title : Crystal structure of apo PsS1\_19B  
Authors : Hettle, A.G.; Boraston, A.B.  
Deposited on : 2019-07-10  
Resolution : 2.50 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

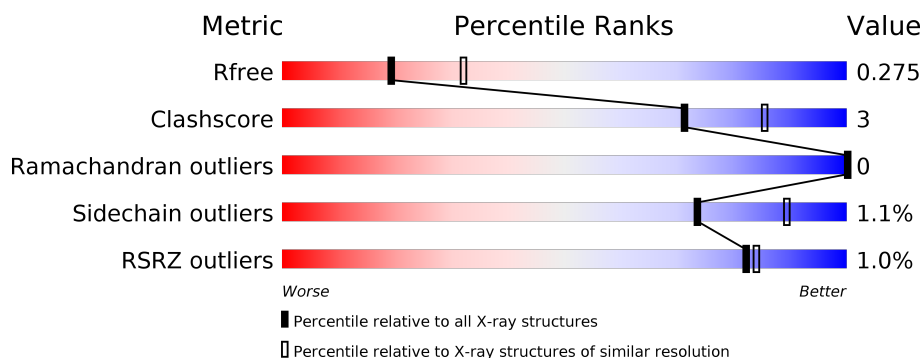
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	469	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	469	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	C	469	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	D	469	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14105 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 exo-4S-kappa carrageenan S1 sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	1	0
			3497	2233	586	668	10			
1	B	447	Total	C	N	O	S	0	1	0
			3497	2232	587	668	10			
1	C	447	Total	C	N	O	S	0	1	0
			3505	2238	589	668	10			
1	D	446	Total	C	N	O	S	0	0	0
			3498	2234	589	665	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

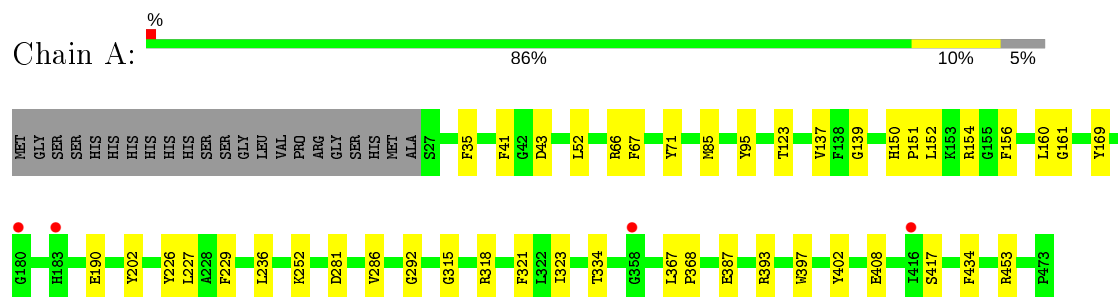
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	28	Total	O	0	0
			28	28		
3	C	24	Total	O	0	0
			24	24		
3	D	32	Total	O	0	0
			32	32		

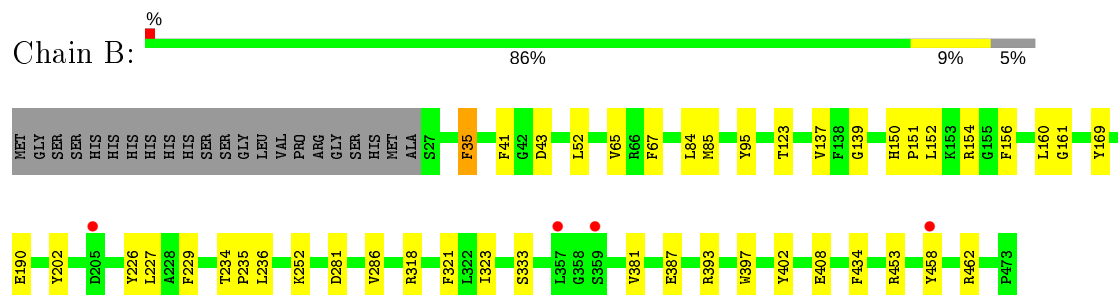
### 3 Residue-property plots [i](#)

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.

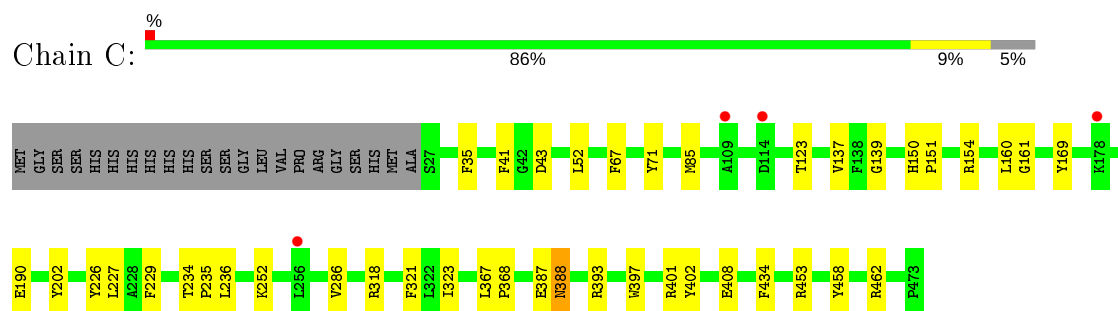
- Molecule 1: exo-4S-kappa carrageenan S1 sulfatase



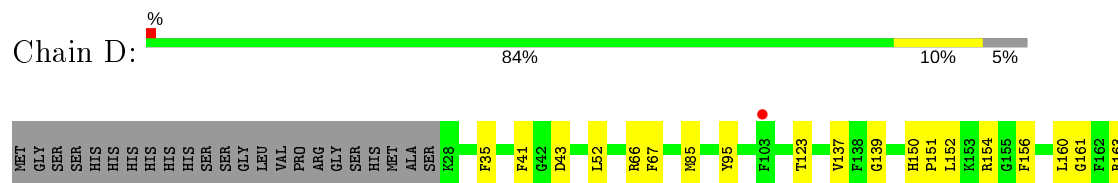
- Molecule 1: exo-4S-kappa carrageenan S1 sulfatase

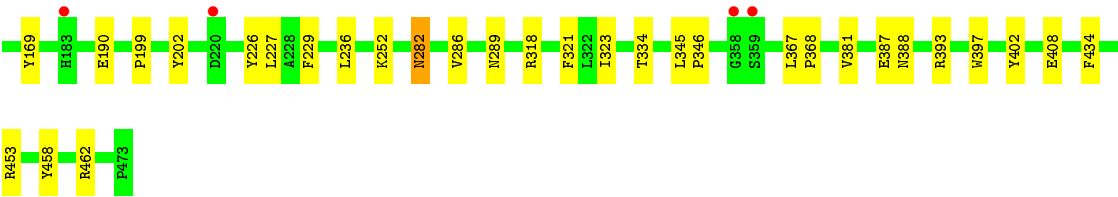


- Molecule 1: exo-4S-kappa carrageenan S1 sulfatase



- Molecule 1: exo-4S-kappa carrageenan S1 sulfatase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.51Å 88.58Å 106.60Å 82.22° 79.85° 84.20°	Depositor
Resolution (Å)	47.60 – 2.50 47.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.60-2.50) 97.9 (47.60-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.238 , 0.273 0.239 , 0.275	Depositor DCC
$R_{free}$ test set	2912 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	14105	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.50% 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: CA

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	0.69	0/3590	0.80	0/4859
1	B	0.68	0/3590	0.80	0/4859
1	C	0.67	0/3598	0.81	0/4867
1	D	0.67	0/3588	0.79	0/4855
All	All	0.68	0/14366	0.80	0/19440

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	3497	0	3308	23	0
1	B	3497	0	3309	22	0
1	C	3505	0	3333	22	0
1	D	3498	0	3325	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	0	0	0
3	C	24	0	0	0	0
3	D	32	0	0	4	0
All	All	14105	0	13275	95	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 (95) 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:367:LEU:HB3	1:C:368:PRO:HD3	1.78	0.66
1:D:367:LEU:HB3	1:D:368:PRO:HD3	1.76	0.65
1:A:367:LEU:HB3	1:A:368:PRO:HD3	1.78	0.65
1:D:282:ASN:CG	1:D:282:ASN:O	2.50	0.50
1:C:123:THR:HG21	1:C:154:ARG:HB3	1.93	0.49
1:D:123:THR:HG21	1:D:154:ARG:HB3	1.94	0.48
1:A:123:THR:HG21	1:A:154:ARG:HB3	1.95	0.48
1:A:417:SER:HB2	3:A:610:HOH:O	2.14	0.48
1:D:286:VAL:HG22	1:D:323:ILE:HG12	1.95	0.48
1:B:43:ASP:HB3	1:B:52:LEU:CD2	2.45	0.47
1:C:41:PHE:CE1	1:C:318:ARG:HG2	2.49	0.47
1:A:43:ASP:HB3	1:A:52:LEU:CD2	2.44	0.47
1:B:123:THR:HG21	1:B:154:ARG:HB3	1.95	0.47
1:D:67:PHE:HB2	1:D:321:PHE:HB3	1.96	0.47
1:D:289:ASN:ND2	3:D:601:HOH:O	2.40	0.47
1:C:236:LEU:CD1	1:C:252:LYS:HG2	2.45	0.47
1:C:43:ASP:HB3	1:C:52:LEU:CD2	2.44	0.47
1:B:150:HIS:CG	1:B:151:PRO:HD2	2.50	0.47
1:C:150:HIS:CG	1:C:151:PRO:HD2	2.50	0.47
1:B:85:MET:CE	1:B:123:THR:HB	2.45	0.47
1:A:41:PHE:CE1	1:A:318:ARG:HG2	2.49	0.47
1:D:236:LEU:CD1	1:D:252:LYS:HG2	2.44	0.47
1:D:150:HIS:CG	1:D:151:PRO:HD2	2.50	0.46
1:B:160:LEU:HA	1:B:190:GLU:O	2.16	0.46
1:A:85:MET:CE	1:A:123:THR:HB	2.46	0.46
1:A:150:HIS:CG	1:A:151:PRO:HD2	2.51	0.46
1:A:169:TYR:HB3	1:A:202:TYR:CE1	2.50	0.46
1:D:402:TYR:OH	1:D:408:GLU:OE1	2.32	0.46
1:D:160:LEU:HA	1:D:190:GLU:O	2.16	0.46
1:C:402:TYR:OH	1:C:408:GLU:OE1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TYR:OH	1:A:408:GLU:OE1	2.32	0.46
1:A:393:ARG:HA	1:A:397:TRP:O	2.15	0.45
1:C:286:VAL:HG22	1:C:323:ILE:HG12	1.98	0.45
1:A:236:LEU:CD1	1:A:252:LYS:HG2	2.47	0.45
1:C:85:MET:HG3	1:C:123:THR:HB	1.99	0.45
1:D:85:MET:HA	1:D:85:MET:HE2	1.99	0.45
1:A:67:PHE:HB2	1:A:321:PHE:HB3	1.99	0.45
1:B:286:VAL:HG22	1:B:323:ILE:HG12	1.98	0.45
1:A:85:MET:HE1	1:A:123:THR:HB	1.99	0.45
1:C:393:ARG:HA	1:C:397:TRP:O	2.17	0.45
1:D:43:ASP:HB3	1:D:52:LEU:CD2	2.47	0.45
1:D:199:PRO:HA	3:D:622:HOH:O	2.17	0.45
1:C:67:PHE:HB2	1:C:321:PHE:HB3	1.99	0.45
1:D:169:TYR:HB3	1:D:202:TYR:CE1	2.51	0.45
1:B:41:PHE:CE1	1:B:318:ARG:HG2	2.51	0.44
1:D:41:PHE:CE1	1:D:318:ARG:HG2	2.51	0.44
1:C:160:LEU:HA	1:C:190:GLU:O	2.17	0.44
1:D:393:ARG:HA	1:D:397:TRP:O	2.18	0.44
1:A:160:LEU:HA	1:A:190:GLU:O	2.17	0.44
1:C:387:GLU:CD	1:C:453:ARG:HH12	2.21	0.44
1:A:286:VAL:HG22	1:A:323:ILE:HG12	1.99	0.44
1:B:393:ARG:HA	1:B:397:TRP:O	2.18	0.44
1:C:169:TYR:HB3	1:C:202:TYR:CE1	2.52	0.44
1:B:137:VAL:HA	1:B:226:TYR:O	2.18	0.43
1:B:387:GLU:CD	1:B:453:ARG:HH12	2.21	0.43
1:B:402:TYR:OH	1:B:408:GLU:OE1	2.33	0.43
1:D:163:ARG:HD3	3:D:627:HOH:O	2.18	0.43
1:B:67:PHE:HB2	1:B:321:PHE:HB3	1.99	0.43
1:C:139:GLY:O	1:C:161:GLY:HA3	2.19	0.43
1:D:387:GLU:CD	1:D:453:ARG:HH12	2.22	0.43
1:B:236:LEU:CD1	1:B:252:LYS:HG2	2.48	0.43
1:D:137:VAL:HA	1:D:226:TYR:O	2.19	0.42
1:A:387:GLU:CD	1:A:453:ARG:HH12	2.23	0.42
1:B:169:TYR:HB3	1:B:202:TYR:CE1	2.54	0.42
1:C:227:LEU:HD21	1:C:229:PHE:CZ	2.55	0.42
1:C:401:ARG:CZ	1:D:388:ASN:HD21	2.32	0.42
1:D:139:GLY:O	1:D:161:GLY:HA3	2.19	0.42
1:B:227:LEU:HD21	1:B:229:PHE:CZ	2.54	0.42
1:B:458:TYR:OH	1:B:462:ARG:NH1	2.53	0.42
1:D:227:LEU:HD21	1:D:229:PHE:CZ	2.55	0.42
1:D:453:ARG:HA	1:D:453:ARG:HE	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLY:O	1:B:161:GLY:HA3	2.20	0.42
1:A:71:TYR:OH	1:A:393:ARG:NH1	2.53	0.41
1:C:137:VAL:HA	1:C:226:TYR:O	2.19	0.41
1:D:150:HIS:HA	3:D:627:HOH:O	2.20	0.41
1:A:66:ARG:O	1:A:334:THR:HA	2.21	0.41
1:D:458:TYR:OH	1:D:462:ARG:NH1	2.54	0.41
1:A:152:LEU:HA	1:A:156:PHE:O	2.20	0.41
1:A:137:VAL:HA	1:A:226:TYR:O	2.19	0.41
1:A:227:LEU:HD21	1:A:229:PHE:CZ	2.56	0.41
1:B:381:VAL:HA	1:B:393:ARG:O	2.20	0.41
1:C:388:ASN:ND2	1:D:388:ASN:OD1	2.53	0.41
1:A:139:GLY:O	1:A:161:GLY:HA3	2.21	0.41
1:B:234:THR:HB	1:B:235:PRO:HA	2.03	0.41
1:D:345:LEU:N	1:D:346:PRO:HD2	2.36	0.41
1:B:35:PHE:CE2	1:B:84:LEU:HD22	2.56	0.41
1:B:152:LEU:HA	1:B:156:PHE:O	2.21	0.41
1:D:66:ARG:O	1:D:334:THR:HA	2.21	0.41
1:D:152:LEU:HA	1:D:156:PHE:O	2.22	0.40
1:A:292:GLY:HA3	1:A:315:GLY:O	2.22	0.40
1:C:234:THR:HB	1:C:235:PRO:HA	2.03	0.40
1:C:458:TYR:OH	1:C:462:ARG:NH1	2.54	0.40
1:C:71:TYR:OH	1:C:393:ARG:NH1	2.55	0.40
1:D:381:VAL:HA	1:D:393:ARG:O	2.22	0.40
1:B:65:VAL:HA	1:B:333:SER:O	2.21	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	446/469 (95%)	424 (95%)	22 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	446/469 (95%)	425 (95%)	21 (5%)	0	100	100
1	C	446/469 (95%)	426 (96%)	20 (4%)	0	100	100
1	D	444/469 (95%)	424 (96%)	20 (4%)	0	100	100
All	All	1782/1876 (95%)	1699 (95%)	83 (5%)	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	356/398 (89%)	352 (99%)	4 (1%)	73	89
1	B	356/398 (89%)	352 (99%)	4 (1%)	73	89
1	C	359/398 (90%)	356 (99%)	3 (1%)	81	93
1	D	357/398 (90%)	353 (99%)	4 (1%)	73	89
All	All	1428/1592 (90%)	1413 (99%)	15 (1%)	73	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	PHE
1	A	95	TYR
1	A	281	ASP
1	A	434	PHE
1	B	35	PHE
1	B	95	TYR
1	B	281	ASP
1	B	434	PHE
1	C	35	PHE
1	C	388	ASN
1	C	434	PHE
1	D	35	PHE
1	D	95	TYR

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Mol	Chain	Res	Type
1	D	282	ASN
1	D	434	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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	447/469 (95%)	0.12	4 (0%) 84 86	17, 32, 50, 77	3 (0%)
1	B	447/469 (95%)	0.14	4 (0%) 84 86	16, 31, 51, 68	1 (0%)
1	C	447/469 (95%)	0.13	4 (0%) 84 86	17, 32, 49, 78	3 (0%)
1	D	446/469 (95%)	0.21	5 (1%) 80 82	17, 34, 55, 87	2 (0%)
All	All	1787/1876 (95%)	0.15	17 (0%) 82 84	16, 33, 52, 87	9 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	358	GLY	3.6
1	C	178	LYS	3.5
1	A	180	GLY	3.2
1	D	220	ASP	2.9
1	B	357	LEU	2.9
1	C	256	LEU	2.8
1	C	109	ALA	2.6
1	A	358	GLY	2.6
1	B	458	TYR	2.5
1	A	416	ILE	2.4
1	D	183	HIS	2.4
1	C	114	ASP	2.2
1	B	205	ASP	2.2
1	B	359	SER	2.1
1	D	359	SER	2.1
1	A	183	HIS	2.0
1	D	103	PHE	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	CA	C	501	1/1	0.91	0.06	44,44,44,44	0
2	CA	A	501	1/1	0.97	0.05	36,36,36,36	0
2	CA	B	501	1/1	0.99	0.05	35,35,35,35	0
2	CA	D	501	1/1	0.99	0.06	32,32,32,32	0

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

There are no such residues in this entry.