Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 02:21 PM JST

PDB ID	:	7YEO
Title	:	Crystal Structure of cystathionine gamma-synthase-like protein C23A1.14c
Authors	:	Zhang, S.J.
Deposited on	:	2022-07-06
Resolution	:	1.70 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 (i) symbol.

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

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

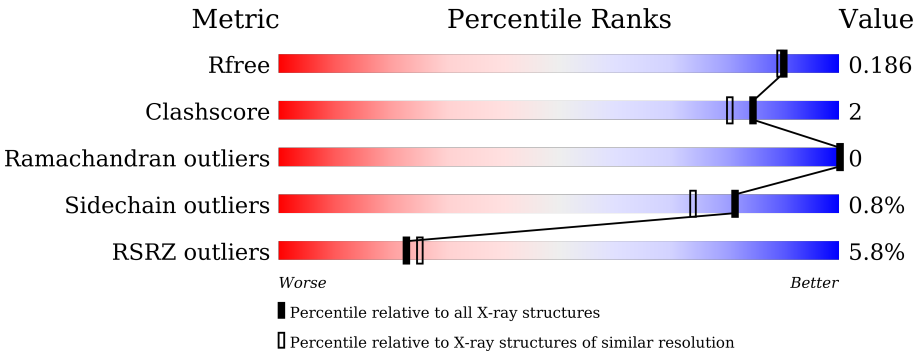
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	398	6% 90% 5%
1	B	398	5% 90% 6%

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	PLP	A	401	-	X	-	-

2 Entry composition

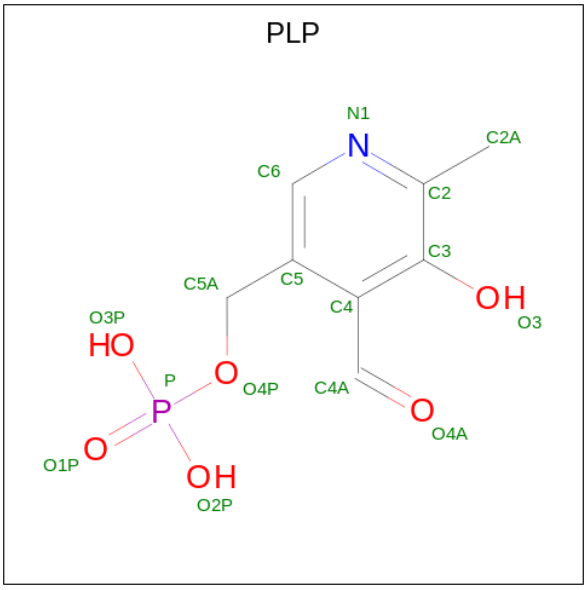
There are 4 unique types of molecules in this entry. The entry contains 6454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 trans-sulfuration enzyme C23A1.14c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	7	0
			2967	1896	500	566	5			
1	B	382	Total	C	N	O	S	0	5	0
			2966	1898	499	564	5			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

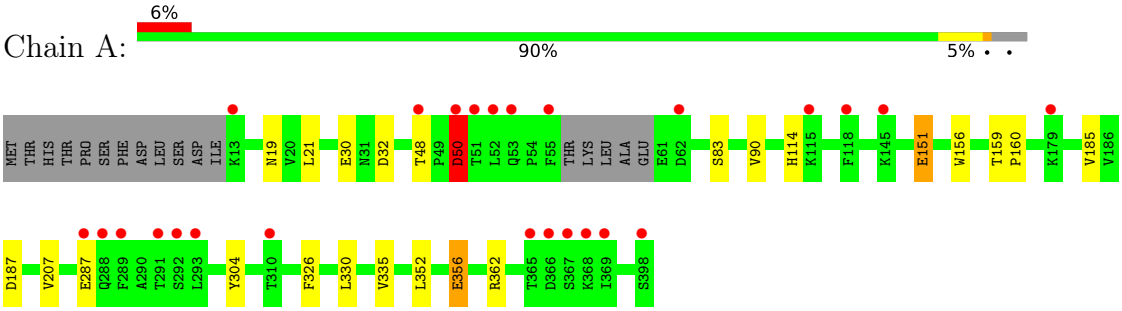
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	237	Total O 237 237	0	0
4	B	252	Total O 252 252	0	0

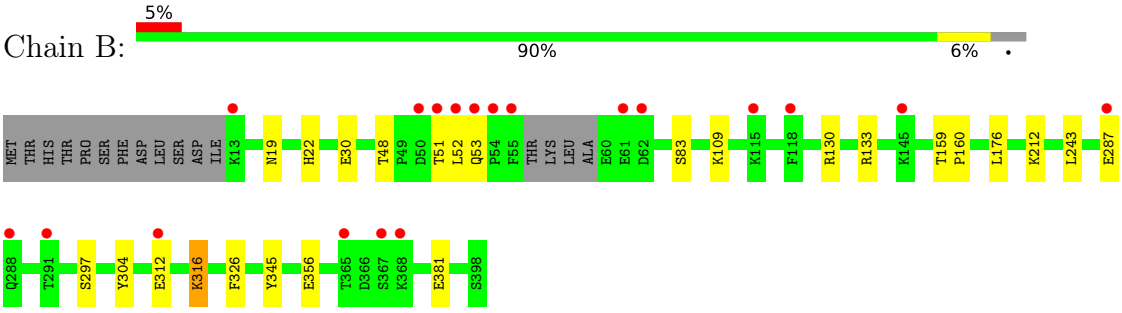
3 Residue-property plots (i)

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: Uncharacterized trans-sulfuration enzyme C23A1.14c



• Molecule 1: Uncharacterized trans-sulfuration enzyme C23A1.14c



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.39Å 106.82Å 82.81Å 90.00° 128.00° 90.00°	Depositor
Resolution (Å)	27.15 – 1.70 27.15 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (27.15-1.70) 98.8 (27.15-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.161 , 0.186 0.161 , 0.186	Depositor DCC
R_{free} test set	4417 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6454	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PLP

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	0.51	0/3031	0.82	8/4123 (0.2%)
1	B	0.53	1/3030 (0.0%)	0.75	4/4122 (0.1%)
All	All	0.52	1/6061 (0.0%)	0.79	12/8245 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	316	LYS	CD-CE	-6.93	1.33	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	GLU	OE1-CD-OE2	-17.14	102.74	123.30
1	A	151	GLU	CG-CD-OE1	13.08	144.46	118.30
1	B	176	LEU	CB-CG-CD2	-10.21	93.64	111.00
1	A	151	GLU	CG-CD-OE2	-9.82	98.66	118.30
1	A	50	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	A	50	ASP	CB-CG-OD1	7.03	124.63	118.30
1	B	109	LYS	CD-CE-NZ	-6.17	97.52	111.70
1	B	312	GLU	CA-CB-CG	6.09	126.81	113.40
1	A	356	GLU	CB-CA-C	-5.98	98.43	110.40
1	B	130	ARG	NE-CZ-NH1	-5.25	117.67	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	A	352	LEU	CB-CG-CD2	5.01	119.52	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	GLU	Sidechain
1	A	287	GLU	Sidechain
1	A	50	ASP	Sidechain

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	2967	0	2967	11	0
1	B	2966	0	2971	17	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	237	0	0	2	0
4	B	252	0	0	7	0
All	All	6454	0	5950	27	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 2.

All (27) 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:48:THR:OG1	1:A:50:ASP:OD1	2.10	0.66
1:B:243[A]:LEU:HD12	4:B:653:HOH:O	1.96	0.66
1:A:356:GLU:HG2	4:B:649:HOH:O	2.02	0.60
1:B:51:THR:O	1:B:53:GLN:HG3	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LYS:HA	1:B:316:LYS:HE2	1.88	0.55
1:A:114:HIS:HD2	4:A:708:HOH:O	1.92	0.53
1:B:345:TYR:OH	4:B:501:HOH:O	2.19	0.51
1:B:48:THR:O	1:B:52:LEU:HB2	2.11	0.50
1:A:21:LEU:HD12	1:B:381:GLU:HG3	1.94	0.50
1:B:133:ARG:NE	4:B:503:HOH:O	2.29	0.49
1:A:187:ASP:HA	1:A:207[B]:VAL:HG23	1.95	0.49
1:B:19:ASN:HB3	1:B:83[A]:SER:OG	2.13	0.48
4:A:647:HOH:O	1:B:22:HIS:HE1	1.97	0.47
1:A:19:ASN:HB3	1:A:83[A]:SER:OG	2.14	0.47
1:B:133:ARG:NH2	4:B:506:HOH:O	2.48	0.46
1:B:133:ARG:CZ	4:B:506:HOH:O	2.63	0.46
1:A:330:LEU:HD13	1:A:335:VAL:HG12	1.99	0.45
1:B:212:LYS:NZ	2:B:401:PLP:O3	2.51	0.43
1:A:187:ASP:HA	1:A:207[B]:VAL:CG2	2.48	0.43
1:B:316:LYS:HE2	1:B:316:LYS:CA	2.49	0.43
1:B:159:THR:HA	1:B:160:PRO:C	2.40	0.42
1:B:304:TYR:O	1:B:326:PHE:HB2	2.20	0.41
1:B:133:ARG:NE	4:B:506:HOH:O	2.52	0.41
1:B:287:GLU:HG2	1:B:297:SER:OG	2.21	0.41
1:A:159:THR:HA	1:A:160:PRO:C	2.40	0.41
1:A:156:TRP:CZ3	1:A:185:VAL:HG11	2.56	0.41
1:A:304:TYR:O	1:A:326:PHE:HB2	2.21	0.41

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	384/398 (96%)	377 (98%)	7 (2%)	0	100	100
1	B	383/398 (96%)	376 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	767/796 (96%)	753 (98%)	14 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	325/334 (97%)	322 (99%)	3 (1%)	78 70
1	B	324/334 (97%)	322 (99%)	2 (1%)	86 80
All	All	649/668 (97%)	644 (99%)	5 (1%)	81 74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	32	ASP
1	A	362	ARG
1	B	30	GLU
1	B	356	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	PLP	A	401	1	15,15,16	2.49	9 (60%)	20,22,23	2.19	10 (50%)
2	PLP	B	401	1	15,15,16	2.47	8 (53%)	20,22,23	2.30	7 (35%)

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
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C5-C4	5.53	1.46	1.40
2	A	401	PLP	P-O3P	-4.16	1.38	1.54
2	A	401	PLP	C5-C4	4.15	1.45	1.40
2	A	401	PLP	P-O2P	-3.74	1.40	1.54
2	B	401	PLP	P-O3P	-3.46	1.41	1.54
2	B	401	PLP	P-O1P	-3.35	1.39	1.50
2	A	401	PLP	O3-C3	-3.26	1.29	1.37
2	A	401	PLP	C4A-C4	-2.80	1.45	1.51
2	B	401	PLP	O3-C3	-2.50	1.31	1.37
2	B	401	PLP	C3-C2	2.44	1.43	1.40
2	B	401	PLP	C3-C4	2.43	1.45	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	P-O2P	-2.28	1.46	1.54
2	B	401	PLP	C4A-C4	-2.26	1.46	1.51
2	A	401	PLP	C3-C2	2.21	1.43	1.40
2	A	401	PLP	C2-N1	-2.11	1.30	1.33
2	A	401	PLP	C3-C4	2.10	1.44	1.40
2	A	401	PLP	C6-N1	-2.05	1.30	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	PLP	C4A-C4-C5	5.71	126.81	120.94
2	A	401	PLP	O4P-C5A-C5	4.61	118.13	109.35
2	B	401	PLP	O4P-C5A-C5	3.76	116.52	109.35
2	B	401	PLP	C4A-C4-C3	-3.43	114.69	120.50
2	A	401	PLP	C6-N1-C2	3.32	125.31	119.17
2	B	401	PLP	C2A-C2-C3	-3.24	116.88	120.89
2	A	401	PLP	C4A-C4-C5	3.24	124.27	120.94
2	B	401	PLP	C2A-C2-N1	2.72	122.98	117.67
2	A	401	PLP	O2P-P-O4P	-2.65	99.68	106.73
2	A	401	PLP	C2A-C2-N1	2.55	122.66	117.67
2	B	401	PLP	C6-C5-C4	-2.53	116.16	118.16
2	B	401	PLP	C6-N1-C2	2.44	123.69	119.17
2	A	401	PLP	C6-C5-C4	-2.34	116.32	118.16
2	A	401	PLP	C2A-C2-C3	-2.18	118.20	120.89
2	A	401	PLP	O3P-P-O4P	2.17	112.50	106.73
2	A	401	PLP	C5A-C5-C6	2.14	122.90	119.37
2	A	401	PLP	C4A-C4-C3	-2.01	117.09	120.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PLP	1	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, 95^{th} 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	381/398 (95%)	0.10	25 (6%)	18	20	17, 27, 48, 73	0
1	B	382/398 (95%)	0.08	19 (4%)	28	32	17, 26, 48, 88	0
All	All	763/796 (95%)	0.09	44 (5%)	23	25	17, 26, 49, 88	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	GLN	7.7
1	B	55	PHE	6.6
1	B	50	ASP	5.9
1	B	62	ASP	5.6
1	A	50	ASP	5.4
1	A	368	LYS	5.0
1	A	55	PHE	4.6
1	B	368	LYS	4.6
1	A	118	PHE	4.5
1	A	288	GLN	4.4
1	A	53	GLN	4.3
1	B	51	THR	3.9
1	A	51	THR	3.9
1	A	367	SER	3.7
1	A	365	THR	3.7
1	B	52	LEU	3.7
1	A	62	ASP	3.5
1	A	310	THR	3.5
1	B	118	PHE	3.4
1	B	54	PRO	3.4
1	B	288	GLN	3.3
1	B	13	LYS	3.3
1	A	287	GLU	3.3
1	A	369	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	3.1
1	A	48	THR	2.9
1	A	291	THR	2.8
1	B	61	GLU	2.8
1	B	367	SER	2.8
1	A	292	SER	2.7
1	B	115	LYS	2.7
1	A	13	LYS	2.5
1	A	115	LYS	2.5
1	B	365	THR	2.3
1	A	179	LYS	2.2
1	A	293	LEU	2.2
1	A	398	SER	2.2
1	B	291	THR	2.2
1	B	145	LYS	2.2
1	B	287	GLU	2.1
1	A	145	LYS	2.1
1	A	366	ASP	2.1
1	B	312	GLU	2.1
1	A	289	PHE	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 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^{th} 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
3	MG	B	402	1/1	0.90	0.09	30,30,30,30	0
3	MG	A	402	1/1	0.97	0.14	29,29,29,29	0
2	PLP	B	401	15/16	0.98	0.07	17,20,25,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	A	401	15/16	0.99	0.08	17,22,26,30	0

6.5 Other polymers (i)

There are no such residues in this entry.