



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:03 PM GMT

PDB ID : 4QPZ  
Title : Crystal structure of the formolase FLS\_v2 in space group P 21  
Authors : Shen, B.W.; Siegel, J.B.; Stoddard, B.L.; Baker, D.  
Deposited on : 2014-06-25  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

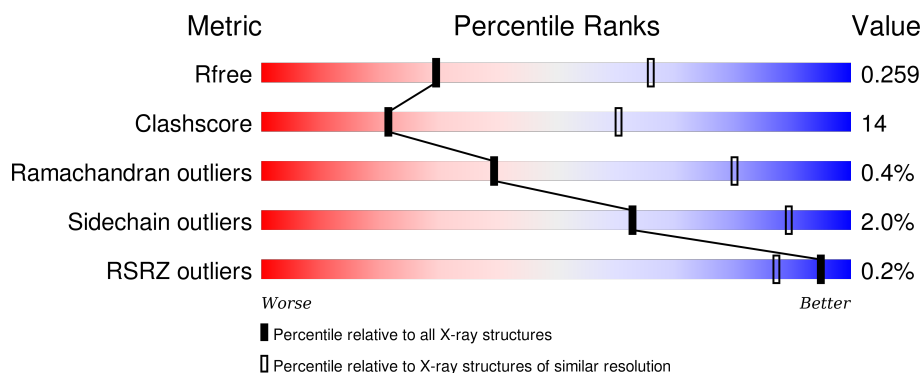
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



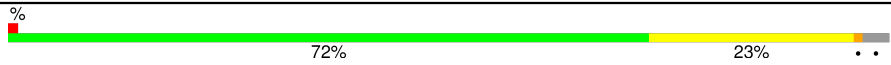


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	582	<div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	B	582	<div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	C	582	<div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	D	582	<div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	E	582	<div> <div>73%</div> <div>23%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	582	
1	G	582	
1	H	582	

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
2	MG	A	601	-	-	-	X
3	TPP	C	602	-	-	X	-
3	TPP	F	602	-	-	X	-
3	TPP	G	602	-	-	X	-
3	TPP	H	602	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33455 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 Formolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4157	2630	734	776	17			
1	B	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	C	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	D	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	E	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	F	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	G	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	H	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ILE	ALA	CONFLICT	UNP Q9F4L3
A	394	GLY	ALA	CONFLICT	UNP Q9F4L3
A	419	ASN	GLY	CONFLICT	UNP Q9F4L3
A	480	TRP	ALA	CONFLICT	UNP Q9F4L3
A	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
A	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
A	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
A	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
A	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
A	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
A	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
A	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
A	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
A	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
A	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
A	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
A	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
A	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
A	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	28	ILE	ALA	CONFLICT	UNP Q9F4L3
B	394	GLY	ALA	CONFLICT	UNP Q9F4L3
B	419	ASN	GLY	CONFLICT	UNP Q9F4L3
B	480	TRP	ALA	CONFLICT	UNP Q9F4L3
B	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
B	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
B	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
B	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
B	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
B	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
B	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
B	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
B	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
B	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
B	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
B	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
B	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
B	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
B	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
B	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	28	ILE	ALA	CONFLICT	UNP Q9F4L3
C	394	GLY	ALA	CONFLICT	UNP Q9F4L3
C	419	ASN	GLY	CONFLICT	UNP Q9F4L3
C	480	TRP	ALA	CONFLICT	UNP Q9F4L3
C	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
C	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
C	566	THR	-	EXPRESSION TAG	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
C	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
C	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
C	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
C	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
C	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
C	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
C	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
C	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
C	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
C	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
C	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
C	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	28	ILE	ALA	CONFLICT	UNP Q9F4L3
D	394	GLY	ALA	CONFLICT	UNP Q9F4L3
D	419	ASN	GLY	CONFLICT	UNP Q9F4L3
D	480	TRP	ALA	CONFLICT	UNP Q9F4L3
D	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
D	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
D	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
D	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
D	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
D	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
D	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
D	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
D	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
D	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
D	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
D	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
D	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
D	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
D	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
D	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	28	ILE	ALA	CONFLICT	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	394	GLY	ALA	CONFLICT	UNP Q9F4L3
E	419	ASN	GLY	CONFLICT	UNP Q9F4L3
E	480	TRP	ALA	CONFLICT	UNP Q9F4L3
E	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
E	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
E	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
E	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
E	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
E	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
E	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
E	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
E	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
E	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
E	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
E	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
E	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
E	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
E	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
E	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	28	ILE	ALA	CONFLICT	UNP Q9F4L3
F	394	GLY	ALA	CONFLICT	UNP Q9F4L3
F	419	ASN	GLY	CONFLICT	UNP Q9F4L3
F	480	TRP	ALA	CONFLICT	UNP Q9F4L3
F	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
F	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
F	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
F	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
F	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
F	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
F	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
F	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
F	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
F	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
F	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
F	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
F	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
F	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
F	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
F	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	28	ILE	ALA	CONFLICT	UNP Q9F4L3
G	394	GLY	ALA	CONFLICT	UNP Q9F4L3
G	419	ASN	GLY	CONFLICT	UNP Q9F4L3
G	480	TRP	ALA	CONFLICT	UNP Q9F4L3
G	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
G	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
G	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
G	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
G	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
G	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
G	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
G	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
G	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3
G	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
G	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
G	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
G	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
G	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
G	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
G	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	28	ILE	ALA	CONFLICT	UNP Q9F4L3
H	394	GLY	ALA	CONFLICT	UNP Q9F4L3
H	419	ASN	GLY	CONFLICT	UNP Q9F4L3
H	480	TRP	ALA	CONFLICT	UNP Q9F4L3
H	564	GLY	-	EXPRESSION TAG	UNP Q9F4L3
H	565	SER	-	EXPRESSION TAG	UNP Q9F4L3
H	566	THR	-	EXPRESSION TAG	UNP Q9F4L3
H	567	GLU	-	EXPRESSION TAG	UNP Q9F4L3
H	568	ASN	-	EXPRESSION TAG	UNP Q9F4L3
H	569	LEU	-	EXPRESSION TAG	UNP Q9F4L3
H	570	TYR	-	EXPRESSION TAG	UNP Q9F4L3
H	571	PHE	-	EXPRESSION TAG	UNP Q9F4L3
H	572	GLN	-	EXPRESSION TAG	UNP Q9F4L3

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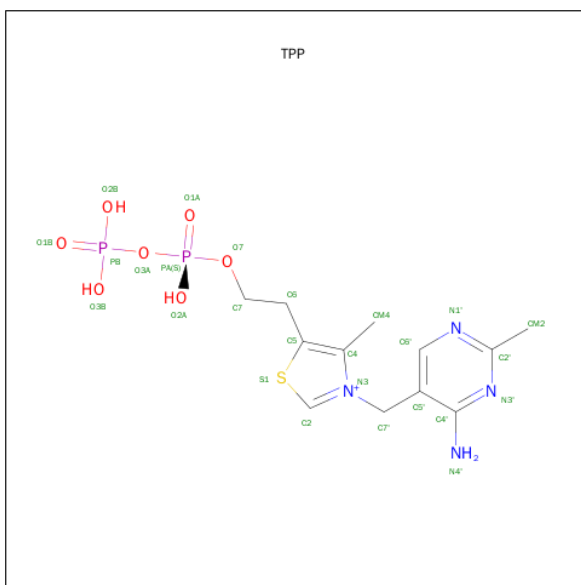
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Chain	Residue	Modelled	Actual	Comment	Reference
H	573	SER	-	EXPRESSION TAG	UNP Q9F4L3
H	574	GLY	-	EXPRESSION TAG	UNP Q9F4L3
H	575	ALA	-	EXPRESSION TAG	UNP Q9F4L3
H	576	LEU	-	EXPRESSION TAG	UNP Q9F4L3
H	577	GLU	-	EXPRESSION TAG	UNP Q9F4L3
H	578	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	579	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	580	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	581	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	582	HIS	-	EXPRESSION TAG	UNP Q9F4L3
H	583	HIS	-	EXPRESSION TAG	UNP Q9F4L3

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	G	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	H	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 4 is water.

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

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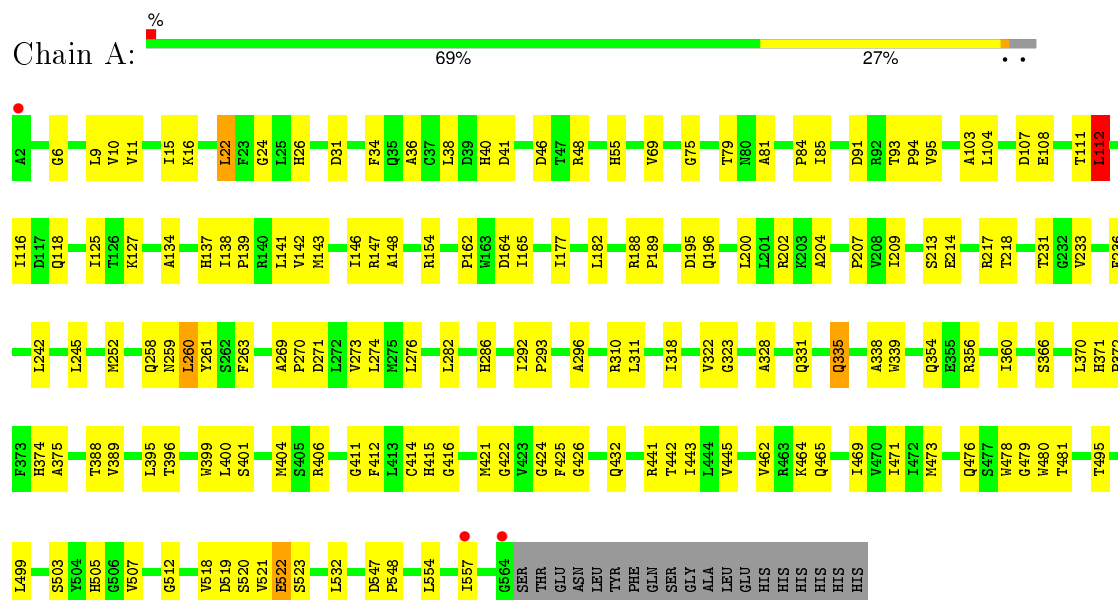
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	3	Total	O	0	0
			3	3		

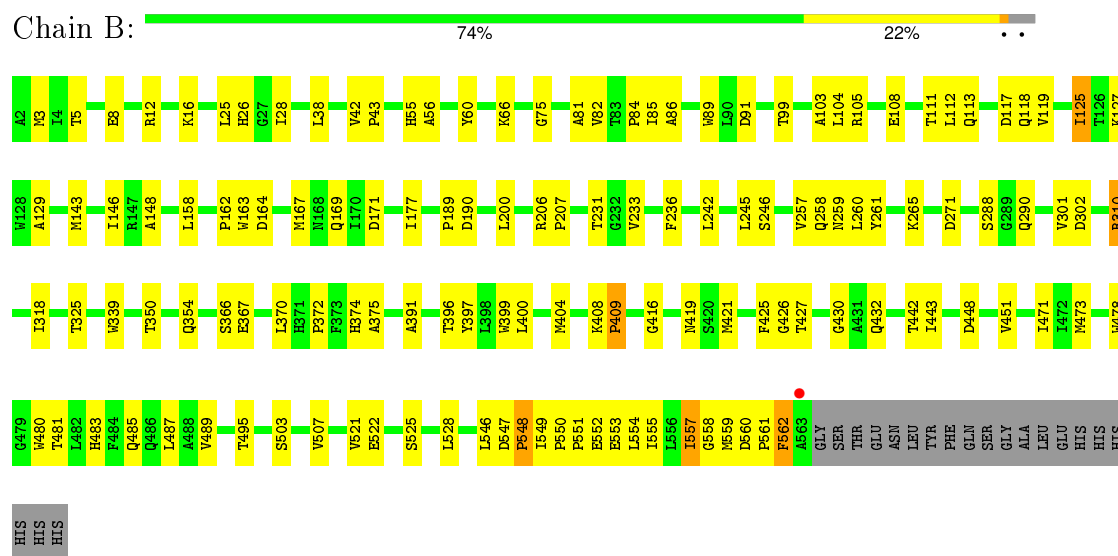
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Formolase



#### • Molecule 1: Formolase

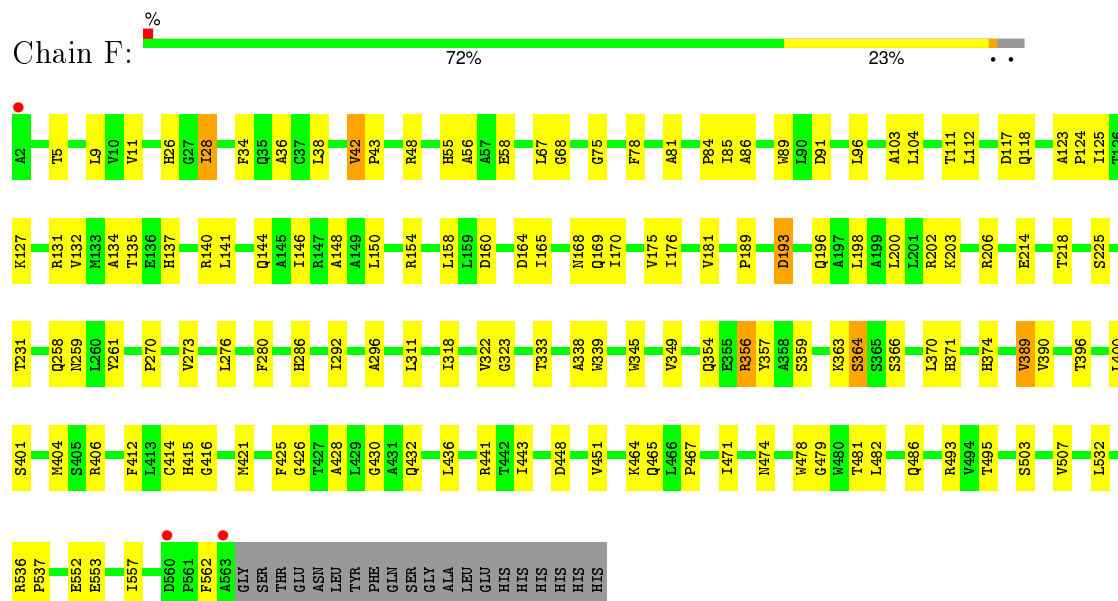


#### • Molecule 1: Formolase

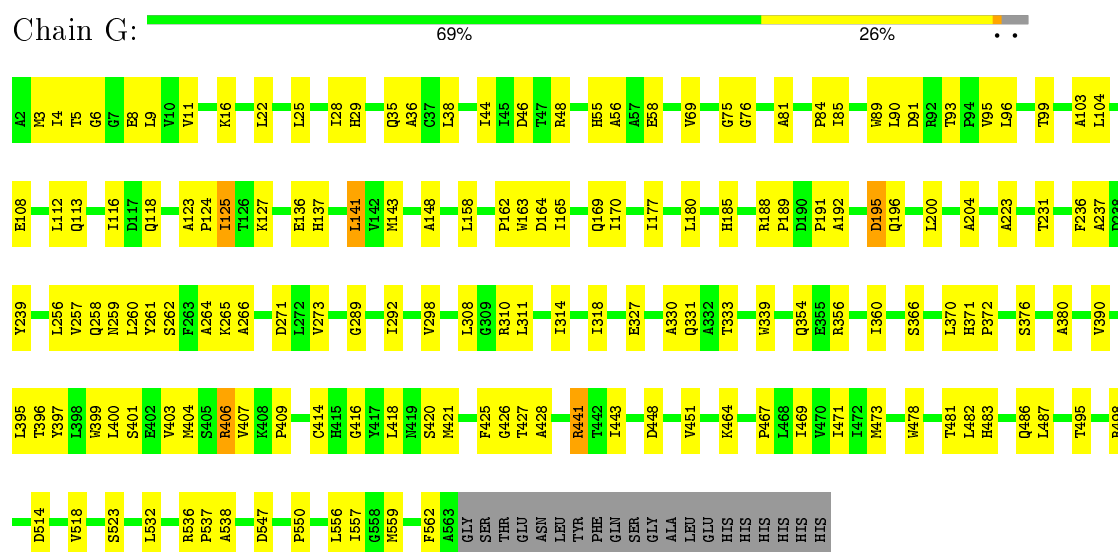


TYR  
PHE  
GLN  
SER  
GLY  
ALA  
LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

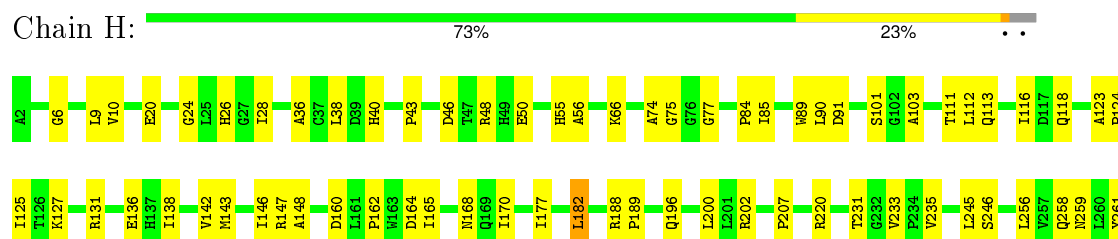
• Molecule 1: Formolase



• Molecule 1: Formolase



• Molecule 1: Formolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.88Å 136.56Å 167.06Å 90.00° 95.36° 90.00°	Depositor
Resolution (Å)	166.33 – 3.00 48.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.4 (166.33-3.00) 89.5 (48.91-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.208 , 0.257 0.212 , 0.259	Depositor DCC
$R_{free}$ test set	4028 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 30.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	4 of 80023 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	33455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.33 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3419e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, TPP

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	0.50	0/4244	0.74	1/5789 (0.0%)
1	B	0.54	1/4240 (0.0%)	0.76	2/5784 (0.0%)
1	C	0.52	0/4240	0.77	0/5784
1	D	0.51	0/4240	0.74	0/5784
1	E	0.52	0/4240	0.76	1/5784 (0.0%)
1	F	0.51	0/4240	0.75	1/5784 (0.0%)
1	G	0.54	0/4240	0.76	1/5784 (0.0%)
1	H	0.53	0/4240	0.79	1/5784 (0.0%)
All	All	0.52	1/33924 (0.0%)	0.76	7/46277 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	PRO	N-CD	-5.57	1.40	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	112	LEU	CA-CB-CG	6.85	131.05	115.30
1	B	117	ASP	CB-CG-OD1	6.44	124.10	118.30
1	E	159	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	H	429	LEU	CB-CG-CD1	-5.40	101.81	111.00
1	F	96	LEU	CA-CB-CG	-5.19	103.36	115.30

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	4157	0	4143	141	0
1	B	4153	0	4140	115	0
1	C	4153	0	4140	109	0
1	D	4153	0	4140	138	0
1	E	4153	0	4140	121	0
1	F	4153	0	4140	116	0
1	G	4153	0	4140	131	0
1	H	4153	0	4140	112	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	26	0	16	8	0
3	B	26	0	16	7	0
3	C	26	0	16	9	0
3	D	26	0	16	6	0
3	E	26	0	16	5	0
3	F	26	0	16	9	0
3	G	26	0	16	10	0
3	H	26	0	16	9	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
4	G	3	0	0	0	0
All	All	33455	0	33251	941	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 14.

The worst 5 of 941 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:E:425:PHE:CZ	1:E:451:VAL:HG23	1.78	1.18
1:F:5:THR:HG22	1:F:169:GLN:HG2	1.27	1.13
1:F:196:GLN:O	1:F:200:LEU:HD13	1.50	1.11
1:G:38:LEU:HD13	1:H:495:THR:HG21	1.20	1.10
1:E:425:PHE:HZ	1:E:451:VAL:HG23	1.08	1.07

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	561/582 (96%)	524 (93%)	35 (6%)	2 (0%)	39	80
1	B	560/582 (96%)	522 (93%)	35 (6%)	3 (0%)	34	76
1	C	560/582 (96%)	529 (94%)	29 (5%)	2 (0%)	39	80
1	D	560/582 (96%)	517 (92%)	39 (7%)	4 (1%)	26	70
1	E	560/582 (96%)	532 (95%)	27 (5%)	1 (0%)	52	88
1	F	560/582 (96%)	531 (95%)	28 (5%)	1 (0%)	52	88
1	G	560/582 (96%)	528 (94%)	27 (5%)	5 (1%)	21	64
1	H	560/582 (96%)	530 (95%)	29 (5%)	1 (0%)	52	88
All	All	4481/4656 (96%)	4213 (94%)	249 (6%)	19 (0%)	39	80

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	PRO
1	C	41	ASP
1	D	265	LYS
1	D	290	GLN
1	F	117	ASP

### 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	421/438 (96%)	412 (98%)	9 (2%)	61	89
1	B	421/438 (96%)	412 (98%)	9 (2%)	61	89
1	C	421/438 (96%)	413 (98%)	8 (2%)	65	90
1	D	421/438 (96%)	416 (99%)	5 (1%)	78	94
1	E	421/438 (96%)	412 (98%)	9 (2%)	61	89
1	F	421/438 (96%)	411 (98%)	10 (2%)	57	87
1	G	421/438 (96%)	412 (98%)	9 (2%)	61	89
1	H	421/438 (96%)	414 (98%)	7 (2%)	68	91
All	All	3368/3504 (96%)	3302 (98%)	66 (2%)	63	89

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	425	PHE
1	E	331	GLN
1	H	177	ILE
1	D	559	MET
1	E	200	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	286	HIS
1	E	258	GLN
1	H	258	GLN
1	D	294	HIS
1	D	432	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	TPP	A	602	2	20,27,27	1.50	4 (20%)	31,40,40	1.93	9 (29%)
3	TPP	B	602	2	20,27,27	1.30	3 (15%)	31,40,40	2.02	11 (35%)
3	TPP	C	602	2	20,27,27	1.47	3 (15%)	31,40,40	1.71	10 (32%)
3	TPP	D	602	2	20,27,27	1.24	1 (5%)	31,40,40	1.93	9 (29%)
3	TPP	E	602	2	20,27,27	1.23	2 (10%)	31,40,40	1.76	10 (32%)
3	TPP	F	602	2	20,27,27	1.38	3 (15%)	31,40,40	1.79	10 (32%)
3	TPP	G	602	2	20,27,27	1.39	4 (20%)	31,40,40	1.95	9 (29%)
3	TPP	H	602	2	20,27,27	1.45	4 (20%)	31,40,40	1.92	9 (29%)

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	TPP	A	602	2	-	0/16/17/17	0/2/2/2
3	TPP	B	602	2	-	0/16/17/17	0/2/2/2
3	TPP	C	602	2	-	0/16/17/17	0/2/2/2
3	TPP	D	602	2	-	0/16/17/17	0/2/2/2
3	TPP	E	602	2	-	0/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	F	602	2	-	0/16/17/17	0/2/2/2
3	TPP	G	602	2	-	0/16/17/17	0/2/2/2
3	TPP	H	602	2	-	0/16/17/17	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	TPP	C6'-C5'	2.08	1.42	1.37
3	C	602	TPP	C6'-C5'	2.22	1.42	1.37
3	B	602	TPP	C6'-C5'	2.22	1.42	1.37
3	E	602	TPP	C7'-C5'	2.30	1.56	1.51
3	H	602	TPP	C4-N3	2.32	1.41	1.39

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TPP	PA-O3A-PB	-4.28	118.32	132.67
3	H	602	TPP	PA-O3A-PB	-4.01	119.23	132.67
3	G	602	TPP	PA-O3A-PB	-3.73	120.16	132.67
3	F	602	TPP	PA-O3A-PB	-3.68	120.32	132.67
3	D	602	TPP	PA-O3A-PB	-3.55	120.77	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	TPP	8	0
3	B	602	TPP	7	0
3	C	602	TPP	9	0
3	D	602	TPP	6	0
3	E	602	TPP	5	0
3	F	602	TPP	9	0
3	G	602	TPP	10	0
3	H	602	TPP	9	0

## 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 [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	563/582 (96%)	-0.45	3 (0%) 91 76	31, 65, 89, 116	0
1	B	562/582 (96%)	-0.49	1 (0%) 95 87	28, 64, 110, 146	0
1	C	562/582 (96%)	-0.50	1 (0%) 95 87	30, 60, 88, 116	0
1	D	562/582 (96%)	-0.46	0 100 100	32, 72, 112, 132	0
1	E	562/582 (96%)	-0.43	0 100 100	31, 69, 115, 149	0
1	F	562/582 (96%)	-0.41	3 (0%) 91 76	32, 66, 97, 136	0
1	G	562/582 (96%)	-0.47	0 100 100	22, 64, 116, 144	0
1	H	562/582 (96%)	-0.47	1 (0%) 95 87	26, 58, 97, 130	0
All	All	4497/4656 (96%)	-0.46	9 (0%) 95 87	22, 64, 107, 149	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	563	ALA	3.3
1	F	563	ALA	3.1
1	A	2	ALA	2.7
1	A	564	GLY	2.6
1	B	563	ALA	2.5

### 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
2	MG	A	601	1/1	0.94	0.21	3.21	56,56,56,56	0
3	TPP	H	602	26/26	0.96	0.19	1.39	52,84,108,121	0
3	TPP	A	602	26/26	0.95	0.19	1.03	55,71,98,114	0
2	MG	G	601	1/1	0.98	0.16	0.91	36,36,36,36	0
3	TPP	D	602	26/26	0.96	0.18	0.53	73,92,112,123	0
3	TPP	B	602	26/26	0.96	0.17	0.39	77,95,120,126	0
2	MG	C	601	1/1	0.99	0.15	0.25	49,49,49,49	0
2	MG	E	601	1/1	0.99	0.16	0.24	62,62,62,62	0
3	TPP	G	602	26/26	0.96	0.17	0.21	55,75,91,94	0
3	TPP	F	602	26/26	0.96	0.17	0.03	61,82,112,119	0
3	TPP	E	602	26/26	0.96	0.17	-0.02	66,73,93,100	0
3	TPP	C	602	26/26	0.97	0.16	-0.13	60,80,103,108	0
2	MG	B	601	1/1	0.98	0.12	-0.19	68,68,68,68	0
2	MG	H	601	1/1	0.97	0.14	-0.25	43,43,43,43	0
2	MG	D	601	1/1	0.96	0.11	-0.85	75,75,75,75	0
2	MG	F	601	1/1	0.99	0.10	-1.62	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.