



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:41 PM GMT

PDB ID : 3VBB  
Title : Crystal Structure of Seryl-tRNA Synthetase from Human at 2.9 angstroms  
Authors : Xu, X.L.; Yang, X.-L.  
Deposited on : 2012-01-02  
Resolution : 2.89 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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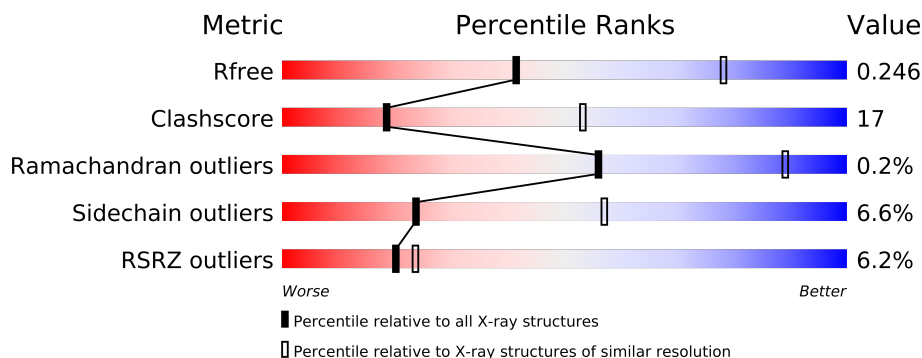
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.89 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	522	
1	B	522	
1	C	522	
1	D	522	
1	E	522	
1	F	522	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	601	-	X
2	MG	B	601	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21387 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Seryl-tRNA synthetase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	5	1	0
			3606	2301	619	668	18			
1	B	454	Total	C	N	O	S	0	1	0
			3625	2311	623	671	20			
1	C	456	Total	C	N	O	S	3	1	0
			3588	2291	609	669	19			
1	D	450	Total	C	N	O	S	7	1	0
			3533	2264	602	649	18			
1	E	440	Total	C	N	O	S	1	1	0
			3469	2216	596	638	19			
1	F	443	Total	C	N	O	S	11	1	0
			3519	2247	604	650	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	515	LEU	-	EXPRESSION TAG	UNP P49591
A	516	GLU	-	EXPRESSION TAG	UNP P49591
A	517	HIS	-	EXPRESSION TAG	UNP P49591
A	518	HIS	-	EXPRESSION TAG	UNP P49591
A	519	HIS	-	EXPRESSION TAG	UNP P49591
A	520	HIS	-	EXPRESSION TAG	UNP P49591
A	521	HIS	-	EXPRESSION TAG	UNP P49591
A	522	HIS	-	EXPRESSION TAG	UNP P49591
B	515	LEU	-	EXPRESSION TAG	UNP P49591
B	516	GLU	-	EXPRESSION TAG	UNP P49591
B	517	HIS	-	EXPRESSION TAG	UNP P49591
B	518	HIS	-	EXPRESSION TAG	UNP P49591
B	519	HIS	-	EXPRESSION TAG	UNP P49591
B	520	HIS	-	EXPRESSION TAG	UNP P49591
B	521	HIS	-	EXPRESSION TAG	UNP P49591
B	522	HIS	-	EXPRESSION TAG	UNP P49591
C	515	LEU	-	EXPRESSION TAG	UNP P49591

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Chain	Residue	Modelled	Actual	Comment	Reference
C	516	GLU	-	EXPRESSION TAG	UNP P49591
C	517	HIS	-	EXPRESSION TAG	UNP P49591
C	518	HIS	-	EXPRESSION TAG	UNP P49591
C	519	HIS	-	EXPRESSION TAG	UNP P49591
C	520	HIS	-	EXPRESSION TAG	UNP P49591
C	521	HIS	-	EXPRESSION TAG	UNP P49591
C	522	HIS	-	EXPRESSION TAG	UNP P49591
D	515	LEU	-	EXPRESSION TAG	UNP P49591
D	516	GLU	-	EXPRESSION TAG	UNP P49591
D	517	HIS	-	EXPRESSION TAG	UNP P49591
D	518	HIS	-	EXPRESSION TAG	UNP P49591
D	519	HIS	-	EXPRESSION TAG	UNP P49591
D	520	HIS	-	EXPRESSION TAG	UNP P49591
D	521	HIS	-	EXPRESSION TAG	UNP P49591
D	522	HIS	-	EXPRESSION TAG	UNP P49591
E	515	LEU	-	EXPRESSION TAG	UNP P49591
E	516	GLU	-	EXPRESSION TAG	UNP P49591
E	517	HIS	-	EXPRESSION TAG	UNP P49591
E	518	HIS	-	EXPRESSION TAG	UNP P49591
E	519	HIS	-	EXPRESSION TAG	UNP P49591
E	520	HIS	-	EXPRESSION TAG	UNP P49591
E	521	HIS	-	EXPRESSION TAG	UNP P49591
E	522	HIS	-	EXPRESSION TAG	UNP P49591
F	515	LEU	-	EXPRESSION TAG	UNP P49591
F	516	GLU	-	EXPRESSION TAG	UNP P49591
F	517	HIS	-	EXPRESSION TAG	UNP P49591
F	518	HIS	-	EXPRESSION TAG	UNP P49591
F	519	HIS	-	EXPRESSION TAG	UNP P49591
F	520	HIS	-	EXPRESSION TAG	UNP P49591
F	521	HIS	-	EXPRESSION TAG	UNP P49591
F	522	HIS	-	EXPRESSION TAG	UNP P49591

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

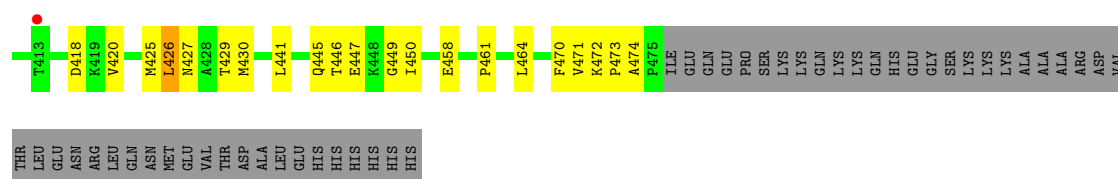


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

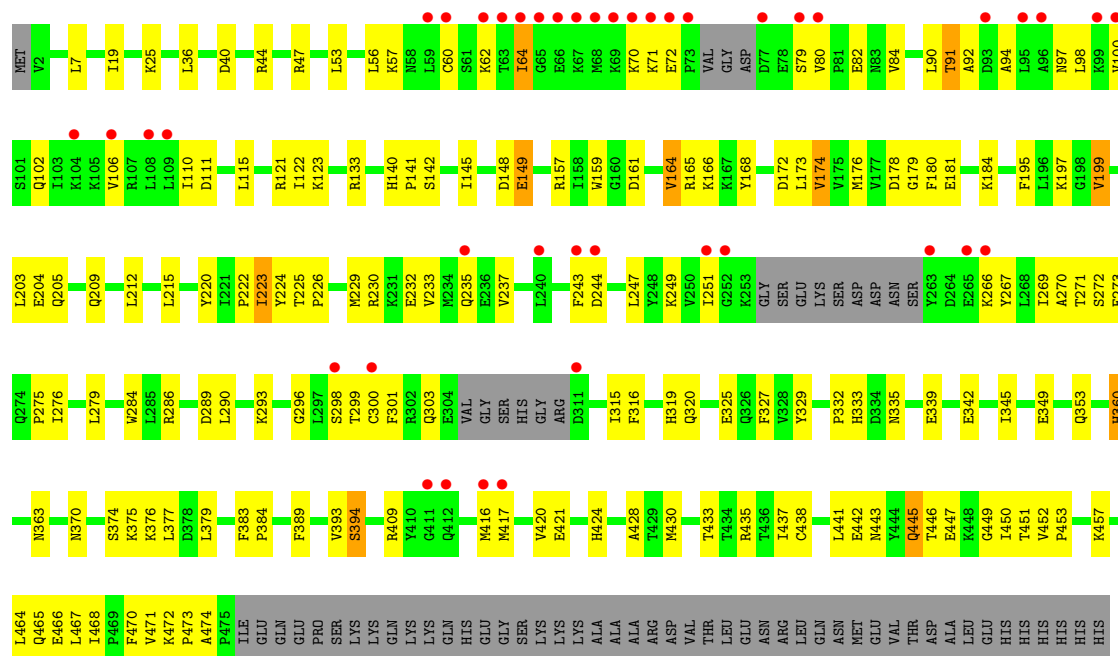
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	3	Total	O	0	0
			3	3		
4	C	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		
4	E	2	Total	O	0	0
			2	2		
4	F	2	Total	O	0	0
			2	2		





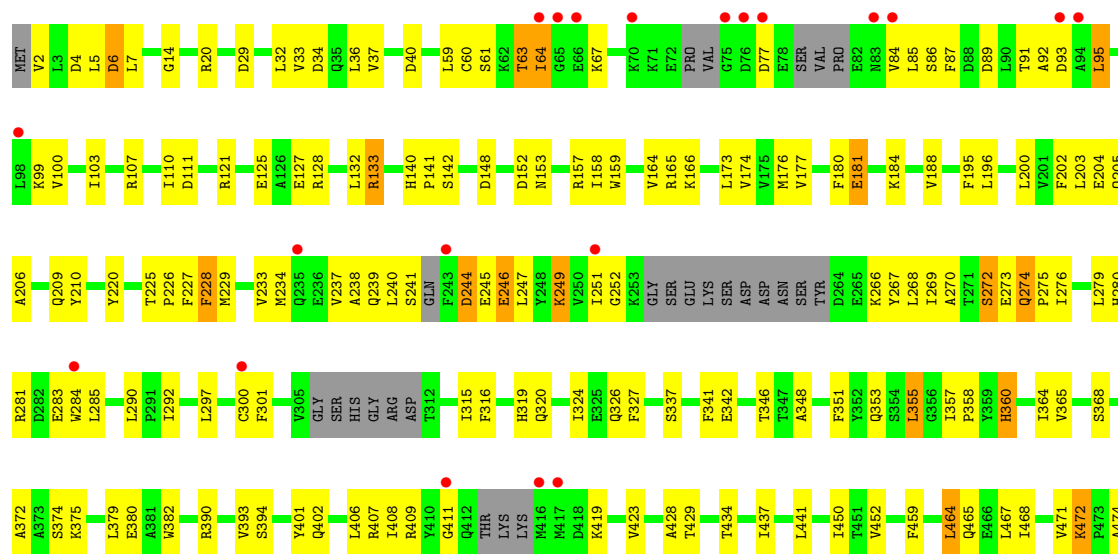
• Molecule 1: Seryl-tRNA synthetase, cytoplasmic

Chain C:



• Molecule 1: Seryl-tRNA synthetase, cytoplasmic

Chain D:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.80Å 189.42Å 230.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.89 48.59 – 2.89	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.59-2.89) 98.7 (48.59-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.194 , 0.250 0.190 , 0.246	Depositor DCC
$R_{free}$ test set	5679 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 113393 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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	0.47	0/3677	0.62	0/4957
1	B	0.49	0/3697	0.64	0/4982
1	C	0.44	0/3661	0.62	0/4949
1	D	0.48	0/3601	0.64	1/4858 (0.0%)
1	E	0.50	0/3539	0.64	0/4777
1	F	0.48	0/3589	0.64	0/4841
All	All	0.48	0/21764	0.63	1/29364 (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	D	6	ASP	N-CA-C	-5.11	97.21	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3606	0	3584	123	0
1	B	3625	0	3600	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3588	0	3506	144	0
1	D	3533	0	3483	122	0
1	E	3469	0	3414	111	0
1	F	3519	0	3465	115	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
All	All	21387	0	21052	712	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

The worst 5 of 712 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:399:THR:HG22	1:E:400:ASP:H	0.97	1.08
1:B:157:ARG:HH11	1:B:157:ARG:HG3	1.20	1.05
1:B:276:ILE:HD12	1:B:327[B]:PHE:CD2	1.93	1.04
1:E:230:ARG:O	1:E:266:LYS:HA	1.58	1.03
1:B:218:ARG:HG3	1:B:218:ARG:HH11	1.27	0.98

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	440/522 (84%)	420 (96%)	20 (4%)	0	100	100
1	B	447/522 (86%)	433 (97%)	14 (3%)	0	100	100
1	C	449/522 (86%)	421 (94%)	27 (6%)	1 (0%)	56	89
1	D	437/522 (84%)	420 (96%)	16 (4%)	1 (0%)	56	89
1	E	431/522 (83%)	422 (98%)	7 (2%)	2 (0%)	38	79
1	F	430/522 (82%)	410 (95%)	20 (5%)	0	100	100
All	All	2634/3132 (84%)	2526 (96%)	104 (4%)	4 (0%)	56	89

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	VAL
1	E	315	ILE
1	E	305	VAL
1	C	420	VAL

### 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	388/461 (84%)	363 (94%)	25 (6%)	25	59
1	B	388/461 (84%)	356 (92%)	32 (8%)	17	44
1	C	379/461 (82%)	359 (95%)	20 (5%)	32	70
1	D	370/461 (80%)	343 (93%)	27 (7%)	20	51
1	E	365/461 (79%)	341 (93%)	24 (7%)	24	57
1	F	373/461 (81%)	351 (94%)	22 (6%)	28	64
All	All	2263/2766 (82%)	2113 (93%)	150 (7%)	24	57

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	199	VAL
1	D	111	ASP
1	F	228	PHE

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Mol	Chain	Res	Type
1	C	243	PHE
1	C	447	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	465	GLN
1	D	353	GLN
1	F	353	GLN
1	D	326	GLN
1	D	402	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z  > 2$
3	PO4	A	602	-	4,4,4	0.15	0	6,6,6	0.30	0
3	PO4	B	602	-	4,4,4	0.20	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	C	601	-	4,4,4	0.16	0	6,6,6	0.30	0
3	PO4	D	601	-	4,4,4	0.12	0	6,6,6	0.31	0
3	PO4	E	601	-	4,4,4	0.11	0	6,6,6	0.31	0
3	PO4	F	601	-	4,4,4	0.15	0	6,6,6	0.31	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	PO4	A	602	-	-	0/0/0/0	0/0/0/0
3	PO4	B	602	-	-	0/0/0/0	0/0/0/0
3	PO4	C	601	-	-	0/0/0/0	0/0/0/0
3	PO4	D	601	-	-	0/0/0/0	0/0/0/0
3	PO4	E	601	-	-	0/0/0/0	0/0/0/0
3	PO4	F	601	-	-	0/0/0/0	0/0/0/0

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.

## 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	451/522 (86%)	0.26	37 (8%)	12 15	47, 74, 146, 167	1 (0%)
1	B	454/522 (86%)	0.18	22 (4%)	29 36	47, 70, 126, 153	0
1	C	456/522 (87%)	0.34	42 (9%)	9 11	52, 78, 147, 165	1 (0%)
1	D	450/522 (86%)	0.18	21 (4%)	30 37	46, 72, 140, 156	3 (0%)
1	E	440/522 (84%)	0.12	20 (4%)	32 39	43, 72, 133, 149	1 (0%)
1	F	443/522 (84%)	0.20	26 (5%)	22 25	50, 71, 152, 176	3 (0%)
All	All	2694/3132 (86%)	0.22	168 (6%)	20 23	43, 73, 142, 176	9 (0%)

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	VAL	6.2
1	F	252	GLY	5.6
1	C	240	LEU	5.5
1	C	311	ASP	5.0
1	D	417	MET	4.9

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	601	1/1	0.70	29.78	90,90,90,90	0
2	MG	A	601	1/1	0.39	5.52	86,86,86,86	0
3	PO4	E	601	5/5	0.20	1.96	125,128,143,154	0
3	PO4	D	601	5/5	0.25	1.57	117,134,150,164	0
3	PO4	C	601	5/5	0.24	0.72	126,131,151,163	0
3	PO4	F	601	5/5	0.25	0.13	121,124,146,155	0
3	PO4	A	602	5/5	0.16	-0.92	115,118,145,154	0
3	PO4	B	602	5/5	0.17	-1.02	134,146,154,159	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.