



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2025 – 04:15 PM JST

PDB ID : 8YRE  
Title : Crystal structure of Arabidopsis VTC1-KJC2  
Authors : Zhang, C.; Liu, L.  
Deposited on : 2024-03-21  
Resolution : 3.54 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

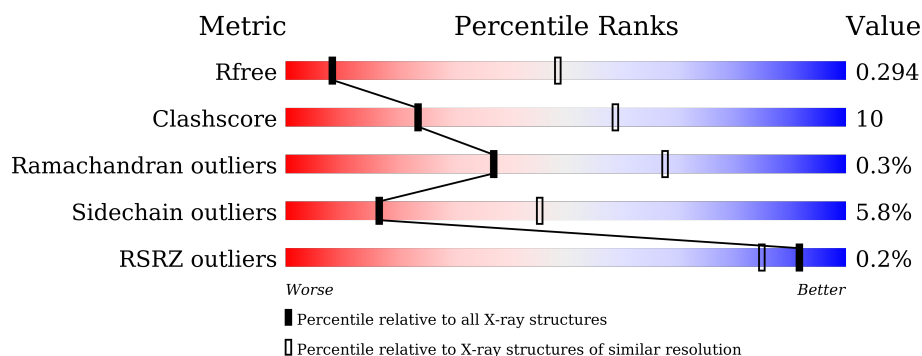
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.54 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))
$R_{free}$	164625	1272 (3.60-3.48)
Clashscore	180529	1360 (3.60-3.48)
Ramachandran outliers	177936	1347 (3.60-3.48)
Sidechain outliers	177891	1348 (3.60-3.48)
RSRZ outliers	164620	1271 (3.60-3.48)

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  $\geq 3$ , 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	A	406	63% 30% • 5%
1	B	406	66% 26% • 5%
1	C	406	67% 24% • 6% %
2	D	361	77% 21% •
2	E	361	77% 20% ••
2	F	361	75% 21% ••

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17197 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 ADP-glucose pyrophosphorylase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2989	1920	506	552	11			
1	B	387	Total	C	N	O	S	0	0	0
			2989	1920	506	552	11			
1	C	381	Total	C	N	O	S	0	0	0
			2919	1870	500	541	8			

- Molecule 2 is a protein called Mannose-1-phosphate guanylyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	361	Total	C	N	O	S	0	0	0
			2771	1782	463	510	16			
2	E	359	Total	C	N	O	S	0	0	0
			2744	1764	461	504	15			
2	F	355	Total	C	N	O	S	0	0	0
			2723	1750	457	500	16			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

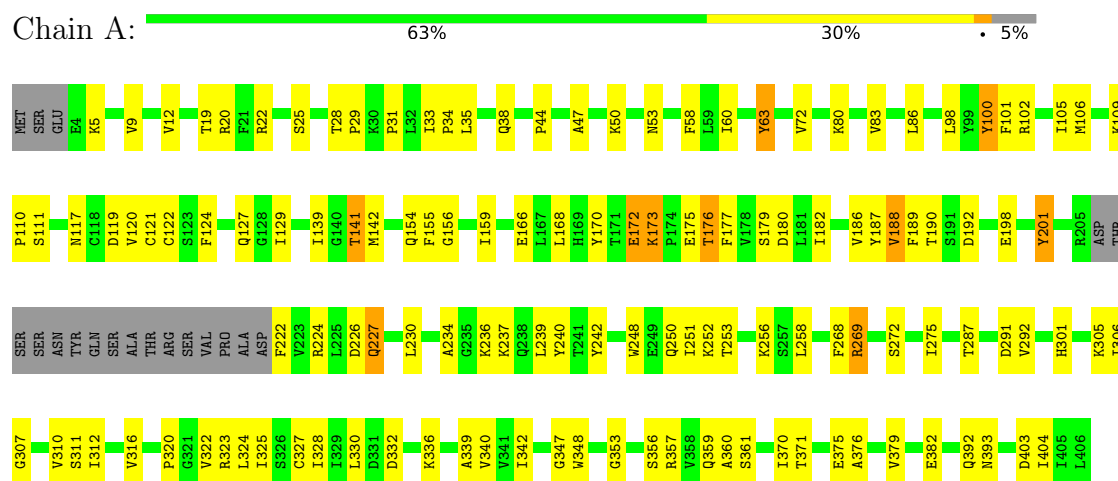
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0

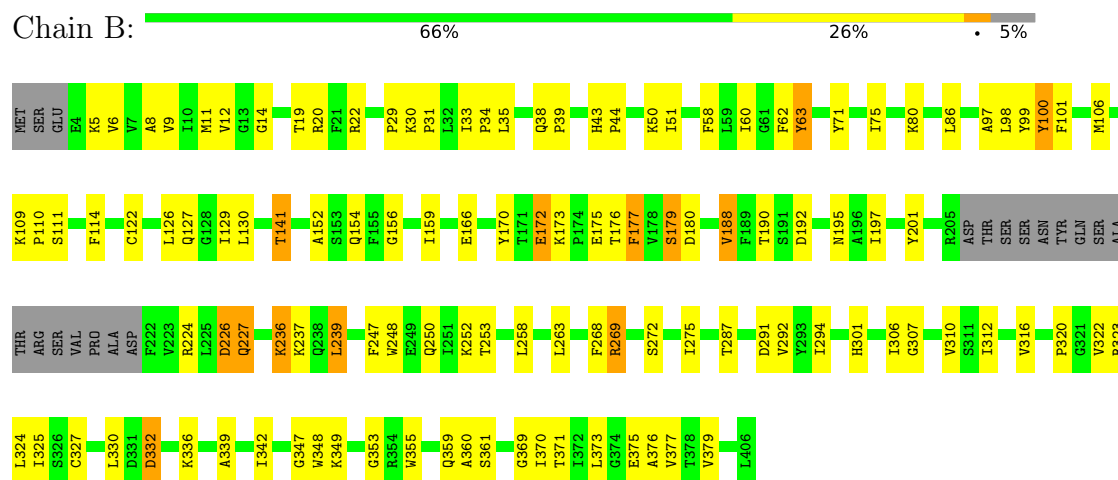
### 3 Residue-property plots

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: ADP-glucose pyrophosphorylase family protein

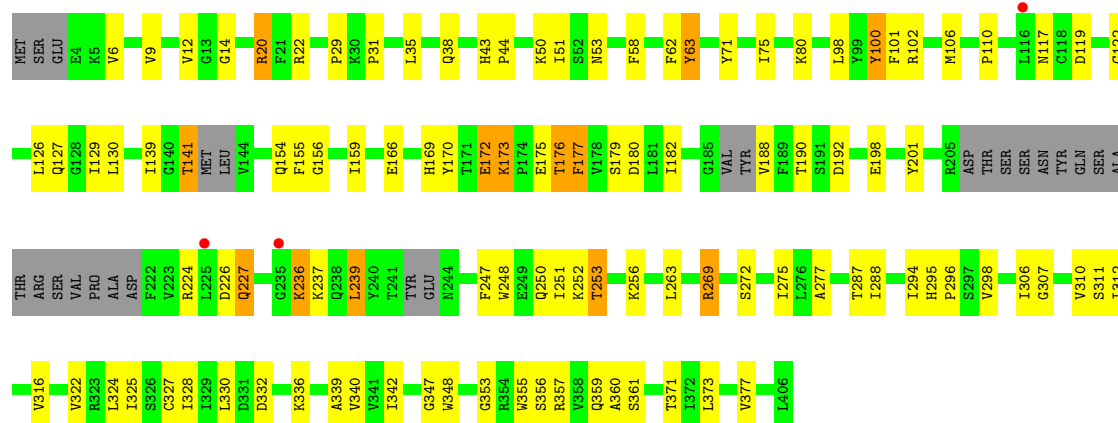


- Molecule 1: ADP-glucose pyrophosphorylase family protein



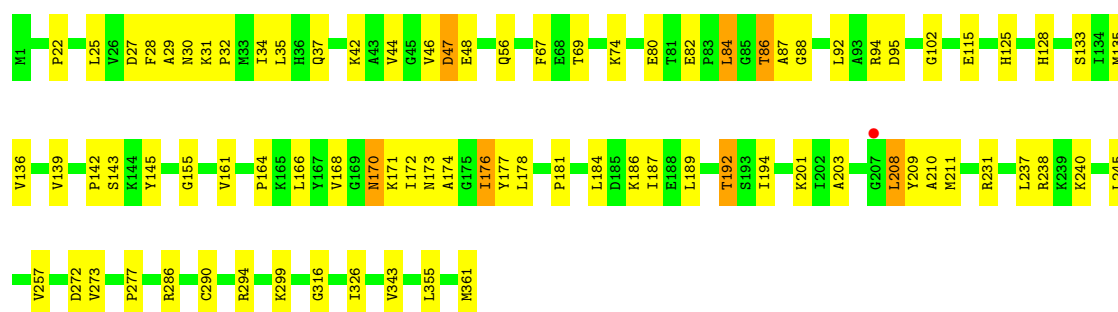
- Molecule 1: ADP-glucose pyrophosphorylase family protein





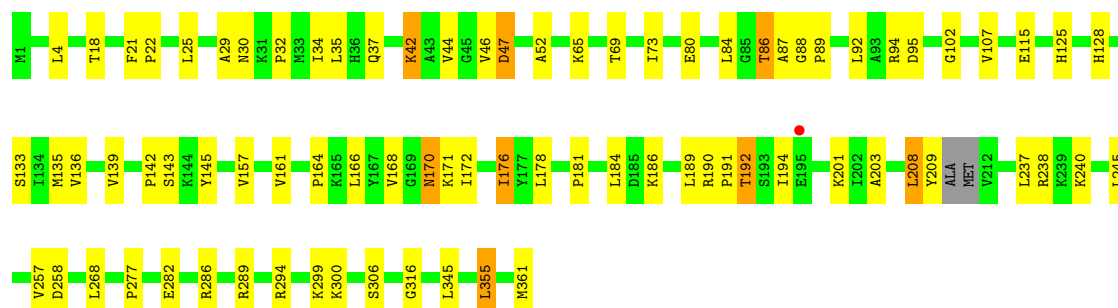
• Molecule 2: Mannose-1-phosphate guanylyltransferase 1

Chain D: 77% 21%



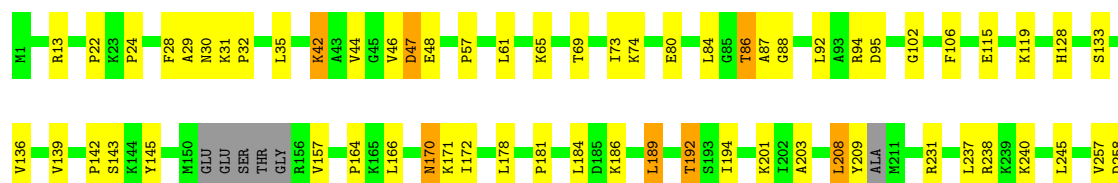
• Molecule 2: Mannose-1-phosphate guanylyltransferase 1

Chain E: 77% 20%



• Molecule 2: Mannose-1-phosphate guanylyltransferase 1

Chain F: 75% 21%



E259	T260	A261	T262	I263	D272	V273	P277	G278	C279	I280	V281	E282	R286	R289	C290	R294	K299	K300	S306	G316	L345	L355	M361
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.27Å 134.99Å 168.47Å 90.00° 117.14° 90.00°	Depositor
Resolution (Å)	149.92 – 3.54 149.92 – 3.54	Depositor EDS
% Data completeness (in resolution range)	96.3 (149.92-3.54) 92.5 (149.92-3.54)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, $R_{free}$	0.261 , 0.295 0.261 , 0.294	Depositor DCC
$R_{free}$ test set	1917 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.4	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 249.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	17197	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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	A	0.26	0/3052	0.44	0/4145
1	B	0.26	0/3052	0.44	0/4145
1	C	0.25	0/2977	0.44	0/4039
2	D	0.26	0/2826	0.44	0/3826
2	E	0.25	0/2797	0.44	0/3787
2	F	0.25	0/2775	0.44	0/3754
All	All	0.25	0/17479	0.44	0/23696

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	A	2989	0	3017	78	0
1	B	2989	0	3017	65	0
1	C	2919	0	2918	62	0
2	D	2771	0	2870	50	0
2	E	2744	0	2840	47	0
2	F	2723	0	2815	47	0
3	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	D	20	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	17197	0	17477	345	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 345 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:SER:HB3	2:D:178:LEU:HB3	1.59	0.84
2:D:84:LEU:HB2	2:D:88:GLY:HA3	1.60	0.83
2:E:133:SER:HB3	2:E:178:LEU:HB3	1.64	0.80
1:A:307:GLY:HA3	1:A:325:ILE:HG22	1.65	0.77
1:C:50:LYS:HE2	1:C:127:GLN:H	1.51	0.74

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/406 (94%)	346 (90%)	35 (9%)	2 (0%)	25	59
1	B	383/406 (94%)	345 (90%)	36 (9%)	2 (0%)	25	59
1	C	371/406 (91%)	335 (90%)	34 (9%)	2 (0%)	25	59
2	D	359/361 (99%)	341 (95%)	18 (5%)	0	100	100
2	E	355/361 (98%)	336 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	349/361 (97%)	333 (95%)	16 (5%)	0	100	100
All	All	2200/2301 (96%)	2036 (92%)	158 (7%)	6 (0%)	37	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	PHE
1	B	177	PHE
1	C	177	PHE
1	A	173	LYS
1	B	173	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/355 (93%)	306 (93%)	23 (7%)	12	39
1	B	329/355 (93%)	306 (93%)	23 (7%)	12	39
1	C	316/355 (89%)	295 (93%)	21 (7%)	14	41
2	D	308/310 (99%)	292 (95%)	16 (5%)	19	48
2	E	304/310 (98%)	290 (95%)	14 (5%)	23	52
2	F	302/310 (97%)	290 (96%)	12 (4%)	27	56
All	All	1888/1995 (95%)	1779 (94%)	109 (6%)	17	45

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	227	GLN
2	D	84	LEU
2	F	69	THR
1	C	239	LEU
1	C	332	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	37	GLN
2	E	37	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	SO4	D	403	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	402	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	F	401	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	E	402	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	F	402	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	D	404	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	E	401	-	4,4,4	0.14	0	6,6,6	0.05	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	387/406 (95%)	-0.60	0	100	100	18, 102, 153, 238	1 (0%)
1	B	387/406 (95%)	-0.58	0	100	100	63, 96, 167, 276	0
1	C	381/406 (93%)	-0.12	3 (0%)	82	64	7, 178, 247, 322	8 (2%)
2	D	361/361 (100%)	-0.30	1 (0%)	90	80	40, 129, 198, 279	1 (0%)
2	E	359/361 (99%)	-0.41	1 (0%)	90	80	46, 146, 235, 368	2 (0%)
2	F	355/361 (98%)	-0.21	0	100	100	8, 152, 216, 322	4 (1%)
All	All	2230/2301 (96%)	-0.37	5 (0%)	92	85	7, 128, 221, 368	16 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	195	GLU	3.3
2	D	207	GLY	2.6
1	C	225	LEU	2.3
1	C	235	GLY	2.1
1	C	116	LEU	2.1

### 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 monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	501	5/5	0.95	0.09	192,192,195,196	0
3	SO4	F	402	5/5	0.95	0.14	153,158,162,165	0
3	SO4	D	403	5/5	0.96	0.13	141,142,150,152	0
3	SO4	E	402	5/5	0.97	0.10	148,149,152,153	0
3	SO4	F	401	5/5	0.97	0.09	151,159,163,170	0
3	SO4	A	502	5/5	0.97	0.09	152,153,158,164	0
3	SO4	A	503	5/5	0.98	0.09	129,130,136,145	0
3	SO4	E	401	5/5	0.98	0.05	124,128,133,135	0
3	SO4	B	501	5/5	0.98	0.13	77,78,83,88	5
3	SO4	D	401	5/5	0.98	0.08	146,147,156,158	0
3	SO4	D	402	5/5	0.98	0.12	131,134,139,141	0
3	SO4	D	404	5/5	0.99	0.06	137,139,148,151	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.