wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 03:41 AM EDT

PDB ID	:	2Q47
Title	:	Ensemble refinement of the protein crystal structure of a putative phosphoprotein phosphatase from Arabidopsis thaliana gene At1g05000
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	:	3.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

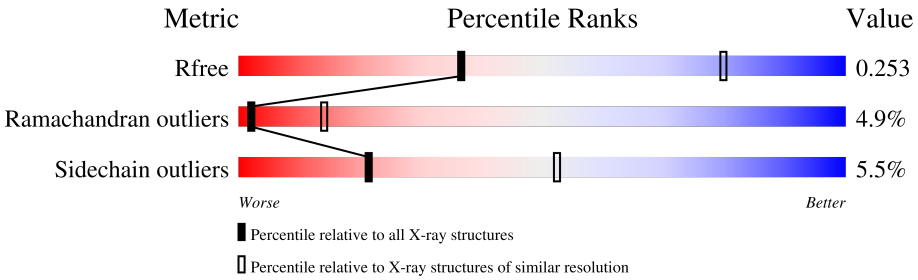
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	1-A	151	91% 8% •
1	1-B	151	91% 9%
1	10-A	151	94% 6%
1	10-B	151	87% 13% •
1	11-A	151	94% 6%
1	11-B	151	92% 7% •
1	12-A	151	93% 7%
1	12-B	151	87% 12% •

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Mol	Chain	Length	Quality of chain
1	13-A	151	89% 11%
1	13-B	151	79% 20%
1	14-A	151	89% 11%
1	14-B	151	84% 15%
1	15-A	151	81% 18%
1	15-B	151	89% 11%
1	16-A	151	82% 17%
1	16-B	151	84% 16%
1	2-A	151	97%
1	2-B	151	93% 7%
1	3-A	151	95% 5%
1	3-B	151	86% 14%
1	4-A	151	91% 9%
1	4-B	151	94% 6%
1	5-A	151	95% 5%
1	5-B	151	89% 11%
1	6-A	151	91% 9%
1	6-B	151	93% 7%
1	7-A	151	92% 7%
1	7-B	151	97%
1	8-A	151	97%
1	8-B	151	93% 7%
1	9-A	151	95% 5%
1	9-B	151	94% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 40448 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 Probable tyrosine-protein phosphatase At1g05000.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	2-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	3-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	4-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	5-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	6-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	7-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	8-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	9-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	10-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	11-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	12-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	13-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	14-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	15-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	16-A	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			

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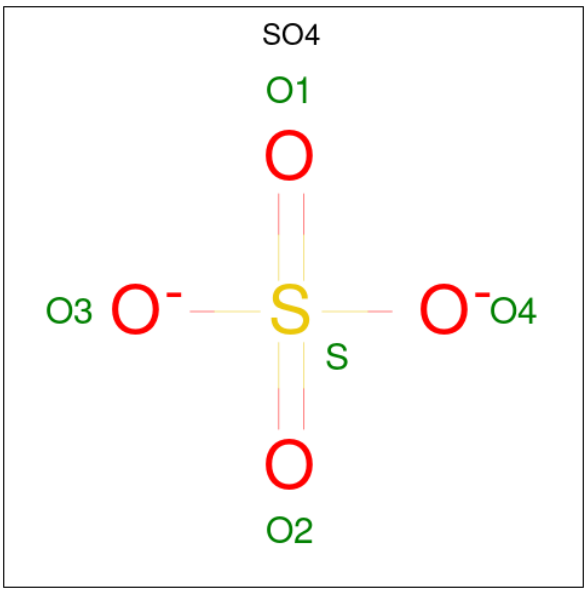
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	2-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	3-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	4-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	5-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	6-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	7-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	8-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	9-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	10-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	11-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	12-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	13-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	14-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	15-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			
1	16-B	151	Total	C	N	O	S	Se	0	0	0
			1224	789	216	211	5	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MSE	MET	modified residue	UNP Q9ZVN4
A	133	MSE	MET	modified residue	UNP Q9ZVN4
A	195	MSE	MET	modified residue	UNP Q9ZVN4
B	61	MSE	MET	modified residue	UNP Q9ZVN4
B	133	MSE	MET	modified residue	UNP Q9ZVN4
B	195	MSE	MET	modified residue	UNP Q9ZVN4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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
2	6-A	1	Total O S 5 4 1	0	0
2	7-A	1	Total O S 5 4 1	0	0
2	8-A	1	Total O S 5 4 1	0	0
2	9-A	1	Total O S 5 4 1	0	0
2	10-A	1	Total O S 5 4 1	0	0
2	11-A	1	Total O S 5 4 1	0	0
2	12-A	1	Total O S 5 4 1	0	0
2	13-A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	14-A	1	Total O S 5 4 1	0	0
2	15-A	1	Total O S 5 4 1	0	0
2	16-A	1	Total O S 5 4 1	0	0
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
2	6-A	1	Total O S 5 4 1	0	0
2	7-A	1	Total O S 5 4 1	0	0
2	8-A	1	Total O S 5 4 1	0	0
2	9-A	1	Total O S 5 4 1	0	0
2	10-A	1	Total O S 5 4 1	0	0
2	11-A	1	Total O S 5 4 1	0	0
2	12-A	1	Total O S 5 4 1	0	0
2	13-A	1	Total O S 5 4 1	0	0
2	14-A	1	Total O S 5 4 1	0	0
2	15-A	1	Total O S 5 4 1	0	0
2	16-A	1	Total O S 5 4 1	0	0
2	1-B	1	Total O S 5 4 1	0	0
2	2-B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	3-B	1	Total O S 5 4 1	0	0
2	4-B	1	Total O S 5 4 1	0	0
2	5-B	1	Total O S 5 4 1	0	0
2	6-B	1	Total O S 5 4 1	0	0
2	7-B	1	Total O S 5 4 1	0	0
2	8-B	1	Total O S 5 4 1	0	0
2	9-B	1	Total O S 5 4 1	0	0
2	10-B	1	Total O S 5 4 1	0	0
2	11-B	1	Total O S 5 4 1	0	0
2	12-B	1	Total O S 5 4 1	0	0
2	13-B	1	Total O S 5 4 1	0	0
2	14-B	1	Total O S 5 4 1	0	0
2	15-B	1	Total O S 5 4 1	0	0
2	16-B	1	Total O S 5 4 1	0	0
2	1-B	1	Total O S 5 4 1	0	0
2	2-B	1	Total O S 5 4 1	0	0
2	3-B	1	Total O S 5 4 1	0	0
2	4-B	1	Total O S 5 4 1	0	0
2	5-B	1	Total O S 5 4 1	0	0
2	6-B	1	Total O S 5 4 1	0	0
2	7-B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	8-B	1	Total O S 5 4 1	0	0
2	9-B	1	Total O S 5 4 1	0	0
2	10-B	1	Total O S 5 4 1	0	0
2	11-B	1	Total O S 5 4 1	0	0
2	12-B	1	Total O S 5 4 1	0	0
2	13-B	1	Total O S 5 4 1	0	0
2	14-B	1	Total O S 5 4 1	0	0
2	15-B	1	Total O S 5 4 1	0	0
2	16-B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	31	Total O 31 31	0	0
3	2-A	31	Total O 31 31	0	0
3	3-A	30	Total O 30 30	0	0
3	4-A	30	Total O 30 30	0	0
3	5-A	29	Total O 29 29	0	0
3	6-A	28	Total O 28 28	0	0
3	7-A	29	Total O 29 29	0	0
3	8-A	29	Total O 29 29	0	0
3	9-A	29	Total O 29 29	0	0
3	10-A	28	Total O 28 28	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	11-A	30	Total O 30 30	0	0
3	12-A	31	Total O 31 31	0	0
3	13-A	29	Total O 29 29	0	0
3	14-A	31	Total O 31 31	0	0
3	15-A	31	Total O 31 31	0	0
3	16-A	31	Total O 31 31	0	0
3	1-B	29	Total O 29 29	0	0
3	2-B	29	Total O 29 29	0	0
3	3-B	30	Total O 30 30	0	0
3	4-B	30	Total O 30 30	0	0
3	5-B	31	Total O 31 31	0	0
3	6-B	32	Total O 32 32	0	0
3	7-B	31	Total O 31 31	0	0
3	8-B	31	Total O 31 31	0	0
3	9-B	31	Total O 31 31	0	0
3	10-B	32	Total O 32 32	0	0
3	11-B	30	Total O 30 30	0	0
3	12-B	29	Total O 29 29	0	0
3	13-B	31	Total O 31 31	0	0
3	14-B	29	Total O 29 29	0	0
3	15-B	29	Total O 29 29	0	0

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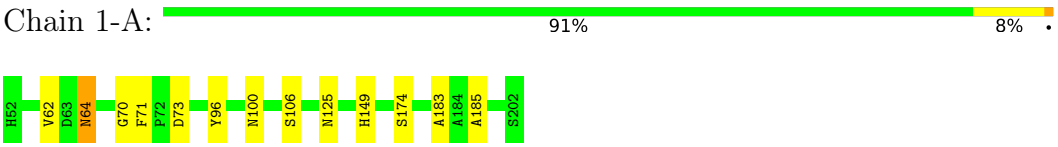
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	16-B	29	29	29	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

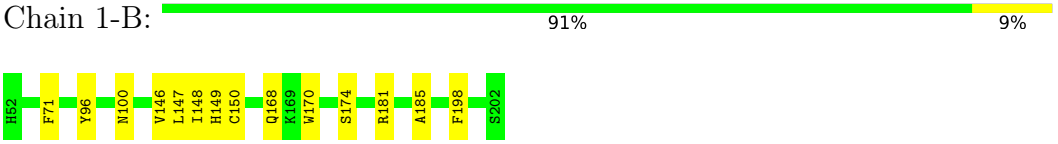
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 1-A:



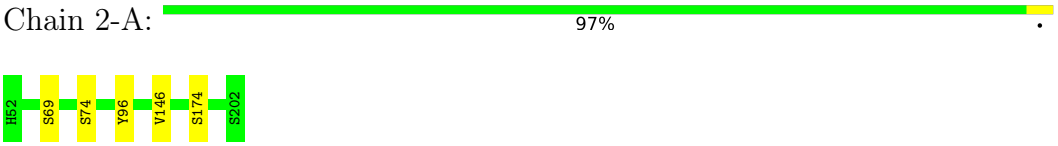
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 1-B:



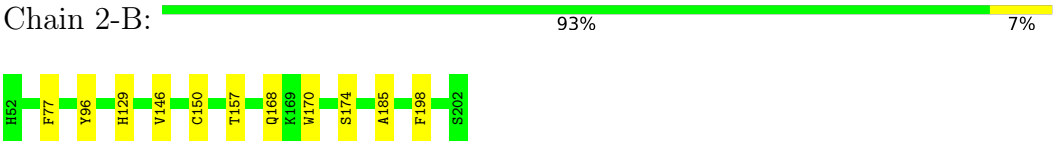
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 2-A:



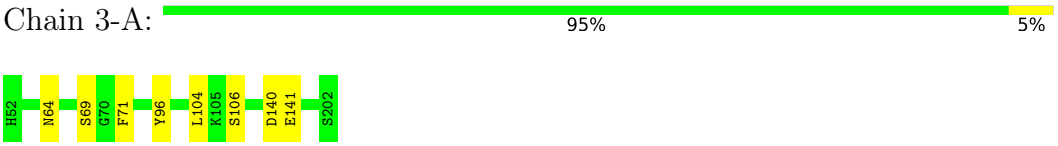
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 2-B:



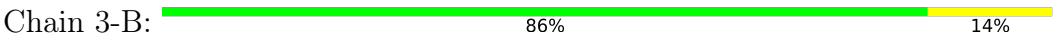
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

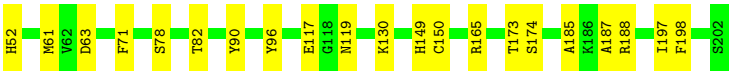
Chain 3-A:



• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 3-B:



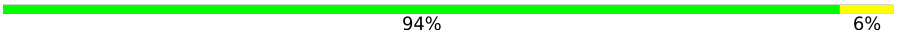


• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 4-A:

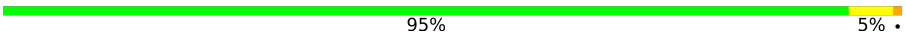
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

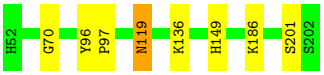
Chain 4-B:



• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 5-A:



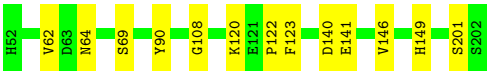


• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 5-B:

• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 6-A:



• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

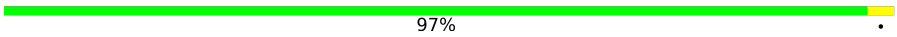
Chain 6-B:

• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 7-A:

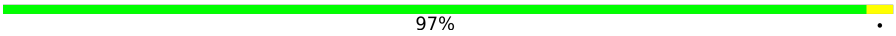
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 7-B:



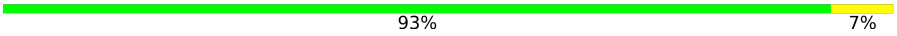
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

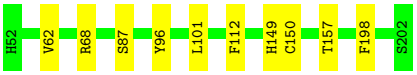
Chain 8-A:



• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

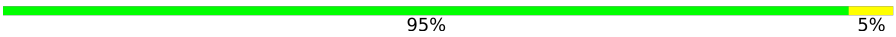
Chain 8-B:

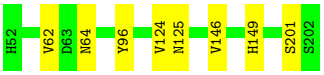




• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

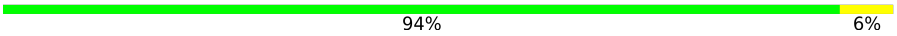
Chain 9-A:





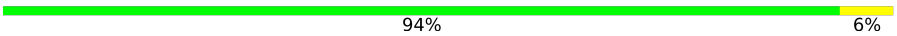
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 9-B:



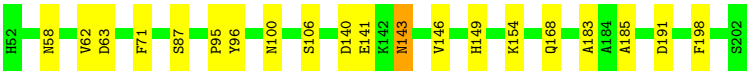
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 10-A:



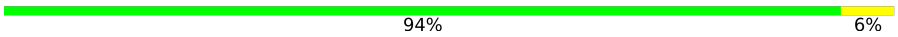
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 10-B:



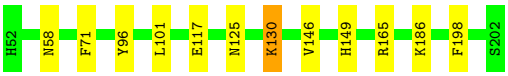
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 11-A:



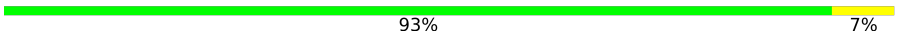
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

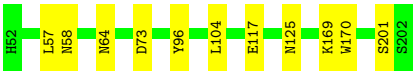
Chain 11-B:



• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 12-A:





• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 12-B:

• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 13-A:

• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

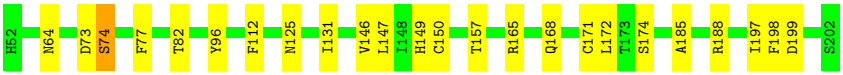
Chain 13-B:

• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 14-A:

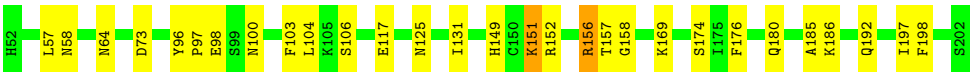
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 14-B:



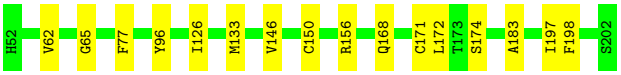
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 15-A:



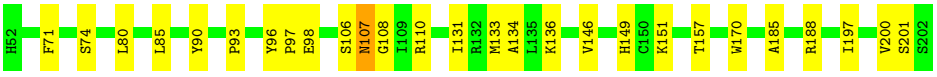
• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 15-B:



• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 16-A:



• Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 16-B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	124.48Å 124.48Å 124.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.50 – 3.30 44.01 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.50-3.30) 99.1 (44.01-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.21 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.160 , 0.234 0.204 , 0.253	Depositor DCC
R_{free} test set	1736 reflections (9.21%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 105.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	40448	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.36	0/1252	0.58	0/1680
1	1-B	0.34	0/1252	0.55	0/1680
1	2-A	0.36	0/1252	0.57	0/1680
1	2-B	0.35	0/1252	0.56	0/1680
1	3-A	0.35	0/1252	0.56	0/1680
1	3-B	0.35	0/1252	0.57	0/1680
1	4-A	0.37	0/1252	0.58	0/1680
1	4-B	0.36	0/1252	0.56	0/1680
1	5-A	0.36	0/1252	0.57	0/1680
1	5-B	0.34	0/1252	0.55	0/1680
1	6-A	0.36	0/1252	0.58	0/1680
1	6-B	0.34	0/1252	0.56	0/1680
1	7-A	0.36	0/1252	0.56	0/1680
1	7-B	0.35	0/1252	0.54	0/1680
1	8-A	0.35	0/1252	0.56	0/1680
1	8-B	0.34	0/1252	0.55	0/1680
1	9-A	0.35	0/1252	0.57	0/1680
1	9-B	0.34	0/1252	0.55	0/1680
1	10-A	0.35	0/1252	0.55	0/1680
1	10-B	0.35	0/1252	0.55	0/1680
1	11-A	0.36	0/1252	0.57	0/1680
1	11-B	0.34	0/1252	0.55	0/1680
1	12-A	0.35	0/1252	0.57	0/1680
1	12-B	0.34	0/1252	0.57	0/1680
1	13-A	0.40	0/1252	0.62	0/1680
1	13-B	0.39	0/1252	0.62	0/1680
1	14-A	0.38	0/1252	0.65	0/1680
1	14-B	0.38	0/1252	0.62	0/1680
1	15-A	0.39	0/1252	0.66	0/1680
1	15-B	0.38	0/1252	0.63	0/1680
1	16-A	0.40	0/1252	0.65	0/1680
1	16-B	0.40	0/1252	0.61	0/1680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.36	0/40064	0.58	0/53760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1224	0	1233	0	0
1	1-B	1224	0	1233	0	0
1	2-A	1224	0	1233	0	0
1	2-B	1224	0	1233	0	0
1	3-A	1224	0	1233	0	0
1	3-B	1224	0	1233	0	0
1	4-A	1224	0	1233	0	0
1	4-B	1224	0	1233	0	0
1	5-A	1224	0	1233	0	0
1	5-B	1224	0	1233	0	0
1	6-A	1224	0	1233	0	0
1	6-B	1224	0	1233	0	0
1	7-A	1224	0	1233	0	0
1	7-B	1224	0	1233	0	0
1	8-A	1224	0	1233	0	0
1	8-B	1224	0	1233	0	0
1	9-A	1224	0	1233	0	0
1	9-B	1224	0	1233	0	0
1	10-A	1224	0	1233	0	0
1	10-B	1224	0	1233	0	0
1	11-A	1224	0	1233	0	0
1	11-B	1224	0	1233	0	0
1	12-A	1224	0	1233	0	0
1	12-B	1224	0	1233	0	0
1	13-A	1224	0	1233	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13-B	1224	0	1233	0	0
1	14-A	1224	0	1233	0	0
1	14-B	1224	0	1233	0	0
1	15-A	1224	0	1233	0	0
1	15-B	1224	0	1233	0	0
1	16-A	1224	0	1233	0	0
1	16-B	1224	0	1233	0	0
2	1-A	10	0	0	0	0
2	1-B	10	0	0	0	0
2	2-A	10	0	0	0	0
2	2-B	10	0	0	0	0
2	3-A	10	0	0	0	0
2	3-B	10	0	0	0	0
2	4-A	10	0	0	0	0
2	4-B	10	0	0	0	0
2	5-A	10	0	0	0	0
2	5-B	10	0	0	0	0
2	6-A	10	0	0	0	0
2	6-B	10	0	0	0	0
2	7-A	10	0	0	0	0
2	7-B	10	0	0	0	0
2	8-A	10	0	0	0	0
2	8-B	10	0	0	0	0
2	9-A	10	0	0	0	0
2	9-B	10	0	0	0	0
2	10-A	10	0	0	0	0
2	10-B	10	0	0	0	0
2	11-A	10	0	0	0	0
2	11-B	10	0	0	0	0
2	12-A	10	0	0	0	0
2	12-B	10	0	0	0	0
2	13-A	10	0	0	0	0
2	13-B	10	0	0	0	0
2	14-A	10	0	0	0	0
2	14-B	10	0	0	0	0
2	15-A	10	0	0	0	0
2	15-B	10	0	0	0	0
2	16-A	10	0	0	0	0
2	16-B	10	0	0	0	0
3	1-A	31	0	0	0	0
3	1-B	29	0	0	0	0
3	2-A	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-B	29	0	0	0	0
3	3-A	30	0	0	0	0
3	3-B	30	0	0	0	0
3	4-A	30	0	0	0	0
3	4-B	30	0	0	0	0
3	5-A	29	0	0	0	0
3	5-B	31	0	0	0	0
3	6-A	28	0	0	0	0
3	6-B	32	0	0	0	0
3	7-A	29	0	0	0	0
3	7-B	31	0	0	0	0
3	8-A	29	0	0	0	0
3	8-B	31	0	0	0	0
3	9-A	29	0	0	0	0
3	9-B	31	0	0	0	0
3	10-A	28	0	0	0	0
3	10-B	32	0	0	0	0
3	11-A	30	0	0	0	0
3	11-B	30	0	0	0	0
3	12-A	31	0	0	0	0
3	12-B	29	0	0	0	0
3	13-A	29	0	0	0	0
3	13-B	31	0	0	0	0
3	14-A	31	0	0	0	0
3	14-B	29	0	0	0	0
3	15-A	31	0	0	0	0
3	15-B	29	0	0	0	0
3	16-A	31	0	0	0	0
3	16-B	29	0	0	0	0
All	All	40448	0	39456	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	149/151 (99%)	116 (78%)	26 (17%)	7 (5%)	2 14
1	1-B	149/151 (99%)	118 (79%)	24 (16%)	7 (5%)	2 14
1	2-A	149/151 (99%)	127 (85%)	21 (14%)	1 (1%)	22 54
1	2-B	149/151 (99%)	122 (82%)	22 (15%)	5 (3%)	3 22
1	3-A	149/151 (99%)	127 (85%)	17 (11%)	5 (3%)	3 22
1	3-B	149/151 (99%)	112 (75%)	29 (20%)	8 (5%)	2 12
1	4-A	149/151 (99%)	114 (76%)	30 (20%)	5 (3%)	3 22
1	4-B	149/151 (99%)	122 (82%)	22 (15%)	5 (3%)	3 22
1	5-A	149/151 (99%)	116 (78%)	28 (19%)	5 (3%)	3 22
1	5-B	149/151 (99%)	116 (78%)	20 (13%)	13 (9%)	1 5
1	6-A	149/151 (99%)	120 (80%)	20 (13%)	9 (6%)	1 10
1	6-B	149/151 (99%)	122 (82%)	23 (15%)	4 (3%)	5 26
1	7-A	149/151 (99%)	130 (87%)	13 (9%)	6 (4%)	3 18
1	7-B	149/151 (99%)	119 (80%)	28 (19%)	2 (1%)	12 40
1	8-A	149/151 (99%)	126 (85%)	21 (14%)	2 (1%)	12 40
1	8-B	149/151 (99%)	119 (80%)	27 (18%)	3 (2%)	7 32
1	9-A	149/151 (99%)	122 (82%)	22 (15%)	5 (3%)	3 22
1	9-B	149/151 (99%)	121 (81%)	24 (16%)	4 (3%)	5 26
1	10-A	149/151 (99%)	118 (79%)	27 (18%)	4 (3%)	5 26
1	10-B	149/151 (99%)	109 (73%)	29 (20%)	11 (7%)	1 7
1	11-A	149/151 (99%)	119 (80%)	26 (17%)	4 (3%)	5 26
1	11-B	149/151 (99%)	113 (76%)	32 (22%)	4 (3%)	5 26
1	12-A	149/151 (99%)	111 (74%)	31 (21%)	7 (5%)	2 14
1	12-B	149/151 (99%)	104 (70%)	32 (22%)	13 (9%)	1 5
1	13-A	149/151 (99%)	115 (77%)	26 (17%)	8 (5%)	2 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	13-B	149/151 (99%)	100 (67%)	32 (22%)	17 (11%)	0 2
1	14-A	149/151 (99%)	109 (73%)	30 (20%)	10 (7%)	1 8
1	14-B	149/151 (99%)	103 (69%)	34 (23%)	12 (8%)	1 6
1	15-A	149/151 (99%)	108 (72%)	26 (17%)	15 (10%)	0 3
1	15-B	149/151 (99%)	115 (77%)	26 (17%)	8 (5%)	2 12
1	16-A	149/151 (99%)	106 (71%)	26 (17%)	17 (11%)	0 2
1	16-B	149/151 (99%)	105 (70%)	36 (24%)	8 (5%)	2 12
All	All	4768/4832 (99%)	3704 (78%)	830 (17%)	234 (5%)	2 14

5 of 234 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	62	VAL
1	2-B	170	TRP
1	3-A	64	ASN
1	3-A	140	ASP
1	3-B	71	PHE

5.3.2 Protein sidechains (i)

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	136/133 (102%)	129 (95%)	7 (5%)	24 54
1	1-B	136/133 (102%)	129 (95%)	7 (5%)	24 54
1	2-A	136/133 (102%)	132 (97%)	4 (3%)	42 69
1	2-B	136/133 (102%)	130 (96%)	6 (4%)	28 59
1	3-A	136/133 (102%)	133 (98%)	3 (2%)	52 74
1	3-B	136/133 (102%)	123 (90%)	13 (10%)	8 29
1	4-A	136/133 (102%)	128 (94%)	8 (6%)	19 49
1	4-B	136/133 (102%)	132 (97%)	4 (3%)	42 69
1	5-A	136/133 (102%)	132 (97%)	4 (3%)	42 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	5-B	136/133 (102%)	133 (98%)	3 (2%)	52 74
1	6-A	136/133 (102%)	132 (97%)	4 (3%)	42 69
1	6-B	136/133 (102%)	128 (94%)	8 (6%)	19 49
1	7-A	136/133 (102%)	128 (94%)	8 (6%)	19 49
1	7-B	136/133 (102%)	134 (98%)	2 (2%)	65 81
1	8-A	136/133 (102%)	133 (98%)	3 (2%)	52 74
1	8-B	136/133 (102%)	129 (95%)	7 (5%)	24 54
1	9-A	136/133 (102%)	133 (98%)	3 (2%)	52 74
1	9-B	136/133 (102%)	131 (96%)	5 (4%)	34 63
1	10-A	136/133 (102%)	131 (96%)	5 (4%)	34 63
1	10-B	136/133 (102%)	126 (93%)	10 (7%)	13 40
1	11-A	136/133 (102%)	131 (96%)	5 (4%)	34 63
1	11-B	136/133 (102%)	127 (93%)	9 (7%)	16 46
1	12-A	136/133 (102%)	132 (97%)	4 (3%)	42 69
1	12-B	136/133 (102%)	127 (93%)	9 (7%)	16 46
1	13-A	136/133 (102%)	126 (93%)	10 (7%)	13 40
1	13-B	136/133 (102%)	119 (88%)	17 (12%)	4 19
1	14-A	136/133 (102%)	130 (96%)	6 (4%)	28 59
1	14-B	136/133 (102%)	123 (90%)	13 (10%)	8 29
1	15-A	136/133 (102%)	120 (88%)	16 (12%)	5 21
1	15-B	136/133 (102%)	128 (94%)	8 (6%)	19 49
1	16-A	136/133 (102%)	125 (92%)	11 (8%)	11 36
1	16-B	136/133 (102%)	120 (88%)	16 (12%)	5 21
All	All	4352/4256 (102%)	4114 (94%)	238 (6%)	21 52

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	11-A	96	TYR
1	16-A	157	THR
1	13-A	90	TYR
1	16-A	146	VAL
1	16-B	165	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-A	129	HIS
1	15-A	180	GLN
1	11-A	192	GLN
1	15-A	155	HIS
1	15-B	192	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

64 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	$\#\|Z\| > 2$
2	SO4	3-A	204	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	6-A	204	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	8-B	203	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	1-A	203	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	6-B	203	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	12-A	203	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	5-B	203	-	4,4,4	0.22	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	11-B	204	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	5-B	204	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	9-B	203	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	7-A	203	-	4,4,4	0.27	0	6,6,6	0.05	0
2	SO4	15-B	204	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	7-A	204	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	3-B	203	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	10-A	203	-	4,4,4	0.21	0	6,6,6	0.07	0
2	SO4	4-A	204	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	9-B	204	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	1-B	204	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	4-A	203	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	5-A	203	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	8-A	203	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	7-B	204	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	7-B	203	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	16-B	203	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	12-B	203	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	11-A	204	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	11-B	203	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	13-B	203	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	16-A	203	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	15-B	203	-	4,4,4	0.21	0	6,6,6	0.06	0
2	SO4	4-B	204	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	12-B	204	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	3-A	203	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	12-A	204	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	16-B	204	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	1-A	204	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	14-A	204	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	10-B	203	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	14-A	203	-	4,4,4	0.22	0	6,6,6	0.07	0
2	SO4	2-A	204	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	16-A	204	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	8-B	204	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	15-A	203	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	15-A	204	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	6-B	204	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	10-A	204	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	9-A	204	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	2-B	203	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	9-A	203	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	11-A	203	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	13-A	204	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	13-A	203	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	1-B	203	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	4-B	203	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	14-B	203	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	2-A	203	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	8-A	204	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	10-B	204	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	6-A	203	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	14-B	204	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	5-A	204	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	2-B	204	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	13-B	204	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	3-B	204	-	4,4,4	0.28	0	6,6,6	0.07	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.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.