



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 06:47 PM EST

PDB ID : 2CXK
Title : Crystal structure of the TIG domain of human calmodulin-binding transcription activator 1 (CAMTA1)
Authors : Pioszak, A.A.; Murayama, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-06-30
Resolution : 1.85 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:

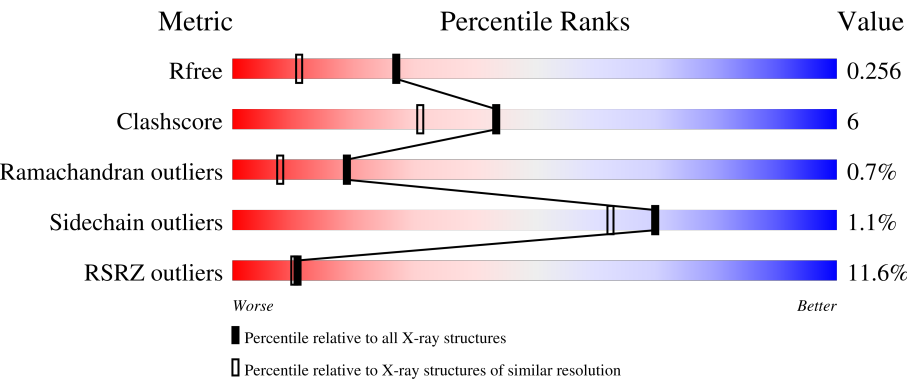
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.85 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	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	A	95	<div><div>11%</div><div><div></div><div>81%</div><div>11%</div><div>8%</div></div></div>
1	B	95	<div><div>7%</div><div><div></div><div>77%</div><div>12%</div><div>•</div><div>11%</div></div></div>
1	C	95	<div><div>5%</div><div><div></div><div>73%</div><div>15%</div><div>•</div><div>11%</div></div></div>
1	D	95	<div><div>15%</div><div><div></div><div>73%</div><div>15%</div><div>•</div><div>12%</div></div></div>
1	E	95	<div><div>14%</div><div><div></div><div>80%</div><div>9%</div><div>•</div><div>9%</div></div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	1005	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3632 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 calmodulin binding transcription activator 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	S	Se	0	0	0
			666	425	106	131	3	1			
1	B	85	Total	C	N	O	S	Se	0	0	0
			654	419	104	127	3	1			
1	C	85	Total	C	N	O	S	Se	0	0	0
			654	419	104	127	3	1			
1	D	84	Total	C	N	O	S	Se	0	0	0
			650	417	103	126	3	1			
1	E	86	Total	C	N	O	S	Se	0	0	0
			662	423	105	130	3	1			

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	865	GLY	-	expression tag	UNP Q5VUE1
A	866	SER	-	expression tag	UNP Q5VUE1
A	867	SER	-	expression tag	UNP Q5VUE1
A	868	GLY	-	expression tag	UNP Q5VUE1
A	869	SER	-	expression tag	UNP Q5VUE1
A	870	SER	-	expression tag	UNP Q5VUE1
A	871	GLY	-	expression tag	UNP Q5VUE1
A	954	SER	-	expression tag	UNP Q5VUE1
A	955	GLY	-	expression tag	UNP Q5VUE1
A	956	PRO	-	expression tag	UNP Q5VUE1
A	957	SER	-	expression tag	UNP Q5VUE1
A	958	SER	-	expression tag	UNP Q5VUE1
A	959	GLY	-	expression tag	UNP Q5VUE1
B	865	GLY	-	expression tag	UNP Q5VUE1
B	866	SER	-	expression tag	UNP Q5VUE1
B	867	SER	-	expression tag	UNP Q5VUE1
B	868	GLY	-	expression tag	UNP Q5VUE1
B	869	SER	-	expression tag	UNP Q5VUE1
B	870	SER	-	expression tag	UNP Q5VUE1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	871	GLY	-	expression tag	UNP Q5VUE1
B	954	SER	-	expression tag	UNP Q5VUE1
B	955	GLY	-	expression tag	UNP Q5VUE1
B	956	PRO	-	expression tag	UNP Q5VUE1
B	957	SER	-	expression tag	UNP Q5VUE1
B	958	SER	-	expression tag	UNP Q5VUE1
B	959	GLY	-	expression tag	UNP Q5VUE1
C	865	GLY	-	expression tag	UNP Q5VUE1
C	866	SER	-	expression tag	UNP Q5VUE1
C	867	SER	-	expression tag	UNP Q5VUE1
C	868	GLY	-	expression tag	UNP Q5VUE1
C	869	SER	-	expression tag	UNP Q5VUE1
C	870	SER	-	expression tag	UNP Q5VUE1
C	871	GLY	-	expression tag	UNP Q5VUE1
C	954	SER	-	expression tag	UNP Q5VUE1
C	955	GLY	-	expression tag	UNP Q5VUE1
C	956	PRO	-	expression tag	UNP Q5VUE1
C	957	SER	-	expression tag	UNP Q5VUE1
C	958	SER	-	expression tag	UNP Q5VUE1
C	959	GLY	-	expression tag	UNP Q5VUE1
D	865	GLY	-	expression tag	UNP Q5VUE1
D	866	SER	-	expression tag	UNP Q5VUE1
D	867	SER	-	expression tag	UNP Q5VUE1
D	868	GLY	-	expression tag	UNP Q5VUE1
D	869	SER	-	expression tag	UNP Q5VUE1
D	870	SER	-	expression tag	UNP Q5VUE1
D	871	GLY	-	expression tag	UNP Q5VUE1
D	954	SER	-	expression tag	UNP Q5VUE1
D	955	GLY	-	expression tag	UNP Q5VUE1
D	956	PRO	-	expression tag	UNP Q5VUE1
D	957	SER	-	expression tag	UNP Q5VUE1
D	958	SER	-	expression tag	UNP Q5VUE1
D	959	GLY	-	expression tag	UNP Q5VUE1
E	865	GLY	-	expression tag	UNP Q5VUE1
E	866	SER	-	expression tag	UNP Q5VUE1
E	867	SER	-	expression tag	UNP Q5VUE1
E	868	GLY	-	expression tag	UNP Q5VUE1
E	869	SER	-	expression tag	UNP Q5VUE1
E	870	SER	-	expression tag	UNP Q5VUE1
E	871	GLY	-	expression tag	UNP Q5VUE1
E	954	SER	-	expression tag	UNP Q5VUE1
E	955	GLY	-	expression tag	UNP Q5VUE1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	956	PRO	-	expression tag	UNP Q5VUE1
E	957	SER	-	expression tag	UNP Q5VUE1
E	958	SER	-	expression tag	UNP Q5VUE1
E	959	GLY	-	expression tag	UNP Q5VUE1

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		

Continued on next page...

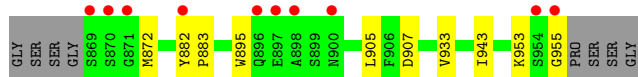
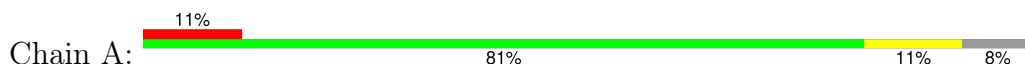
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	60	Total 60	O 60	0	0
3	C	68	Total 68	O 68	0	0
3	D	56	Total 56	O 56	0	0
3	E	65	Total 65	O 65	0	0

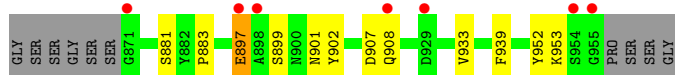
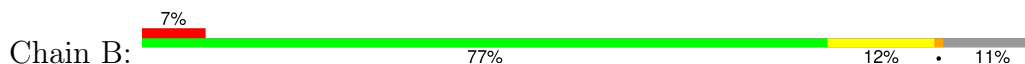
3 Residue-property plots [i](#)

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 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.

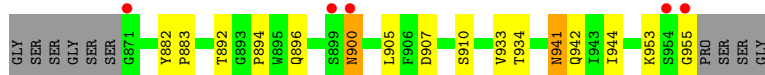
- Molecule 1: calmodulin binding transcription activator 1



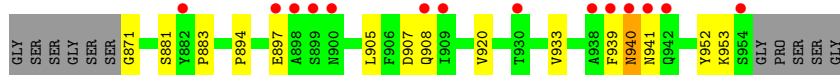
- Molecule 1: calmodulin binding transcription activator 1



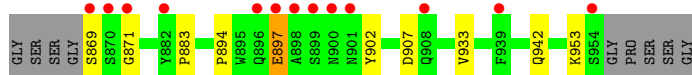
- Molecule 1: calmodulin binding transcription activator 1



- Molecule 1: calmodulin binding transcription activator 1



- Molecule 1: calmodulin binding transcription activator 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.88Å 88.88Å 107.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.01 – 1.85 46.01 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.9 (46.01-1.85) 93.0 (46.01-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	21.40 (at 1.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.259 0.223 , 0.256	Depositor DCC
R_{free} test set	1748 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3632	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% 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 [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	0.36	0/683	0.65	0/933
1	B	0.35	0/671	0.64	0/917
1	C	0.38	0/671	0.64	0/917
1	D	0.34	0/667	0.62	0/912
1	E	0.35	0/679	0.62	0/928
All	All	0.36	0/3371	0.63	0/4607

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	666	0	635	8	0
1	B	654	0	625	7	0
1	C	654	0	625	11	0
1	D	650	0	622	9	0
1	E	662	0	632	7	0
2	A	5	0	0	0	0
2	B	5	0	0	0	6
2	C	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10	0	0	0	0
3	A	67	0	0	0	0
3	B	60	0	0	0	0
3	C	68	0	0	1	0
3	D	56	0	0	0	0
3	E	65	0	0	0	0
All	All	3632	0	3139	39	6

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 6.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:ASP:O	1:B:908:GLN:HG2	1.81	0.80
1:A:905:LEU:HD12	1:A:943:ILE:HD11	1.71	0.73
1:C:883:PRO:HD3	1:C:953:LYS:O	1.88	0.73
1:E:883:PRO:HD3	1:E:953:LYS:O	1.89	0.72
1:A:882:TYR:CE1	1:A:955:GLY:HA3	2.26	0.71
1:D:871:GLY:HA2	1:D:894:PRO:HG3	1.73	0.70
1:B:907:ASP:HB2	1:B:933:VAL:HB	1.74	0.69
1:C:907:ASP:HB2	1:C:933:VAL:HB	1.76	0.67
1:C:882:TYR:CE1	1:C:955:GLY:HA3	2.28	0.67
1:D:907:ASP:HB2	1:D:933:VAL:HB	1.81	0.63
1:E:907:ASP:HB2	1:E:933:VAL:HB	1.84	0.59
1:A:883:PRO:HD3	1:A:953:LYS:O	2.02	0.59
1:D:883:PRO:HD3	1:D:953:LYS:O	2.04	0.57
1:A:872:MSE:HE1	1:C:933:VAL:O	2.05	0.56
1:C:894:PRO:O	1:C:896:GLN:HG2	2.06	0.56
1:A:872:MSE:SE	1:C:934:THR:HG22	2.56	0.55
1:E:942:GLN:NE2	1:E:942:GLN:HA	2.22	0.55
1:A:905:LEU:CD1	1:A:943:ILE:HD11	2.39	0.52
1:B:883:PRO:HD3	1:B:953:LYS:O	2.10	0.52
1:E:942:GLN:HA	1:E:942:GLN:HE21	1.75	0.51
1:D:905:LEU:N	1:D:905:LEU:HD12	2.26	0.51
1:D:939:PHE:O	1:D:940:ASN:HB2	2.12	0.49
1:C:905:LEU:CD2	1:C:910:SER:HB2	2.44	0.47
1:A:907:ASP:HB2	1:A:933:VAL:HB	1.97	0.46
1:B:897:GLU:HB2	1:B:902:TYR:CE2	2.51	0.46
1:C:900:ASN:ND2	3:C:48:HOH:O	2.45	0.45
1:C:942:GLN:O	1:C:944:ILE:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:TYR:CD1	1:A:955:GLY:HA3	2.52	0.44
1:E:897:GLU:HB2	1:E:902:TYR:CZ	2.52	0.43
1:B:899:SER:OG	1:B:901:ASN:OD1	2.37	0.43
1:B:899:SER:HB3	1:B:939:PHE:HZ	1.83	0.43
1:D:940:ASN:O	1:D:941:ASN:HB2	2.19	0.43
1:D:907:ASP:O	1:D:908:GLN:HB2	2.18	0.42
1:E:869:SER:HA	1:E:894:PRO:O	2.20	0.42
1:C:941:ASN:HD22	1:C:941:ASN:HA	1.71	0.42
1:D:881:SER:O	1:D:952:TYR:HA	2.20	0.42
1:E:871:GLY:HA3	1:E:894:PRO:HG3	2.02	0.41
1:C:892:THR:HG21	1:D:920:VAL:HG11	2.01	0.41
1:B:881:SER:O	1:B:952:TYR:HA	2.20	0.41

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1005:SO4:O1	2:B:1005:SO4:O3[8_666]	1.33	0.87
2:B:1005:SO4:O2	2:B:1005:SO4:O3[8_666]	1.34	0.86
2:B:1005:SO4:S	2:B:1005:SO4:O3[8_666]	1.42	0.78
2:B:1005:SO4:S	2:B:1005:SO4:O1[8_666]	1.52	0.68
2:B:1005:SO4:S	2:B:1005:SO4:O2[8_666]	1.52	0.68
2:B:1005:SO4:O1	2:B:1005:SO4:O2[8_666]	1.60	0.60

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	85/95 (90%)	83 (98%)	2 (2%)	0	100	100
1	B	83/95 (87%)	80 (96%)	2 (2%)	1 (1%)	11	3
1	C	83/95 (87%)	80 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	82/95 (86%)	77 (94%)	4 (5%)	1 (1%)	11	3
1	E	84/95 (88%)	81 (96%)	2 (2%)	1 (1%)	11	3
All	All	417/475 (88%)	401 (96%)	13 (3%)	3 (1%)	19	8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	897	GLU
1	B	897	GLU
1	D	897	GLU

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	76/80 (95%)	75 (99%)	1 (1%)	65	55
1	B	74/80 (92%)	74 (100%)	0	100	100
1	C	74/80 (92%)	72 (97%)	2 (3%)	40	25
1	D	74/80 (92%)	73 (99%)	1 (1%)	62	53
1	E	76/80 (95%)	76 (100%)	0	100	100
All	All	374/400 (94%)	370 (99%)	4 (1%)	70	62

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	895	TRP
1	C	900	ASN
1	C	941	ASN
1	D	940	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	900	ASN
1	A	940	ASN
1	A	942	GLN
1	B	900	ASN
1	B	940	ASN
1	B	941	ASN
1	C	900	ASN
1	C	940	ASN
1	C	941	ASN
1	D	908	GLN
1	D	940	ASN
1	D	941	ASN
1	E	896	GLN
1	E	901	ASN
1	E	941	ASN
1	E	942	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](#)

6 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	D	1002	-	4,4,4	1.07	0	6,6,6	1.29	1 (16%)
2	SO4	A	1006	-	4,4,4	1.03	0	6,6,6	1.38	1 (16%)
2	SO4	C	1004	-	4,4,4	1.03	0	6,6,6	1.38	1 (16%)
2	SO4	C	1001	-	4,4,4	1.07	0	6,6,6	1.35	1 (16%)
2	SO4	B	1005	-	4,4,4	1.03	0	6,6,6	1.38	1 (16%)
2	SO4	D	1003	-	4,4,4	1.06	0	6,6,6	1.34	1 (16%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1005	SO4	O4-S-O3	3.05	125.34	108.54
2	C	1004	SO4	O4-S-O3	3.04	125.32	108.54
2	A	1006	SO4	O4-S-O3	3.04	125.29	108.54
2	C	1001	SO4	O4-S-O3	2.96	124.88	108.54
2	D	1003	SO4	O4-S-O3	2.95	124.80	108.54
2	D	1002	SO4	O4-S-O3	2.84	124.21	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1005	SO4	0	6

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	A	86/95 (90%)	0.23	10 (11%) 11 10	8, 16, 42, 49	0
1	B	84/95 (88%)	0.45	7 (8%) 19 19	9, 18, 38, 52	0
1	C	84/95 (88%)	0.40	5 (5%) 29 31	10, 19, 39, 50	0
1	D	83/95 (87%)	0.73	14 (16%) 5 4	10, 21, 42, 50	0
1	E	85/95 (89%)	0.64	13 (15%) 6 6	11, 20, 43, 53	0
All	All	422/475 (88%)	0.49	49 (11%) 11 10	8, 19, 42, 53	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	897	GLU	4.9
1	C	955	GLY	4.8
1	E	897	GLU	4.8
1	B	955	GLY	4.7
1	E	898	ALA	4.5
1	E	899	SER	4.5
1	A	955	GLY	4.2
1	D	954	SER	4.1
1	B	954	SER	3.9
1	E	954	SER	3.6
1	D	941	ASN	3.5
1	B	871	GLY	3.4
1	E	871	GLY	3.3
1	C	954	SER	3.3
1	A	954	SER	3.3
1	A	870	SER	3.2
1	E	870	SER	3.2
1	B	897	GLU	3.2
1	A	898	ALA	3.2
1	E	882	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	898	ALA	3.0
1	D	899	SER	2.9
1	D	900	ASN	2.9
1	E	896	GLN	2.8
1	A	869	SER	2.7
1	D	942	GLN	2.7
1	B	929	ASP	2.7
1	D	939	PHE	2.6
1	D	897	GLU	2.6
1	B	908	GLN	2.5
1	B	898	ALA	2.5
1	D	882	TYR	2.5
1	D	930	THR	2.5
1	C	900	ASN	2.5
1	E	869	SER	2.4
1	A	871	GLY	2.4
1	A	900	ASN	2.4
1	C	871	GLY	2.4
1	E	900	ASN	2.3
1	D	908	GLN	2.3
1	D	909	ILE	2.3
1	E	939	PHE	2.2
1	A	882	TYR	2.2
1	D	940	ASN	2.1
1	A	896	GLN	2.1
1	E	908	GLN	2.1
1	C	899	SER	2.1
1	E	901	ASN	2.1
1	D	938	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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, 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(\AA^2)	Q<0.9
2	SO4	A	1006	5/5	0.87	0.25	55,57,84,109	5
2	SO4	C	1001	5/5	0.88	0.12	21,32,39,46	0
2	SO4	C	1004	5/5	0.89	0.13	27,29,59,67	0
2	SO4	D	1003	5/5	0.89	0.14	32,37,57,61	0
2	SO4	D	1002	5/5	0.93	0.13	27,35,41,47	0
2	SO4	B	1005	5/5	0.96	0.21	18,29,53,54	2

6.5 Other polymers [i](#)

There are no such residues in this entry.