



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:30 PM UTC

PDB ID : 2Q47 / pdb_00002q47
Title : Ensemble refinement of the protein crystal structure of a putative phospho-protein 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 Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

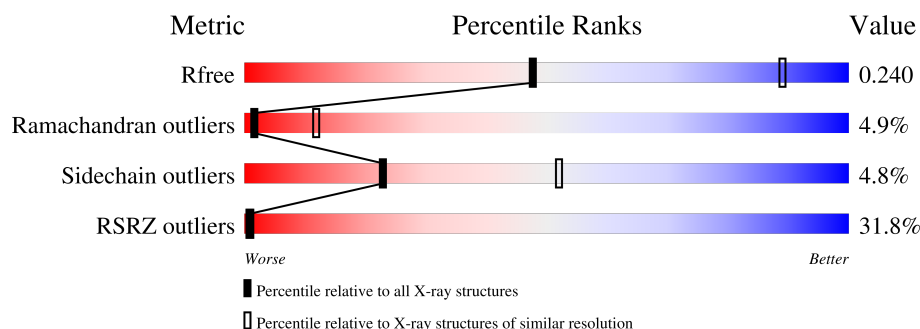
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



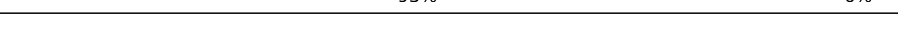
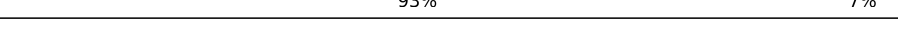
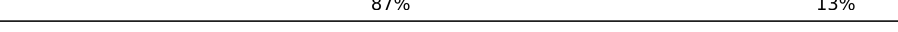
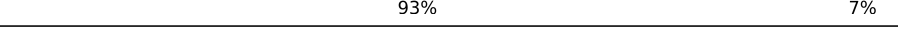
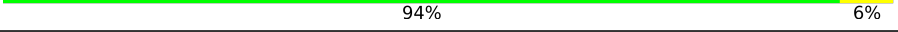
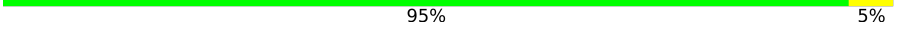
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	1-A	151	35% 91% 9%
1	1-B	151	27% 91% 9%
1	10-A	151	93% 7%
1	10-B	151	88% 12%
1	11-A	151	93% 7%
1	11-B	151	93% 7%
1	12-A	151	91% 9%

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Mol	Chain	Length	Quality of chain
1	12-B	151	 87% 12%
1	13-A	151	 91% 9%
1	13-B	151	 85% 15%
1	14-A	151	 89% 11%
1	14-B	151	 87% 13%
1	15-A	151	 86% 14%
1	15-B	151	 90% 10%
1	16-A	151	 85% 15%
1	16-B	151	 90% 10%
1	2-A	151	 95% 5%
1	2-B	151	 92% 8%
1	3-A	151	 93% 7%
1	3-B	151	 91% 9%
1	4-A	151	 93% 6%
1	4-B	151	 92% 8%
1	5-A	151	 93% 7%
1	5-B	151	 87% 13%
1	6-A	151	 90% 10%
1	6-B	151	 93% 7%
1	7-A	151	 92% 8%
1	7-B	151	 94% 6%
1	8-A	151	 95% 5%
1	8-B	151	 93% 7%
1	9-A	151	 93% 6%
1	9-B	151	 93% 7%

2 Entry composition

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 (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
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	9-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		

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

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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		
2	9-B	1	Total	O	S	0	0
			5	4	1		
2	10-B	1	Total	O	S	0	0
			5	4	1		
2	11-B	1	Total	O	S	0	0
			5	4	1		
2	12-B	1	Total	O	S	0	0
			5	4	1		
2	13-B	1	Total	O	S	0	0
			5	4	1		
2	14-B	1	Total	O	S	0	0
			5	4	1		
2	15-B	1	Total	O	S	0	0
			5	4	1		
2	16-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		

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

- Molecule 3 is water.

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

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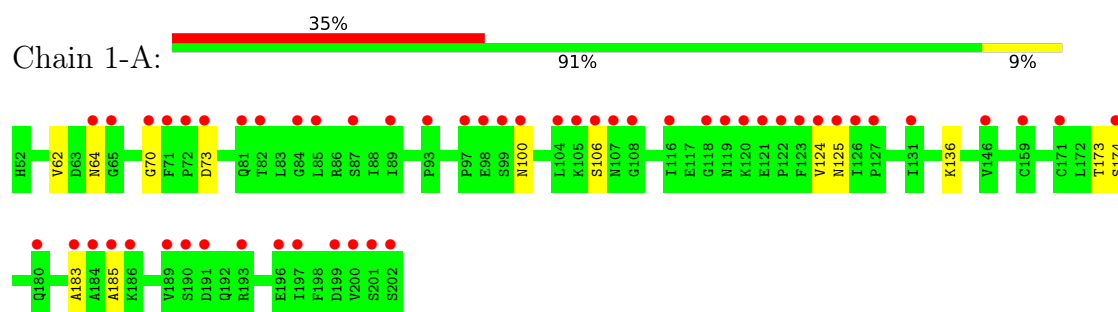
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	16-B	29	Total	O	0	0
			29	29		

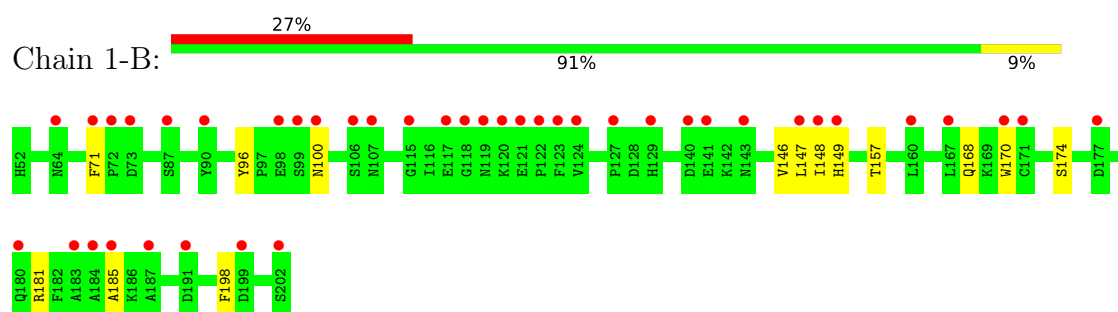
3 Residue-property plots

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 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.

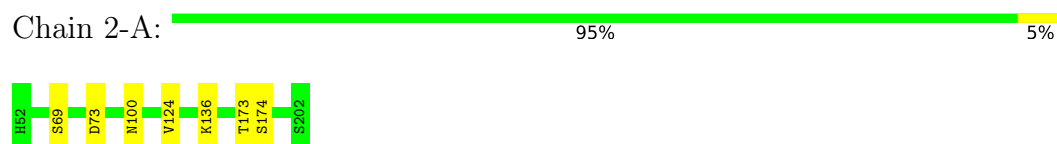
- Molecule 1: Probable tyrosine-protein phosphatase At1g05000



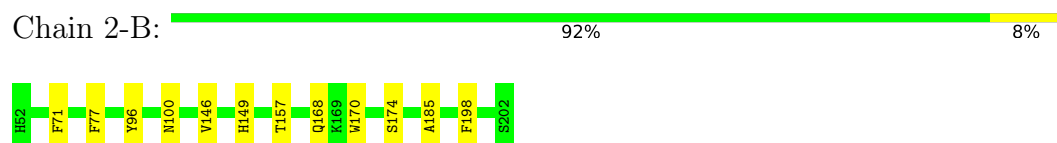
- Molecule 1: Probable tyrosine-protein phosphatase At1g05000



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 3-A:  93% 7%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 3-B:  91% 9%



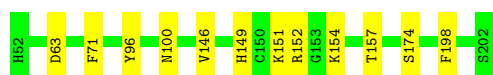
- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 4-A:  93% 6%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 4-B:  92% 8%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 5-A:  93% 7%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 5-B:  87% 13%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 6-A:  90% 10%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 6-B:  93% 7%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 7-A:  92% 8%

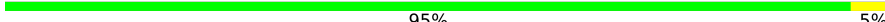


- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 7-B:  94% 6%

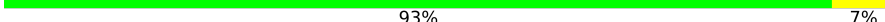


- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 8-A:  95% 5%

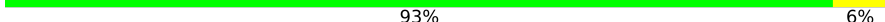


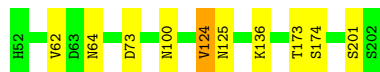
- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 8-B:  93% 7%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 9-A:  93% 6%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 9-B:  93% 7%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 10-A:  93% 7%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 10-B:  88% 12%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 11-A:  93% 7%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 11-B:  93% 7%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 12-A:  91% 9%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 12-B:  87% 12%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 13-A:  91% 9%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 13-B:  85% 15%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 14-A:  89% 11%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 14-B:  87% 13%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 15-A:  86% 14%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 15-B:  90% 10%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 16-A:  85% 15%



- Molecule 1: Probable tyrosine-protein phosphatase At1g05000

Chain 16-B:  90% 10%



4 Data and refinement statistics

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 41.50 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.50-3.30) 98.3 (41.50-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.21 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.160 , 0.234 0.192 , 0.240	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)	0.02 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.81	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.20	0/1252	0.36	0/1680
1	1-B	0.17	0/1252	0.35	0/1680
1	2-A	0.20	0/1252	0.36	0/1680
1	2-B	0.17	0/1252	0.35	0/1680
1	3-A	0.20	0/1252	0.36	0/1680
1	3-B	0.17	0/1252	0.35	0/1680
1	4-A	0.20	0/1252	0.36	0/1680
1	4-B	0.17	0/1252	0.35	0/1680
1	5-A	0.20	0/1252	0.36	0/1680
1	5-B	0.17	0/1252	0.35	0/1680
1	6-A	0.20	0/1252	0.36	0/1680
1	6-B	0.17	0/1252	0.35	0/1680
1	7-A	0.20	0/1252	0.36	0/1680
1	7-B	0.17	0/1252	0.35	0/1680
1	8-A	0.20	0/1252	0.36	0/1680
1	8-B	0.17	0/1252	0.35	0/1680
1	9-A	0.20	0/1252	0.36	0/1680
1	9-B	0.17	0/1252	0.35	0/1680
1	10-A	0.20	0/1252	0.36	0/1680
1	10-B	0.17	0/1252	0.35	0/1680
1	11-A	0.20	0/1252	0.36	0/1680
1	11-B	0.17	0/1252	0.35	0/1680
1	12-A	0.20	0/1252	0.36	0/1680
1	12-B	0.17	0/1252	0.35	0/1680
1	13-A	0.20	0/1252	0.36	0/1680
1	13-B	0.17	0/1252	0.35	0/1680
1	14-A	0.20	0/1252	0.36	0/1680
1	14-B	0.17	0/1252	0.35	0/1680
1	15-A	0.20	0/1252	0.36	0/1680
1	15-B	0.17	0/1252	0.35	0/1680
1	16-A	0.20	0/1252	0.36	0/1680
1	16-B	0.17	0/1252	0.35	0/1680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.19	0/40064	0.36	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

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 ⓘ

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	149/151 (99%)	116 (78%)	26 (17%)	7 (5%)	2	12
1	1-B	149/151 (99%)	118 (79%)	24 (16%)	7 (5%)	2	12
1	2-A	149/151 (99%)	127 (85%)	21 (14%)	1 (1%)	18	49
1	2-B	149/151 (99%)	122 (82%)	22 (15%)	5 (3%)	3	18
1	3-A	149/151 (99%)	127 (85%)	17 (11%)	5 (3%)	3	18
1	3-B	149/151 (99%)	112 (75%)	29 (20%)	8 (5%)	1	10
1	4-A	149/151 (99%)	114 (76%)	30 (20%)	5 (3%)	3	18
1	4-B	149/151 (99%)	122 (82%)	22 (15%)	5 (3%)	3	18
1	5-A	149/151 (99%)	116 (78%)	28 (19%)	5 (3%)	3	18
1	5-B	149/151 (99%)	116 (78%)	20 (13%)	13 (9%)	0	4
1	6-A	149/151 (99%)	120 (80%)	20 (13%)	9 (6%)	1	9
1	6-B	149/151 (99%)	122 (82%)	23 (15%)	4 (3%)	4	22
1	7-A	149/151 (99%)	130 (87%)	13 (9%)	6 (4%)	2	15
1	7-B	149/151 (99%)	119 (80%)	28 (19%)	2 (1%)	9	35
1	8-A	149/151 (99%)	126 (85%)	21 (14%)	2 (1%)	9	35
1	8-B	149/151 (99%)	119 (80%)	27 (18%)	3 (2%)	6	27
1	9-A	149/151 (99%)	122 (82%)	22 (15%)	5 (3%)	3	18
1	9-B	149/151 (99%)	121 (81%)	24 (16%)	4 (3%)	4	22
1	10-A	149/151 (99%)	118 (79%)	27 (18%)	4 (3%)	4	22
1	10-B	149/151 (99%)	109 (73%)	29 (20%)	11 (7%)	1	6
1	11-A	149/151 (99%)	119 (80%)	26 (17%)	4 (3%)	4	22
1	11-B	149/151 (99%)	113 (76%)	32 (22%)	4 (3%)	4	22
1	12-A	149/151 (99%)	111 (74%)	31 (21%)	7 (5%)	2	12
1	12-B	149/151 (99%)	104 (70%)	32 (22%)	13 (9%)	0	4
1	13-A	149/151 (99%)	115 (77%)	26 (17%)	8 (5%)	1	10

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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	7
1	14-B	149/151 (99%)	103 (69%)	34 (23%)	12 (8%)	1	5
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%)	1	10
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%)	1	10
All	All	4768/4832 (99%)	3704 (78%)	830 (17%)	234 (5%)	1	12

All (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
1	5-B	74	SER
1	5-B	151	LYS
1	5-B	183	ALA
1	6-A	123	PHE
1	6-A	140	ASP
1	7-A	74	SER
1	8-A	201	SER
1	10-B	87	SER
1	10-B	95	PRO
1	10-B	183	ALA
1	10-B	198	PHE
1	12-A	64	ASN
1	12-A	170	TRP
1	13-A	142	LYS
1	13-A	143	ASN
1	13-B	68	ARG
1	13-B	71	PHE
1	13-B	78	SER
1	13-B	83	LEU
1	13-B	85	LEU
1	13-B	111	LEU
1	14-B	197	ILE
1	15-A	57	LEU

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Mol	Chain	Res	Type
1	15-A	64	ASN
1	15-A	98	GLU
1	15-A	106	SER
1	15-A	151	LYS
1	15-A	185	ALA
1	15-A	197	ILE
1	15-B	62	VAL
1	16-A	98	GLU
1	16-A	106	SER
1	16-A	151	LYS
1	16-A	170	TRP
1	16-A	185	ALA
1	16-A	188	ARG
1	16-A	197	ILE
1	16-A	201	SER
1	16-B	186	LYS
1	1-A	70	GLY
1	1-A	106	SER
1	1-A	125	ASN
1	1-A	185	ALA
1	1-B	147	LEU
1	1-B	181	ARG
1	1-B	185	ALA
1	2-B	185	ALA
1	2-B	198	PHE
1	3-A	69	SER
1	3-B	198	PHE
1	4-A	186	LYS
1	4-B	63	ASP
1	4-B	151	LYS
1	4-B	152	ARG
1	5-A	70	GLY
1	5-A	119	ASN
1	5-A	201	SER
1	5-B	120	LYS
1	5-B	185	ALA
1	5-B	198	PHE
1	6-A	64	ASN
1	6-A	120	LYS
1	6-A	201	SER
1	6-B	185	ALA
1	6-B	201	SER

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Mol	Chain	Res	Type
1	8-B	198	PHE
1	9-A	64	ASN
1	9-A	201	SER
1	9-B	85	LEU
1	10-A	201	SER
1	10-B	62	VAL
1	10-B	168	GLN
1	10-B	185	ALA
1	11-A	70	GLY
1	11-A	125	ASN
1	11-B	198	PHE
1	12-A	57	LEU
1	12-A	58	ASN
1	12-A	125	ASN
1	12-A	201	SER
1	12-B	87	SER
1	12-B	103	PHE
1	12-B	198	PHE
1	13-A	63	ASP
1	13-A	74	SER
1	13-A	125	ASN
1	13-A	170	TRP
1	13-B	73	ASP
1	13-B	74	SER
1	13-B	86	ARG
1	13-B	108	GLY
1	13-B	150	CYS
1	13-B	154	LYS
1	13-B	185	ALA
1	14-A	62	VAL
1	14-A	80	LEU
1	14-A	168	GLN
1	14-B	74	SER
1	14-B	77	PHE
1	14-B	172	LEU
1	14-B	185	ALA
1	14-B	188	ARG
1	14-B	198	PHE
1	14-B	199	ASP
1	15-A	58	ASN
1	15-A	103	PHE
1	15-A	125	ASN

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Mol	Chain	Res	Type
1	15-A	186	LYS
1	15-B	77	PHE
1	15-B	168	GLN
1	15-B	197	ILE
1	15-B	198	PHE
1	16-A	74	SER
1	16-B	63	ASP
1	16-B	185	ALA
1	1-A	183	ALA
1	1-B	168	GLN
1	2-A	69	SER
1	2-B	77	PHE
1	2-B	168	GLN
1	3-A	106	SER
1	3-A	141	GLU
1	3-B	185	ALA
1	4-A	64	ASN
1	4-B	154	LYS
1	4-B	198	PHE
1	5-A	97	PRO
1	5-B	115	GLY
1	5-B	117	GLU
1	5-B	125	ASN
1	5-B	168	GLN
1	5-B	188	ARG
1	6-B	188	ARG
1	7-A	69	SER
1	7-A	97	PRO
1	7-A	186	LYS
1	8-A	69	SER
1	9-B	117	GLU
1	10-A	64	ASN
1	10-A	125	ASN
1	10-A	150	CYS
1	10-B	106	SER
1	10-B	140	ASP
1	11-A	64	ASN
1	11-A	186	LYS
1	11-B	130	LYS
1	11-B	186	LYS
1	12-B	117	GLU
1	12-B	146	VAL

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Mol	Chain	Res	Type
1	12-B	147	LEU
1	12-B	185	ALA
1	13-B	57	LEU
1	13-B	130	LYS
1	14-A	74	SER
1	14-A	185	ALA
1	14-B	125	ASN
1	15-B	65	GLY
1	15-B	172	LEU
1	15-B	183	ALA
1	16-A	80	LEU
1	16-A	97	PRO
1	16-A	107	ASN
1	16-B	74	SER
1	1-A	64	ASN
1	1-B	170	TRP
1	1-B	198	PHE
1	3-B	82	THR
1	3-B	130	LYS
1	4-A	97	PRO
1	5-A	186	LYS
1	6-A	122	PRO
1	6-A	141	GLU
1	7-A	63	ASP
1	7-A	200	VAL
1	9-A	62	VAL
1	10-B	143	ASN
1	10-B	154	LYS
1	11-B	125	ASN
1	12-B	90	TYR
1	12-B	125	ASN
1	12-B	197	ILE
1	13-A	117	GLU
1	13-A	186	LYS
1	13-B	93	PRO
1	14-A	70	GLY
1	14-A	98	GLU
1	14-A	198	PHE
1	14-B	82	THR
1	14-B	168	GLN
1	15-A	156	ARG
1	15-A	198	PHE

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Mol	Chain	Res	Type
1	16-A	108	GLY
1	16-A	133	MSE
1	16-A	134	ALA
1	16-B	56	PRO
1	16-B	111	LEU
1	3-B	63	ASP
1	3-B	187	ALA
1	4-A	173	THR
1	5-B	150	CYS
1	7-B	168	GLN
1	8-B	87	SER
1	9-A	125	ASN
1	9-B	86	ARG
1	9-B	191	ASP
1	12-A	169	LYS
1	12-B	106	SER
1	13-B	201	SER
1	14-B	131	ILE
1	15-A	97	PRO
1	15-A	158	GLY
1	4-A	65	GLY
1	6-B	173	THR
1	7-B	143	ASN
1	12-B	148	ILE
1	1-B	148	ILE
1	5-B	122	PRO
1	14-A	158	GLY
1	16-B	93	PRO
1	6-A	62	VAL
1	12-B	56	PRO
1	14-A	108	GLY
1	16-B	145	PRO
1	6-A	108	GLY
1	3-B	197	ILE
1	9-A	124	VAL
1	16-A	200	VAL
1	8-B	62	VAL
1	16-A	93	PRO

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	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	1-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	2-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	2-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	3-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	3-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	4-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	4-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	5-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	5-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	6-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	6-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	7-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	7-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	8-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	8-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	9-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	9-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	10-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	10-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	11-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	11-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	12-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	12-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	13-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	13-B	136/133 (102%)	129 (95%)	7 (5%)	21	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	14-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	14-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	15-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	15-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
1	16-A	136/133 (102%)	130 (96%)	6 (4%)	25	54
1	16-B	136/133 (102%)	129 (95%)	7 (5%)	21	50
All	All	4352/4256 (102%)	4144 (95%)	208 (5%)	23	52

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	73	ASP
1	1-A	100	ASN
1	1-A	124	VAL
1	1-A	136	LYS
1	1-A	173	THR
1	1-A	174	SER
1	1-B	71	PHE
1	1-B	96	TYR
1	1-B	100	ASN
1	1-B	146	VAL
1	1-B	149	HIS
1	1-B	157	THR
1	1-B	174	SER
1	2-A	73	ASP
1	2-A	100	ASN
1	2-A	124	VAL
1	2-A	136	LYS
1	2-A	173	THR
1	2-A	174	SER
1	2-B	71	PHE
1	2-B	96	TYR
1	2-B	100	ASN
1	2-B	146	VAL
1	2-B	149	HIS
1	2-B	157	THR
1	2-B	174	SER
1	3-A	73	ASP
1	3-A	100	ASN
1	3-A	124	VAL

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Mol	Chain	Res	Type
1	3-A	136	LYS
1	3-A	173	THR
1	3-A	174	SER
1	3-B	71	PHE
1	3-B	96	TYR
1	3-B	100	ASN
1	3-B	146	VAL
1	3-B	149	HIS
1	3-B	157	THR
1	3-B	174	SER
1	4-A	73	ASP
1	4-A	100	ASN
1	4-A	124	VAL
1	4-A	136	LYS
1	4-A	173	THR
1	4-A	174	SER
1	4-B	71	PHE
1	4-B	96	TYR
1	4-B	100	ASN
1	4-B	146	VAL
1	4-B	149	HIS
1	4-B	157	THR
1	4-B	174	SER
1	5-A	73	ASP
1	5-A	100	ASN
1	5-A	124	VAL
1	5-A	136	LYS
1	5-A	173	THR
1	5-A	174	SER
1	5-B	71	PHE
1	5-B	96	TYR
1	5-B	100	ASN
1	5-B	146	VAL
1	5-B	149	HIS
1	5-B	157	THR
1	5-B	174	SER
1	6-A	73	ASP
1	6-A	100	ASN
1	6-A	124	VAL
1	6-A	136	LYS
1	6-A	173	THR
1	6-A	174	SER

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Mol	Chain	Res	Type
1	6-B	71	PHE
1	6-B	96	TYR
1	6-B	100	ASN
1	6-B	146	VAL
1	6-B	149	HIS
1	6-B	157	THR
1	6-B	174	SER
1	7-A	73	ASP
1	7-A	100	ASN
1	7-A	124	VAL
1	7-A	136	LYS
1	7-A	173	THR
1	7-A	174	SER
1	7-B	71	PHE
1	7-B	96	TYR
1	7-B	100	ASN
1	7-B	146	VAL
1	7-B	149	HIS
1	7-B	157	THR
1	7-B	174	SER
1	8-A	73	ASP
1	8-A	100	ASN
1	8-A	124	VAL
1	8-A	136	LYS
1	8-A	173	THR
1	8-A	174	SER
1	8-B	71	PHE
1	8-B	96	TYR
1	8-B	100	ASN
1	8-B	146	VAL
1	8-B	149	HIS
1	8-B	157	THR
1	8-B	174	SER
1	9-A	73	ASP
1	9-A	100	ASN
1	9-A	124	VAL
1	9-A	136	LYS
1	9-A	173	THR
1	9-A	174	SER
1	9-B	71	PHE
1	9-B	96	TYR
1	9-B	100	ASN

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Mol	Chain	Res	Type
1	9-B	146	VAL
1	9-B	149	HIS
1	9-B	157	THR
1	9-B	174	SER
1	10-A	73	ASP
1	10-A	100	ASN
1	10-A	124	VAL
1	10-A	136	LYS
1	10-A	173	THR
1	10-A	174	SER
1	10-B	71	PHE
1	10-B	96	TYR
1	10-B	100	ASN
1	10-B	146	VAL
1	10-B	149	HIS
1	10-B	157	THR
1	10-B	174	SER
1	11-A	73	ASP
1	11-A	100	ASN
1	11-A	124	VAL
1	11-A	136	LYS
1	11-A	173	THR
1	11-A	174	SER
1	11-B	71	PHE
1	11-B	96	TYR
1	11-B	100	ASN
1	11-B	146	VAL
1	11-B	149	HIS
1	11-B	157	THR
1	11-B	174	SER
1	12-A	73	ASP
1	12-A	100	ASN
1	12-A	124	VAL
1	12-A	136	LYS
1	12-A	173	THR
1	12-A	174	SER
1	12-B	71	PHE
1	12-B	96	TYR
1	12-B	100	ASN
1	12-B	146	VAL
1	12-B	149	HIS
1	12-B	157	THR

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Mol	Chain	Res	Type
1	12-B	174	SER
1	13-A	73	ASP
1	13-A	100	ASN
1	13-A	124	VAL
1	13-A	136	LYS
1	13-A	173	THR
1	13-A	174	SER
1	13-B	71	PHE
1	13-B	96	TYR
1	13-B	100	ASN
1	13-B	146	VAL
1	13-B	149	HIS
1	13-B	157	THR
1	13-B	174	SER
1	14-A	73	ASP
1	14-A	100	ASN
1	14-A	124	VAL
1	14-A	136	LYS
1	14-A	173	THR
1	14-A	174	SER
1	14-B	71	PHE
1	14-B	96	TYR
1	14-B	100	ASN
1	14-B	146	VAL
1	14-B	149	HIS
1	14-B	157	THR
1	14-B	174	SER
1	15-A	73	ASP
1	15-A	100	ASN
1	15-A	124	VAL
1	15-A	136	LYS
1	15-A	173	THR
1	15-A	174	SER
1	15-B	71	PHE
1	15-B	96	TYR
1	15-B	100	ASN
1	15-B	146	VAL
1	15-B	149	HIS
1	15-B	157	THR
1	15-B	174	SER
1	16-A	73	ASP
1	16-A	100	ASN

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Mol	Chain	Res	Type
1	16-A	124	VAL
1	16-A	136	LYS
1	16-A	173	THR
1	16-A	174	SER
1	16-B	71	PHE
1	16-B	96	TYR
1	16-B	100	ASN
1	16-B	146	VAL
1	16-B	149	HIS
1	16-B	157	THR
1	16-B	174	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	64	ASN
1	1-A	81	GLN
1	1-A	143	ASN
1	1-A	180	GLN
1	1-B	81	GLN
1	1-B	100	ASN
1	1-B	107	ASN
1	1-B	113	GLN
1	1-B	129	HIS
1	2-A	102	GLN
1	2-A	192	GLN
1	2-B	76	ASN
1	2-B	113	GLN
1	2-B	168	GLN
1	2-B	192	GLN
1	3-A	119	ASN
1	3-A	129	HIS
1	3-A	168	GLN
1	3-B	52	HIS
1	3-B	64	ASN
1	3-B	107	ASN
1	3-B	119	ASN
1	3-B	180	GLN
1	3-B	192	GLN
1	4-A	76	ASN
1	4-A	102	GLN
1	4-A	119	ASN

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Mol	Chain	Res	Type
1	4-A	129	HIS
1	4-A	143	ASN
1	4-A	144	HIS
1	4-A	192	GLN
1	4-B	100	ASN
1	4-B	107	ASN
1	4-B	143	ASN
1	4-B	168	GLN
1	4-B	180	GLN
1	5-A	119	ASN
1	5-A	143	ASN
1	5-A	180	GLN
1	5-B	113	GLN
1	5-B	168	GLN
1	5-B	180	GLN
1	5-B	192	GLN
1	6-A	64	ASN
1	6-A	102	GLN
1	6-A	144	HIS
1	6-A	149	HIS
1	6-B	52	HIS
1	6-B	113	GLN
1	6-B	149	HIS
1	6-B	180	GLN
1	6-B	192	GLN
1	7-A	76	ASN
1	7-A	102	GLN
1	7-A	107	ASN
1	7-A	113	GLN
1	7-A	129	HIS
1	7-A	143	ASN
1	7-A	180	GLN
1	7-B	81	GLN
1	7-B	107	ASN
1	7-B	113	GLN
1	7-B	180	GLN
1	8-A	102	GLN
1	8-B	64	ASN
1	8-B	81	GLN
1	8-B	143	ASN
1	8-B	168	GLN
1	8-B	180	GLN

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Mol	Chain	Res	Type
1	8-B	192	GLN
1	9-A	64	ASN
1	9-A	76	ASN
1	9-A	81	GLN
1	9-A	102	GLN
1	9-A	107	ASN
1	9-A	119	ASN
1	9-A	129	HIS
1	9-B	113	GLN
1	9-B	192	GLN
1	10-A	102	GLN
1	10-A	113	GLN
1	10-A	144	HIS
1	10-A	155	HIS
1	10-B	100	ASN
1	10-B	107	ASN
1	10-B	113	GLN
1	11-A	64	ASN
1	11-A	119	ASN
1	11-A	129	HIS
1	11-A	144	HIS
1	11-A	168	GLN
1	11-A	180	GLN
1	11-B	81	GLN
1	11-B	107	ASN
1	11-B	129	HIS
1	11-B	143	ASN
1	11-B	192	GLN
1	12-A	58	ASN
1	12-A	64	ASN
1	12-A	143	ASN
1	12-A	180	GLN
1	12-B	52	HIS
1	12-B	107	ASN
1	12-B	113	GLN
1	12-B	192	GLN
1	13-A	76	ASN
1	13-A	81	GLN
1	13-A	102	GLN
1	13-A	129	HIS
1	13-A	168	GLN
1	13-A	192	GLN

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Mol	Chain	Res	Type
1	13-B	58	ASN
1	13-B	64	ASN
1	13-B	102	GLN
1	13-B	113	GLN
1	13-B	192	GLN
1	14-A	102	GLN
1	14-A	129	HIS
1	14-A	168	GLN
1	14-B	64	ASN
1	14-B	81	GLN
1	14-B	107	ASN
1	14-B	143	ASN
1	14-B	168	GLN
1	15-A	76	ASN
1	15-A	100	ASN
1	15-A	107	ASN
1	15-A	129	HIS
1	15-A	155	HIS
1	15-A	180	GLN
1	15-A	192	GLN
1	15-B	64	ASN
1	15-B	113	GLN
1	15-B	143	ASN
1	15-B	168	GLN
1	15-B	180	GLN
1	16-A	64	ASN
1	16-A	81	GLN
1	16-A	107	ASN
1	16-A	155	HIS
1	16-A	192	GLN
1	16-B	76	ASN
1	16-B	107	ASN
1	16-B	113	GLN
1	16-B	144	HIS
1	16-B	155	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	7-B	204	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	5-B	204	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	10-B	203	-	4,4,4	0.37	0	6,6,6	0.05	0
2	SO4	11-B	204	-	4,4,4	0.35	0	6,6,6	0.11	0
2	SO4	12-B	204	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	12-A	203	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	16-B	203	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	5-A	203	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	3-A	203	-	4,4,4	0.34	0	6,6,6	0.09	0
2	SO4	6-A	204	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	12-B	203	-	4,4,4	0.35	0	6,6,6	0.07	0
2	SO4	5-B	203	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	9-A	203	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	7-A	204	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	11-A	203	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	1-B	204	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	13-A	203	-	4,4,4	0.35	0	6,6,6	0.09	0
2	SO4	16-A	204	-	4,4,4	0.36	0	6,6,6	0.16	0
2	SO4	4-A	203	-	4,4,4	0.35	0	6,6,6	0.10	0
2	SO4	4-B	204	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	14-B	203	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	6-B	204	-	4,4,4	0.38	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	7-A	203	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	1-A	203	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	1-B	203	-	4,4,4	0.35	0	6,6,6	0.07	0
2	SO4	3-A	204	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	5-A	204	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	10-A	203	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	8-B	203	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	14-A	204	-	4,4,4	0.38	0	6,6,6	0.16	0
2	SO4	8-A	203	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	2-B	204	-	4,4,4	0.37	0	6,6,6	0.11	0
2	SO4	4-A	204	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	15-A	203	-	4,4,4	0.38	0	6,6,6	0.13	0
2	SO4	2-A	204	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	11-B	203	-	4,4,4	0.35	0	6,6,6	0.09	0
2	SO4	13-B	203	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	15-B	204	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	4-B	203	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	9-A	204	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	10-B	204	-	4,4,4	0.38	0	6,6,6	0.10	0
2	SO4	13-A	204	-	4,4,4	0.38	0	6,6,6	0.16	0
2	SO4	16-A	203	-	4,4,4	0.35	0	6,6,6	0.09	0
2	SO4	6-B	203	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	11-A	204	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	7-B	203	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	3-B	203	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	10-A	204	-	4,4,4	0.37	0	6,6,6	0.05	0
2	SO4	14-B	204	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	2-A	203	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	1-A	204	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	14-A	203	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	15-A	204	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	13-B	204	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	2-B	203	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	15-B	203	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	8-B	204	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	9-B	204	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	6-A	203	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	8-A	204	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	12-A	204	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	16-B	204	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	9-B	203	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	3-B	204	-	4,4,4	0.39	0	6,6,6	0.09	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

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, 95th 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 ²)	Q<0.9
1	1-A	148/151 (98%)	1.83	53 (35%)  	1, 2, 4, 7	148 (100%)
1	1-B	148/151 (98%)	1.53	41 (27%)  	1, 2, 5, 6	148 (100%)
1	2-A	0/151	-	-	-	-
1	2-B	0/151	-	-	-	-
1	3-A	0/151	-	-	-	-
1	3-B	0/151	-	-	-	-
1	4-A	0/151	-	-	-	-
1	4-B	0/151	-	-	-	-
1	5-A	0/151	-	-	-	-
1	5-B	0/151	-	-	-	-
1	6-A	0/151	-	-	-	-
1	6-B	0/151	-	-	-	-
1	7-A	0/151	-	-	-	-
1	7-B	0/151	-	-	-	-
1	8-A	0/151	-	-	-	-
1	8-B	0/151	-	-	-	-
1	9-A	0/151	-	-	-	-
1	9-B	0/151	-	-	-	-
1	10-A	0/151	-	-	-	-
1	10-B	0/151	-	-	-	-
1	11-A	0/151	-	-	-	-
1	11-B	0/151	-	-	-	-
1	12-A	0/151	-	-	-	-
1	12-B	0/151	-	-	-	-
1	13-A	0/151	-	-	-	-
1	13-B	0/151	-	-	-	-
1	14-A	0/151	-	-	-	-
1	14-B	0/151	-	-	-	-
1	15-A	0/151	-	-	-	-
1	15-B	0/151	-	-	-	-
1	16-A	0/151	-	-	-	-
1	16-B	0/151	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	296/4832 (6%)	1.68	94 (31%) 1 1	1, 2, 5, 7	296 (100%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	185	ALA	11.5
1	1-A	184	ALA	9.9
1	1-B	148	ILE	7.2
1	1-A	123	PHE	7.0
1	1-A	100	ASN	5.5
1	1-A	202	SER	5.3
1	1-B	123	PHE	5.3
1	1-B	120	LYS	5.2
1	1-B	171	CYS	4.9
1	1-B	124	VAL	4.7
1	1-A	190	SER	4.5
1	1-A	200	VAL	4.4
1	1-A	104	LEU	4.3
1	1-A	122	PRO	4.2
1	1-B	121	GLU	4.2
1	1-B	199	ASP	4.2
1	1-A	186	LYS	4.1
1	1-A	119	ASN	4.0
1	1-A	99	SER	4.0
1	1-A	201	SER	4.0
1	1-A	105	LYS	4.0
1	1-A	108	GLY	3.9
1	1-B	180	GLN	3.9
1	1-A	70	GLY	3.9
1	1-B	100	ASN	3.7
1	1-B	202	SER	3.6
1	1-B	147	LEU	3.6
1	1-A	81	GLN	3.6
1	1-A	82	THR	3.6
1	1-A	97	PRO	3.5
1	1-B	183	ALA	3.5
1	1-A	107	ASN	3.4
1	1-B	73	ASP	3.4
1	1-B	119	ASN	3.3
1	1-A	116	ILE	3.2
1	1-A	193	ARG	3.2
1	1-B	177	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-B	117	GLU	3.1
1	1-A	65	GLY	3.1
1	1-A	120	LYS	3.1
1	1-A	98	GLU	3.1
1	1-B	122	PRO	3.0
1	1-A	183	ALA	3.0
1	1-B	98	GLU	3.0
1	1-A	72	PRO	3.0
1	1-A	189	VAL	3.0
1	1-A	127	PRO	2.9
1	1-A	73	ASP	2.9
1	1-A	64	ASN	2.9
1	1-B	71	PHE	2.8
1	1-B	115	GLY	2.8
1	1-A	197	ILE	2.7
1	1-B	87	SER	2.7
1	1-B	149	HIS	2.7
1	1-A	196	GLU	2.6
1	1-B	160	LEU	2.6
1	1-A	125	ASN	2.6
1	1-B	64	ASN	2.6
1	1-A	171	CYS	2.6
1	1-B	129	HIS	2.6
1	1-B	127	PRO	2.6
1	1-B	106	SER	2.6
1	1-A	118	GLY	2.6
1	1-B	184	ALA	2.6
1	1-B	90	TYR	2.5
1	1-B	72	PRO	2.5
1	1-A	174	SER	2.5
1	1-B	141	GLU	2.4
1	1-A	93	PRO	2.4
1	1-A	71	PHE	2.4
1	1-A	159	CYS	2.4
1	1-B	143	ASN	2.3
1	1-B	191	ASP	2.3
1	1-B	107	ASN	2.3
1	1-A	191	ASP	2.3
1	1-A	84	GLY	2.3
1	1-B	185	ALA	2.3
1	1-A	124	VAL	2.3
1	1-A	106	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	89	ILE	2.2
1	1-B	118	GLY	2.2
1	1-B	170	TRP	2.2
1	1-B	99	SER	2.2
1	1-B	187	ALA	2.1
1	1-B	140	ASP	2.1
1	1-A	180	GLN	2.1
1	1-A	121	GLU	2.1
1	1-A	85	LEU	2.1
1	1-A	131	ILE	2.1
1	1-A	146	VAL	2.1
1	1-A	199	ASP	2.1
1	1-A	126	ILE	2.1
1	1-B	167	LEU	2.0
1	1-A	87	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	SO4	1-A	204	5/5	0.49	0.32	54,54,54,55	5
2	SO4	2-A	203	5/5	-	-	36,37,37,38	5
2	SO4	3-A	203	5/5	-	-	28,30,30,30	5
2	SO4	4-A	203	5/5	-	-	36,37,38,38	5
2	SO4	5-A	203	5/5	-	-	36,37,38,38	5
2	SO4	6-A	203	5/5	-	-	36,36,37,37	5
2	SO4	7-A	203	5/5	-	-	37,37,38,38	5
2	SO4	8-A	203	5/5	-	-	37,37,38,38	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	9-A	203	5/5	-	-	33,34,35,35	5
2	SO4	10-A	203	5/5	-	-	37,38,38,38	5
2	SO4	11-A	203	5/5	-	-	37,37,38,38	5
2	SO4	12-A	203	5/5	-	-	36,36,38,38	5
2	SO4	13-A	203	5/5	-	-	36,37,38,39	5
2	SO4	14-A	203	5/5	-	-	26,29,29,29	5
2	SO4	15-A	203	5/5	-	-	38,38,38,39	5
2	SO4	16-A	203	5/5	-	-	38,38,38,39	5
2	SO4	1-B	204	5/5	0.83	0.21	54,54,55,56	5
2	SO4	2-A	204	5/5	-	-	55,55,56,57	5
2	SO4	3-A	204	5/5	-	-	49,50,50,51	5
2	SO4	4-A	204	5/5	-	-	54,54,54,55	5
2	SO4	5-A	204	5/5	-	-	55,55,56,56	5
2	SO4	6-A	204	5/5	-	-	53,54,54,55	5
2	SO4	7-A	204	5/5	-	-	53,53,54,55	5
2	SO4	8-A	204	5/5	-	-	53,53,54,54	5
2	SO4	9-A	204	5/5	-	-	49,50,50,51	5
2	SO4	10-A	204	5/5	-	-	36,38,39,39	5
2	SO4	11-A	204	5/5	-	-	51,51,51,52	5
2	SO4	12-A	204	5/5	-	-	53,53,54,54	5
2	SO4	13-A	204	5/5	-	-	52,52,53,53	5
2	SO4	14-A	204	5/5	-	-	48,49,50,50	5
2	SO4	15-A	204	5/5	-	-	34,36,37,38	5
2	SO4	16-A	204	5/5	-	-	46,46,47,47	5
2	SO4	1-B	203	5/5	0.89	0.16	36,36,36,37	5
2	SO4	2-B	203	5/5	-	-	37,37,37,38	5
2	SO4	3-B	203	5/5	-	-	40,40,41,42	5
2	SO4	4-B	203	5/5	-	-	35,35,36,36	5
2	SO4	5-B	203	5/5	-	-	38,38,38,39	5
2	SO4	6-B	203	5/5	-	-	37,37,38,38	5
2	SO4	7-B	203	5/5	-	-	35,36,36,36	5
2	SO4	8-B	203	5/5	-	-	35,36,36,37	5
2	SO4	9-B	203	5/5	-	-	36,36,36,37	5
2	SO4	10-B	203	5/5	-	-	36,37,38,38	5
2	SO4	11-B	203	5/5	-	-	39,39,40,40	5
2	SO4	12-B	203	5/5	-	-	36,36,37,37	5
2	SO4	13-B	203	5/5	-	-	38,38,39,40	5
2	SO4	14-B	203	5/5	-	-	41,41,42,43	5
2	SO4	15-B	203	5/5	-	-	41,41,41,42	5
2	SO4	16-B	203	5/5	-	-	40,40,41,42	5
2	SO4	1-A	203	5/5	0.92	0.17	37,37,38,39	5
2	SO4	2-B	204	5/5	-	-	54,55,56,57	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	3-B	204	5/5	-	-	52,52,54,54	5
2	SO4	4-B	204	5/5	-	-	53,53,54,54	5
2	SO4	5-B	204	5/5	-	-	37,39,39,39	5
2	SO4	6-B	204	5/5	-	-	55,56,56,57	5
2	SO4	7-B	204	5/5	-	-	55,55,56,56	5
2	SO4	8-B	204	5/5	-	-	54,54,55,56	5
2	SO4	9-B	204	5/5	-	-	51,51,52,52	5
2	SO4	10-B	204	5/5	-	-	56,56,57,57	5
2	SO4	11-B	204	5/5	-	-	37,38,39,40	5
2	SO4	12-B	204	5/5	-	-	55,55,56,57	5
2	SO4	13-B	204	5/5	-	-	49,50,52,52	5
2	SO4	14-B	204	5/5	-	-	54,54,55,56	5
2	SO4	15-B	204	5/5	-	-	54,55,56,56	5
2	SO4	16-B	204	5/5	-	-	1,6,7,7	5

6.5 Other polymers [i](#)

There are no such residues in this entry.