



# wwPDB X-ray Structure Validation Summary Report

Apr 4, 2014 – 12:04 PM BST

PDB ID : 2Q4X  
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At3g16990  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.10 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>

---

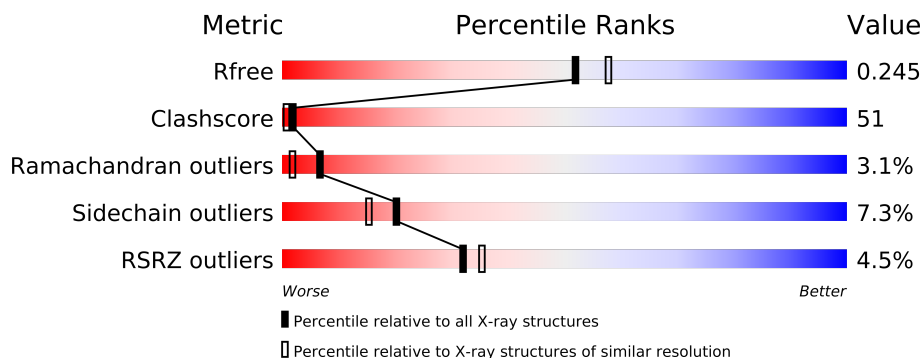
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23015  
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) : stable23015

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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.



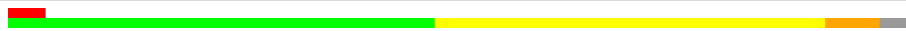
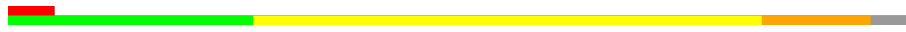
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	1-A	221	
1	1-B	221	
1	2-A	221	
1	2-B	221	
1	3-A	221	
1	3-B	221	
1	4-A	221	
1	4-B	221	
1	5-A	221	
1	5-B	221	
1	6-A	221	
1	6-B	221	
1	7-A	221	
1	7-B	221	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	8-A	221	
1	8-B	221	

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	SO4	1-A	1403	-	X
2	SO4	1-B	1404	-	X
2	SO4	2-B	1403	-	X
2	SO4	2-B	1404	-	X
2	SO4	3-B	1403	-	X
2	SO4	3-B	1404	-	X
2	SO4	4-B	1403	-	X
2	SO4	4-B	1404	-	X
2	SO4	5-B	1403	-	X
2	SO4	5-B	1404	-	X
2	SO4	6-B	1403	-	X
2	SO4	6-B	1404	-	X
2	SO4	7-B	1403	-	X
2	SO4	7-B	1404	-	X
2	SO4	8-B	1403	-	X
2	SO4	8-B	1404	-	X
3	HMH	1-A	1300	X	X
3	HMH	1-B	1301	X	-
3	HMH	2-A	1300	X	X
3	HMH	3-A	1300	X	X
3	HMH	3-B	1301	X	-
3	HMH	4-A	1300	X	X
3	HMH	4-B	1301	X	-
3	HMH	5-A	1300	X	X
3	HMH	5-B	1301	X	-
3	HMH	6-A	1300	-	X
3	HMH	6-B	1301	X	-
3	HMH	7-A	1300	X	X
3	HMH	7-B	1301	X	-
3	HMH	8-A	1300	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30952 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.

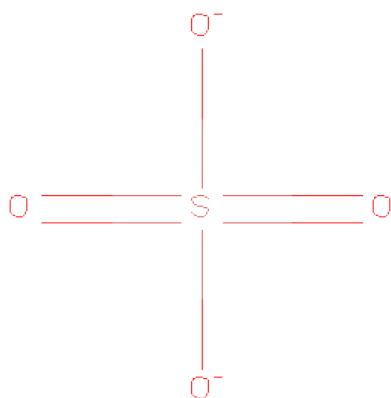
- Molecule 1 is a protein called Seed maturation protein PM36 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	2-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	3-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	4-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	5-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	6-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	7-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	8-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	1-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	2-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	3-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	4-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	5-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	6-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	7-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	8-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
A	21	ALA	SER	ENGINEERED	UNP Q9ASY9
A	75	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
A	123	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
A	133	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
A	216	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
B	21	ALA	SER	ENGINEERED	UNP Q9ASY9
B	75	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
B	123	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
B	133	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9
B	216	MSE	MET	MODIFIED RESIDUE	UNP Q9ASY9

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	1	Total O S 5 4 1	0	0
2	2-A	1	Total O S 5 4 1	0	0
2	3-A	1	Total O S 5 4 1	0	0
2	4-A	1	Total O S 5 4 1	0	0
2	5-A	1	Total O S 5 4 1	0	0

*Continued on next page...*

*Continued from previous page...*

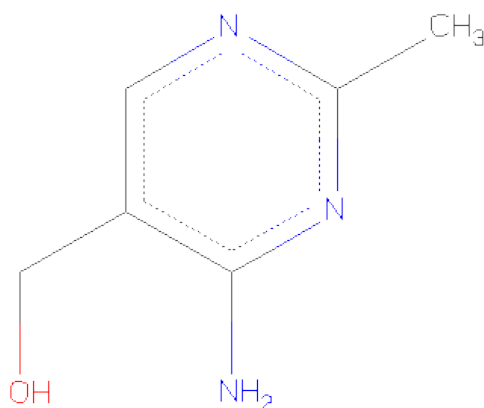
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	1-B	1	Total	O	S	0	0
			5	4	1		
2	2-B	1	Total	O	S	0	0
			5	4	1		
2	3-B	1	Total	O	S	0	0
			5	4	1		
2	4-B	1	Total	O	S	0	0
			5	4	1		
2	5-B	1	Total	O	S	0	0
			5	4	1		
2	6-B	1	Total	O	S	0	0
			5	4	1		
2	7-B	1	Total	O	S	0	0
			5	4	1		
2	8-B	1	Total	O	S	0	0
			5	4	1		
2	1-B	1	Total	O	S	0	0
			5	4	1		
2	2-B	1	Total	O	S	0	0
			5	4	1		
2	3-B	1	Total	O	S	0	0
			5	4	1		
2	4-B	1	Total	O	S	0	0
			5	4	1		
2	5-B	1	Total	O	S	0	0
			5	4	1		
2	6-B	1	Total	O	S	0	0
			5	4	1		
2	7-B	1	Total	O	S	0	0
			5	4	1		
2	8-B	1	Total	O	S	0	0
			5	4	1		
2	1-B	1	Total	O	S	0	0
			5	4	1		
2	2-B	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	3-B	1	Total	O	S	0	0
			5	4	1		
2	4-B	1	Total	O	S	0	0
			5	4	1		
2	5-B	1	Total	O	S	0	0
			5	4	1		
2	6-B	1	Total	O	S	0	0
			5	4	1		
2	7-B	1	Total	O	S	0	0
			5	4	1		
2	8-B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-AMINO-5-HYDROXYMETHYL-2-METHYLPYRIMIDINE (three-letter code: HMH) (formula: C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	2-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	3-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	4-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	5-A	1	Total	C	N	O	0	0
			10	6	3	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	6-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	7-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	8-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	1-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	2-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	3-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	4-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	5-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	6-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	7-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	8-B	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	213	Total	O	0	0
			213	213		
4	2-A	214	Total	O	0	0
			214	214		
4	3-A	214	Total	O	0	0
			214	214		
4	4-A	214	Total	O	0	0
			214	214		
4	5-A	213	Total	O	0	0
			213	213		
4	6-A	214	Total	O	0	0
			214	214		
4	7-A	214	Total	O	0	0
			214	214		
4	8-A	214	Total	O	0	0
			214	214		

*Continued on next page...*



*Continued from previous page...*

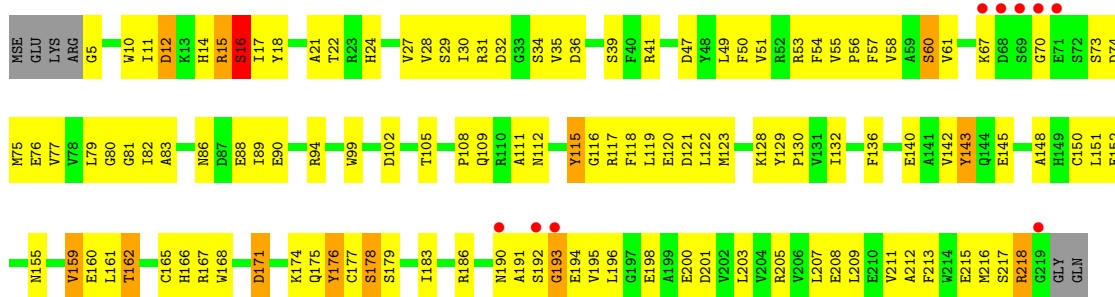
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-B	214	Total 214	O 214	0	0
4	2-B	213	Total 213	O 213	0	0
4	3-B	213	Total 213	O 213	0	0
4	4-B	213	Total 213	O 213	0	0
4	5-B	214	Total 214	O 214	0	0
4	6-B	213	Total 213	O 213	0	0
4	7-B	213	Total 213	O 213	0	0
4	8-B	213	Total 213	O 213	0	0

### 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.

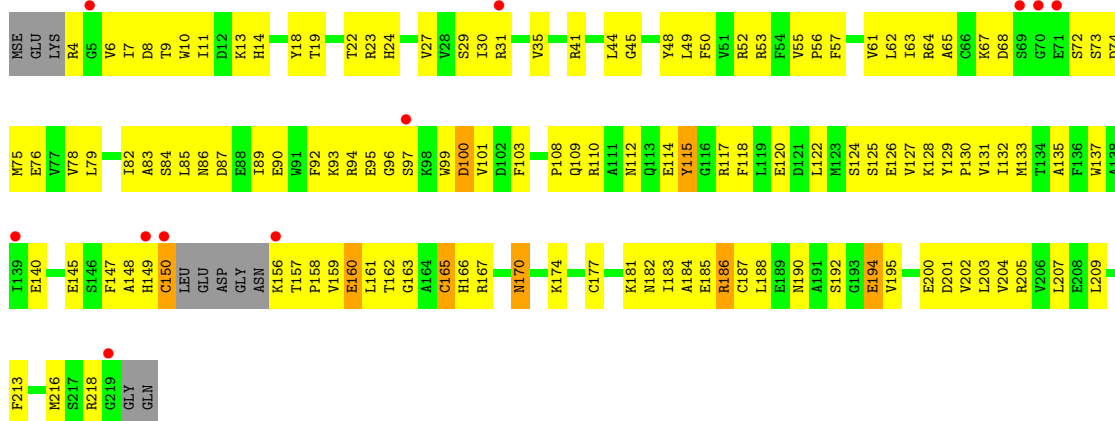
- Molecule 1: Seed maturation protein PM36 homolog

Chain 1-A:



- Molecule 1: Seed maturation protein PM36 homolog

Chain 1-B:



- Molecule 1: Seed maturation protein PM36 homolog

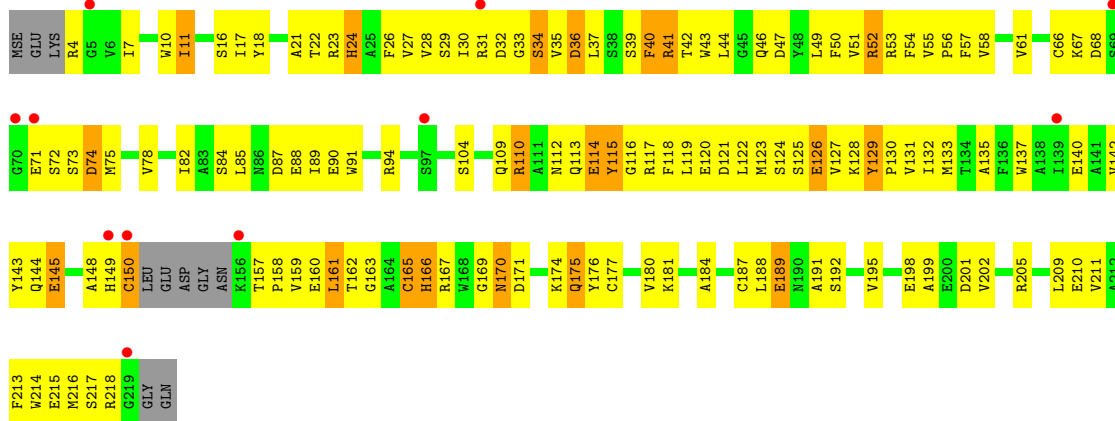
Chain 2-A:





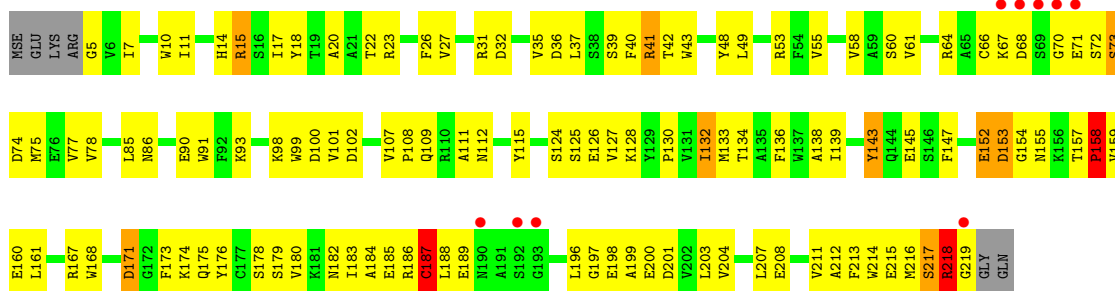
- Molecule 1: Seed maturation protein PM36 homolog

Chain 2-B:



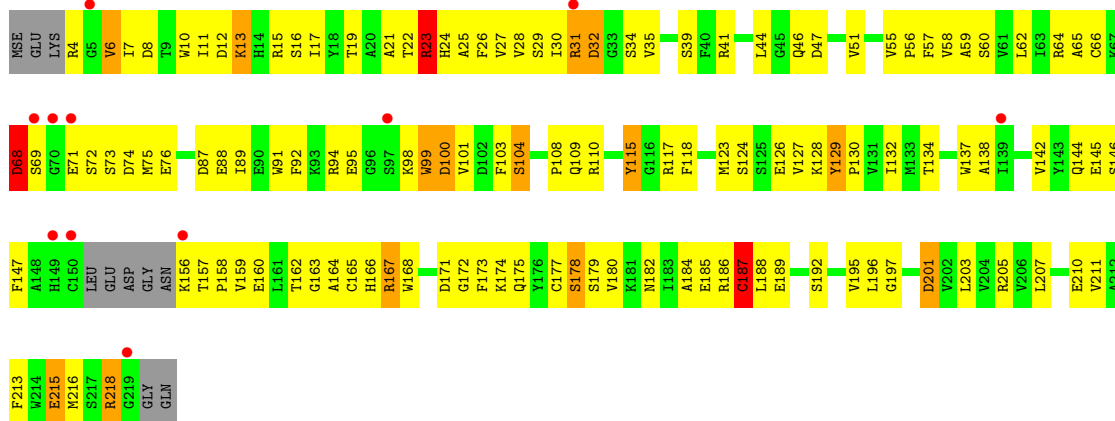
- Molecule 1: Seed maturation protein PM36 homolog

Chain 3-A:

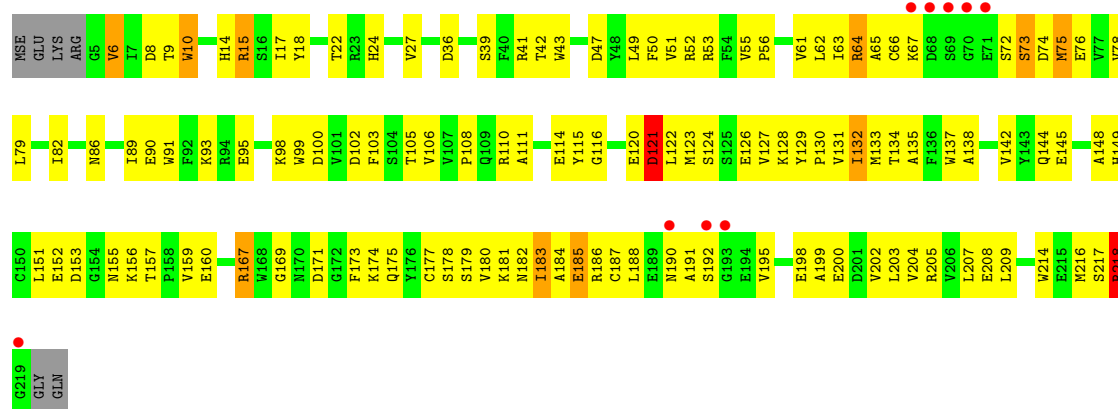


- Molecule 1: Seed maturation protein PM36 homolog

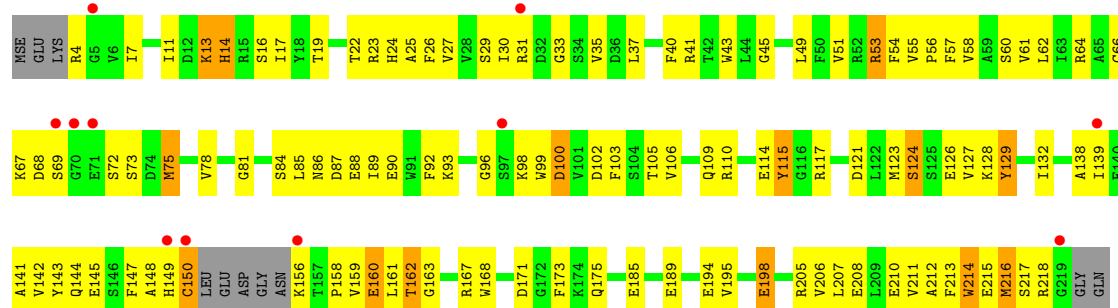
Chain 3-B:



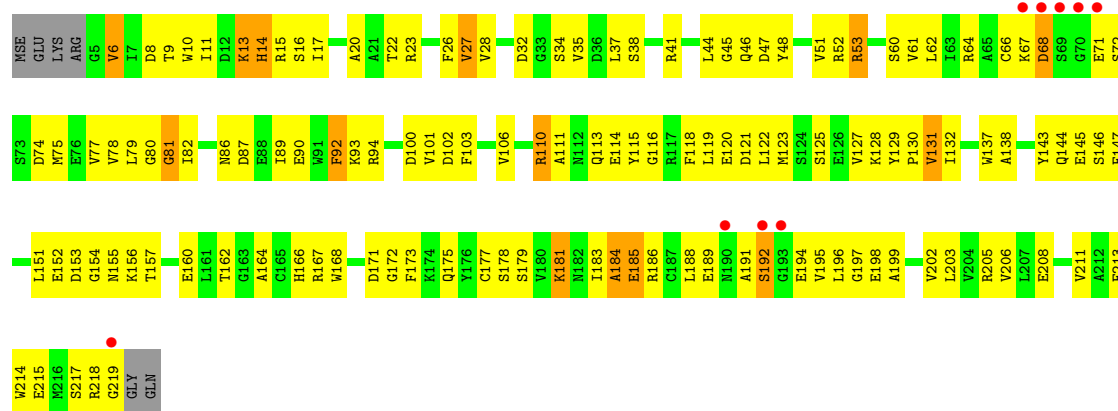
- Molecule 1: Seed maturation protein PM36 homolog

Chain 4-A: 

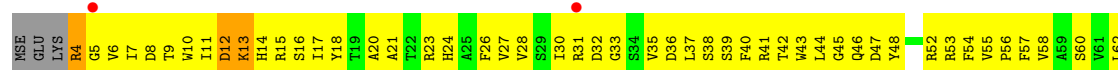
- Molecule 1: Seed maturation protein PM36 homolog

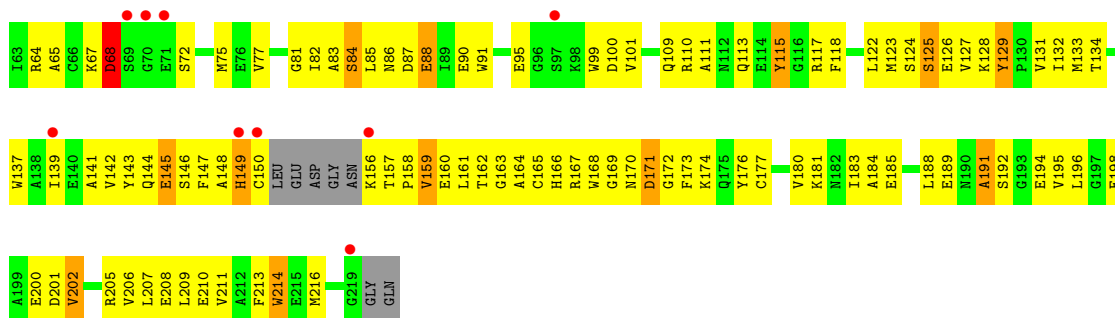
Chain 4-B: 

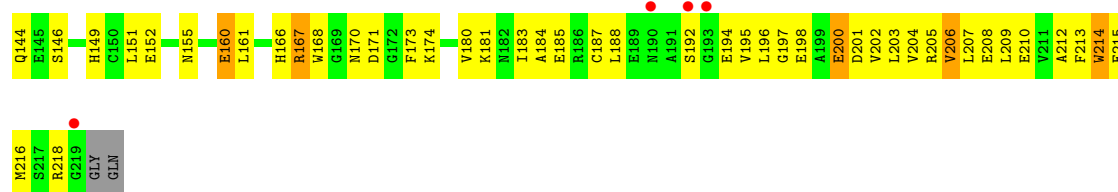
- Molecule 1: Seed maturation protein PM36 homolog

Chain 5-A: 

- Molecule 1: Seed maturation protein PM36 homolog

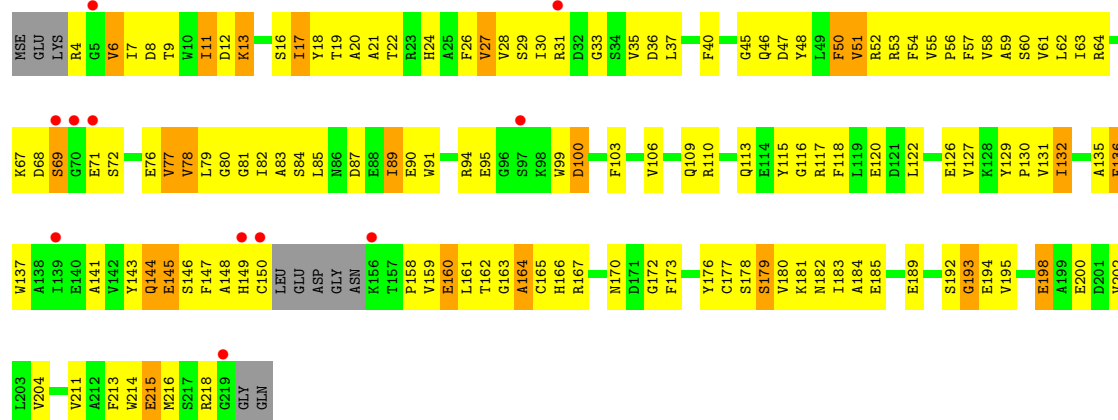
Chain 5-B: 





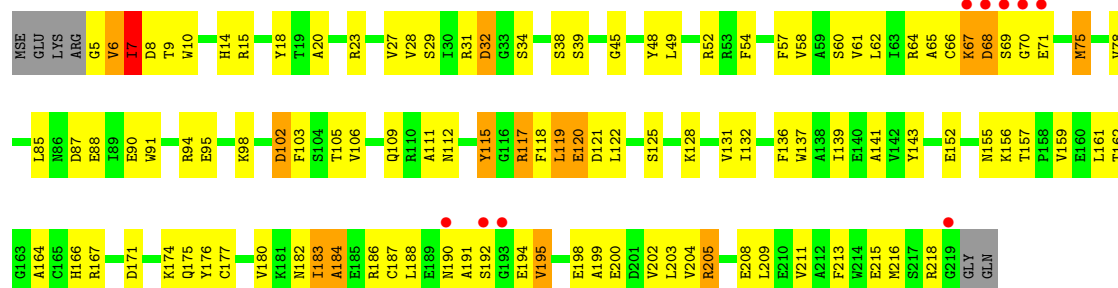
- Molecule 1: Seed maturation protein PM36 homolog

Chain 7-B:



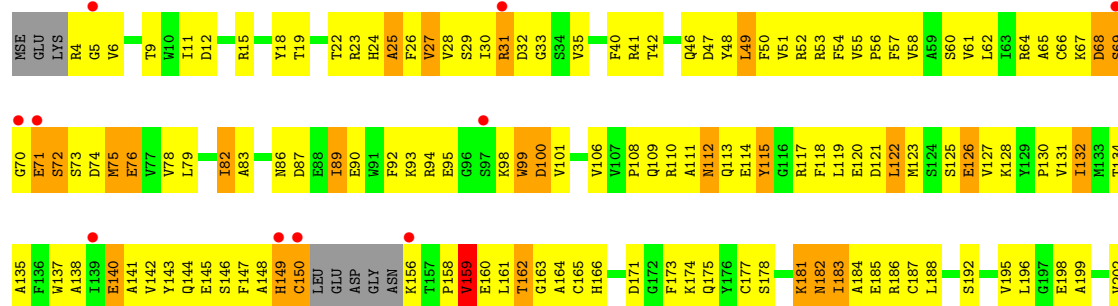
- Molecule 1: Seed maturation protein PM36 homolog

Chain 8-A:



- Molecule 1: Seed maturation protein PM36 homolog

Chain 8-B:



L203	V204	R205	V206	L207	E208	L209	E210	V211	A212	F213	W214	E215	M216	S217	R218	G219	GLY	GLN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

●

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.70Å 62.70Å 287.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.04 – 2.10 28.04 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.4 (28.04-2.10) 86.5 (28.04-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.46 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.136 , 0.231 0.152 , 0.245	Depositor DCC
$R_{free}$ test set	1519 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30054 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	30952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: HMH, 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	1-A	0.86	0/1749	0.85	0/2362
1	1-B	0.90	0/1722	0.85	1/2323 (0.0%)
1	2-A	0.91	1/1749 (0.1%)	0.90	0/2362
1	2-B	0.91	0/1722	0.89	2/2323 (0.1%)
1	3-A	0.86	0/1749	0.84	1/2362 (0.0%)
1	3-B	0.90	0/1722	0.87	1/2323 (0.0%)
1	4-A	0.87	0/1749	0.88	1/2362 (0.0%)
1	4-B	0.90	0/1722	0.85	0/2323
1	5-A	1.00	1/1749 (0.1%)	1.00	3/2362 (0.1%)
1	5-B	1.01	1/1722 (0.1%)	0.98	0/2323
1	6-A	0.94	0/1749	0.93	3/2362 (0.1%)
1	6-B	0.98	0/1722	0.96	5/2323 (0.2%)
1	7-A	1.02	3/1749 (0.2%)	1.00	4/2362 (0.2%)
1	7-B	1.06	2/1722 (0.1%)	0.97	3/2323 (0.1%)
1	8-A	0.93	0/1749	0.95	2/2362 (0.1%)
1	8-B	0.99	1/1722 (0.1%)	0.95	3/2323 (0.1%)
All	All	0.94	9/27768 (0.0%)	0.92	29/37480 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-A	0	1
1	2-B	0	1
1	3-B	0	1
1	4-B	0	1
1	5-B	0	1
1	6-A	0	1
All	All	0	6

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-B	215	GLU	CD-OE1	14.97	1.42	1.25
1	7-A	88	GLU	CG-CD	7.26	1.62	1.51
1	5-B	88	GLU	CB-CG	6.82	1.65	1.52
1	7-A	187	CYS	CB-SG	-6.58	1.71	1.82
1	2-A	114	GLU	CG-CD	6.48	1.61	1.51

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	117	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	7-B	215	GLU	OE1-CD-OE2	8.75	133.80	123.30
1	7-B	215	GLU	CG-CD-OE2	-8.34	101.62	118.30
1	8-A	117	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	2-B	74	ASP	CB-CG-OD1	7.23	124.80	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-A	176	TYR	Sidechain
1	2-B	129	TYR	Sidechain
1	3-B	129	TYR	Sidechain
1	4-B	129	TYR	Sidechain
1	5-B	129	TYR	Sidechain

## 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	1-A	1714	0	1642	127	0
1	1-B	1688	0	1624	152	1
1	2-A	1714	0	1642	144	1
1	2-B	1688	0	1624	209	0
1	3-A	1714	0	1642	130	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-B	1688	0	1624	152	2
1	4-A	1714	0	1642	146	2
1	4-B	1688	0	1624	166	1
1	5-A	1714	0	1642	154	2
1	5-B	1688	0	1624	222	3
1	6-A	1714	0	1642	184	1
1	6-B	1688	0	1624	212	2
1	7-A	1714	0	1642	172	2
1	7-B	1688	0	1624	200	0
1	8-A	1714	0	1642	139	1
1	8-B	1688	0	1624	216	0
2	1-A	5	0	0	0	0
2	1-B	15	0	0	3	0
2	2-A	5	0	0	0	0
2	2-B	15	0	0	0	0
2	3-A	5	0	0	0	0
2	3-B	15	0	0	1	0
2	4-A	5	0	0	1	0
2	4-B	15	0	0	1	0
2	5-A	5	0	0	0	0
2	5-B	15	0	0	3	0
2	6-A	5	0	0	1	0
2	6-B	15	0	0	0	0
2	7-A	5	0	0	2	0
2	7-B	15	0	0	4	0
2	8-A	5	0	0	1	0
2	8-B	15	0	0	1	0
3	1-A	10	0	8	1	0
3	1-B	10	0	9	0	0
3	2-A	10	0	8	1	0
3	2-B	10	0	9	1	0
3	3-A	10	0	8	1	0
3	3-B	10	0	9	2	0
3	4-A	10	0	8	0	0
3	4-B	10	0	8	1	0
3	5-A	10	0	9	5	0
3	5-B	10	0	9	1	0
3	6-A	10	0	9	1	0
3	6-B	10	0	8	2	0
3	7-A	10	0	8	0	0
3	7-B	10	0	9	2	0
3	8-A	10	0	8	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8-B	10	0	9	3	0
4	1-A	213	0	0	29	2
4	1-B	214	0	0	45	1
4	2-A	214	0	0	23	1
4	2-B	213	0	0	61	2
4	3-A	214	0	0	29	3
4	3-B	213	0	0	45	3
4	4-A	214	0	0	27	2
4	4-B	213	0	0	34	3
4	5-A	213	0	0	37	3
4	5-B	214	0	0	81	2
4	6-A	214	0	0	51	4
4	6-B	213	0	0	52	1
4	7-A	214	0	0	41	1
4	7-B	213	0	0	57	3
4	8-A	214	0	0	43	1
4	8-B	213	0	0	60	2
All	All	30952	0	26264	2728	27

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 51.

The worst 5 of 2728 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:ARG:NH2	1:B:100:ASP:HB2	1.45	1.30
1:A:27:VAL:HG23	4:A:1410:HOH:O	1.30	1.27
1:B:150:CYS:SG	4:B:1542:HOH:O	1.95	1.25
1:B:72:SER:HA	4:B:1596:HOH:O	1.40	1.22
1:A:70:GLY:HA3	4:A:1525:HOH:O	1.40	1.22

The worst 5 of 27 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	Distance(Å)	Clash(Å)
1:A:126:GLU:OE1	4:B:1432:HOH:O[5_555]	1.79	0.41
4:A:1597:HOH:O	4:B:1560:HOH:O[5_555]	1.90	0.30
4:A:1597:HOH:O	4:B:1560:HOH:O[5_555]	1.90	0.30
4:A:1597:HOH:O	4:B:1560:HOH:O[5_555]	1.90	0.30
4:A:1597:HOH:O	4:B:1560:HOH:O[5_555]	1.90	0.30

## 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	1-A	213/221 (96%)	192 (90%)	15 (7%)	6 (3%)	8	2
1	1-B	207/221 (94%)	190 (92%)	14 (7%)	3 (1%)	16	9
1	2-A	213/221 (96%)	203 (95%)	8 (4%)	2 (1%)	25	17
1	2-B	207/221 (94%)	179 (86%)	20 (10%)	8 (4%)	5	1
1	3-A	213/221 (96%)	181 (85%)	26 (12%)	6 (3%)	8	2
1	3-B	207/221 (94%)	175 (84%)	23 (11%)	9 (4%)	4	1
1	4-A	213/221 (96%)	186 (87%)	19 (9%)	8 (4%)	5	1
1	4-B	207/221 (94%)	184 (89%)	21 (10%)	2 (1%)	22	14
1	5-A	213/221 (96%)	191 (90%)	16 (8%)	6 (3%)	8	2
1	5-B	207/221 (94%)	184 (89%)	18 (9%)	5 (2%)	9	3
1	6-A	213/221 (96%)	190 (89%)	15 (7%)	8 (4%)	5	1
1	6-B	207/221 (94%)	181 (87%)	17 (8%)	9 (4%)	4	1
1	7-A	213/221 (96%)	188 (88%)	21 (10%)	4 (2%)	12	5
1	7-B	207/221 (94%)	165 (80%)	28 (14%)	14 (7%)	2	0
1	8-A	213/221 (96%)	188 (88%)	19 (9%)	6 (3%)	8	2
1	8-B	207/221 (94%)	179 (86%)	20 (10%)	8 (4%)	5	1
All	All	3360/3536 (95%)	2956 (88%)	300 (9%)	104 (3%)	7	2

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	190	ASN
1	1-A	193	GLY
1	2-B	170	ASN
1	3-B	124	SER
1	4-A	73	SER

### 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	1-A	184/184 (100%)	169 (92%)	15 (8%)	17	11
1	1-B	181/184 (98%)	171 (94%)	10 (6%)	30	26
1	2-A	184/184 (100%)	179 (97%)	5 (3%)	57	60
1	2-B	181/184 (98%)	165 (91%)	16 (9%)	14	9
1	3-A	184/184 (100%)	170 (92%)	14 (8%)	19	14
1	3-B	181/184 (98%)	166 (92%)	15 (8%)	16	11
1	4-A	184/184 (100%)	172 (94%)	12 (6%)	24	20
1	4-B	181/184 (98%)	168 (93%)	13 (7%)	21	16
1	5-A	184/184 (100%)	170 (92%)	14 (8%)	19	14
1	5-B	181/184 (98%)	166 (92%)	15 (8%)	16	11
1	6-A	184/184 (100%)	169 (92%)	15 (8%)	17	11
1	6-B	181/184 (98%)	167 (92%)	14 (8%)	18	13
1	7-A	184/184 (100%)	173 (94%)	11 (6%)	27	22
1	7-B	181/184 (98%)	173 (96%)	8 (4%)	39	36
1	8-A	184/184 (100%)	169 (92%)	15 (8%)	17	11
1	8-B	181/184 (98%)	160 (88%)	21 (12%)	8	4
All	All	2920/2944 (99%)	2707 (93%)	213 (7%)	20	15

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4-B	162	THR
1	5-B	82	ILE
1	8-B	72	SER
1	4-B	216	MSE
1	5-A	115	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	4-A	182	ASN
1	5-B	182	ASN
1	8-B	112	ASN
1	4-B	182	ASN
1	5-A	113	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 ⓘ

48 ligands are modelled in this entry.

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	HMH	1-A	1300	-	10,10,10	2.12	7 (70%)	13,13,13	3.06	9 (69%)
2	SO4	1-A	1403	-	4,4,4	0.53	0	6,6,6	0.29	0
3	HMH	1-B	1301	-	10,10,10	1.62	3 (30%)	13,13,13	2.42	8 (61%)
2	SO4	1-B	1401	-	4,4,4	0.43	0	6,6,6	0.30	0
2	SO4	1-B	1402	-	4,4,4	0.32	0	6,6,6	0.15	0
2	SO4	1-B	1404	-	4,4,4	0.38	0	6,6,6	0.23	0
3	HMH	2-A	1300	-	10,10,10	2.10	4 (40%)	13,13,13	2.97	10 (76%)
2	SO4	2-A	1401	-	4,4,4	0.36	0	6,6,6	0.33	0
3	HMH	2-B	1301	-	10,10,10	1.80	3 (30%)	13,13,13	2.19	7 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	2-B	1402	-	4,4,4	0.52	0	6,6,6	0.30	0
2	SO4	2-B	1403	-	4,4,4	0.50	0	6,6,6	0.11	0
2	SO4	2-B	1404	-	4,4,4	0.34	0	6,6,6	0.17	0
3	HMH	3-A	1300	-	10,10,10	2.24	4 (40%)	13,13,13	3.06	8 (61%)
2	SO4	3-A	1401	-	4,4,4	0.31	0	6,6,6	0.35	0
3	HMH	3-B	1301	-	10,10,10	1.47	2 (20%)	13,13,13	2.49	9 (69%)
2	SO4	3-B	1402	-	4,4,4	0.30	0	6,6,6	0.12	0
2	SO4	3-B	1403	-	4,4,4	0.49	0	6,6,6	0.25	0
2	SO4	3-B	1404	-	4,4,4	0.51	0	6,6,6	0.21	0
3	HMH	4-A	1300	-	10,10,10	2.11	7 (70%)	13,13,13	2.99	9 (69%)
2	SO4	4-A	1401	-	4,4,4	0.70	0	6,6,6	0.40	0
3	HMH	4-B	1301	-	10,10,10	1.36	2 (20%)	13,13,13	2.41	9 (69%)
2	SO4	4-B	1402	-	4,4,4	0.20	0	6,6,6	0.18	0
2	SO4	4-B	1403	-	4,4,4	0.42	0	6,6,6	0.28	0
2	SO4	4-B	1404	-	4,4,4	0.40	0	6,6,6	0.21	0
3	HMH	5-A	1300	-	10,10,10	2.42	4 (40%)	13,13,13	2.83	8 (61%)
2	SO4	5-A	1401	-	4,4,4	0.44	0	6,6,6	0.23	0
3	HMH	5-B	1301	-	10,10,10	2.07	4 (40%)	13,13,13	2.53	8 (61%)
2	SO4	5-B	1402	-	4,4,4	0.47	0	6,6,6	0.12	0
2	SO4	5-B	1403	-	4,4,4	0.26	0	6,6,6	0.24	0
2	SO4	5-B	1404	-	4,4,4	0.56	0	6,6,6	0.14	0
3	HMH	6-A	1300	-	10,10,10	2.33	3 (30%)	13,13,13	2.45	7 (53%)
2	SO4	6-A	1401	-	4,4,4	0.28	0	6,6,6	0.33	0
3	HMH	6-B	1301	-	10,10,10	1.70	4 (40%)	13,13,13	2.59	9 (69%)
2	SO4	6-B	1402	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	6-B	1403	-	4,4,4	0.48	0	6,6,6	0.15	0
2	SO4	6-B	1404	-	4,4,4	0.58	0	6,6,6	0.13	0
3	HMH	7-A	1300	-	10,10,10	2.22	4 (40%)	13,13,13	2.87	9 (69%)
2	SO4	7-A	1401	-	4,4,4	0.57	0	6,6,6	0.31	0
3	HMH	7-B	1301	-	10,10,10	1.72	3 (30%)	13,13,13	2.49	9 (69%)
2	SO4	7-B	1402	-	4,4,4	0.31	0	6,6,6	0.12	0
2	SO4	7-B	1403	-	4,4,4	0.60	0	6,6,6	0.23	0
2	SO4	7-B	1404	-	4,4,4	0.12	0	6,6,6	0.24	0
3	HMH	8-A	1300	-	10,10,10	2.26	5 (50%)	13,13,13	2.96	8 (61%)
2	SO4	8-A	1401	-	4,4,4	0.74	0	6,6,6	0.29	0
3	HMH	8-B	1301	-	10,10,10	1.60	3 (30%)	13,13,13	2.10	7 (53%)
2	SO4	8-B	1402	-	4,4,4	0.47	0	6,6,6	0.26	0
2	SO4	8-B	1403	-	4,4,4	0.55	0	6,6,6	0.33	0
2	SO4	8-B	1404	-	4,4,4	0.42	0	6,6,6	0.18	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	HMH	1-A	1300	-	-	0/2/2/2	0/1/1/1
2	SO4	1-A	1403	-	-	0/0/0/0	0/0/0/0
3	HMH	1-B	1301	-	-	0/2/2/2	0/1/1/1
2	SO4	1-B	1401	-	-	0/0/0/0	0/0/0/0
2	SO4	1-B	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	1-B	1404	-	-	0/0/0/0	0/0/0/0
3	HMH	2-A	1300	-	-	0/2/2/2	0/1/1/1
2	SO4	2-A	1401	-	-	0/0/0/0	0/0/0/0
3	HMH	2-B	1301	-	-	0/2/2/2	0/1/1/1
2	SO4	2-B	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	2-B	1403	-	-	0/0/0/0	0/0/0/0
2	SO4	2-B	1404	-	-	0/0/0/0	0/0/0/0
3	HMH	3-A	1300	-	-	0/2/2/2	0/1/1/1
2	SO4	3-A	1401	-	-	0/0/0/0	0/0/0/0
3	HMH	3-B	1301	-	-	0/2/2/2	0/1/1/1
2	SO4	3-B	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	3-B	1403	-	-	0/0/0/0	0/0/0/0
2	SO4	3-B	1404	-	-	0/0/0/0	0/0/0/0
3	HMH	4-A	1300	-	-	0/2/2/2	0/1/1/1
2	SO4	4-A	1401	-	-	0/0/0/0	0/0/0/0
3	HMH	4-B	1301	-	-	0/2/2/2	0/1/1/1
2	SO4	4-B	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	4-B	1403	-	-	0/0/0/0	0/0/0/0
2	SO4	4-B	1404	-	-	0/0/0/0	0/0/0/0
3	HMH	5-A	1300	-	-	0/2/2/2	0/1/1/1
2	SO4	5-A	1401	-	-	0/0/0/0	0/0/0/0
3	HMH	5-B	1301	-	-	0/2/2/2	0/1/1/1
2	SO4	5-B	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	5-B	1403	-	-	0/0/0/0	0/0/0/0
2	SO4	5-B	1404	-	-	0/0/0/0	0/0/0/0
3	HMH	6-A	1300	-	-	0/2/2/2	0/1/1/1
2	SO4	6-A	1401	-	-	0/0/0/0	0/0/0/0
3	HMH	6-B	1301	-	-	0/2/2/2	0/1/1/1
2	SO4	6-B	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	6-B	1403	-	-	0/0/0/0	0/0/0/0
2	SO4	6-B	1404	-	-	0/0/0/0	0/0/0/0
3	HMH	7-A	1300	-	-	0/2/2/2	0/1/1/1
2	SO4	7-A	1401	-	-	0/0/0/0	0/0/0/0
3	HMH	7-B	1301	-	-	0/2/2/2	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	7-B	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	7-B	1403	-	-	0/0/0/0	0/0/0/0
2	SO4	7-B	1404	-	-	0/0/0/0	0/0/0/0
3	HMH	8-A	1300	-	-	0/2/2/2	0/1/1/1
2	SO4	8-A	1401	-	-	0/0/0/0	0/0/0/0
3	HMH	8-B	1301	-	-	0/2/2/2	0/1/1/1
2	SO4	8-B	1402	-	-	0/0/0/0	0/0/0/0
2	SO4	8-B	1403	-	-	0/0/0/0	0/0/0/0
2	SO4	8-B	1404	-	-	0/0/0/0	0/0/0/0

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6-A	1300	HMH	C4A-N3A	4.71	1.42	1.35
3	5-A	1300	HMH	C6A-N1A	4.07	1.43	1.34
3	3-A	1300	HMH	C4A-N3A	3.86	1.41	1.35
3	7-A	1300	HMH	C4A-N3A	3.86	1.41	1.35
3	8-A	1300	HMH	C4A-N3A	3.84	1.41	1.35

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-A	1300	HMH	N4A-C4A-N3A	5.39	124.68	116.99
3	5-A	1300	HMH	CM2-C2A-N1A	5.36	123.41	117.02
3	2-A	1300	HMH	N4A-C4A-N3A	5.32	124.59	116.99
3	6-A	1300	HMH	N4A-C4A-N3A	5.05	124.20	116.99
3	1-A	1300	HMH	CM2-C2A-N1A	4.92	122.88	117.02

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	1-A	215/221 (97%)	-0.21	9 (4%) 35 39	11, 22, 34, 59	215 (100%)
1	1-B	211/221 (95%)	-0.03	11 (5%) 26 29	6, 22, 44, 59	211 (100%)
1	2-A	215/221 (97%)	-0.21	9 (4%) 35 39	11, 22, 34, 59	215 (100%)
1	2-B	211/221 (95%)	-0.03	11 (5%) 26 29	6, 22, 44, 59	211 (100%)
1	3-A	215/221 (97%)	-0.21	9 (4%) 35 39	11, 22, 34, 59	215 (100%)
1	3-B	211/221 (95%)	-0.03	11 (5%) 26 29	6, 22, 44, 59	211 (100%)
1	4-A	215/221 (97%)	-0.21	9 (4%) 35 39	11, 22, 34, 59	215 (100%)
1	4-B	211/221 (95%)	-0.03	11 (5%) 26 29	6, 22, 44, 59	211 (100%)
1	5-A	215/221 (97%)	-0.21	9 (4%) 35 39	11, 22, 34, 59	215 (100%)
1	5-B	211/221 (95%)	-0.03	11 (5%) 26 29	6, 22, 44, 59	211 (100%)
1	6-A	215/221 (97%)	-0.21	9 (4%) 35 39	11, 22, 34, 59	215 (100%)
1	6-B	211/221 (95%)	-0.03	11 (5%) 26 29	6, 22, 44, 59	211 (100%)
1	7-A	215/221 (97%)	-0.21	9 (4%) 35 39	11, 22, 34, 59	215 (100%)
1	7-B	211/221 (95%)	-0.03	11 (5%) 26 29	6, 22, 44, 59	211 (100%)
1	8-A	215/221 (97%)	-0.21	9 (4%) 35 39	11, 22, 34, 59	215 (100%)
1	8-B	211/221 (95%)	-0.03	11 (5%) 26 29	6, 22, 44, 59	211 (100%)
All	All	3408/3536 (96%)	-0.12	160 (4%) 32 33	6, 22, 41, 59	3408 (100%)

The worst 5 of 160 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	70	GLY	9.3
1	2-B	70	GLY	9.3
1	3-B	70	GLY	9.3
1	4-B	70	GLY	9.3
1	5-B	70	GLY	9.3

## 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	SO4	7-B	1404	5/5	0.18	11.48	63,64,67,67	5
2	SO4	5-B	1404	5/5	0.18	11.23	66,67,68,68	5
2	SO4	3-B	1404	5/5	0.18	10.83	68,68,68,69	5
2	SO4	6-B	1404	5/5	0.18	10.83	67,67,68,69	5
2	SO4	2-B	1404	5/5	0.18	9.45	65,67,68,68	5
2	SO4	8-B	1404	5/5	0.18	9.19	64,66,67,68	5
2	SO4	1-B	1404	5/5	0.18	9.10	66,67,68,69	5
2	SO4	4-B	1404	5/5	0.18	9.06	66,67,68,69	5
2	SO4	2-B	1403	5/5	0.17	4.73	58,58,59,59	5
2	SO4	6-B	1403	5/5	0.17	4.73	57,57,58,58	5
2	SO4	4-B	1403	5/5	0.17	4.66	61,62,62,63	5
2	SO4	8-B	1403	5/5	0.17	4.49	61,61,62,63	5
2	SO4	7-B	1403	5/5	0.17	4.49	61,62,63,63	5
2	SO4	1-A	1403	5/5	0.17	4.12	62,62,62,63	5
3	HMH	5-A	1300	10/10	0.23	2.76	21,25,27,29	10
3	HMH	6-A	1300	10/10	0.23	2.76	14,23,26,27	10
3	HMH	4-A	1300	10/10	0.23	2.65	17,23,25,25	10
3	HMH	1-A	1300	10/10	0.23	2.65	19,24,25,26	10
3	HMH	7-A	1300	10/10	0.23	2.64	16,21,23,31	10
3	HMH	3-A	1300	10/10	0.23	2.63	21,24,26,28	10
3	HMH	8-A	1300	10/10	0.23	2.63	21,24,26,26	10
3	HMH	2-A	1300	10/10	0.23	2.61	17,23,25,26	10
2	SO4	3-B	1403	5/5	0.17	2.25	60,60,61,61	5
2	SO4	5-B	1403	5/5	0.17	2.02	58,61,61,61	5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HMH	8-B	1301	10/10	0.19	1.77	3,20,23,24	10
3	HMH	7-B	1301	10/10	0.19	1.58	21,25,28,31	10
3	HMH	3-B	1301	10/10	0.19	1.56	23,25,29,32	10
3	HMH	6-B	1301	10/10	0.19	1.51	19,24,26,26	10
3	HMH	4-B	1301	10/10	0.19	1.48	19,21,25,26	10
3	HMH	1-B	1301	10/10	0.19	1.47	15,19,23,33	10
3	HMH	5-B	1301	10/10	0.19	1.45	17,19,21,24	10
3	HMH	2-B	1301	10/10	0.19	1.38	15,17,21,34	10
2	SO4	5-A	1401	5/5	0.10	-0.03	24,25,27,27	5
2	SO4	3-A	1401	5/5	0.10	-0.03	28,30,31,32	5
2	SO4	7-A	1401	5/5	0.10	-0.04	26,28,29,29	5
2	SO4	6-A	1401	5/5	0.10	-0.05	26,28,30,31	5
2	SO4	2-A	1401	5/5	0.10	-0.05	27,30,30,31	5
2	SO4	4-A	1401	5/5	0.10	-0.05	29,35,36,36	5
2	SO4	8-A	1401	5/5	0.10	-0.11	25,25,26,28	5
2	SO4	5-B	1402	5/5	0.07	-0.22	21,25,26,27	5
2	SO4	8-B	1402	5/5	0.07	-0.29	21,22,23,25	5
2	SO4	1-B	1401	5/5	0.09	-0.31	29,29,30,31	5
2	SO4	2-B	1402	5/5	0.07	-0.34	23,24,26,26	5
2	SO4	3-B	1402	5/5	0.07	-0.41	22,22,23,24	5
2	SO4	6-B	1402	5/5	0.07	-0.43	22,22,25,25	5
2	SO4	4-B	1402	5/5	0.07	-0.44	24,24,26,26	5
2	SO4	7-B	1402	5/5	0.07	-0.45	22,23,25,25	5
2	SO4	1-B	1402	5/5	0.07	-0.45	21,21,22,23	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.