



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:20 AM UTC

PDB ID : 3TX3 / pdb_00003tx3
Title : CysZ, a putative sulfate permease
Authors : Assur, Z.; Liu, Q.; Hendrickson, W.A.; Mancina, F.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : 2011-09-22
Resolution : 2.30 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

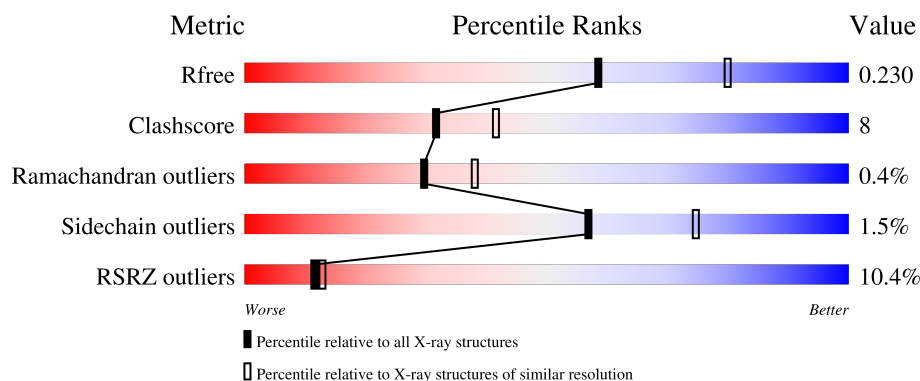
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	249	10% 74% 16% • 9%
1	B	249	8% 78% 13% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4078 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 Uncharacterized protein involved in cysteine biosynthesis.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1849	1236	297	306	10			
1	B	226	Total	C	N	O	S	0	0	0
			1828	1219	295	304	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5QUJ8
A	-1	TYR	-	expression tag	UNP Q5QUJ8
A	0	VAL	-	expression tag	UNP Q5QUJ8
B	-2	SER	-	expression tag	UNP Q5QUJ8
B	-1	TYR	-	expression tag	UNP Q5QUJ8
B	0	VAL	-	expression tag	UNP Q5QUJ8

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

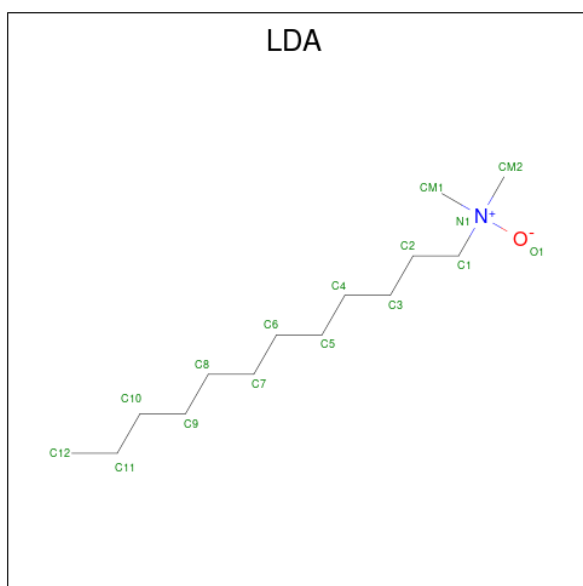


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	5	0
			16	14	1	1		
4	A	1	Total	C	N	O	5	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	5	0
			16	14	1	1		
4	A	1	Total	C	N	O	5	0
			16	14	1	1		
4	A	1	Total	C	N	O	5	0
			16	14	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	3	0
			16	14	1	1		
4	B	1	Total	C	N	O	5	0
			16	14	1	1		
4	B	1	Total	C	N	O	5	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	5	0
			16	14	1	1		
4	B	1	Total	C	N	O	5	0
			16	14	1	1		
4	B	1	Total	C	N	O	5	0
			16	14	1	1		

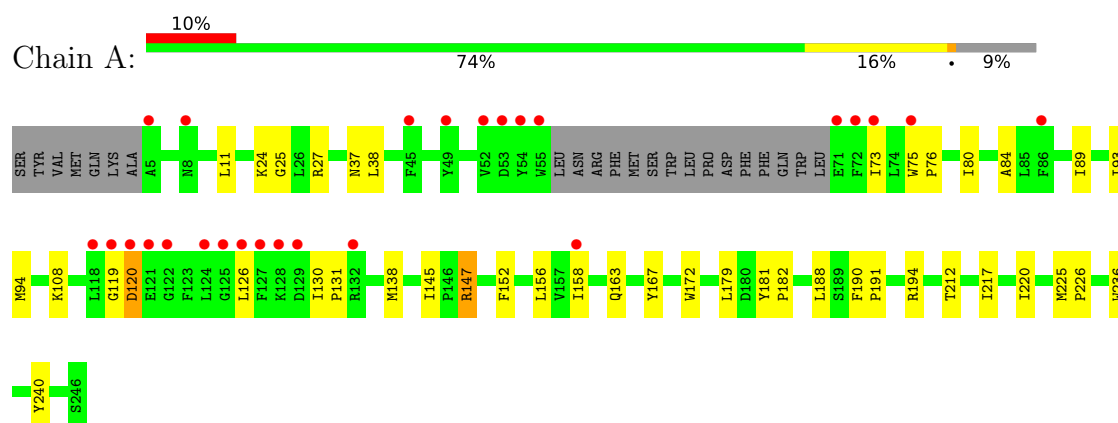
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	85	Total	O	0	0
			85	85		

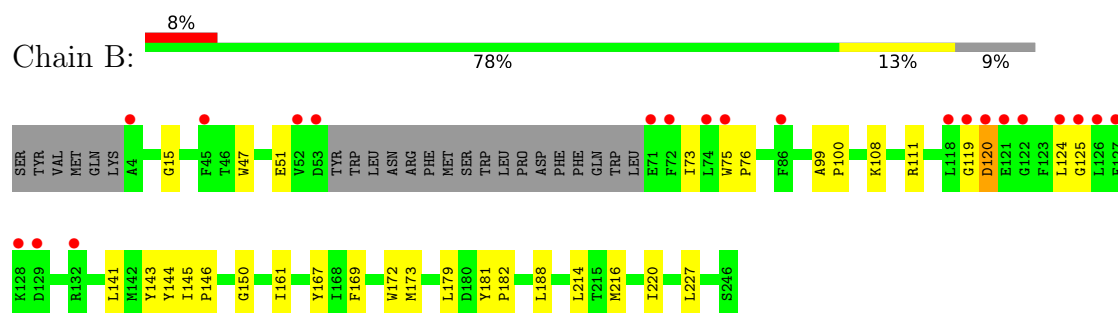
3 Residue-property plots [i](#)

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: Uncharacterized protein involved in cysteine biosynthesis



- Molecule 1: Uncharacterized protein involved in cysteine biosynthesis



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.85Å 81.99Å 100.38Å 90.00° 125.12° 90.00°	Depositor
Resolution (Å)	29.17 – 2.30 29.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.17-2.30) 96.8 (29.17-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.200 , 0.238 0.192 , 0.230	Depositor DCC
R_{free} test set	1948 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.8	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	0.94	EDS
Total number of atoms	4078	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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: CL, LDA, 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	0.43	0/1901	0.77	2/2580 (0.1%)
1	B	0.46	0/1877	0.75	1/2546 (0.0%)
All	All	0.44	0/3778	0.76	3/5126 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ASP	N-CA-C	-6.91	102.84	112.45
1	B	120	ASP	N-CA-C	-6.54	103.43	111.40
1	A	158	ILE	N-CA-C	5.44	113.42	107.60

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	1849	0	1899	32	0
1	B	1828	0	1885	30	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	112	0	217	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	128	0	248	9	0
5	A	67	0	0	0	0
5	B	85	0	0	0	0
All	All	4078	0	4249	65	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 8.

All (65) 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:A:76:PRO:HG3	4:A:604:LDA:H92	1.61	0.81
1:B:111:ARG:HH12	1:B:120:ASP:HB2	1.44	0.80
1:A:167:TYR:HB3	4:A:603:LDA:H102	1.66	0.77
1:A:194:ARG:HH22	4:A:605:LDA:H12	1.51	0.76
1:A:145:ILE:HG23	4:A:606:LDA:H123	1.67	0.75
1:B:144:TYR:HD1	1:B:173:MET:HE3	1.56	0.70
1:A:194:ARG:NH2	4:A:605:LDA:H12	2.07	0.70
1:B:143:TYR:CD2	1:B:173:MET:HE1	2.30	0.67
1:B:144:TYR:CD1	1:B:173:MET:HE3	2.31	0.66
1:A:80:ILE:HD11	4:B:603:LDA:H91	1.77	0.65
1:B:15:GLY:HA3	4:B:602:LDA:H51	1.80	0.64
1:B:108:LYS:HZ1	1:B:120:ASP:HB3	1.63	0.64
1:B:169:PHE:CZ	1:B:173:MET:HE2	2.34	0.61
1:B:108:LYS:NZ	1:B:120:ASP:HB3	2.16	0.61
1:A:147:ARG:HD3	4:A:605:LDA:H31	1.84	0.59
1:B:75:TRP:HB3	1:B:76:PRO:HD3	1.82	0.59
1:A:84:ALA:HB2	1:B:216:MET:HE1	1.85	0.59
1:A:24:LYS:HG2	1:A:27:ARG:HH21	1.69	0.58
1:B:73:ILE:C	1:B:76:PRO:HD2	2.29	0.57
1:B:99:ALA:HB3	1:B:100:PRO:HD3	1.89	0.54
1:A:11:LEU:HD23	1:A:11:LEU:O	2.08	0.53
4:A:604:LDA:H121	4:B:603:LDA:H112	1.90	0.53
1:B:145:ILE:HB	1:B:146:PRO:HD3	1.93	0.51
1:A:73:ILE:C	1:A:76:PRO:HD2	2.35	0.51
1:B:73:ILE:O	1:B:76:PRO:HD2	2.10	0.51
1:B:141:LEU:O	1:B:145:ILE:HG12	2.10	0.51
1:B:167:TYR:HB3	4:B:603:LDA:H82	1.93	0.51
1:A:24:LYS:HD3	1:A:25:GLY:N	2.28	0.49
1:B:161:ILE:H	1:B:161:ILE:HD12	1.78	0.49
1:A:138:MET:HA	1:A:138:MET:HE2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HH11	4:A:605:LDA:H31	1.77	0.48
1:A:152:PHE:CZ	1:A:156:LEU:HD11	2.49	0.48
1:B:143:TYR:HD2	1:B:173:MET:HE1	1.77	0.48
1:B:145:ILE:HG23	4:B:606:LDA:H122	1.96	0.47
1:A:163:GLN:HE22	4:A:606:LDA:HM12	1.80	0.46
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.98	0.46
1:A:225:MET:HB3	1:A:226:PRO:CD	2.46	0.46
1:B:150:GLY:HA3	4:B:610:LDA:H112	1.98	0.46
1:A:212:THR:HG22	4:A:603:LDA:H62	1.98	0.45
1:B:143:TYR:CE2	1:B:173:MET:HE1	2.51	0.45
1:B:181:TYR:N	1:B:182:PRO:HD2	2.32	0.45
1:B:169:PHE:CZ	1:B:173:MET:CE	3.00	0.45
1:A:108:LYS:NZ	1:A:120:ASP:HB3	2.33	0.44
1:A:37:ASN:CG	1:A:94:MET:HE2	2.42	0.44
1:B:172:TRP:CE3	4:B:605:LDA:H71	2.52	0.44
4:B:606:LDA:HM13	4:B:606:LDA:H21	1.67	0.44
1:A:11:LEU:HD23	1:A:11:LEU:C	2.42	0.44
4:B:605:LDA:HM13	4:B:605:LDA:H21	1.59	0.43
1:A:217:ILE:HD12	1:A:220:ILE:HD12	2.00	0.43
1:B:227:LEU:O	1:B:227:LEU:HD23	2.18	0.43
1:A:190:PHE:HB3	1:A:191:PRO:HD3	2.01	0.43
1:A:172:TRP:CD1	4:A:605:LDA:H71	2.54	0.42
4:A:606:LDA:HM22	4:A:606:LDA:H22	1.68	0.42
1:A:75:TRP:HB2	1:A:76:PRO:HD3	2.02	0.42
1:A:236:TRP:HA	1:A:240:TYR:HB2	2.02	0.42
1:B:214:LEU:HB3	1:B:220:ILE:HG21	2.02	0.42
1:A:75:TRP:CB	1:A:76:PRO:HD3	2.50	0.41
1:A:89:ILE:O	1:A:93:ILE:HG12	2.21	0.41
1:A:126:LEU:C	1:A:126:LEU:HD23	2.45	0.41
1:B:227:LEU:HD23	1:B:227:LEU:C	2.46	0.41
1:A:181:TYR:N	1:A:182:PRO:HD2	2.36	0.41
1:B:124:LEU:HD12	1:B:125:GLY:N	2.35	0.41
1:B:161:ILE:HD12	1:B:161:ILE:N	2.36	0.41
1:A:37:ASN:HA	1:A:94:MET:HE2	2.02	0.41
1:B:47:TRP:CZ2	1:B:51:GLU:HG3	2.56	0.41

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	A	223/249 (90%)	219 (98%)	3 (1%)	1 (0%)	30	38
1	B	222/249 (89%)	217 (98%)	4 (2%)	1 (0%)	24	31
All	All	445/498 (89%)	436 (98%)	7 (2%)	2 (0%)	30	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLY
1	B	119	GLY

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	199/220 (90%)	195 (98%)	4 (2%)	48	67
1	B	197/220 (90%)	195 (99%)	2 (1%)	68	82
All	All	396/440 (90%)	390 (98%)	6 (2%)	57	75

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	147	ARG
1	A	179	LEU
1	A	188	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	179	LEU
1	B	188	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	B	199	GLN
1	B	221	ASN

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](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

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	$\# Z > 2$
4	LDA	B	603	-	13,15,15	2.46	2 (15%)	14,17,17	0.49	0
2	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.15	0
4	LDA	A	604	-	13,15,15	2.47	2 (15%)	14,17,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	A	607	-	13,15,15	2.45	2 (15%)	14,17,17	0.49	0
4	LDA	B	608	-	13,15,15	2.45	2 (15%)	14,17,17	0.47	0
4	LDA	B	606	-	13,15,15	2.43	2 (15%)	14,17,17	0.53	0
4	LDA	B	602	-	13,15,15	2.47	2 (15%)	14,17,17	0.50	0
4	LDA	A	605	-	13,15,15	2.47	2 (15%)	14,17,17	0.57	0
4	LDA	B	610	-	13,15,15	2.49	2 (15%)	14,17,17	0.51	0
4	LDA	A	602	-	13,15,15	2.44	2 (15%)	14,17,17	0.42	0
4	LDA	A	601	-	13,15,15	2.46	2 (15%)	14,17,17	0.48	0
4	LDA	A	603	-	13,15,15	2.45	2 (15%)	14,17,17	0.48	0
4	LDA	B	601	-	13,15,15	2.43	2 (15%)	14,17,17	0.47	0
4	LDA	B	605	-	13,15,15	2.48	2 (15%)	14,17,17	0.53	0
4	LDA	A	606	-	13,15,15	2.50	2 (15%)	14,17,17	0.56	0
4	LDA	B	609	-	13,15,15	2.47	2 (15%)	14,17,17	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	B	603	-	-	9/13/13/13	-
4	LDA	A	607	-	-	7/13/13/13	-
4	LDA	A	604	-	-	7/13/13/13	-
4	LDA	B	608	-	-	6/13/13/13	-
4	LDA	B	606	-	-	3/13/13/13	-
4	LDA	B	602	-	-	7/13/13/13	-
4	LDA	A	605	-	-	7/13/13/13	-
4	LDA	B	610	-	-	6/13/13/13	-
4	LDA	A	602	-	-	6/13/13/13	-
4	LDA	A	601	-	-	7/13/13/13	-
4	LDA	A	603	-	-	6/13/13/13	-
4	LDA	B	601	-	-	7/13/13/13	-
4	LDA	B	605	-	-	6/13/13/13	-
4	LDA	A	606	-	-	4/13/13/13	-
4	LDA	B	609	-	-	6/13/13/13	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	608	LDA	O1-N1	-6.85	1.25	1.42
4	B	602	LDA	O1-N1	-6.85	1.25	1.42
4	A	606	LDA	O1-N1	-6.83	1.25	1.42
4	A	607	LDA	O1-N1	-6.82	1.25	1.42
4	A	601	LDA	O1-N1	-6.82	1.25	1.42
4	B	603	LDA	O1-N1	-6.82	1.25	1.42
4	B	610	LDA	O1-N1	-6.82	1.25	1.42
4	A	603	LDA	O1-N1	-6.81	1.25	1.42
4	B	605	LDA	O1-N1	-6.80	1.25	1.42
4	A	602	LDA	O1-N1	-6.80	1.25	1.42
4	A	605	LDA	O1-N1	-6.80	1.25	1.42
4	B	609	LDA	O1-N1	-6.79	1.25	1.42
4	B	601	LDA	O1-N1	-6.79	1.25	1.42
4	A	604	LDA	O1-N1	-6.78	1.25	1.42
4	B	606	LDA	O1-N1	-6.77	1.25	1.42
4	A	606	LDA	C1-N1	-5.86	1.45	1.51
4	B	610	LDA	C1-N1	-5.78	1.45	1.51
4	B	605	LDA	C1-N1	-5.73	1.45	1.51
4	A	604	LDA	C1-N1	-5.73	1.45	1.51
4	B	609	LDA	C1-N1	-5.72	1.45	1.51
4	A	605	LDA	C1-N1	-5.70	1.45	1.51
4	B	603	LDA	C1-N1	-5.63	1.45	1.51
4	B	602	LDA	C1-N1	-5.62	1.45	1.51
4	A	601	LDA	C1-N1	-5.60	1.45	1.51
4	A	603	LDA	C1-N1	-5.58	1.45	1.51
4	A	607	LDA	C1-N1	-5.55	1.45	1.51
4	B	606	LDA	C1-N1	-5.52	1.45	1.51
4	B	608	LDA	C1-N1	-5.51	1.45	1.51
4	A	602	LDA	C1-N1	-5.49	1.45	1.51
4	B	601	LDA	C1-N1	-5.46	1.45	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	LDA	C2-C1-N1-O1
4	A	602	LDA	C2-C1-N1-CM1
4	A	602	LDA	C2-C1-N1-CM2
4	A	603	LDA	C2-C1-N1-CM1
4	A	603	LDA	C2-C1-N1-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	605	LDA	C2-C1-N1-O1
4	A	605	LDA	C2-C1-N1-CM1
4	A	601	LDA	C2-C1-N1-CM1
4	A	601	LDA	C2-C1-N1-CM2
4	A	604	LDA	C2-C1-N1-O1
4	A	604	LDA	C2-C1-N1-CM1
4	A	604	LDA	C2-C1-N1-CM2
4	A	607	LDA	C2-C1-N1-O1
4	A	607	LDA	C2-C1-N1-CM1
4	A	607	LDA	C2-C1-N1-CM2
4	B	601	LDA	C2-C1-N1-O1
4	B	601	LDA	C2-C1-N1-CM1
4	B	601	LDA	C2-C1-N1-CM2
4	B	602	LDA	C2-C1-N1-O1
4	B	602	LDA	C2-C1-N1-CM1
4	B	602	LDA	C2-C1-N1-CM2
4	B	603	LDA	C2-C1-N1-CM1
4	B	603	LDA	C2-C1-N1-CM2
4	B	608	LDA	C2-C1-N1-O1
4	B	608	LDA	C2-C1-N1-CM1
4	B	608	LDA	C2-C1-N1-CM2
4	B	609	LDA	C2-C1-N1-O1
4	B	609	LDA	C2-C1-N1-CM1
4	B	609	LDA	C2-C1-N1-CM2
4	B	610	LDA	C2-C1-N1-CM1
4	B	610	LDA	C2-C1-N1-CM2
4	A	601	LDA	C7-C8-C9-C10
4	B	603	LDA	C3-C4-C5-C6
4	A	607	LDA	C7-C8-C9-C10
4	B	601	LDA	C4-C5-C6-C7
4	B	603	LDA	C7-C8-C9-C10
4	B	606	LDA	C7-C8-C9-C10
4	B	608	LDA	C7-C8-C9-C10
4	A	605	LDA	C4-C5-C6-C7
4	B	602	LDA	C1-C2-C3-C4
4	B	609	LDA	C7-C8-C9-C10
4	A	606	LDA	C7-C8-C9-C10
4	A	604	LDA	C1-C2-C3-C4
4	B	603	LDA	C1-C2-C3-C4
4	B	601	LDA	C1-C2-C3-C4
4	A	602	LDA	C7-C8-C9-C10
4	B	603	LDA	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	610	LDA	C7-C8-C9-C10
4	A	603	LDA	C7-C8-C9-C10
4	B	605	LDA	C7-C8-C9-C10
4	A	606	LDA	C9-C10-C11-C12
4	B	606	LDA	C4-C5-C6-C7
4	A	602	LDA	C9-C10-C11-C12
4	A	603	LDA	C4-C5-C6-C7
4	B	610	LDA	C1-C2-C3-C4
4	A	604	LDA	C2-C3-C4-C5
4	B	605	LDA	C9-C10-C11-C12
4	B	605	LDA	C4-C5-C6-C7
4	B	603	LDA	C5-C6-C7-C8
4	A	602	LDA	C11-C10-C9-C8
4	B	609	LDA	C1-C2-C3-C4
4	A	606	LDA	C1-C2-C3-C4
4	A	604	LDA	C11-C10-C9-C8
4	A	604	LDA	C9-C10-C11-C12
4	A	605	LDA	C2-C1-N1-CM2
4	B	603	LDA	C4-C5-C6-C7
4	A	603	LDA	C1-C2-C3-C4
4	B	609	LDA	C9-C10-C11-C12
4	A	601	LDA	C5-C6-C7-C8
4	A	601	LDA	C2-C1-N1-O1
4	B	605	LDA	C2-C3-C4-C5
4	A	607	LDA	C4-C5-C6-C7
4	A	605	LDA	C7-C8-C9-C10
4	B	603	LDA	C9-C10-C11-C12
4	B	608	LDA	C11-C10-C9-C8
4	A	607	LDA	C9-C10-C11-C12
4	A	601	LDA	C9-C10-C11-C12
4	B	610	LDA	C9-C10-C11-C12
4	A	605	LDA	C9-C10-C11-C12
4	B	602	LDA	C4-C5-C6-C7
4	B	605	LDA	C1-C2-C3-C4
4	A	607	LDA	C1-C2-C3-C4
4	B	601	LDA	C7-C8-C9-C10
4	B	605	LDA	C5-C6-C7-C8
4	B	608	LDA	C1-C2-C3-C4
4	A	606	LDA	C4-C5-C6-C7
4	A	601	LDA	C6-C7-C8-C9
4	B	601	LDA	C5-C6-C7-C8
4	B	602	LDA	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	606	LDA	C1-C2-C3-C4
4	A	605	LDA	C5-C6-C7-C8
4	B	602	LDA	C5-C6-C7-C8
4	A	603	LDA	C2-C1-N1-O1
4	B	610	LDA	C2-C1-N1-O1

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	LDA	3	0
4	A	604	LDA	2	0
4	B	606	LDA	2	0
4	B	602	LDA	1	0
4	A	605	LDA	5	0
4	B	610	LDA	1	0
4	A	603	LDA	2	0
4	B	605	LDA	2	0
4	A	606	LDA	3	0

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	227/249 (91%)	0.61	26 (11%)	9 10	25, 43, 96, 158	0
1	B	226/249 (90%)	0.31	21 (9%)	14 16	23, 41, 85, 130	0
All	All	453/498 (90%)	0.46	47 (10%)	11 13	23, 43, 91, 158	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	GLY	8.5
1	A	124	LEU	7.6
1	A	55	TRP	7.4
1	A	125	GLY	7.2
1	A	122	GLY	6.4
1	A	127	PHE	6.4
1	A	71	GLU	5.7
1	B	127	PHE	5.5
1	A	120	ASP	5.4
1	A	54	TYR	5.3
1	A	121	GLU	5.0
1	B	124	LEU	4.8
1	A	73	ILE	4.6
1	B	71	GLU	4.5
1	B	72	PHE	4.4
1	B	45	PHE	4.4
1	A	45	PHE	3.9
1	B	121	GLU	3.8
1	A	75	TRP	3.8
1	B	125	GLY	3.8
1	B	53	ASP	3.6
1	A	128	LYS	3.6
1	B	119	GLY	3.6
1	A	52	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	129	ASP	3.5
1	B	4	ALA	3.5
1	A	72	PHE	3.5
1	A	126	LEU	3.5
1	B	75	TRP	3.3
1	B	122	GLY	3.2
1	A	129	ASP	3.2
1	B	120	ASP	2.9
1	A	132	ARG	2.9
1	A	118	LEU	2.9
1	B	74	LEU	2.8
1	A	53	ASP	2.8
1	A	8	ASN	2.7
1	B	86	PHE	2.5
1	B	132	ARG	2.4
1	B	128	LYS	2.3
1	B	126	LEU	2.3
1	B	52	VAL	2.3
1	A	86	PHE	2.2
1	B	118	LEU	2.2
1	A	5	ALA	2.2
1	A	49	TYR	2.2
1	A	158	ILE	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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LDA	A	602	16/16	0.59	0.40	56,70,105,106	5
4	LDA	A	607	16/16	0.72	0.33	91,93,96,96	5
4	LDA	B	609	16/16	0.77	0.28	89,94,98,99	5
4	LDA	B	608	16/16	0.79	0.28	67,86,89,91	5
4	LDA	B	605	16/16	0.79	0.27	52,73,118,118	0
4	LDA	A	606	16/16	0.80	0.32	76,90,100,103	0
4	LDA	A	601	16/16	0.80	0.23	57,72,99,100	5
4	LDA	B	602	16/16	0.81	0.25	54,59,87,87	5
4	LDA	A	603	16/16	0.83	0.19	51,61,70,71	5
4	LDA	B	603	16/16	0.84	0.20	40,53,86,86	5
4	LDA	B	606	16/16	0.85	0.25	73,85,97,100	0
4	LDA	B	601	16/16	0.85	0.26	58,81,106,106	3
4	LDA	A	605	16/16	0.85	0.29	48,83,123,123	0
4	LDA	B	610	16/16	0.86	0.23	60,70,75,75	5
4	LDA	A	604	16/16	0.87	0.20	40,63,72,72	5
2	SO4	A	301	5/5	0.94	0.18	45,60,66,80	0
3	CL	B	402	1/1	0.97	0.12	46,46,46,46	0
3	CL	A	402	1/1	0.97	0.09	54,54,54,54	0
3	CL	A	401	1/1	0.98	0.07	43,43,43,43	0
3	CL	B	401	1/1	0.99	0.04	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.