



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2017 – 09:06 PM EDT

PDB ID : 4WXG  
Title : Crystal structure of L-Serine Hydroxymethyltransferase in complex with a mixture of L-allo-Threonine and Glycine  
Authors : Hernandez, K.; Zelen, I.; Petrillo, G.; Uson, I.; Wandtke, C.; Bujons, J.; Joglar, J.; Parella, T.; Clapes, P.  
Deposited on : unknown  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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 : rb-20029824  
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) : rb-20029824

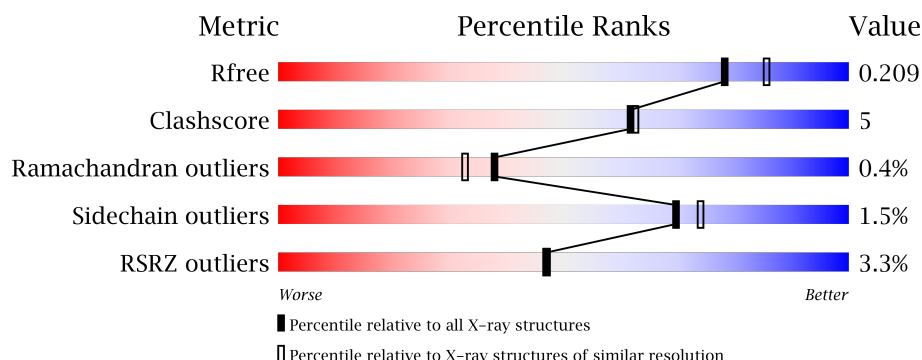
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	428	
1	C	428	

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
4	GOL	A	503	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6742 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.

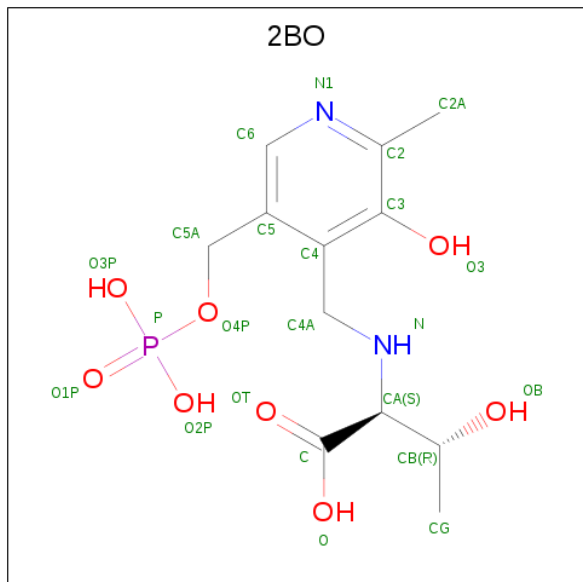
- Molecule 1 is a protein called Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	4	0
			3143	1991	538	605	9			
1	C	410	Total	C	N	O	S	0	4	0
			3143	1991	538	605	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q5M0B4
A	-16	ARG	-	expression tag	UNP Q5M0B4
A	-15	GLY	-	expression tag	UNP Q5M0B4
A	-14	SER	-	expression tag	UNP Q5M0B4
A	-13	HIS	-	expression tag	UNP Q5M0B4
A	-12	HIS	-	expression tag	UNP Q5M0B4
A	-11	HIS	-	expression tag	UNP Q5M0B4
A	-10	HIS	-	expression tag	UNP Q5M0B4
A	-9	HIS	-	expression tag	UNP Q5M0B4
A	-8	HIS	-	expression tag	UNP Q5M0B4
A	-7	GLY	-	expression tag	UNP Q5M0B4
A	-6	SER	-	expression tag	UNP Q5M0B4
C	-17	MET	-	initiating methionine	UNP Q5M0B4
C	-16	ARG	-	expression tag	UNP Q5M0B4
C	-15	GLY	-	expression tag	UNP Q5M0B4
C	-14	SER	-	expression tag	UNP Q5M0B4
C	-13	HIS	-	expression tag	UNP Q5M0B4
C	-12	HIS	-	expression tag	UNP Q5M0B4
C	-11	HIS	-	expression tag	UNP Q5M0B4
C	-10	HIS	-	expression tag	UNP Q5M0B4
C	-9	HIS	-	expression tag	UNP Q5M0B4
C	-8	HIS	-	expression tag	UNP Q5M0B4
C	-7	GLY	-	expression tag	UNP Q5M0B4
C	-6	SER	-	expression tag	UNP Q5M0B4

- Molecule 2 is N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)-L-threonine (three-letter code: 2BO) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			27	14	2	10	1		
2	C	1	Total	C	N	O	P	0	1
			27	14	2	10	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

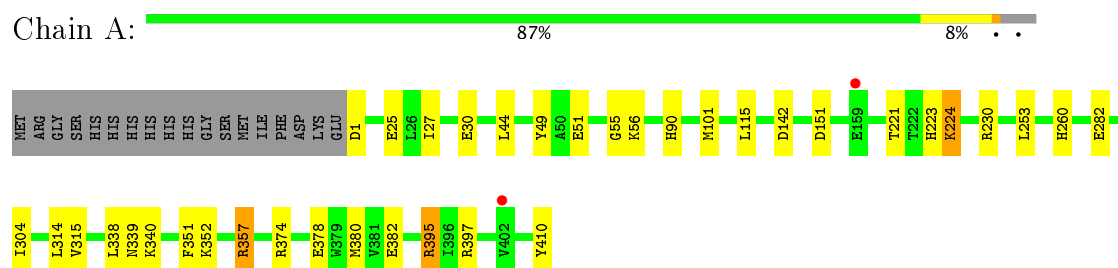
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	229	Total	O	0	1
			230	230		
5	C	163	Total	O	0	1
			164	164		

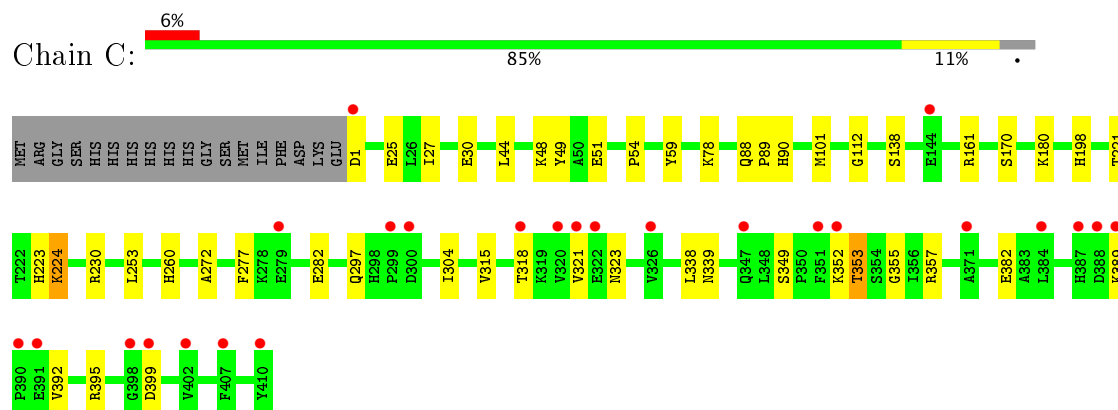
### 3 Residue-property plots

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: Serine hydroxymethyltransferase



- Molecule 1: Serine hydroxymethyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.43 Å   115.43 Å   191.48 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.43 – 2.00 45.44 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.43-2.00) 98.6 (45.44-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.171   ,   0.203 0.181   ,   0.209	Depositor DCC
$R_{free}$ test set	4344 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.6	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	0.97	EDS
Total number of atoms	6742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: 2BO, GOL, NA

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	0.96	2/3225 (0.1%)	1.02	14/4377 (0.3%)
1	C	0.92	2/3225 (0.1%)	0.98	7/4377 (0.2%)
All	All	0.94	4/6450 (0.1%)	1.00	21/8754 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	GLU	CD-OE1	-6.42	1.18	1.25
1	A	410	TYR	CE1-CZ	6.04	1.46	1.38
1	C	59	TYR	CE1-CZ	5.30	1.45	1.38
1	C	59	TYR	CG-CD2	5.06	1.45	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	395	ARG	NE-CZ-NH1	-9.57	115.51	120.30
1	A	230	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	223[A]	HIS	N-CA-C	8.18	133.09	111.00
1	A	223[B]	HIS	N-CA-C	8.18	133.09	111.00
1	A	230	ARG	CG-CD-NE	-8.05	94.89	111.80
1	A	395	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	A	151	ASP	CB-CG-OD1	7.13	124.72	118.30
1	C	223[A]	HIS	N-CA-C	6.99	129.86	111.00
1	C	223[B]	HIS	N-CA-C	6.99	129.86	111.00
1	C	230	ARG	CG-CD-NE	-6.41	98.34	111.80
1	C	161	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	357	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	142	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	A	223[A]	HIS	CB-CA-C	-5.71	98.98	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223[B]	HIS	CB-CA-C	-5.71	98.98	110.40
1	A	380	MET	CG-SD-CE	-5.66	91.15	100.20
1	C	230	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	142	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	397	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	180	LYS	CD-CE-NZ	-5.16	99.83	111.70

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	3143	0	3117	31	0
1	C	3143	0	3117	32	0
2	A	27	0	8	0	0
2	C	27	0	8	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	6	0	8	0	0
5	A	230	0	0	8	1
5	C	164	0	0	7	0
All	All	6742	0	6258	64	1

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 (64) 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:349:SER:HB3	1:C:352:LYS:HD3	1.35	1.07
1:C:382:GLU:OE2	1:C:395:ARG:NH1	2.02	0.93
1:C:304:ILE:HG12	5:C:651:HOH:O	1.79	0.82
1:A:25[A]:GLU:HG3	5:A:604:HOH:O	1.79	0.80
1:C:1:ASP:OD1	5:C:601:HOH:O	2.05	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ILE:HD13	5:A:602:HOH:O	1.94	0.67
1:A:339:ASN:HD21	1:A:357:ARG:HH21	1.42	0.67
1:C:349:SER:HB3	1:C:352:LYS:CD	2.19	0.65
1:C:395:ARG:NH2	1:C:399:ASP:OD2	2.30	0.64
1:C:90:HIS:HD2	5:C:674:HOH:O	1.82	0.63
1:C:101:MET:HE1	1:C:253:LEU:HD21	1.82	0.61
1:C:51:GLU:OE2	5:C:602[A]:HOH:O	2.17	0.60
1:A:101:MET:HE1	1:A:253:LEU:HG	1.84	0.60
1:C:260:HIS:CD2	1:C:260:HIS:H	2.21	0.58
1:A:1:ASP:HB3	5:A:797:HOH:O	2.03	0.58
1:A:260:HIS:CD2	1:A:260:HIS:H	2.22	0.58
1:A:51:GLU:OE2	5:A:601[A]:HOH:O	2.18	0.57
1:A:340:LYS:HE3	1:A:351:PHE:O	2.06	0.55
1:A:339:ASN:ND2	1:A:357:ARG:HH21	2.05	0.54
1:A:304:ILE:HG12	1:A:314:LEU:HB2	1.90	0.53
5:A:608:HOH:O	1:C:48:LYS:HE3	2.09	0.51
1:A:221:THR:HG21	1:A:224[A]:LYS:NZ	2.26	0.51
1:C:304:ILE:CD1	5:C:651:HOH:O	2.59	0.50
1:C:25[B]:GLU:HG3	5:C:719:HOH:O	2.11	0.50
1:C:339:ASN:HD21	1:C:357:ARG:HH21	1.60	0.49
1:C:389:LYS:HB3	1:C:392:VAL:HG23	1.95	0.48
1:A:101:MET:HE1	1:A:253:LEU:CG	2.44	0.47
1:A:25[B]:GLU:OE1	1:A:30[B]:GLU:OE1	2.33	0.46
1:A:90:HIS:HD2	5:A:686:HOH:O	1.98	0.46
1:C:318:THR:HA	1:C:321:VAL:O	2.16	0.46
1:A:374:ARG:O	1:A:378:GLU:HG2	2.16	0.46
1:A:315:VAL:HA	5:A:602:HOH:O	2.15	0.45
1:A:304:ILE:CD1	5:A:602:HOH:O	2.61	0.45
1:A:115:LEU:HG	1:A:115:LEU:H	1.47	0.45
1:C:88:GLN:N	1:C:89:PRO:CD	2.80	0.45
1:C:170:SER:HA	1:C:198:HIS:CD2	2.52	0.45
1:A:27:ILE:HG13	1:A:338:LEU:HA	1.99	0.45
1:C:101:MET:HB2	1:C:101:MET:HE2	1.86	0.44
1:A:382:GLU:OE2	1:A:395:ARG:NH1	2.46	0.44
1:A:101:MET:HB2	1:A:101:MET:HE2	1.75	0.43
1:C:221:THR:HG21	1:C:224[A]:LYS:NZ	2.34	0.43
1:C:101:MET:HE3	1:C:253:LEU:HD11	2.00	0.42
1:C:101:MET:CE	1:C:253:LEU:HD21	2.49	0.42
1:A:55:GLY:O	1:A:56:LYS:HG3	2.19	0.42
1:C:349:SER:CB	1:C:352:LYS:HD3	2.24	0.42
1:A:260:HIS:CD2	1:A:260:HIS:N	2.88	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ILE:HB	1:C:30[A]:GLU:CG	2.50	0.41
1:C:112:GLY:O	1:C:138:SER:HA	2.20	0.41
1:C:101:MET:HE1	1:C:253:LEU:CD2	2.49	0.41
1:C:323:ASN:HB2	1:C:353:THR:O	2.21	0.41
1:A:260:HIS:H	1:A:260:HIS:HD2	1.66	0.40
1:C:315:VAL:O	1:C:355:GLY:HA2	2.21	0.40
1:C:272:ALA:HA	1:C:277:PHE:CG	2.56	0.40
1:C:260:HIS:HD2	1:C:260:HIS:H	1.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:802:HOH:O	5:A:802:HOH:O[7_555]	2.05	0.15

## 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	412/428 (96%)	400 (97%)	10 (2%)	2 (0%)	32	26
1	C	412/428 (96%)	398 (97%)	11 (3%)	3 (1%)	25	18
All	All	824/856 (96%)	798 (97%)	21 (2%)	5 (1%)	38	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224[A]	LYS
1	A	224[B]	LYS
1	C	224[A]	LYS
1	C	224[B]	LYS
1	C	353	THR

### 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	331/343 (96%)	328 (99%)	3 (1%)	82	87
1	C	331/343 (96%)	324 (98%)	7 (2%)	59	62
All	All	662/686 (96%)	652 (98%)	10 (2%)	70	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	49	TYR
1	A	352	LYS
1	C	44	LEU
1	C	49	TYR
1	C	54	PRO
1	C	78	LYS
1	C	282	GLU
1	C	297	GLN
1	C	338	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	90	HIS
1	A	260	HIS
1	A	297	GLN
1	A	335	ASN
1	A	339	ASN
1	A	341	ASN
1	A	347	GLN
1	C	11	ASN
1	C	88	GLN
1	C	90	HIS
1	C	260	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	329	ASN
1	C	339	ASN
1	C	341	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	2BO	A	501[A]	-	20,23,23	1.79	4 (20%)	26,33,33	4.15	10 (38%)
2	2BO	A	501[B]	-	17,20,23	1.45	3 (17%)	23,28,33	2.36	9 (39%)
4	GOL	A	503	-	5,5,5	1.79	2 (40%)	5,5,5	1.61	1 (20%)
2	2BO	C	501[A]	-	20,23,23	1.73	3 (15%)	26,33,33	3.53	11 (42%)
2	2BO	C	501[B]	-	17,20,23	1.47	2 (11%)	23,28,33	2.00	7 (30%)

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	2BO	A	501[A]	-	-	0/15/19/19	0/1/1/1
2	2BO	A	501[B]	-	-	0/10/12/19	0/1/1/1
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	2BO	C	501[A]	-	-	0/15/19/19	0/1/1/1
2	2BO	C	501[B]	-	-	0/10/12/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	2BO	C4A-N	-5.12	1.31	1.46
2	C	501[A]	2BO	C4A-N	-5.05	1.31	1.46
2	C	501[A]	2BO	C3-C2	-3.77	1.38	1.40
2	C	501[B]	2BO	C3-C2	-3.77	1.38	1.40
2	A	501[B]	2BO	C4A-N	-3.07	1.31	1.46
2	A	501[B]	2BO	O4P-C5A	-3.03	1.33	1.44
2	A	501[A]	2BO	O4P-C5A	-3.03	1.33	1.44
2	C	501[B]	2BO	C4A-N	-3.03	1.31	1.46
2	A	501[B]	2BO	C3-C4	2.15	1.43	1.40
2	A	501[A]	2BO	C3-C4	2.15	1.43	1.40
2	C	501[A]	2BO	CB-CA	2.21	1.60	1.53
4	A	503	GOL	O2-C2	2.36	1.50	1.43
4	A	503	GOL	O1-C1	2.81	1.54	1.42
2	A	501[A]	2BO	CB-CA	3.12	1.63	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[A]	2BO	CB-CA-N	-5.59	96.92	111.82
2	A	501[B]	2BO	O2P-P-O4P	-4.11	95.81	106.73
2	A	501[A]	2BO	O2P-P-O4P	-4.11	95.81	106.73
2	C	501[A]	2BO	O2P-P-O4P	-4.09	95.85	106.73
2	C	501[B]	2BO	O2P-P-O4P	-4.09	95.85	106.73
2	A	501[B]	2BO	C5A-C5-C6	-4.09	112.30	119.33
2	A	501[A]	2BO	C5A-C5-C6	-4.09	112.30	119.33
2	A	501[B]	2BO	C3-C4-C5	-3.76	115.00	118.71
2	A	501[A]	2BO	C3-C4-C5	-3.76	115.00	118.71
2	A	501[B]	2BO	C-CA-N	-3.31	106.18	111.91
2	C	501[A]	2BO	CB-CA-N	-3.27	103.12	111.82
2	C	501[A]	2BO	OB-CB-CG	-2.02	103.39	109.70
2	C	501[A]	2BO	C2A-C2-C3	2.08	123.45	120.96
2	C	501[B]	2BO	C2A-C2-C3	2.08	123.45	120.96
2	C	501[A]	2BO	C4-C4A-N	2.08	117.52	111.78
2	C	501[A]	2BO	O2P-P-O1P	2.28	119.42	110.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501[B]	2BO	O2P-P-O1P	2.28	119.42	110.50
2	C	501[A]	2BO	C4A-C4-C5	2.36	121.91	119.75
2	C	501[B]	2BO	C4A-C4-C5	2.36	121.91	119.75
2	C	501[A]	2BO	OB-CB-CA	2.40	114.28	109.15
2	A	501[B]	2BO	C4-C4A-N	2.61	116.43	111.91
2	A	501[B]	2BO	O4P-P-O1P	2.65	113.90	106.47
2	A	501[A]	2BO	O4P-P-O1P	2.65	113.90	106.47
2	C	501[A]	2BO	CG-CB-CA	2.72	118.21	112.34
4	A	503	GOL	O2-C2-C1	2.85	122.28	108.84
2	A	501[B]	2BO	O4P-C5A-C5	3.12	115.60	109.32
2	A	501[A]	2BO	O4P-C5A-C5	3.12	115.60	109.32
2	C	501[B]	2BO	C4-C4A-N	3.23	117.52	111.91
2	A	501[B]	2BO	C4A-N-CA	3.33	119.61	112.18
2	A	501[A]	2BO	OB-CB-CA	3.37	116.36	109.15
2	C	501[B]	2BO	C4A-N-CA	3.72	120.48	112.18
2	A	501[A]	2BO	CG-CB-CA	3.79	120.51	112.34
2	A	501[B]	2BO	C4A-C4-C5	3.84	123.27	119.75
2	A	501[A]	2BO	C4A-C4-C5	3.84	123.27	119.75
2	C	501[A]	2BO	O4P-C5A-C5	4.98	119.33	109.32
2	C	501[B]	2BO	O4P-C5A-C5	4.98	119.33	109.32
2	C	501[A]	2BO	C4A-N-CA	14.99	134.54	113.78
2	A	501[A]	2BO	C4A-N-CA	16.86	137.13	113.78

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

### 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	410/428 (95%)	-0.19	2 (0%) 90 90	22, 30, 50, 74	0
1	C	410/428 (95%)	0.07	25 (6%) 22 22	22, 36, 65, 86	0
All	All	820/856 (95%)	-0.06	27 (3%) 47 47	22, 33, 59, 86	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	318	THR	3.7
1	C	388	ASP	3.6
1	C	351	PHE	3.2
1	C	322	GLU	3.2
1	C	390	PRO	3.1
1	C	300	ASP	2.9
1	A	402	VAL	2.8
1	C	407	PHE	2.8
1	C	384	LEU	2.8
1	C	321	VAL	2.7
1	C	299	PRO	2.7
1	C	391	GLU	2.6
1	C	389	LYS	2.6
1	C	347	GLN	2.6
1	C	402	VAL	2.6
1	C	144	GLU	2.6
1	C	387	HIS	2.4
1	C	352	LYS	2.4
1	C	326	VAL	2.4
1	A	159	GLU	2.3
1	C	279	GLU	2.1
1	C	398	GLY	2.1
1	C	371	ALA	2.1
1	C	320	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	399	ASP	2.1
1	C	410	TYR	2.0
1	C	1	ASP	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 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(Å <sup>2</sup> )	Q<0.9
4	GOL	A	503	6/6	0.83	0.24	5.02	36,42,49,54	0
3	NA	C	502	1/1	0.91	0.23	0.76	60,60,60,60	0
2	2BO	C	501[B]	20/23	0.97	0.14	0.69	26,35,40,43	4
2	2BO	C	501[A]	23/23	0.97	0.14	0.69	26,36,43,49	7
2	2BO	A	501[A]	23/23	0.97	0.17	0.57	25,32,38,45	7
2	2BO	A	501[B]	20/23	0.97	0.17	0.29	25,32,41,45	4
3	NA	A	502	1/1	0.97	0.10	-0.15	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.